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Mémoire présenté en vue de l'obtention de l'
HABILITATION A DIRIGER DES RECHERCHES

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Numerical paleontology and its application to Ammonoidea

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Contents

Abstract

This dissertation to obtain the French diploma HDR ("Habilitation à Diriger des Recherches") summarizes my research activities in paleontology since my PhD defense (2004). During these years, my research was characterized by two major threads: 1) the study of ammonoids (extinct, externally shelled cephalopods), and 2) the application and development of modern quantitative methods to study these organisms. In addition to the classical taxonomic works, three major themes characterize my research: quantitative biostratigraphy/biochronology, computer-assisted 3D morphometrics, and macroevolution (based on taxonomic richness and morphological disparity).

With regard to ammonoids, I conducted classical, but essential, taxonomic studies, along with field-work, preparation, storing, and systematic description of the collected material, in order to increase the knowledge of ammonoids in space and time. I worked in the Devonian (419–359 Ma), Triassic (252–201 Ma), and Cretaceous (145–66 Ma) in various geographic areas (Nevada, Southern Alps, France). Also, I conducted studies on the evaluation of the intraspecific variation of ammonoid shell characters and their non-random patterns of covariation (coined "Buckman's rules").

The ammonoids are well-known to be a powerful tool to correlate and date marine sediments. Facing the abundance of biostratigraphic data and the need for higher-resolved and more robust biochronological scales, a large part of my research was to apply and critically evaluate the various quantitative methods of biochronology (such as the UAs, CONOP, and RASC), their computer implementation, and also to highlight their critical points and possible improvements.

The external shell of ammonoids is the fundamental element for their discrimination and to study their evolution. The largest part of the morphological differences among ammonoid species corresponds to subtle changes of shell geometry. Therefore, I created a non-destructive method to reconstruct and quantify the 3D morphology of the conch through ontogeny, particularly by means of micro-computed tomography to acquire the data, by numerical creation of 3D models, and by geometric analyses implemented in Matlab and R scientific languages.

The ammonoids are also a powerful tool to quantify and evaluate macro-evolutionary (biodiversity, disparity, trends) and macro-ecological patterns. A large part of my research focuses on the biosphere–geosphere relationships by investigating biodiversity changes (taxonomic richness) and the repetitive patterns of disparity (morphological disparity). In the context of the current concern about the global warming and its consequences, I studied the Cenomanian/Turonian boundary mass extinction (93.5 Ma) initially interpreted to be caused by the spreading of anoxic waters. My research highlighted a more protracted extinction, which started before the anoxic event and which better correlates with the global warming culminating in the lower Turonian. I also contributed to investigate the biotic recovery after the biggest mass extinction of the Permian/Triassic boundary (252 Ma). The major highlighted result is the much shorter duration of the biotic recovery (1 Myr instead of 10 Myr) suggesting a quick re-establishment of ecosystems.

With regard to patterns of morphological disparity, part of my research investigated the macroevolution of ammonoids and underlined its chaotic behavior with repetitive patterns partly related to the covariation of some shell features, which facilitated convergences and parallel trends. In this context, I applied and developed modern quantitative methods (implemented in R) in order to explore and statistically test the phenotypic trajectories of phylogenetic lineages or stratigraphic sequences in morphospace.

Finally, since several years, I am developing an R package (called “epaleo”), which contains series of functions to apply various quantitative, explorative and statistical methods in the field of taxonomic biodiversity, long-term morphological trends, taxonomy and morphometrics (1D, 2D, and 3D), and community analyses. With regard to this package, all functions have already been used for published analyses, and its reporting orientation enables to easily repeat and reproduce the analyses.

In conclusion, my research enables me to acquire skills in various paleobiological topics from alpha taxonomy to macroevolution that are recognized by the paleontological community, as illustrated by my recent invited contribution of six on twenty chapters for a comprehensive book (605 pp) reviewing the current knowledge of ammonoids (*Klug et al 2015, Ammonoid Paleobiology: from macroevolution to paleogeography, Topics in Geobiology 44, Springer*).

Keywords

Ammonoids • Famennian • Anisian • Cenomanian/Turonian • Biochronology • Biostratigraphy • Correlation • Morphometrics • Intraspecific variation • Ontogeny • Allometry • Shell geometry • 3D reconstruction • Tomography • Macroevolution • Macroecology • Long-term evolutionary trends • Cope's rule • Taxonomic biodiversity • Mass extinction • Morphological disparity • Numerical tools • Image analysis • Mesh analysis • Quantitative methods • Multivariate and statistical analyses • R project

Résumé

Ce mémoire pour l'obtention de l'HDR (Habilitation à Diriger des Recherches) résume mes activités de recherche depuis ma soutenance de thèse de doctorat (2004). Aux cours de ces années, mes travaux de recherche se sont caractérisés par deux fils conducteurs principaux : 1) l'étude des ammonoïdes (céphalopodes marins, fossiles, à coquille externe) et 2) l'application/développement de méthodes quantitatives modernes pour l'étude de ces organismes. En plus des travaux de base, trois thématiques majeures se dégagent de mes travaux de recherche : la biochronologie quantitative, la morphométrie 3D assistée par ordinateur, et la macroévolution (basée sur les signaux taxonomique et morphologique).

En ce qui concerne les ammonoïdes, j'ai effectué des travaux taxonomiques, classiques et essentiels en paléontologie, avec fouilles de terrain, préparation, archivage et description systématique du matériel, afin d'élargir les connaissances spatio-temporelles et taxonomiques de ces organismes ; plus particulièrement au Dévonien (419–359 Ma), Trias (252–201 Ma) et Crétacé (146–66 Ma), et dans les régions du Nevada, des Alpes italiennes, et du SE de la France. J'ai aussi dirigé des travaux sur l'évaluation de la variation intraspécifique de ces animaux et la caractérisation de motifs particuliers ("lois de Buckman") dus à la covariation de certains caractères.

Les ammonoïdes constituent un outil de datation relative très performant des sédiments marins. Face à l'abondance de données biostratigraphiques et le besoin croissant d'échelles de datation robustes, une part importante de mes travaux de recherche a été d'appliquer et d'évaluer de manière critique diverses méthodes de biochronologie quantitative (UAs, CONOP, RASC), leur implémentation algorithmique sur ordinateur, et la mise en évidence des points critiques et des améliorations possibles. De manière tout aussi originale, ces travaux ont permis de quantifier le diachronisme, souvent négligé, des ammonoïdes étudiés et d'évaluer la corrélation automatique de biozonations de bassin distants.

La coquille externe des ammonoïdes constitue l'élément clé pour les discriminer et étudier leur évolution. L'essentiel des différences correspondant à des changements subtils dans la forme géométrique, j'ai développé des méthodes non destructrices pour pouvoir reconstruire et quantifier la morphologie 3D de ces coquilles, notamment avec acquisition de données par micro-tomographie, reconstruction de modèles 3D (réseau de triangles) par traitement numérique, et enfin analyse géométrique par programmation sous Matlab et R. Ces méthodes permettent l'accès à des paramètres volumiques inédits et de modéliser/tester l'hydrodynamisme des coquilles.

Les ammonoïdes se révèlent aussi un très bon outil pour évaluer et quantifier les motifs macro-évolutifs (diversité, disparité, tendances) et macro-écologiques. Une part importante de mes travaux de recherche s'est focalisée, d'une part sur l'interaction biosphère-géosphère notamment au travers des variations de biodiversité (signal taxonomique), et d'autre part sur les motifs récurrents dans l'évolution de la forme de ces ammonoïdes (signal morphologique). Dans le contexte actuel de réchauffement climatique et de ses conséquences, j'ai étudié l'extinction de masse du Cénomanien/Turonien (93.5 Ma) dont le développement brusque d'eaux anoxiques était considéré comme la cause principale. Mes travaux ont mis en évidence une crise de biodiversité sur le long terme, et non abrupte, qui précède cette anoxie et suit plutôt le réchauffement climatique globale de l'époque. J'ai aussi contribué à l'étude de la récupération biotique faisant suite à la plus grande extinction de masse du Phanérozoïque (la limite Permien/Trias, 252 Ma). Le résultat majeur est la mise en évidence d'une récupération biotique qui ne dure qu'1 million d'années plutôt que les 10 préalablement reconnues.

Sur le plan macro-évolutif du signal morphologique, certains de mes travaux ont analysé l'évolution des ammonoïdes, qui s'avère être de type chaotique avec des motifs récurrents dus à la covariation entre certains modules, conduisant souvent à des tendances évolutives persistantes (comme la loi de Cope), à des convergences et à des évolutions parallèles. Dans ce contexte, j'ai appliqué et développé des méthodes (programmées sous R) pour évaluer et tester statistiquement les trajectoires phylogénétiques ou stratophénétiques dans des espaces morphologiques.

Enfin, depuis quelques années, je développe un package ("epaleo") pour l'environnement de calcul scientifique R. Ce package reprend l'ensemble des méthodes quantitatives appliquées et/ou développées en ce qui concerne notamment l'analyse de la biodiversité taxonomique, des tendances morphologiques, de la taxonomie/morphométrie (1D, 3D), et l'analyse des communautés. Les différentes fonctions de ce package ont déjà été utilisées dans des analyses publiées et l'accès libre et orienté "reporting" de ce package permet de reproduire aisément les analyses.

En conclusion, mes travaux de recherche m'ont permis d'acquérir une expertise reconnue par la communauté dans ces thématiques. J'ai d'ailleurs été récemment invité à écrire six chapitres (parmi vingt) pour un livre de synthèse majeur (605 pp) sur les connaissances des ammonoïdes et publié récemment (*Klug et al 2015, Ammonoid Paleobiology: from macroevolution to paleogeography, Topics in Geobiology 44, Springer*).

Mots clés

Ammonoïdes • Famennien • Anisien • Cénomanien/Turonien • Biochronologie • Biostratigraphie • Corrélation • Morphométrie • Variation intraspécifique • Ontogénie • Allométrie • Géométrie de la coquille • Reconstruction 3D • Tomographie • Macroévolution • Macroécologie • Tendances évolutives à long-terme • Loi de Cope • Biodiversité taxonomique • Extinction de masse • Disparité morphologique • Outils numériques • Analyses d'images • Méthodes quantitatives • Analyses multivariées et statistiques • Projet R

Acknowledgments

This dissertation is the result of years of research, of supervising students, of teaching, and of leading short and long-term projects in paleontology. If they reflect my own interests and opportunities, they also result from the influence and interaction with many colleagues. All the studies started several years ago were made possible thanks to support from a number of people and to fruitful collaboration based on the exchange of contrasted ideas characterizing any scientific construction. While writing this report, I think therefore above all to everyone, colleagues and friends, who have marked my path, trusted me, and enable me to progress in my scientific research.

Professionally, it all started at the University of Lyon (France). I like to start this list with my thesis supervisor, Hugo Bucher (Zürich), who helped me take my first steps in research and supported me for many years, first in Lyon and then in Zürich. I owe him for introducing me to the beautiful world of ammonoids and to the complex world of quantitative biochronology. Among other people from Lyon, I am also indebted to Serge Ferry (Lyon) for its snack heads in sequence stratigraphy and its prolific introduction to field-work in geology, as well as Gilles Carbonnel (Lyon) for the discovery of quantitative geology and paleontology. Last but not least, I want to thank Gilles Escarguel (Lyon) for its always relevant advices and for being an inspiration to apply and develop numerical tools, and to investigate patterns in macroevolution and macroecology.

Some contingencies led me to lead various research projects at the University of Zürich (Switzerland) during almost ten years. The welcome and the atmosphere within the PIMUZ (Paläontologisches Institut und Museum der Universität Zürich) was a real asset and a pleasure throughout these years, therefore, I deeply thank them all, especially for their administrative and scientific support and for their discussion (scientific or not) during coffee breaks and lunches. I also think especially to Peter Brack and Hans Rieber (Zürich) who made me discover the stratigraphy and ammonoids of the Alpine Triassic. I am also indebted to Christoph Zollikofer (Zürich) for his patience and for initiating me to the acquisition of 3D data by means of tomography and digital processing. Last but not least, I thank particularly Christian Klug (Zürich) for its friendship, introduction to Devonian ammonoids, and for indirectly forcing me to delve into R.

Then my peregrination led me to a position of “research engineer” (IR) at the University of Lille (France). I thank the team of paleontology for his welcome, and especially Thomas Servais (Lille) who contacted me to apply on this position and drove me to do this dissertation. Also, I thank all the students that I have enjoyed coaching and that, for some, now fly on their own.

I want to thank the jury members who have agreed to evaluate this report despite their overloaded schedule: Catherine Crônier (Lille), Taniel Danelian (Lille), Gilles Escarguel (Lyon), Pascal Neige (Dijon), Paula Noble (Reno), and Xavier Vekemans (Lille).

Finally, my research also benefited more particularly from some people for their enthusiasm, their help on the field and in research, and/or their friendship: Fabrizio Cecca (Paris), Kenneth De Baets (Erlangen), Jim Jenks (Salt Lake City), and, last but not least, Arnaud Brayard (Dijon). Finally, as research is not everything and I need to refresh my mind from time to time, I end these thanks by my family for its help and support.

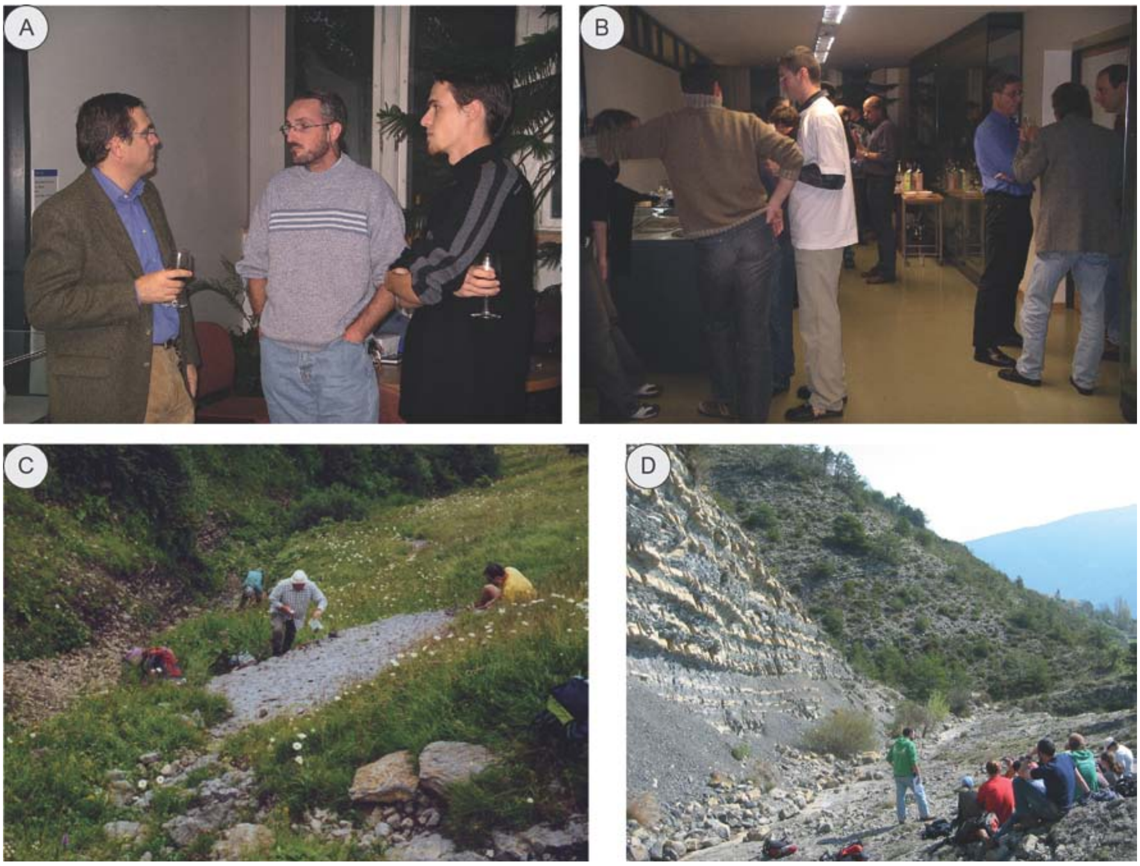


***Figure** – Some of my colleagues and friends who influenced my research (from left to right). **A)** Fabrizio Cecca, Gilles Escarguel, and Arnaud Brayard at the PIMUZ. **B)** Séverine Urdy, Nicolas Goudemand, me, Peter Brack, Peter Hochuli, Wolfgang Weitschat, and Hugo Bucher at the PIMUZ. **C)** Peter Brack, Hans Rieber, and Hugo Bucher (field-trip in Southern Alps). **D)** Kenneth De Baets (green guy) and Christian Klug (orange guy) during a field-trip for Master students in SE France.*

Ammonoids

Ammonoids are the model fossil I am working on to investigate questions in evolutionary biology. Hence, a brief overview of these organisms follows. For another short overview of ammonoids, see De Baets et al (2016), for exhaustive reviews of their anatomy and ecology, see Klug et al (2015a), and for their biostratigraphy, biogeography and macroevolution, see Klug et al (2015b). Ammonoids (Mollusca: Cephalopoda: Ammonoidea) are an extinct group of marine, nektonic (mobile, active swimmers within the water column) invertebrates with an external shell. They were cephalopods, and hence closely related to modern cuttlefish, squid, octopuses and the pearly nautilus. The Ammonoidea as a whole lived from the Early Devonian (ca. 400 Ma) to the Cretaceous/Tertiary boundary (ca. 66 Ma), covering more than 300 Myr of history. Due to the large diversity (taxonomic richness), disparity (morphological richness), nearly global distribution and abundance of their shells in the fossil record, ammonoids have been valued by geologists, paleontologists, and fossil collectors alike. They displayed rapid rates of evolution (with individual species typically persisting no more than one million year) and, thus, have been particularly useful for studies of biodiversity and for correlating and assigning relative ages to rocks. Ammonoids have also proved valuable for studying the processes and patterns of evolution, because they seemingly and repeatedly evolved towards peculiar patterns (Kennedy 1977; Neige et al 2009).

Shell morphology

With regard to ammonoids, almost only their shells (aka. conchs) are found in the fossil record. Conchs from adult ammonoids range from about 5 mm to 2 m in diameter. This conch is typically coiled in a plane, and as such classified as monomorph (*Fig 1C*). There is, however, a great variety of ammonoid conch forms, ranging from tightly coiled, through loosely coiled to uncoiled, irregularly or trochospirally coiled. These are called heteromorph shapes (*Fig 1D*). Whatever the shape, the conch of all ammonoids can be subdivided into a body chamber containing the soft parts, and a phragmocone consisting of individual chambers separated by walls called septa and connected by an organic tube called the siphuncle (*Fig 1A*). The junction of the septa and the outer shell forms a suture line. The shape/outline of the suture lines is complex and not random. There is a trend toward increasing septal complexity over ammonoid evolution, from goniatitic (septa describe a series of tight curves), over ceratitic (series of tight curves with a single series of smaller curves superimposed at apices), to ammonitic (septa extremely complex at multiple scales). The shell may bear ornamentation consisting of ribs, tubercles, spines, constrictions, or keels, among others. Several characters can be used to describe the ammonoid shell (Arkell et al 1957; Dommergues et al 1996; Korn 2010; Klug et al 2015a); its morphology can be separated into three major sets of characters, which are the geometry of the shell tube (including whorl shape and degree of involution), its ornamentation, and the suture shape.

The ammonite shell grows by continually adding layers of calcium carbonate to the leading edge or aperture of the conch, so that their entire life history is recorded in their shells, from embryo to adult (Fig 1B). The calcareous shell is secreted by the mantle and composed of three layers: thin outer organic periostracum; thick calcareous prismatic layer; thin innermost nacreous layer made of thin sheets of aragonite. Different ontogenetic stages are often marked by constrictions, or changes in conch shape, shell thickness and ornamentation. In many species, particularly during the Jurassic period, sexual dimorphism was often very pronounced (differences in size, shape, and ornamentation), whereas in others, it seems to have been insignificant or absent.

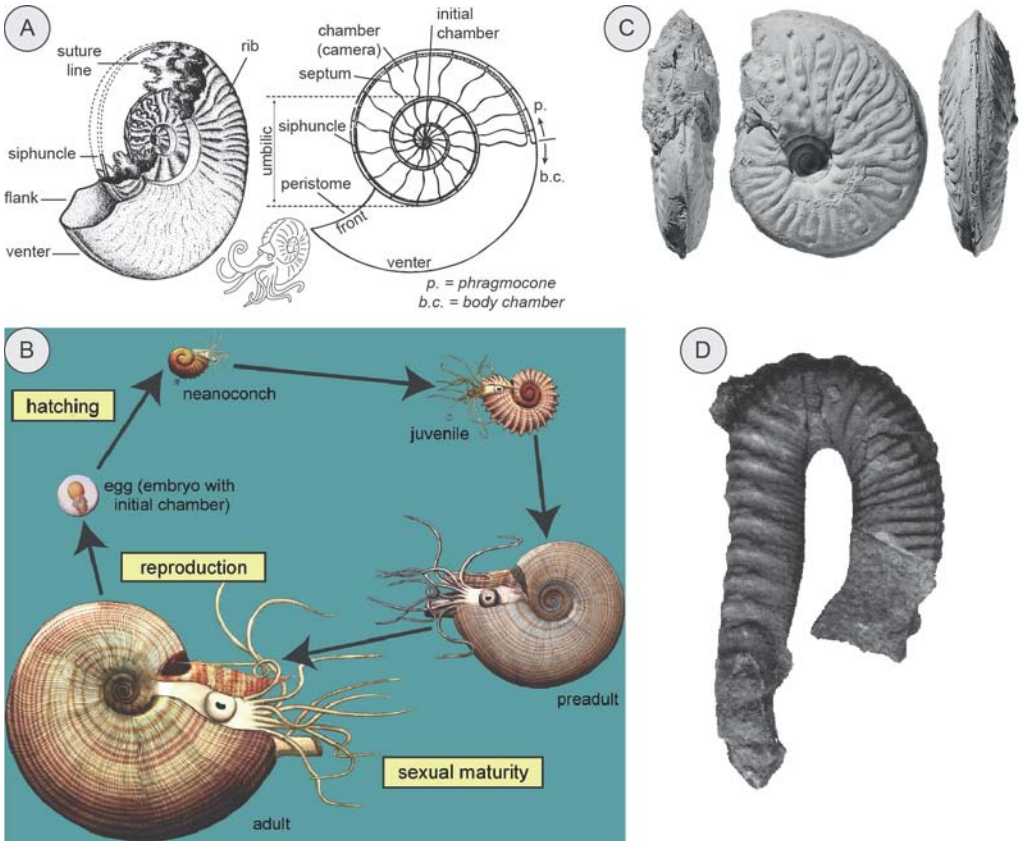


Figure 1 –** The ammonoid shell terminology and reconstruction.* ***A) *Terminology of the conch.* ***B)*** *Life cycle of an ammonoid, exemplified with the Devonian genus* Manticoceras *(modified after Korn & Klug 2007).* ***C)*** *A monomorph ammonoid: the keeled and ribbed Anisian* Eutomoceras *(Nevada, USA).* ***D)*** *A heteromorph ammonoid: the ribbed and hooked Albian* Anisoceras *(Montlaux, SE France).*

Anatomy

Ammonoids probably had a large variety of life modes and reproductive strategies, but despite the widespread attention that they have received, there are still several controversies concerning their anatomy and paleoecology. This results mainly from the very scarce and incomplete preservation of soft tissues of ammonoids in the fossil record. Nevertheless, a few exceptionally preserved specimens have offered insights into some aspects of their anatomy and mode of life.

Ammonoids possess, initially, upper and lower jaws, which consisted mainly of chitin material, and superficially resembled the jaws of modern cephalopods. Between the jaws was a structure called the radula, which is a tongue-like organ with minute chitinous teeth to grasp and transport food particles (similarly to aquatic gastropods). These teeth were arranged in rows, and attached on top of a long, thin ribbon; the tooth rows were lined up across this tongue-shaped structure. During the Jurassic, the lower jaw in some groups became split into two shovel-like valves (aka. *Aptychus*) covered with calcite. By analogy with their phylogenetic relatives, ammonoids probably had also ten arms. The anus is directed into a mantle cavity, which houses the gills. Whereas nautilids lack an ink-sack, fossils indicate its presence in ammonoids. Also, whereas nautilids have few, large eggs that develop directly into adults and do not become part of the plankton, ammonoids may have been different, with small, abundant, planktonic larvae.

Ecology

Hypotheses about mode of life of ammonoids have often been based on the morphology and strength of their mineralized parts (conchs and septa), as well as the depositional environment (facies) of the rocks they are found in. Although still speculative and general, the functional interpretation of ammonoids is constrained by the presence of this external conch. The phragmocone of ammonoids and other chambered, now-extinct, cephalopods functioned as a buoyancy apparatus, as in extant *Nautilus* or *Spirula*, and implies a mode of life of floating in the water column. Also, the chambers of the phragmocone are separated by septa and filled with gas and connected to the living organism by the siphuncle. The siphuncle and the living membranes lining the chambers regulate the secretion of gasses into the chambers, allowing them to be used to maintain neutral buoyancy. Therefore, conch geometry and streamlining are important for hydrodynamic properties of ammonoids.

One of the most famous models (correct or not, because it is based on a set of ad hoc hypotheses, which might not be true for at least some species) is probably that of Westermann (1996), who linked external morphology, both for normally coiled ammonoids and for heteromorph forms, to different modes of life (*Fig 2B*). Interestingly, the distance between the centre of gravity and the centre of buoyancy determines the hydrodynamic stability of ammonoids when swimming, propelled by the water jet out of its funnel. The positions of these centers, coupled with the conch shape, are directly related to the orientation of the aperture. Furthermore, the positions of both centers are mainly controlled by the length of the body chamber. Because of the interplay between the center of gravity and center of buoyancy, modifications in conch morphology have often been correlated with changes in maximum swimming velocity and maneuverability (*Fig 2A*; Klug & Korn 2004). A more recent approach assessing possible functional aspects of conch shape applies a technique called Pareto Optimization to the range of known ammonoid morphologies (Tendler et al 2015). It assumes that ammonoid shapes can never fully be optimized for a single function (such as swimming) because of trade-offs between different tasks, including swimming (hydrodynamics), growth and compactness of the conch (a small conch is advantageous because it reduces embryo size, and makes the conch less vulnerable to predator attacks). By analogy to the classical viewpoint of a fitness landscape in which phenotypes are arranged along the slopes near the peak of a fitness hill maximum, the Pareto viewpoint suggests a tradeoff between functional tasks of the ammonoid conch (*Fig 2C*). Based on the classical Raupian parameters, the approach yields a pyramid with five vortices, each representing one archetype optimized for one task.

The occasional preservation of stomach contents from Mesozoic specimens contained planktonic crinoids, ammonoids, bivalves, gastropods, foraminifers, ostracods, isopods, sponges, and ophiuroids (Kruta et al 2011). This variety of organisms suggests that ammonoids could pick up food items from the sea floor or fish them from the entire water column. Modern reconstructions of ammonoid conchs based on various tomographic data have allowed determining that around 20% of the chamber volumes filled by water is necessary to achieve neutral buoyancy. Ammonoids were probably active migrants through the water column; besides, the living *Nautilus* is known to reach depth of about 700 m. Also, many modern cephalopods migrate from shallower to deeper waters (and vice versa) during their lifetime, as well as from close to shore to further from it. Isotope studies corroborate that various species of ammonoids live at various water depth from the sea-floor to the surface (Ritterbush et al 2014; Lukeneder et al 2010; Sessa et al 2015).

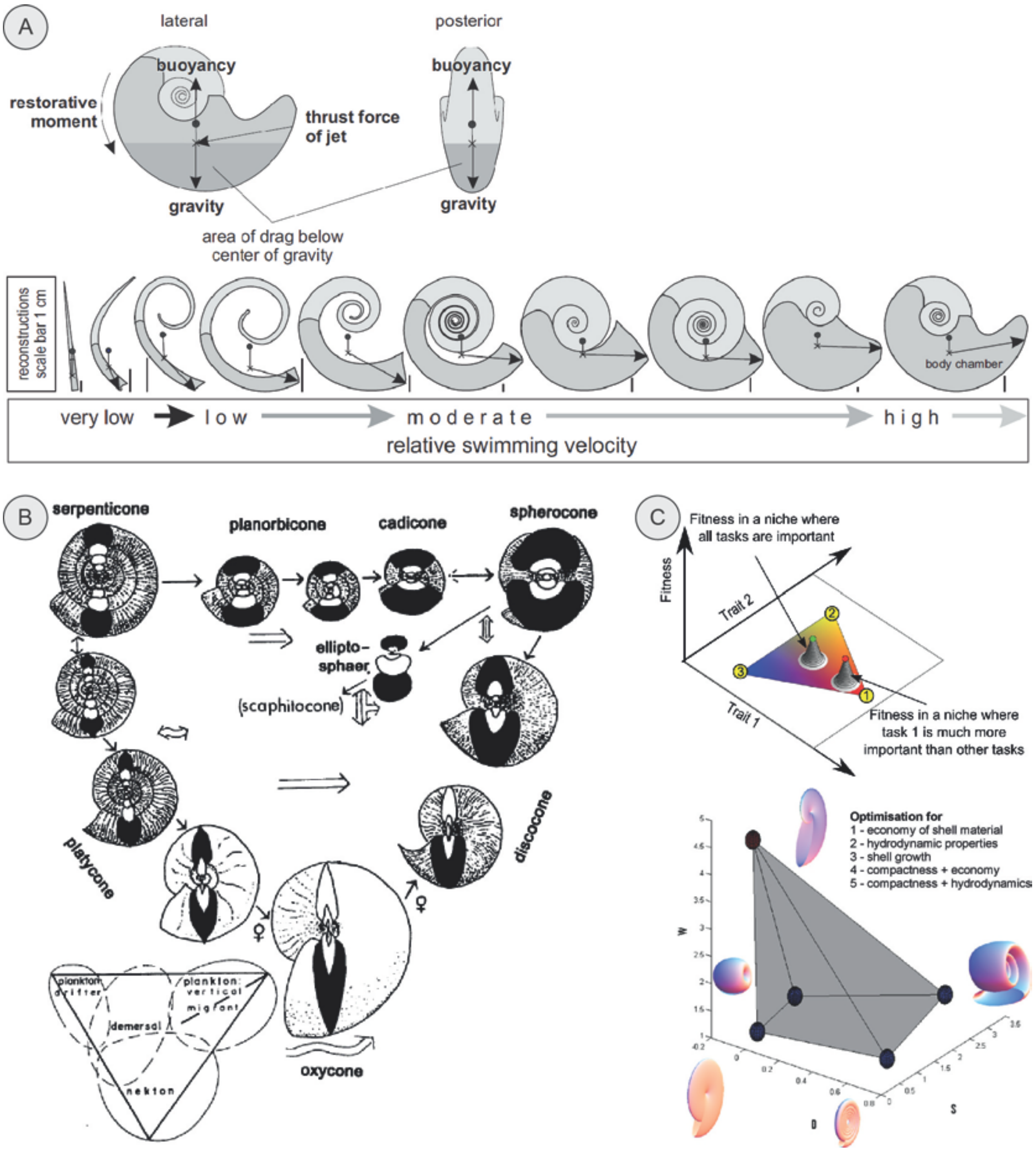


Figure 2 – Ammonoid shell shape and mode of life. ***A)*** *Forces operating on ammonoids during swimming (after Klug & Korn 2004 and Jacobs & Chamberlain 1996). The thrust force produced by the jet which is expelled by the hyponome acts on the centre of gravity. This causes an oblique downward momentum which is opposed by the restorative moment (resulting from buoyancy and gravity) and the drag. At relatively high velocities, this might result in a fairly stable horizontal movement in some derived ammonoids. Evolution of coiled ammonoid shells from straight shells and the consequences for body-chamber length, aperture orientation, thrust angle of the jet they use to move, hydrodynamic stability and interpretations for swimming capabilities (after Klug & Korn 2004).* ***B)*** *The basic planispiral shapes and their habitats according to Westermann (1996).* ***C)*** *The Pareto viewpoint suggests a tradeoff between tasks in a similar way to the classical viewpoint of a fitness landscape in which phenotypes are arranged along the slopes near the peak of a fitness hill maximum. Ammonoid morphospace after Tendler et al (2015) using the Raupian parameters W, S and D (Raup 1966).*

Macroevolution and phylogeny

The oldest ammonoids come from the Early Devonian period (Emsian: 408 to 393 Ma) of Germany, China and Morocco. Ammonoids had a successful evolutionary history, spanning nearly 350 million years, and surviving the Late Devonian, Permian–Triassic and Triassic–Jurassic extinction events (*Fig 3*). Only a few genera survived these mass extinctions, but they rapidly recovered and re-diversified. This could be attributed to their low position in food webs, as well as their opportunistic reproductive strategy ("r-strategist"). Despite being one of the most-studied fossil groups, the evolutionary relationships (phylogeny) of ammonoids are still not fully resolved. This is largely because their phylogeny is based on their conchs, which have a limited amount of strongly varying characters (conch morphology, septa, ornamentation).

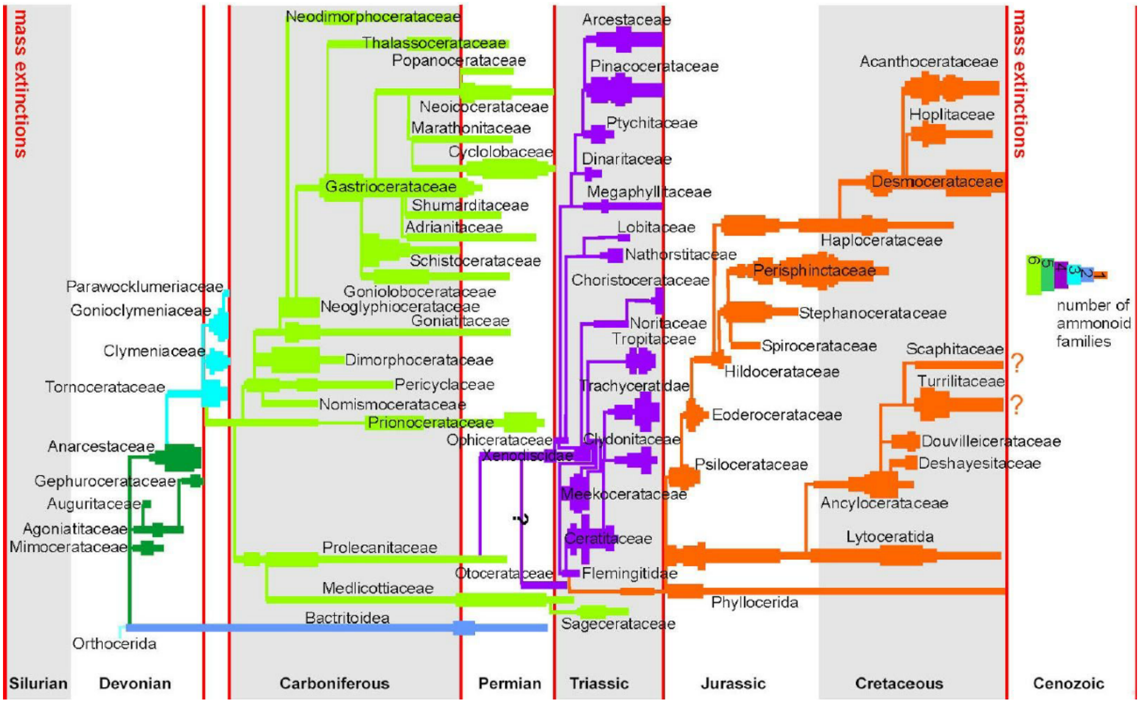
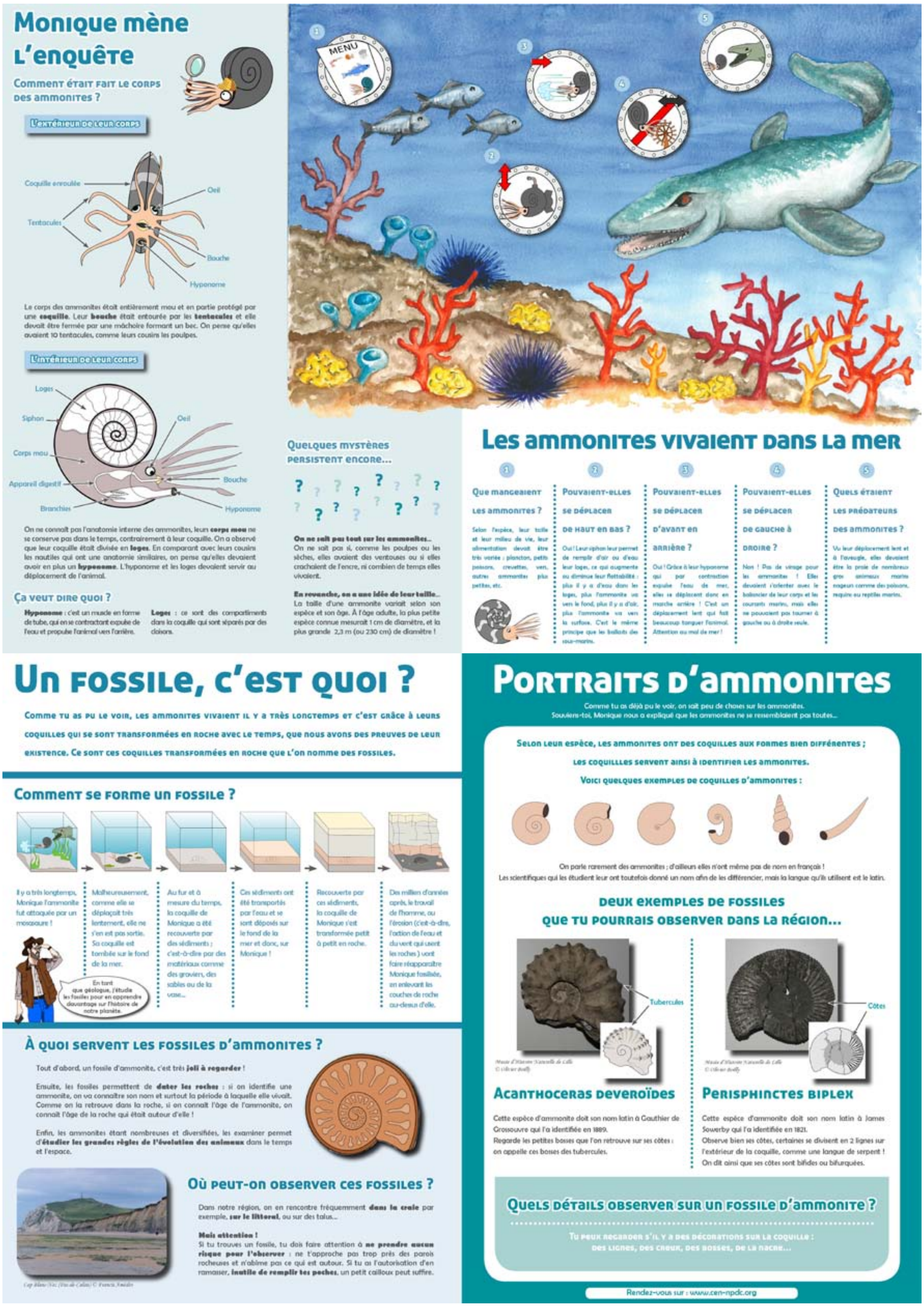


***Figure 3 –** Ammonoid phylogeny (after De Baets et al 2016 who modified House & Senior 1981).*

Despite centuries of study, interest in ammonoids has hardly diminished, leaving room for multiple new discoveries. More exceptionally preserved specimens are necessary to better constrain the anatomy of both internal and external soft tissues of ammonoids. Furthermore, new material will allow for quantitative study of their shells in space and time, which will help to better understand their macroevolution and macroecology.



Monique mène l'enquête

Comment était fait le corps des ammonites ?

L'extérieur de leur corps

Le corps des ammonites était entièrement mou et en partie protégé par une **coquille**. Leur **bouche** était entourée par les **tentacules** et elle devait être fermée par une mâchoire formant un bec. On pense qu'elles avaient 10 tentacules, comme leurs cousins les poulpes.

L'intérieur de leur corps

On ne connait pas l'anatomie interne des ammonites, leurs **corps mou** ne se conserve pas dans le temps, contrairement à leur coquille. On a observé que leur coquille était divisée en **loges**. En comparant avec leurs cousins les nautiles qui ont une anatomie similaires, on pense qu'elles devaient avoir en plus un **hyponome**. L'hyponome et les loges devaient servir au déplacement de l'animal.

Ça veut dire quoi ?

Hyponome : c'est un muscle en forme de tube, qui en se contractant expulse de l'eau et propulse l'animal vers l'arrière.

Loges : ce sont des compartiments dans la coquille qui sont séparés par des cloisons.

Quelques mystères persistent encore...

On ne sait pas tout sur les ammonites...
On ne sait pas si, comme les poulpes ou les sèches, elles avaient des ventouses ou si elles crachaient de l'encre, ni combien de temps elles vivaient.

En revanche, on a une idée de leur taille...
La taille d'une ammonite variait selon son espèce et son âge. À l'âge adulte, la plus petite espèce connue mesurait 1 cm de diamètre, et la plus grande 2,3 m (ou 230 cm) de diamètre !

Les ammonites vivaient dans la mer

① Que mangeaient les ammonites ?	② Pouvaient-elles se déplacer de haut en bas ?	③ Pouvaient-elles se déplacer d'avant en arrière ?	④ Pouvaient-elles se déplacer de gauche à droite ?	⑤ Quels étaient les prédateurs des ammonites ?
Selon l'espèce, leur taille et leur milieu de vie, leur alimentation devait être très variée : plancton, petits poissons, crevettes, vers, autres ammonites plus petites, etc.	Oui ! Leur siphon leur permet de remplir d'air ou d'eau leur loges, ce qui augmente ou diminue leur flottabilité : plus il y a d'eau dans les loges, plus l'ammonite va vers le fond, plus il y a d'air, plus l'ammonite va vers la surface. C'est le même principe que les ballasts des sous-marins.	Oui ! Grâce à leur hyponome qui par contraction expulse l'eau de mer, elles se déplacent donc en marche arrière ! C'est un déplacement lent qui fait beaucoup tanguer l'animal. Attention au mal de mer !	Non ! Pas de virage pour les ammonites ! Elles devaient s'orienter avec le balancier de leur corps et les courants marins, mais elles ne pouvaient pas tourner à gauche ou à droite seule.	Vu leur déplacement lent et à l'aveugle, elles devaient être la proie de nombreux gros animaux marins nageurs comme des poissons, requins ou reptiles marins.

Un fossile, c'est quoi ?

Comme tu as pu le voir, les ammonites vivaient il y a très longtemps et c'est grâce à leurs coquilles qui se sont transformées en roche avec le temps, que nous avons des preuves de leur existence. Ce sont ces coquilles transformées en roche que l'on nomme des fossiles.

Comment se forme un fossile ?

Il y a très longtemps, Monique l'ammonite fut attaquée par un mosasaure !

Malheureusement, comme elle se déplaçait très lentement, elle ne s'en est pas sortie. Sa coquille est tombée sur le fond de la mer.

Au fur et à mesure du temps, la coquille de Monique a été recouverte par des sédiments ; c'est-à-dire par des matériaux comme des graviers, des sables ou de la vase...

Ces sédiments ont été transportés par l'eau et se sont déposés sur le fond de la mer et donc, sur Monique !

Recouverte par ces sédiments, la coquille de Monique s'est transformée petit à petit en roche.

Des millions d'années après, le travail de l'homme, ou l'érosion (c'est-à-dire, l'action de l'eau et du vent qui usent les roches) vont faire réapparaître Monique fossilisée, en enlevant les couches de roche au-dessus d'elle.

En tant que géologue, j'étudie les fossiles pour en apprendre davantage sur l'histoire de notre planète.

À quoi servent les fossiles d'ammonites ?

Tout d'abord, un fossile d'ammonite, c'est très **joli à regarder** !

Ensuite, les fossiles permettent de **dater les roches** : si on identifie une ammonite, on va connaître son nom et surtout la période à laquelle elle vivait. Comme on la retrouve dans la roche, si on connait l'âge de l'ammonite, on connait l'âge de la roche qui était autour d'elle !

Enfin, les ammonites étant nombreuses et diversifiées, les examiner permet d'**étudier les grandes règles de l'évolution des animaux** dans le temps et l'espace.

Où peut-on observer ces fossiles ?

Dans notre région, on en rencontre fréquemment **dans la craie** par exemple, **sur le littoral**, ou sur des talus...

Mais attention !
Si tu trouves un fossile, tu dois faire attention à **ne prendre aucun risque pour l'observer** : ne t'approche pas trop près des parois rocheuses et n'abîme pas ce qui est autour. Si tu as l'autorisation d'en ramasser, **inutile de remplir tes poches**, un petit cailloux peut suffire.

Portraits d'ammonites

Comme tu as déjà pu le voir, on sait peu de choses sur les ammonites.
Souviens-toi, Monique nous a expliqué que les ammonites ne se ressemblaient pas toutes...

Selon leur espèce, les ammonites ont des coquilles aux formes bien différentes ;
les coquillles servent ainsi à identifier les ammonites.
Voici quelques exemples de coquilles d'ammonites :

On parle rarement des ammonites ; d'ailleurs elles n'ont même pas de nom en français !
Les scientifiques qui les étudient leur ont toutefois donné un nom afin de les différencier, mais la langue qu'ils utilisent est le latin.

Deux exemples de fossiles que tu pourrais observer dans la région...

Acanthoceras deveroïdes

Cette espèce d'ammonite doit son nom latin à Gauthier de Grossouvre qui l'a identifiée en 1889.
Regarde les petites bosses que l'on retrouve sur ses côtes : on appelle ces bosses des tubercules.

Perisphinctes biplex

Cette espèce d'ammonite doit son nom latin à James Sowerby qui l'a identifiée en 1821.
Observe bien ses côtes, certaines se divisent en 2 lignes sur l'extérieur de la coquille, comme une langue de serpent !
On dit ainsi que ses côtes sont bifides ou bifurquées.

Quels détails observer sur un fossile d'ammonite ?

Tu peux regarder s'il y a des décorations sur la coquille :
des lignes, des creux, des bosses, de la nacre...

Rendez-vous sur : www.cen-npdc.org

***Figure 4 –** Extract of a booklet (in French) to explain and illustrate ammonoids to children that I am currently creating in collaboration with the* Conservatoire d'Espaces Naturels du Nord Pas-de-Calais.

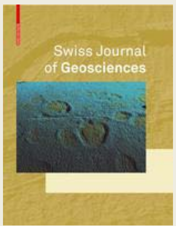
Taxonomy and Morphometry of Ammonoids

Alpha taxonomy

Related publications:

Monnet & Bucher 2005; **Monnet** et al 2008, 2010, 2013; De Baets et al 2013; Jattiot et al 2016; unpublished data

Appended publication:



Monnet C, Brack P, Bucher H, Rieber H (**2008**)
Ammonoids of the middle/late Anisian boundary (Middle Triassic) and the transgression of the Prezzo Limestone in eastern Lombardy-Giudicarie (Italy).
***Swiss J Geosci* 101:61–84**
(doi: 10.1007/s00015-008-1251-7)

A primary and fundamental work in paleontology is alpha taxonomy. It is the discipline of collecting, describing, and classifying new species, as well as revising the classification of previously described species. It is among the most tedious of all biological endeavors, involving intensive collecting and detailed observation, preparation, description, measurement, and illustration. Nowadays there is little incentive to gain training in alpha taxonomy because it is often viewed as old fashioned, although this discipline is fundamental to all other branches of biology. Fortunately, it can be done in such a way as to simultaneously provide crucial data on ecology, evolution, biodiversity, and biogeography, among other research areas. Functioning at the professional level in alpha taxonomy in paleontology requires extensive training, because it is an information-intensive field: it requires detailed knowledge of centuries of previous literature, of the existing classification, and of the morphology and evolution of a particular group.

Part of my research focuses on conducting alpha taxonomy of ammonoids belonging to several periods (Cretaceous, Triassic, and more recently Devonian) covering the entire time interval of existence of these extinct, shell-bearing, marine animals (ca. 400 to 65 Ma). For each studied chronostratigraphic interval (e.g. Anisian, Cenomanian), I compiled and created an exhaustive database of all described ammonoid species. For instance, my PhD thesis reports a form for each Cenomanian genus of Acanthoceratidae with the definition, description, comparison, and illustration of their species. In order to contribute to the taxonomic and biostratigraphic knowledge of ammonoids, I conducted field studies in various places of the world, such as in southeastern France, Southern Alps (Italy), and Nevada (USA). As a case in point, I published several papers of alpha taxonomy that described new species and new genera of ammonoids. This erection of new taxa remains a small part of the amount of described taxa. Indeed, my own feeling is that ammonoid taxonomy is globally rather well documented (even if there is still room to discover new faunas at particular time intervals) with relatively few new taxa created, compared to the amount of described taxa in their biostratigraphic context. Therefore, ammonoid taxonomy reached a mature state characterized by a rather stable taxonomy, at least at the genus level. In addition to their biostratigraphic content, nowadays, most taxonomic studies of ammonoids try to account for the large intraspecific variation of the conch. Hence, this often leads to lump previously defined taxa instead of describing new ones. All of my works on ammonoid alpha taxonomy are clearly framed by this context, especially with regard to peculiar patterns of covariation of some shell characters, the so-called "Buckman's rules of covariation" (see corresponding chapter).

In taxonomic studies, ammonoid shells are historically described by qualitative characters (Arkell et al 1957; Dommergues et al 1996; Korn 2010; Klug et al 2015a) and usually quantified by linear distances, leading to datasets composed of measured parameters and ratios for studied specimens.

Each set of measurements includes classical geometric parameters of the ammonoid conch (*Fig 1A*) such as the shell diameter (D) and corresponding whorl height (H), whorl width (W) and umbilical diameter (U). To assess the variability of these parameters for each species, they are usually analyzed as a ratio with the size-related parameter D (H/D, W/D and U/D) to remove in part the influence of growth. In addition to these three ratios, the ratio W/H is also used as a simple, rough descriptor of the whorl section shape. These measurements and ratios can be processed by univariate and multivariate quantitative analyses and used to further constraints the qualitative, empirical hypotheses. This is an important aspect of ammonoid taxonomy, because the ammonoid conch is characterized by a very large intraspecific variation when large samples are available, leading to similar forms for the slender variants of different species.

With regard to my own research, several descriptive, exploratory and multivariate analyses of the biometric ratios are usually computed by means of the free scientific and statistical environment R (R Core Team 2016) and with my own package *epaleo* (unpublished; see corresponding chapter). These quantitative approaches are convenient tools to investigate taxonomy and morphometry more objectively than classical, comparative, qualitative approaches.

For instance, box plots can be constructed to illustrate the univariate distribution of the conch ratios for each studied morphological group. These graphs display a visual comparison of the distribution of quantitative parameters with its median value (horizontal line), its 25th and 75th percentiles (the box that contains half of the values around the median), its extended interquartile range (marked by the whiskers) and its eventual outliers (isolated dots). These plots allow determining whether the morphological groups differ by their biometric parameters as indicated by the amount of overlap between them (*Fig 1D*).

In addition, the normality of the H/D, U/D, W/D and W/H parameters is often graphically assessed by means of a quantile–quantile plot and statistically tested by means of a Lilliefors test. This test evaluates the null hypothesis that the investigated data have a normal distribution with unspecified mean and variance (at a confidence level of 95%). Also, the Q–Q plot is an exploratory graphic used to check the validity of a distributional assumption for a data set. In general, the basic idea is to compute and compare the theoretically expected value for each data point based on the distribution in question. On a Q–Q plot, if the data conform to a normal distribution, the data will all lie quite close to a line. Normality of the data is also empirically evaluated by means of a standard histogram of the values. In this context, the outline of the chart is expected to closely approximate a bell shape.

The growth trajectories of H/D, W/D, U/D and W/H ratios are also explored by means of scatter diagrams (*Fig 1B*) and by fitting an allometric curve (*Fig 1C*) to the data with respect to shell diameter in order to evaluate the differences in size-based allometries of the geometry of the shell. Because allometric growth conforms to an exponential-like equation, the values of each parameter are fitted by a power equation by means of a linear regression of log-transformed data. The isometric versus allometric state is tested by a Z-test with the null hypothesis that the allometric exponent is equal to 1 (i.e. isometric growth) at a confidence level of 95%.

Finally, these ratios H/D, U/D, W/D and W/H can be investigated by means of standard multivariate analyses (*Fig 2*). For instance, a linear discriminant analysis (LDA) can been performed in order to graphically evaluate how the studied morphotypes of a taxon can be more or less well distinguished based on these ratios. Briefly, the purpose of this standard ordination method is to project the multidimensional dataset (composed here of the conch ratios) onto newly constructed axes, which maximize the discrimination between given groups and which are ordered by decreasing importance. This method is thus a convenient tool for finding differences between groups (taxa) in the function of the parameters and of the value of each parameter. This method enables investigation of the patterns of morphological variation in the studied species or morphological groups.

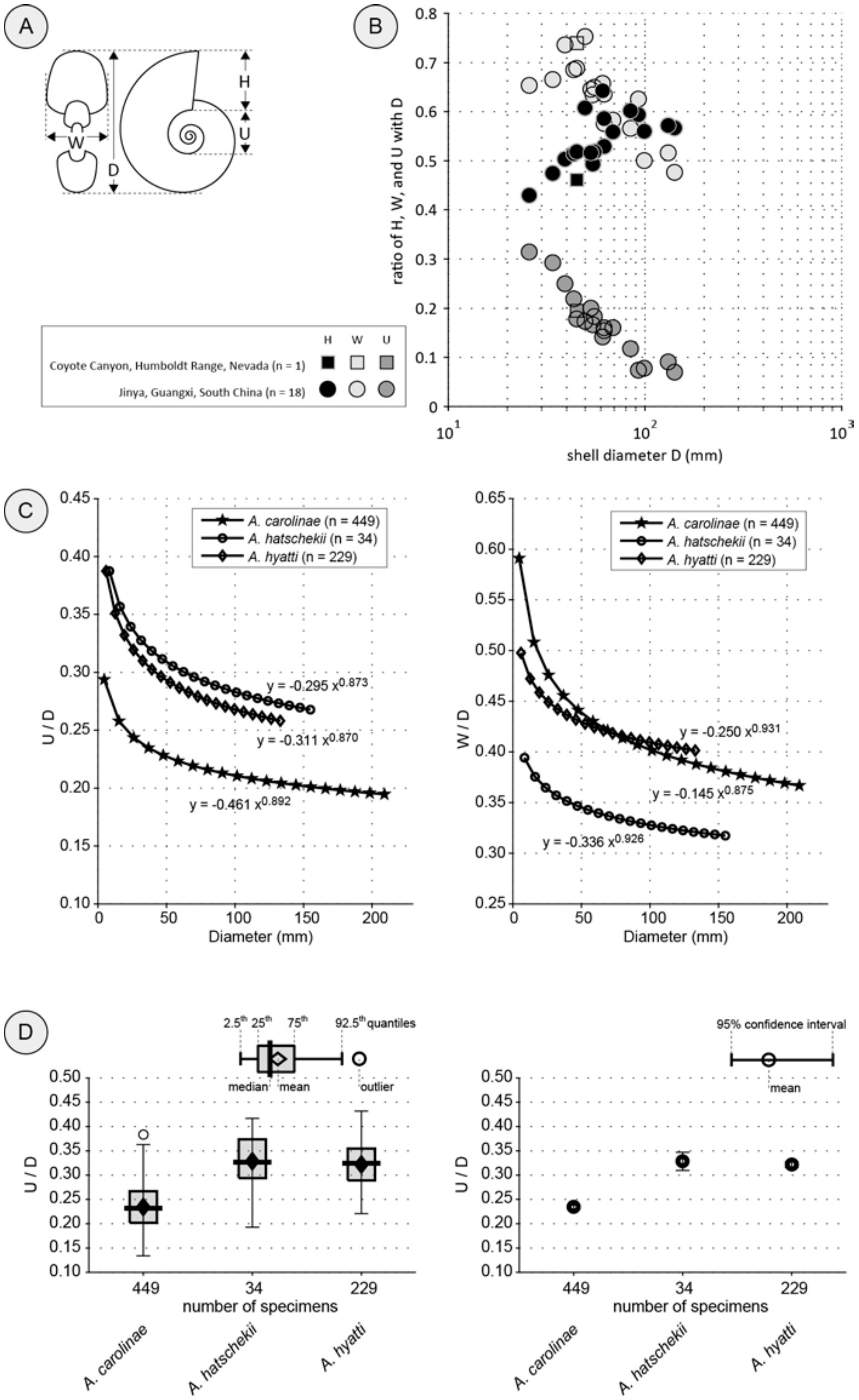


***Figure 1** – Example descriptive univariate analyses of the standard ammonoid shell measurements. **A)** Illustration of the four commonly used linear parameters of the ammonoid conch: D, shell diameter; U, umbilical width of the shell along D; H, whorl height along D; and W, whorl width along H. **B)** Scatter plot of the measurements of the classical geometric parameters of the ammonoid shell for* Globacrochordiceras transpacificum *from Guangxi (South China) and Nevada (USA) (after Monnet et al 2013). **C)** Allometric curves of some shell shape ratios for the revised species of* Acrochordiceras *from Nevada (after Monnet et al 2010). D) Box and mean plots of a shell shape ratio for the revised species of* Acrochordiceras *from Nevada (after Monnet et al 2010).*

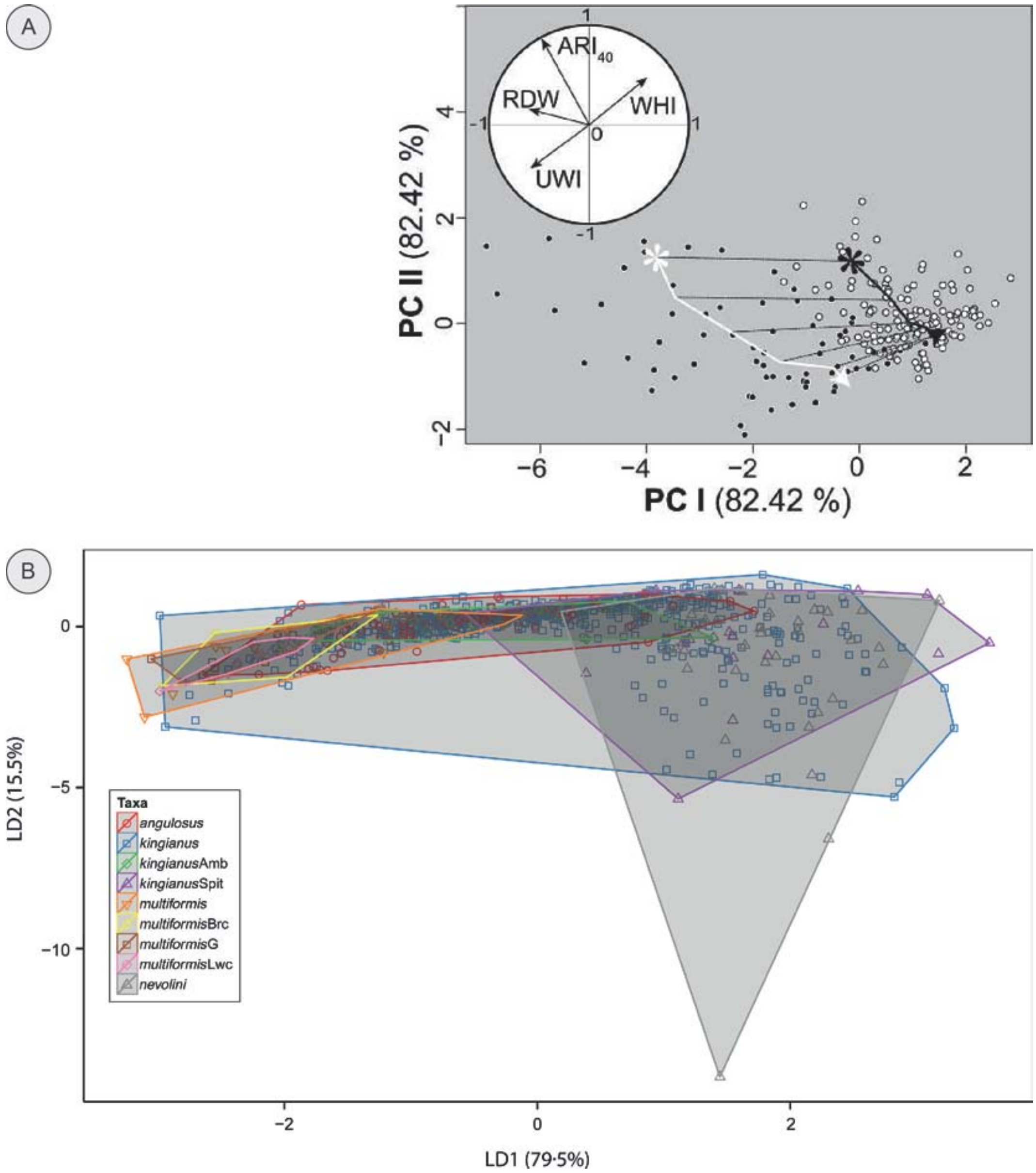


Figure 2 *– Example descriptive multivariate analyses of standard shell measurements.* ***A)*** *Biplot of the principal component analysis of the Devonian ammonoids* Anetoceras *(black dots) and* Erbenoceras *(white dots) (after De Baets et al 2013). The first two principal components account for about 96% of the variation. The projection of the ontogenetic trajectory of each group (from the asterisk to the arrow) is underlined by six common size classes for* Anetoceras *(white) and* Erbenoceras *(black). The circle shows the loadings of original parameters in relation with the first (PCI) and second principal component (PCII).* ***B)*** *Biplot (with convex hull of the taxa) of the linear discriminant analysis of the morphotypes of* Anasibirites *(after Jattiot et al 2016). The first and second discriminant axes account for about 95% of the total variation. The first axis is mostly controlled by the W/H and W/D ratios, with the highest values (depressed whorls) towards the right and the lowest values (compressed whorls) towards the left.*

CRETACEOUS OF SE FRANCE

Since several decades, I am sampling the ammonoid faunas of the Albian, Cenomanian and Turonian (Cretaceous) in southeastern France (aka. the Vocontian Basin; *Fig 3*). The purposes of this long-term work are mainly to document the Cenomanian (and its Albian and Turonian boundaries) ammonoid species, their intraspecific variation, and their biostratigraphic information, especially along a proximal-to-distal transect within the basin in order to cover all major environments recording ammonoids. In this context, the Vocontian Basin is a well-known and important basin for studying the taxonomy, biostratigraphy, and evolution of marine organisms during the Mesozoic. This basin is also at the paleogeographic interface between the Boreal and Tethyan realms and consequently constitutes a critical region for biostratigraphic correlation and climatic studies (Thomel 1992b). Furthermore, this region is a key area with, for instance, the GSSP of the base of the Cenomanian, which is defined at Mont Risou near Rosans (Gale et al 1996; Kennedy et al 2004).

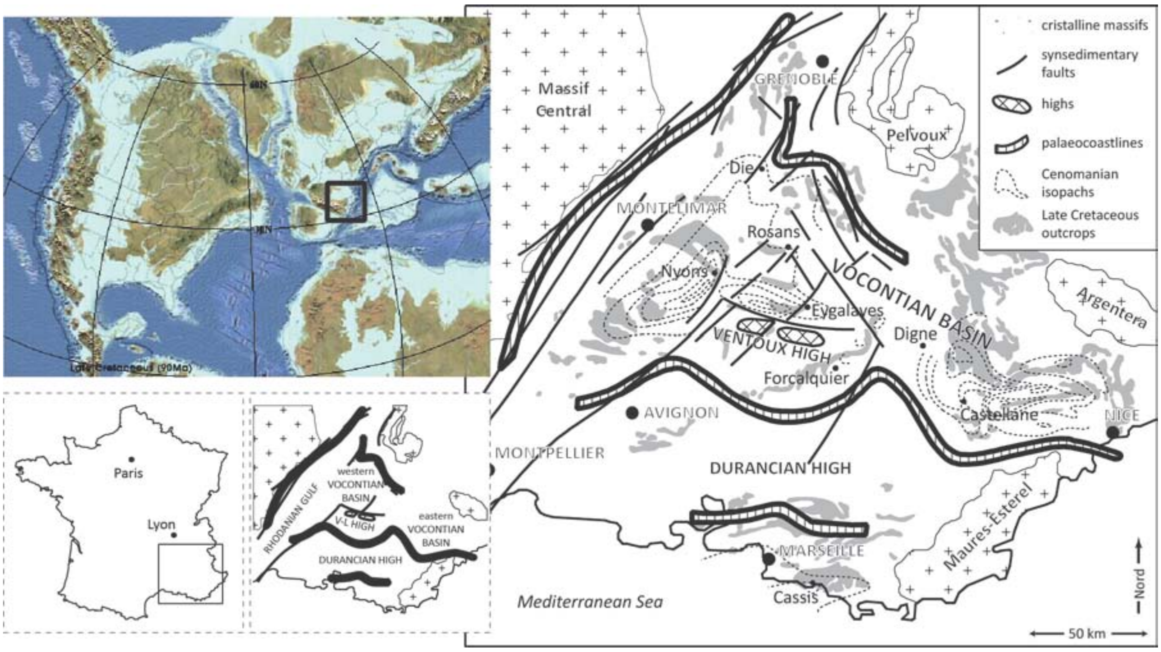


Figure 3 – *Cenomanian paleogeography of SE France (modified after Porthault 1978 and Thomel 1992b).*

Although a monographic treatment of several thousands of specimens of ammonoids collected in tens of outcrops is still in preparation, the biostratigraphic data resulting from this long-term sampling have already been exploited, especially to revise the Cenomanian ammonoid biochronology by means of quantitative methods (see corresponding chapter).

My field works focus on two major paleogeographic areas, the western and eastern part of the basin, respectively. In both areas, the Cenomanian marks the transition between the marl-dominated sediments of the Aptian and Albian to the limestone-dominated sediments of the Turonian (*Fig 4*).

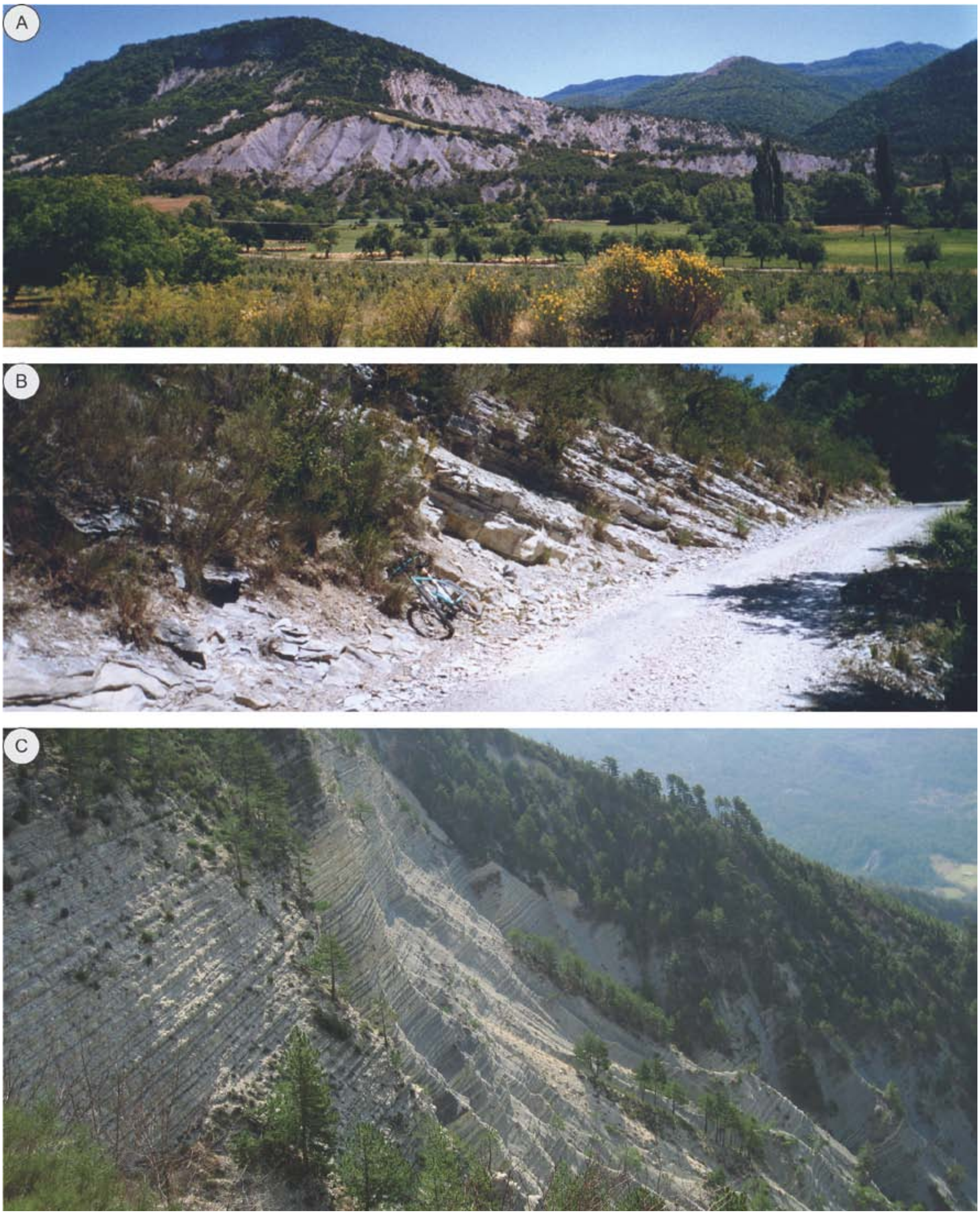


Figure 4 – *Some Cretaceous outcrops in SE France.* ***A)*** *The Albian to Turonian interval near Pommerol (the Marnes Bleues Formation of the Albian are in front and the hill is topped with the Turonian limestones).* ***B)*** *The lower Turonian limestones near Pommerol (the bike gives the scale and illustrates my major transport in the field).* ***C)*** *The Cenomanian–Turonian interval characterized by black shales near Vergons.*

Western Vocontian Basin

Most of my field works focuses on the western part of the Vocontian Basin. This area occupies an intermediate location between the continental and littoral clastic sediments of the Rhodanian Gulf to the west and the hemipelagic alternating marls and limestones of the eastern Vocontian Basin to the east (*Fig 3*). Hence, the studied fauna and their biostratigraphic content are critical for correlation at least at the basin scale (e.g. for sequence stratigraphic analyses). Contrary to the eastern Vocontian Basin, the western part is poorly studied for its macro-faunas although some areas appeared rather rich in ammonoids.

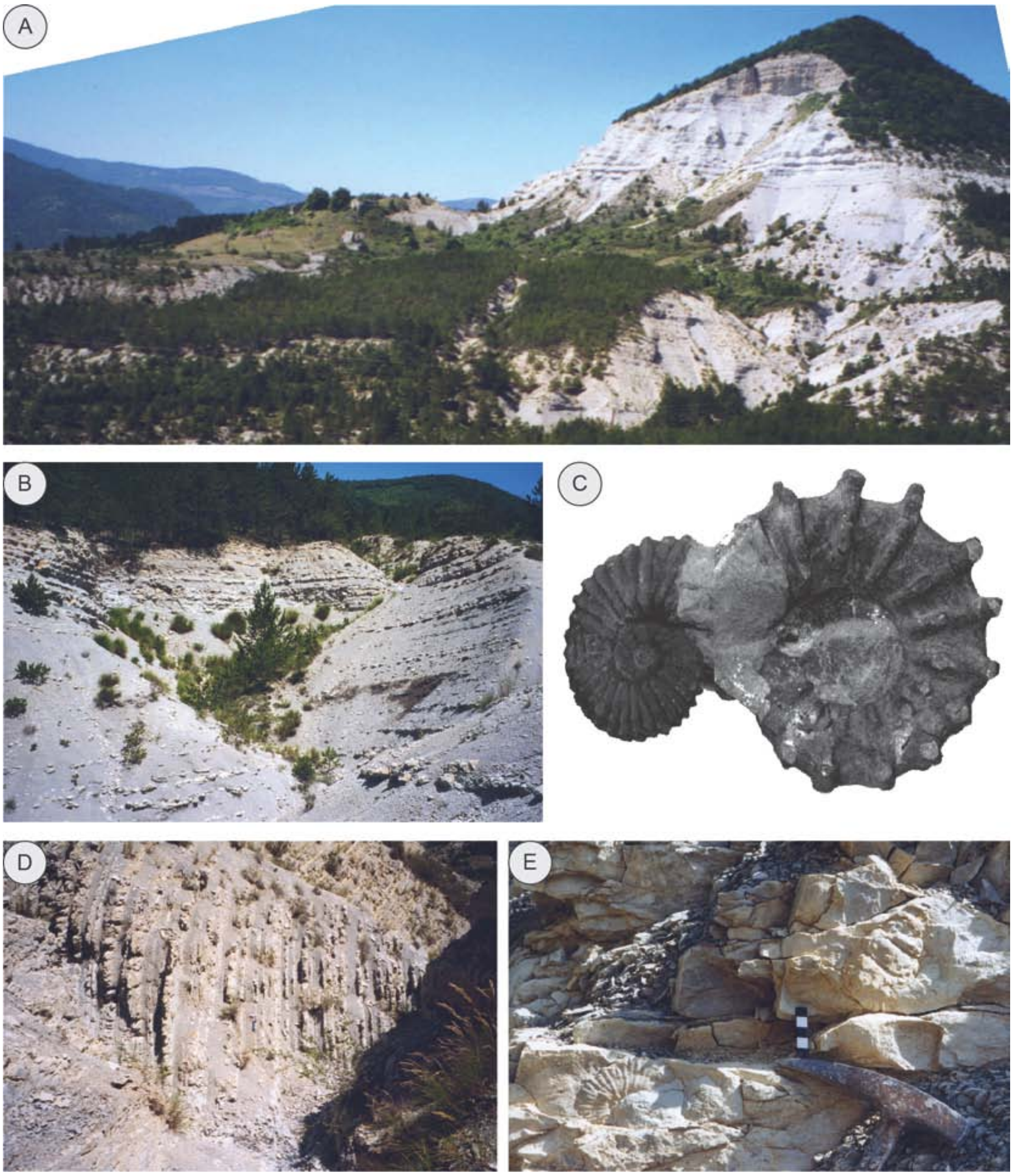


Figure 5 –** The Meouge syncline.* ***A) *The middle Cenomanian–lower Turonian outcrop of la Geneste near Gonson.* ***B)*** *The middle Cenomanian outcrop of Trisson.* ***C)*** *The ammonoids* Calycoceras *(left) and* Cunningtoniceras *(right) found in the layers illustrated in* ***B****.* ***D)*** *The lower Cenomanian outcrop of Serre Gervais.* ***E)*** *The ammonoids* Mantelliceras *(left) and* Hypoturrilites *(right) found in layers illustrated in* ***D****.*

The subalpine ranges of the western Vocontian Basin are constituted by large marl-dominated synclines elongated west–east and short limestone-dominated anticlines. Generally, the Cenomanian is a thick series of silty grey marls irregularly alternating with clayey, silty and glauconious limestones. The Cenomanian outcrops in several synclines (e.g. Eygaliers, Méouge, Chauvac, Rosans, la Charce, and Nyons). However, only the Rosans and the Méouge areas contain abundant Cenomanian ammonoid faunas. The former area is critical, especially with the GSSP of the base of the Cenomanian stage, which is defined near Rosans. The latter area is also important, because it is rich in Cenomanian ammonoids, thus complementing the work of Thomel in the eastern part of the Vocontian Basin (*Fig 5*).

Another important area of the western part of the Vocontian Basin is the Ventoux–Lure High near Forcalquier (*Fig 6*). Indeed, this area is well-known from collectors for expanded sections of the Albian/Cenomanian boundary, rich in well-preserved ammonoids. This area is thus a key area for studying this interval, especially to compensate for the drawbacks of the GSSP, which contains only flattened and small ammonoids.

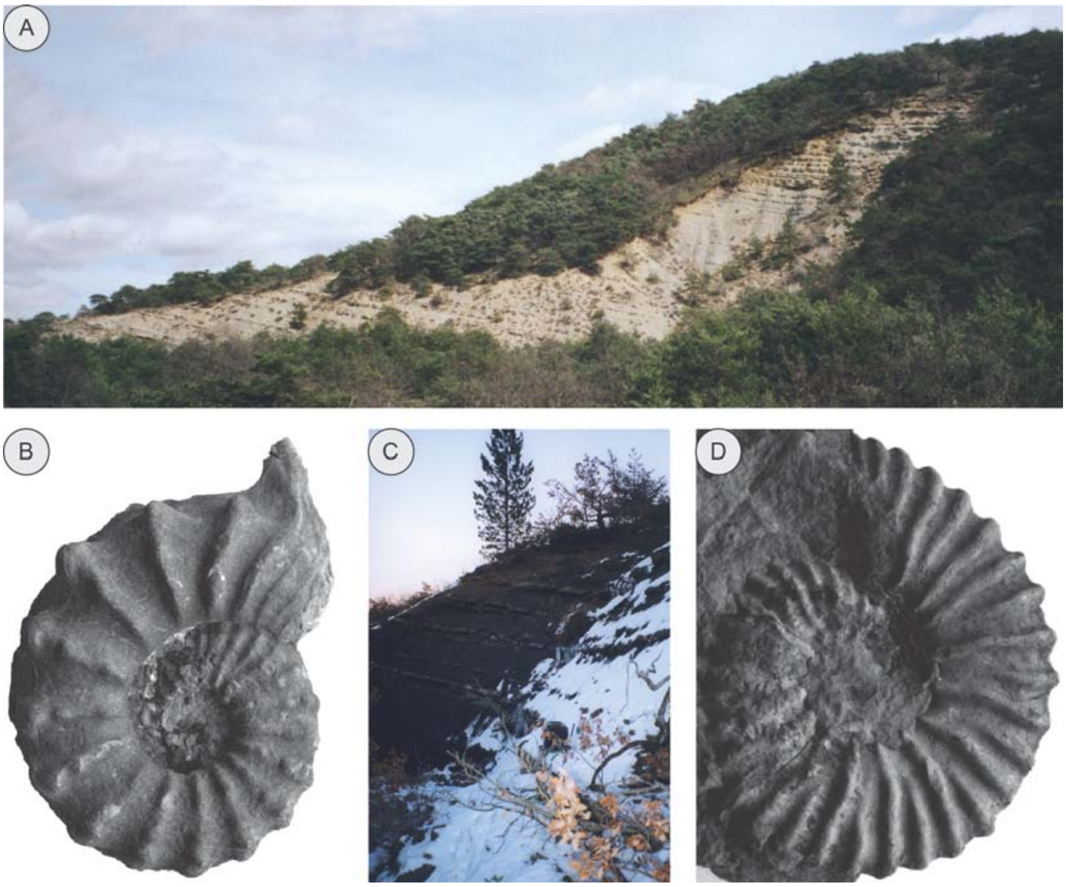


Figure 6 – *The Lure area.* ***A)*** *The uppermost Albian (Vraconian)–lower Cenomanian outcrop of Gipières.* ***B)*** *The Vraconian ammonoid* Mortoniceras rostratum *with its mature hook, deeply researched by collectors.* ***C)*** *The snowy Vraconian strata of les Vaches containing this ammonoid.* ***D)*** *The ammonoid* Mantelliceras picteti *from the lower Cenomanian of Gipières.*

Eastern Vocontian Basin

In contrast to the western area, the ammonoid faunas of the eastern Vocontian Basin are well-known thanks to more than thirty years of field works by G Thomel who focused his research on this part of the basin and published two major monographs (Thomel 1972, 1992a, b). Despite this tremendous field-work, the Cenomanian ammonoid faunas of SE France still require to be intensively revised, because the taxonomy of Thomel is flawed by over-splitting and misunderstanding compared to the standard taxonomy leaded by WJ Kennedy (Wright & Kennedy 1984, 1987, 1990). Hence, one major goal of my research in SE France was to sample and revise ammonoid faunas, especially by accounting for intraspecific variation. In addition, the published biostratigraphy of Thomel contains major discrepancies with other well-sampled and described areas such as England and Germany, and my works was also to evaluate the reality of these biostratigraphic differences (which now appear mainly due to taxonomic misidentification).

Another major purpose of my research in this area is to focus on the Cenomanian/Turonian boundary. Indeed, this basin is well-known to record the Oceanic Anoxic Event 2 (OAE2), which is associated to a moderate mass extinction and characterized by the sedimentation of black shales. But the major point is that this basin is one of the rare basins in the world to record this OAE2 in different settings and to have expanded sections of thousands of meters straddling this interval. Therefore, the Vocontian Basin is a key area for the Cenomanian/Turonian boundary, and in addition to the collection of ammonoids during this interval, my field works enabled me to actually assess the extant and impact (or not) of this event (see macroevolution chapter).

In this context, my research focuses on two major outcrops, which are characterized by two different paleoenvironments: The Vergons section with deep, basinal series, and the la Foux section with typical shelf break series.

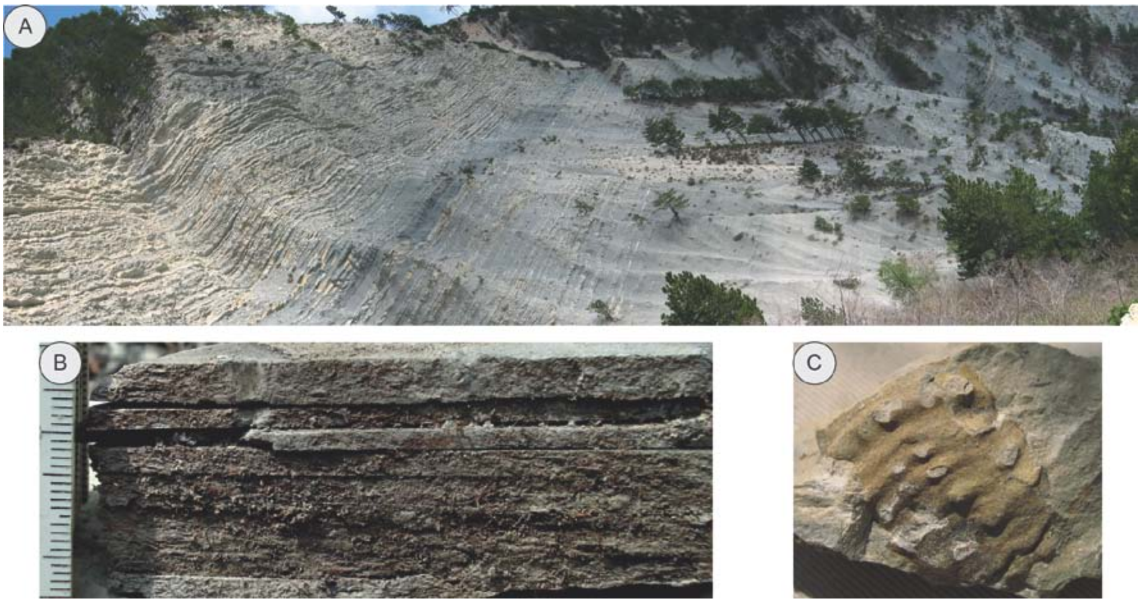


Figure 7** – The Vergons section.* ***A) *Top of the outcrop with the black shales at the Cenomanian/Turonian boundary.* ***B)*** *The black shales marking the OAE2.* ***C)*** *The ammonoid* Euomphaloceras septemseriatum *of the uppermost Cenomanian (base of the OAE2).*

The Vergons section is a worldwide, well-known and studied section with black shales characterizing the OAE2 (*Fig 7*). Although a key section for the study of this anoxic event, it remains poor in ammonoids around the Cenomanian/Turonian boundary.

The la Foux – les Lattes area near Castellane is less known than the Vergons area, but probably more important. In this area, the Cenomanian/Turonian boundary outcrops abundantly and in expanded sections with abundant macro-faunas, but it is devoid of black shales (*Fig 8*).

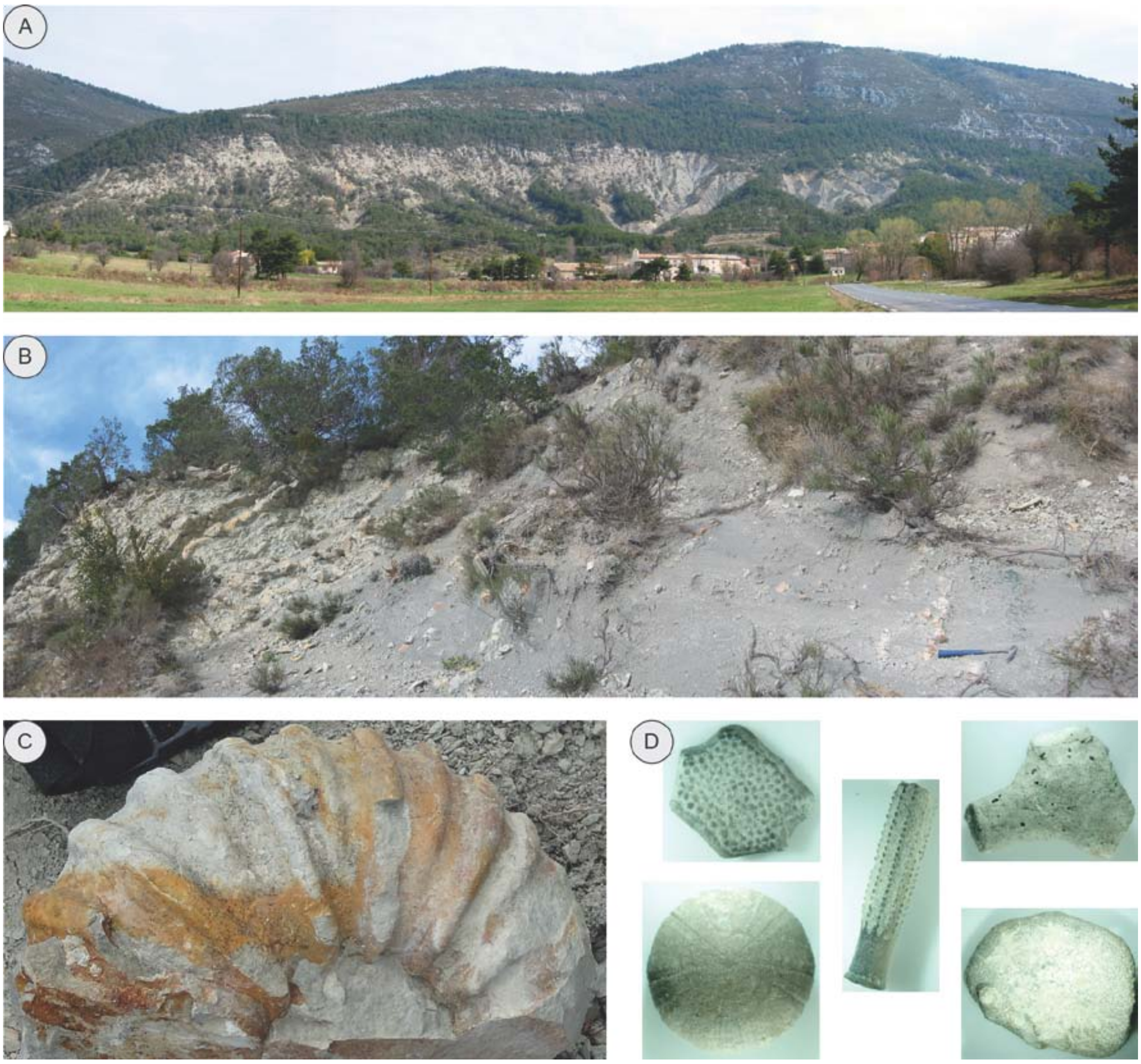


***Figure 8 –** The la Foux – les Lattes area. **A)** The Cenomanian/Turonian boundary at la Foux. **B)** The Cenomanian/Turonian boundary at les Lattes; this interval is the age-equivalent to the black shales of Vergons; note the green glauconious level marked by the hammer. **C)** The ammonoid* Calycoceras *of the lower upper Cenomanian. **D)** Some of the fossils (starfish, echinoids, bryozoans, and sponge) found in the layers equivalent to the OAE2 (above the glauconious level underlined by the hammer in **B**).*

The comparison of the stratigraphic record of the Cenomanian/Turonian boundary (CTB) between these two contrasted areas has been published (Monnet & Bucher 2007a). It enabled me demonstrating that the impact of the OAE2 on the extinction event of this interval is over-rated. Indeed, this study reveals and emphasizes several important results: (1) in both, the Anglo-Paris and Vocontian basins, the occurrence of oxygen-depleted water masses are confined to the deepest parts and limited in time to the *geslinianum* and *juddii* Zones (latest Cenomanian); (2) in both basins shelf environments were fully oxygenated as demonstrated by oxygen and carbon isotope studies in the Anglo-Paris Basin and by abundant and highly diverse benthic and planktonic faunas in the Vocontian Basin; and (3) in both basins the major changes of ammonoid faunas (diversity decline, evolutionary changes, taxonomic restructuring) started around the middle/late Cenomanian boundary (the *guerangeri* Zone), one ammonoid zone before the onset of the spreading of anoxic water masses in the deeper settings (the *geslinianum* Zone). Therefore, although I agree that there is extensive evidence for widespread anoxia during the CTB interval in deep-water environments, my field work investigation and biodiversity analyses (Monnet et al 2003) rule out anoxia as the cause of the ammonoid crisis in northwest Europe. The latter predates by about 0.75 Myr the evidence of anoxia in these basins. This lag is long enough to preclude anoxia as a killing-mechanism for ammonoids. Moreover, available data challenge the classic hypothesis that anoxia spread onto shelves during the late Cenomanian. Therefore, other causative mechanisms must have initiated the moderate CTB mass extinction, although the OAE2 had contributed to the disruption of marine ecosystems and consequently to extinctions. These results show the need to reassess the widely invoked causal link between anoxia and the moderate mass extinction at the Cenomanian/Turonian boundary (see macroevolution chapter).

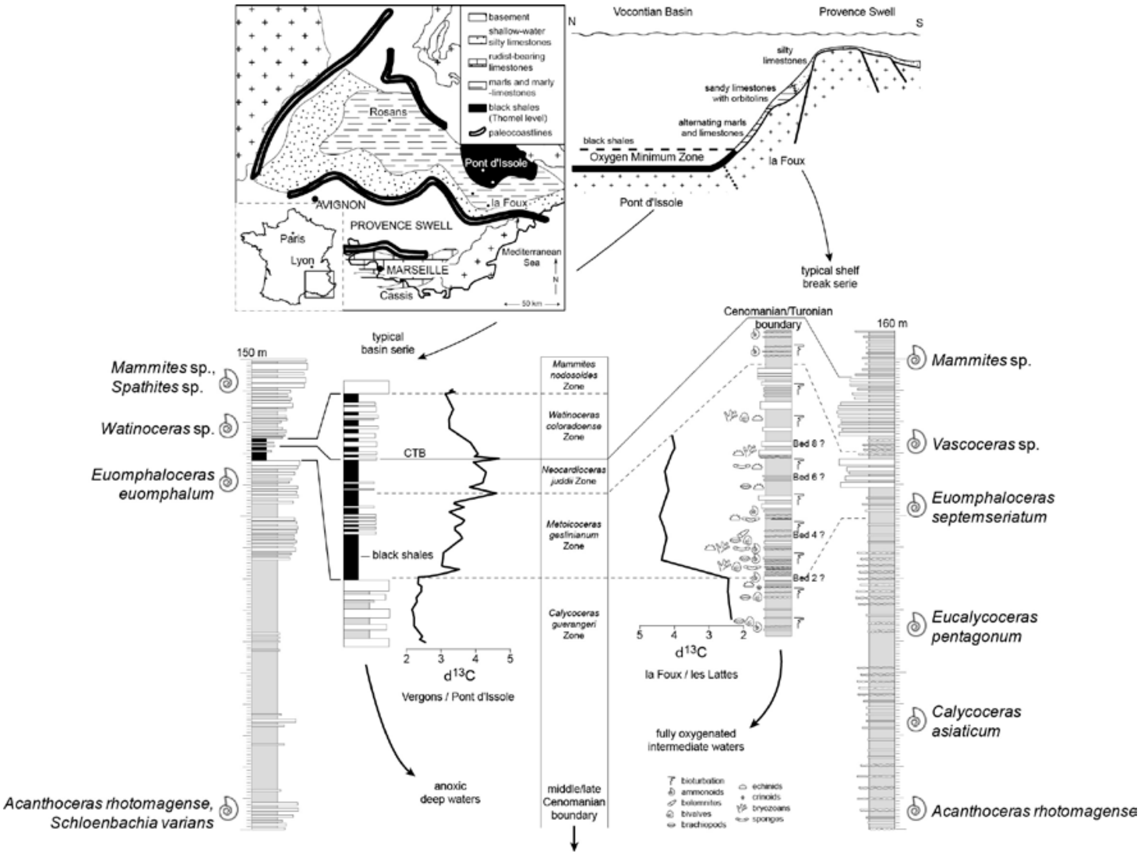


Figure 9 – *Carbon isotope stratigraphy and ammonoid biostratigraphy of the la Foux and Vergons sections in the Vocontian Basin (modified after Monnet & Bucher 2007a).*

In conclusion, the Vocontian Basin is a key area to study the Cenomanian/Turonian interval, not only for macro- and micro-fossils, but also for geochemical and sedimentary analyses. For instance, in this context, I helped other researchers to conduct their studies on the geochemy of this CTB in SE France (see Frau 2012). Also, I directed and organized several field-trips for Master students in geology and paleontology.

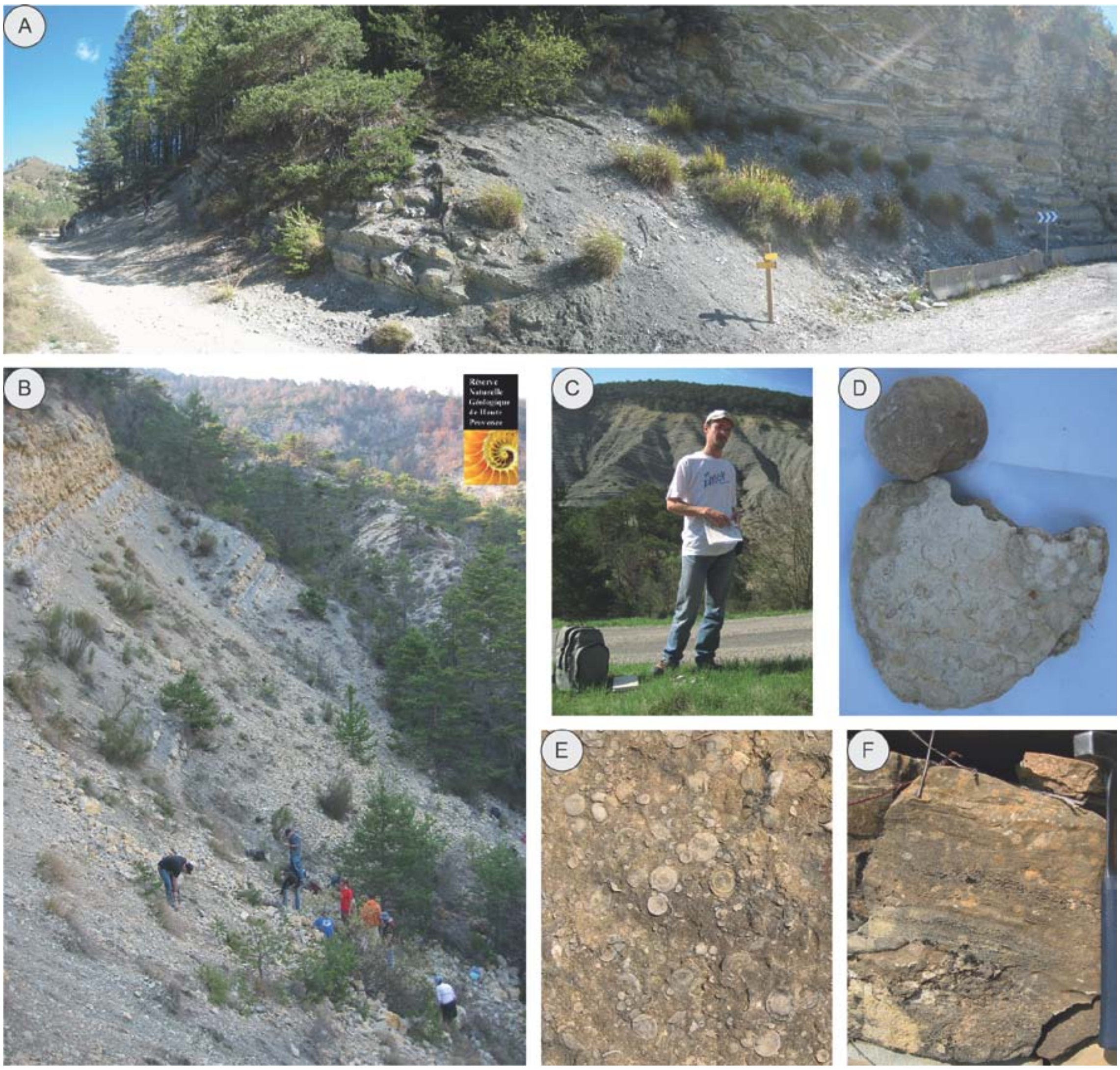


Figure 10 – A) *The Cenomanian/Turonian boundary at Pont d'Issole with a Burgundy team collecting samples for geochemical studies (C Thomazo, A Brayard, C Frau).* ***B)*** *The middle Cenomanian near le Bourguet with a PIMUZ team supervising Master students.* ***C)*** *Me, talking about facies correlation in front of the lower Cenomanian near le Bourguet.* ***D)*** *Lower Turonian ammonoids (*Fagesia*,* Choffaticeras*) from le Bourguet.* ***E)*** *The centimetric alveolinids (benthic Foraminifera) of the lower Cenomanian of le Bourguet that often underline HCS sedimentary structures (****F****).*

TRIASSIC OF NEVADA AND SOUTHERN ALPS

A second important part of my research in alpha taxonomy is the monographic description of Anisian ammonoid faunas from north-western Nevada (USA) and the Southern Alps (Italy). Similarly to my researches on the mid-Cretaceous, such taxonomic works also lead to biostratigraphic data enabling quantitative revision of the biochronological zonation of the studied interval (see corresponding chapter).

Anisian of Nevada

The base of my research in Triassic ammonoids results from several field-trips in Nevada (USA) that led to a published monograph (Monnet & Bucher 2005). This work focusing on the middle/late Anisian interval complements the study of Bucher (1989, 1992a, b) covering the lower and middle Anisian and the study of Silberling & Nichols (1982) covering the late Anisian.

Monnet & Bucher (2005) conducted an intensive investigation of the Fossil Hill Member in the Augusta Mountains (north-western Nevada) leading to the recognition of new ammonoid faunas that bracket the middle/late Anisian boundary. These faunas are of great significance for biochronological correlation across the low paleolatitude belt from the eastern Pacific to the western end of the Tethys. Three new sections in the Augusta Mountains have yielded a rich faunal succession, whose upper part correlates with the resampled lower portion of the classic Fossil Hill section in the Humboldt Range.

Eleven genera (*Chiratites*, *Billingsites*, *Dixieceras*, *Jenksites*, *Rieppelites*, *Rieberites*, *Marcouxites*, *Silberlingia*, *Ceccaceras*, *Brackites*, *Oxylongobardites*) and fifteen species (*Balatonites hexatuberculatus*, *Chiratites retrospinosus*, *C. bituberculatus*, *Billingsites cordeyi*, *B. escargueli*, *Gymnotoceras weitschati*, *G. mimetus*, *Jenksites flexicostatus*, *Rieppelites boletzkyi*, *R. shevyrevi*, *Rieberites transiformis*, *Silberlingia praecursor*, *Ceccaceras stecki*, *Brackites spinosus*, *Oxylongobardites acutus*) have been newly described. "*Ceratites*" *lawsoni* and "*Ceratites*" *spinifer*, as previously described by Smith (1914) and subsequently synonymized by Silberling & Nichols (1982), were recognized as valid species and assigned to the new genera *Dixieceras* and *Marcouxites*, respectively. Some of these new taxa have been subsequently collected in other basins such as in Southern Alps and South China (Monnet et al 2008; Stiller & Bucher 2008), therefore corroborating the validity of these taxa and their worldwide utility.

In the new biostratigraphic sequence, the scope of the latest middle Anisian *Shoshonensis* Zone is expanded by the introduction of a new uppermost subdivision, namely the *Bulogites mojsvari* Subzone, which correlates with the Grossreifling fauna of the western Tethys. The *Gymnotoceras weitschati* Zone and *Gymnotoceras mimetus* Zone are introduced at the base of the Late Anisian, in ascending order. The *Weitschati* Zone, composed of the *Billingsites cordeyi* and *Rieberites transiformis* subzones, is approximately equivalent to the ill-defined *Trinodosus* Zone of the Tethyan realm. Included in the *Mimetus* Zone are the *Dixiceras lawsoni* and *Marcouxites spinifer* subzones. The *Gymonotoceras rotelliformis* Zone, which was formerly considered as a correlative of the *Trinodosus* Zone, was previously subdivided into five subzones, mainly on the basis of various species referred to as "*Paraceratites*". These species, whose respective ranges are shown to largely overlap, are reassigned to the new genera *Silberlingia*, *Ceccaceras*, and *Brackites*. Hence, the number of subdivisions of the *Rotelliformis* Zone is reduced to two, namely the *Brackites vogdesi* and *Gymnotoceras blakei* subzones, in ascending order. Some of these new ammonoid zones are now documented also in other areas (Southern Alps and South China; Monnet et al 2008; Stiller & Bucher 2008), therefore corroborating the newly established biozonation.

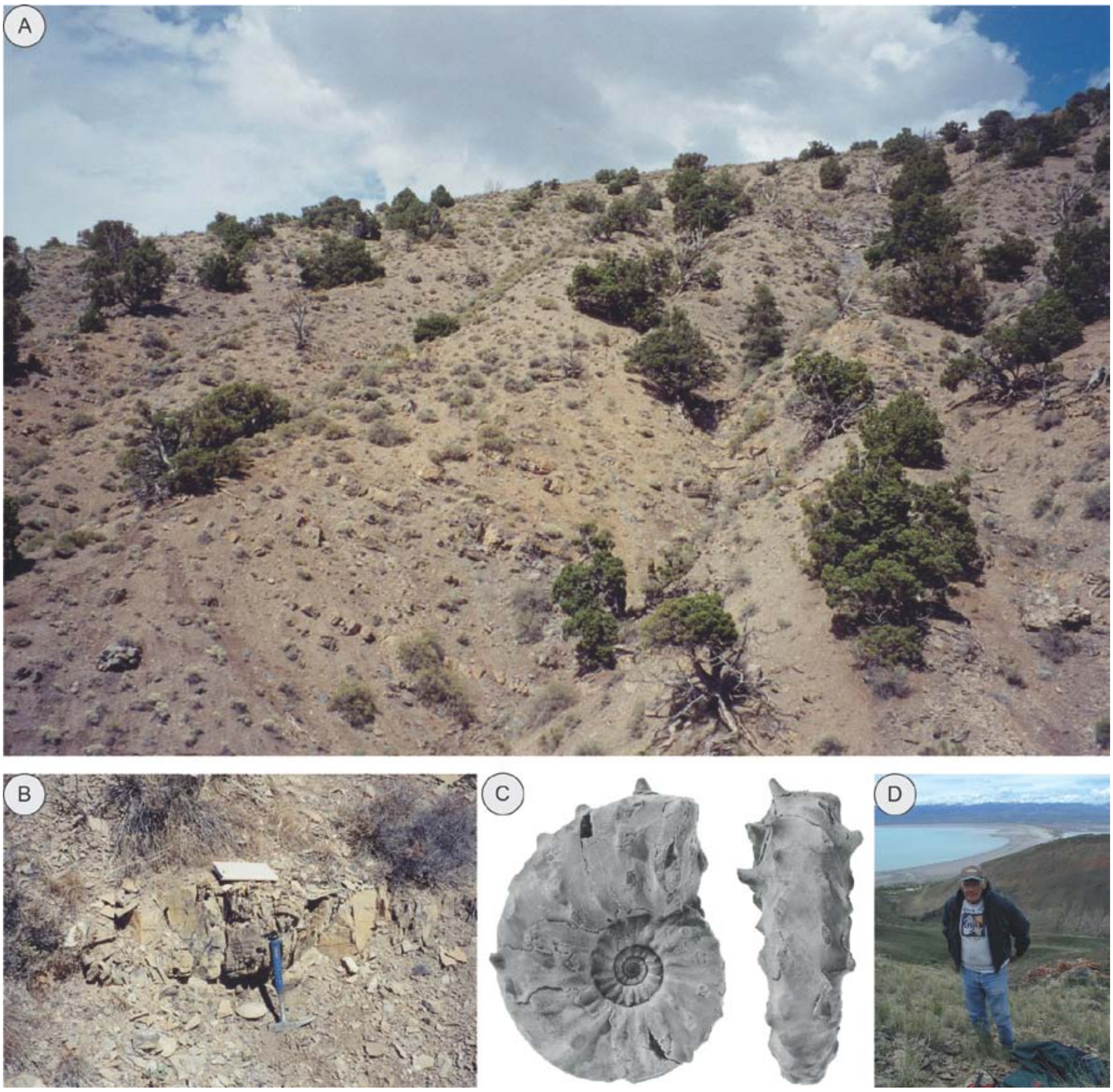


Figure 11 – *The Augusta Mountains (Nevada, USA).* ***A)*** *The upper Anisian outcrop of Fergusson Canyon.* ***B)*** *The bed HB2016 of Rieber Gulch outcrop.* ***C)*** *The newly described ammonoid* Brackites vogdesi *characteristic of the newly erected late Anisian subzone* Vogdesi. ***D)*** *Jim Jenks whose assistance in the field of Triassic rocks in the USA and friendship are invaluable.*

Anisian of Southern Alps

The ammonoid biostratigraphy of the middle/late Anisian boundary has a long and controversial history (Assereto 1971; Tozer 1984) marked by the famous *binodosus* and *trinodosus* zones starting from the key work of Mojsisovics et al (1895). My previous studies in Nevada allowed establishing a new ammonoid scheme and taxonomy independently of the old Tethyan data. Therefore, one consequence was to confront the two areas in order to resolve, at least in part, some of the known discrepancies. Therefore, I conducted several field-works in classical Tethyan localities of Southern Alps, leading to the publication of Monnet et al (2008). In this context, this research complements the works of Balini (1992a, b).

Monnet et al (2008) sampled ammonoids with a precise stratigraphic control at the middle/late Anisian (Pelsonian/Illyrian) boundary from a new locality in eastern Lombardy-Giudicarie (Monte Guglielmo) and from classical sections in Giudicarie (Stabol Fresco, Malga Avalina, Corno Vecchio). These ammonoid faunas allow revising the taxonomic interpretation of *Ceratites cimeganus* Mojsisovics, 1882 and of the genus *Paraceratites* Hyatt, 1900. *Ceratites cimeganus* is here assigned to the North American genus *Rieppelites* Monnet & Bucher, 2005.

In eastern Lombardy-Giudicarie, *R. cimeganus* is diagnostic of a distinct biochronological unit (*cimeganus* Zone) bracketed between the older *Bulogites zoldianus* Zone and the younger *Judicarites euryomphalus*–*Paraceratites trinodosus* zones. The recognition of this *cimeganus* Zone significantly improves worldwide correlation since it is recognized in several other Tethyan basins (Dolomites, Northern Calcareous Alps) as well as in North America (Nevada). These new data allow a redefinition of the middle/late Anisian boundary in the western Tethys, which is here intercalated between the *zoldianus* and *cimeganus* zones. This limit is marked by a clear ammonoid turnover (disappearance of *Acrochordiceras* and *Balatonites*, appearance of *Rieppelites*).

Finally, the presence of sections including the *cimeganus* Zone in eastern Lombardy-Giudicarie allow the establishment of local gaps in sedimentation, which may reflect the regional and important transgression of the pelagic Prezzo Limestone over the shallow water platform carbonates of a “Camorelli-Dosso dei Morti barrier”, as also underlined by the spatial distribution of brachiopod lumachellas (for further details, see Monnet et al 2008).

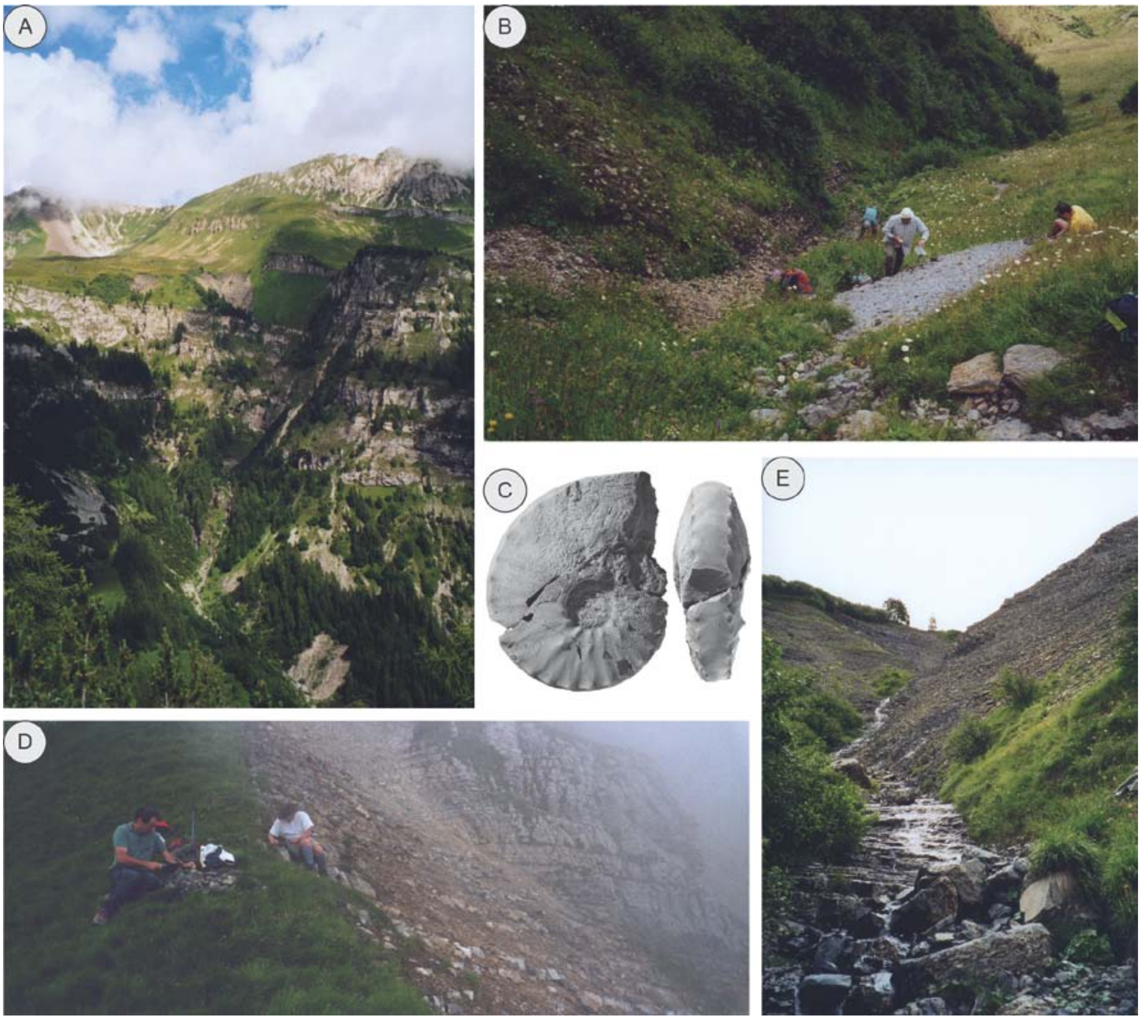


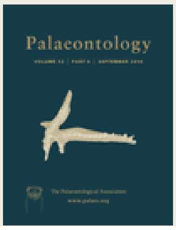
Figure 12 –** The Anisian of Southern Alps.* ***A) *The Stabol Frasco outcrop in the middle of nowhere.* ***B)*** *A PIMUZ team sampling the bone bed of the Monte Gugliemo section.* ***C)*** *The upper Anisian ammonoid* Rieppelites cimeganus *from Monte Guglielmo.* ***D)*** *Hugo Bucher and Stéphane Bouchet digging for ammonoids on the foggy Corno Vecchio section.* ***E)*** *The Stabol Fresco section with the* Bulogites *beds at the bottom.*

Intraspecific variation and covariation

Related publications:

Monnet & Bucher 2005; **Monnet** et al 2010, 2015b; De Baets et al 2013, 2015; Jattiot et al 2016; unpublished data

Appended publication:



Monnet C, Bucher H, Wasmer M, Guex J (**2010**) Revision of the genus *Acrochordiceras* Hyatt, 1877 (Ammonoidea, Middle Triassic): morphology, biometry, biostratigraphy and intraspecific variability.
***Palaeontology* 53:961–996**
(doi: 10.1111/j.1475-4983.2010.00956.x)

Many ammonoid taxa have long been known to show a huge degree of morphological variation of their conch (Kennedy & Cobban 1976; De Baets et al 2015). Morphological variability is an important subject in evolutionary studies because genetic variation and thus its morphological reflection is one of the driving factors of evolution. To some extent, intraspecific morphological variability reflects the evolvability of species and their evolutionary dynamics by promoting diversification and by protecting against extinction (West-Eberhard 1989, 2003; Wagner & Altenberg 1996; Sniegowski & Murphy 2006; Kolbe et al 2011). High levels of morphological variability have been attributed to ecological and developmental mechanisms, including selection for ecological generalists in an unstable environment (Simpson 1944; Parsons 1987; but see Sheldon 1993), adaptation to a variable hydrodynamic regime (Jacobs et al 1994), inherent developmental plasticity (Yacobucci 1999), and the lack of competitors (Erwin et al 1987; Valentine 1995).

This very broad range of shell shapes of many ammonoid species continues to present a challenge for delimiting and distinguishing species, which becomes even more important when it concerns taxa widely used in biostratigraphy (Reeside & Cobban 1960; Kennedy & Cobban 1976; Dzik 1985). Analysis of intraspecific variability is thus a prerequisite for many paleobiological and evolutionary studies. Therefore, one important aspect of my research in alpha taxonomy is to account for and evaluate intraspecific variation of the ammonoid shell as thoroughly as possible and by means of quantitative analyses of the standard shell parameters (Monnet & Bucher 2005; Monnet et al 2010; Jattiot et al 2016). Besides, I recently co-authored a thorough review of intraspecific variation of ammonoids (De Baets et al 2015). Also, one striking feature that emerges when studying the intraspecific variation of the ammonoid shell at the species rank is that aspects of intraspecific variation of ammonoid shell features are often not random and covary in determinate patterns, which I recently reviewed (Monnet et al 2015b).

INTRASPECIFIC VARIATION

Mollusks in general and ammonoids in particular are known to display a sometimes profound morphological intraspecific variability of their shell. Although this phenomenon is of greatest importance, it is rarely investigated and quantified. It is especially crucial for taxonomy and incidentally for macroevolutionary analyses to account for it (e.g. in biodiversity the number of described species might exceed that of actual species within any group).

For ammonoids, the studies of intraspecific variability published so far focused mainly on Mesozoic taxa of coiled ammonoids (Reeside & Cobban 1960; Westermann 1966; Kennedy & Cobban 1976; Hohenegger & Tatzreiter 1992; Dagys & Weitschat 1993; Checa et al 1996; Dagys et al 1999; Morard & Guex 2003; Monnet & Bucher 2005; Weitschat 2008). All of these studies documented a large intraspecific variability in coiling (degree of involution), whorl shape, and ribbing (spacing, strength). They revealed a continuous spread of morphotypes between two extreme variants, with an intermediate shell shape being the most common.

My works on intraspecific variation of ammonoids are here illustrated by two papers: Monnet et al 2010 and De Baets et al 2013, which deal with monomorph and heteromorph ammonoids, respectively, by means of quantitative analyses in addition to the classical, empirical comparative approach.

Monomorphs

Monnet et al (2010) investigated in details the family Acrochordiceratidae, which ranges in age from latest Spathian to the late Anisian, and which represents a major component of ammonoid faunas during that time. The middle Anisian genus *Acrochordiceras* is the most widespread taxon of the family and occurs abundantly worldwide within the low paleolatitude belt. However, there is a profusion of species names available for *Acrochordiceras*. This excessive diversity at the species level essentially results from the fact that sufficiently large samples were not previously available, thus leading to a typological approach of its taxonomy.

Based on new extensive collections obtained from the Anisian (Middle Triassic) Fossil Hill Member (Star Peak Group, north-west Nevada) for which a high resolution biostratigraphic frame is available (Monnet & Bucher 2005), the taxonomy and biostratigraphy of the genus *Acrochordiceras* Hyatt, 1877 has been revised with respect to its intraspecific variation. Morphological and biometric studies (ca. 550 bedrock-controlled specimens were measured) showed that only one species occurs in each stratigraphic level. Continuous ranges of intraspecific variation of studied specimens enable to synonymize *Haydenites* Diener, 1907, *Silesiacrochordiceras* Diener, 1916 and *Epacrochordiceras* Spath, 1934 with *Acrochordiceras* Hyatt, 1877. Three stratigraphically successive species have been recognized in the low paleolatitude middle Anisian faunas from Nevada: *A. hatschekii* (Diener, 1907), *A. hyatti* Meek, 1877 and *A. carolinae* Mojsisovics, 1882.

Moreover, an assessment of intraspecific variation of the adult size range does not support recognition of a dimorphic pair (*Acrochordiceras* and *Epacrochordiceras*) as previously suggested by other workers (compare Dzik 1990 and Monnet et al 2010): *Epacrochordiceras* is the compressed and weakly ornamented end-member variant of *Acrochordiceras* (*Fig 1*). The successive middle Anisian species of *Acrochordiceras* form an anagenetic lineage characterized by increasing involution, adult size and intra-specific variation. This taxonomic revision based on new bedrock-controlled collections was thus an important prerequisite before studying the evolution of the group (Monnet et al 2012, 2013).

Figure 1 – *Intergrading morphological series illustrating the covariation pattern between ornamentation robustness, whorl section, and degree of involution for a paleo-population of* Acrochordiceras carolinae *from a single stratigraphic bed (after Monnet et al 2010, 2015b).*

Heteromorphs

De Baets et al (2013) investigated in details the intraspecific variation of some Devonian heteromorph ammonoids from Morocco. These early ammonoids typically suffer from a splitting bias. For instance, most specimens from the same layer and the same region (e.g. the *Erbenoceras* beds of the Moroccan Anti-Atlas studied in this paper) differ morphologically from each other. Depending on the importance given to certain morphological characters, therefore, one could create a new species for almost every specimen.

In this study, nearly 100 specimens from a restricted stratigraphic interval were measured and used to quantify the shell variability. This study illustrates that some of the earliest ammonoids exhibit great intraspecific variability, which hampers comparison between samples with few specimens. The data suggest the presence of at least two taxonomic groups within the studied beds, both of which are highly variable in coiling and rib spacing and have transitional forms between extreme variants. In Group II (*Erbenoceras*), which has the most specimens, the unimodal frequency distribution in conch parameters and rib spacing for several size classes throughout ontogeny corroborates the group's status as a single very variable species (*Fig 2*). The variants fall on a spectrum from forms with coarser and more widely spaced ribs and tighter coiling (''*E. solitarium*'') to forms with coarse and more densely space ribs, and often looser coiling (''*E. advolvens*''). In both groups, coiling as expressed by the whorl interspace index (comparable to the whorl imprint zone in coiled ammonoids) is the most variable character, followed by rib spacing and whorl height index, and the umbilical width index is the least variable of the parameters.

When ontogenetic trajectories of the Moroccan specimens are compared with coeval faunas from other regions (assigned to other species), a strong overlap between the morphospace occupied by these taxa becomes apparent. The justification of some of these latter species is thus questionable even if their mean values in some conch parameters differ considerably from the mean values of the Moroccan species. At least three previously described Moroccan species of *Erbenoceras* fall in the range of morphological variability of a single species, and four species of *Erbenoceras* defined outside of Morocco fall in the range of variability of the Moroccan specimens (Group II). In Group I (*Anetoceras*), the frequency distribution is not unequivocally unimodal, which might reflect either the presence of multiple species or the lower sample size. The ranges of variability from the *Anetoceras* specimens from southern China do not overlap completely with those of the two Moroccan taxa. This supports a taxonomic separation. However, a firm conclusion is hampered by the comparisons of samples, which might be too small to show the continuous range of variation, and more non-Moroccan specimens are necessary to further test these hypotheses and formally synonymize these taxa. Hence, the number of currently valid species of these loosely coiled early ammonoids is probably much too high. Extreme caution must therefore be taken when examining the diversity of groups in which the intraspecific variability is poorly known.

The above results reflect the importance of thorough examinations of intraspecific variability in taxonomy, which has always been and commonly still is neglected. This often causes over-splitting of taxa, i.e. the erection of taxa whose systematic justification cannot be tested. Although single species can show a great variability in coiling or ribbing, they may still be separated by using their entire ontogeny and comparing the frequency distribution of certain parameters through ontogeny. Also, whether or not the large variability in heteromorph ammonoids is caused by the poorer morphological constraints because of their loose coiling must be tested further (ongoing work).

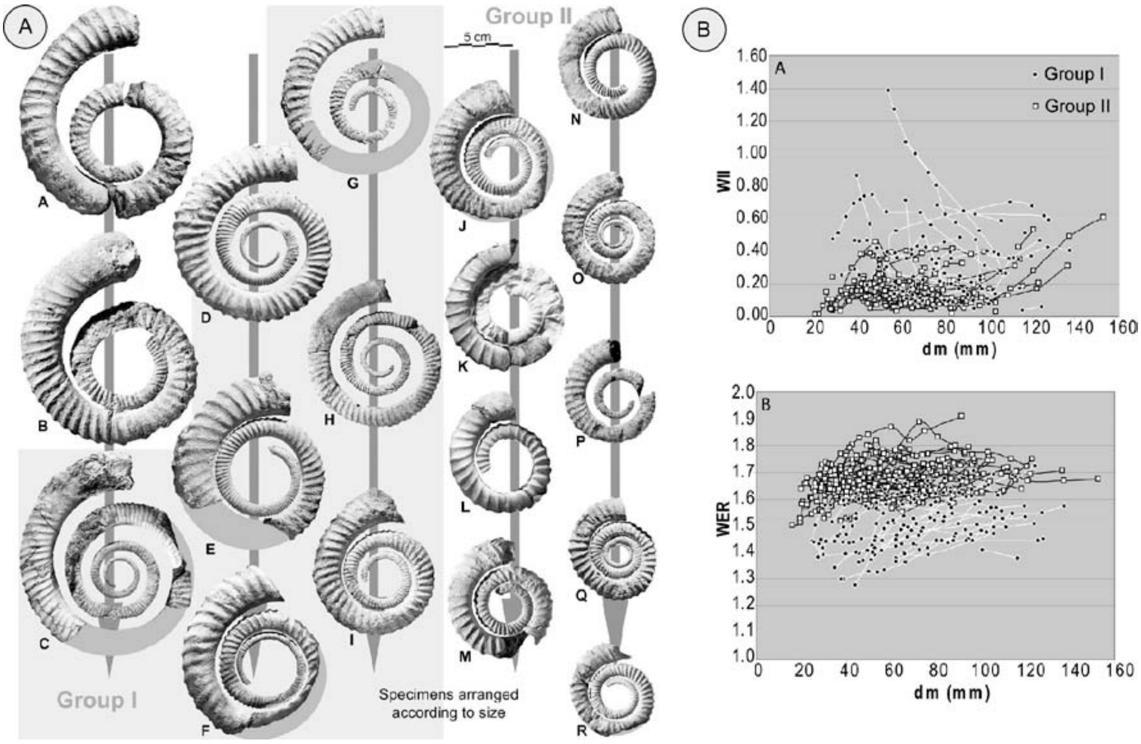


***Figure 2 –** Shell variability of heteromorphs (after De Baets et al 2013). **A)** Some specimens of Group I (''*Anetoceras''*) and Group II (''*Erbenoceras''*) arranged according to size. **B)** Bivariate plots of whorl interspace index (WII) and whorl expansion rate (WER) for all Moroccan specimens of Group I (black fillings, white lines) and Group II (white fillings, black lines); multiple measurements of the same specimen through ontogeny are connected by a line.*

COVARIATION PATTERNS

As illustrated above, ammonoids display a sometimes profound morphological intraspecific variation of their shell. One striking aspect of this intraspecific variation is that it is very often not randomly distributed and characterized by the covariation of determinate shell features. The morphology of the ammonoid shell can be separated into three major sets of characters, which are the geometry of the shell tube (including whorl shape and degree of involution), its ornamentation, and the suture shape. These three categories all display patterns of covariation, which were first described over a century ago (Buckman 1892; Jayet 1929; Haas 1946) and more recently have been used to characterize the intraspecific variation of ammonoids. These patterns have been coined as the Buckman's rules of covariation (Westermann 1966). I recently published a review (Monnet et al 2015b) with regard to these covariation patterns. The major points highlighted by this review are summarized below.

The rules

Buckman’s first rule of covariation was coined by Westermann (1966) for the interdependence between the basic shell geometry (involution of the shell and shape of the whorl section) and the coarseness of shell ornamentation. In other words, the more evolute, the more depressed and the more ornamented the ammonoid shell is (*Fig 1*). As initially defined, this pattern of covariation holds within a species (i.e. intraspecific variation) of ammonoids. Indeed, many authors have characterized a species as a variable species ranging from compressed forms that have dense, fine ribs and small tubercles to more robust forms that have fewer but more robust ribs and more rounded tubercles (e.g. the classical example of the Cenomanian *Acanthoceras*: Kennedy & Hancock 1970; Wright & Kennedy 1987). This law was recently reformulated by Hammer & Bucher (2005): ‘‘size of lateral and ventral ornamentation correlates with size of the aperture (in width and height respectively)’’; however, some counter examples exist, so this correlation needs to be further tested. This is, however, hard to quantify, because the upper part of the ribs are easily damaged during preparation and rib strength/relief is difficult to measure (Yacobucci 2004).

Buckman’s second rule of covariation was coined by Westermann (1966) for the interdependence between the geometry of the whorl section and suture frilling: the more compressed the whorl section, the more frilled the suture line. Contrary to the first rule, which is abundantly recognized in large samples, the second rule between shell geometry and suture frilling may not necessarily hold in all these cases (Dagys et al 1999; Dagys 2001) or may be muted by larger constraints on suture pattern than shell shape (Yacobucci & Manship 2011).

These patterns of covariation of specific shell characters have been abundantly documented in very different taxonomic groups and throughout the entire evolutionary history of ammonoids (see references in Monnet et al 2015b). However, the recognition of these patterns requires an abundant material, relatively well-preserved; hence, these rules are not always identified, especially in the Paleozoic and for heteromorphs. Furthermore, even with abundant material, intraspecific variation of ammonoids often depart from these rules (De Baets et al 2015). As noted by Bert (2013), it appears that Buckman's rules of covariation are not the only covariation patterns of intraspecific variation of ammonoids, although these rules may be more common.

Quantification

Although frequently described, these patterns of covariation are rarely assessed quantitatively, even though such an approach could be used to evaluate species delimitations and investigate the evolution of intraspecific variation. The covariation pattern involves the conch geometry (shape and coiling) and the shell ornamentation (robustness and density). The ammonoid shell geometry can be quantified by using the classical linear measurements usually supplied with systematic descriptions of ammonoid species (*Fig 3*): D, shell diameter; H, whorl height; U, umbilical diameter; and W, whorl width. Conch geometry can be then approximated with the following ratios: degree of compression of whorl section (ratio H/W; ellipsoid of whorl shell aperture), and degree of involution (ratio U/D; amount of overlap between successive whorls). These ratios provide a relative metric, which allow shells of different size to be compared. Note, though, that these ratios are known to change through ontogeny. The ornamentation of the ammonoid shell is a very important diagnostic character. Ornamental characters may be relatively diverse but are described mostly as qualitative, discrete characters. The degree of ornamentation can be approximated by the density of these ornaments and by their thickness. The former (often available in the literature) can be expressed as the number of (ventral) ribs (and/or tubercles) per whorl or half-whorl at a distinct diameter (R/D). The latter (rarely available in the literature) can be characterized by the difference of height and width of the whorl section (H and W) measured exactly on top of a rib and between two consecutive ribs (RH and RW, respectively; see Hammer & Bucher 2005). Note that ribbing density and strength of ornamentation are mostly negatively correlated (compare Bert 2013; De Baets et al 2015).

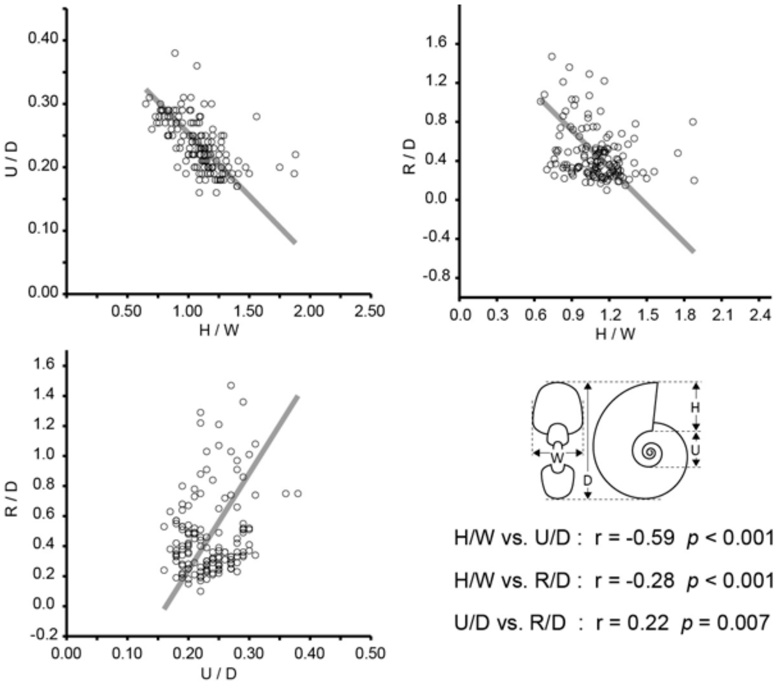


Figure 3 – *Quantification of the Buckman's first rule of covariation within* Acrochordiceras carolinae *(Anisian) for 146 specimens from the same stratigraphic bed (after Monnet et al 2015b). The rule is assessed by means of linear fitting (reduced major axis) of the three character sets (ornamentation is here evaluated by means of rib density). R varies from 0 to 1 and indicates the amount of correlation;* p *indicates the statistical significance of the correlation)*

Buckman's first rule of covariation of ammonoid shells is thus the statement of a regular relationship between three characters: negative correlation between whorl compression and strength of ornamentation, as well as negative correlation between whorl involution and strength of ornamentation. This kind of correlation can be evaluated by means of standard linear regression models for each pair of characters. These analyses and their graphic outputs are standard (for methodological descriptions, see e.g. Davis 2002; Hammer & Harper 2006; for a detailed application see Bert 2013). Monnet et al (2015b) illustrated this pattern of covariation for the ammonoid species *Acrochordiceras carolinae* from the Anisian of Nevada (*Fig 3*; dataset from Monnet et al 2010). The linear regression analysis of the covariation pattern for this species (146 specimens from a single stratigraphic bed) indicates that the three character sets are significantly correlated (*p* value lower than 0.01). Whorl section (H/W) and degree of involution (U/D) are more strongly correlated (r = 0.59), whereas density of ornamentation (R/D) is less correlated with the two other characters (r = 0.25). One important conclusion of this study is that, although the covariation patterns are corroborated, there are not as strongly correlated as could have been expected empirically.

Causes of covariation

The Buckman's rules of covariation involve three major sets of characters: shell shape, ornamentation, and suture patterns. What mechanism could produce such consistent and pervasive covariation across the ammonoid body plan? A helpful way to think about constraints on form was provided by Seilacher (1970) in what has come to be known as "Seilacher's Triangle" (Gould 2002). The three corners of the triangle represent three categories of constraint that limit the types of forms organisms take: 1) historical/phylogenetic, 2) functional/adaptive, and 3) constructional/ morphogenetic. All three types of constraint are likely to influence the anatomical forms of organisms and entangling these in fossil samples is not straightforward. Given the pervasiveness of Buckman's covariation across a variety of ammonoid clades, phylogenetic constraints are not likely to explain the phenomenon. Several authors, though, have attempted to explain Buckman's rules in terms of either functional or constructional constraints.

The various forms of the ammonoid shell have been largely interpreted in terms of functional needs (Dietl 1978; Jacobs 1992; Jacobs et al 1994; Jacobs & Chamberlain 1996; Hewitt 1996; Westermann 1996; Klug & Korn 2004; Saunders et al 2004, 2008; Klug et al 2008; see other references therein), mostly in order to reconstruct the modes of life and habitats of this extinct group (Kennedy & Cobban 1976; Westermann 1996; Ritterbush & Bottjer 2012; Ritterbush et al 2014). Although parts of these adaptive interpretations remain debated, the ammonoid shell has defense properties and is undoubtedly a buoyancy apparatus, which along with shell shape, structure, and ornamentation impose hydrodynamic limits on the animal's swimming abilities (Saunders & Shapiro 1986; Elmi 1993; Jacobs 1992; Jacobs & Chamberlain 1996; Seki et al 2000; De Blasio 2008; Ifrim 2013). However, the sometimes extreme intraspecific variation and covariation of characters of ammonoids challenge current and past ideas about a close correlation between mode of life and shell morphology in ammonoids (Dagys & Weitschat 1993; Dagys et al 1999).

Checa et al (1997) calculated that, despite the extreme morphological variation, hydrostatic (orientation) and hydrodynamic (stability) properties of the various intraspecific morphotypes remained within narrow limits, therefore supporting the adaptive/functional constraint. Some researchers argued that Buckman's rules of covariation may result from an ecophenotypic response to different energy habitats. They documented that compressed forms tend to inhabit high-energy sandy inner shelf environments and depressed forms tend to occur in low-energy offshore mud facies (Kawabe 2003; Landman & Waage 1993; Jacobs et al 1994). However, some authors reported the exact opposite pattern, with more depressed and heavily ornamented forms in shallower water (compare Wilmsen & Mosavinia 2011), thus questioning this functional interpretation. In contrast to the previous interpretations, Westermann (1966) and Reyment (1988) argued against any adaptive cause of this intraspecific covariation pattern. They maintained that the occurrence of such a large morphological variation within a single species and its abundant presence in distantly related groups through time and space is unlikely to reflect ecophenotypism. Paleogeographic differences also do not seem to impact the covariation patterns: e.g. the low paleolatitudinal *Acrochordiceras* and high paleolatitudinal *Czekanowskites* (Anisian) show similar patterns of covariation (compare Dagys & Weitschat 1993 and Monnet et al 2010). With regard to covariation of septal spacing and indentation to whorl compression and shell ornamentation, respectively, several functional explanations have also been proposed (retain neutral buoyancy and resistance to hydrostatic pressure, respectively; Westermann 1966; Hammer & Bucher 2006). However, the function of the septal folding is still the subject of much debate and several hypotheses have been proposed (for details, see Klug & Hoffmann 2015); hence, it is difficult to confirm this biomechanical relationship.

Instead of, or in complement to, adaptive constraints, covariation patterns of the ammonoid shell have been explained in terms of constructional and/or developmental constraints. For instance, Guex et al (2003) simulated the covariation pattern by a reaction/diffusion model of shell morphogenesis (similarly to models reproducing color patterns of mollusks; Meinhardt 1995; Boettiger et al 2009) that fits strength of ornamentation to strength of whorl shape curvature. In contrast to this still speculative model of shell morphogenesis, other researchers (Checa 1987, 1994; Checa & Westermann 1989) argued for the opposite causal link, noting that the formation of more robust ribs during shell growth could cause the shell to automatically become more inflated and depressed. Hammer & Bucher (2005) also argued that the first rule of covariation is “simply” a statement of proportionality that needs no special explanation; ornamentation being proportional to the amount of soft parts. While morphogenetic pre-patterns can probably be translated into pigmentation patterns more or less directly (Fowler et al 1992; Meinhardt 1995; Hammer & Bucher 1999; Boettiger et al 2009), ribbing and other three-dimensional shell features involve growth, folding and stretching of tissues, implying strong developmental constraints in terms of growth rates, mechanics and geometry. In this context, the ratios of proportionality can vary across species (some species have stronger lateral ribs relative to shell width than others) and consequently weaken the interspecific correlation between ornamentation and whorl shape (Hammer & Bucher 2005). Anyway, a better understanding of shell morphogenesis is required to really gain insights on this topic.

Buckman’s second rule of covariation (more compressed shell, more frilled sutures) can also be explained as a case of constructional constraint. Although the function of septal folding is subject of much debate, it has been suggested that septal formation behaves like “viscously fingering” liquids (Checa & Garcia-Ruiz 1996). According to this model, the degree of suture indentation depends on the space and shape available for the suture during its formation (“domain effect”): with equal mantle length secreting the septum, the more compressed the shell, the less space is available for the mantle, and therefore the more constrained the suture shape will be. This domain effect on suture pattern has also been invoked to explain the common evolutionary trends in suture complexity coupled with trends in involution and size increase (Monnet et al 2011a, 2015c). This effect is also clearly illustrated by increasing indentation of suture line during ontogeny (Swinnerton & Trueman 1917; Wiedmann 1966a, b; Korn & Klug 2003; Pérez-Claros et al 2007).

Yacobucci (2004) studied the correlation between the amount of variation of shell shape and of ornamentation (rib thickness and spacing). With respect to Buckman’s first rule of covariation, one can expect that species with variable shell shapes would also have variable patterns of ornamentation. However, her study documented a different pattern in the Cenomanian acanthoceratids of the Western Interior: those groups with especially large shape variation are not those with the most intense variation in ornamentation. Hence, ammonoid shell morphogenesis is complex with some character sets more constrained than others, probably due to a different impact of developmental, constructional, and environmental, as well as functional processes.

In conclusion, the exact causes of Buckman’s rules of covariation for the ammonoid shell are still debated. Constructional and adaptive constraints are not mutually exclusive: both can contribute to the fabrics of structured intraspecific variation for ammonoid shells (Seilacher 1970). The recurrence of particular combinations of morphology, which are commonly regarded as strong arguments for functional constraints, can also represent “fabricational noise” (Seilacher 1970, 1973). Additional studies are required to test quantitatively the various hypotheses (e.g. the proportionality hypothesis of Hammer & Bucher 2005 is so far confirmed only by a single dataset). Additional insights may be found in comparative studies on the morphogenesis of living mollusks as well as from theoretical models of shell morphogenesis (Urdy et al 2010a, b; Moulton et al 2012, 2015; Chirat et al 2013).

Extent of Buckman’s rules of covariation

Buckman’s rules of covariation appear to be a pervasive pattern characterizing the intraspecific variation of planispirally and regularly coiled (non-heteromorphic) Mesozoic ammonoids to varying degrees. However, a number of questions still remain to be investigated: Does each component of the co-varying character set equally contribute to the global covariation pattern? Is the degree of covariance constant during growth? Is the degree of covariance constant through time during anagenetic changes? Do dimorphic pairs show similar covariance? Does the covariation pattern apply equally within different taxonomic groups? Does the extent of covariation vary through time and phylogeny? Does it change with environmental factors and, if so, which ones? Is it related to environmental instability, developmental flexibility, or competition? For discussion and perspectives with regard to these questions, see Monnet et al (2015b); just a few are discussed here.

Concerning covariation patterns within heteromorph species, few studies are available and their results vary. It has often been stated that heteromorph ammonoids have a higher degree of intraspecific variation than normally coiled ammonoids (Kakabadze 2004). However, the phenomenon has only been rarely quantified (Urreta & Riccardi 1988; Tsujino et al 2003; De Baets et al 2013; Knauss & Yacobucci 2014). Interestingly, De Baets et al (2013) reported a negative correlation between coiling and ribbing, such that more loosely coiled variants had a more densely spaced, finer ribbing, as opposed to Mesozoic coiled ammonoids where the relationship is reversed (denser, finer ribbing for more coiled variants). Therefore, it is not possible in the present state of knowledge to generalize a single rule of covariation patterns of ammonoids. They can partially follow some of Buckman’s rules or completely diverge from them.

With regard to the relative contribution of each character set into the global covariation pattern, no comparative study has yet been conducted to our knowledge. Nevertheless, as can been seen with the example of *Acrochordiceras* (*Fig 3*), pair components of the extended rule (the more evolute, the more depressed, the more coarsely ornamented, the less densely ornamented, the less frilled the sutures, and the less densely septate) are not equally correlated, as shown by the various values of the linear correlation coefficient. Since these pair components (e.g. involution–whorl compression or suture frilling–whorl compression) can be explained by different causes, not only are these different contributions expected, but their detailed investigation can help decipher which explanations best fit observed patterns and consequently are the most likely explanations for Buckman's rules of covariation.

Another question in evolutionary biology pertains to whether intraspecific variation can lead to interspecific differentiation (West-Eberhard 1989, 2003, 2005), because anatomical variations within populations increase the range of ecologically relevant variation that can fuel speciation (Schluter 2000, 2001; Butler et al 2007; Nosil 2012), especially by means of heterochronic processes (Spicer et al 2011; Tills et al 2011). In this context, Yacobucci (2004) described a Buckman-like pattern of covariation not within a single species but within a Late Cretaceous clade of acanthoceratid ammonites. Entire genera could be categorized as compressed, involute, and lightly ornamented (e.g. *Metoicoceras*, *Neocardioceras*) while other, closely related genera were depressed, involute, and more heavily ornamented (e.g. *Acanthoceras*, *Plesiacanthoceras*). Similarly, within a genus, different species showed either a more compressed morph (e.g. *Metoicoceras praecox*) or a more depressed morph (e.g. *Metoicoceras geslinianum*), along with the corresponding coiling and ornamentation. Therefore, Buckman's rules of covariation may uphold above the species level, but additional datasets and studies are required to better understand this phenomenon. Particularly, such studies may help to determine whether patterns of covariation are constrained by phylogenetic heritage.

Documenting the existence of Buckman-like covariation patterns among various related groups of ammonoid species and genera will help us better understand the underlying cause(s) of these correlations. Therefore, construction of datasets (especially for ornamentation and suture) and their quantitative analyses is the next step in order to investigate and test the various still unresolved questions about covariation rules of the ammonoid shell.

IMPACT ON SYSTEMATICS

Because only hard tissues are typically fossilized for ammonoids, paleontologists necessarily define morphological species and do not have access neither to the inter-breeding criterion of biological species, nor to their DNA barcodes. Two major and opposite approaches have been used to define fossil morphospecies (for reviews on ammonoids, see Tozer 1971; Dzik 1985, 1990; Chandler & Callomon 2009; De Baets et al 2015). The first concept ("typological approach") puts emphasis on every (even slight) difference in morphological characters; such an approach leads to the multiplication of species ("oversplitting") and is encouraged by the concept of the holotype as well as by the utility of ammonoid "species" as stratigraphic markers. However, many living species are known to not have such a narrow morphological variation. The second concept ("population approach") takes the present-day biological species' structure into account by allowing a certain degree of morphological variation. The notion of species as an array of intergrades separated from another series of organism between which intermediates are absent or at least rare has been formally known at least since Dobzhansky (1937). Hence, a set of specimens showing a continuous inter-gradation of characters fitting a continuous and unimodal distribution should be interpretable as variants of a single species. The recognition of Buckman's rules of covariation can then serve as an aid to discriminate between ammonoid morphospecies, which may correspond to biospecies. Note that some discrepancies between reproductive isolation and distribution of morphological characters may inevitably occur, such as in sibling/cryptic species (Mayr 1948; Knowlton 1993; Boyle & Rodhouse 2005), and fossil populations are often biased by several geological and taphonomic processes (e.g. temporal and vertical mixing/averaging: Bush et al 2002; Kidwell & Holland 2002; Hunt 2004).

Ammonoids, perhaps more than any other group, have suffered from taxonomic splitting (Tozer 1971; Kennedy & Cobban 1976), and authors have frequently divided intergrading populations into a whole range of typological species and even genera, which belong to what can now be regarded as a single variable species (compare Buckman 1892 and Westermann 1966). This problem results from the truly remarkable intraspecific variation seen among many ammonite groups (see De Baets et al 2015). Note that in some groups, end-member variants may show extreme morphological distance and, in the absence of sufficiently large samples, may be attributed to different species or genera (Monnet et al 2010). The two extreme forms can be very different in their morphological proportions, but are always linked by (more frequent) intermediate forms (Weitschat 2008; De Baets et al 2015). It is therefore critical to assess intraspecific variation from large assemblages. Recognition of this variation has led to significant simplification of the nomenclature in several cases (Reeside & Cobban 1960; Kennedy & Cobban 1976; Silberling & Nichols 1982; Wright & Kennedy 1984, 1987, 1990; Hohenegger & Tatzreiter 1992; Weitschat 2008; Monnet et al 2010; Bert 2013). Neglecting the population concept can lead erroneous ecological and biostratigraphic interpretations (Dagys & Weitschat 1993), as well as overestimated values of past taxonomic richness. As a consequence, ammonoid workers have to accept that a single specimen may not necessarily be sufficient for unequivocal species identification and/or description. This evaluation also requires that the studied assemblages are derived from a single bed in order to minimize the mixing of forms that evolved through time or that lived in different environmental settings (Kidwell & Holland 2002).

The most famous case study of the impact of population versus typological approach in defining ammonoid species is the genus *Sonninia*, by recognizing that the observed range of fossil forms was, in fact, due to intraspecific variation rather than species-level differences. Based on a careful re-study of *Sonninia* from the Jurassic of Dorset, which Buckman (1892) split in 64 typological species, Westermann (1966) clearly documented the pattern of covariation between the geometry of shell tube and strength of the ornamentation, and recognized a single (highly) variable species. Although a large degree of intraspecific variation in *Sonninia* is still accepted, Westermann (1966) lumped together specimens from various stratigraphic levels (Callomon 1985; Sandoval & Chandler 2000) and this stratigraphic "lumping" should be avoided at the risk of synonymizing species with temporal anagenetic changes (compare Monnet et al 2010 and Dzik 1990). Another relevant case has been described by Dagys & Weitschat (1993), who documented an impressive case of marked intraspecific variation in a large sample of 600 specimens of *Czekanowskites rieberi* from a single concretion of Anisian age (Middle Triassic) from Arctic Siberia. Morphologically, specimens of *C. rieberi* grade from keeled, narrowly umbilicate, smooth suboxycones to widely umbilicate subcadicones with bullate, straight ribs. Dagys & Weitschat (1993) illustrated that this morphological variation has a roughly normal distribution, which suggests that all specimens belong to a single population.

A recent example of the impact of Buckman's rules of covariation on ammonoid taxonomic nomenclature has been described by Monnet et al (2010). Based on bed-by-bed ammonoid collections in north-west Nevada, this study revised the species of *Acrochordiceras*, which is one of the most important genera of both Tethyan and North American ammonoid faunas of the Anisian (Middle Triassic). However, there was a profusion of species in the literature included in *Acrochordiceras*, mainly because of the typological taxonomic concept, which is often based on small samples and usually characterized by slight morphological differences such as a more compressed shell, coarser ribbing, or absence of tuberculation. A careful examination of these co-occurring "species" erected applying the classical typological concept reveals the presence of intermediate forms among them, thus suggesting the existence of only one highly variable species. This pattern is illustrated by the distribution of the degree of coiling (U/D) for various sizes of *Acrochordiceras carolinae* from north-west Nevada, with inclusion of values for the holotype of other synonymized species (*Fig 4A*; for more details, see Monnet et al 2010). The figure clearly shows that *A. carolinae* has a wide range of intraspecific variation with a continuous unimodal distribution and that each old typological "species" falls within this variation. Hence, the wide range of morphological variation exhibited by acrochordiceratids illustrates Buckman's first rule of covariation quite well. A similar example has been more recently published by Jattiot et al (2016), who synonymized the 60 available species names of the Smithian *Anasibirites* in only two valid species based on comprehensive morphological and biometric studies of more than 900 specimens from a new extensive collection from Timor.

It is noteworthy that, when additional material is acquired through more sampling with better preserved and/or better stratigraphically controlled material, the revision of ammonoid species accounting for intraspecific variation usually significantly decreases species richness of ammonoid genera (De Baets et al 2015). Study of additional specimens more rarely leads to the erection of additional species or the re-establishment of older ones based on previously overlooked differences in ontogeny or morphology (e.g. *Rieppelites cimeganus* in Monnet et al 2008; *Sonninia* in De Baets et al 2015). Therefore, the history of species taxonomy for an ammonoid genus usually is characterized by an initial rapid increase in taxonomic richness as a result of taxonomic oversplitting related to a strict typological approach, followed by a plateau with the accumulation of data, and then a decline in diversity when a better numerical grasp on intraspecific variation and finer stratigraphic resolution is achieved. The taxonomic history of the genus *Acrochordiceras* illustrates this pattern quite well (*Fig 4B*). Note also that the confusion between "dimorphism" and continuous intraspecific variation is not uncommon; particularly when only a small sample size is available (e.g. compare Dzik 1990 and Monnet et al 2010). Nevertheless, continuous intraspecific variation does not rule out dimorphism (see Wright & Kennedy 1984 for example of dimorphic species in *Mantelliceras* for which each dimorph follows Buckman's rule of covariation).

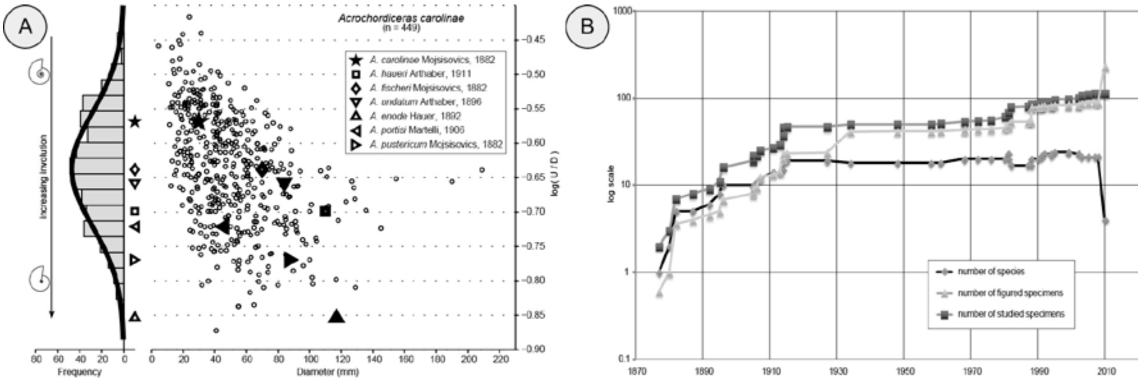


Figure 4 –** Impact of Buckman's rules of covariation on ammonoid taxonomic nomenclature.* ***A) *Distribution of degree of coiling (U/D) for* Acrochordiceras carolinae *in the middle Anisian from Nevada (modified after Monnet et al 2010). This diagram shows the normal distribution of U/D and the position of each species synonymized with* A. carolinae*, thus illustrating the continuous range of degree of coiling for all of the old typological species.* ***B)*** *Numbers of species, specimens figured and specimens studied of the genus* Acrochordiceras *through time in the literature (after Monnet et al 2015b).*

Morphometrics and virtual paleontology

Related publications:

Monnet et al 2009; Naglik et al 2015a

Appended publication:

Monnet C, Zollikofer C, Bucher H, Goudemand N (**2009**) Three-dimensional morphometric ontogeny of mollusc shells by micro-computed tomography and geometric analysis. ***Palaeontol Electron*** **12(3)12A:1–13** (http://palaeo-electronica.org/2009_3/183/)

Morphometrics (or morphometry) refers to the quantitative analysis of form, a concept that encompasses size and shape. Morphometric analyses are commonly performed on organisms, and are useful in analyzing their fossil record, the impact of mutations on shape, developmental changes in form, covariance between ecological factors and shape, as well for estimating genetic parameters of shape. Morphometrics can be used to quantify a trait of evolutionary significance, and by detecting changes in the shape, deduce something of their ontogeny, function or evolutionary relationships. A major objective of morphometrics is to statistically test hypotheses about the factors that affect shape. Morphometrics is one of the most dynamic and popular fields on the contemporary biological scene. Focusing on the quantitative characterization and analysis of morphological data, morphometrics is now a necessary complement to molecular studies in the quests to understand the origin and maintenance of biodiversity. Moreover, morphometrics has recently been shown to have direct utility in phylogenetic contexts, by both finding new, and sharpening the definition of old, character states. Nowadays, three major sets of methods can be distinguished in morphometrics. First, traditional morphometrics rely on the multivariate analysis of linear measurements and ratios, and is this characterized by distances between pairs of points, which roughly describe the shape of the studied object. Second, the recent development of the field of geometric morphometrics marked a "revolution" in morphometrics (Rohlf & Marcus 1993) that is characterized by the coordinates of sets of homologous landmarks, which describe in more details the key structures of the studied object. Third, forms can be characterized by the modeling of their shapes by fitting mathematical models (e.g. elliptical Fourier analysis) or by creating models of shape genesis (e.g. Raup's model of mollusk shells) that also lead to the field of theoretical morphology. All these various fields of morphometrics yield shape variables, which can be used to quantify the morphological disparity of studied organisms in morphospaces.

Since now several years, thanks to increasing computing power and more affordable material for the non-destructive numerical acquisition of three-dimensional anatomical data such as computed tomography (CT), morphometrics of (fossil) organisms has gained a renewed interest and many new insights are provided by this ability to access and quantify the third dimension. Indeed, using these approaches to build up digital visualizations of a fossil's anatomy, it is possible to gain a better understanding of the paleobiology of a wide range of organisms. The field of paleontology has thus been revolutionized by the development of what is more and more commonly called "virtual paleontology". These virtual representations are opening a number of new possibilities for the analysis of specimens. Most notably, precise quantitative analysis of inaccessible internal structures (including small structures such as the middle and inner ears, bony tables, vascular foramina, etc.) and comparison of these structures with living references. Such techniques also make studies through techniques such as geometric morphometrics easier (especially for 3D analyses), and open a range of other computer-based options for assessing the fossil. These include finite element analysis (e.g. to map the stresses and strains of actions such as chewing or running onto an organism's shape) and approaches such as computational fluid dynamics, which models fluid flow around marine organisms.

With regard to my research, I often performed traditional morphometrics on the ammonoid shell, especially in the context of taxonomic descriptions and quantification of variation (see previous chapters). In addition, I actively participate to the fields of 3D morphometrics and of virtual paleontology. Indeed, my post-doctoral position at the Anthropological Museum and Institute of the University of Zürich enabled me to acquire strong experience in various areas of three-dimensional data: 1) manipulation of a medical micro-computed tomograph and acquisition of the digital 2D data gray-scaled images, 2) numerical treatment of the 2D stacked images (filtering, segmentation) to reconstruct 3D models (tessellation), 3) 3D geometric analysis and mesh analysis (extraction of centerline, computation and extraction of cross-sections along this skeleton) by means of scripting under the environment MATLAB and implementation of computer tools with the C language, and 4) application of 2D geometric morphometrics (elliptical Fourier analysis of cross-sections).

In this context, I created a method allowing acquisition of quantitative morphometric parameters, which describe the geometry of coiled mollusk shells throughout their ontogeny (Monnet et al 2009). The proposed morphometric approach has been established with gastropods, but can be easily extended to ammonoids. Although still rarely exploited (acquisition of data remains time-consuming), my method has been recently slightly improved (Noshita 2014; Noshita et al 2016) and the still ever-growing speed of computers will enable to apply it more largely in the future. Therefore, I summarized below this multi-stepped approach, which requires multiple expertise in data acquisition, image analysis, mesh analysis, and geometric morphometrics. Also, my research in 3D morphometrics and virtual paleontology involves the investigation of 3D biometric parameters such as volumes and the insights they can provide into ammonoid paleobiology/morphometry (Naglik et al 2015a).

SHELL MODELING

Significant advances in the quantitative and three-dimensional characterization of the mollusk shell have been first achieved by the pioneer work of Raup (Raup & Michelson 1965; Raup 1966, 1967). Raup (1966) demonstrated that the nearly self-similar accretionary growth of the mollusk shell allows for simulation of most shell shapes by varying only four geometric parameters (*Fig 1*). This model enables constructing a theoretical morphospace of mollusk shells that can be filled with real specimens, because its geometric parameters are easy to acquire. Consequently, the coiled conic shell of mollusks is a well-known case study of theoretical morphology (McGhee 1999, 2007).

Although highly successful, the Raup's model is a simplification of shell geometry, especially of aperture shape, based on 2D measurements. The most important set of morphological characters of ammonoids resides in the geometry of their shell, which is difficult to capture by conventional descriptive, qualitative and discrete approaches. For instance, the investigation of shell geometry has largely been limited to two-dimensional measurements such as width of aperture, shell diameter, or apical angle. Such characters are efficient to characterize the general shell geometry, but poorly capture the subtle differences of shell geometry among species and individuals. Also, in Raup's model, ontogeny is reduced to the relative position of aperture centroid and therefore carries no information about aperture shape, and it is also restricted to regularly coiled shells. Clearly, as such, the approach focuses on only one facet of shell morphology (coiling geometry).

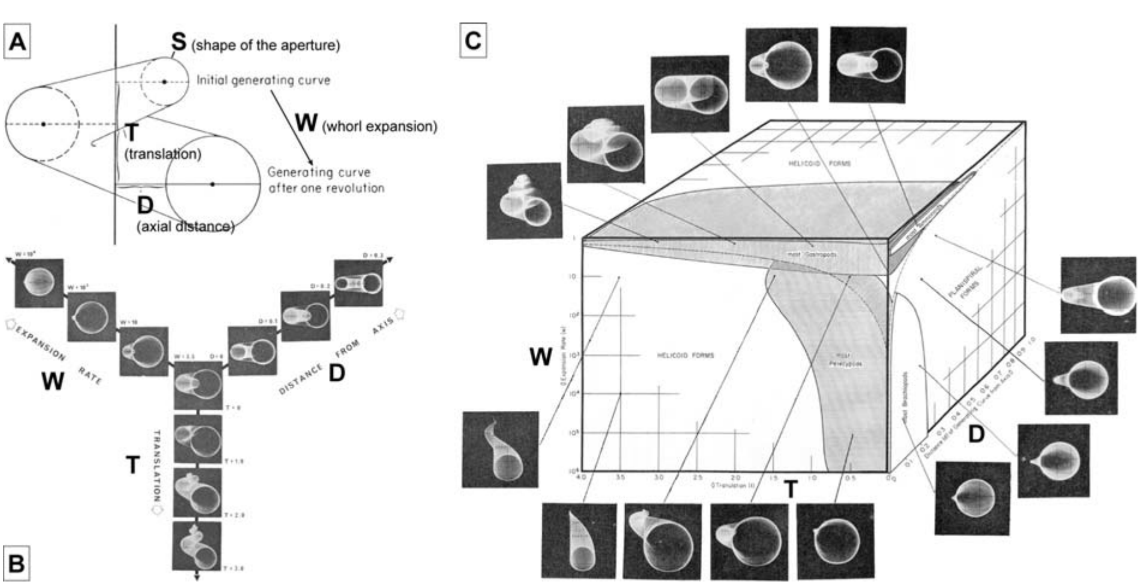


***Figure 1 –** Raup's model (1966) for mollusk shells. **A)** The four geometric parameters, which are defined around a coiling axis: W (whorl expansion rate), T (translation rate along the coiling axis), D (axial distance), and S (aperture shape). **B)** Illustration of the influence of each parameter separately. **C)** These variables enable constructing a theoretical morphospace of mollusk shells and investigating its filling with regard to real specimens.*

In contrast, more complex theoretical models of ammonoid shells, that can intrinsically simulate any aperture shape and changes in settings during growth, have been subsequently proposed (Okamoto 1988; Ackerly 1989; Urdy 2010a). However, the parameters of these models were not measurable on real shells until recently with the approach of Monnet et al (2009). The purpose of this study was to propose a method, which captures the 3D morphology of the coiled mollusk shell and exploits quantitative and continuous characters throughout ontogeny, thanks to continuing improvements in non-destructive, three-dimensional computed image acquisition and analysis. The approach proposed includes the following major steps: 1) acquisition of digital three-dimensional data of the shell; 2) quantitative modeling of shell geometry; 3) extraction of shell geometry through ontogeny; and 4) quantification by geometric morphometrics.

In this approach, the acquisition of digital 3D data of mollusk shells is performed with a micro-computed tomograph (*Fig 2*). This leads to a series of grey-scaled, parallel, 2D images with a micrometric resolution. This process may take hours and produce data of several Go, depending on the size of the studied organism and selected resolution of the scanning process. Anatomical structures of interest must now be traced between adjacent images; stacking those sliced structures on top of each other reveals an approximation of their three-dimensional shape.

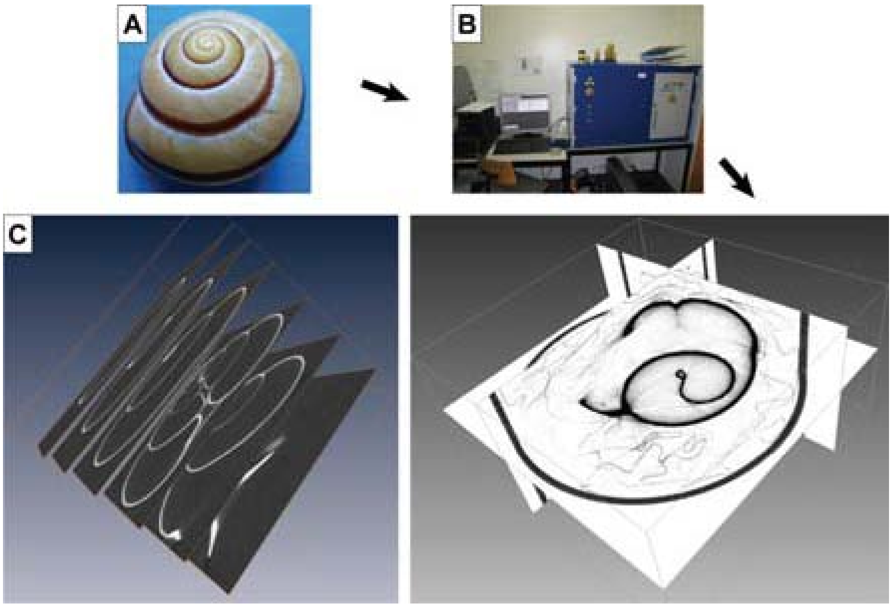


Figure 2 –** Acquisition of the 3D digital data.* ***A) *Gastropod shell of* Cepaea nemoralis*.* ***B)*** *The medical Scanco® micro-CT 80 of the Anthropological Institute of Zürich.* ***C)*** *The raw data are stored as a stack of noisy, grey-scaled 2D images.*

The next step is to reconstruct a 3D, numerically exact descriptive model of the scanned shell by several treatments on the images; this step is called segmentation (*Fig 3*). For this purpose, the series of images is transferred into a computer visualization system (such as the commercial software Avizo®, which is a convenient and interactive system for 3D data analysis, visualization and geometry reconstruction; Stalling et al 2005). To ease this segmentation process, the stacked images are previously treated with various filters and dilation/erosion processes. Because raw scanned images may contain "noisy" background values and additional objects of non-interest, the stacked images must be segmented, that is selecting/identifying voxels and divided them into different segments for 3D reconstruction (the label fields). At this step, the gastropod shell is represented by a 3D matrix of integer values (aka. the voxel grid) indicating to which segment each voxel belongs to. Now, the different segments of the shell (here, the shell itself, the stopper at the mature constriction, and the internal volume of the shell) can be accurately reconstructed by tessellating their boundary surfaces from the 3D image data. Tessellation consists in representing the segmented structure by a rather large set of interconnected triangles. For instance, the internal volume of the shell is described by a triangular mesh, which basically is a connected network of 3D triangles placed at its surface.

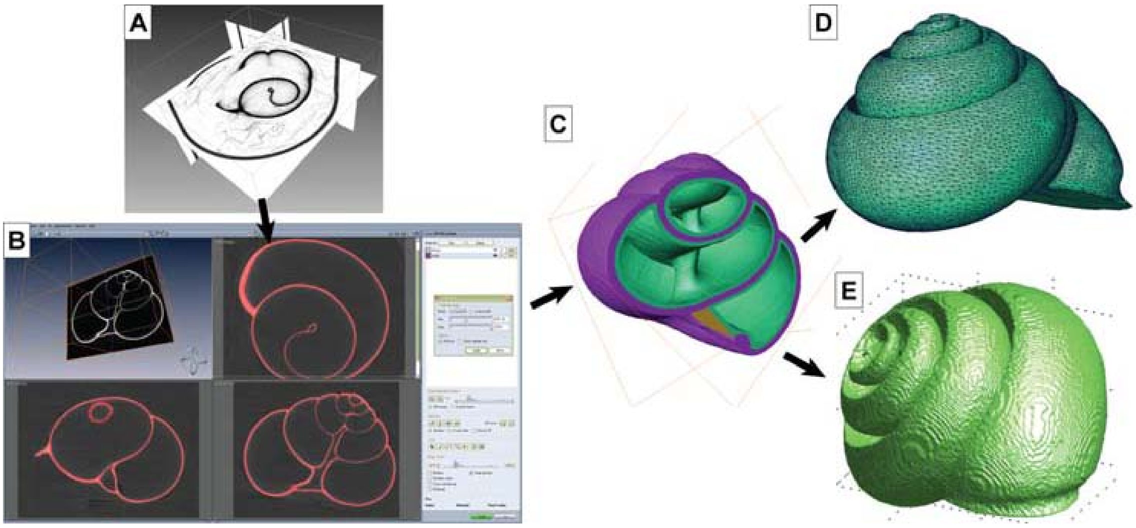


***Figure 3** – Reconstruction of the shell 3D model. **A)** The stacked images. **B)** Segmentation of the shell with the segmentation module of Avizo®, which enables marking and classifying image areas in any of the three orthogonal views with an immediate feedback in all other views including a three-dimensional visualization. **C)** The studied gastropod shell is segmented into three parts (the shell itself, a stopper in the plane of the mature constriction, and the internal volume of the shell). **D)** The segmented data can be used to produce a triangular mesh describing the surface of each segment. **E)** The segmented data can also be used to produce a numerical matrix characterizing each segment (aka. voxel grid).*

The next part of the method is the extraction of shell geometry throughout ontogeny. I proposed to recover the ontogenetic changes of the shell geometry by reconstructing and using a curve-skeleton. A curve-skeleton (aka. centerline, medial axis, or central path) is a compact 1D representation of 3D objects, which is conceptually defined as the locus of centre voxels in the object. In this approach, the curve-skeleton is expected to be placed at the centre of the shell aperture at each increment of growth. Due to its compact shape representation, skeletonization has been studied for a long time in pattern recognition (Trahanias 1992), in medicine (Sorantin et al 2002; Deschamps & Cohen 2001) and in computer graphics (Blanding et al 2000). The extraction of a curve-skeleton in 3D remains a challenging task and there exist several methods; I selected the potential field method (Cornea et al 2005, 2007). Practically the curve-skeleton is a series of 3D points, which are extracted from the voxel grid. For this curve-skeleton extraction, I programmed software in C language. The curve-skeleton of a mollusk shell is a very useful tool. It can be compared with the aperture trajectory (Stone 1995) or generating curve of Raup's model (1966), although defined and calculated in a different way. It can be used as a guide to extract the geometry of a succession of whorl sections in an automated navigation throughout ontogeny of the shell. The same idea is widely applied in medicine such as in virtual colonoscopy. For this purpose, successive cross-sections, centered on and perpendicular to the curve-skeleton, are computed along the curve-skeleton, by calculating the intersection of the corresponding cutting plane with the triangular mesh (*Fig 4*). The result is an ontogenetic series of successive outlines representing shell geometry. For this extraction of aperture shape through ontogeny, I programmed scripts in Matlab language.

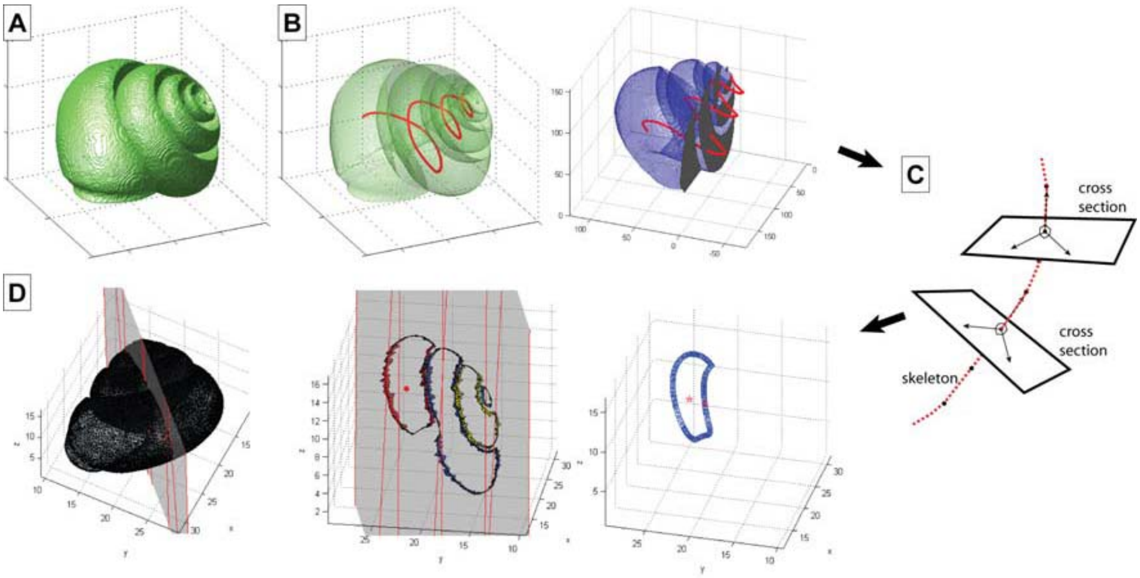


Figure 4 – *Extraction of shell shape aperture through ontogeny.* ***A)*** *Voxel grid of the internal shell segment.* ***B)*** *Curve-skeleton of the internal volume of the gastropod shell reconstructed by means of the potential field method.* ***C)*** *Illustration of two successive cross-sectioning planes perpendicular to and placed along the curve-skeleton.* ***D)*** *Results of a cross-sectioning plane (left figure shows the triangular mesh of the shell and the cutting plane; middle figure shows the triangles of the mesh which intersect the cutting plane; and right figure shows the resulting outline of the whorl section at each examined ontogenetic stage).*

Now, the 3D geometry of the shell can be quantified by two sets of parameters. The first set is the displacement vector between two successive cross-sectioning planes. This vector records the translation and rotation coefficients between the origins of two successive cross-sectioning planes. The second set is the successive outlines of whorl sections through ontogeny. These two datasets can be transposed both in Raup's model and in moving frame models in order to combine theoretical and real mollusk shell morphology. The outlines of aperture shape thru growth can be quantified by standard morphometric methods such as elliptical Fourier analysis (Lestrel 1997; Haines & Crampton 1998). Fourier analysis can be thought of as supplying the coefficients of a trigonometric function that reproduces as closely as possible a sample curve. The number of harmonics (terms of the function) necessary to reconstruct an outline depends on the complexity of this outline, but usually does not exceed 20 for mollusk shells. The series of coefficients of the selected harmonics are then used as a mathematical characterization of the geometry of whorl sections. The calculated coefficients of harmonics of a whorl section of the shell, coupled with the displacement vector (translation and rotation) between two successive cross-sectioning planes, constitute an n-dimensional morphometric space. The successive values of these harmonics and of the displacement vector of a single shell through ontogeny constitute a morphometric ontogenetic trajectory in this n-D space. The ontogenetic trajectories of each specimen and species can thus be analyzed and compared quantitatively within this n-D space. The geometry of a shell is thus quantified by a set of multivariate data. The analysis of such datasets is standard in morphometrics (usually by means of a principal component analysis; *Fig 5*) (one can found methodological developments and examples in Zelditch et al 2004, among others).

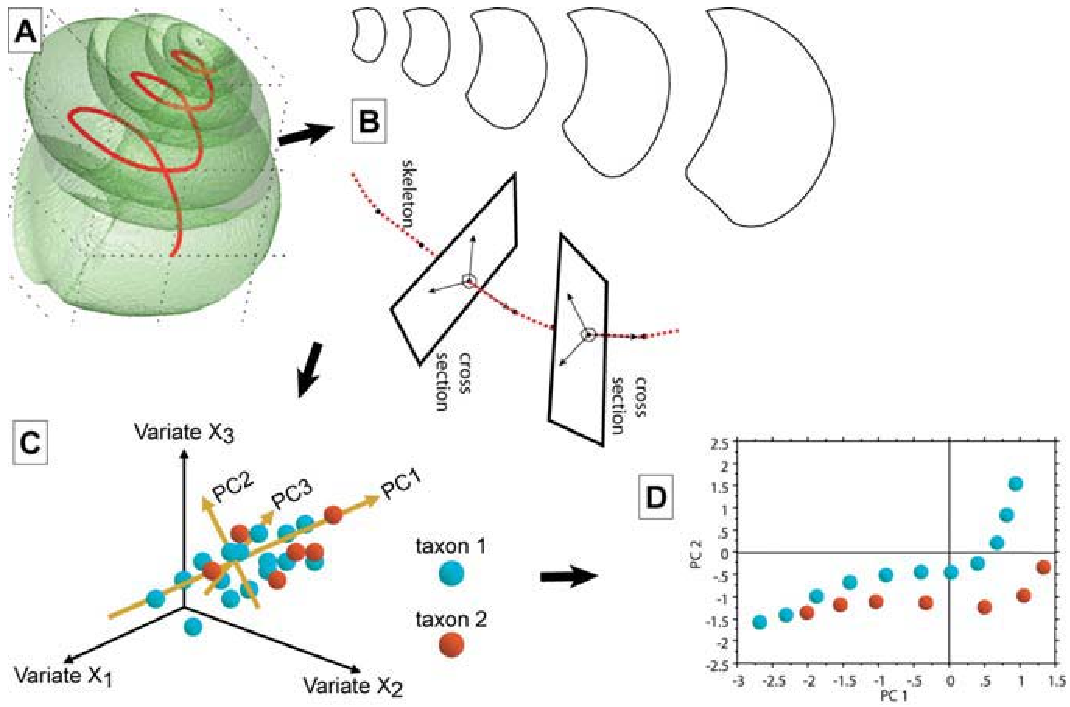


Figure 5 – *Quantification of shell morphology through ontogeny.* ***A)*** *Voxel grid and curve-skeleton of the shell.* ***B)*** *Successive aperture shapes based on cross-sectioning along the curve-skeleton.* ***C, D)*** *Investigation of these data by standard multivariate analyses (principal component analysis).*

In conclusion, my study (Monnet et al 2009) proposed a quantitative, non-destructive and semi-automatic method to quantify the geometry of the mollusk shell through its ontogeny, by means of micro-computed tomography, 3D image analyses (segmentation), 3D modeling (tessellation producing a triangular mesh and a voxel grid), mesh analysis (extraction of a centerline of the shell, which serves as a guide to slice the shell throughout ontogeny and extract the successive outlines of the whorl sections), and geometric morphometric analysis (quantification of aperture shape through ontogeny and comparison of specimens/taxa in a morphospace).

CHAMBER VOLUMES

Mollusks such as ammonoids record their growth in their accretionary shells, making them ideal for the study of evolutionary changes in ontogeny through time. Standard methods usually focus on two-dimensional data and do not quantify empirical changes in shell and chamber volumes through ontogeny, which can possibly be important to disentangle phylogeny, interspecific variation and paleobiology of these extinct cephalopods. Tomographic and computational methods offer the opportunity to empirically study volumetric changes in shell and chamber volumes through ontogeny of major ammonoid sub-clades in three dimensions (3D).

In their study, Naglik et al (2015a) documented the growth of chamber and septal volumes through ontogeny, and differences in ontogenetic changes between species from each of three major sub-clades of Paleozoic ammonoids throughout their early phylogeny. The data used are three-dimensional reconstructions of specimens that have been subjected to grinding tomography. The following species were studied (*Fig 6*): the agoniatitid *Fidelites clariondi* and anarcestid *Diallagites lenticulifer* (Middle Devonian) and the Early Carboniferous goniatitid *Goniatites multiliratus*.

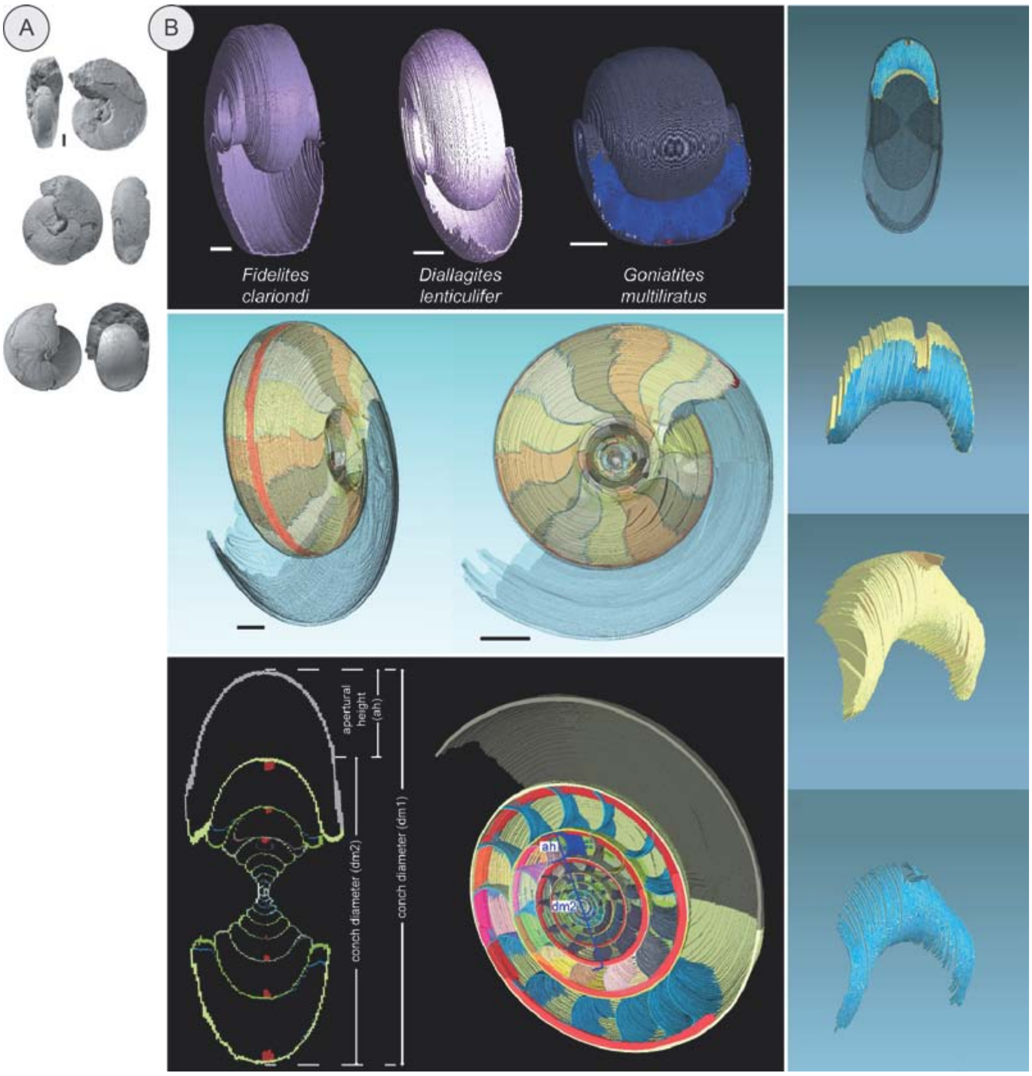


Figure 6 –** 3D reconstruction of ammonoids and their chambers (Naglik et al 2015a).* ***A) *The studied specimens before grinding tomography (*Fidelites clariondi*,* Diallagites lenticulifer*, and* Goniatites multiliratus*).* ***B)*** *Reconstructions of the studied specimens: apertural oblique views of the generated 3D*

models of the specimens; colored inner elements of Diallagites lenticulifer *(chambers, septa, siphuncle) with transparent shell, example of a complex chamber/septum, and classical one-dimensional parameters in cross-section compared to the 3D measurements.*

Chamber and septum volumes were plotted against the septum number and the shell diameter (proxies for growth) in the three species (*Fig 7*); although differences are small, the trajectories are more similar among the most derived *Diallagites* and *Goniatites* compared with the more widely umbilicate *Fidelites*. There is a good correlation between the 3D and the 2D measurements. In all three species, both volumes follow exponential trends with deviations in very early ontogeny (resolution artefacts) and near maturity (mature modifications in shell growth). Additionally, they analyzed the intraspecific differences in the volume data between two specimens of *Normannites* (Middle Jurassic).

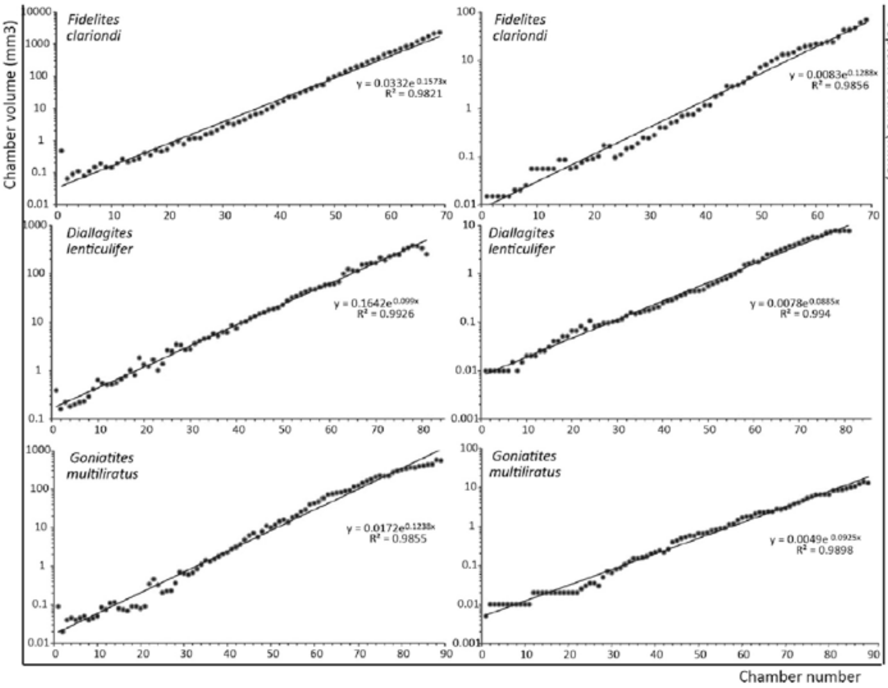


***Figure 7 –** Volumetric data plotted versus chamber numbers (Naglik et al 2015a). In the left column, the volumes of the chambers are represented and show an exponential trend for each specimen. The exponential regression equations as well as their R^2 values are displayed on the graphs. Concerning the last chambers, a decrease in volumes is visible in* Diallagites lenticulifer *corresponding to the mature stage. In the right column, similar trends are seen in the evolution of the septum volumes through ontogeny. Generally, values are more similar between* D. lenticulifer *and* G. multiliratus *compared with* F. clariondi.

Quantitative Biostratigraphy of Ammonoids

Methods

Related publications:

Monnet & Bucher 1999, 2002, 2006, 2007b; **Monnet** et al 2011b, 2015a

Appended publication:

Monnet C, Klug C, Goudemand N, De Baets K, Bucher H (**2011**b) Quantitative biochronology of Devonian ammonoids from Morocco and proposals for a refined unitary association method. ***Lethaia* 44:469–489**
(doi: 10.1111/j.1502-3931.2010.00256.x)

Biostratigraphy is the branch of stratigraphy which focuses on correlating and assigning relative ages of rock strata by using the fossil assemblages contained within them. Usually the aim is correlation, demonstrating that a particular horizon in one geological section represents the same period of time as another horizon at some other section. The fossils are useful because sediments of the same age can look completely different because of local variations in the sedimentary environment. Biostratigraphy originated in the early 19th century, where geologists recognized that the correlation of fossil assemblages between rocks of similar type but different age decreased as the difference in age increased. Consequently, biostratigraphy has a long history of empirical establishment. Most traditionalist biostratigraphers have, and still, resisted, stubbornly the use of numerical methods and the construction of biochronological time scales has sometimes been perceived as an “art” by some scientists who were distant from the field (Brower 1982). However, biostratigraphy can best harness the full potential of vast amount of spatial and temporal distribution data of fossil organisms by using quantitative, computer-assisted techniques. Following notable forerunners such as the graphic correlation method (Shaw 1964), modern quantitative stratigraphy then developed spectacularly (Gradstein et al 1985; Guex 1991; Kemple et al 1995) in response to the personal computer revolution enabling to run sophisticated algorithms on large amount of raw stratigraphic data (Palfy 2007). Gradually gaining popularity, a wide range of quantitative stratigraphic methods is now available. Because of their high evolutionary rates, broad paleogeographic distributions, and frequent preservation in marine deposits, ammonoids are one of the prime fossil groups for dating Paleozoic and Mesozoic marine strata (House 1985). Therefore, given the amount of available biostratigraphic data, ammonoid is a suitable model to apply and test quantitative methods of biochronology.

Quantitative biostratigraphy is probably the part of my works that best characterized my research. Indeed, a large part of my research focused and still focuses (see prospects) on 1) applying quantitative biostratigraphic approaches to construct more robust biozonations of ammonoids, and 2) on critically analyzing the advantages, drawbacks and algorithms of these methods. Also, one original characteristic of my research in biochronology is the development of empirical procedures to evaluate the robustness of the UA solution and to get some feedback on the quality of used data and on the origin of the biostratigraphic contradictions. For instance, I always check that the automatic correction of cycles is parsimonious and identify which part of the data caused these cycles, notably to evaluate if taxonomic inconsistencies or sedimentary/taphonomic biases could be responsible (see Monnet et al 2011b).

I recently published a review (Monnet et al 2015a), which synthesizes the studies I conducted during several years, not only on the application of quantitative methods in ammonoid biostratigraphy/ biochronology, but also on the critical evaluation of the theoretical aspects of these methods (more particularly the unitary association method). This review also illustrates my concerns in applying quantitative methods for paleontological data analysis. In addition, I published (Monnet et al 2011b) a thorough application of the unitary associations and a critical assessment of the method. The following text summarizes the principal results discussed mostly in these two publications.

BIOCHRONOLOGY AND BIOSTRATIGRAPHIC CONTRADICTIONS

Over the last decades, quantitative biochronology has seen a consolidation of methods and a better understanding of their advantages and limitations has emerged. These methods are robust and allow resolving the numerous problems encountered in dating and correlating fossiliferous strata, be it at a global scale, across different basins, within a single basin, or within an oil field. The construction of robust and highly resolved biozonations is a necessary prerequisite both in academic and in oil and mining studies using fossils for dating and correlating sections. To achieve these goals of accuracy and precision, a number of quantitative biochronological methods have been developed during the last decades (Hay & Southam 1978; Guex 1979; Cubitt & Reyment 1982; Gradstein et al 1985; Boulard 1993; Sadler 2004). All these methods utilize strict and well-defined algorithms that allow processing large datasets. Computerized methods ensure a rigorous, exhaustive, and consistent treatment of the biostratigraphic data. They often produce better-resolved biozonations than empirical studies (Boulard 1993; Monnet & Bucher 2002; Sadler 2004). However, these quantitative methods often lead to partly different results (Baumgartner 1984; Agterberg 1985; Boulard 1993; Galster et al 2010; Monnet et al 2011b). Such divergences are expected, because these methods are based on different types of available biostratigraphic data (coexistence vs. apparition/extinction of taxa), on different theoretical assumptions and practical algorithms (probabilistic vs. deterministic approaches) in how to resolve the biostratigraphic contradictions, and on the expected type of results (continuous vs. discrete biozonations). Therefore, the biostratigrapher doing a quantitative biochronological analysis must make a choice based on his/her data and expectations in agreement with the advantages and constraints of each method (compare Gradstein 2012).

Among the existing quantitative biochronological methods, the three most popular nowadays are Ranking and Scaling (RASC: Agterberg & Nel 1982a, b; Agterberg & Gradstein 1999; Gradstein et al 1999), Constrained Optimization (CONOP: Kemple et al 1989, 1995; Sadler & Cooper 2003; Cody et al 2008; Sheets et al 2012), and Unitary Associations (UAs: Guex 1977, 1991; Galster et al 2010; Monnet et al 2011b). All these methods have computer software either separately or altogether (but often with less options) in the widely used free software of paleontological data analysis PAST (Hammer et al 2001). A complete review of all available quantitative methods in biostratigraphy is beyond the scope of this study, and the reader is referred to previously cited references for further details and applications (for a short overview, see Gradstein 2012; Monnet et al 2015a). Finally, note that the UAs stands in sharp contrast to RASC and CONOP: UAs are based on the co-occurrences of taxa in successive levels, resolve biostratigraphic contradictions by focusing on coexistences and inferring virtual coexistences, and yield discrete biozonations; RASC and CONOP are based on the bioevents of studied taxa spotted on profiles, resolve biostratigraphic contradictions by focusing on the relative range of taxa and by modifying these ranges, and produce continuous biozonations made of interval zones based on the first and/or last occurrences of index taxa.

The fossil record is clearly incomplete and cannot be read at its face value. Sedimentary successions do not necessarily faithfully reflect the true relative order of evolutionary events (origination = First Appearance Datum/FAD; extinction = Last Appearance Datum/LAD) through time because of a whole array of primary and secondary causes that may blur their actual succession (e.g. ecological/ environmental constraints, selective preservation, sedimentary gap or reworking, taxonomic vagaries, sampling effort, or amount of available exposures). Therefore, both first and last local occurrences of a taxon (FOs, LOs) in the rock record may result from a wealth of causes other than true evolutionary speciation or extinction (FADs, LADs), which remain intrinsically restricted biological processes in space and time.

The crucial effect of all these parameters is the creation of conflicting stratigraphic positions between taxa across several sections; the so-called biostratigraphic contradictions (*Fig 1*). Indeed, each taxon is characterized by a very irregular and complex paleogeographic distribution in space, which is in turn altered through time (*Fig 1A*). Since biostratigraphic data are obtained from a necessarily finite number of sections, they represent only a small fraction of the true distribution in time and space of the studied taxa. Because of all the factors that degrade the true time and space distribution of species, real data usually contain contradictions, i.e. inconsistent superposition relationships between FOs and LOs, which make it impossible to obtain a unique order of species ranges along the time axis (*Fig 1B*). Some of those biostratigraphic contradictions may result from virtual coexistences, i.e. species that actually co-existed in time but not in space (*Fig 1C*).

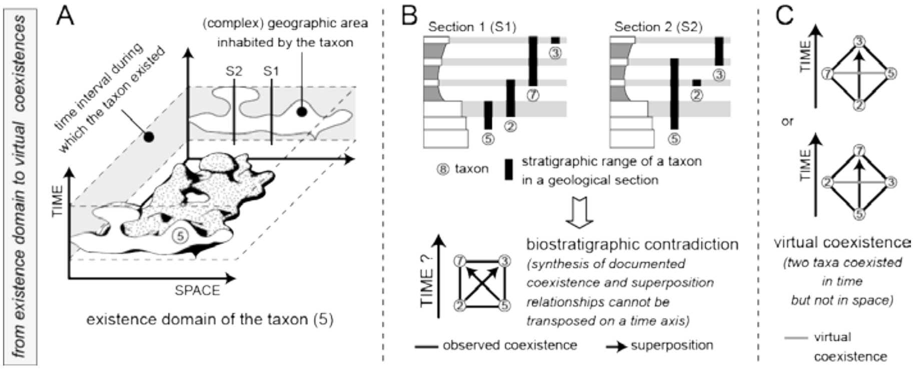


Figure 1 *– Notions of existence domain (**A**), biostratigraphic contradiction (**B**), and virtual coexistence (**C**).*

With increasing size of biostratigraphic datasets including larger numbers of taxa and sections, the number of contradictions usually grows exponentially. The major goal of biochronological methods is to extract biostratigraphic units (biozones) and their temporal relationships from the description of the stratigraphic distribution of fossils along geological sections. Because these data are usually unevenly and sparsely distributed, all biochronological methods must cope with and resolve the (often large amount of) biostratigraphic contradictions in order to recover the actual time ranges of fossils.

CORE CONCEPTS OF THE UAS

Among the modern quantitative methods in biostratigraphy, my preferred choice goes to the UAs. This selection is mainly driven by the theoretical and practical properties of the UAs (e.g. production of discrete biozones and preservation of all observed co-occurrences), by its efficiency in resolving complicated biochronological problems produced by taxonomic groups with very different completeness of their fossil record and as shown by comparative studies (Baumgartner 1984; Boulard 1993; Galster et al 2010; Monnet et al 2011b), and last but not least, by its panel of supplementary tools enabling critical assessment of the studied dataset. Despite an ever increasing number of datasets and the need of higher resolved correlations, there are still few studies applying these quantitative and robust biochronological methods to ammonoids. This is unfortunate since quantitative stratigraphic approaches produce results with a much higher resolution potential than empirical zonations (Boulard 1993; Monnet & Bucher 1999, 2002, 2007b; Sadler 2004; Cody et al 2008). Even if ammonoids have a long-standing reputation as excellent age biomarkers, ammonoid biozonations can be significantly improved by using these quantitative methods. Among these, it appears that UAs are most commonly used with ammonoids (Pálfy et al 1997, 2003; Pálfy & Vörös 1998; Galfetti et al 2007; Pálfy 2007; Brühwiler et al 2010; Guex et al 2012). Also it allows a subsequent, objective assessment of the diachronism of the studied taxa and the choice of actual characteristic taxa of each zone (compare Pálfy & Vörös 1998; Pálfy 2007). Finally, Escarguel & Bucher (2004) demonstrated that the unknown duration of the discrete UA-based biozones does not introduce a significant bias when using UA-zones as time bins for counts of species richness. Therefore, the UAs are a very powerful method to resolve biochronological problems, to rapidly produce robust zonations, and to assess critically the quality of the dataset.

The UAs was developed by Guex (1977, 1991) and its analytical algorithms evolved since. The last implementation is available as the stand-alone software called UA-graph or within the paleontological software PAST (Hammer et al 2001). For typical applications with UA-graph, see Carter et al (2010), Galster et al (2010), Monnet et al (2011b), or Guex et al (2012). The UAs is a deterministic approach based on the observed coexistences of studied taxa (and not their bioevents) by preserving in the outputs all raw documented associations of taxa (coexistence in space). It takes advantage of the fact that the intrinsic nature of biostratigraphic data (association, superposition, unknown relation) is identical with the kind of data processed by the mathematical graph theory founded by Euler (1741), thus enabling a formal and logical treatment of the biochronological "problem". This approach resolves the biostratigraphic contradictions by inferring virtual associations. A virtual association is defined as the coexistence of taxa in time, but not in space (*Fig 1*). The biozonations constructed by means of the UAs are consequently composed by an ordered sequence of discrete units (the UAs), which are unique maximum sets of coexisting (really or virtually) taxa. The major challenging requirement of UAs is that it forces the biostratigrapher to think in four dimensions (space and time) instead of the usual one dimension of a section or a time axis. It is also less intuitive for biostratigraphers used to work with continuous scales such as interval zones (as stimulated by stage boundaries defined on the FAD of index taxa).

I am currently the only author who provided a detailed and illustrated application of the method and its computer implementation UA-graph, although I am not involved in its development. Hence, follows a personal overview of the current algorithmic state of the UAs. For a recent and exhaustive application of the method on ammonoids by means of the graphic user interface and use of its supplementary tools, see Monnet et al (2011b, 2015a). The major principles and steps of the UAs are here illustrated with an imaginary and simple example, based on the occurrences of eight taxa within four sections (*Fig 2A*). The first step is the construction of the biostratigraphic graph (*Fig 2B*), which compiles and represents all observed biostratigraphic relationships. Its vertices represent the taxa, its edges represent their documented association, and its arcs represent their superposition.

The next step is the extraction of all unique maximal sets (a set is maximal if not contained in a larger set) of mutually coexisting species, called “maximal cliques” (*Fig 2C*). The example proposed here contains 6 maximal cliques among which one (“mc4”, *Fig 2C*) includes taxa 3, 5 and 7 that coexist altogether in time (but not necessarily in the same section). Then, the method resolves the superpositional relationships between these maximal cliques by the comparison of documented stratigraphic relationships of taxa in the biostratigraphic graph between each pair of cliques (*Fig 2D*). Usually, conflicting stratigraphic relationships occur between some of the taxa (“biostratigraphic contradictions”). For instance, the figure reports: one case in which the superpositional relationships between the taxa are congruent (arcs in the same direction); and another one in which the relationships are contradictory (arcs of opposed directions). The method solves such conflicting stratigraphic relationships by assuming that one of these contradictory arcs is wrong and is in fact generated by a virtual coexistence (i.e. inter-taxa coexistence that is real in time but not observed physically in the stratigraphic samples). The choice of the supposed badly oriented arc (or set of arcs) follows a “majority rule” (Galster et al 2010, p. 244). This rule counts the number of arcs and their frequency in each direction separately, and then considers the most frequently observed direction as the correct stratigraphic order (*Fig 2D*). Once all superpositional relationships between the maximal cliques have been resolved, one can construct a graph that exactly represents all these relationships (*Fig 2E*).

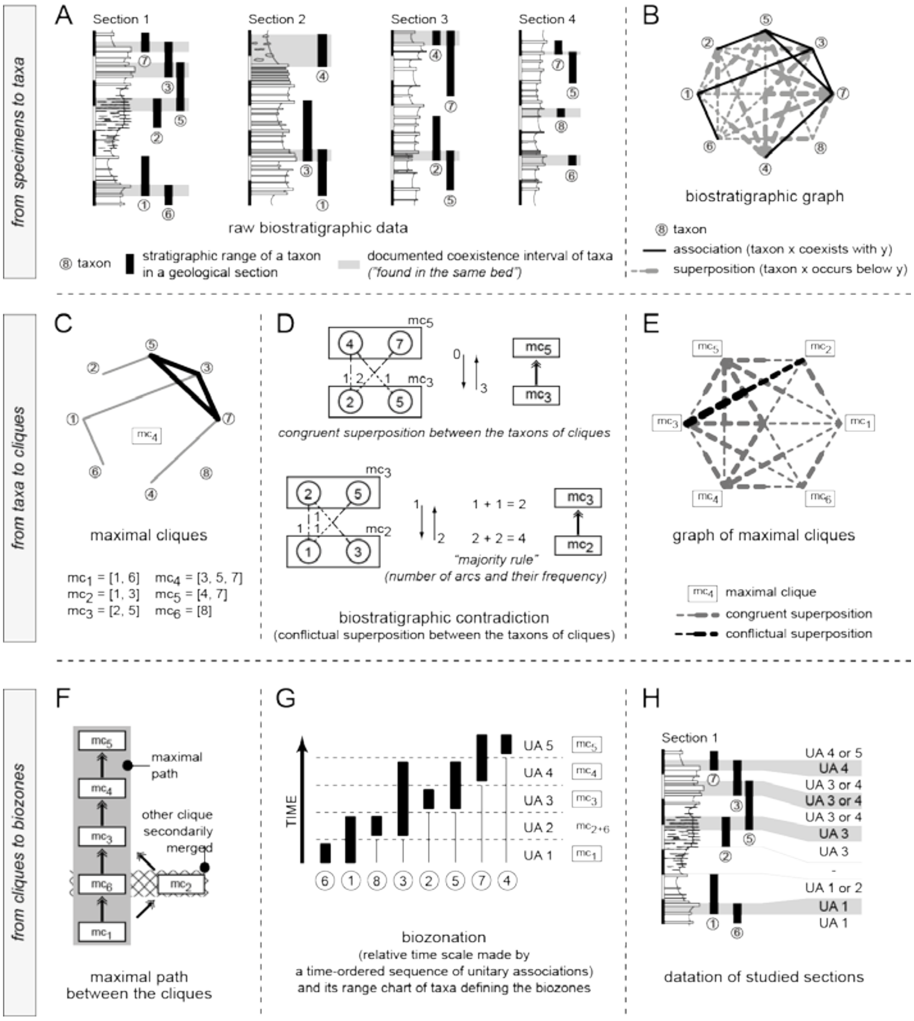


Figure 2 – *Flow chart of the major analytical steps of the UAs (see text for explanation).*

Next, the method extracts the longest sequence (path) of superposed maximal cliques (*Fig 2F*). Maximal cliques, which do not belong to the longest path, are merged (if possible) with contemporary maximal cliques of the path. Finally, one can transcribe the sequence of maximal cliques into the sequence of unitary associations (*Fig 2G*). A unitary association is thus defined as a maximal set of mutually coexisting species, be it actually or virtually. The sequence of UAs is called the "protoreferential" and along with the reproducibility matrix (a sections vs. UAs matrix), they constitute the zonation used to correlate the fossiliferous content of studied sections (*Fig 2H*). Note that a strict association zone such as produced by the UAs is characterized either by the taxa occurring only within this zone or by the intersecting ranges of taxa observed within the zone: the FADs and LADs per se do not matter.

CRITICAL ASSESSMENT OF THE UAS

The unitary association method is a powerful method to resolve biochronological problems, to produce robust zonations quickly, and to assess critically the quality of the dataset. The basic principle of the method (conflicting stratigraphic relationships are interpretable as virtual coexistences) is concordant with the raw state of the biostratigraphic data (occurrences of taxa; FOs/LOs and superposition relationships are already interpretation). Furthermore, its integration in the mathematical frame of the graph theory ensures a rigorous and consistent treatment of the data. However, the implementation of a theory in practical algorithms is not straightforward and selected solutions and their intrinsic uncertainties must be assessed and not ignored.

One important part of my research in biochronology is devoted to the critical assessment of the various quantitative methods (with a special focus on UAs). This aspect of my research is relatively unique, because most biostratigraphers are concerned with the direct application of the various quantitative methods and not with their development. Although not implicated in the development of UAs, I highlighted (Monnet et al 2011b) some weaknesses in the algorithms of some steps of the method that led the authors of the computer-based approach (UA-graph, PAST; J. Guex and O. Hammer) to modify some of their algorithms. This chapter lists some possible improvements that can be applied to the UAs. These propositions result from several years of experiment on applying and evaluating this method. This experience enabled me to create artificial datasets from scratch that push the various quantitative methods to their limits. Some of these provocative ideas have been published in Monnet et al (2011b) and are just summarized here (for an opposite view, see Guex 2011). As pointed out in my study, the crucial points are the resolution of the conflicting stratigraphic relationships between the maximal cliques, and the treatment of cycles involved between maximal cliques. The UAs could also be supplemented with two other sets of information: multiple solutions originating from the merging of "isolated" maximal cliques, and relative order of the bioevents of taxa.

Cliques, contradictions, and cycles

In the UAs and its UA-graph computer implementation, the conflicting stratigraphic relationships between the maximal cliques are solved by a “majority rule”, which minimizes the number of superposition replaced by virtual coexistences. This solution is globally and generally sufficient. However, if the data are too loosely constrained, most superpositional relationships are nearly indeterminate with a ratio of the majority rule close to 1. In such cases, the single solution adopted by the UAs is nearly arbitrary. Yet, the UAs offer no test or alternative algorithm to handle this problem, and the different solutions must be checked empirically and manually. A “cascade effect” can thus be generated when dealing with under-constrained data. One error in the superpositional relationship between two maximal cliques is likely to propagate as a cycle in the sequencing of maximal cliques. For instance, this effect is illustrated in the correction of cycles (see the treatment of the Devonian ammonoid dataset analyzed by Monnet et al 2011b). One solution proposed to avoid this problem is to calculate all possible relationships of the conflicting superposition and to select subsequently the most parsimonious solution in terms of virtual coexistences created. Interestingly, this problem is real and not just theoretical, because it has been detected in the real Devonian ammonoid dataset analyzed by Monnet et al (2011b).

Another source of uncertainties can arise from the case of data leading to cycles between the maximal cliques (“strongly connected components”). Unfortunately, such cycles occur frequently in poorly constrained data and again their destruction can be nearly arbitrary (Guex 1991; Savary & Guex 1999). UA-graph currently solves these contradictions by using the “weakest link” rule (i.e. the clique superposition supported by the fewest inter-taxon relationships is destroyed; Guex 1991, p. 82). Given the uncertainties related to this type of solution, the unique result produced by the UAs is likely to be partly wrong. I created an imaginary example containing cycles between its maximal cliques where the automatic resolution by the software UA-graph yields a result, which is clearly not the most parsimonious compared to what can be found empirically (*Fig 3*). This example clearly illustrates and demonstrates that the “weakest link” rule is not adequate in such cases. One way to avoid this problem is to calculate all possible minimal sets of clique superpositional relationships necessary to break the cycles and then select the most parsimonious solution in terms of reconstructed virtual coexistences. Besides, this is the empirical approach that I have personally adopted since several years (Monnet & Bucher 2007b; Monnet et al 2011b).

As seen above, there are several sources of uncertainties when processing poorly constrained datasets and equally parsimonious solutions (different sets of virtual coexistences) may sometimes compete against one another. However, the current implementation of the method yields necessarily a single solution without further indication. Because the method should rather not become to some kind of a “black box”, I suggested that the software should provide the user with the possible solutions of a biochronological problem, thus clearly indicating all uncertainties associated with each solution. In the case of multiple solutions, the UAs should be completed with tools that calculate consensus solutions and confidence intervals on the ranges of studied taxa by means of bootstrapping on the raw data. The purposes of these additional tools are intended to help users to assess both the robustness of the results and the quality of the data. It is likely that the differences among the set of solutions will pinpoint the problematic occurrences of taxa and, hence, help the user to judge his data or at least encourage treating those occurrences with more caution. The UAs was already differing from other quantitative methods by allowing the user to evaluate the origin of the conflicting stratigraphic relationships and will thus be even more powerful by allowing the user to evaluate robust and weak parts of the produced zonation. Nevertheless, the implementation of the proposed solutions is not trivial. Indeed, finding all solutions between the conflicting superpositional relationships is well-known to be a difficult combinatorial approach (Guex & Davaud 1984), which may be impossible to solve if too many taxa are involved. However, using heuristic approaches may still be relevant and able to find a solution more parsimonious than the one currently produced by the UAs in the case of under-constrained data. These tools are routinely used in phylogenetic reconstructions and they would be equally useful implements for the UAs.

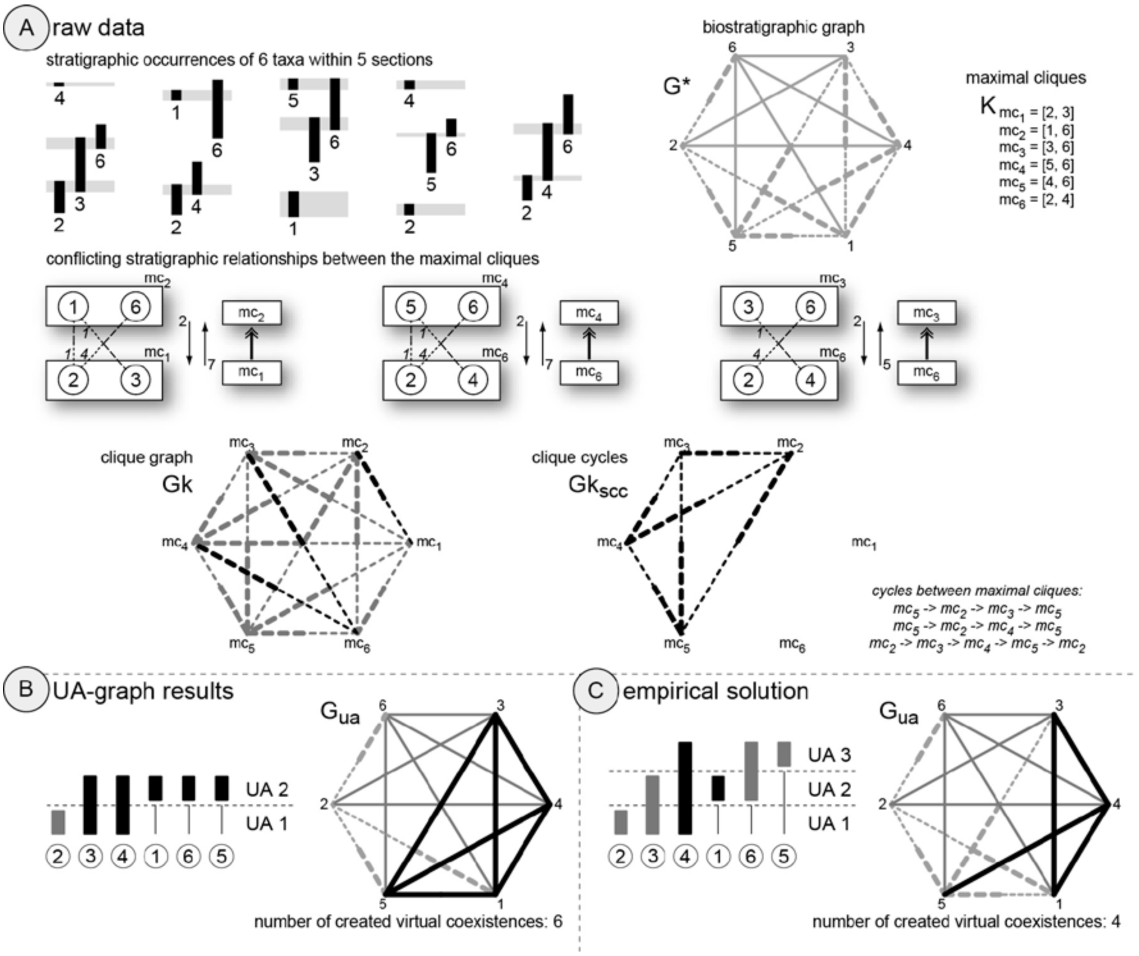


Figure 3 – *Imaginary biostratigraphic dataset containing cycles between its maximal cliques (after Monnet et al 2011b). It illustrates that in the case of poorly constrained superpositional relationships between the taxa (**A**), the solution produced by UA-graph (**B**) is not the most parsimonious as evidenced by the empirical solution showed here (**C**).*

UAs and derived information

The UAs focuses on associations of taxa to reconstruct a biochronological zonation. Given the incompleteness of the fossil record and thus of the stratigraphic raw data, this may be a better approach than focusing on FOs and LOs as currently done in other methods (Guex 1991). Yet, although FOs and LOs are highly susceptible to diachronism, also for ammonoids (Monnet & Bucher 2002, 2007b), their relative order can still be partly congruent in a dataset. Hence, instead of discarding this information, the UAs could report at least a majority consensus of the relative order of these bioevents with their confidence intervals (their reproducibility should be tested) in order to present the most complete results. For instance, Monnet et al (2011b) processed this empirically after the UAs run.

It often happens that several maximal cliques do not belong to the longest sequence *L* of superposed maximal cliques from *Gk* because of indeterminate superposition relationships (*Fig 4*). Generally, there are parallel paths and even disconnected maximal cliques. The solution adopted by the UAs is to merge (if possible) the cliques, which are not contained in the longest path, with cliques in the longest path based on a “best fit” criterion (Guex 1991) such that a clique is merged with its most similar clique in *L* if it is also bracketed between cliques of *L* (*Fig 2F*). This step of the method (called here the “full-merging approach”) intrinsically induces the creation of virtual coexistences between all taxa belonging to the merged cliques. However, this solution can lead to the creation of more virtual coexistences than necessary. I created an imaginary example (*Fig 4A*) and the corresponding result of UA-graph (*Fig 4B*). In this case, it induces the virtual coexistence of taxon 8 with taxa 1 and 3. However, there exist two other possible solutions if one creates virtual coexistences only between some of the taxa involved (called here the “partial-merging approach”): either taxon 8 remains below taxon 3 and coexists with taxon 1, or taxon 8 remains above taxon 1 and coexists with taxon 3 (*Fig 4C*). These two solutions involve the creation of a single virtual coexistence instead of two for the solution of the UAs. Hence, the “full-merging approach” has the advantage of providing a single solution to the user, but this procedure does not yield the most parsimonious solution in terms of the number of created virtual coexistences and more importantly, it does not reflect the fact that multiple solutions (assuming different sets of virtual coexistences) exist. Note that from a purely biochronological point of view, the proposed partial-merging approach provides no additional power of correlation. However, it has an important influence on the diversity counts, which can be derived from the zonation provided by the method. For instance, in the previous example (*Fig 4*), it appears that the taxon richness of UA 2 may be overestimated and that only two taxa really coexisted. The partial-merging approach can thus provide the user an index of potential errors in the derived diversity curves.

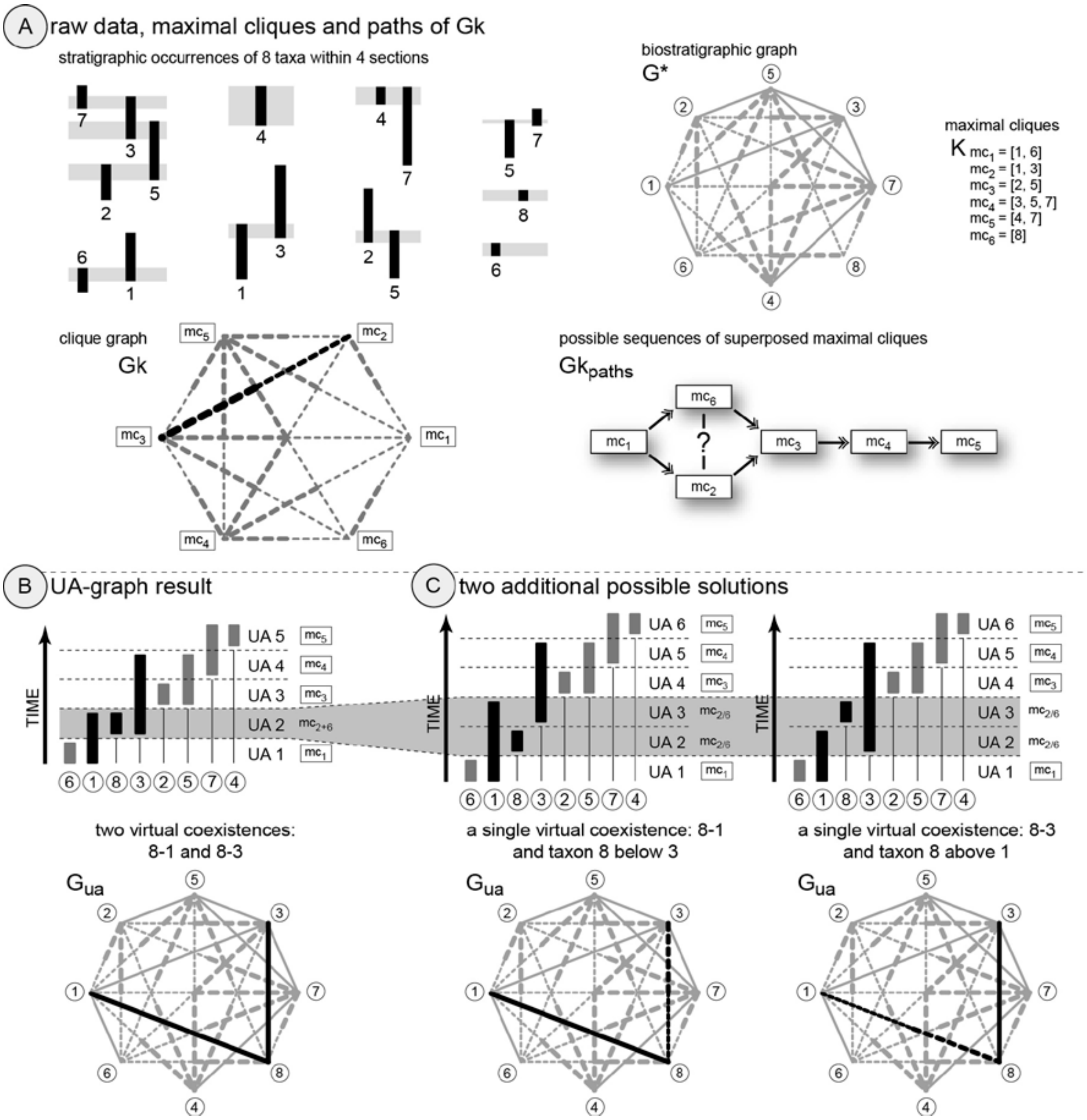


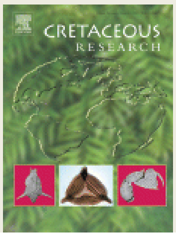
***Figure 4** – Imaginary biostratigraphic dataset containing several possible sequences of superposed maximal cliques (after Monnet et al 2011b). It illustrates that UA-graph selects a single solution by creating a virtual coexistence between all taxa implied by the merging of isolated maximal cliques. However, two additional interpretations are possible and illustrate the underlying uncertainties of specific parts of the results.*

Applications

Related publications:

Monnet & Bucher 1999, 2002, 2006, 2007b; **Monnet** et al 2011b, 2015a

Appended publication:



Monnet C, Bucher H (**2007**) Ammonite-based correlations in the Cenomanian-lower Turonian of north-west Europe, central Tunisia and the Western Interior (North America).
Cretaceous Res **28:1017–1032**
(doi: 10.1016/j.cretres.2007.01.007)

My expertise on the quantitative biochronological methods results from several years of their critical application to ammonoid datasets of various extent (basin-, regional-, to global-scale) and for very different periods (Early–Middle Devonian, Middle Triassic, and Late Cretaceous). This chapter summarizes some of these various applications.

All of the studies I directed in biostratigraphy are characterized primarily by applying quantitative methods in order to obtain more objective biozonations by using consistent approaches that enable treating the large amount of biostratigraphic data and which are not biased by the *a priori* empirical selection of supposedly index taxa.

In addition, my works are not a blind application; they are characterized by identifying and accounting for the diachronism of ammonoids. Although this is usually completely ignored by biostratigraphers, the accuracy and reliability of the geological time scale can be enhanced if the biochronological correlation error is fully assessed in its construction. Computer-assisted methods (UAs, CONOP, RASC) are amenable to quantify the uncertainty which cannot be neglected in long-distance correlation involving different continents or ancient ocean basins. Another original aspect of my research is the use of tools to detect the origin of the biostratigraphic contradictions in order to get some feedback on the quality of the data and on the origin of the biostratigraphic contradictions.

MIDDLE DEVONIAN AMMONOIDS

Monnet et al (2011b) revised the regional late Emsian and Eifelian (Early–Middle Devonian) ammonoid biozonation of Morocco. They focused on the Devonian sedimentary successions from the Tafilalt (eastern Anti-Atlas, Morocco) and analyzed a rich dataset of 53 species from 15 sections (data after Klug 2002). This dataset has been processed with the automatic and quantitative unitary association method (UA-graph). It led to the construction of a sequence of 17 UAs (maximal sets of actually or virtually coexisting taxa), which are grouped into 10 laterally reproducible association zones (*Fig 1*). This biozonation is the result of an empirical post-treatment of the UA result, notably to overcome inconsistencies in the resolution of cycles (see previous chapter), as well as the reintegration of singleton species and taxonomic uncertainties

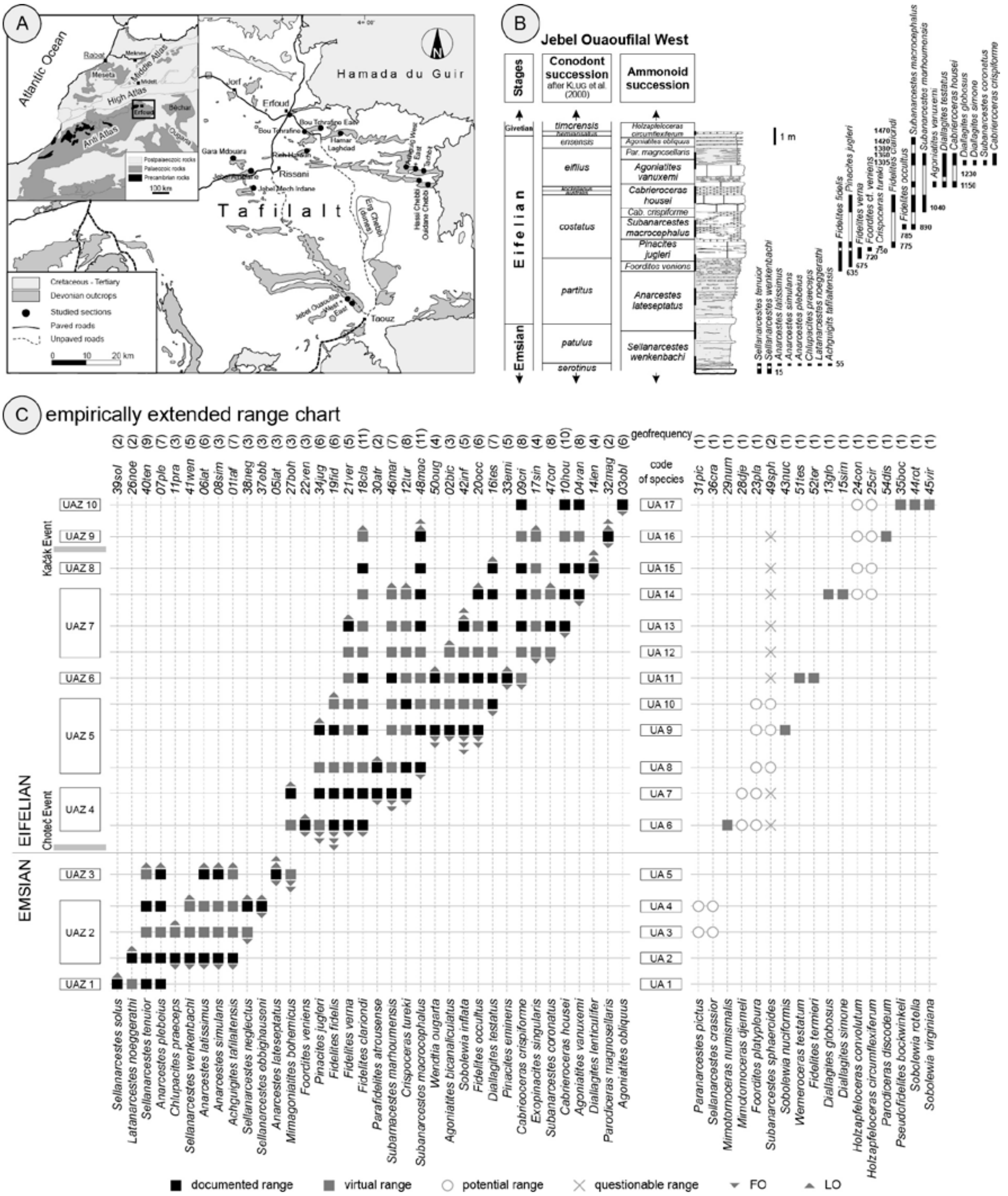


Figure 1 – A) *Geological map of the eastern Anti-Atlas (Morocco) showing the sections analyzed for the biochronological revision of Devonian ammonoids (Klug 2002).* ***B)*** *Example of raw biostratigraphic data: occurrences of taxa along a section (Klug 2002).* ***C)*** *The extended range chart constituting the revised biozonation of Monnet et al (2011b); the relative order of first occurrences or last occurrences (FOs⁄LOs) for each taxon has been checked and a consensus is reported on the figure.*

The revised biostratigraphic subdivision of the studied interval is in some parts finer than the classically used empirical stratigraphic scheme (compare Klug 2002). Interestingly, this zonation is also compared to a previous zonation erected using the graphic correlation method. In addition to providing supplementary biochronological subdivisions, the UAs enabled to underline one drawback of graphic correlation: it often artificially lengthens the stratigraphic range of species and thus creates unnecessary virtual coexistences between some species (*Fig 2*).

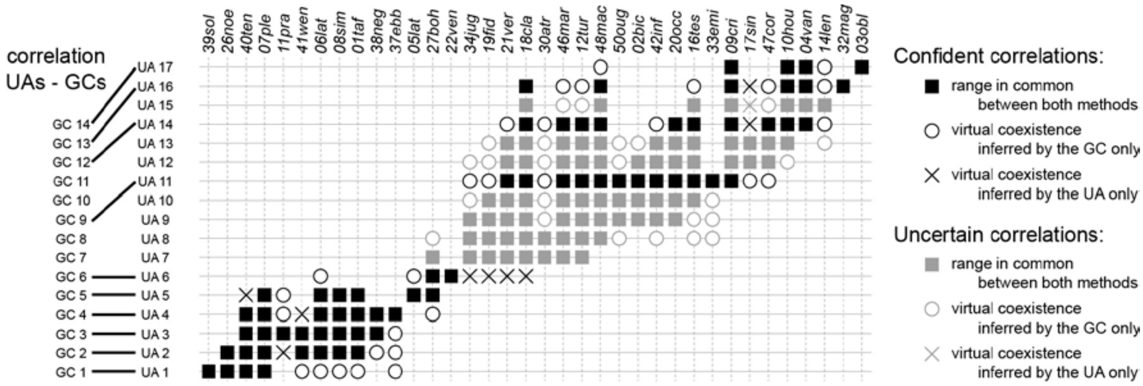


***Figure 2** – Comparison of the graphic correlation (GC) results with the unitary associations (UA) in terms of reconstructed virtual coexistences (Monnet et al 2011b): squares = coexistence documented by both methods; crosses = virtual coexistence inferred by the UA but not by the GC; circles = virtual coexistence inferred by the GC but not by the UA. Grey markers indicate uncertain correlations between the two methods.*

Finally, based on the resulting species ranges of the 17 UAs from late Emsian to Eifelian, this study quantified the regional ammonoid diversity of this interval in detail. This enabled to document several regional and global diversity patterns, especially between anarcestids and agoniatitids: 1) a late Emsian anarcestid radiation; 2) a late Emsian anarcestid extinction; 3) an early Eifelian agoniatitid radiation (Choteč event); 4) an early to middle Eifelian anarcestid radiation; and 5) a late Eifelian ammonoid diversity decrease (Kačák event).

MIDDLE TRIASSIC AMMONOIDS

Monnet & Bucher (2005, 2006) synthesized and revised the ammonoid zonations of the Anisian (Middle Triassic) from North America. Their study focused on three basins, which were distributed along a latitudinal gradient (*Fig 3B*): western Nevada (low paleolatitude, USA), British Columbia (mid paleolatitude, Canada), and the Sverdrup Basin (high paleolatitude, Canada). They applied the UAs method to reconstruct an ammonoid biozonation for each of the three basins, as well as the correlation between the three basins in a second, hierarchical step. This biochronological study benefited from recent and thorough taxonomic updates of Anisian ammonoids (Silberling & Nichols 1982; Bucher 1989, 1992a, b; Tozer 1994b; Monnet & Bucher 2005).

Based on this quantitative analysis, the Anisian in the studied areas contains 13, 10, and 3 zones and a total of 174, 90, and 7 species, for western Nevada, British Columbia and the Sverdrup Basin, respectively (*Fig 3A*). The use of such quantitative biochronological methods lead to new and more precise correlation. For instance, the *Buddhaites hagei* Zone (Canada) correlates only with the *Intornites mctaggarti* Subzone (Nevada) and not with the entire *Acrochordiceras hyatti* Zone (Nevada) as previously empirically assumed by other authors (compare *Figs 3A, C*). The *Tetsaoceras hayesi* Zone (Canada) appears to correlate with the *Unionvillites hadleyi* Subzone (Nevada) of the *hyatti* Zone and not with the *Nevadisculites taylori* Zone. The *Hollandites minor* Zone (Canada) correlates with the *taylori* Zone (Nevada), not with the *Balatonites shoshonensis* Zone as is usually acknowledged (see Tozer 1994a).

The UAs also enabled quantifying the diachronism of studied taxa. It appears that about 67% of the genera and 18% of the species common to Nevada and British Columbia have diachronous FOs or LOs (*Fig 3D*). Therefore, this diachronism is significant and its impact on correlation should not be overlooked.

Finally, these revised biochronological zonations enabled quantifying the biodiversity of Anisian ammonoids from North America, with for instance, the highlight of a major diversity peak during the early Middle Anisian exact correlatives *hadleyi* Subzone in Nevada and *hayesi* Subzone in British Columbia that is concomitant with short-lived faunal exchanges between the usually latitudinally restricted middle and late Anisian faunas (for more details, see Monnet & Bucher 2006).

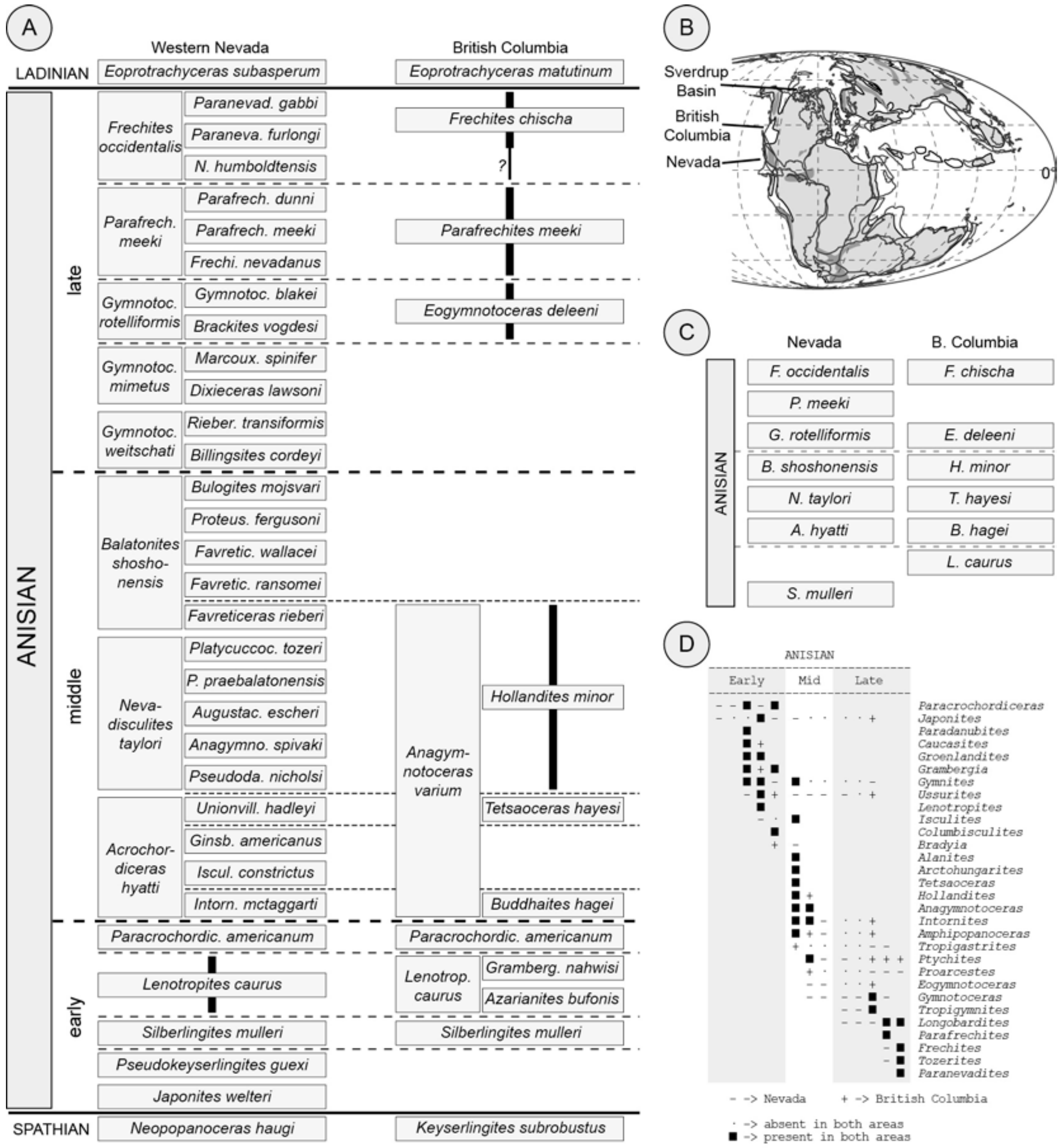


***Figure 3 –** Ammonoid biochronology of the Anisian (Middle Triassic). **A)** Ammonoid zonations and correlation of Nevada and British Columbia (after Monnet & Bucher 2006); compare with (C). Thick vertical black bars indicate poorly constrained correlation with their length representing the maximum amount of uncertainty. **B)** Paleogeographic location of Nevada and British Columbia. **C)** Correlation of Nevada and British Columbia ammonoid zones after Tozer (1994a). **D)** Biostratigraphic ranges and diachronism of Anisian ammonoid genera between Nevada and British Columbia at the zone level (after Monnet & Bucher 2006).*

LATE CRETACEOUS AMMONOIDS

The marine Cenomanian–Turonian is one of the best-studied stratigraphic intervals of the Cretaceous, prompted by the occurrence of several biotic and abiotic events (see Monnet 2009). Hence, the biostratigraphic distribution of major ammonoid genera and species during the Cenomanian–Turonian is relatively well documented, and empirical ammonoid zonation have been established in details in various basins, but with sometimes important discrepancies in the position of supposedly key index taxa: Anglo-Paris Basin (Wright & Kennedy 1981, 1984), the Vocontian Basin (SE France; Thomel 1972, 1992a, b), the Münster Basin (Kaplan et al 1998), central Tunisia (Robaszynski et al 1994), and the Western Interior (Cobban 1984; Kennedy & Cobban 1991; Kennedy et al 2005).

For my research, I revised thoroughly and quantitatively the Cenomanian ammonoid zonation by means of the UAs (Biograph) in order to improve correlation and understand the origin of the discrepancies (Monnet & Bucher 1999, 2002, 2007b). These revisions were based on a taxonomic homogenization of ammonoid faunas among the studied areas. Interestingly, these analyses were successively performed from basin-, regional-, to global geographic scale. Only the last analysis is illustrated here.

Based on a large number of sections and species, the Cenomanian and early Turonian comprises 30 UA-zones in north-west Europe, 24 UA-zones in central Tunisia and 23 UA-zones in the middle Cenomanian–early Turonian of the Western Interior Basin (*Fig 4A*). The quantitative, revised zonation and correlation are in relative good agreement with the empirical, standard zonation of the three study areas (*Fig 4*). The few discrepancies were about the position of the middle–upper Cenomanian boundary in the Western Interior and in Tunisia compared to Europe. Note that these revised zonations define discrete association (not interval) zones. It implies that the interval zones proposed by Gale (1995) are not recognized since the two concepts are not compatible. For instance, the *Cunningtoniceras inerme* Zone defines the base of the middle Cenomanian by the appearance of the species *C. inerme*. However, from the assemblage point of view, this species coexists with younger ammonoids of the *Acanthoceras rhotomagense* Zone and does not belong to a distinct association, and therefore does not deserve a distinct biochronozone.

The UAs leads to a two-fold increase in resolution of these ammonoid zonations compared to the standard, empirical schemes. These correlations enable the designation of a new global marker for the middle/late Cenomanian boundary, which is characterized by the disappearance of the genera *Turrilites*, *Acanthoceras* and *Cunningtoniceras* and by the appearance of *Eucalycoceras*, *Pseudocalycoceras* and *Euomphaloceras*.

Interestingly, I used an original approach to semi-automatically correlate the studied areas by considering each regional biozonation as a section. This approach enabled to objectively correlate the three areas and to evaluate the diachronism of studied taxa. The correlation between the studied areas highlight the variable completeness and resolution of the faunal record through space and time, and reveal a significant number of diachronous taxa (*Fig 4C*). The only synchronous datum known to date is the last occurrence (LO) of *Turrilites acutus*, which may thus be potentially used as a marker for the middle/late Cenomanian boundary, provided that it does not turn out to be diachronous in the light of any new data.

Finally, these revised quantitative ammonoid biozonations enabled precise investigation of biodiversity patterns of ammonoids during the Cenomanian–Early Turonian in these areas and to evaluate these in the face of known abiotic changes during this time interval (Monnet et al 2003b; Monnet 2009).

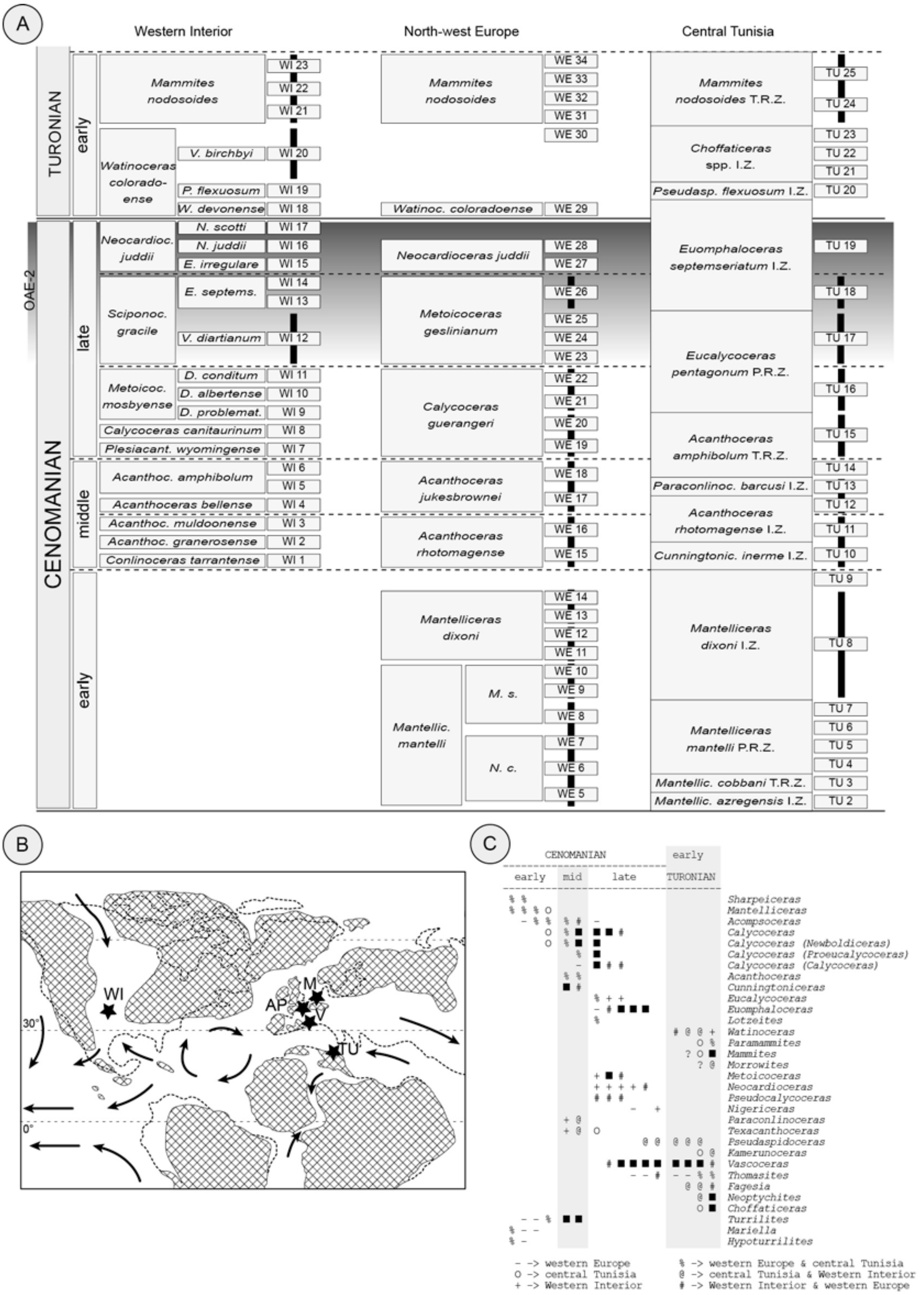


Figure 4 – *Ammonoid biochronology of the Cenomanian–early Turonian (after Monnet & Bucher 2007b).* ***A)*** *Ammonoid zonations and correlation) between the three studied areas and between the previous empirical zonations and the reconstructed UAs.* ***B)*** *Paleogeographic location of the three studied areas (Western Interior, Central Tunisia, and north-west Europe, which includes the Anglo-Paris, Vocontian, and Münster Basins).* ***C)*** *Biostratigraphic ranges and diachronism of ammonoid genera between the three studied areas.*

BIOSTRATIGRAPHY OF TRIASSIC AMMONOIDS

In addition to being a proponent of quantitative biostratigraphy, I am also trained on traditional, empirical correlation. Indeed, my expertise enabled me to lead a review paper on the entire Triassic ammonoid biostratigraphy and the correlation of biozonations between the major areas in the world (Jenks et al 2015). In addition to review the historical and geographic development of the Triassic ammonoid biostratigraphy, the major outcome of this review is the construction of correlation tables of all major existing ammonoid biozonations in space and time (*Fig 5*).

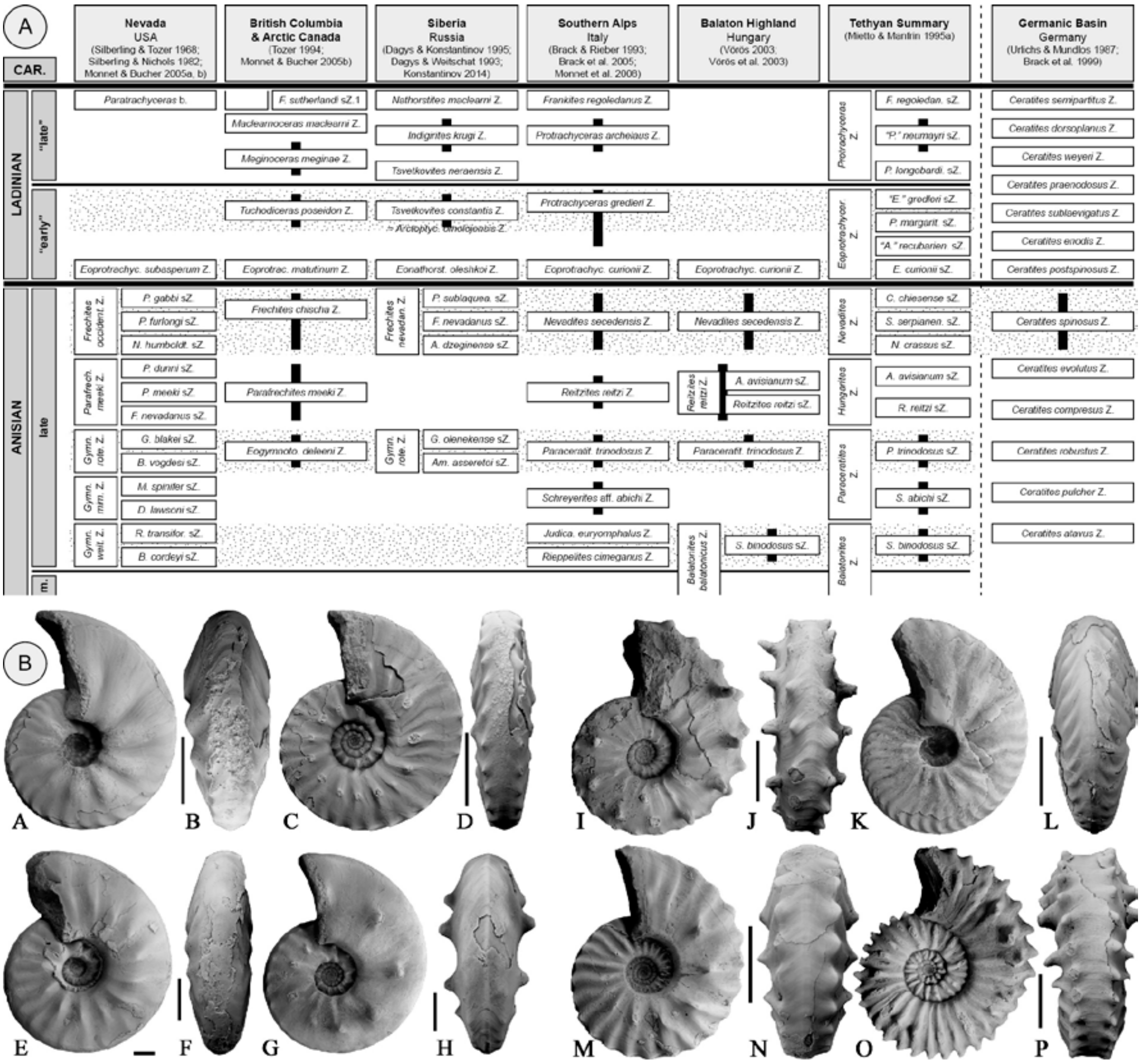


***Figure 5** – Example outcome of the recently revised Triassic ammonoid biostratigraphy (after Jenks et al 2015). **A)** Late Anisian and Ladinian (Middle Triassic) ammonoid zones and correlation (vertical bars indicate poorly constrained correlation; Z zone, sZ subzone, b beds). **B)** Some characteristic ammonoids of the late Anisian: a, b,* Dixieceras lawsoni*; c, d,* Rieppelites shevyrevi*; e, f,* Gymnotoceras blakei*; g, h,* Silberlingitoides cricki*; i, j,* Brackites vogdesi*; k, l,* Parafrechites meeki*; m, n,* Frechites nevadanus*; o, p,* Nevadites hyatti. *Scale bars = 2 cm. All specimens from JF Jenks collection (Nevada).*

This review of Triassic ammonoid biostratigraphy (historical development and current state of knowledge) demonstrates that the correlation of ammonoid zones through time and space is very irregular. This situation reflects the complex and very long history of Triassic ammonoid biochronology, which has been conditioned by the evolutionary history of ammonoids in space and time, such as biogeographic endemism/cosmopolitanism. For instance, latitudinal differentiation among ammonoids varied significantly during the Triassic, thus making clear and unambiguous global correlation more difficult at times (Dagys 1988; Brayard et al 2006, 2009a, 2015). Furthermore, the personalities of some ammonoid workers as well as their respective theories and practices regarding taxonomy have produced some rather strongly diverging opinions and approaches (Brack & Rieber 1996; Mietto et al 2004), which sometimes may have hindered more accurate and dependable correlation. Famous examples such as *Ceratites binodosus* (Hauer) and *Ceratites reitzi* Böckh have been reviewed by Balini et al (2010); Tozer (1971) has also emphasized some of these taxonomic problems.

By tradition, ammonoids have always been regarded as the best marine guide fossils for the Triassic system (Mojsisovics et al 1895; Tozer 1984; Balini et al 2010; Lucas 2010, 2013). However, in Triassic biostratigraphic studies, there are two different (but not conflicting) approaches to the use of ammonoids (and other fossils) as time markers: one is based on bioevents (FADs and LADs), and the other on coexistences. The former is often linked to a body of strata and it fits well with the concept of GSSPs, which are defined by such bioevents that lead to continuous, interval zones, often focused on a single section. The latter is a more abstract concept, independent of rocks, and characterized by discrete, association (or assemblage) biozones, often encompassing as many sections as possible. This dual concept may sometimes confuse correlation and dating of sections if not clearly defined. Nevertheless, quantitative methods exist for treating both data types that lead to robust biozonation. Because bioevents (FADs and LADs) are biased by many factors, caution should be exercised when using them to define biozones and GSSPs in order to avoid as much as possible the problems related to the non-negligible proportion of diachronic taxa (Monnet & Bucher 2002, 2006, 2007b). Because of the tendency that began in the last few decades to define GSSPs by the FADs of conodonts, it is here stressed that such problems hold not only for ammonoids, but for all fossils including conodonts; see Shevyrev 2006; Goudemand et al 2012; Lucas 2013; Zhang et al 2014).

The resolution of the various Triassic ammonoid biochronological schemes is highly variable (as is the duration of the stages). This variability is well illustrated by the average duration of ammonoid biochronozones (ca. 0.74 Myr for the zone level), which varies from 60 kyr for the Smithian to over 0.43 Myr for the Anisian to 2.70 Myr for the Norian. Thus, resolution is seen to not only be variable, but it also obviously decreases significantly during the Triassic. Although this decline can be readily correlated with the decreasing turnover of ammonoids during the Triassic (see Brayard et al 2009a), it is also probably influenced somewhat by the relative lack of studies in the Late Triassic. These values are comparable in magnitude with those of Milankovitch cycles (20 kyr for the precession cycles, 100 and 400 kyr for the eccentricity cycles; see Brack et al 1996; Szurlies 2007; Ikeda et al 2010; Tanner 2010) and with the validated magnetozones (mean reversal of 250 kyr for the Early–Middle Triassic; see Hounslow & Muttoni 2010).

The current approach in biochronostratigraphy tends toward global correlation and integrated studies, which is well exemplified by the definition of the GSSPs. Indeed, the definition of GSSPs emphasizes the reproducible correlation of events (e.g. various fossil groups, magnetostratigraphy, and isotope analysis) by cross-comparison (see e.g. Brack et al 2005; Mietto et al 2012; Hillebrandt et al 2013). In this context, the role of ammonoids for the definition of Triassic stages and substages has thus been further corroborated and enlarged. The comparison of ammonoid biostratigraphy to conodont, radiolarian, pelagic bivalve and palynomorph biostratigraphies demonstrates, without doubt, that the ammonoids are the fossil group with the potential to reach the highest temporal resolution within Triassic marine environments.

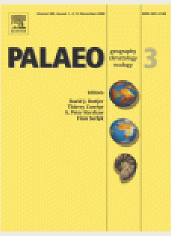
Macroevolutionary Patterns of Ammonoids

Biodiversity

Related publications:

Monnet et al 2003; **Monnet** & Bucher 2007a; **Monnet** 2009; Brayard et al 2009b

Appended publication:



Monnet C (2009) The Cenomanian-Turonian boundary mass extinction (Late Cretaceous): new insights from ammonoid biodiversity patterns of Europe, Tunisia and the Western Interior (North America).
***Palaeogeogr Palaeoclimatol Palaeoecol* 282:88–104**
(doi: 10.1016/j.palaeo.2009.08.014)

One major outcome of paleontology is the description of past biodiversity and its fluctuations in space and deep time. It is famously exemplified by the Sepkoski's (1984, 1993) biodiversity curves of the number of marine taxa through the Phanerozoic. These resulted from his global compendia of marine animal families and genera, and have been used to and still continue to motivate a tremendous amount of paleobiological research. Among many examples, such biodiversity curves enabled identifying the major ("Big Five") mass extinctions, the three "Great Evolutionary Faunas" that sequentially replaced one another as dominant groups during the Phanerozoic, possible periodicity in biodiversity fluctuations, and also the major biodiversification events such as the "Cambrian Explosion" and the "Great Ordovician Biodiversification Event". Beginning with the work of Phillips (1860), paleontologists have intuited that counts of fossil taxa through the geological record provide a metronome of the pace of large-scale evolution. The deep-time history of life on Earth results from background originations and extinctions defining a steady-state, nonstationary equilibrium occasionally perturbed by biotic crises and ‘‘explosive’’ diversifications. As a direct consequence, in a physically heterogeneous and ever-changing world, spatial and temporal fluctuations of biodiversity are the rule since the origin of life on Earth, thus legitimating two main questions (Escarguel et al 2011): how does biodiversity vary through time, and how does biodiversity vary through space?

Biodiversity generally refers to the variety and variability of life on Earth; this can refer to genetic variation, ecosystem variation, or species variation (number of species) within an area at a certain time (Sepkoski 1997). In deep time, the most commonly applied approach due to its easier access relies on the Linnaean hierarchical classification, leading to a biodiversity estimate based on taxonomic richness.

Because the fossil record is the only direct witness of past biodiversity, reconstructing biodiversity curves is an important task, which has seen the development of multiple metrics to account for the various facets of biodiversity. The quality of our understanding of the biases and weaknesses in paleontological data has also progressed markedly. Questions of quality involve completeness of the fossil record, accuracy of taxonomy, precision of correlation and dating, and temporal biases in the amount of study, quantity of sediment, and quality of preservation.

Continuing study of data compiled from the fossil record is providing a consistent picture of the history of biodiversity in the geological past (Alroy et al 2008). Data for marine animal genera look much like data for families with differences being largely predictable. This supports the idea that paleontological data are of sufficient quality to make general statements about how large-scale biodiversity has evolved and how it has behaved during crises of extinction.

With regard to my own research, I directed studies on the Cenomanian/Turonian boundary event (CTBE: Monnet et al 2003; Monnet & Bucher 2007a; Monnet 2009). All these studies on biodiversity are based on a revised taxonomy and a revised biochronological frame (see corresponding chapter) in order to minimize the related biases. I also collaborated on the investigation of the Permian/Triassic boundary (PTB: Brayard et al 2009b) and the concomitant biodiversity dynamics of ammonoids (for further details, see Escarguel et al 2011; Brayard & Bucher 2015).

BIODIVERSITY METRICS

The calculation of biodiversity indices is one of the cornerstones of ecological analysis and paleontology. It is also an excessively bewildering field, with an impressive list of potential indices. This diversity of diversity indices thus implies that diversity can be defined in many ways. Unfortunately, it is impossible to point to any single index as being best for any given kind of data or any particular investigation. Magurran (1988) gave a thorough introduction to these techniques, and Hill (1973) provided a unifying theoretical framework for several diversity indices. Also, in paleontology, most commonly used biodiversity approaches are described by Hammer & Harper (2006). In paleontology, biodiversity indices are used for several purposes, but especially diversity can be plotted as a function of time in order to identify events and trends.

In paleontology, two types of data, each with two states, characterized the bunch of possible biodiversity indices/estimators: 1) presence/absence (incidence) *versus* counts of individuals (abundance), and 2) one set of information *versus* data from several samples.

The simplest possible diversity index is the number of species present in one sample, known as species richness. This can be generalized to genera or higher taxonomic levels. Species richness is a useful index that is easy to understand, and it can be used also with only incidence data. Because, a count of species in a sample will usually be an underestimate of the species richness even in the preserved part of the biota from which the sample was taken, species richness will generally increase with sample size. Therefore, several other indices have been proposed that attempt to compensate for this effect. On the one hand, some approaches are based on abundance data from a single sample: several indices weight the richness by sample size (Margalef 1958; Menhinick 1964); others rely on the comparison of rarefaction curves (Foote 1992). On the other hand, there exists richness estimators based on incidence data from several samples: in this case the *Chao2* (Chao 1987) seems to perform particularly well (Colwell & Coddington 1994). Finally, based on both abundance data from multiple samples, the most modern approach called *SQS* (shareholder quorum subsampling) has been developed by Alroy (2010) and estimates how many species can be expected given fixed coverage of the underlying abundance distribution (coverage is the sum of the frequencies of the species sampled).

Also, in complement to taxonomic richness, there exists a series of biodiversity indices, which attempt to incorporate relative abundance/proportion of taxa, leading to the concept of dominance or evenness: Berger–Parker index, or Simpson index, among others (Simpson 1949; Magurran 1988).

With regard to my research, several metrics are used to extract and analyze ammonoid biodiversity patterns. The species richness is defined here as the number of species occurring within a given zone.

Origination and extinction values correspond to the number of taxa appearing and disappearing between two successive zones. The turnover is defined as the sum of the number of originations and extinctions. For each index, the relative proportion and the time ratio is also computed; e.g. the percentage of origination is defined as origination divided by the total number of taxa occurring in the next overlying zone.

With regard to my research, I often include also less conventional biodiversity metrics such as poly-cohort analysis and taxonomic distinctness. Poly-cohort survivorship analysis (Van Valen 1973, 1979; Raup 1978, 1986) is a tool used to graphically investigate and compare survivorship through time. A poly-cohort survivorship curve is a plot of the percentage of all taxa from a community defined at time *t* still existing at time *t+dt*. The poly-cohort curves' log-linearity is statistically tested using two distinct approaches involving the Epstein's test for straightness (Epstein 1960a, b; Raup 1975) and a statistical procedure developed by Escarguel (in Monnet et al 2003). This procedure is based on a Monte-Carlo procedure of random re-sampling with replacement (bootstrap) in order to estimate the confidence intervals linked to the observed survivorship percentages. It allows to test the departure of observed curves from the null expectation that, for a given ammonoid community, survivorship percentages are log-linearly arranged, i.e. that extinction risk is stochastically constant through time within poly-cohort.

The taxonomic distinctness (TD) method (Warwick & Clarke 1995) processes presence/absence data with two univariate indices (the Average Taxonomic Distinctness index, AvTD, Clarke & Warwick 1998; and the Variation in Taxonomic Distinctness index, VarTD, Clarke & Warwick 2001). These two indices reflect the hierarchical structure underlying the studied assemblage of taxa by calculating the 'taxonomic distance' of all pairs of taxa from the studied assemblage. AvTD reflects the 'taxonomic disparity' of the sample, i.e. if each taxonomic level is equally represented. VarTD is a measure of taxonomic unevenness, i.e. if species are distributed at the same taxonomic rank or at all ranks. These two robust indices can also be statistically tested by bootstrapping to detect non-random taxonomic structures in the studied assemblages, i.e. taxonomical assemblages with AvTD and/or VarTD values significantly higher or lower than what might be expected if taxa were randomly distributed through samples. The TD indices could be biologically and ecologically meaningful if the taxonomic structure of the studied group reflects an ecological and adaptive hierarchy (see Warwick & Clarke 1998; Clarke & Warwick 2001).

THE CENOMANIAN/TURONIAN BOUNDARY EVENT (CTBE)

The Cenomanian/Turonian boundary witnessed one of the ten most severe biotic crises of life's history (Raup & Sepkoski 1986) with the extinction of approximately 26% of marine animal genera. It is characterized by a worldwide diversity drop of a number of groups, such as benthic and planktonic foraminifers (Jarvis et al 1988; Kaiho 1994; Peryt & Lamolda 1996; Tur 1996; Groshény & Malartre 1997), calcareous nannoplankton (Leckie et al 2002), ostracods (Babinot et al 1998), radiolarians (Erbacher & Thurow 1997; O'Dogherty & Guex 2002), aragonitic rudist bivalves (Johnson & Kauffman 1990; Philip & Airaud-Crumière 1991; Steuber & Löser 2000), and ammonoids (Elder 1989; Hirano et al 2000). For example, in the Western Interior, Harries & Little (1999) reported the extinction of 79% of macro-invertebrate species and Elder (1989) of 74% of ammonoid species.

The description of several sections around the world highlighted the occurrence of many, more or less interwoven, abiotic events around this mass extinction (*Fig 1*). The Cenomanian–Turonian boundary recorded the highest sea level of the Mesozoic (Haq et al 1988), some of the highest atmospheric CO_2 concentrations (Berner 1994; Bice & Norris 2002), a global warming (Jenkyns et al 1994; Clarke & Jenkyns 1999; Huber et al 2002), a global oceanic anoxic event (Jenkyns 1980; Arthur et al 1987; Schlanger et al 1987), and a global major positive $\delta^{13}C$ excursion (Scholle & Arthur 1980; Accarie et al 1996; Tsikos et al 2004; Groshény et al 2006; Jarvis et al 2006) coupled with massive deposition of organic-rich sediments (Herbin et al 1986; Schlanger et al 1987). Therefore, the Cenomanian–Turonian interval represents an ideal context to study the interactions between biotic and abiotic events.

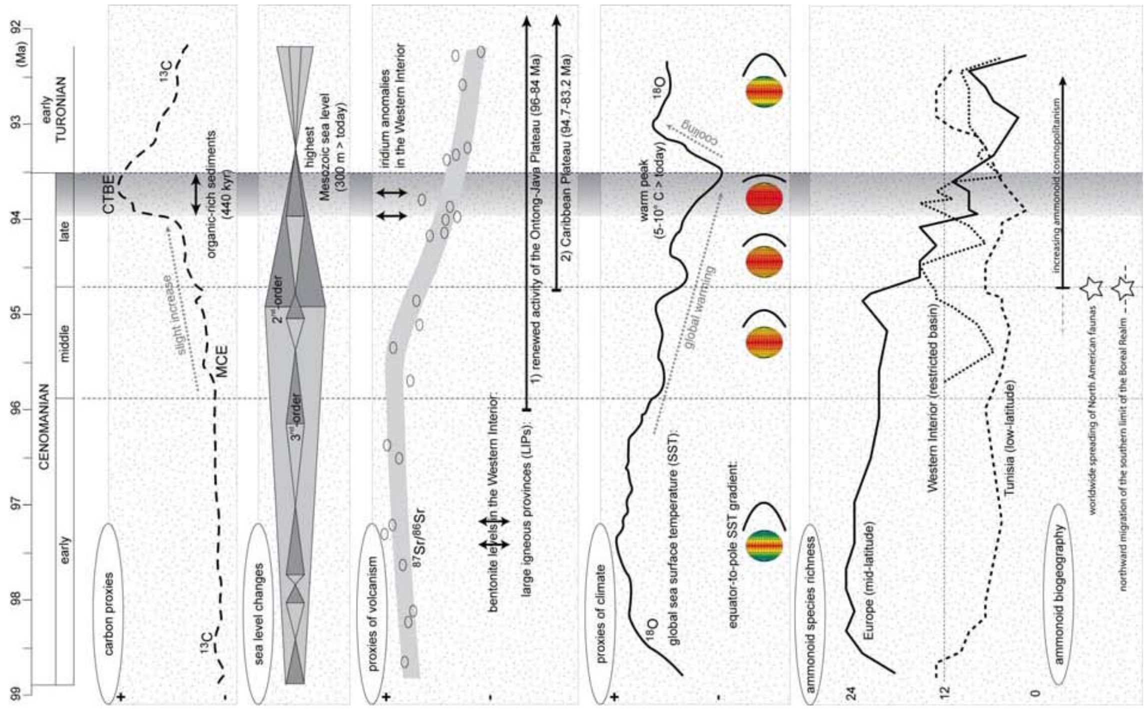


Figure 1 *– Major environmental markers during the Cenomanian–Turonian (Monnet 2009).*

The uppermost Cenomanian is characterized by the worldwide spreading of hypoxic/anoxic waters, the so-called Oceanic Anoxic Event 2 (OAE2). This event has been considered the major cause of the Cenomanian–Turonian boundary mass extinction and the killing-mechanism for numerous species (Kauffman & Hart 1995). However, several authors questioned the existence of this mass extinction (Corfield et al 1990; Banerjee & Boyajian 1996; Gale et al 2000; Smith et al 2001). The goal of my research during several years was to document the biodiversity patterns of ammonoids throughout the entire Cenomanian from three major areas (Europe, Tunisia, and the Western Interior) and to evaluate the relationships between ammonoid biodiversity patterns and abiotic factors during the Cenomanian–Turonian interval.

Therefore, based on the previously revised taxonomy and biochronology of the Cenomanian–Turonian ammonoids (see corresponding chapter), I evaluated ammonoid biodiversity patterns first at a local scale (the Vocontian Basin: Monnet & Bucher 1999), then at a regional scale (north-west Europe: Monnet et al 2003), and finally at a rather global scale by including the Western Interior (USA) and Tunisia (Monnet 2009), therefore including all basins with a complete ammonoid record for this interval.

The biodiversity patterns of ammonoids (species richness, origination/extinction, turnover, poly-cohort survivorship, and taxonomic distinctness) highlight that the mass extinction of the

Cenomanian/Turonian boundary is restricted to Europe (*Fig 2*), as far as ammonoids are concerned. Only Europe documents an actual decrease of species richness during the late Cenomanian, which results mainly from decreasing originations. This result is also supported by the absence of statistically significant changes in the extinction probabilities of poly-cohorts during the entire Cenomanian (no simultaneous extinction event between several poly-cohorts). In Tunisia, where the onset of anoxic waters is synchronous with Europe, species richness increases during the late Cenomanian and reaches its highest values in the early Turonian. The Western Interior records relatively high species richness during the late Cenomanian with only a single minor extinction event. Because the duration of the upper Cenomanian is estimated to about 1.2 myr (Obradovitch 1993; Gale 1995), the consistent decrease of species richness appears as a general protracted trend, which initiated at the middle–upper Cenomanian boundary. As noted by Thomel (1992b), a marked and abrupt decrease in absolute abundance of ammonoids also occurred during the upper Cenomanian of Europe. Furthermore, major changes in biodiversity patterns of ammonoids occurred around the middle/upper Cenomanian boundary, i.e. about 0.75 Myr before the onset of the Oceanic Anoxic Event 2 (OAE2).

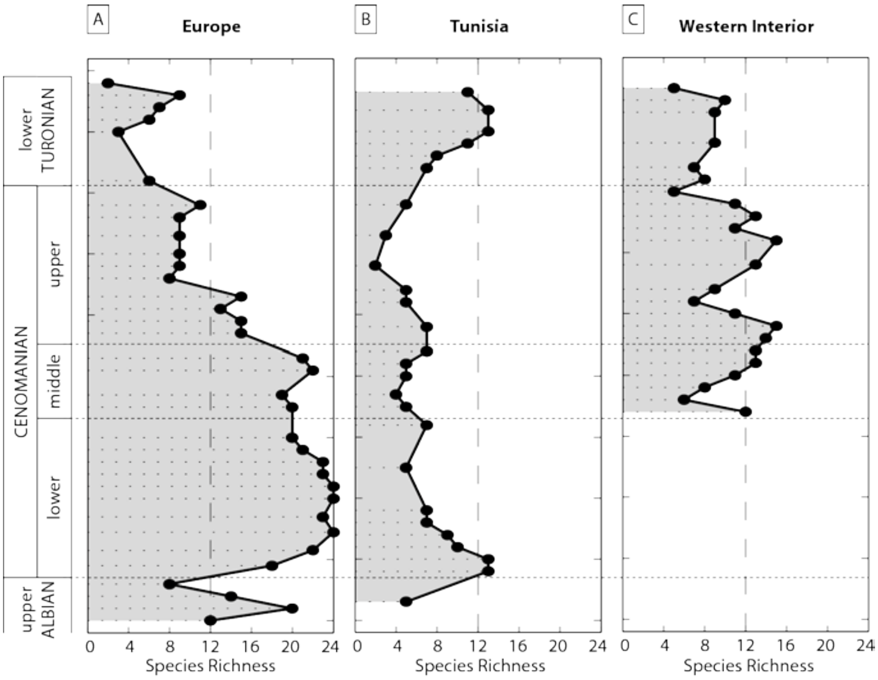


Figure 2 – *Species richness of Cenomanian–lower Turonian ammonoids (Monnet 2009) from Europe (**A**), Tunisia (**B**), and the Western Interior (**C**). Species richness is the number of different species in each biostratigraphic unit.*

The two essential components of the Cenomanian ammonoid community are the acanthoceratids (predominantly nekto-benthic species) and the heteromorphs (predominantly pelagic species) (*Fig 3*). Others families have too low percentages for any reliable recognition of trends during the Cenomanian. Hence, trends in species richness appear to be mainly governed by acanthoceratids and heteromorphs. Separate analyses of species richness for these two groups reveal that heteromorphs declined before the acanthoceratids (middle–upper Cenomanian boundary and mid-upper Cenomanian, respectively). In Europe, the local disappearance of the Turrilitidae largely accounts for this dropdown among the heteromorphs at the middle–upper Cenomanian boundary.

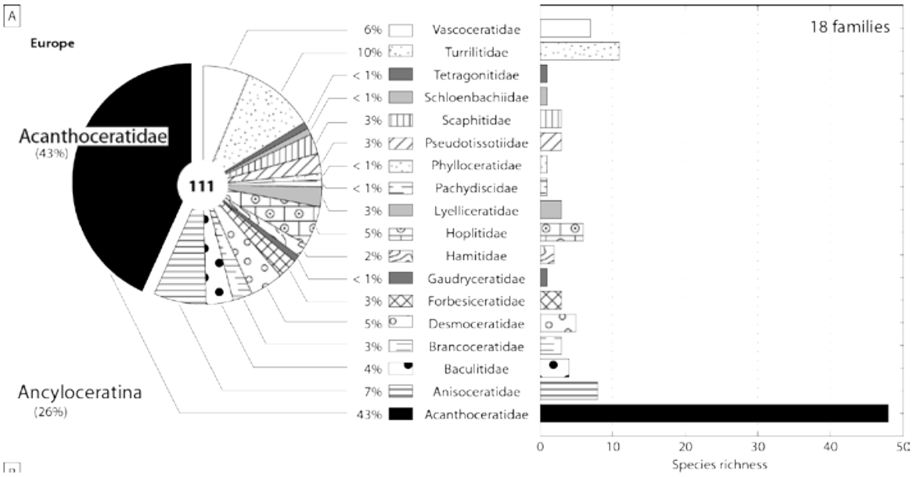


***Figure 3 –** Proportions and species richness of ammonoid families for the entire Cenomanian in Europe.*

Changes of taxonomic distinctness through time and the curves of confidence intervals simulated by bootstrapping show that AvTD values are significantly lower than expected throughout the entire upper Cenomanian (*Fig 4*). These low AvTD values of the lower-upper Cenomanian suggest that there are exceedingly few familial and supra-familial taxa in comparison to the number of species. This fact corresponds to the extinction of most heteromorphs and families such as Schloenbachiidae and Forbesiceratidae. Indeed, the Acanthoceratidae almost exclusively dominates ammonoid assemblages of the upper Cenomanian.

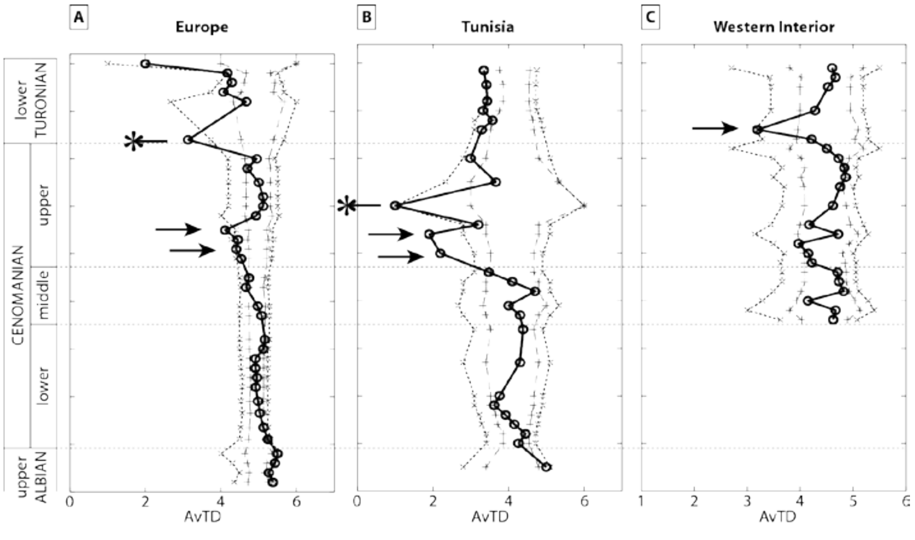


***Figure 4 –** Average taxonomic distinctness of ammonoids for the Cenomanian–lower Turonian of Europe (**A**), Tunisia (**B**), and the Western Interior (**C**). The average taxonomic distinctness (AvTD) reflects the taxonomic disparity.*

Although there is extensive evidence for widespread anoxia during the Cenomanian/Turonian boundary interval in deep sea environments, the biodiversity patterns of ammonoids in Europe, Tunisia, and the Western Interior rule out global anoxia as a direct causal mechanism for changes in ammonoid diversity (Monnet & Bucher 2007a; Monnet 2009). These biodiversity patterns also question the global scale character of the so-called Cenomanian/Turonian mass extinction.

The paleobiogeographic patterns of Cenomanian–lower Turonian ammonoids are currently poorly known, mostly because they have not yet been analyzed quantitatively and by means of a standardized taxonomy. Nevertheless, a major change in the biogeographic distribution of ammonoids is recorded around the middle–upper Cenomanian boundary. This substage boundary is characterized in several basins by the immigration of faunas of different biogeographic affinities. For instance, assemblages with *Texacanthoceras*, *Paraconlinoceras*, and *Tarrantoceras* (previously considered endemic to the Western Interior) have been discovered in Tunisia, Nigeria, Japan, Morocco, and Spain. The unusual widespread occurrence of these species probably reflects new migratory pathways and re-organization of oceanic currents near the middle–upper Cenomanian boundary. Furthermore, the extent of the Boreal realm was strongly reduced during the upper Cenomanian and lower Turonian compared to the lower–middle Cenomanian as suggested by the presence of supposed endemic and Tethyan ammonoids in Europe since the middle–upper Cenomanian boundary (*Fig 5*).

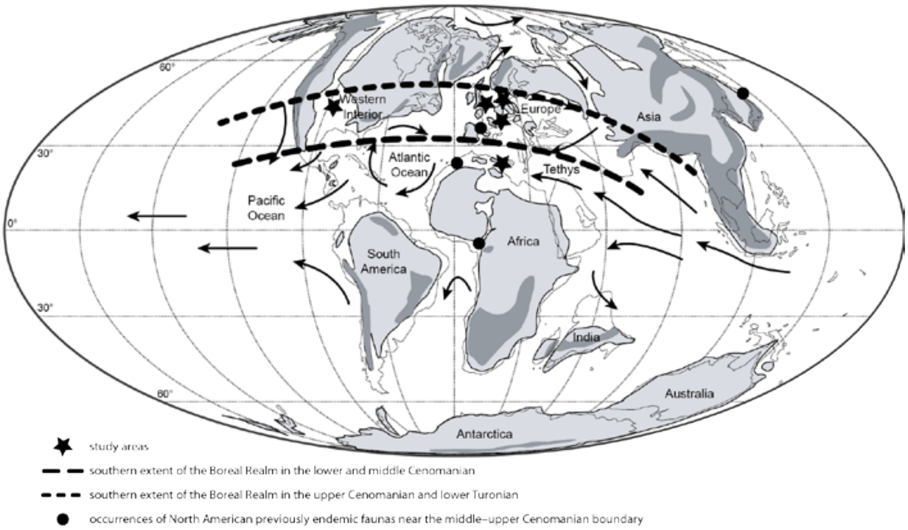


Figure 5 *– Paleogeographic distribution of so-called North-American endemic faunas at the middle–upper Cenomanian boundary (see text) and southern boundary of the Boreal realm (according to ammonoids) in the lower–middle Cenomanian and in the upper Cenomanian–lower Turonian.*

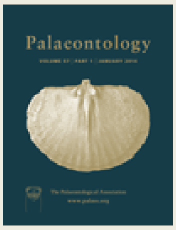
Among all documented abiotic changes (spreading of anoxic marine waters, comet shower, sea level changes, global warming, enhanced volcanic activity) during the Cenomanian–Turonian (see review in Monnet 2009), the observed biodiversity patterns of ammonoids seem to support the global warming of the late Cenomanian as evidenced by the northward migration of taxa typical of the Tethyan Realm. Changes in ammonoid diversity are compatible with the exceptional high sea level occurring at that time and with concomitant regional climate changes (*Fig 1*; Monnet 2009). These abiotic changes may be triggered by increased volcanic activity but their relations in time and space remain to be more precisely elucidated. The so-called Cenomanian–Turonian boundary mass extinction appears to result from the complex interplay of different environmental changes acting at different scales in space and time. This mass extinction is not restricted to an anoxic event, changes occurred before, and these must be accounted for when studying global diversity changes.

Long-term morphological trends

Related publications:

Monnet et al 2011a, 2012, 2013, 2015c

Appended publication:



Monnet C, Bucher H, Guex J, Wasmer M (**2012**) Large-scale evolutionary trends of Acrochordiceratidae Arthaber, 1911 (Ammonoidea, Middle Triassic) and Cope's rule. ***Palaeontology*** **55:87–107** (doi: 10.1111/j.1475-4983.2011.01112.x)

This paper has been selected by Clarkson (2014) as one of nine papers for a virtual issue of the journal *Paleontology* that best characterize the development of concepts in ammonoid paleobiology from 1965 onwards.

An important part of my research focuses on investigating patterns and processes in the long-term evolution of ammonoid shell morphology such as Cope’s rule. Evolutionary trends among ammonoids have been frequently documented, but usually from a qualitative point of view. One important aspect of my research is thus 1) to acquire quantitative datasets, 2) to quantify these trends, 3) to test the randomness and pervasiveness of the identified patterns, and 4) to evaluate the processes leading to such trends.

Rcently, I published a thorough review of quantitative methods, which can be used in the topic of long-term phenotypic evolution, and their application to ammonoids (Monnet et al 2015c). This paper reviews my view on the macroevolution, and more particularly the repeated long-term morphological evolutionary trends, which often characterize the evolution of ammonoids, whose evolution is well-known to operate as “variation on a theme”. On the one hand, this review surveys and synthesizes the studies that I directed during several years on this theme of macroevolutionary trends, such as the famous Cope’s rule. On the other hand, this review also emphasizes my concerns in conducting researches by means of quantitative analyses with the application of standard exploratory and statistical analyses, as well as the development of new approaches when necessary. Because this review is the culminating point of my research in this topic, the following text is reproduced and adapted from this paper.

INTRODUCTION

Ammonoids are characterized by high evolutionary rates. Because their taxa evolved and became extinct rapidly, ammonoids are extremely useful tools for dating strata. For instance, due to their high turnover rates, ammonoid species can often enable the construction of biozones spanning less than 100 kyr duration (House 1985; Jenks et al 2015). In addition to this outstanding time marker property, ammonoids also can provide significant insights into evolutionary biology. They have repeatedly been proven valuable study objects to develop or test evolutionary hypotheses and to investigate patterns of biodiversity (Schindewolf 1933, 1940, 1950; Kennedy 1977, 1989; Kennedy & Wright 1985; Landman 1988; Korn 2003; House 1996; Saunders et al 1999; Guex 2001, 2003, 2006; Korn & Klug 2003; Gerber et al 2008; Neige et al 2009; Brayard et al 2009b; Monnet et al 2011a; De Baets et al 2012; Korn et al 2013). Seilacher (1988, p. 67) correctly summarized this fact in his phrase stating that ammonoids "*are for paleontologists what Drosophila is in genetics*". This is the result of exceptional properties such as their high abundance, widespread occurrence, high evolutionary rates, high taxonomic diversity and morphological disparity, usually well-known stratigraphic framework (Stanley 1979; Sepkoski 1998; Foote & Sepkoski 1999), and their accretionary mode of shell growth that records the complete development (ontogeny) of the animals from the embryonic and juvenile stages to adulthood. In the fossil record, ammonoids are well-known to display major evolutionary patterns in shell morphology. They often evolved homeomorphic lineages and experienced numerous long-term (often several million years) morphological evolutionary trends, many of which were iterative or even parallel over time. This review will focus on these two points.

Homeomorphy has been recognized frequently among ammonoids (Schindewolf 1933, 1940; Haas 1942; Reyment 1955; Kennedy & Cobban 1976; Kennedy 1977; Wright & Kennedy 1979; Bayer & McGhee 1984; Kennedy & Wright 1985; Hewitt 1989; Page 1996; Bujtor 2010). Homeomorphy can be defined as the result of the evolution of close morphological similarities between species that are not closely related, or as the recurrence of phenotypic similarity within unrelated clades that evolved independently (Neville 1962; Lauder 1981; Wake 1991; Sanderson & Hufford 1996; Hall 2007; Futuyma 2009; McGhee 2011). It is generally thought to result from adaptation to similar modes of life or similar functions in different organisms or parts of organisms (but not always; Reyment 1955). Homeomorphy can be the outcome of convergent evolution (McGhee 2011) when animals exploit similar habitats/ecological niches in similar ways and thus likely arrive at morphologically similar solutions independently. The wings of birds, bats and pterosaurs are a classic example of homeomorphy, having evolved independently in three separate lineages from joint ancestors lacking this character as a means of achieving the functional requirements of flight.

Among animals with an external shell, convergent evolution leading to homeomorphic taxa has always been common and thus has been abundantly documented (Rudwick 1965; Horne 2005). For ammonoids, which are limited to a tubular external shell with finite limits of variation in coiling, ornament and suture imposed by constructional constraints, evolutionary convergence is widespread (*Fig 1*). In the most extreme cases, Mesozoic forms developed "atavistic" shell shapes reminiscent of Paleozoic ammonoids. Some examples (out of countless) are the shell shapes or suture lines of Triassic Arcestina resembling Paleozoic Goniatitina (Page 1996), or members of the Cretaceous Flickiidae with a simplified suture line and shell form similar to some Devonian Anarcestina (Wright & Kennedy 1979). These morphological similarities are no evidence for phylogenetic relationships but of convergent evolution. In some cases, ammonoids have developed very similar morphologies in most aspects generally accepted to be of diagnostic, taxonomic value that can lead to erroneous phylogenetic inferences or classification when not taking into account the stratigraphic gap separating these taxa. The situation is even more precarious when these forms co-occur or follow each other closely in time and where homeomorphic characters might be used to infer phylogenetic relationships.

Among ammonoids, examples of long-term morphological evolutionary trends are numerous (Haas 1942; Guex 1992, 2001, 2006; Kennedy 1977; Thierry 1982; Bayer & McGhee 1984, 1985; Kennedy & Wright 1985; Dommergues et al 1989; Dommergues 1990; Neige et al 1997; Korn & Klug 2003; Klug et al 2005; Monnet et al 2011a, 2013; De Baets et al 2012). These long-term phenotypic evolutionary trends are persistent and directed changes of morphological characters through significant periods of geological time (often several million years) within a monophyletic group (Gould 1988, 1990). Furthermore, these repeated trends can be independent, but often are organized in convergent, iterative and parallel patterns over time (Haas 1942; Guex 2001, 2003). Last but not least, all these patterns can contribute in a major way to the understanding of homeomorphic characters in ammonoid shells.

Parallel evolution (Serb & Eernisse 2008) can be defined as the independent evolution of similar biological traits in at least two different lineages having similar phenotypic trajectories driven by common (developmental) constraints. Parallel evolution is often confused with convergence (Webb 1994) since both can result in taxa with highly similar characters, but the two concepts remain distinct (Serb & Eernisse 2008) even if there may be a continuum between parallelism and convergence (Gould 2002; Donoghue 2005). On the one hand, superficially similar features are formed by different developmental pathways in convergence. On the other hand, parallel evolution is thought to involve similar developmental modifications that evolved independently (often in closely related organisms). Parallel evolution is a moderately common phenomenon in extinct and extant lineages (Averoff & Patel 1997) and often assumed to be the product of adaptation by means of natural selection. The literature on ammonoid evolution contains several references to parallel evolution or “parallelism” (parallelism is sometimes used in a slightly different meaning: Monnet et al 2011a), but many of these studies are spurious because they do not account for dimorphism and intraspecific variability and they rely only on qualitative description (Kennedy 1977). However, there are now convincing examples based on data for which their taxonomy, stratigraphy and phylogeny have been revised by quantitative methods (Meister 1993; Monnet et al 2011a).

Homeomorphic character states can evolve convergently or in parallel. They are major patterns of phenotypic evolution. Such examples of homoplasy (Lankester 1870) present opportunities to discover the foundations of morphological traits and determine processes and mechanisms of evolution (Wake et al 2011). Furthermore, understanding what is driving the high degree of homeomorphy within ammonoids is of great importance for taxonomy (Hewitt 1989; Webb 1994) and phylogeny as it might result in a high degree of homoplasy (Wake 1991; Yacobucci 2012). Understanding the long-term morphological trends is also of prime importance as they are at least partially responsible for the high degree of homeomorphism among ammonoids and may provide significant insights into evolutionary constraints operating on the ammonoid shell. However, the processes behind these common evolutionary patterns are still not well understood. As noted by Kennedy & Wright (1985, p. 142), the evolution of Cretaceous ammonoids shows “repeated patterns that reflect the selection of features whose adaptive significance in most cases escapes the observer”. For ammonoids, this situation may partly arise from two major sources of noise. First, the phylogeny of ammonoids at the species rank is only rarely reconstructed by means of state-of-the-art, recent phylogenetic methods (Neige et al 2009; Yacobucci 2012) and consequently prevent the valuable use of ammonoids in evolutionary studies despite having a huge potential. Second, studies on ammonoid evolution are very often carried out using qualitative/descriptive approaches without real quantification and statistical testing. However, these phenotypic evolutionary patterns can only be confidently assessed by novel quantitative and statistical methods. The major aim of this chapter is to review some of these methods and their application to ammonoids, which reflect the potential of ammonoids for providing insights into evolutionary patterns and processes.

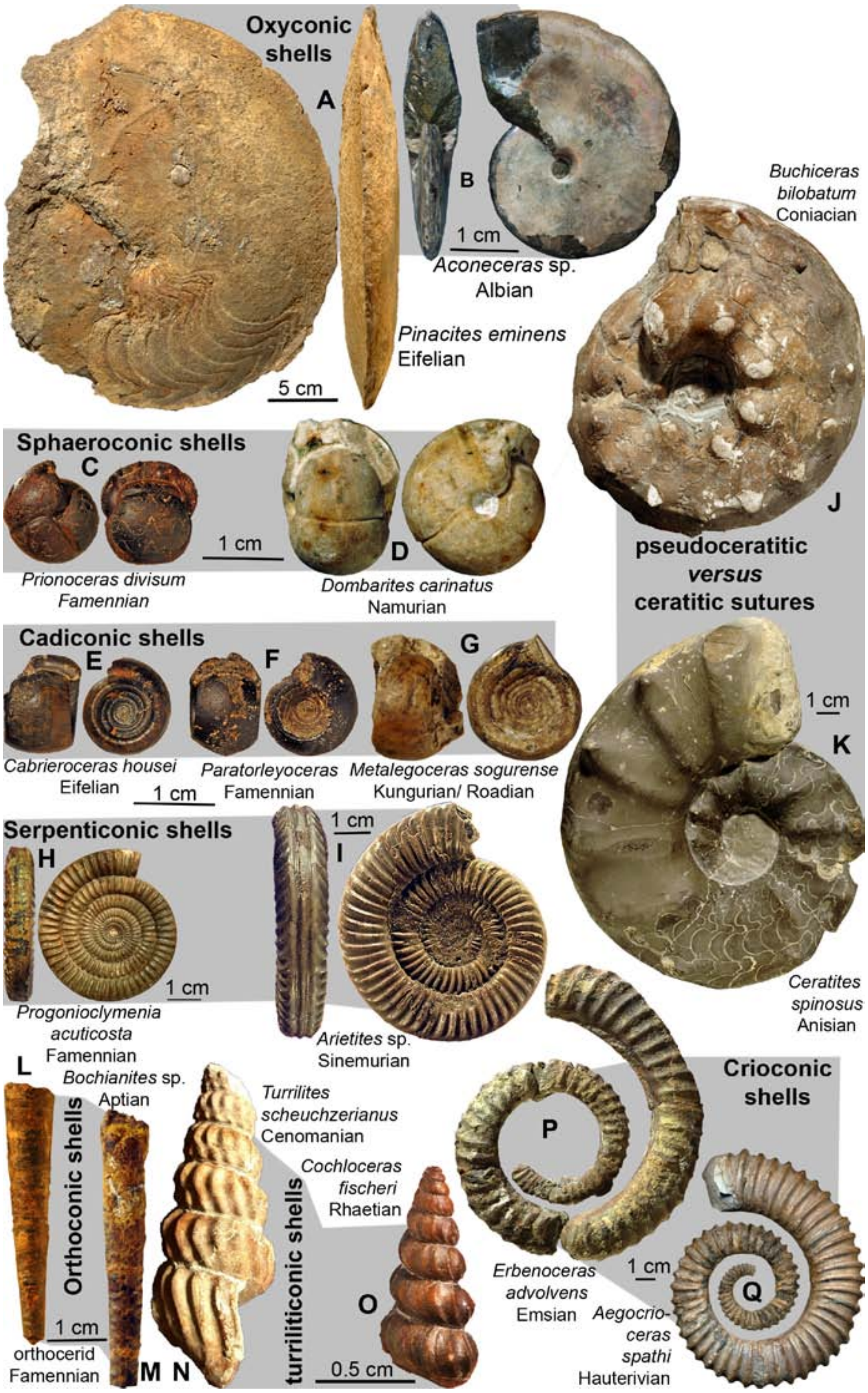


Figure 1 – *Some cases of convergence in shell form and suture line course (Monnet et al 2015c).*

MACROEVOLUTIONARY TRENDS

Definition

"*One of the crowning achievements of paleontology, and of surpassing importance in the development of evolutionary theory, has been the discovery of innumerable graded morphological series of fossils showing progressive change as we ascend the geological scale of time. Many of the evolutionary modifications follow simple patterns, or trends, which recur again and again in related or even unrelated stocks.*" (Newell 1949, p. 103)

One of the intriguing outcomes of biological evolution (as described by Newell above) is the frequent occurrence of long-term evolutionary trends. These patterns are persistent and directed changes of morphological characters through significant periods of geological time within a monophyletic group (*Fig 2*; Simpson 1953; Gould 1988, 1990; McKinney 1990; McShea 1994; McNamara 2006). The fossil record displays numerous examples of lineages persistently evolving during several million years toward greater “complexity” and/or toward larger body size (Cope 1887, 1896; Depéret 1909; Matthew 1926; Newell 1949; Simpson 1953; Rensch 1959; Stanley 1973; Hallam 1975; Kennedy & Wright 1985; Fisher 1986; MacFadden 1986, 1992, 2005; Gould 1988, 1990, 1996, 1997; Jablonski 1987, 1997; McShea 1991, 1994, 1996; Boyajian & Lutz 1992; Valentine et al 1994; Kaiser & Boucot 1996; Wagner 1996; Trammer & Kaim 1999; Alroy 1998, 2000; Saunders et al 1999; Adami et al 2000; Wang 2001; Gould & MacFadden 2004; Guex 2006; Hunt & Roy 2006; Adamowicz et al 2008; Novack-Gottshall & Lanier 2008; McGhee 2011). Such trends occur in almost all metazoan groups and probably reflect a pervasive pattern of evolution. This sustained directionality of morphological evolution is one of the oldest and most important aspects of evolution, and is therefore an important research program in paleobiology (McNamara 1990). The occurrence, generality and causes of long-term evolutionary trends have been intensively studied and debated, and have significant implications for an overall understanding of patterns and processes of evolution.

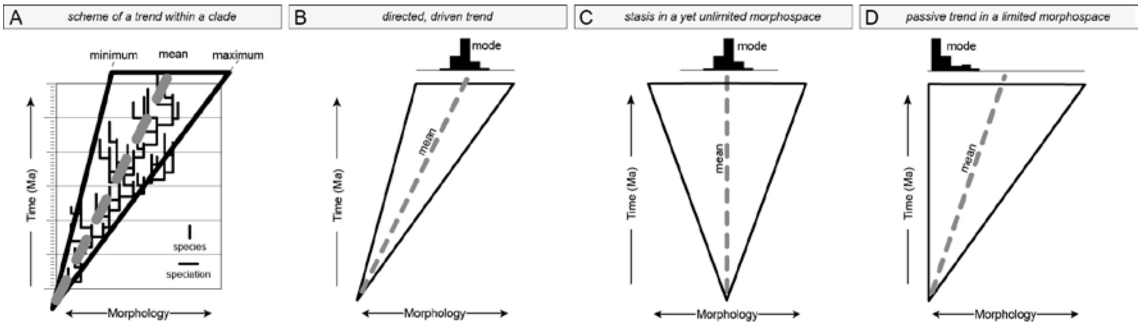


Figure 2 – *Schemes of long-term phenotypic macroevolutionary trends of a lineage through time (modified after McShea 1994 and Monnet et al 2015c).* ***A)*** *The vagaries of the morphology (origination and extinction of species) of a clade through time are mainly characterized by its mean and range in its phenotypic space.* ***B)*** *A long-term trend is characterized by a protracted shift of the entire range and mean morphology of the studied group.* ***C)*** *Absence of changes in this morphological mean illustrates stasis.* ***D)*** *A seemingly trend may occur in a phenotypic space limited by physical/constructional boundaries, but in this case the most abundant forms still remain similar to the root of the clade (compare with* ***B****).*

Phenotypic trends in shell characters

Ammonoids are characterized by a septate, univalved, usually coiled shell, basically conic, with or without an external sculptured ornamentation. This shell can be described by multiple qualitative (for a list of ammonoid characters, see Arkell et al 1957; Dommergues et al 2002; Korn 2010) and quantitative characters, some of which will be illustrated here (for their definition, see Monnet et al 2011a). Among quantified ammonoid shell characters, there are four that commonly display long-term evolutionary trends through time: adult body size, degree of involution (coiling), strength (or spacing) of ornamentation, and indentation of suture line (Kennedy 1977; Kennedy & Wright 1985; Dommergues 1990; Saunders 1995; Saunders & Work 1996; Saunders et al 1999; Guex 2001, 2006; Korn & Klug 2003; Klug & Korn 2004; Monnet et al 2011a and references therein). The general tendency for body size to increase during the evolution of a group of animals is known as Cope's rule (Rensch 1948) or as the law of phyletic increase in size (Depéret 1909). With regard to ammonoids, several authors have illustrated and discussed examples of increasing shell size (Stanley 1973; Hallam 1975; Thierry 1982; Kennedy & Wright 1985; Guex 2003; Dommergues et al 2002; Monnet et al 2011a, 2012; De Baets et al 2012). For instance, Hallam (1975) described Cope's rule in some Jurassic ammonoid families but he focused only on maximum shell size, whereas Dommergues et al (2002) documented no preponderant trends (but without phylogenetic data) in an almost exhaustive compendium (more than 1000 species) of Early Jurassic ammonoids. Furthermore, trends of decreasing shell size might also occur (Korn 1995).

Another repeatedly documented evolutionary trend within ammonoids is that from an openly umbilicate ancestral group (evolute) toward a descendant group with a smaller or closed umbilicus (involute; *Fig 3A*). Such trends have been documented already by Hyatt (1889) for Liassic arietitids. This pattern has even been documented in the earliest history of ammonoids: during the Early Devonian, ammonoids showed a progressive coiling from straight orthocerids via curved bactritoids to coiled ammonoids (Erben 1966; Wiedmann 1966; Klug 2001; Klug & Korn 2004; De Baets et al 2009, 2012). This increasing shell involution (protracted closure of the umbilicus by increasing overlap of the whorls) is also the most commonly described long-term morphological trend among more derived ammonoids (Hyatt 1889; Schindewolf 1940; Haas 1942; Guex 1992; Bayer & McGhee 1984, 1985; Dommergues 1990; De Baets et al 2009, 2012; Klug et al 2010; Monnet et al 2012, 2013; see also Monnet et al 2011a and references therein). Note that uncoiling of ammonoids has also been documented repeatedly (Wiedmann 1969; Cecca 1997).

With regard to shell ornamentation, various authors (Ward 1981, 1996; Vermeij 1987; Westerman 1996) showed that the whole ammonoid clade reveals a trend toward more ornamented forms (*Fig 3B*). Although the authors interpreted this pattern as a response to the evolution of increasing numbers of shell crushing predators, the qualitative data of Ward (1981) suggest a passive trend constrained by a left-wall effect. For instance, convergent evolution of spines in marine mollusk shells have classically been interpreted as having repeatedly evolved as a defense in response to shell-crushing predators (Vermeij 1987; Kröger 2005; Ifrim 2013), but other interpretations are also available (Ifrim 2013). Recent studies (Moulton et al 2012, 2015; Chirat et al 2013) have demonstrated that a large diversity of ornamentation and spine structures can be accounted for through small variations in control parameters of the mechanical interaction between the secreting mantle edge and the calcified shell edge, which suggests that convergent evolution of spines can also be understood through a generic morphogenetic process without selective pressures. By contrast, simplification of shell ornament through the evolution of a clade was also frequently observed at a lower taxonomic scale (Bayer & McGhee 1984, 1985; Kenney & Wright 1985).

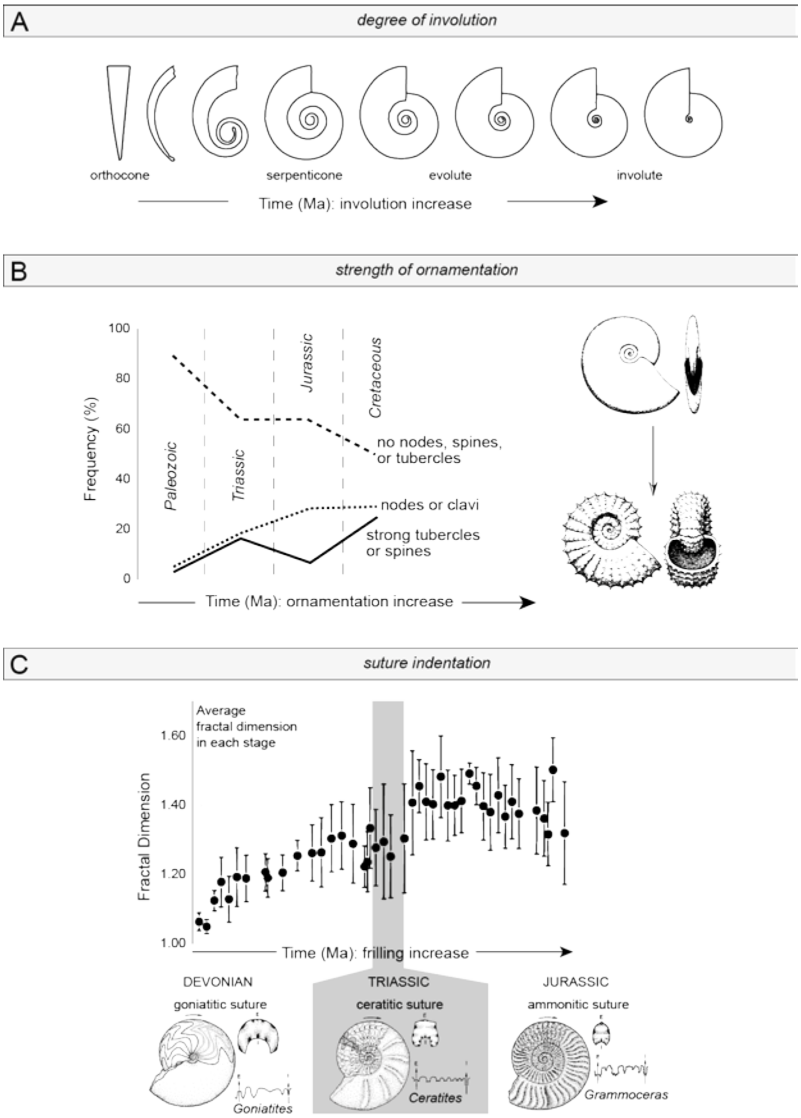


***Figure 3** – Global long-term evolutionary trends of the ammonoid conch. **A)** Scheme of the initial trend in the degree of involution within Devonian early ammonoids (modified after Wiedmann 1966). **B)** Scheme of the trend toward more ornamented shells (modified after Ward 1981). **C)** Scheme of the trend toward greater complexity of the suture line (modified after Boyajian and Lutz 1992).*

Finally, ammonoid evolution is also characterized by an overall increase in the intensity of indentation of adult sutures (= frilling or “complexity”) (*Fig 3C*): from agoniatitic (smooth lobes and saddles), via goniatitic (smooth lobes, pointed saddles), to ceratitic (smooth saddles, denticulate lobes), and to ammonitic (frilled lobes and saddles). This increasing suture indentation has been quantified by fractal or Fourier analyses by several authors (García-Ruiz et al 1990; Boyajian & Lutz 1992; Saunders & Work 1996, 1997; Saunders et al 1999; Pérez-Claros et al 2002, 2007). For instance, Saunders et al (1999) documented a bias in the direction of speciation toward more indented sutures (within 475 ancestor/descendant pairs; descendants were more than twice as likely to be more complex than their ancestors). They also noted that mass extinctions acted in opposition to this long-term trend by eliminating more indented forms and thus resetting the trend (which might be linked with the elimination of extreme morphologies like oxycones and cadicones, which tend to have more sutural elements). Interestingly, this role of lineage sorting by means of increased extinction rates of particular morphologies has also been emphasized either as resetting trends (Guex 2001, 2006) or as strengthening trends (De Baets et al 2012). At lower taxonomic ranks and shorter time intervals, evolutionary trends in suture indentation are also common and include not only patterns of increasing indentation, but also decreasing indentation and smoothing of sutures (Kennedy & Wright 1985; Checa 1987). In addition, this statement holds for every character (size, ornamentation, coiling, and suture): both increasing and decreasing trends have been documented (Kennedy & Wright 1985).

Interestingly, the morphological trends described above often happened simultaneously. This lead to a particular evolutionary pattern characterized by lineages originating with small, ornamented, evolute and depressed forms, which more or less progressively changed and ended with large, smooth, involute and compressed shells (*Fig 4*; Silberling & Nichols 1980; Bayer & McGhee 1984, 1985; Klinger & Kennedy 1984; Guex 2001, 2003, 2006; Monnet et al 2012). These trends are also recognized to occur successively several times within a clade leading to a repetitive pattern of similar trends (“evolutionary cycles” of Haas 1942). The frequency, combination and proportion of these morphological trends within the evolution of ammonoids remain however to be investigated. Moreover, Kennedy & Wright (1985) recognized that Late Cretaceous ammonoids experienced almost all combinations of trends and it is not yet clear if one pattern predominates or not.

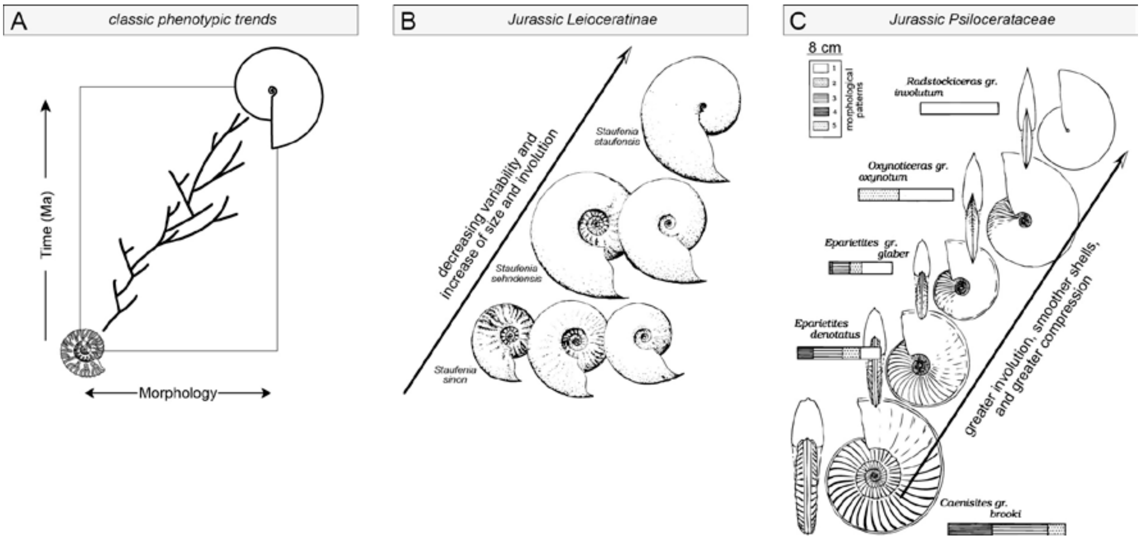


***Figure 4 –** Examples of long-term phenotypic evolutionary trends of the ammonoid shell within lineages. **A)** Scheme of the most frequently described ammonoid trend: it starts with more evolute, more depressed, and more ornamented shells and evolves toward more involute, more compressed, and smoother shells. **B)** Morphological trend of Staufenia during the Jurassic of Germany (modified after Bayer & McGhee 1985). **C)** Peramorphic trend of Psilocerataceae (modified after Dommergues 1990).*

UNIVARIATE PHENOTYPIC TRENDS IN AMMONOIDS

Classic descriptive stratophenetics

Evolutionary changes of the ammonoid shell through time are classically investigated by means of a stratophenetic approach (Gingerich 1979, 1993; Raup & Crick 1981, 1982; Bookstein 1988; Roopnarine et al 1999) regardless of its phylogenetic interpretation. It usually includes a graphic illustration of the morphological range of a character through successive time slices such as beds or biozones (Raup & Crick 1981; Thierry 1982; Bayer & McGhee 1984; Kennedy & Wright 1985; Dommergues et al 1989; Dommergues 1990; Klug et al 2005; Monnet et al 2011a, 2012; De Baets et al 2012). Patterns of phenotypic evolution of quantitative characters are usually examined separately by means of bivariate plots depicting their quantile distribution (or descriptive statistics such as mean, minimum, maximum, median and/or quartiles). These plots enable an empirical evaluation of the presence or absence of directed evolutionary changes (trends) for each character.

A recent example of morphological trends of the ammonoid shell investigated by a classic stratophenetic approach has been published by Monnet et al (2012). Therein, details of the long-term phenotypic evolution of Acrochordiceratidae during the Anisian (Middle Triassic) were analyzed. Morphological changes of the acrochordiceratid shell were quantified based on large collections (more than 700 specimens) from Nevada (USA). This study showed (*Fig 5A*) that the monophyletic clade of Acrochordiceratidae (i) underwent a significant increase (possibly with several steps) of its adult shell diameter (i.e. Cope's rule), (ii) showed an evolute to involute evolutionary trend (i.e. an increase of the degree of shell involution), and (iii) experienced a qualitative increase of indentation of its suture line. The protracted changes in shell morphology of the Acrochordiceratidae are robust and non-random (Monnet et al 2012). They can be interpreted as being constrained by the persistent, common selection pressure on this mostly anagenetic lineage with relatively moderate evolutionary rates during an ecologically stable period (*Fig 5C*). As discussed by Monnet et al (2011a), such trends of morphological evolution in the ammonoid shell may suggest that their morphology is mainly controlled by adaptive and constructional constraints. Interestingly, not all quantified characters showed trends such as whorl shape compression and ribbing density (*Fig 5B*).

Passive and driven trends and lineage sorting

The ammonoid literature is rich in descriptions of phenotypic trends through time (see references above). However, a crucial question is whether these evolutionary trajectories are robust and not just random fluctuations in phenotypic space. Indeed, the classic stratophenetic approach is a subjective graphic approach, which impedes distinguishing random fluctuations from persistent trends (Roopnarine et al 1999; Hunt 2006). The method has been criticized because it lacks a means of evaluating the robustness of the documented pattern. This is not always straightforward in fossil organisms due to, e.g., low sample size combined with large variation in fossil groups (De Baets et al 2015). The absence of quantitative methods adapted to the study of the incomplete and time-averaged fossil record lead in the past to biased descriptive studies. In addition, Gould (1988, 1990) pointed out two major common misinterpretations of stratophenetic trends: (i) biases may result from the systematic search of gradual evolution between species by arbitrary picking out only part of a clade and ignoring the entire complex phylogenetic tree ("anagenesis faith"); (ii) other biases may arise from a focus on extreme values (maximum) instead of accounting for the entire variance. Furthermore, Raup et al (1973) showed that trends can be simulated even if both direction and frequency of speciation and extinction are allowed to vary randomly. To overcome such problems, several approaches have been developed and/or used during the past decades for evaluating trends, especially for stratophenetic data and with or without a phylogenetic framework.

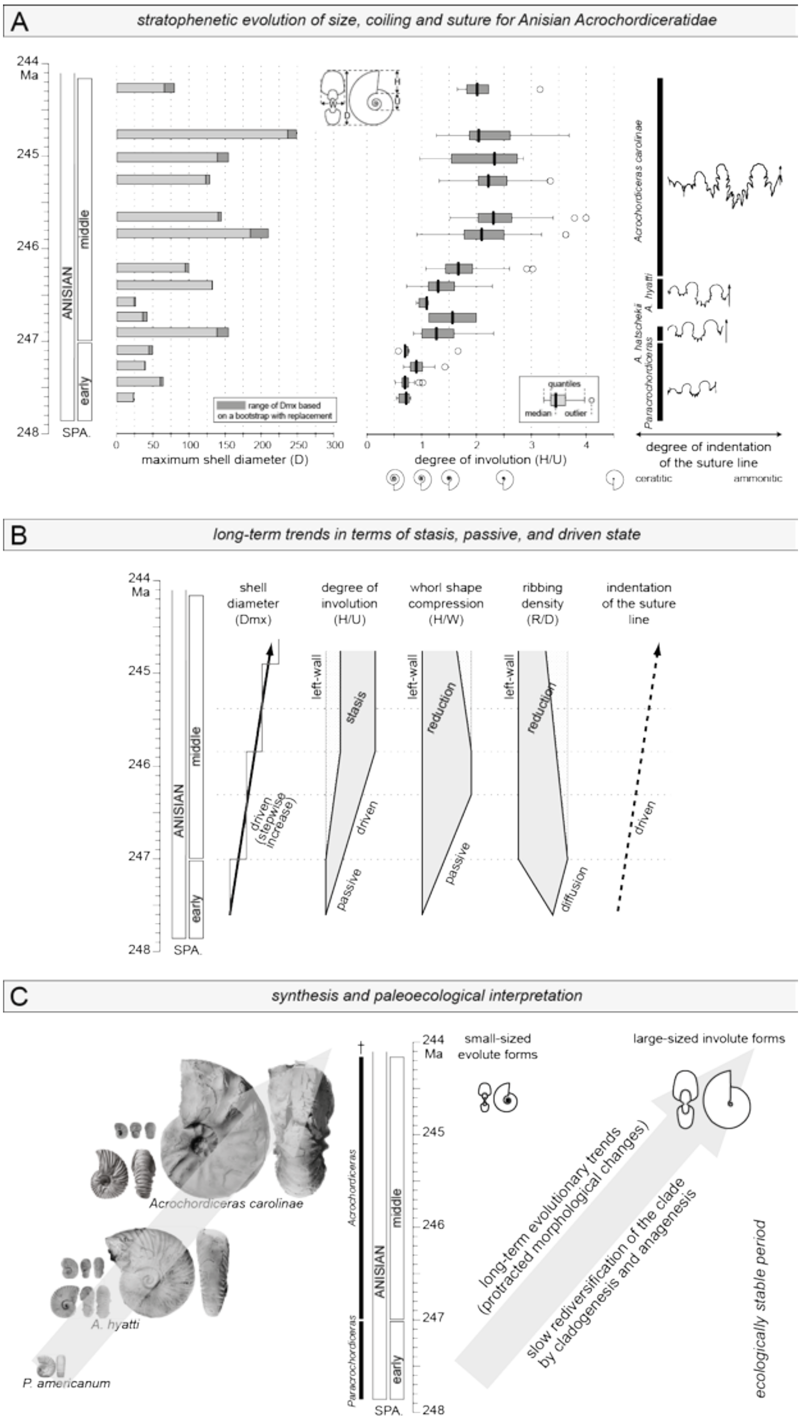


***Figure 5** – Evolution of maximum shell diameter, degree of involution and suture shape for Acrochordiceratidae during the Anisian (Middle Triassic) (modified after Monnet et al 2012). **A)** Stratophenetic patterns of some conch characters showing a trend of their mean. **B)** The corresponding patterns in terms of long-term trends (stasis, left-wall effect, directed shift) showing that some characters have very different evolutionary patterns. **C)** Interpretation of the typical documented pattern (illustrated ammonoids are at the same scale).*

One major advance in the understanding of trends came with the recognition of the "left-wall effect" (Stanley 1973; Gould 1988; McShea 1994). Indeed, many patterns could arise via (random) fluctuations from a fixed boundary, as when a clade originates near a minimum viable morphology (*Fig 1D*); in this case, the mean of the studied lineage can increase because change in one direction is blocked by a boundary in some region of the morphological space. For instance, the coiling of ammonoids is bounded on one side by "straight conch" and on the other side by "fully occluded umbilicus". Such boundary-limited trends were referred to as "passive" in opposition to "active" trends, which display a shift of the entire range of the morphology (McShea 1994; see also discussion of Alroy 2000). Note that "passive" is not identical with "random", because a passive trend can still result from different processes acting independently and heterogeneously (McShea 1994). Since such passive trends arise owing to the topography of the adaptive landscape (Kaplan 2008; Pigliucci 2008), it is useful to identify them in order to avoid overinterpretation (usually adaptive) of the patterns and help discriminate the limiting effects of structural constraints from natural selection (Gould 1988).

Long-term phenotypic changes can arise by means of a wide range of mechanisms, and different dynamics can operate simultaneously, in opposition or in concert, at different levels (Stanley 1973; Vrba & Gould 1986; Gould 1988, 2002; McNamara 1990; McShea 1994; Foote & Miller 2007). For instance, a trend may be underlain by transformation of its constituent species, by preferential origination of new species, by random speciation followed by differential survival or proliferation in the direction of the trend, or by any combination of these very different processes (Stanley 1973; Gould 1988; Jablonski 2007). For example, Gould (1988) showed that one process or the combination of several processes might cause a driven process (*Fig 6*): (i) a bias in the direction of speciation ("branching bias": is the number of speciation events equally distributed among decreasing and increasing phenotypic changes?); (ii) a bias in the magnitude of speciation ("fertility bias": are speciation rates similar throughout the morphospace?); (iii) a bias in the amount of extinction ("longevity bias": do species located in a particular part of the morphospace survive longer?).

Evolutionary trends can also result from mechanisms acting at different hierarchical levels, leading to the concept of "lineage sorting" (Vrba & Gould 1986): (i) trends can be driven by organism-level traits (within-lineage sorting) such as body size or habitat preferences that can also be translated into patterns of among species evolution (Vrba 1980, 1983, 1984); or (ii) trends can be driven by emergent properties at the species level (among-lineage sorting) such as geographic range, speciation rates, or longevity (Stanley 1979; Gould 2002). From a methodological viewpoint, several authors discussed several tests to discriminate passive and driven trends, globally for a clade (Gould 1988; McShea 1994; Wagner 1996; Wang 2001, 2005), mainly by focusing on the biases listed above. Alroy (2000) also proposed additional approaches to analyze phenotypic macroevolutionary trends. However, none of these tests have been applied to ammonoids.

Another major approach to quantify the relative proportion of passive and driven trends within a lineage is that of Jablonski (1997) (see also Trammer & Kaim 1999). He proposed the "quadrant" method as a graphic approach to evaluate the relative proportion of evolutionary changes between the minimum and maximum of the range of a character (*Fig 7A*). This approach thus focuses on changes in variance (*sensu* Gould 1988) and can accommodate stratophenetic series or phylogenetic sequences. In this approach, a graph reports and synthesizes the complete series within a clade of the differences of morphological values of some characters either between an ancestor and its descendant or between two successive stratigraphic intervals. The four quadrants represent four possible trends in character evolution. This enables the comparison of the relative proportion of increases, stases, and decreases within the studied clade and thus evaluates if one macroevolutionary pattern dominates or not. By accounting for the changes at the lower and upper phenotypic bounds, these analyses essentially correspond to the test based on "the behavior of the minimum" for distinguishing passive from active (directional) trends. Jablonski (1997) applied the method to evaluate Cope's rule within Cretaceous mollusks and found no support for a predominance of body size increase. For ammonoids, Dommergues et al (2002) applied the method also to evaluate the pervasiveness of Cope's rule in the Jurassic. Their study highlighted the absence of sustained trends for shell size and even emphasizes the predominance of random fluctuations in shell size (*Fig 7B*).

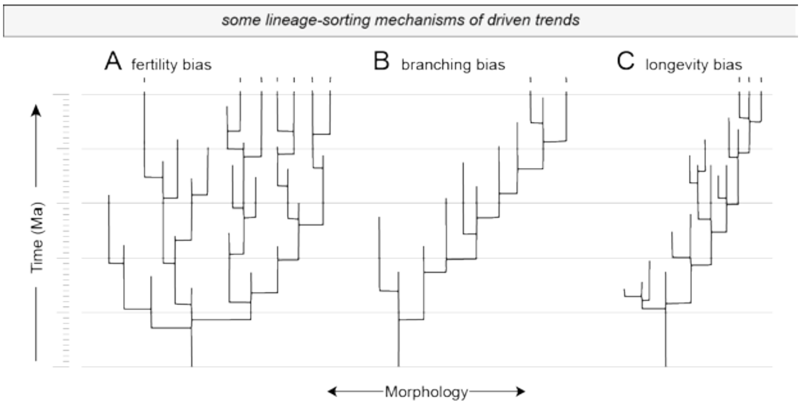


Figure 6 – *Some lineage-sorting mechanisms leading to phenotypic patterns of among-species, driven trends (modified after Gould 1988).* ***A)*** *The trend results from a higher speciation rate of a part of the morphospace of the studied lineage.* ***B)*** *The trend is triggered by a preferred direction of speciation.* ***C)*** *The trend is induced by longer persistence of species from a particular part of the morphospace.*

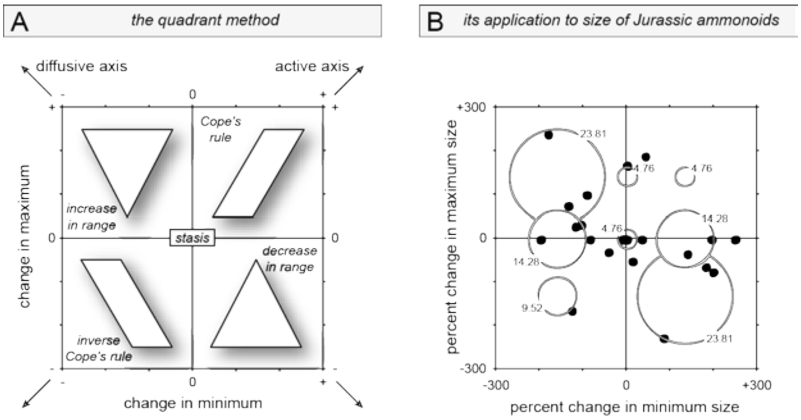


Figure 7 – *The quadrant method and its application to quantify the relative proportion of passive and driven trends within a linage.* ***A)*** *The quadrant method of Jablonski (1997) reports phenotypic changes between pairs of successive stratigraphic intervals or phylogenetic data in terms of changes in variance. The top right quadrant corresponds to an increase in the studied morphology, the bottom left quadrant to a decrease, the top left quadrant to an increase in range, and the bottom right quadrant to a decrease in range.* ***B)*** *Styles of size change in Early Jurassic ammonoids (black circles are the difference between two successive sets of biozones; circle diameter is proportional to frequency in the corresponding quadrant) (modified after Dommergues et al 2002).*

Random walks and univariate phenotypic trajectory analysis

Previously described approaches aim to describe and quantify the relative phenotypic changes of a lineage through time and phylogeny, usually at the species rank. However, trends in evolutionary series can be produced randomly (Raup & Gould 1974; Raup & Crick 1981; Bookstein 1987, 1988; Raup 1997; Roopnarine et al 1999; Sheets & Mitchell 2001). Hence, previously empirically identified evolutionary trends must be tested statistically before examining the discrimination of patterns and processes of macroevolutionary trends. For this purpose, several methods exist, which are based on random walk models, to test and characterize observed trends and to distinguish the three modes of evolutionary change commonly considered in paleontological studies: directional change (GRW, general random walk), random walk (URW, unbiased random walk), and stasis (Gingerich 1993; Roopnarine 2001; Sheets & Mitchell 2001; Hunt 2006). The evolutionary changes of each character can be evaluated by means of the maximum likelihood method of Hunt (2004, 2006, 2007) and Hunt et al (2008). The method performs well even when evolutionary sequences are incompletely sampled, which is likely for empirical sequences of fossils (Hunt 2006). It has been implemented as a package ("paleoTS"; Hunt 2006) in the scientific environment R. The method evaluates the maximum likelihood of producing the observed trends for the three evolutionary modes (GRW, URW, stasis). The relative support of each of these three models is assessed using statistical means such as Akaike weights (Anderson et al 2000; Hunt 2004, 2006; Hunt et al 2008). Methods to study phenotypic evolution and evolutionary trends in a phylogenetic framework have also been developed (Hunt & Carrano 2010).

For ammonoids, a recent application of random walk methods is the study of Monnet et al (2011a). Therein, the evolution of two lineages of Early to Middle Devonian age (405–395 Ma) was investigated. Eight quantitative shell characters were analyzed (Monnet et al 2011a). The stratophenetic evolution of some of these shell characters for the lineage that includes the Pinacitidae is shown (*Fig 8A*). Within this lineage, the maximum adult shell size (Dmx), the number of lobes of the suture (NLb), their relative depth of the lateral lobe (OLb), as well as the acuteness of the venter (FCI) increased simultaneously, especially among the more derived species. The umbilical width index (UWI) and the imprint zone rate (IZR) also display trends but these occur only among the more primitive species. Evolutionary changes of whorl shape compression (WSC) and whorl expansion rate (WER) display different, slightly more complex evolutionary patterns: a quick increase in the most primitive species, an abrupt reset and then a slight increase in the most derived species, giving the trend a sigmoid course.

This ammonoid lineage thus displays empirical morphological evolutionary trends of some shell characters. The statistical evaluation of the three evolutionary modes (directional trend, random walk, and stasis) by means of the method of Hunt (2006) is illustrated (*Fig 8B*). Among the three tested evolutionary patterns, the studied quantitative characters are mainly characterized by random trends and/or stasis (Akaike weights > 0.5). The only well-supported directional trend is for UWI (increasing degree of involution). Two other shell characters may display possible directed trends (Dmx, NLb), which have negligible values for stasis and moderate values for random walks. Thus, the studied ammonoid lineage displays directed trends for UWI with certainty, and probably for Dmx and NLb, while all other characters remain devoid of directional trends. In other words, through time and phylogeny, pinacitids acquired larger, more involute and oxyconic shells and more complex sutures. With the appearance of the umbilical lid (an extension of the lateral shell wall covering the umbilicus), the trends toward greater involution (decreasing UWI) leveled off (*Fig 8A*). This leveling off corresponds to a "left-wall effect": the trend cannot go further once the umbilicus is closed because this marks a constructional boundary (successive whorls completely overlap). Given the variety of patterns illustrated by the various quantitative shell characters studied, this example illustrates the necessity to test statistically for the likelihood of the three evolutionary modes. This prerequisite test is crucial to avoid over-interpretation of the evolutionary patterns and their suspected causes. Studies of phenotypic evolution of ammonoid shells can thus greatly benefit from these recent quantitative approaches (see below).

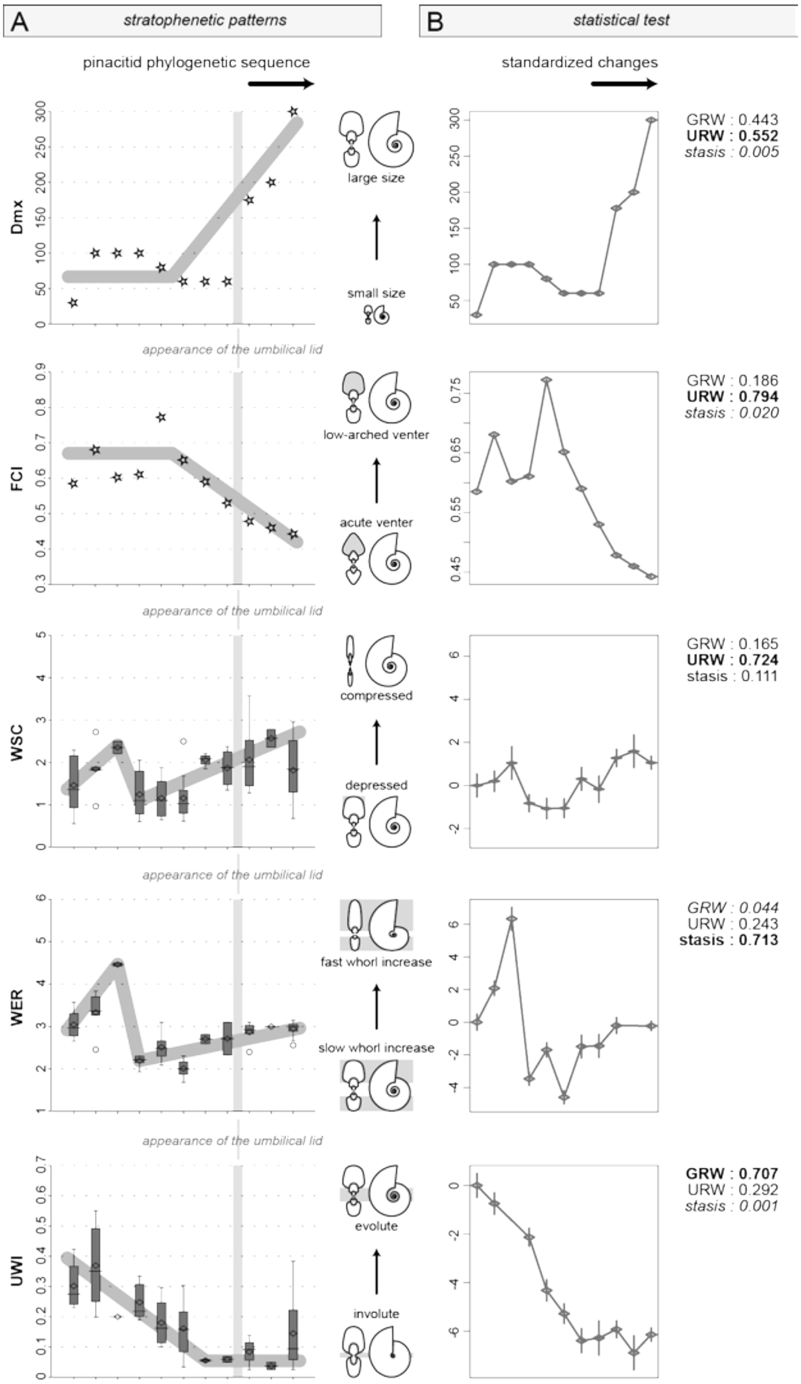


Figure 8 – *Phenotypic trajectory analysis of univariate shell characters of Devonian ammonoids (modified after Monnet et al 2011a). A) Stratophenetic patterns of some conch parameters and sketch of the impact on the ammonoid shell. Boxes represent the inter-quartile range of individual values for each character and species. B) Statistical assessment of the trends by means of the random walk method of Hunt (2006). Akaike values of the three tested evolutionary modes (GRW – directional trend, URW – random walk, and stasis) are reported and significant when greater than a half unit.*

MULTIVARIATE PHENOTYPIC TRENDS IN AMMONOIDS

Investigating morphological macroevolution of a lineage through time by focusing on a single character (univariate) enables one to distinguish two major patterns: either stasis (absence of significant changes), or trend (directional or random walk; *Fig 9A*). Based on these two primary patterns of morphological evolution, a series of additional patterns can be distinguished based on the relative evolution among multiple trends (multivariate): convergence, divergence, and parallel evolution (*Fig 9B*). In a phenotypic space, convergence and divergence describe that the youngest forms are closest and farthest from the oldest forms, respectively; magnitude, shape, and direction of this change do not have to be similar. Parallel evolution is defined as the independent evolution of similar biological traits in at least two different lineages having similar magnitude, shape, and direction of their phenotypic trajectories. Cases of convergence and divergence are frequent but the concepts are broad. Demonstrated cases of parallel evolution are less frequent but concern a more precise pattern. Assessing quantitatively the significance and robustness of any of these evolutionary patterns is a difficult task, for which two statistical methods became available recently. The difficulty is to model and compare curves (evolutionary trajectories) within a multidimensional space constituted by the studied morphological characters (morphospace). These two methods were applied to ammonoids to test for parallel evolution.

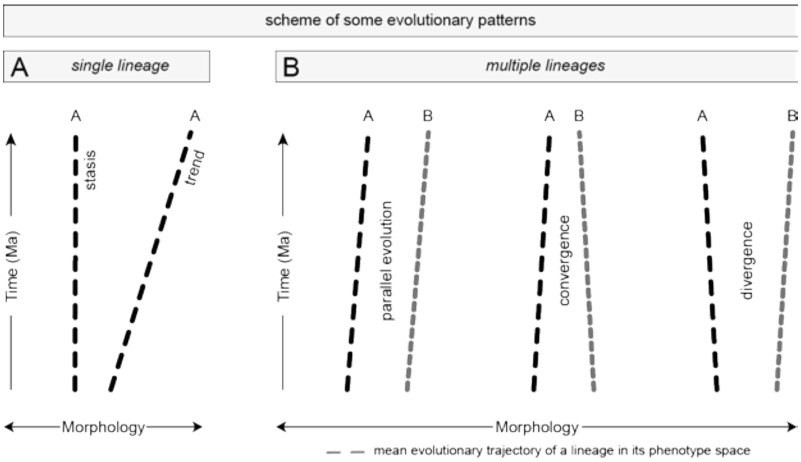


Figure 9 – *Scheme of some macroevolutionary patterns of a lineage in its morphological space.* ***A)*** *Accounting for a single character enables distinction of stasis and directed/random trend.* ***B)*** *Accounting for multiple characters enables distinction of convergence, divergence, and parallel evolution.*

The relative evolution of a subset of characters within a morphological space can be evaluated by a method developed by Adams & Collyer (2009) for comparing evolutionary trajectories of phenotypic change (Collyer & Adams 2013). According to this method, the phenotypic evolution of a lineage is defined as a trajectory across a set of evolutionary levels in a multivariate morphological space. Attributes of these trajectories (magnitude, direction and shape) are quantified and statistically compared across pairs of taxa by means of a residual randomization permutation method (Collyer & Adams 2007, 2013; Adams & Collyer 2009), and a summary statistic is used to determine the extent to which patterns of phenotypic evolution are concordant. This method is very powerful since it can be used to evaluate various evolutionary patterns. One constraint is that it currently requires the same number of comparable evolutionary levels (e.g. the same number of species) between the two compared lineages. Within this method, parallel evolution of two lineages can be defined by a similar origin in the morphological space, and by similar magnitude and direction of their evolutionary trajectories.

A second method to test parallel evolution of two lineages has been proposed by Monnet et al (2011a). It follows an approach proposed by Mitteroecker et al (2005) for comparing ontogenetic trajectories. This method is a permutation test based on within-lineage multivariate regression of the characters hypothesized to be involved in the parallel evolution. If the two lineages evolved in parallel, then their phylogenetic trajectories are identical in the morphological space defined by the subset of characters involved. This hypothesis is tested by comparing the summed squared distances of a linear total least square regression for each lineage separately between the two original lineages and for random series of two lineages obtained by permutation of species. If the two studied lineages evolved in parallel, the original test statistic should not be an outlier in the permutation distribution of summed squared distances (Mitteroecker et al 2005; Monnet et al 2011a). In other words, the affiliation of permuting specimens does not increase the residuals of the multivariate regressions and this is possible only if specimens of both families are close together in the studied morphological space. The major constraint of this method is that it assumes a linear trajectory of the evolution of studied lineages in the phenotypic space, but evolutionary steps are not required to be comparable and of the same quantity as opposed to the first method (Adams & Collyer 2009).

For ammonoids, the multivariate phenotypic trajectory analysis and permutation test were applied by Monnet et al (2011a) for the first time by investigating the evolution of eight shell characters for two Devonian lineages (Auguritidae, Pinacitidae). This period was a time of major changes in the marine ecosystems with the major diversification of several important nektonic groups such as jawed fishes and ammonoids (Klug et al 2010). In time and through phylogenetic order of appearance, both lineages display morphological directed trends toward more involute coiling, larger adult body size, more sutural elements, and the development of an umbilical lid in the most derived taxa (*Figs 8, 10A*).

The hypothesis of parallel evolution of the quantified characters under consideration has been tested by the two previously described permutation methods based on the character subset including UWI, Dmx and NLb (*Fig 10B*). These three characters were selected because they were previously demonstrated to follow directed trends and not just random walks (see above; *Fig 8*). Using the phenotypic trajectory analysis approach of Adams & Collyer (2009), it appears that there are no significant differences in the magnitude (MDsize = 0.103, Psize = 0.920) and in the direction (θdir = 14.735, Pdir = 0.087) of phenotypic evolution between the two lineages (*Fig 10B*). However, there are significant differences in the shape of the two evolutionary trajectories (Dshape = 0.586, Pshape = 0.001). This difference is, however, expected because the taxa in each lineage are not truly equivalent and do not necessarily represent the same evolutionary steps. Using the linear regression approach of Monnet et al (2011a), it appears that the hypothesis of parallel trajectories of the two studied lineages cannot be rejected (p = 0.019), but the value is low (*Fig 10C*). Hence, it appears likely that auguritids and pinacitids evolved in parallel with respect to increasing involution, adult size, suture indentation and construction of an umbilical lid.

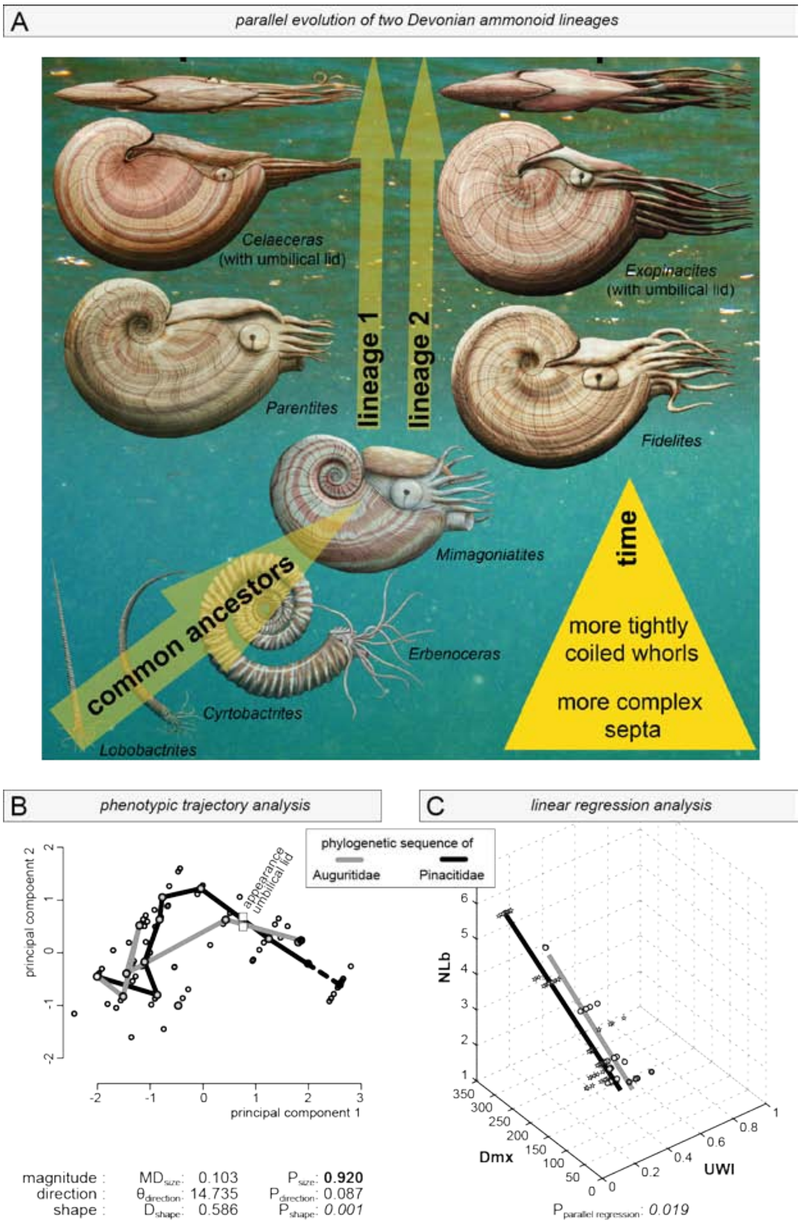


***Figure 10 –** Parallel evolution of two Devonian ammonoid families (Auguritidae and Pinacitidae) during the most intense phase of the "Devonian Nekton Revolution" (modified after Monnet et al 2011a). **A)** Illustration of this parallel evolution with reconstructions of the loosely coiled ancestors and two representatives of the two lineages under consideration. **B)** Statistical evaluation of the parallel evolution by means of the trajectory approach of Adams & Collyer (2009). Plot of the first and second principal components estimated from the correlation matrix for auguritids and pinacitids based on the three standardized characters UWI, Dmx, and NLb. There are no significant differences in magnitude and direction of the trajectories, but they are different in shape. **C)** Statistical evaluation of the parallel evolution by means of the regression approach of Monnet et al (2011). The phylogenetic trajectory of each lineage is fitted by a linear total least square regression. The* p-value *of the test is low, but the hypothesis of parallel trajectories could not be rejected by the permutation test.*

DISCUSSION

Adaptation (functional constraints)

Among the documented morphological evolutionary trends of ammonoids, the trends of increasing involution, increased adult shell diameter, and increased suture indentation are the most frequent. In the context of the neo-Darwinian theory of evolution, all these phenotypic trends have been and still can be interpreted as reflecting increasing adaptation of shell morphology to environmental factors and/or inter-/intra-specific competition. The various forms of the ammonoid shell have thus been interpreted in terms of functional needs, mostly in order to reconstruct the modes of life and habitats of this extinct group (Kennedy & Cobban 1976; Westermann 1996; Ritterbush & Bottjer 2012; Lukeneder 2015).

With regard to increasing adult body size, several advantages have been enumerated, such as increased defense against predation, increased food competition, increased success in mating and reproduction, increased individual longevity, and better energy use (Newell 1949; Simpson 1953; Rensch 1959; Gould 1966; Stanley 1973; Brown & Maurer 1986; Hone & Benton 2005; Korn & Klug 2007; Monnet et al 2011a; De Baets et al 2012). Hence, trends toward larger shell diameter have traditionally been interpreted to reflect persistent adaptive selection within long-ranging lineages. Trends toward smaller size, often interpreted by paedomorphosis, are also documented (Wright & Kennedy 1979; Kennedy & Wright 1985; Korn 1995a; Korn et al 2013a).

With regard to trends of increasing involution, their abundance and recurrence among numerous and distantly related ammonoid clades suggest that it may have an adaptive significance due to functional constraints (Dietl 1973, 1978; Westermann 1996; Klug & Korn 2004; Saunders et al 2004, 2008). Although hydrodynamic capabilities of these extinct animals are impossible to measure, it appears reasonable to assume that they were no enduring high-speed swimmers (Chamberlain 1980; Jacobs 1992). This interpretation is corroborated by mechanical experiments on shell models and analytical calculations of shell hydrodynamics (Chamberlain 1976, 1980; Saunders & Shapiro 1986; Elmi 1991, 1993; Jacobs 1992; Jacobs & Chamberlain 1996; Seki et al 2000; De Blasio 2008; Naglik et al 2015b), as well as by analogy with recent nautilids (the only extant cephalopod with a chambered external shell; Ward 1988; Jacobs & Landman 1993). It has been widely demonstrated that, for shells with oxyconic shell shapes (involute and compressed), the energy consumption for swimming is the lowest and potential maximal swimming speed is the highest (decreasing drag, increasing streamlining, etc.; Schmidt 1930; Raup 1967; Chamberlain 1976, 1980; Chamberlain & Westermann 1976; Jacobs 1992; Jacobs & Chamberlain 1996; Hassan et al 2002; Klug & Korn 2004; Klug et al 2008; Naglik et al 2015b). Increased involution of the shell therefore appears to represent an adaptation toward improved hydrodynamic properties of the shell (*Fig 11*; but for alternative interpretations including sea-level changes and predatory pressure, see Bayer & McGhee 1984, 1985; McGhee et al 1991; Neige et al 1997; Olóriz et al 1997, 1999; Kröger 2005; Wilmsen & Mosavinia 2011). For example, the gradual shift during the Devonian from marine communities dominated by organisms with openly-coiled shells to communities dominated by tightly coiled shells in distantly related organisms (nautilids, ammonoids, gastropods) was probably caused by predatory selective forces (Nützel & Frýda 2003; Kröger 2005; Klug et al 2010), assuming that open coiling makes shells weak and vulnerable to attack and force but also, they are simply larger (this selection pressure is also linked with swimming abilities).

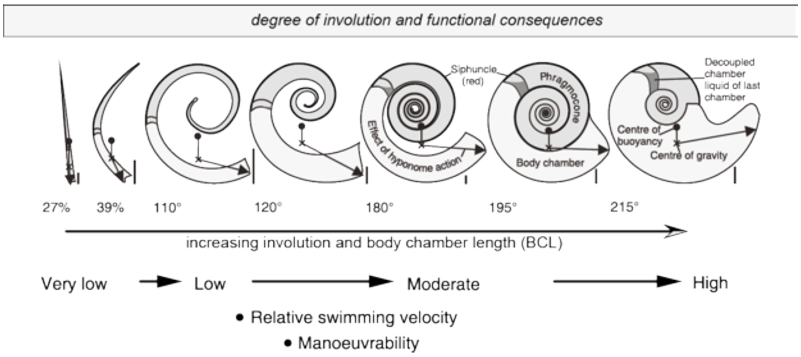


Figure 11 – *Degree of involution of the ammonoid conch and functional interpretation. Phylogenetic change in orientation of the conchs and swimming velocity of Bactritida and primitive Ammonoidea during the Devonian (modified after Klug & Korn 2004; Klug et al 2008). Outlines of the conchs with body chamber lengths (BCL), orientation of the aperture (OA), and relative swimming speed. Centre of gravity is indicated by a cross and the centre of buoyancy by a circle.*

With regard to trends of increasing suture frilling, the function of septal folding is subject of much debate (Kennedy & Cobban 1976; Saunders 1995; Hewitt & Westermann 1997; Daniel et al 1997; Lewy 2002; Checa 2003; Klug & Hoffmann 2015). The classic morpho-functional interpretation is that increasing suture frilling reduces the risk of implosion by providing buttressing against hydrostatic pressure on the phragmocone (Pfaff 1911; Westermann 1971, 1975; Hewitt & Westermann 1986, 1997; Seilacher 1988; Jacobs 1990; Hewitt 1996; Daniel et al 1997; Hassan et al 2002; De Blasio 2008). By contrast, available quantitative analyses of the ammonoid fossil record reveal no correlation between suture frilling and supposed water depths (Olóriz & Palmqvist 1995; Olóriz et al 1997, 1999). The evidence for paleobathymetric reconstruction is, however, commonly poor, thus making the hypothesis of depth-controlled suture frilling difficult to test. Ammonoids were mostly epipelagic organisms inhabiting the uppermost part of the marine water column (< 300 m; Westermann 1996; Lukeneder 2015). Wells (1999) even thought that this payed a role in their extinction, because nautilids (simple septa) can sustain pressures in depths up to 700 m (Ward 1988; Dunstan et al 2011). In any case, septum shape has also a strong developmental component (suture frilling increases through growth and is significantly correlated with the space available; Klug & Hoffmann 2015).

Iterative evolution and evolutionary jumps

Numerous examples of morphological long-term trends have been described in the literature within ammonoid cephalopods (see above). These repeated trends in phenotypic traits are commonly regarded as evidence of adaptation under common selection pressures (Simpson 1953; Endler 1986; Schluter 2000), therefore illustrating natural selection's major role in shaping morphological evolution and repeatability of evolutionary processes.

In this context, repetitive sedimentary sequences reflecting cyclic environmental changes (e.g. sea level, climate) have been suggested as a major trigger of morphological evolutionary trends of the ammonoid shell by means of similar morphofunctional adaptive responses. For instance, Bayer & McGhee (1984, 1985) studied the morphological evolution of several ammonoid lineages during the Jurassic and they identified "iterative repetition of identical evolutionary courses" in the ammonite faunas (*Fig 4B*). They argued that these iterative morphological changes were in response to cyclic changes in the physical marine environment: "similar environments were inhabited by ammonite faunas of similar morphology, and moreover, similar directional changes in the physical environment are mirrored by similar morphological changes in the ammonite faunas" (Bayer & McGhee 1984). Both endemic forms, which evolved in situ and migrant forms from the Tethyan realm, were equally affected. The phenomenon of iterative evolution in ammonoids is well known and several authors noted that these morphological sequences are repeated in groups separated both in time and taxonomy (Schindewolf 1940, 1950; Haas 1942; Arkell et al 1957; Wiedmann 1973; Kennedy & Cobban 1976). However, most discussions in the literature concern taxonomic and biostratigraphic consequences of the implied homeomorphies. This view of iterative evolution led to the concept that ammonoids repeatedly evolved from long-lived generalist lineages mainly inhabiting distal environments toward short-lived opportunistic lineages inhabiting shallower environments (Wiedmann 1973; Jacobs et al 1994).

In contrast, Guex (1992, 2001, 2003, 2006) qualitatively examined these iterative patterns for Mesozoic ammonoids. He argued that during stable periods, ammonoid lineages experience classic long-term evolutionary trends of their shell (e.g., increase of shell size, involution, compression, as well as increase of suture frilling) and that during extinction periods, relatively tightly coiled ammonites can give rise to highly evolute forms or heteromorphs with simple ornamentation and almost ceratitic suture line. He dubbed this sudden evolutionary change, which is at variance with previous long-term changes, an "evolutionary jump". He pointed out that these evolutionary jumps are characterized by the appearance of forms, which are partly homeomorphic with remote ancestors of their own lineage and interpreted these newly evolved homeomorphic taxa as being atavistic. He called also this phenomenon "proteromorphosis" because it cannot be explained by normal paedomorphic transformations. Monnet et al (2013) recently described such a potential evolutionary jump within a lineage of Triassic ammonoids. Guex (1992, 2001, 2006) also argued that episodes of strong environmental stress are at the origin of many new ammonoid lineages by promoting the abrupt appearance of significantly different forms by means of such evolutionary jumps.

The most extreme case of iterative evolution is probably the recurrent appearance of loosely coiled, uncoiled and trochospirally coiled heteromorph ammonoids, which have not only been linked to periods of environmental stress (Guex 2006), but also to advantageous trophic conditions (Nesis 1986; Cecca 1997) or sea-level changes (Keupp 2000). Such heteromorphic ammonoids were long seen as evolutionary dead ends and irreversible, phylogenetic end-forms (for a review, see Wiedmann 1969). Before this time, the belief in Dollo's law of irreversibility was deeply entrenched in the thoughts of natural scientists, stating that the re-evolution of any complex character like the coiled ammonoid shell was considered unlikely or impossible. Besides methodological problems with interpreting uncoiled as less "complex" than coiled shells (Urdy & Chirat 2006), there are additional reasons to see heteromorphic ammonoids as anything but evolutionary dead ends. Heteromorphs were highly successful (diverse and abundant) during some periods (Cretaceous), and diverse heteromorphic lineages gave rise to coiled representatives, which counter-act these ideas (Wiedman 1969; Cecca 1997; Bert & Bersac 2013). Contra-intuitively involute forms have also been seen as phylogenetic end-forms. For instance, this seems to be the case of the Devonian Auguritidae and Pinacitidae (Monnet et al 2011a), Triassic Sagecerataceae and Pinacocerataceae (Diener 1917; McGowan & Smith 2007; Korn 2012), and Jurassic Amaltheidae (Meister 1988), among others. However, some lineages with oxyconic forms have also successfully given rise to less coiled descendants.

The major characteristic of all these models of macroevolution of the ammonoid shell is that they rely on two widespread views among ammonitologists: (i) the ammonoid conch is shaped by its functional needs only and thus reflects environmental changes, and (ii) ammonoids evolved toward particular morphologies, which correspond to adaptive peaks in the ammonoid phenotypic landscape. By contrast, the widespread adaptive interpretations of the ammonoid conch are ad hoc explanations in many cases, partially because their behavior cannot be observed (e.g. swimming speeds, habitat depths, vertical movements; compare Ritterbush et al 2014, Naglik et al 2015b). This is a common problem in paleontology (Ebbighausen & Korn 2013), strongly limiting the range and number of falsifiable hypotheses. In some cases, iterative intricate evolutionary patterns or morphological characteristics allow speculations with a certain degree of plausibility, which justifies their description and discussion.

Moreover, natural selection is one possible and important, although commonly over-rated, trigger and driver among several others in the fabric of evolutionary trends. Interestingly, evolutionary trends are never global and opposite patterns are also common: usually, they occur only in specific clades, while other coexisting clades still retain or evolve very different shell morphologies. For instance, crioconic, serpenticonic and platyconic forms coexisted with the highly involute auguritids and pinacitids (Klug 2002; Korn & Klug 2003). Representatives with very complex and very simple suture lines were found together (e.g. *Beloceras* and *Archoceras*: Korn et al 2013a; *Metoicoceras* and *Euomphaloceras*: Cobban et al 1989). Micromorphic and large-sized ammonoids also co-occured (e.g. *Nannometoicoceras* and *Metoicoceras*: Kennedy 1989), and very involute and compressed forms coexisted with evolute and/or depressed forms (e.g. *Oxylongobardites*, *Tropigastrites* and *Proarcestes*; Monnet & Bucher 2005). Furthermore, quantitative analyses of the correlation between the supposed adaptive shell characters and environmental factors produced variable results (Bayer & McGhee 1985; Donovan 1985; Cariou & Hantzpergue 1988; Batt 1989; Jacobs et al 1994; Westermann 1996; Neige et al 1997; Olóriz et al 1997, 1999, 2002; Vörös 2002; Kawabe 2003). But it must be acknowledged that environmental parameters (e.g. bathymetry, temperature) are usually difficult to assess and quantify in the past and in most cases, evidence for the ammonoids' actual habitats is weak because they might have lived anywhere in the water column above where they are found (De Baets et al 2015) and their shells could easily be transported (Wani & Gupta 2015). Nevertheless, some indication of their habitat can be constrained by combining multiple lines of evidence (Ritterbush et al 2014; Naglik et al 2015b), including predator–prey interactions (Keupp 2006; Kruta et al 2011; Hoffmann & Keupp 2015; Tanabe et al 2015) and stable isotopes of their shells (Lécuyer & Bucher 2006; Lukeneder et al 2010; Lukeneder 2015). Interestingly, the co-occurrence in time of different evolutionary trends leading to very disparate co-existing morphologies may reflect the existence of multiple adaptive peaks in the ammonoid phenotypic landscape and/or that the triggers of these trends are not global and not only adaptive. The model of Guex (2001, 2006) assumed that trends are reset during periods of high environmental stress. This remains to be tested but enables us to ask about the distribution, influence and frequency of trends within/among space, time, taxonomy, and phylogeny, as well as the proportion of adaptation, covariation and chance generating these trends. Furthermore, rates of morphological change depend on the observed time interval, so that these first need to be quantified to speak about evolutionary jump as opposed to normal evolutionary trends.

Covariation (constructional constraints)

Evolution of shell shape driven by adaptation, although reasonable from a mechanical point of view, is certainly not the sole driving mechanism behind long-term evolutionary trends in ammonoids. To explain how certain organisms have evolved certain features, evolutionary biologists emphasized the role of constructional/developmental constraints on evolution (Williamson 1981; Alberch 1982; Charlesworth & Lande 1982; Holder 1983; Maynard-Smith et al 1985; Raff 1987; Goldsmith 1990; Arnold 1992; Tabin 1992). Maynard-Smith et al (1985, p. 266) defined a developmental constraint as "*a bias on the production of various phenotypes caused by the structure, character, composition, or dynamics of the developmental system*". Correlations between characters belong to the most common patterns attributed to developmental constraints. Such correlations may result from interactions between tissues during the development or the involvement of the same genes or developmental pathways in multiple morphogenetic processes. Although it is difficult to rule out selective (functional) constraints (adaptation), constructional, developmental and/or genetic constraints can also explain common evolutionary patterns (Morita 1993, 2003; Wagner & Erwin 2006).

In this context, it is here suggested that many of the described long-term morphological evolutionary trends of ammonoids can be explained, in part, by other constraints than selective ones. Indeed, some of the documented trends of the ammonoid shell can be produced by constructional constraints (Seilacher 1973; Urdy et al 2010a, 2010b; Monnet et al 2011a) referred to as covariation. In other words, some morphological trends of specific characters of the ammonoid shell can result from trends in other traits because the way the shell is constructed (morphogenesis) involves the covariation (scaling, usually by means of allometric rules) of several shell characters. It is important to identify such aspects of covariation, because in this case, it is unnecessary to search for an adaptive explanation.

Covariation of shell characters is well known from ammonoids. For instance, the intraspecific variation of an ammonoid species is usually expressed by the following gradient: the more evolute the shell, the thicker the whorl shape (large whorl width to whorl height ratio), and the more robust the ornamentation. It is referred to as Buckman's first rule of covariation (Reeside & Cobban 1960; Westermann 1966; Dagys & Weitschat 1993; Morard & Guex 2003; Yacobucci 2004; Hammer & Bucher 2005; Monnet et al 2010, 2015b; Bert & Bersac 2013; De Baets et al 2013, De Baets et al 2015). This covariation pattern concerns intraspecific variability and differs from the type of covariation discussed below. Among phenotypic directed evolutionary trends of ammonoids, the concept that some of these trends can be due to scaling effects is discussed below for the two most frequent morphological trends: increasing involution and increasing suture indentation.

A striking pattern of ammonoid evolution is that trends of increasing adult shell diameter are commonly, but not systematically, associated with trends of increasing involution and increasing suture indentation. These trends in size are usually interpreted to exemplify Cope's rule. However, these trends concern the adult shell diameter, not the volume of the soft tissues. Soft tissues of ammonoid cephalopods are insufficiently known and consequently also their relation with conch size. Nevertheless, we can reasonably assume that their soft body scales with the volume of the body chamber (Arkell et al 1957; Doguzhaeva & Mutvei 1991; De Baets et al 2012, De Baets et al 2015). Yet, from a morphogenetic point of view, what would happen if a studied ammonoid clade followed a size-increase of its soft body? It appears that increasing body size (volume of soft tissues in the body chamber) can be accommodated in several ways (Guex 2001, 2003): increasing arc length of the body chamber, increasing whorl width, or increasing whorl height, which can result in increasing shell diameter and/or involution (*Fig 12*). We stress that several trends in ammonoid shell geometry can be explained by increasing adult body size as an alternative to functional explanations (Guex 2003), because both changes in shell diameter and shell involution are two possible paths for ammonoids to accommodate soft body size increase. Although shell diameter is usually assumed to reflect body size, it does not suffice and even is not required to identify a case of body size increase for ammonoids. For example, increasing whorl width or increasing involution without changes in shell diameter still can be induced by an increasing adult body size (*Fig 12*). Therefore, an evolutionary increase of ammonoid soft body size can indirectly trigger several trends in ammonoid geometry.

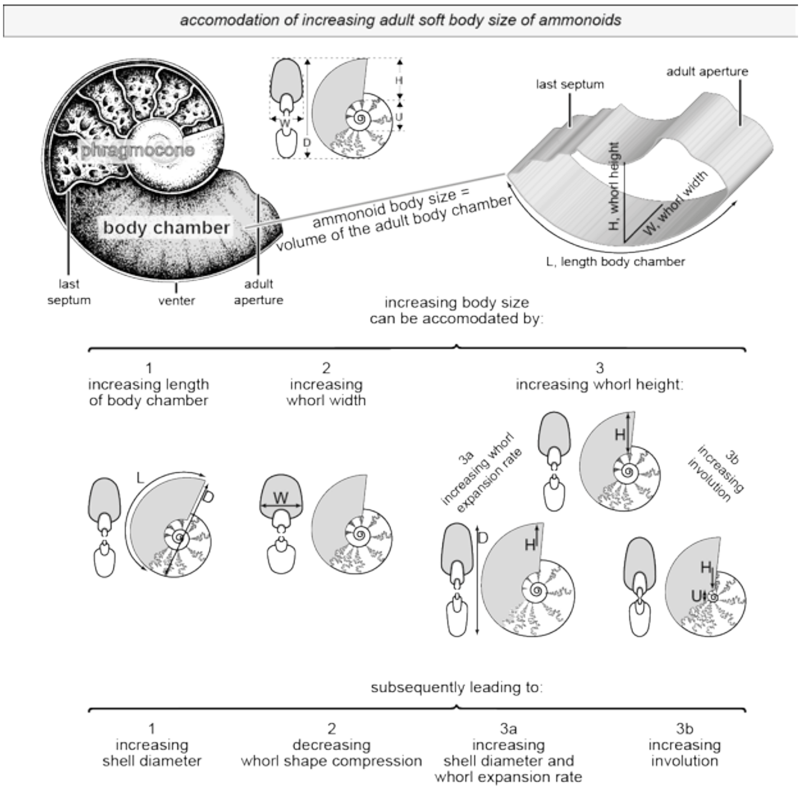


***Figure 12** – Illustration of the various ways how an increase of adult soft body size of ammonoids can be accommodated by the geometry of their external shell. Increase in ammonoid soft body size can be expressed in terms of three basic alternatives, which are not mutually exclusive and can be accumulated in various combinations and proportions: increasing arc length of body chamber, increasing whorl width, and/or increasing whorl height. This three accommodating changes can lead to four increasing phenotypic trends of shell geometry: in shell diameter, in whorl shape depression, in whorl expansion rate, and in involution (compare Figs 5, 8).*

Bearing this distinction in mind is essential because morphological trends of the ammonoid shell are quite often interpreted by more or less ad hoc adaptive and morpho-functional explanations. With regard to trends of increasing involution, it may well result solely from an increase in body size, and not directly from a selection pressure on the coiling itself and its associated swimming advantage; increase in body size may itself be a swimming-related factor, because it provides the possibility for a larger volume of propulsive muscles and hydrodynamic properties change with body size as well (Naglik et al 2015b). Therefore, some conclusions on improved hydrodynamics of the shell may be speculative and represent secondary adaptations (Gould & Lewontin 1979; but see Levinton 2001). The role of hydrodynamic efficiency in ammonoid shell shape, argued by several authors, may have been overestimated (Weitschat & Bandel 1991). This is also supported by large intraspecific variability in shell shape in several ammonoid lineages (Dagys & Weitschat 1993; De Baets et al 2015). With regard to trends of increasing suture indentation, it may also result from an increase in body size, and not directly from selection pressure on the suture frilling. Although knowledge of the morphogenesis of ammonoid septa remains incomplete (Klug & Hoffmann 2015), septal patterns display similarities with structures that developed under a "domain effect" by a "viscous fingering" phenomenon (see also review of Checa & García-Ruiz 1996). In this morphogenetic model, details of the suture pattern depend on the space and shape available for the suture during its formation (septa are secreted after the surrounding shell). This is supported by the widely documented significant increase in suture indentation throughout ontogeny of the ammonoid shell (the number of suture elements increases with whorl height of the shell; Swinnerton & Trueman 1917; Erben

1966; Korn & Klug 2003; Pérez-Claros et al 2007). In this context, as for involution, folding and fluting of the septal mantle are an additional means to accommodate body size increase (Guex 2003; compare Illert & Reverberi 1988). Interestingly, even if some trends in ammonoid shell geometry can be triggered by an increase of ammonoid soft body size and thus result from constructional constraints as stressed above, adaptive pressure can still operate indirectly: An increase in soft body size coupled with a constant shell diameter will induce a loss of buoyancy, which can be compensated in several ways (e.g. decrease of body chamber length or decrease of shell thickness, which both influence shell orientation). Hence, positive or negative adaptive feedback can enhance or minimize the impact of constructional constraints.

The comparison of these theoretical investigations with the previously described long-term evolution of Triassic acrochordiceratids and Devonian auguritids and pinacitids (*Figs 5, 8*) is striking. The three lineages are characterized by directed trends toward increasing involution and suture indentation concomitant with increasing adult shell size (Monnet et al 2011a, 2012). Following the previous reasoning, it appears that these trends can be induced by covariation (constructional constraints) with evolutionary changes in soft body volume. They may be secondary trends and as such their interpretation in terms of adaptation should be cautious. Notably, these trends in the three studied ammonoid lineages are not associated with any trend in whorl shape compression whereas it is one of the possible ways of accommodating increased soft body volume (compare *Figs 5, 8, 12*). This observation highlights the view that the relative influence of these different possible covariation patterns remains to be elucidated and investigated, as well as why certain evolutionary trajectories are favored or not (possibly by means of adaptive feedbacks induced by some constructional constraints). Therefore, it is stressed that long-term phenotypic trends in ammonoid shell form must be tested rigorously and conjointly. This remains to be done, but such an effort is crucial because it is not really possible to interpret the adaptive value of trends in ammonoid shell form without accounting for such possible constructional constraints. An additional problem is that there may be other constructional or even adaptive constraints that are not yet understood because of missing data, non-preservation or simply the historic aspect (i.e. behavior). In the case of the degree of septal frilling, it has to be understood that not all aspects of septal growth and construction are fully understood yet. This situation strongly limits the scientifically correct approaches to identify potential evolutionary drivers triggering the evolution of ammonoid septa.

In conclusion, from a theoretical point of view, long-term phenotypic evolutionary trends of the ammonoid shell can result from adaptation (selective constraints), from covariation (constructional constraints) or a combination of these and other factors. For instance, both increasing involution and suture indentation can just be scaling effect of within-lineage size-increase (if soft body volume is considered and not shell diameter); similarly, seeming simplification of sutures might have originated in size-reduction or changes in whorl cross section or development. The respective relative role of these non-mutually exclusive, possible drivers of evolutionary trends in shaping ammonoid evolution has not been investigated sufficiently yet. Furthermore, morphogenesis of the ammonoid shell (and other mollusk shells) is still insufficiently known. More and new information on mollusk shell morphogenesis could provide crucial insights on patterns and processes of mollusk evolution. In this context, it is not surprising that previous studies trying to evaluate the prevalence of Cope’s rule or increasing complexity of life resulted in unclear and controversial results. Indeed, such studies have to differentiate between adaptive trends and covariation, be it driven by scaling effects or other factors.

Developmental constraints and heterochrony

Constraints on evolutionary trends are not limited to adaptive selection and constructional covariation. Naturally, there are also developmental and genetic constraints. The latter cannot be assessed in ammonoid cephalopods since it is an extinct group and DNA of that age is unknown, but these factors may have an important role. For instance, the repeated evolution of a shell character may speculatively result from the repetitive loss of the expression of regulatory Hox-genes (Averoff & Patel 1997; Prud'homme et al 2006) or the repeated recruiting of developmental genes (Lindsey 1962; Colosimo et al 2005). Sudies on extant shell-bearing mollusks such as gastropods are one of the only ways to provide clues about this kind of constraints on the evolution of ammonoids.

Major evolutionary changes in a trend are often constrained by morphological and functional trade-offs, with one structure improving at the expense of another. Many such trade-offs have a developmental basis and have arisen from heterochrony (McNamara 1997). Heterochrony (i.e. developmental change in the timing of events, leading to changes in size and shape) is a fundamental aspect of evolution, supported by a vast biological and paleontological literature. It has been argued that heterochrony plays an important role in evolutionary trends (McNamara 1982, 1990), including both anagenetic and cladogenetic trends, and both micro- and macro-evolutionary trends (McNamara & McKinney 2005). Briefly, heterochrony can be described in the form of paedomorphosis and peramorphosis that occur between an ancestor and its descendant: on the one hand, paedomorphosis can be observed when a descendent retains in its reproductive, adult stage the juvenile traits of its ancestor taxon, and on the other hand, peramorphosis is delayed maturation and extended periods of growth (*Fig 13*). It must, however, be kept in mind that in fossil organisms like ammonoids only size and shape is available, while the duration (age) and the rate of growth are mostly unknown (Landman & Geyssant 1993; allometric heterochrony *sensu* McKinney 1988). A relationship between evolutionary trends and heterochrony arises because evolutionary trends are, like ontogenetic trajectories, unidirectional. For trends to develop, in addition to the intrinsic factor of heterochrony, extrinsic factors are also critical. Selection of either progressively more paedomorphic or more peramorphic traits must take place along an environmental gradient, such as in the aquatic environment from deep to shallow water, or from coarse to fine-grained sediments (McNamara 1982, 2006). An evolutionary trend from ancestors to descendants that show increasingly more paedomorphic characters is called a paedomorphocline. If the trend shows increasing peramorphic descendants, it is called a peramorphocline (McNamara 1982, 1990). Collectively these are called heterochronoclines. Many examples of heterochronoclines have been described in ammonoids and for various characters and in various directions in their shell morphospace (Gould 1977; Dommergues et al 1986, 1989; Landman 1988, 1989; Meister 1988; Dommergues & Meister 1989; McNamara 1990; Dommergues 1990; Korn 1992, 1995a, b; Landman & Geyssant 1993; Gerber 2011; Korn et al 2013a; *Fig 4*). Hence, not only developmental constraints play a significant role in ammonoid evolution, but also this role can be evaluated thanks to the accretionary mode of growth of mollusk shells, which provides an invaluable access to individual ontogenetic development in individual ammonoids. In this context, the recurrence of morphological evolutionary trends within ammonoids can be seen as the repetitive and preferential selection of the same heterochronic process because of similar environmental conditions/gradients and intrinsic constraints that canalize the evolution of ammonoid clades (Dommergues et al 1989; McNamara 1990).

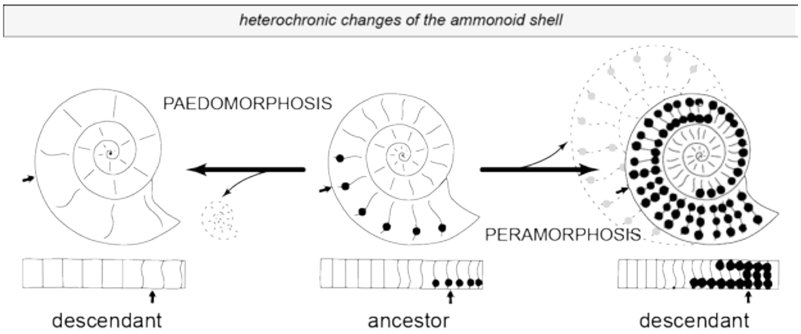


Figure 13 *– Scheme illustrating the paedomorphosis and peramorphosis of an ancestral ammonoid with regard to the presence and number of rows of tubercles (modified after Landman & Geyssant 1993).*

Heterochronoclines *ipso facto* induce a rough parallel trend between phylogeny and ontogeny that has been frequently described in ammonoid evolution. However, within the same lineages, the chronocline evolution of the different ammonoid shell characters is a mosaic pattern characterized by various trends and stases that are often at variance. For instance, in the case of the previously discussed Triassic acrochordiceratids, one important ontogenetic pattern is that several shell characters show significant and persistent shift during ontogeny (Monnet et al 2012, *Fig 11*). Members of this lineage became more involute, developed more compressed whorl sections, and reduced the number of ribs during development. Interestingly, while the ontogenetic trends in coiling and ribbing density mirror their long-term stratophenetic trend (this can be described as a size-based or allometric peramorphocline; McKinney 1988; Dommergues et al 1989; McKinney & McNamara 1991), no ontogenetic trend in whorl shape compression could be found in the evolution of this group during the Anisian. Hence, evolutionary trends of the Anisian Acrochordiceratidae parallel their ontogenetic developments in part only. This partial concordance between the evolution of the group and its ontogenetic changes poses the question whether the direction of evolutionary change at the phenotypic level may be a product of the within-individual dynamics of development and/or of the within-population dynamics of natural selection. In other words, was the morphological evolutionary trend of increasing coiling of ammonoids driven by natural selection, by a developmental constraint, or by a combination of both (Arthur 2001, 2004)? Paleontologists and neontologists sometimes underestimate developmental constraints in the shaping of anagenetic morphological trends (McKinney 1990). Since the evolution of organisms is an equilibrium between various mutually interacting processes (Waddington 1941), what is the relative influence of the various constraints (selective, constructional, developmental, chance, etc.) on the evolution of the ammonoid shell? The exact contribution of each type of constraints remains to be investigated and also requires a better understanding of the morphogenesis of the ammonoid shell. Crucial information may come from the ongoing development of quantitative and theoretical modeling of the mollusk shell (Raup 1966; Ubukata et al 2008; Monnet et al 2009; Urdy et al 2010a; Parent et al 2010, 2012; Moulton et al 2012, 2015; Chirat et al 2013), as well as from the comparison with growth-monitored individuals in the wild or in aquaria (Urdy et al 2010b).

Prospects on long-term phenotypic trends

Understanding the patterns of evolution requires identifying the processes that shape these patterns and in which context they apply. Currently, the knowledge and understanding of the fabrics and dynamics of long-term morphological evolutionary trends is complicated by two major sources of bias.

Natural selection as a driver of phenotypic evolution tends to be overrated, or, in the words of Graffin & Olson (2010), there is a “false idol of natural selection”. Although adaptation has been historically overestimated, the existence of adaptation and selection as drivers of evolution with a much smaller role than originally thought appears reasonable. A fundamental epistemological problem of both is the near impossibility to prove the causal relationship between, e.g., an ecological factor and a morphological change. However, it is legitimate and stimulating to seek correlations between evolutionary change in ammonoid morphology and other factors such as ecological factors, paleogeography, predation patterns, and particular evolutionary patterns. At some degree of correlation between evolutionary patterns and ecological processes, randomness of evolutionary change becomes increasingly implausible, allowing near-hypothetical speculations on aspects of adaptation and selection influencing evolution.

A first example has been discussed in great detail above, namely the parallel evolution of two distantly related lineages of Devonian Auguritidae and Pinacitidae (Monnet et al 2011a). It appears unlikely that several morphological traits including highly unusual ones such as the umbilical lid evolve in parallel over millions of years without the slightest aspect of adaptation or selective mechanism as evolutionary driver. It is undoubted that covariation explains a significant part of the evolutionary change, but explaining the entire course of this case of parallel evolution would mean circular reasoning. At some point, adaptation or selection must have a played a role, even if only gently. Sexual selection is well-known to play an important role in extant organisms, but is hard to prove for extinct ones; it is well conceivable that sexual selection is also responsible for some evolutionary trends in ammonoid evolution (compare Knell et al 2013).

A second example is a number of distinct evolutionary trends (although a left wall effect cannot be entirely ruled out in these cases) in early ammonoid evolution (Korn & Klug 2003; Klug & Korn 2004; De Baets et al 2012; Klug et al 2015a), which are well documented for the embryonic shell (De Baets et al 2012). These include a reduction in ammonitella size, increase in coiling of the ammonitella (Erben 1966; House 1996; De Baets et al 2012, 2013b) but also of post-embryonic whorls (Klug & Korn 2004), the decrease of the size of the umbilical window until its closure (House 1996; De Baets et al 2012) as well as an increase of the whorl expansion and soft-part volume (Korn & Klug 2003; Klug & Korn 2004). Several alternative explanations for these trends present themselves: (i) ammonitella-size decreased simultaneously with increasing soft-body size, suggesting increasing reproductive rates (and reduced survivorship of offspring) (discussion in De Baets et al 2012); (ii) in the Early Devonian, an increase in coiling is documented from several clades (Ammonoidea, Dacryoconarida, Orthocerida) synchronous with a decrease in embryonic or larval shell size (Gastropoda, Ammonoidea)—a random coincidence appears less likely than selective pressure from profound macroecological pressures (Klug et al 2010); (iii) with increasing coiling, the orientation of the aperture changed from vertically downward via oblique to horizontally upward (Korn & Klug 2003; Klug & Korn 2004)—a random evolutionary change appears, again, unreasonable, since it makes perfect sense from a hydrodynamic point of view (a more or less horizontal aperture enhances maneuverability and swimming; see discussion in Klug & Korn 2004); and (iv) increased coiling and improved swimming capabilities do make sense in the light that more or less synchronously the gnathostome fish underwent an explosive radiation, thus suggesting a selective pressure from evolving mobile predators, probably progressively occupying the same habitats as the ammonoids (compare Klug et al 2010, 2015a).

Therefore, it appears easier and reasonable to keep hands off adaptive explanations for evolutionary change among ammonoids, but selection and adaptation must have played a role of unknown proportion in ammonoid evolution. Its denial is of no help in under-standing ammonoid evolution, but great care and openness towards criticism and discussion is essential.

A major second source of biases in the analysis of long-term trends is rooted in the data available and the approaches used to these analyses. Most studies are partly biased by one or a combination of the following aspects: absence of a rigorous phylogenetic framework, insufficient consideration of anagenetic and ontogenetic changes, insufficient taxonomic coverage, insufficient consideration of morphogenetic constraints, absence of comparison with simulated evolutionary patterns (specially to evaluate the impact of chance alone), among others. For instance, evolutionary changes in size were documented to apply to several ammonoid groups, but there are no quantitative data covering all ammonoid taxa (rather than specific clades) of a distinct time interval, with a robust phylogenetic framework and with integration of covariation patterns of the diverse shell characters (compare Hallam 1975 and Dommergues et al 2002). In this context, several questions on evolutionary patterns and processes remain to be investigated. What is the proportion between adaptive (selective constraints) and scaled (constructional constraints) morphological long-term evolutionary trends among ammonoids? Under which conditions did these trends occur? Are trends (be it adaptive and/or a secondary effect) restricted in time and space and clades? What is the influence of origination and extinction events on the fabrics of evolutionary trends (see Guex 2006)? All these questions among many others remain to be investigated and await adequate data collection and subsequent quantitative analyses.

Finally, the impact of chance on the frequency of ammonoid evolutionary trends remains also to be assessed. Theoretically, evolutionary trends in involution and suture indentation can be adaptive and/or scaling effects of size changes. Since apparent trends in evolutionary series can be produced randomly (Raup & Gould 1974; Raup & Crick 1981; Bookstein 1987, 1988; Raup 1997; Roopnarine et al 1999; Hunt 2006), are these documented trends more frequent than what can be expected just by sheer random evolution? All morphological characters have lower and upper viable limits. Hence, the location of origination of a clade or taxon in its phenotype space directly influences the chance of having a trend among its descendants. Indeed, the chance of a taxon having a larger descendant (or with a more involute shell, or with a more indented suture, etc.) may be related to the distance from the limits of the considered character in the morphological space of the studied group. Hence, it remains to be seen whether documented evolutionary trends of the ammonoid shell are caused (and in which proportion) by random evolution constrained by the constructional limits of the shell (left-wall effect).

Now, if we consider shell characters in the biological concept of adaptive landscapes (Wright 1932; McGhee 1999, 2007; Wilson 2013), shell form can be expected to exhibit repeated trends in some characters given the functional properties of the ammonoid shell (buoyancy device containing soft-tissues). In this case, is the distribution in time and space of trends concordant with adaptive hypotheses? Can we derive a morphological adaptive landscape of the ammonoid shell? Finally, in this context of evolutionary trends and morphological landscapes, several questions remain to be investigated. Are kinds of trends randomly distributed among shell characters (for instance, are cases of size trends restricted to particular morphologies)? Do trends originate at random locations in the morphospace of the studied group? New data delivering answers to these questions will provide insights on patterns and processes of long-term phenotypic trends of the ammonoid conch such as convergence, divergence, and parallel evolution.

CONCLUSIONS

Long-term morphological evolutionary trends of ammonoid cephalopods are numerous and suggest the existence of common processes acting regularly to mold their macroevolution. Although ammonoid cephalopods are extinct, their high evolutionary rates and the excellent fossil record of their shells make them superb study objects to reveal insights into patterns and processes of long-term phenotypic evolutionary trends. Unfortunately, quantitative studies are still rare and often lack a phylogenetic framework. As acknowledged by Jablonski (2000): "*only a few studies have met the necessary protocols for the analysis of evolutionary tempo and mode at the species level, and so the distribution of evolutionary patterns among clades, environments, and modes of life remains poorly understood*".

From the few existing studies, it appears that constructional (covariation) and adaptive constraints are not mutually exclusive. Both can contribute to the fabrics of evolutionary trends for ammonoid lineages. This underlines that evolutionary and developmental morphogenesis, and the controls upon them, can never be truly understood in separation from functional adaptation and constructional covariation. Distinction between covariation and adaptation in evaluating evolutionary trends is essential in order to avoid over-interpretation of the evolutionary patterns. For instance, the frequent increase in suture indentation is probably not a primary adaptation to water depth against implosion, but likely represents a secondary trend caused partly by an increase of adult shell size and shape due to covariation (constructional constraints). Hence, recurrence of particular combinations of morphology, which are commonly regarded as strong arguments for functional constraints, can also represent "fabricational noise" (Seilacher 1970, 1973). It is thus crucial for evolutionary analyses to understand the driving factors behind evolutionary morphological modifications.

Selective (adaptation) and constructional (covariation) constraints do occur in the evolution of the ammonoid shell. Taken separately, they do not explain every evolutionary trend, and their respective contribution to ammonoid evolution remains to be quantified. Understanding the underlying processes of directed evolution still require further research. Answers to such questions strongly needs adequate quantitative datasets framed with robust phylogenies, comparison against simulated random evolution (to evaluate the prevalence of constraints or chance in generating trends), a better knowledge of shell morphogenesis (to precisely quantify the expectable covariation between measured shell characters), and accounting for both anagenetic and cladogenetic changes.

We expect that further discoveries and the application of quantitative methods and better knowledge of mollusk shell morphogenesis will continue to reveal information on the evolutionary history of this major marine extinct group, the ammonoids, and contribute to the understanding of patterns and processes in macroevolution. If ammonitologists do so, they can become nomothetic scientists, which Stephen Jay Gould would probably have appreciated.

Numerical Tools
in
Paleontology

NUMERICAL TOOLS IN PALEONTOLOGY

Related publications:
Monnet et al 2003a; unpublished programs and scripts

Paleontology is often viewed as a dusty discipline, which is restricted to collecting bones with a brush and storing them in dusty drawers in old museums. However, advances in statistical methods and computer technology provide paleontologists with a variety of techniques for collecting, managing, and evaluating large volumes of data. Paleontology has proven invaluable to provide significant insights in topics such as macroevolution as illustrated by the famous biodiversity curves of the Phanerozoic. Paleontology is also a leading discipline with regard to morphometrics and managing incomplete data, among others. With the advent of ever-growing and large worldwide collaborative databases, paleontology is nowadays a dynamic discipline, which is largely supported and pulled up by quantitative analyses.

From a personal viewpoint, I always have enjoyed fossils and have fun playing with numbers and computer programs. Therefore, it is logical for me to perform quantitative analyses on paleontological data, and my position as a "research engineer" in Lille clearly suits these two passions. Historically, this is this aspect, which convinced me to be a professional paleontologist, especially the aspect of solving brain teaser by means of computer. This began with the implementation of a computer tool with the BASIC language to extract forbidden subgraphs for the unitary associations, under a Apple IIc with floppy disks of 128 ko when I was in Master (1st year, Lyon). The following chapter will thus review my contribution in the development of computer tools to perform quantitative analyses of paleontological data.

MATLAB – THE SCRIPTS ISOPAQ AND AMMOPAL

I started writing computer softwares with the scientific language Matlab: first to develop a program to perform isopach mapping of sedimentary and stratigraphic data (Monnet et al 2003a), and second to develop a program to characterize and quantify variation of ammonoids with their classic shell measurements (unpublished).

Isopaq

The three-dimensional reconstruction of basin sediments is a major topic in earth sciences and is now a necessary step for modeling and understanding the depositional context of sediments. Because data are generally scattered, the construction of any irregular, continuous surface involves the interpolation of a large number of points over a regular grid. However, interpolation is a highly technical specialty that is still somewhat of a black art for most people. The lack of multi-platform contouring software that is easy to use, fast and automatic, without numerous abstruse parameters, motivated the programming of the software called ISOPAQ.

This program is an interactive desktop tool for spatial analysis, interpolation and display (location, contour and surface mapping) of earth science data, especially stratigraphic data. It handles four-dimensional datasets, where the dimensions are usually longitude, latitude, thickness and time, stored in a single text file. The program uses functions written for the MATLAB language (*Fig 1A*). Data are managed by means of a user-friendly graphic interface, which allows the user to interpolate and generate maps for stratigraphic analyses (*Fig 1B*), as well as geological sections around a precise stratigraphic boundary (*Fig 1C*). This program can process and compare several interpolation methods (nearest neighbor, linear and cubic triangulations, inverse distance and surface splines) and some stratigraphic treatments, such as the decompaction of sediments. Moreover, the window interface helps the user to easily change some parameters like coordinates, grid cell size, and equidistance of contour lines and scale between files. Primarily developed for non-specialists of interpolation thanks to the graphic user interface, practitioners can also easily append the program with their own functions, since it is written in the MATLAB open language.

As an example, the program has been applied to the Bajocian stratigraphic sequences of eastern France (Thiry-Bastien 2002).

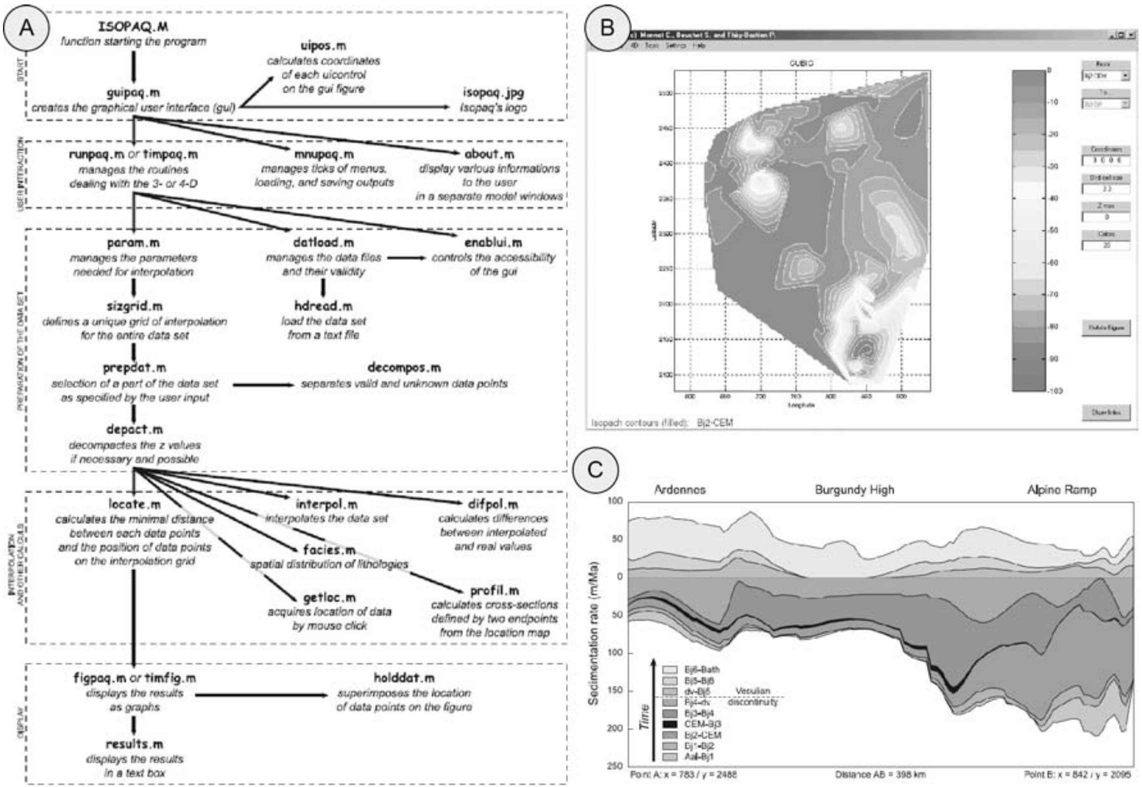


Figure 1 – *ISOPAQ and its application to the Bajocian of France (Monnet et al 2003a).* ***A)*** *Flow chart and goals of ISOPAQ's functions (code was written for MATLAB 6 without additional toolbox).* ***B)*** *Graphic user interface of ISOPAQ with output of the isopach map of the Bj2-CEM stratigraphic interval.* ***C)*** *Cross-section of the stratigraphic sequences from Paris Basin to southward Jura during the Bajocian (output of ISOPAQ).*

Ammopal

Systematic descriptions of ammonoid faunas are always illustrated with plots depicting the classical shell measurements and their derived ratios for each studied taxon. In order to standardize this kind of output and to automatically generate the various plots, as well as to process uni- and multi-variate analyses of these biometric data, I also programmed a series of scripts called AMMOPAL with the MATLAB language. Although this package has not been published, it has been abundantly used by the ammonoid workers of the PIMUZ team (*Fig 2A–B*; Monnet & Bucher 2005, 2010; Monnet et al 2008; Brühwiler et al 2010a, 2012; Ware et al 2015).

Also, this package contained scripts to compute basic biodiversity analyses of incidence data (taxonomic richness, origination, extinction and turnover rates). This part is also unpublished but has been used for several publications (*Fig 2C*; Monnet et al 2003b; Monnet & Bucher 2006; Monnet 2009; Brühwiler et al 2010b; Ware et al 2015).

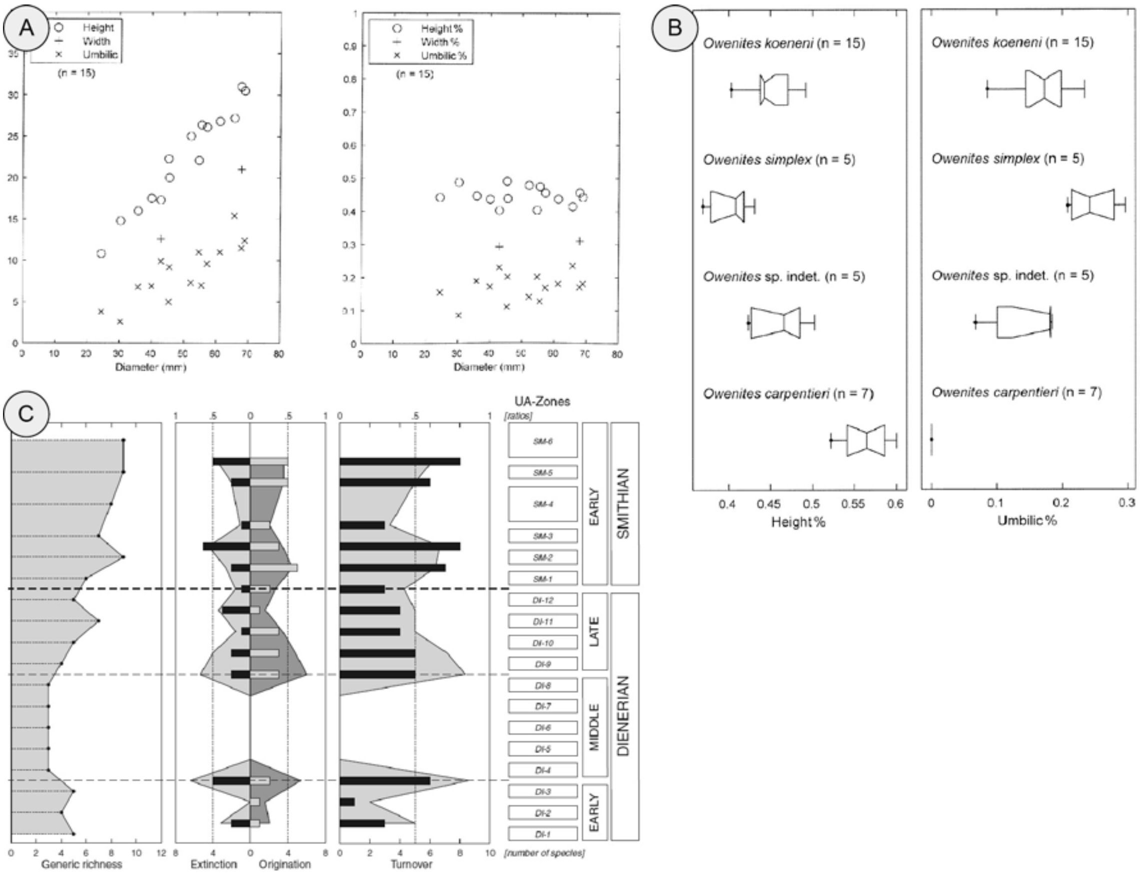


Figure 2 – *AMMOPAL and example applications.* ***A)*** *Scatter diagram of H, W, and U, and of their ratios with D for the Smithian Owenites koeneni (Brühwiler et al 2012).* ***B)*** *Box plots of H/D and U/D for the species of the Smithian* Owenites *(Brühwiler et al 2012).* ***C)*** *Generic richness, origination, extinction and turnover throughout the Dienerian and early Smithian of the Northern Indian Margin (Ware et al 2015).*

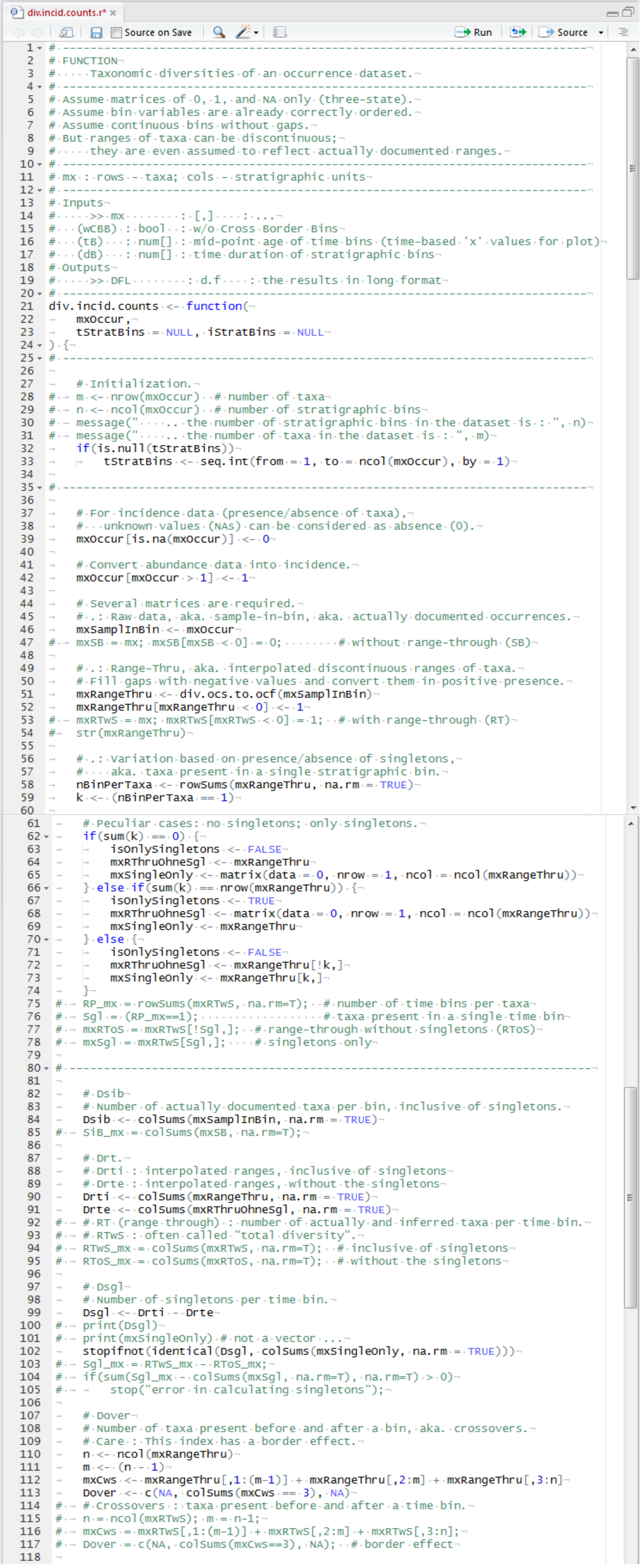
R – THE PACKAGE EPALEO

In paleontology, there is already excellent software to perform a very large variety of uni- to multivariate analyses: PAST (Hammer et al 2001), coupled with the excellent book "*Paleontological data analysis*" (Hammer & Harper 2006). Although this is the software I am using for teaching, this program lacks tools to manage the data, as well as enough control on the settings of the methods, and there are still many methods (especially the recent ones), which are not yet available.

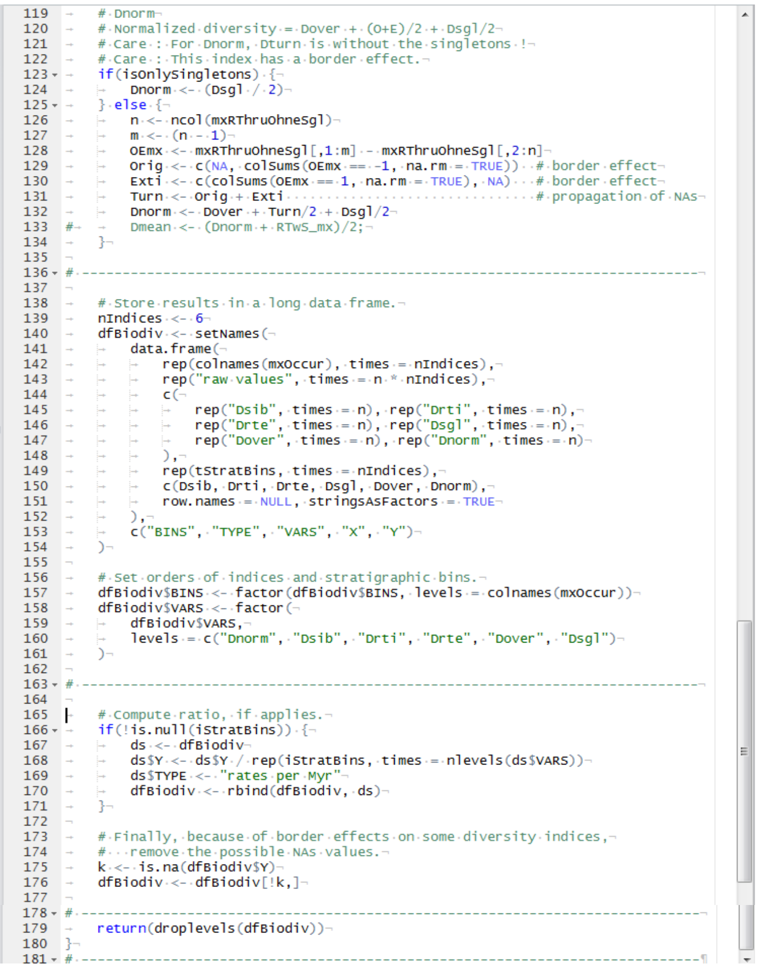
Therefore, since several years, I am using the scientific environment R (https://www.r-project.org/) in order to perform various paleontological data analyses with the settings, which fit the purposes of the processed analyses. R is a user-friendly, open source, flexible computer language, which has recently gained a lot of popularity in academia. Since its release in the mid-1990s, R has become one of the most commonly used statistical environments. Within the field of paleontology, R has become a common tool for a wide range of analyses including: trait evolution (Hunt 2007; Young et al 2011); rates of morphological evolution (Lloyd et al 2012); the quality of the rock record (Benson & Mannion 2012), and geometric morphometrics (Adams & Otarola-Castillo 2013; Arbour & Brown 2014), among others. It has several advantages that make it a valuable statistical package for academics at least. Firstly and importantly it is open source, freely available and supported on UNIX, Mac and Windows operating systems. Secondly, the graphics package within R allows for the creation of publication-quality vector figures that can be quickly and easily changed without the need for fiddling around with other graphics software. To illustrate the popularity and efficiency of R, the *Newsletter* of the British *Palaeontological Association* started to publish a tutorial series on R in paleontology (Bell 2014, and following years), and the journal "*Methods in Ecology and Evolution*" publishes at least one paper describing a new package for R in every issue.

One of the most useful features of R is the package system, allowing users to create libraries of functions for specific purposes ranging from plotting functions to more complex analytical toolkits. Therefore, since several years, I am implementing an R package (unpublished) called EPALEO. This package is a collection of scripts, which are independent functions, devoted each to process a specific task. My collection of functions cover a vast range of paleontological data analyses: from phenetics, over 3D morphometrics, to biodiversity and macroevolutionary trends. Currently the package contains about one hundred functions and about 10 000 lines of commented code (*Fig 3*).

One original aspect of my package is also the development of so-called "vignettes". These are peculiar scripts to output an automatic report of the analysis with the description/interpretation of the processed methods and inclusion of the results and their graphical outputs. Currently the package contains ten vignettes with each about 1 000 lines of code.



```r
# --------------------------------------------------------------------------
# FUNCTION
#     Taxonomic diversities of an occurrence dataset.
# --------------------------------------------------------------------------
# Assume matrices of 0, 1, and NA only (three-state).
# Assume bin variables are already correctly ordered.
# Assume continuous bins without gaps.
# But ranges of taxa can be discontinuous;
#     they are even assumed to reflect actually documented ranges.
# --------------------------------------------------------------------------
# mx : rows - taxa; cols - stratigraphic units
# --------------------------------------------------------------------------
# Inputs
#     >> mx        : [,]    : ...
#   (wCBB) : bool  : w/o Cross Border Bins
#   (tB)   : num[] : mid-point age of time bins (time-based 'x' values for plot)
#   (dB)   : num[] : time duration of stratigraphic bins
# Outputs
#     >> DFL        : d.f    : the results in long format
# --------------------------------------------------------------------------
div.incid.counts <- function(
    mxOccur,
    tStratBins = NULL, iStratBins = NULL
) {
# --------------------------------------------------------------------------

    # Initialization.
#   m <- nrow(mxOccur)  # number of taxa
#   n <- ncol(mxOccur)  # number of stratigraphic bins
#   message("     .. the number of stratigraphic bins in the dataset is : ", n)
#   message("     .. the number of taxa in the dataset is : ", m)
    if(is.null(tStratBins))
        tStratBins <- seq.int(from = 1, to = ncol(mxOccur), by = 1)

# --------------------------------------------------------------------------

    # For incidence data (presence/absence of taxa),
    #   unknown values (NAs) can be considered as absence (0).
    mxOccur[is.na(mxOccur)] <- 0

    # Convert abundance data into incidence.
    mxOccur[mxOccur > 1] <- 1

    # Several matrices are required.
    # .: Raw data, aka. sample-in-bin, aka. actually documented occurrences.
    mxSamplInBin <- mxOccur
#   mxSB = mx; mxSB[mxSB < 0] = 0;        # without range-through (SB)

    # .: Range-Thru, aka. interpolated discontinuous ranges of taxa.
    # Fill gaps with negative values and convert them in positive presence.
    mxRangeThru <- div.ocs.to.ocf(mxSamplInBin)
    mxRangeThru[mxRangeThru < 0] <- 1
#   mxRTwS = mx; mxRTwS[mxRTwS < 0] = 1;  # with range-through (RT)
#   str(mxRangeThru)

    # .: Variation based on presence/absence of singletons,
    #    aka. taxa present in a single stratigraphic bin.
    nBinPerTaxa <- rowSums(mxRangeThru, na.rm = TRUE)
    k <- (nBinPerTaxa == 1)

    # Peculiar cases: no singletons; only singletons.
    if(sum(k) == 0) {
        isOnlySingletons <- FALSE
        mxRThruOhneSgl <- mxRangeThru
        mxSingleOnly <- matrix(data = 0, nrow = 1, ncol = ncol(mxRangeThru))
    } else if(sum(k) == nrow(mxRangeThru)) {
        isOnlySingletons <- TRUE
        mxRThruOhneSgl <- matrix(data = 0, nrow = 1, ncol = ncol(mxRangeThru))
        mxSingleOnly <- mxRangeThru
    } else {
        isOnlySingletons <- FALSE
        mxRThruOhneSgl <- mxRangeThru[!k,]
        mxSingleOnly <- mxRangeThru[k,]
    }
#   RP_mx = rowSums(mxRTwS, na.rm=T);  # number of time bins per taxa
#   Sgl = (RP_mx==1);                  # taxa present in a single time bin
#   mxRToS = mxRTwS[!Sgl,];  # range-through without singletons (RToS)
#   mxSgl = mxRTwS[Sgl,];    # singletons only

# --------------------------------------------------------------------------

    # Dsib
    # Number of actually documented taxa per bin, inclusive of singletons.
    Dsib <- colSums(mxSamplInBin, na.rm = TRUE)
#   SiB_mx = colSums(mxSB, na.rm=T);

    # Drt.
    # Drti : interpolated ranges, inclusive of singletons
    # Drte : interpolated ranges, without the singletons
    Drti <- colSums(mxRangeThru, na.rm = TRUE)
    Drte <- colSums(mxRThruOhneSgl, na.rm = TRUE)
#   # RT (range through) : number of actually and inferred taxa per time bin.
#   # RTwS : often called "total diversity".
#   RTwS_mx = colSums(mxRTwS, na.rm=T);  # inclusive of singletons
#   RToS_mx = colSums(mxRToS, na.rm=T);  # without the singletons

    # Dsgl
    # Number of singletons per time bin.
    Dsgl <- Drti - Drte
#   print(Dsgl)
#   print(mxSingleOnly) # not a vector ...
    stopifnot(identical(Dsgl, colSums(mxSingleOnly, na.rm = TRUE)))
#   Sgl_mx = RTwS_mx - RToS_mx;
#   if(sum(Sgl_mx - colSums(mxSgl, na.rm=T), na.rm=T) > 0)
#       stop("error in calculating singletons");

    # Dover
    # Number of taxa present before and after a bin, aka. crossovers.
    # Care : This index has a border effect.
    n <- ncol(mxRangeThru)
    m <- (n - 1)
    mxCws <- mxRangeThru[,1:(m-1)] + mxRangeThru[,2:m] + mxRangeThru[,3:n]
    Dover <- c(NA, colSums(mxCws == 3), NA)
#   # Crossovers : taxa present before and after a time bin.
#   n = ncol(mxRTwS); m = n-1;
#   mxCws = mxRTwS[,1:(m-1)] + mxRTwS[,2:m] + mxRTwS[,3:n];
#   Dover = c(NA, colSums(mxCws==3), NA);  # border effect

```



```r
    # Dnorm
    # Normalized diversity = Dover + (O+E)/2 + Dsgl/2
    # Care : For Dnorm, Dturn is without the singletons !
    # Care : This index has a border effect.
    if(isOnlySingletons) {
        Dnorm <- (Dsgl / 2)
    } else {
        n <- ncol(mxRThruOhneSgl)
        m <- (n - 1)
        OEmx <- mxRThruOhneSgl[,1:m] - mxRThruOhneSgl[,2:n]
        Orig <- c(NA, colSums(OEmx == -1, na.rm = TRUE))  # border effect
        Exti <- c(colSums(OEmx == 1, na.rm = TRUE), NA)   # border effect
        Turn <- Orig + Exti                               # propagation of NAs
        Dnorm <- Dover + Turn/2 + Dsgl/2
#       Dmean <- (Dnorm + RTwS_mx)/2;
    }

# ----------------------------------------------------------------------------

    # Store results in a long data frame.
    nIndices <- 6
    dfBiodiv <- setNames(
        data.frame(
            rep(colnames(mxOccur), times = nIndices),
            rep("raw values", times = n * nIndices),
            c(
                rep("Dsib", times = n), rep("Drti", times = n),
                rep("Drte", times = n), rep("Dsgl", times = n),
                rep("Dover", times = n), rep("Dnorm", times = n)
            ),
            rep(tStratBins, times = nIndices),
            c(Dsib, Drti, Drte, Dsgl, Dover, Dnorm),
            row.names = NULL, stringsAsFactors = TRUE
        ),
        c("BINS", "TYPE", "VARS", "X", "Y")
    )

    # Set orders of indices and stratigraphic bins.
    dfBiodiv$BINS <- factor(dfBiodiv$BINS, levels = colnames(mxOccur))
    dfBiodiv$VARS <- factor(
        dfBiodiv$VARS,
        levels = c("Dnorm", "Dsib", "Drti", "Drte", "Dover", "Dsgl")
    )

# ----------------------------------------------------------------------------

    # Compute ratio, if applies.
    if(!is.null(iStratBins)) {
        ds <- dfBiodiv
        ds$Y <- ds$Y / rep(iStratBins, times = nlevels(ds$VARS))
        ds$TYPE <- "rates per Myr"
        dfBiodiv <- rbind(dfBiodiv, ds)
    }

    # Finally, because of border effects on some diversity indices,
    #   remove the possible NAs values.
    k <- is.na(dfBiodiv$Y)
    dfBiodiv <- dfBiodiv[!k,]

# ----------------------------------------------------------------------------
    return(droplevels(dfBiodiv))
}
# ----------------------------------------------------------------------------
```

***Figure 3 –** The R package EPALEO: script of one function of the package.*

Although my package EPALEO is not yet published, quantitative analyses of paleontological data (not only ammonoids) performed using this package have already been published and for various topics (taxonomy and variation: Monnet et al 2013; De Baets et al 2013; Colpaert et al 2015; Jattiot et al 2016; biodiversity: Nowak et al 2015; community analysis: Maillet et al 2013; Tetard et al 2015; Amberg et al 2016). Other tools are already available in my package and concern biogeography, cenograms, 3D morphometrics (*Fig 4*), and macroevolutionary trends (Monnet et al 2011a), among others.

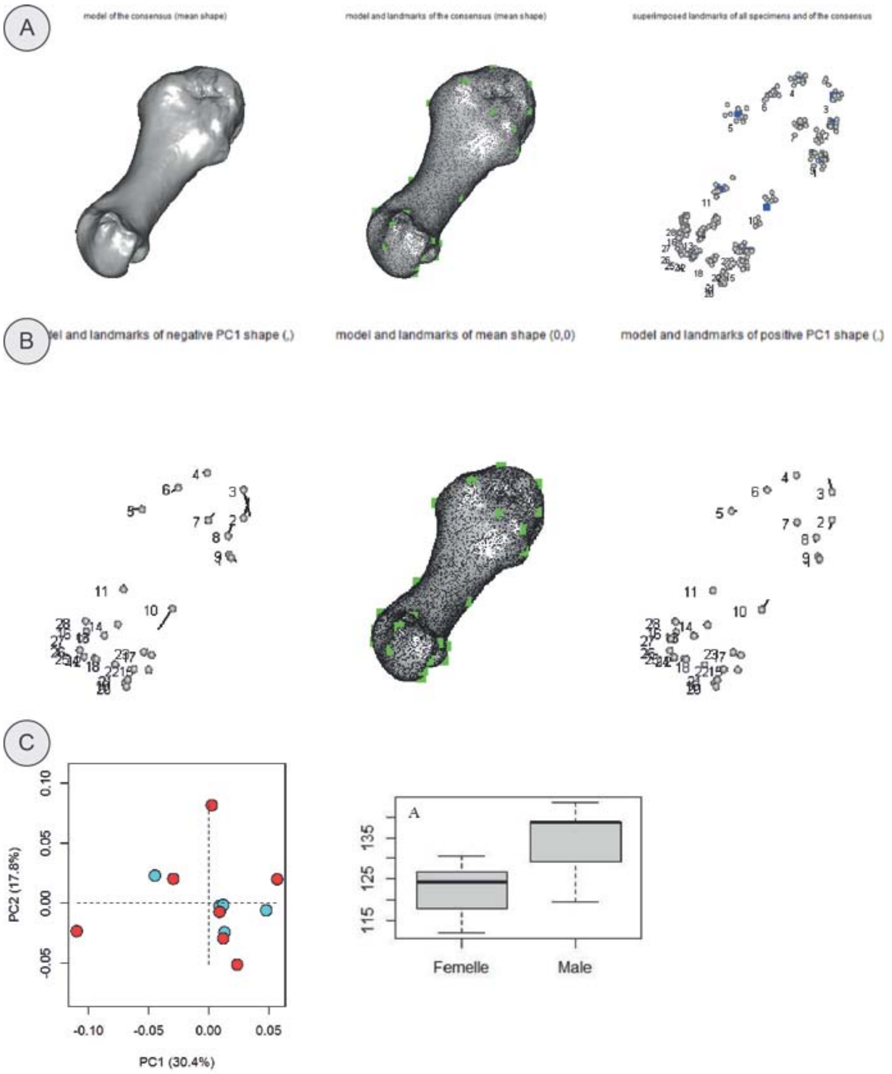


Figure 4 – *Example outputs of a 3D morphometric analysis of* Ursus *metacarpials with the R package EPALEO (Auguste et al, in prep).* ***A)*** *The model and landmarks of the consensus.* ***B)*** *Vector maps of the landmarks along the first principal component.* ***C)*** *Comparison of males and females with regard to shape (left) and centroid size (right).*

One example report (still under construction for some parts) is reproduced afterwards. It concerns the analysis of biodiversity of an incidence dataset of Silurian radiolarians (Tetard et al, in prep).

Biodiversity : Taxonomic : Incidence

Claude Monnet (University of Lille, France)

Fri Sep 09 17:20:43 2016

> **EPALEO - PALEONTOLOGICAL DATA ANALYSIS with R**
> (Copyright © Claude Monnet, University of Lille, France)

1 Taxonomic Biodiversity Analysis of Incidence Data

PURPOSE.- Describe and depict various indices of taxonomic diversity of a time-ordered chronostratigraphic occurrence matrix reconstructed from incidence/abundance of taxa within samples.

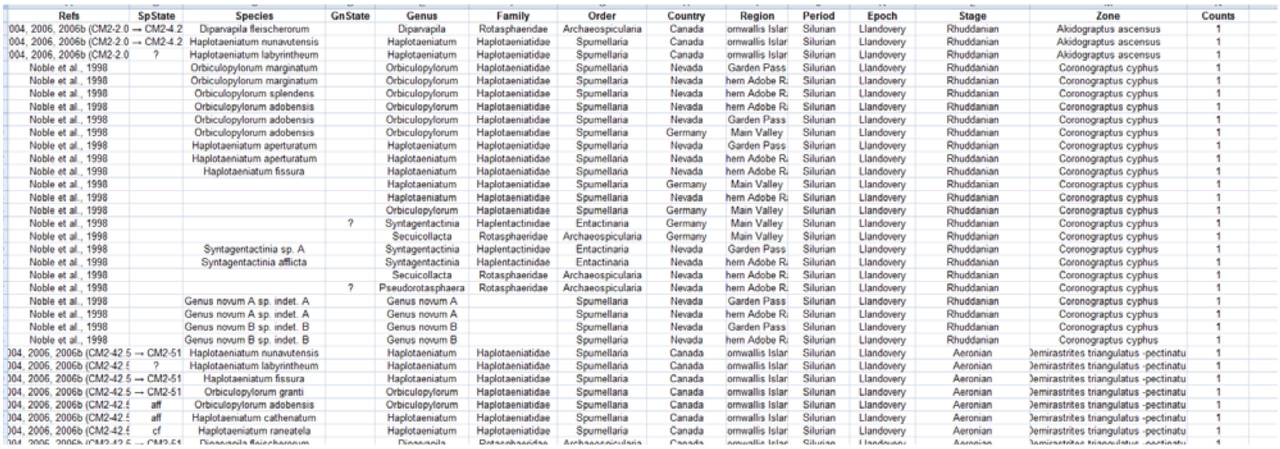
COMMENTS.-

- Biodiversity. Very large meaning. Multiple indices. Here, focus on indices based on taxonomy.
- There are numerous studies that evaluate biodiversity estimators. Unfortunately, no estimator performs well in all situations.

2 Set the Data and the Report

PURPOSE.- Load, check, process and save the data in an adapted format for subsequent analyses. Initially, the data must be stored in a main sample-based datafile. Also, this part outputs the list of variables and their levels (*list of the different values for categorical variables*). The user must carefully read how the data are treated and agree with these options. Text files with a 'log' extension are saved frequently in order to help the user in this task.

MAIN SAMPLE-based DATAFILE.- Matrix (*aka. 2D-array, table, or wide data frame*) of numeric or categorical values of variables/parameters /factors (*in columns*) for observations characterizing samples (*in rows*). Typical dataset: an occurrence matrix (*counts of taxa in samples*). These data are read from a text-based datafile (*tab- or comma-delimited; '.TXT' or '.CSV', respectively*). The content and format of this datafile must respect the following constraints. The names of variables must be unique and in the first row. Columns of variables can contain numeric or categorical values. Unknwon values are left empty. Decimal values are marked by a dot. Use preferentially only base characters (*a, …, z*) and avoid special characters (*e.g., " ' / : ! ? , ; **); also, avoid accents and white spaces, especially for column names.



Refs	SpState	Species	GnState	Genus	Family	Order	Country	Region	Period	Epoch	Stage	Zone	Counts
004, 2006, 2006b (CM2-2.0	→ CM2-4.2	Diparvapila fleischerorum		Diparvapila	Rotasphaeridae	Archaeospicularia	Canada	ornwallis Islar	Silurian	Llandovery	Rhuddanian	Akidograptus ascensus	1
004, 2006, 2006b (CM2-2.0	→ CM2-4.2	Haplotaeniatum nunavutensis		Haplotaeniatum	Haplotaeniatidae	Spumellaria	Canada	ornwallis Islar	Silurian	Llandovery	Rhuddanian	Akidograptus ascensus	1
004, 2006, 2006b (CM2-2.0	?	Haplotaeniatum labyrintheum		Haplotaeniatum	Haplotaeniatidae	Spumellaria	Canada	ornwallis Islar	Silurian	Llandovery	Rhuddanian	Akidograptus ascensus	1
Noble et al., 1998		Orbiculopylorum marginatum		Orbiculopylorum	Haplotaeniatidae	Spumellaria	Nevada	Garden Pass	Silurian	Llandovery	Rhuddanian	Coronograptus cyphus	1
Noble et al., 1998		Orbiculopylorum marginatum		Orbiculopylorum	Haplotaeniatidae	Spumellaria	Nevada	hem Adobe R	Silurian	Llandovery	Rhuddanian	Coronograptus cyphus	1
Noble et al., 1998		Orbiculopylorum splendens		Orbiculopylorum	Haplotaeniatidae	Spumellaria	Nevada	hem Adobe R	Silurian	Llandovery	Rhuddanian	Coronograptus cyphus	1
Noble et al., 1998		Orbiculopylorum adobensis		Orbiculopylorum	Haplotaeniatidae	Spumellaria	Nevada	hem Adobe R	Silurian	Llandovery	Rhuddanian	Coronograptus cyphus	1
Noble et al., 1998		Orbiculopylorum adobensis		Orbiculopylorum	Haplotaeniatidae	Spumellaria	Nevada	Garden Pass	Silurian	Llandovery	Rhuddanian	Coronograptus cyphus	1
Noble et al., 1998		Orbiculopylorum adobensis		Orbiculopylorum	Haplotaeniatidae	Spumellaria	Germany	Main Valley	Silurian	Llandovery	Rhuddanian	Coronograptus cyphus	1
Noble et al., 1998		Haplotaeniatum aperturatum		Haplotaeniatum	Haplotaeniatidae	Spumellaria	Nevada	Garden Pass	Silurian	Llandovery	Rhuddanian	Coronograptus cyphus	1
Noble et al., 1998		Haplotaeniatum aperturatum		Haplotaeniatum	Haplotaeniatidae	Spumellaria	Nevada	hem Adobe R	Silurian	Llandovery	Rhuddanian	Coronograptus cyphus	1
Noble et al., 1998		Haplotaeniatum fissura		Haplotaeniatum	Haplotaeniatidae	Spumellaria	Nevada	hem Adobe R	Silurian	Llandovery	Rhuddanian	Coronograptus cyphus	1
Noble et al., 1998				Haplotaeniatum	Haplotaeniatidae	Spumellaria	Germany	Main Valley	Silurian	Llandovery	Rhuddanian	Coronograptus cyphus	1
Noble et al., 1998				Haplotaeniatum	Haplotaeniatidae	Spumellaria	Nevada	hem Adobe R	Silurian	Llandovery	Rhuddanian	Coronograptus cyphus	1
Noble et al., 1998				Orbiculopylorum	Haplotaeniatidae	Spumellaria	Germany	Main Valley	Silurian	Llandovery	Rhuddanian	Coronograptus cyphus	1
Noble et al., 1998			?	Syntagentactinia	Haplentactinidae	Entactinaria	Germany	Main Valley	Silurian	Llandovery	Rhuddanian	Coronograptus cyphus	1
Noble et al., 1998				Secuicollacta	Rotasphaeridae	Archaeospicularia	Germany	Main Valley	Silurian	Llandovery	Rhuddanian	Coronograptus cyphus	1
Noble et al., 1998		Syntagentactinia sp. A		Syntagentactinia	Haplentactinidae	Entactinaria	Nevada	Garden Pass	Silurian	Llandovery	Rhuddanian	Coronograptus cyphus	1
Noble et al., 1998		Syntagentactinia afflicta		Syntagentactinia	Haplentactinidae	Entactinaria	Nevada	hem Adobe R	Silurian	Llandovery	Rhuddanian	Coronograptus cyphus	1
Noble et al., 1998				Secuicollacta	Rotasphaeridae	Archaeospicularia	Nevada	hem Adobe R	Silurian	Llandovery	Rhuddanian	Coronograptus cyphus	1
Noble et al., 1998			?	Pseudorotasphaera	Rotasphaeridae	Archaeospicularia	Nevada	hem Adobe R	Silurian	Llandovery	Rhuddanian	Coronograptus cyphus	1
Noble et al., 1998		Genus novum A sp. indet. A		Genus novum A		Spumellaria	Nevada	Garden Pass	Silurian	Llandovery	Rhuddanian	Coronograptus cyphus	1
Noble et al., 1998		Genus novum A sp. indet. A		Genus novum A		Spumellaria	Nevada	hem Adobe R	Silurian	Llandovery	Rhuddanian	Coronograptus cyphus	1
Noble et al., 1998		Genus novum B sp. indet. B		Genus novum B		Spumellaria	Nevada	Garden Pass	Silurian	Llandovery	Rhuddanian	Coronograptus cyphus	1
Noble et al., 1998		Genus novum B sp. indet. B		Genus novum B		Spumellaria	Nevada	hem Adobe R	Silurian	Llandovery	Rhuddanian	Coronograptus cyphus	1
04, 2006, 2006b (CM2-42.5	→ CM2-51	Haplotaeniatum nunavutensis		Haplotaeniatum	Haplotaeniatidae	Spumellaria	Canada	ornwallis Islar	Silurian	Llandovery	Aeronian	emirastrites triangulatus -pectinatu	1
04, 2006, 2006b (CM2-42.5	?	Haplotaeniatum labyrintheum		Haplotaeniatum	Haplotaeniatidae	Spumellaria	Canada	ornwallis Islar	Silurian	Llandovery	Aeronian	emirastrites triangulatus -pectinatu	1
04, 2006, 2006b (CM2-42.5	→ CM2-51	Haplotaeniatum fissura		Haplotaeniatum	Haplotaeniatidae	Spumellaria	Canada	ornwallis Islar	Silurian	Llandovery	Aeronian	emirastrites triangulatus -pectinatu	1
04, 2006, 2006b (CM2-42.5	→ CM2-51	Orbiculopylorum granti		Orbiculopylorum	Haplotaeniatidae	Spumellaria	Canada	ornwallis Islar	Silurian	Llandovery	Aeronian	emirastrites triangulatus -pectinatu	1
04, 2006, 2006b (CM2-42.5	aff	Orbiculopylorum adobensis		Orbiculopylorum	Haplotaeniatidae	Spumellaria	Canada	ornwallis Islar	Silurian	Llandovery	Aeronian	emirastrites triangulatus -pectinatu	1
04, 2006, 2006b (CM2-42.5	aff	Haplotaeniatum cathenatum		Haplotaeniatum	Haplotaeniatidae	Spumellaria	Canada	ornwallis Islar	Silurian	Llandovery	Aeronian	emirastrites triangulatus -pectinatu	1
04, 2006, 2006b (CM2-42.5	cf	Haplotaeniatum raneatela		Haplotaeniatum	Haplotaeniatidae	Spumellaria	Canada	ornwallis Islar	Silurian	Llandovery	Aeronian	emirastrites triangulatus -pectinatu	1
04, 2006, 2006b (CM2-42.5	→ CM2-51	Diparvapila fleischerorum		Diparvapila	Rotasphaeridae	Archaeospicularia	Canada	ornwallis Islar	Silurian	Llandovery	Aeronian	emirastrites triangulatus -pectinatu	1

FIGURE : Preview of a typical sample-based dataset.

WARNING.- …

SETTINGS.- Computing environment (EV) : Data basename = ***Rad.Silur.2016.09.09.MT***. Mandatory parameters (AG) : Taxonomic rank of the analysis : ***Species***; Chronostratigraphic interval to focus on : ***Stage, Rhuddanian, Pridoli stage*** Variable containing groups to compare =

Country. Vignette options (AG) : Triplet used to filter data = ***n/a***; Hierarchical classification = ***no***.

- Option of the vignette : A **‘group’** variable will be considered if indicated. This categorical variable will be used to subset the dataset into smaller datasets (e.g., if the analysis need to be performed independently for different regions), which will be analyzed separately.
- A chronostratigraphic chart must be provided, and without gaps.

TODO : rm empty cells of ‘Counts’ ? and zero values ? yes

assume a ID and COUNT columns ?

- Currently, samples with unknown values are removed from the dataset.

!!! lines with NAs and 0s of ‘Count’ and sRank are removed !!!

! warning. - Species must be labelled with their Linnaean binomial !

A chronostratigraphic chart must be provided, *and without gaps*.

assume a basename.myr file

assume a column named Type, one named Base, and another one named Duration, and a first one named Name

data are subset by groups ; a margin is automatically added

!!! ASSUME and CONVERT to CONTINUOUS BINS (absence of gaps) !!!

CURRENTLY, abundance data are automatically converted to incidence (within ‘ocm.to.ocs’)

Convert the data into expected format: from sample-based abundance/properties matrix to taxon-based stratigraphic-bins matrix. Then, identify stratigraphic gaps in the dataset(s) and reshape them in consequence.

TODO : check if the generic process has deleted some levels of the evaluated factors

```
DATA - LOAD THE MAIN DATASET
    .. Rad.Silur.2016.09.09.MT <DFW>
        .. number of rows (observations)    : 459 (complete: 0; ca. 0 %)
        .. number of columns (variables)    : 16
        .. number of missing values (cells) : 1220 (among 7344; ca. 16.6 %)
    .. classes/types of the variables in the dataset
        .. variables of type 'FACTOR'  : 15 : Ref, Sample, Region, Country, Zone, Stage, Epoch, Period, Species, S
pecies.Origin, Species.State, Genus, GnState, Family, Order
        .. variables of type 'NUMERIC' : 1 : Count
        .. variables of other type(s)  : 0
```

```
               Ref Sample         Region    Country                 Zone    Stage  Epoch   Period Count
1 Amon et al. 1995   <NA> Southern Urals Kazakhstan Lobograptus scanicus Gorstian Ludlow Silurian     1
2 Amon et al. 1995   <NA> Southern Urals Kazakhstan Lobograptus scanicus Gorstian Ludlow Silurian     1
3 Amon et al. 1995   <NA> Southern Urals Kazakhstan Lobograptus scanicus Gorstian Ludlow Silurian     1
4 Amon et al. 1995   <NA> Southern Urals Kazakhstan Lobograptus scanicus Gorstian Ludlow Silurian     1
5 Amon et al. 1995   <NA> Southern Urals Kazakhstan Lobograptus scanicus Gorstian Ludlow Silurian     1
6 Amon et al. 1995   <NA> Southern Urals Kazakhstan Lobograptus scanicus Gorstian Ludlow Silurian     1
                       Species            Species.Origin Species.State             Genus GnState
1     Labyrinthosphaera lancia  Labyrinthosphaera lancia          <NA> Labyrinthosphaera    <NA>
2          Secuicollacta cassa       Secuicollacta cassa          <NA>     Secuicollacta    <NA>
3    Palaeoephippium echinatum Palaeoephippium echinatum          <NA>   Palaeoephippium    <NA>
4      Palaeoephippium radices   Palaeoephippium radices          <NA>   Palaeoephippium    <NA>
5     Palaeoephippium bifurcum  Palaeoephippium bifurcum          <NA>   Palaeoephippium    <NA>
6 Palaeoscenidium rarispinosum   Goodbodium rarispinosum          <NA>        Goodbodium    <NA>
             Family             Order
1  Haplotaeniatidae       Spumellaria
2    Rotasphaeridae Archaeospicularia
3 Palaeoscenidiidae      Entactinaria
4 Palaeoscenidiidae      Entactinaria
5 Palaeoscenidiidae      Entactinaria
6 Palaeoscenidiidae      Entactinaria
```

```
DATA - GENERIC PROCESS
    .. filter dataset
        .. n/a
    .. report names of all variables for manual checking (see log files)
            .. Rad.Silur.2016.09.09.MT-Names.of.Factors.log
            .. Rad.Silur.2016.09.09.MT-Names.of.Numerics.log
    .. report levels of categorical variables for checking (see log files)
            .. Rad.Silur.2016.09.09.MT-Levels.of.Ref.log
            .. Rad.Silur.2016.09.09.MT-Levels.of.Sample.log
            .. Rad.Silur.2016.09.09.MT-Levels.of.Region.log
            .. Rad.Silur.2016.09.09.MT-Levels.of.Country.log
            .. Rad.Silur.2016.09.09.MT-Levels.of.Zone.log
            .. Rad.Silur.2016.09.09.MT-Levels.of.Stage.log
            .. Rad.Silur.2016.09.09.MT-Levels.of.Epoch.log
            .. Rad.Silur.2016.09.09.MT-Levels.of.Period.log
            .. Rad.Silur.2016.09.09.MT-Levels.of.Species.log
            .. Rad.Silur.2016.09.09.MT-Levels.of.Species.Origin.log
            .. Rad.Silur.2016.09.09.MT-Levels.of.Species.State.log
            .. Rad.Silur.2016.09.09.MT-Levels.of.Genus.log
            .. Rad.Silur.2016.09.09.MT-Levels.of.GnState.log
            .. Rad.Silur.2016.09.09.MT-Levels.of.Family.log
            .. Rad.Silur.2016.09.09.MT-Levels.of.Order.log
    .. remove rows with unknown values (NA) for indicated variables
        .. variable in focus : Country
            .. YES : all rows are without NAs
        .. variable in focus : Count
            .. NO : some rows have NAs : 1 : these rows are removed (see log file)
            .. Rad.Silur.2016.09.09.MT-Rows.w.NAs.for.Count.log
        .. variable in focus : Species
            .. NO : some rows have NAs : 49 : these rows are removed (see log file)
            .. Rad.Silur.2016.09.09.MT-Rows.w.NAs.for.Species.log
        .. variable in focus : Stage
            .. YES : all rows are without NAs
    .. remove rows with values of zero (0) for indicated variables
        .. variable in focus : Count
            .. YES : all rows are without 0s
    .. save processed dataset in wide format
            .. Rad.Silur.2016.09.09.MT-DFW.dat
```

```
'data.frame':   409 obs. of  16 variables:
 $ Ref           : Factor w/ 20 levels "Amon et al. 1995",..: 1 1 1 1 1 1 1 1 1 1 ...
 $ Sample        : Factor w/ 20 levels "CM2-106.5 to CM2-107.0",..: NA NA NA NA NA NA NA NA NA NA ...
 $ Region        : Factor w/ 14 levels "Brittany","Canadian Arctic archipelago",..: 13 13 13 13 13 13 13 13 13 13
...
 $ Country       : Factor w/ 10 levels "Alaska","Canada",..: 7 7 7 7 7 7 7 7 7 7 ...
 $ Zone          : Factor w/ 21 levels "Akidograptus ascensus",..: 10 10 10 10 10 10 10 10 10 10 ...
 $ Stage         : Factor w/ 8 levels "Aeronian","Gorstian",..: 2 2 2 2 2 2 2 2 2 2 ...
 $ Epoch         : Factor w/ 4 levels "Llandovery","Ludlow",..: 2 2 2 2 2 2 2 2 2 2 ...
 $ Period        : Factor w/ 1 level "Silurian": 1 1 1 1 1 1 1 1 1 1 ...
 $ Count         : int  1 1 1 1 1 1 1 1 1 1 ...
 $ Species       : Factor w/ 161 levels "Bipylospongia rudosa",..: 51 118 77 83 76 91 88 3 42 84 ...
 $ Species.Origin: Factor w/ 166 levels "Bipylospongia rudosa",..: 61 129 83 89 82 34 32 4 51 90 ...
 $ Species.State : Factor w/ 3 levels "?","aff","cf": NA NA NA NA NA NA NA NA NA 3 ...
 $ Genus         : Factor w/ 51 levels "Bipylospongia",..: 27 47 33 33 33 16 16 3 20 33 ...
 $ GnState       : Factor w/ 1 level "?": NA NA NA NA NA NA NA NA NA NA ...
 $ Family        : Factor w/ 9 levels "Ceratoikiscidae",..: 4 8 7 7 7 7 7 1 1 7 ...
 $ Order         : Factor w/ 4 levels "Albaillellaria",..: 4 2 3 3 3 3 3 1 1 3 ...
```

```
DATA - APPEND CHRONOSTRAT
    .. load the chronostratigraphic dataset <CST$dfChron> ..
        .. Rad.Silur.2016.09.09.MT.myr
        .. number of rows (observations)    : 42 (complete: 42; ca. 100 %)
        .. number of columns (variables)    : 4
        .. number of missing values (cells) : 0 (among 168; ca. 0 %)
    .. recall the chronostratigraphic constraints <AG$Chronos> ..
        .. Stage, Rhuddanian, Pridoli stage
    .. extract the chronostratigraphic scale and units to focus on <CST$dfFocus> ..
        .. Stage : 8 units : Rhuddanian, Aeronian, Telychian, Sheinwoodian, Homerian, Gorstian, Ludfordian, Pridol
i stage
    .. set time limits to constrain future outputs <CST$iLimits> ..
        .. [-443.8, -419.2]
    .. filter the main dataset to include only the selected stratigraphic units <DFW>
        .. selected rows : 409 of 409
    .. merge the main- and the chronostratigraphic- datasets <DFW>
    .. set back original order of 'stratigraphic units' <DFW>
```

```
'data.frame':   42 obs. of  4 variables:
 $ Name    : Factor w/ 42 levels "Aeronian","Akidograptus ascensus",..: 37 14 42 17 31 34 1 41 36 12 ...
 $ Type    : Factor w/ 4 levels "Epoch","Period",..: 2 1 1 1 1 3 3 3 3 3 ...
 $ Lower   : num  -444 -444 -433 -427 -423 ...
 $ Duration: num  24.6 10.4 6 4.4 3.8 3 2.3 5.1 2.9 3.1 ...
```

```
'data.frame':   409 obs. of  20 variables:
 $ Stage        : Factor w/ 8 levels "Rhuddanian","Aeronian",..: 2 2 2 2 2 2 2 2 2 2 ...
 $ Ref          : Factor w/ 20 levels "Amon et al. 1995",..: 8 8 8 8 8 8 16 16 8 8 ...
 $ Sample       : Factor w/ 20 levels "CM2-106.5 to CM2-107.0",..: 3 3 3 3 3 3 10 10 3 3 ...
 $ Region       : Factor w/ 14 levels "Brittany","Canadian Arctic archipelago",..: 3 3 3 3 3 3 1 1 3 3 ...
 $ Country      : Factor w/ 10 levels "Alaska","Canada",..: 2 2 2 2 2 2 4 4 2 2 ...
 $ Zone         : Factor w/ 21 levels "Akidograptus ascensus",..: 7 7 7 7 7 7 8 8 7 7 ...
 $ Epoch        : Factor w/ 4 levels "Llandovery","Ludlow",..: 1 1 1 1 1 1 1 1 1 1 ...
 $ Period       : Factor w/ 1 level "Silurian": 1 1 1 1 1 1 1 1 1 1 ...
 $ Count        : int  1 1 1 1 1 1 1 1 1 1 ...
 $ Species      : Factor w/ 161 levels "Bipylospongia rudosa",..: 28 35 34 60 59 33 133 117 8 10 ...
 $ Species.Origin: Factor w/ 166 levels "Bipylospongia rudosa",..: 46 44 43 67 66 42 141 128 9 11 ...
 $ Species.State : Factor w/ 3 levels "?","aff","cf": 3 1 NA NA 2 2 NA NA NA NA ...
 $ Genus        : Factor w/ 51 levels "Bipylospongia",..: 19 19 19 29 29 19 47 47 5 5 ...
 $ GnState      : Factor w/ 1 level "?": NA NA NA NA NA NA NA NA NA NA ...
 $ Family       : Factor w/ 9 levels "Ceratoikiscidae",..: 4 4 4 4 4 4 8 8 8 8 ...
 $ Order        : Factor w/ 4 levels "Albaillellaria",..: 4 4 4 4 4 4 2 2 2 2 ...
 $ Lower        : num  -441 -441 -441 -441 -441 ...
 $ Duration     : num  2.3 2.3 2.3 2.3 2.3 2.3 2.3 2.3 2.3 2.3 ...
 $ Upper        : num  -438 -438 -438 -438 -438 ...
 $ Mid          : num  -440 -440 -440 -440 -440 ...
```

```
     Stage                        Ref               Sample            Region Country
1 Aeronian MacDonald 2004 2006a 2006b CM2-42.5 to CM2-51.2 Cornwallis Island  Canada
2 Aeronian MacDonald 2004 2006a 2006b CM2-42.5 to CM2-51.2 Cornwallis Island  Canada
3 Aeronian MacDonald 2004 2006a 2006b CM2-42.5 to CM2-51.2 Cornwallis Island  Canada
4 Aeronian MacDonald 2004 2006a 2006b CM2-42.5 to CM2-51.2 Cornwallis Island  Canada
5 Aeronian MacDonald 2004 2006a 2006b CM2-42.5 to CM2-51.2 Cornwallis Island  Canada
6 Aeronian MacDonald 2004 2006a 2006b CM2-42.5 to CM2-51.2 Cornwallis Island  Canada
                                     Zone      Epoch   Period Count                     Species
1 Demirastrites triangulatus <U+0096> pectinatus Llandovery Silurian     1       Gyrosphaera raneatela
2 Demirastrites triangulatus <U+0096> pectinatus Llandovery Silurian     1 Haplotaeniatum labyrintheum
3 Demirastrites triangulatus <U+0096> pectinatus Llandovery Silurian     1      Haplotaeniatum fissura
4 Demirastrites triangulatus <U+0096> pectinatus Llandovery Silurian     1      Orbiculopylorum granti
5 Demirastrites triangulatus <U+0096> pectinatus Llandovery Silurian     1   Orbiculopylorum adobensis
6 Demirastrites triangulatus <U+0096> pectinatus Llandovery Silurian     1   Haplotaeniatum cathenatum
               Species.Origin Species.State           Genus GnState           Family       Order  Lower
1    Haplotaeniatum raneatela            cf  Haplotaeniatum    <NA> Haplotaeniatidae Spumellaria -440.8
2 Haplotaeniatum labyrintheum             ?  Haplotaeniatum    <NA> Haplotaeniatidae Spumellaria -440.8
3      Haplotaeniatum fissura          <NA>  Haplotaeniatum    <NA> Haplotaeniatidae Spumellaria -440.8
4      Orbiculopylorum granti          <NA> Orbiculopylorum    <NA> Haplotaeniatidae Spumellaria -440.8
5   Orbiculopylorum adobensis           aff Orbiculopylorum    <NA> Haplotaeniatidae Spumellaria -440.8
6   Haplotaeniatum cathenatum           aff  Haplotaeniatum    <NA> Haplotaeniatidae Spumellaria -440.8
  Duration  Upper     Mid
1      2.3 -438.5 -439.65
2      2.3 -438.5 -439.65
3      2.3 -438.5 -439.65
4      2.3 -438.5 -439.65
5      2.3 -438.5 -439.65
6      2.3 -438.5 -439.65
```

```
DATA - FINALIZATION
    .. save processed dataset in wide format <DFW>
            .. Rad.Silur.2016.09.09.MT-DFW.dat
    .. subset the data by groups <DFS>
        .. [Country]: 10 : Alaska, Canada, England, France, Germany, Japan, Kazakhstan, Nevada, Sweden, Texas
    .. recover the stratigraphic range of the subset(s) <CST$dfRanges>
    .. and re-order groups by stratigraphic completeness
        .. [Country]: 11 : COUNTRY, Canada, Japan, Texas, Sweden, Alaska, England, France, Germany, Kazakhstan, Ne
vada
        .. [completeness]: 8, 1, 6, 1, 1, 1, 3, 1, 1, 2, 3
    .. keep only groups with an enough complete record (>= 50%)
        .. COUNTRY, Canada
    .. convert data from sample-based to taxon-based stratigraphic-units <DFT>
        .. for 2 groups : COUNTRY, Canada
```

```
List of 2
 $ COUNTRY:'data.frame':    409 obs. of  20 variables:
 $ Canada :'data.frame':    193 obs. of  20 variables:
'data.frame':   16 obs. of  3 variables:
 $ Group: Factor w/ 2 levels "COUNTRY","Canada": 1 1 1 1 1 1 1 1 2 2 ...
 $ Strat: Factor w/ 8 levels "Rhuddanian","Aeronian",..: 1 2 3 4 5 6 7 8 1 2 ...
 $ X    : num  1 1 1 1 1 1 1 1 1 1 ...
```

3 Stratigraphic Occurrences

PURPOSE.- Investigate data distribution and properties.

TODO : order taxa by FAD and group them by families/orders TODO : add bubble maps TODO : add refs ranges

```
STRATIGRAPHIC OCCURRENCES
```

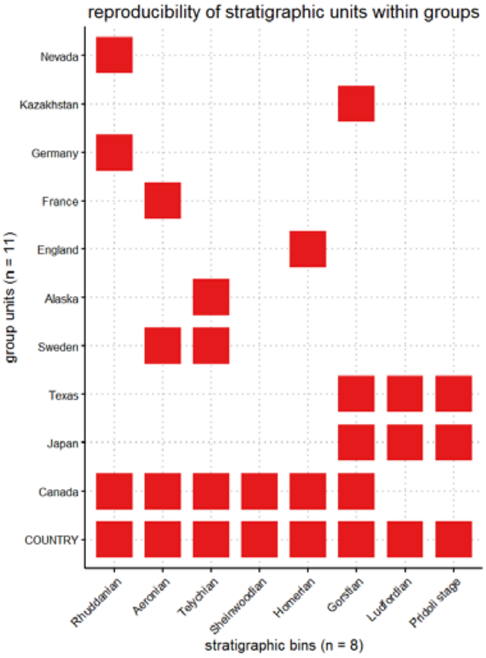


FIGURE : Reproducibility of stratigraphic units within groups.

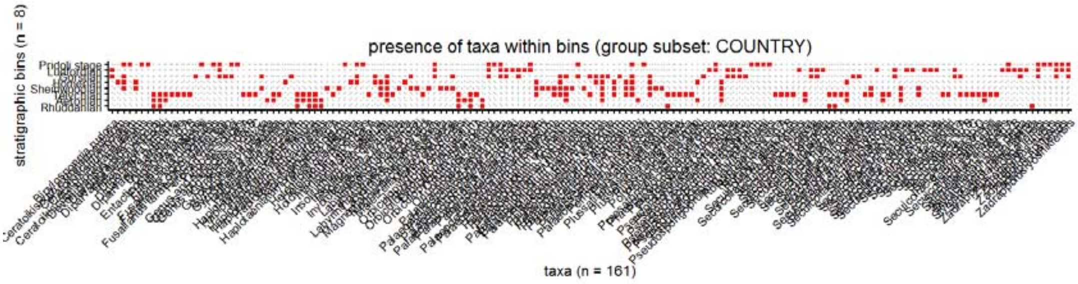


FIGURE : Presence of taxa within stratigraphic bins.

4 Taxonomic Richness

PURPOSE.-

- Available estimates on the trajectories of diversities are based on a taxic approach, that is, they count the distinct names of a specific taxonomic rank (e.g. species, genera, families) irrespective of their phylogenetic relationships. These estimates are thus coined as 'taxonomic richness' indices.

- Taxonomic richness is here presented by classic biodiversity curves against the succession of studied time-ordered stratigraphic intervals (e.g. samples, beds, assemblages, biozones, stages). The goal is to produce reliable trajectories of biodiversity through time close to the true diversity in a given time (aka. the 'standing diversity').

METHODS.- Diversity through time can be measured in several ways, and especially differently for incidence (presence/absence of taxa) and abundance (counts of individuals within taxa) data. For incidence data, the most commonly used indices are:

- "Sampled in Bin" (Dsib) : the most straightforward method, which just counts every taxa in a given time/stratigraphic interval/bin (thus, inclusive of singletons).
- "Singletons" (Dsgl) : singletons are taxa known from only one bin. Due to potential biases (e.g., exceptional preservation and/or sampling size), these can be included or excluded in other diversity indices (see below).
- "Range-Through" (Drt.) : the traditional method, which estimates diversity from counting everything that is known to occur in an interval (e.g. first and last occurrences) plus everything that is inferred to be present (Difr) (e.g. recorded before and after the considered stratigraphic interval). With this approach, singletons can be included (Drti) or excluded (Drte), the former being known also as 'total diversity'. $Drti = Drte + Dsgl$ $Drti = Dsib + Difr$
- "Crossovers" (Dover) : the number of taxa that are knwon before and after the considered stratigraphic interval.
- "Normalized diversity" (Sepkoski 1975) (Dnorm) : sum of species that range from the interval below to the interval above, plus half the number of species that originate and/or become extinct within the interval, plus half of those that are confined to the interval itself.

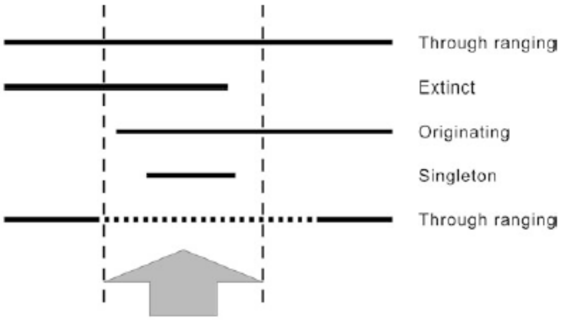


FIG.- .

COMMENTS.-

- Singletons : these can be either genuinely short-lived taxa or represent artefacts (e.g. monographic, preservational). In the context of global diversity studies, singletons are usually omitted because the artifactual patterns are thought to prevail (Pease 1985; Alroy 1998; Foote 2000). Even if a singleton represented a biological reality its inclusion would tell us little about standing diversity within an interval, that is, the number of taxa that coexisted at any one time (Pease 1985). This is because singletons can be spread through an interval without overlap.

REFERENCES.-

4.1 Standard Indices of Taxonomic Richness

PURPOSE.- Compute the most common diversity indices based on presence/absence data.

COMMENTS.- Continuity of stratigraphic bins : if focused stratigraphic intervals contain gaps of record, be care on the interpretation of the curves at and around these gaps. Changes in taxonomic diversity are artefactually enhanced at these points.

CARE.- Sampling bias : It is well-known that the number of recovered taxa within samples depends on the number of collected individuals. Hence, for incidence data (presence/absence of taxa), this potential bias cannot be assessed and data must be interpreted with this in mind.

TODO : add curve number of completed ranges per strat bin TODO : add ribbon Dnorm-Drti

```
RICHNESS - STANDARD INDICES
    .. for 2 groups : COUNTRY, Canada
```

```
'data.frame':   176 obs. of  6 variables:
 $ BINS : Factor w/ 8 levels "Rhuddanian","Aeronian",..: 1 2 3 4 5 6 7 8 1 2 ...
 $ TYPE : Factor w/ 2 levels "raw values","rates per Myr": 1 1 1 1 1 1 1 1 1 1 ...
 $ VARS : Factor w/ 6 levels "Dnorm","Dsib",..: 2 2 2 2 2 2 2 2 3 3 ...
 $ X    : num  -442 -440 -436 -432 -429 ...
 $ Y    : num  13 25 65 33 21 45 36 32 13 28 ...
 $ GROUP: Factor w/ 2 levels "COUNTRY","Canada": 1 1 1 1 1 1 1 1 1 1 ...
```

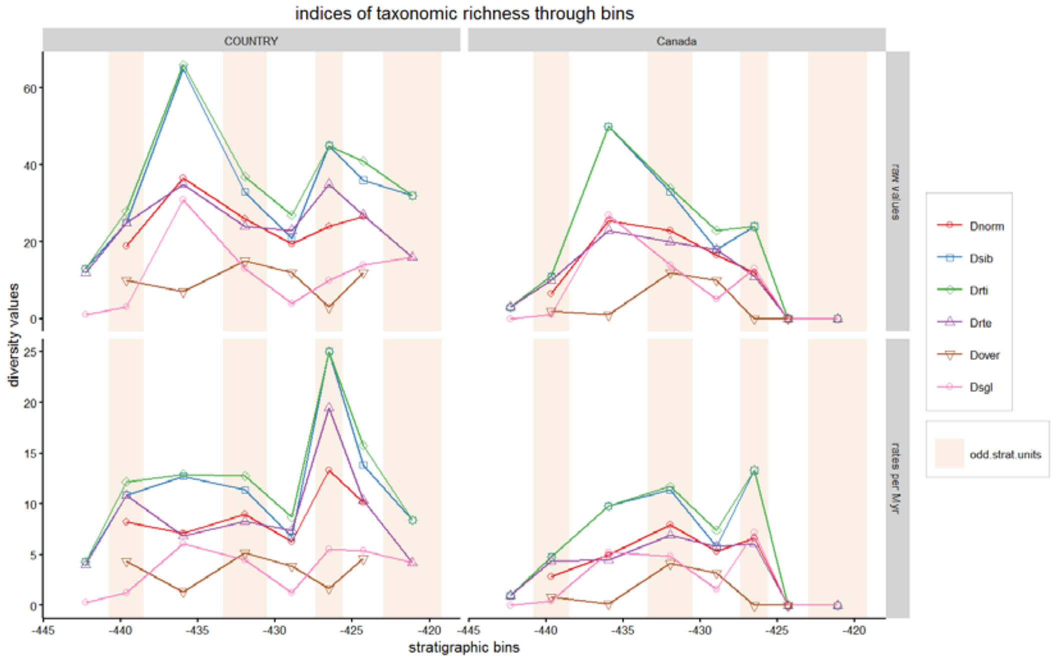


FIGURE : Taxonomic richness through bins by indices.

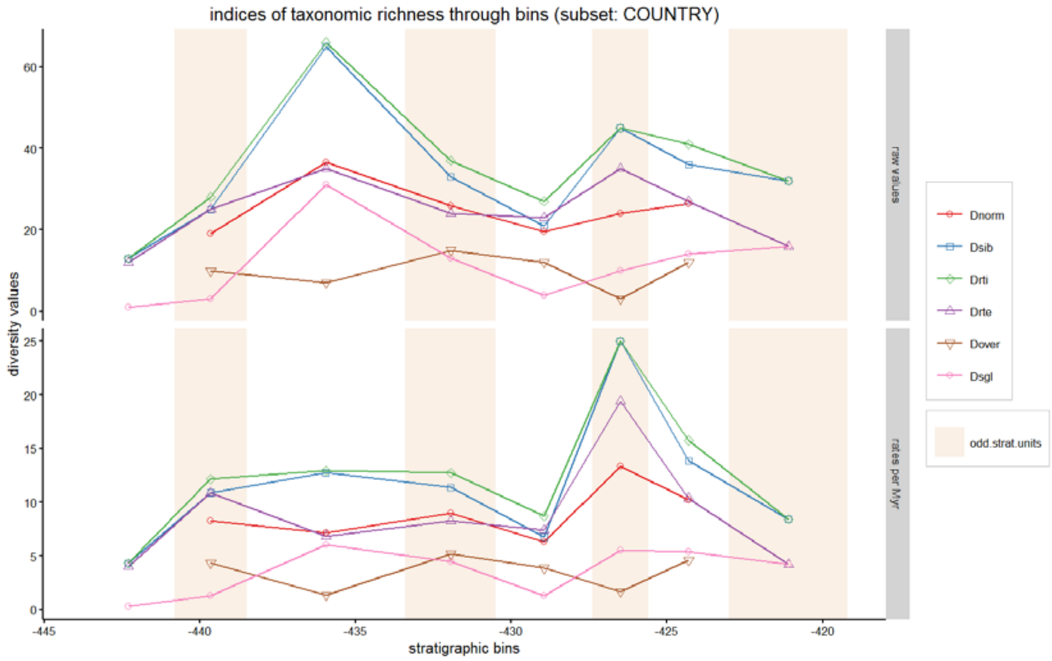


FIGURE : Taxonomic richness through bins by indices for each group.

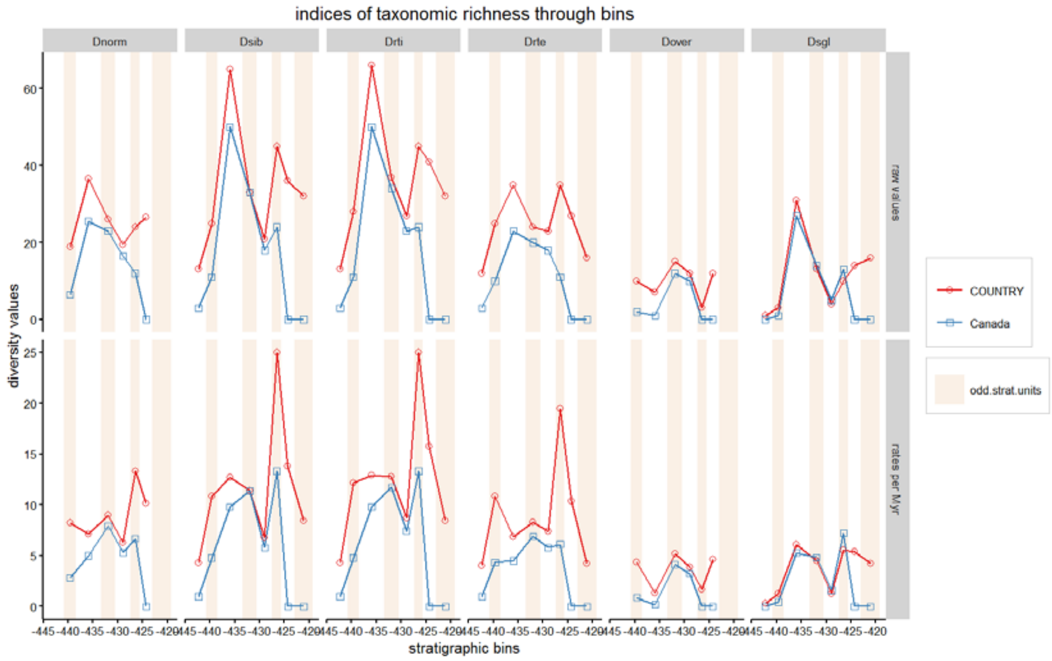


FIGURE : Taxonomic richness through bins by groups.

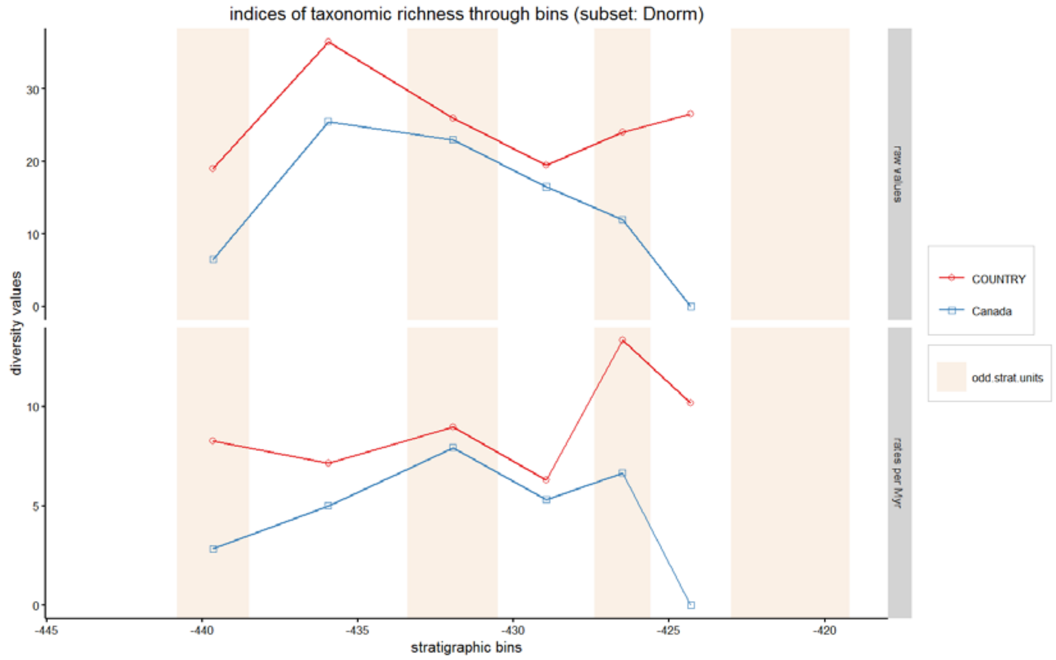


FIGURE : Taxonomic richness through bins by groups for each index.

4.2 Phase Diagrams of Taxonomic Richness

PURPOSE.- ...

COMMENTS.- ...

TEMPORARY NOTES : * Trends in taxonomic diversity can be represented by a phase diagram. This graph displays the diversity at time *t* against diversity at time *t+1*, and thus reflects the relative trend of taxonomic diversity through time.

Purpose: * This representation makes it easier to visualize any dynamical trend of taxonomic diversity during the entire studied time interval. * It can be used to evaluate dynamics of taxonomic diversity, and more precisely dynamical trends and carrying capacity. In paleontology, a phase diagrams often display fluctuations of species richness in time separated in two non-overlapping clusters. If there is a continuous species turnover, such two clusters suggest the presence of two successive dynamical equilibria separated by a threshold, which is strongly reminiscent of the logistic growth model of diversification (e.g. Carr & Kitchell 1980; Gotelli 1998; Kot 2001). According to this model, a dynamical equilibrium of species richness may reflect the carrying capacity of the studied area. In this context, the logistic model predicts that a sudden shift toward lower equilibrium values can be interpreted as a thresholded response caused by a decreasing carrying capacity. * It can be used also to evaluate the pace of changes between any dynamical equilibria as reflected by the number of time units separating two dynamical equilibria (assuming that the time bins are separated by the same amount of time, otherwise this may just reflect documentation gaps).

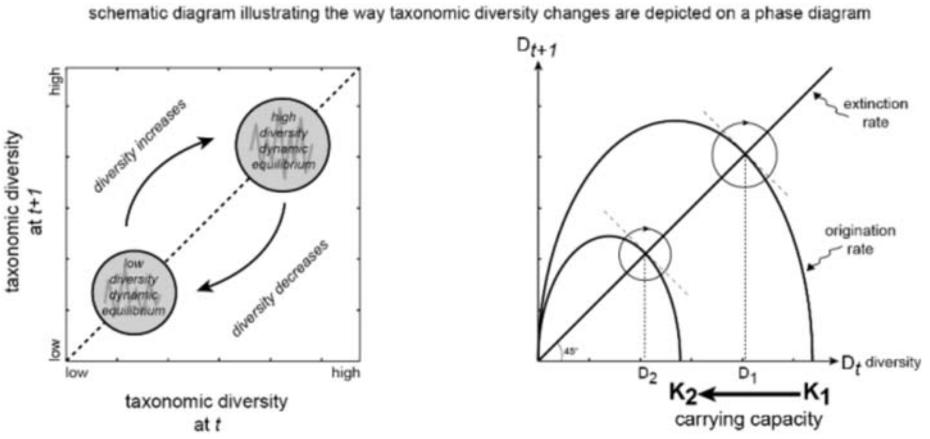


FIG.- .

Method: * See Monnet et al (2003). * Basically: scatterplot of TRn = f(TRn+1)

Applications: * Phase diagrams of taxonomic diversity have been applied to various fossil groups: e.g. Cretaceous and Triassic ammonoids (Monnet et al 2003; Brayard et al 2009).

TODO : order colors by age TODO : add a connecting line when ordered TODO : re-order groups as original

```
RICHNESS - PHASE DIAGRAMS
    .. for 2 groups : COUNTRY, Canada
```

```
'data.frame':   152 obs. of  7 variables:
 $ BINS : Factor w/ 7 levels "Aeronian-Telychian",..: 1 7 6 3 2 5 1 7 6 3 ...
 $ TYPE : Factor w/ 2 levels "rates per Myr",..: 2 2 2 2 2 2 2 2 2 2 ...
 $ VAR  : Factor w/ 6 levels "Dnorm","Dover",..: 1 1 1 1 1 6 6 6 6 6 ...
 $ X    : num  19 36.5 26 19.5 24 13 25 65 33 21 ...
 $ Y    : num  36.5 26 19.5 24 26.5 25 65 33 21 45 ...
 $ Z    : num  1 2 3 4 5 1 2 3 4 5 ...
 $ GROUP: Factor w/ 2 levels "COUNTRY","Canada": 1 1 1 1 1 1 1 1 1 1 ...
```

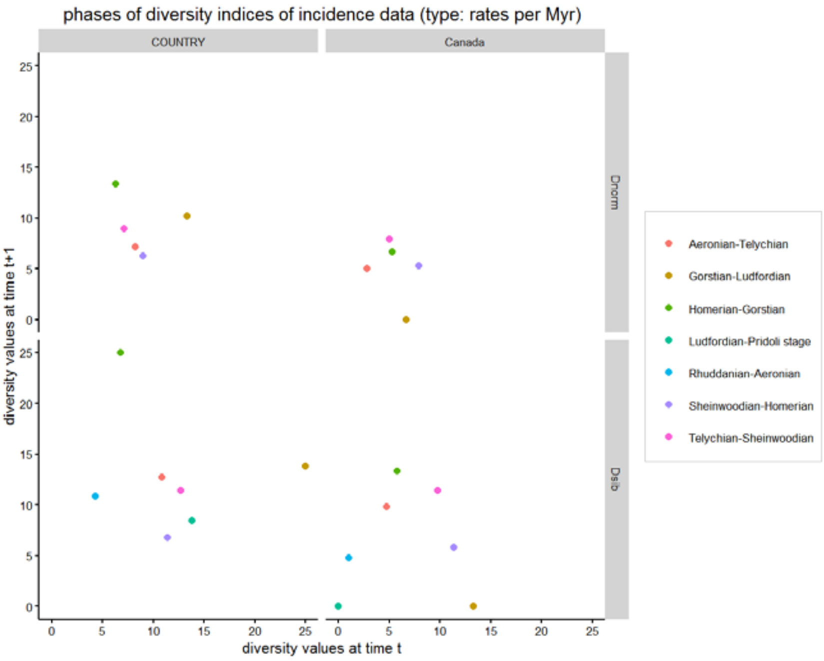


FIGURE : Phases of diversity indices of incidence data.

5 Taxonomic Changes

PURPOSE.- ...

5.1 Standard Indices of Changes in Taxonomic Richness

TEMPORARY NOTES : Origination and extinction correspond to the number of species appearing (First Occurrence, FO) and disappearing (Last Occurrence, LO) between two successive time-ordered intervals (samples, biozones).

This approach to calculate origination and extinction is adapted to discrete time intervals, not continuous scales. In the former case, FOs and LOs are included into the separation interval between two consecutive time intervals (samples, biozones).

The percentage of origination is defined as the number of FOs divided by the total number of taxa occurring in the next overlying time interval. For example, in a pair of two consecutive biozones (bzl, bz2), with bzl containing the set of species {a, b. c, d. e, f} and bz2 containing the set of species {d, e, f, g, h}, the percentage of origination is 2/5=0.4 and the percentage of extinction is 3/6=0.5.

The turnover is defined as the sum of the number of origination and the number of extinction (i.e. 5 in this arbitrary example). The percentage of turnover corresponds to the turnover divided by the total number of distinct species present in the two bracketing biozones (i.e. 5/8=0.625 in the arbitrary example). The turnover is a measure of the intensity of the restructuration of the entire community, but alternatively, it may also be artificially increased by the presence of documentation gaps in the faunal successions.

CARE : Singletons are removed before computing indices of taxonomic changes.

- Erte : extinction of range-thru excluding singletons
- Orte : origination of range-thru excluding singletons
- Trte : turnover (origination + extinction) of range-thru excluding singletons
- Dover : number of taxa present before and after (hence, indicative of no changes)
- Esbe : extinction of sampled-in-bin excluding singletons
- Osbe : origination of sampled-in-bin excluding singletons
- Tsbe : turnover (origination + extinction) of sampled-in-bin excluding singletons

- Crte : net changes (origination - extinction)
- Csbe : net changes (origination - extinction)

TODO : see Alroy's comments TODO : see Foote's comments

```
CHANGES - STANDARD INDICES
    .. groups : 2 : COUNTRY, Canada
```

```
'data.frame':   232 obs. of  6 variables:
 $ BIN  : Factor w/ 8 levels "Rhuddanian","Aeronian",..: 2 3 4 5 6 7 8 2 3 4 ...
 $ TYPE : Factor w/ 2 levels "values.per.bin",..: 1 1 1 1 1 1 1 1 1 1 ...
 $ VAR  : Factor w/ 9 levels "Erte","Orte",..: 7 7 7 7 7 7 7 2 2 2 ...
 $ X    : num  -440 -436 -432 -429 -426 ...
 $ Y    : num  13 15 5 5 26 4 5 13 12 5 ...
 $ GROUP: Factor w/ 2 levels "COUNTRY","Canada": 1 1 1 1 1 1 1 1 1 1 ...
```

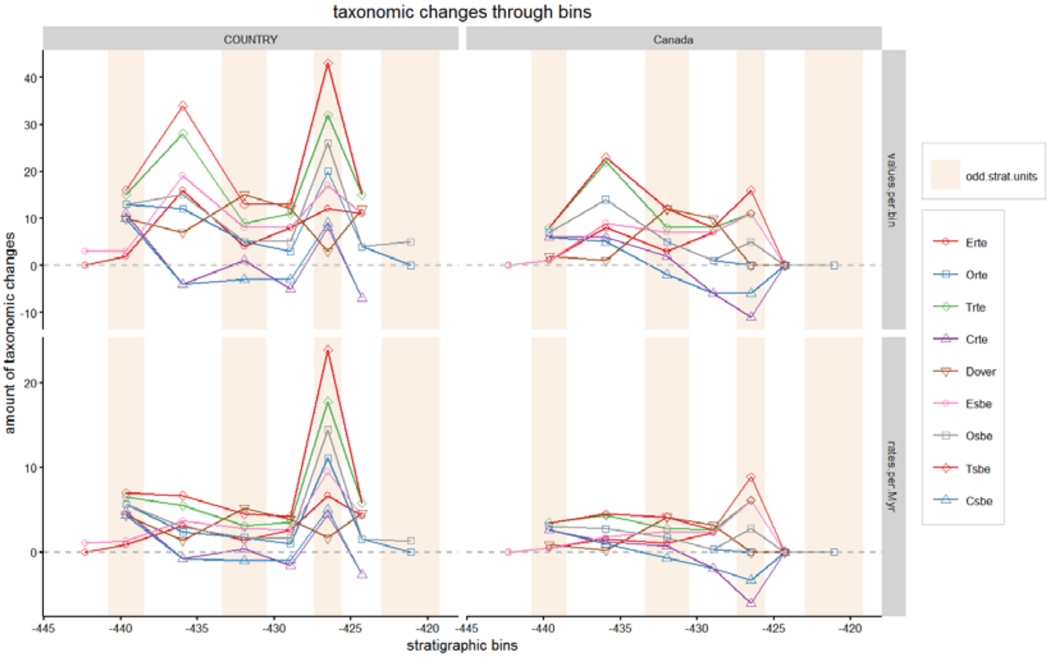


FIGURE : Taxonomic changes through bins by indices.

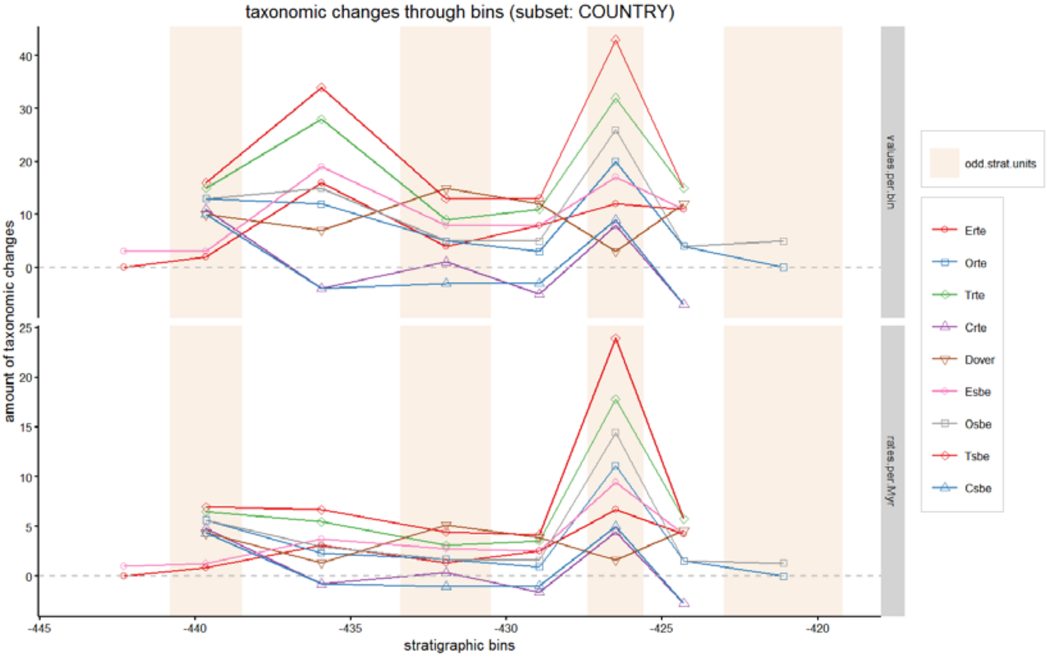


FIGURE : Taxonomic changes through bins by indices for each group.

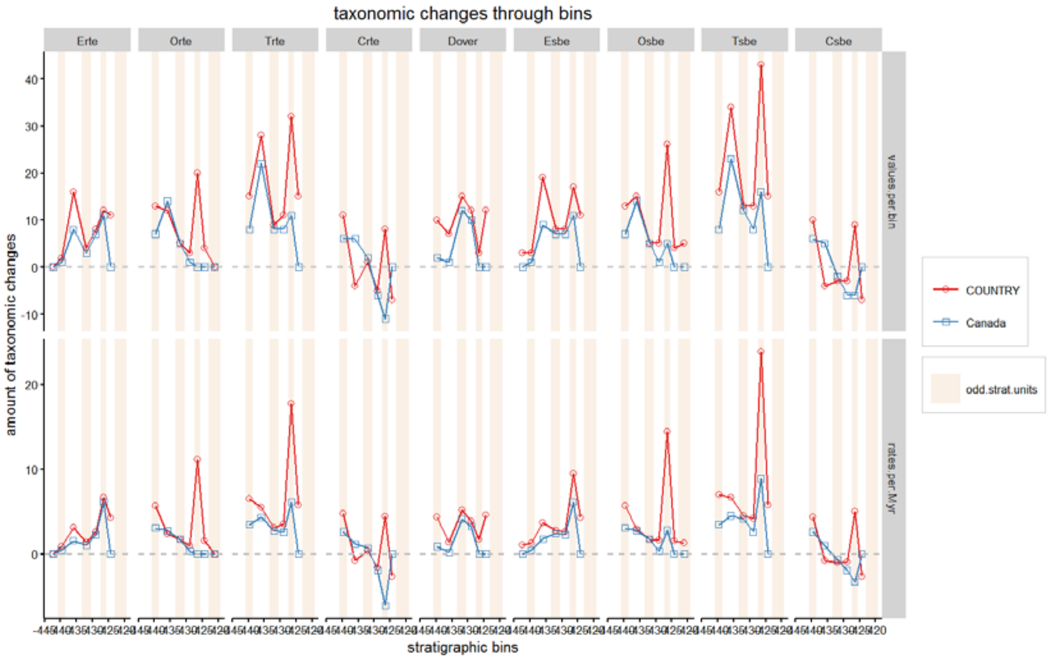


FIGURE : Taxonomic changes through bins by groups.

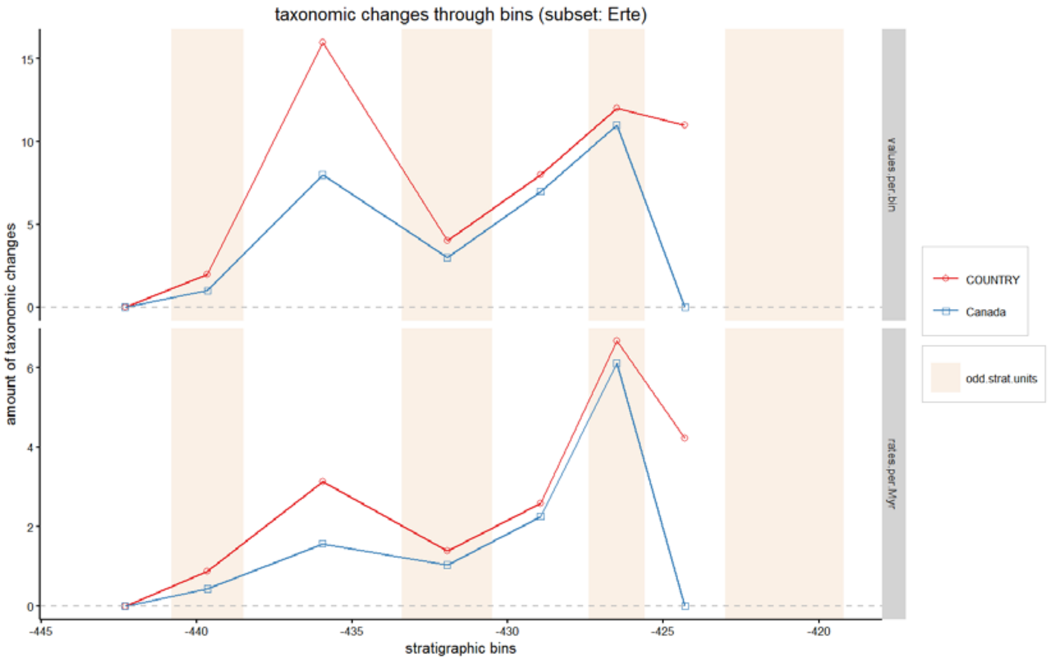


FIGURE : Taxonomic changes through bins by groups for each index.

5.2 Poly-Cohorts Analysis

PURPOSE.- …

COMMENTS.- …

TEMPORARY NOTES : Purpose: * Poly-cohort analysis is a classic analytic tool routinely used to graphically investigate and compare survivorship (and by opposition prenascence) of taxonomic assemblages through time. It investigates the log-linearity through successive time slices of changes in extinction and origination, and particularly their departure from random fluctuations. * Test relative constancy of extinction and origination rates through time intervals (assumed to be of equal duration).

Definition and Method: * A poly-cohort is an assemblage of taxa from a time unit, whatever the taxonomic affinities of these taxa. A poly-cohort survivorship curve is a plot of the percentage of all taxa from a community defined at time *t* still existing at time *t+dt* (Van Valen 1973, 1979; Raup 1978,1986). Survivorship and prenascence are thus the proportion of taxa surviving and originating, respectively, within poly-cohorts, separately, through time. * For a complete description of the method, see, among others, Monnet et al (2003). * The poly-cohort curves' log-linearity is statistically tested using two distinct approaches involving (i) the Epstein's test for straightness (Epstein 1960a, b; see Raup 1975), and (ii) a statistical procedure developed by G.E. and which will be thoroughly described elsewhere. This new procedure, close to that already proposed by Foote (1988), is based on a Monte-Carlo procedure of random re-sampling with replacement (non-parametric bootstrap) in order to estimate the confidence intervals linked to the observed survivorship percentages. As for the Epstein's test, it first allows to globally test the departure of observed curves from the null expectation that, for a given community, survivorship percentages are log-linearly arranged, i.e. that within poly-cohort extinction risk is stochastically constant through time. Then, if the alternate hypothesis is accepted, the event(s) of significant departure from stochastic fluctuations in observed survivorship percentages could be identified, thus providing additional information of interest not given by Epstein's method. * Finally, the timing of the fluctuations of percentages of extinction/origination across all poly-cohorts can be evaluated by means of a contour plot.

Applications: * Poly-cohort analyses of survivorship and prenascence have been applied to various fossil groups, especially in the context of mass extinction and their recovery: e.g. Cretaceous and Triassic ammonoids (Monnet et al 2003; Brayard et al 2009).

Figures: * The first and second figures report the survivorship and prenascence curves, respectively, of each individual poly-cohorts of the successive time intervals. * The third figure displays the contour intervals of the percentage of survivorship and prenascence through time. This graph assesses the synchronism of fluctuations of percentages of extinction and origination across all poly-cohorts. Such a plot implies that if all poly-cohorts have a constant extinction/origination rate through time, then all contour lines should be statistically parallel to the time axis (diagonal). On the other hand, horizontal contour intervals imply a concomitant increase of percentages of extinction across several poly-cohorts.

(TODO) : For each poly-cohort, the two statistical methods used to test for log-linearity of survivorship curves demonstrate that all poly-cohorts of the entire studied time interval are not significantly non log-linear (Ho not rejected), which implies that, for a given polycohort, the extinction risk is stochastically constant through time (earlier taxa have statistically the same risk of extinction as do later taxa). Consequently, these tests indicate that no statistically significant extinction phase can be detected during xxxxx times on the basis of the poly-cohorts analysis.

Remark : discontinuous ranges are completed, and NAs by absence !

TODO : log-scale ?

```
CHANGES - POLY-COHORTS
    .. groups : 2 : COUNTRY, Canada
```

```
'data.frame':   108 obs. of  6 variables:
 $ BIN   : Factor w/ 8 levels "Rhuddanian","Aeronian",..: 1 2 3 4 2 3 4 5 6 7 ...
 $ COHORT: Factor w/ 8 levels "Rhuddanian","Aeronian",..: 1 1 1 1 2 2 2 2 2 2 ...
 $ Y     : num  100 100 83.3 0 100 ...
 $ X     : num  -442 -440 -436 -432 -440 ...
 $ TYPE  : Factor w/ 2 levels "survivorship",..: 1 1 1 1 1 1 1 1 1 1 ...
 $ GROUP : Factor w/ 2 levels "COUNTRY","Canada": 1 1 1 1 1 1 1 1 1 1 ...
```

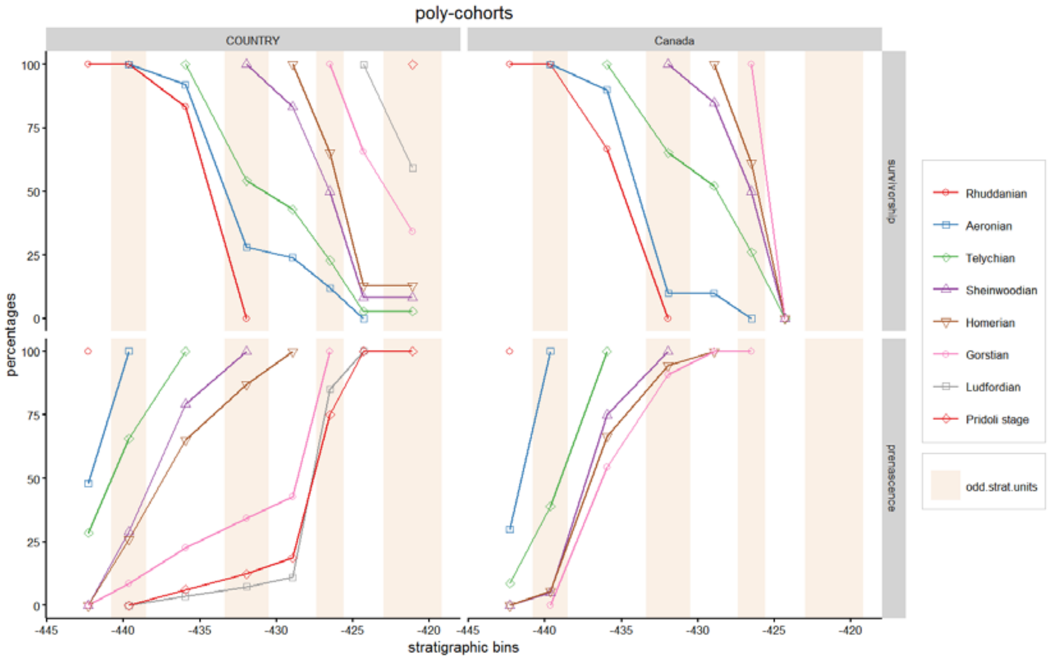


FIGURE : Poly-cohorts through bins by indices.

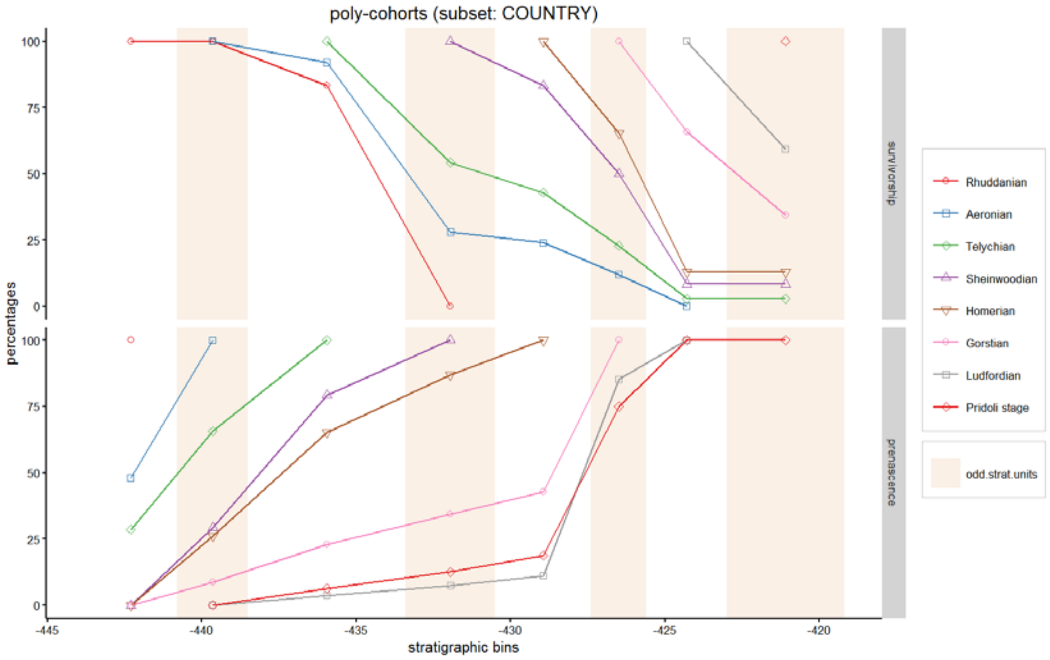


FIGURE : Poly-cohorts through bins by indices for each group.

6 Taxonomic Composition

PURPOSE : Investigate changes in taxonomic composition (aka. similarities and differences) through time (instead of taxonomic richness).

6.1 Taxonomic Similarities

relative area chart of the number of specimens/number of samples per zone for each order, families, genera, etc.

taxonomic components

- Dcom : number of common taxa between two successive stratigraphic bins
- Dric : number of taxa over two successive stratigraphic bins
- Dcop : proportion of common taxa between two successive stratigraphic bins relative to the taxonomic richness of the two bins

create a second facet for the percentages ... ?

TODO : add area chart of rihcness at another taxonomic rank (e.g. families) ? TODO : add raup & crick index

```
COMPOSITION - SIMILARITIES
    .. groups : 2 : COUNTRY, Canada
```

```
'data.frame':   41 obs. of  6 variables:
 $ BIN  : Factor w/ 7 levels "Rhuddanian-Aeronian",..: 1 2 3 4 5 6 7 1 2 3 ...
 $ TYPE : Factor w/ 2 levels "rates.per.unit",..: 2 2 2 2 2 2 2 2 2 2 ...
 $ VAR  : Factor w/ 3 levels "Dcom","Dric",..: 1 1 1 1 1 1 1 2 2 2 ...
 $ X    : num  -441 -439 -433 -430 -427 ...
 $ Y    : num  12 23 19 20 15 23 16 25 37 40 ...
 $ GROUP: Factor w/ 2 levels "COUNTRY","Canada": 1 1 1 1 1 1 1 1 1 1 ...
```

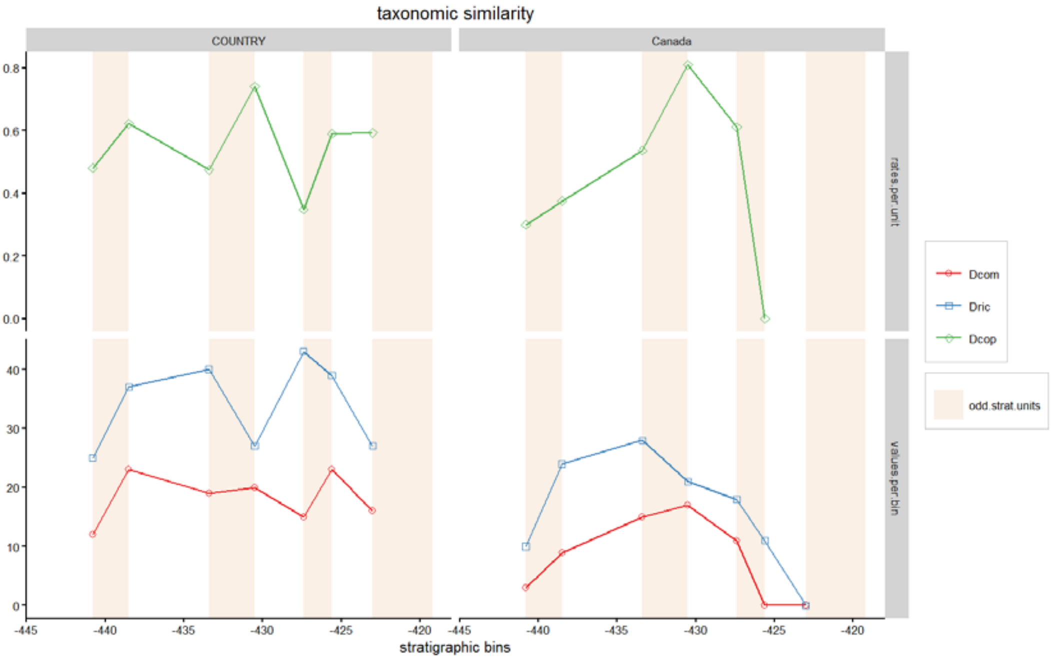


FIGURE : Similarities through bins by indices.

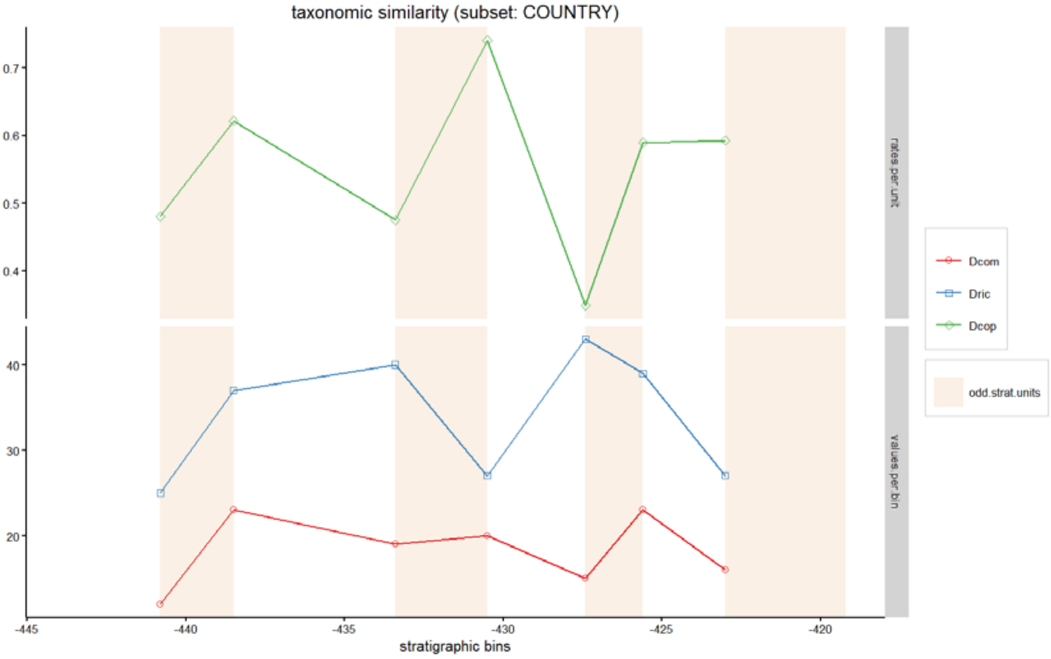


FIGURE : Similarities through bins by indices for each group.

6.2 Taxonomic Distinctness

PURPOSE : ...

```
COMPOSITION - DISTINCTNESS
    .. not yet implemented
```

6.3 Statistical Tests (ANOSIM)

PURPOSE : ...

ANOSIM and PERMANOVA

```
COMPOSITION - ANOSIM
    .. not yet implemented
```

7 Biases

Purpose : ...

7.1 Authorship

Purpose : …

Influence of Authorship on Taxonomic Diversity as number of references used to construct the database

linear correlations of nb studies vs nb taxa

up-down correlation

- Range chart of References: coverage of time bins by included publications.
- Diversities of References (Dsib).
- Reproducibility of References.
- Correlation of Taxonomic Diversities with Monographic Diversities.

```
BIAS - AUTHORSHIP
    .. for 2 groups : COUNTRY, Canada
    .. construct range chart of references ..
```

```
'data.frame':   16 obs. of  7 variables:
 $ BINS : Factor w/ 8 levels "Rhuddanian","Aeronian",..: 1 2 3 4 5 6 7 8 1 2 ...
 $ TYPE : Factor w/ 1 level "raw values": 1 1 1 1 1 1 1 1 1 1 ...
 $ VARS : Factor w/ 1 level "Dsib": 1 1 1 1 1 1 1 1 1 1 ...
 $ Z    : num  -442 -440 -436 -432 -429 ...
 $ Y    : num  2 3 5 4 4 4 2 6 1 1 ...
 $ GROUP: Factor w/ 2 levels "COUNTRY","Canada": 1 1 1 1 1 1 1 1 2 2 ...
 $ X    : num  13 25 65 33 21 45 36 32 3 11 ...
          GROUP  VAR       TYPE X Y N rho.val  rho.p tau.val  tau.p
COUNTRY COUNTRY Dsib raw values 0 6 8   0.381 0.3524   0.309 0.3044
Canada   Canada Dsib raw values 0 6 8   0.870 0.0050   0.762 0.0133
                                                                 NOTE
COUNTRY n = 8\nR.rho = 0.381 ; p = 0.3524\nR.tau = 0.309 ; p = 0.3044
Canada  n = 8\nR.rho = 0.870 ; p = 0.0050\nR.tau = 0.762 ; p = 0.0133
```

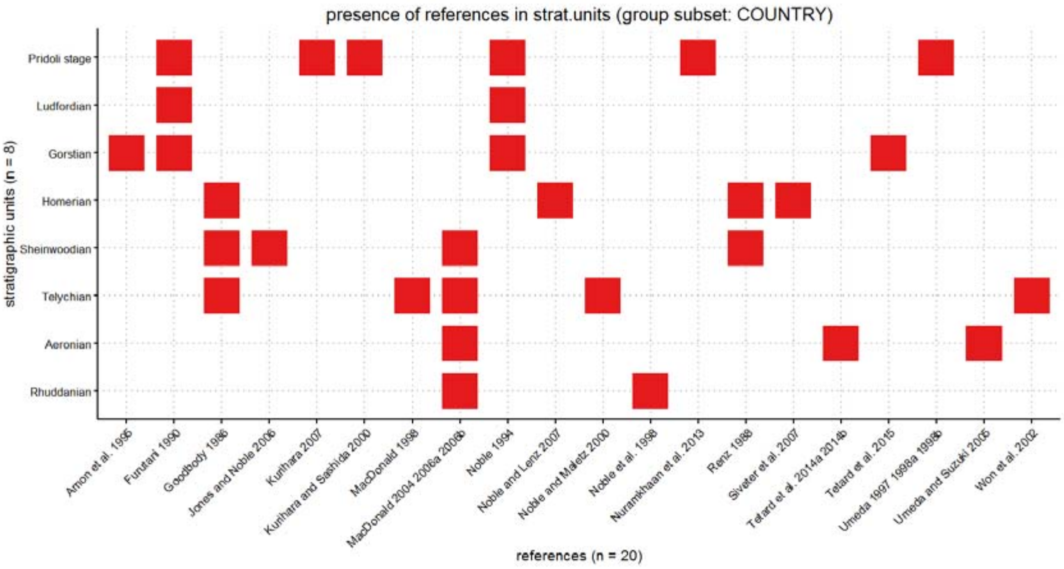


FIGURE : Presence of references within the stratigraphic bins.

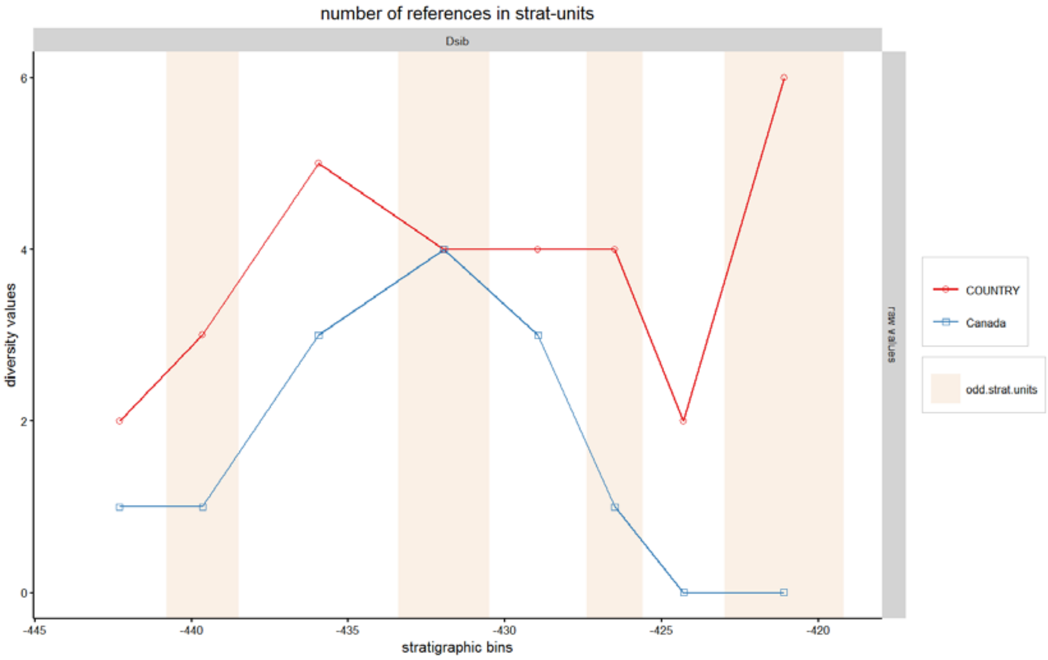


FIGURE : Number of references in strat-units by groups.

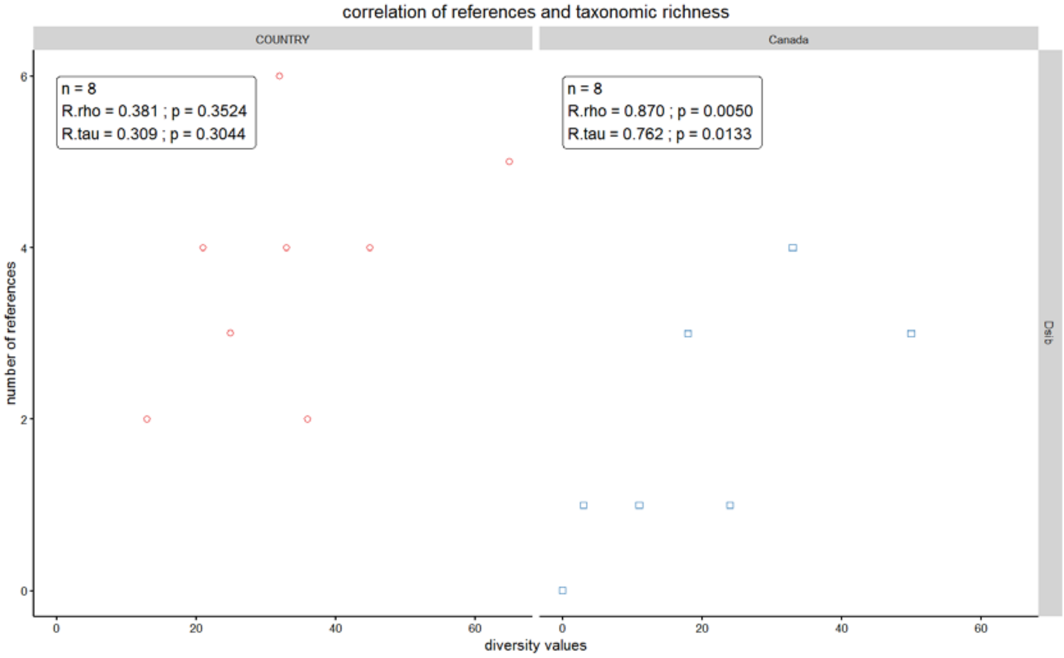


FIGURE : Correlation of references and taxonomic richness.

7.2 Sampling

```
BIAS - SAMPLING
    .. not yet implemented
```

7.3 Taxonomic Uncertainties

```
BIAS - NOMENCLATURE
    .. groups : 2 : COUNTRY, Canada
```

```
'data.frame':   8 obs. of  3 variables:
 $ STATE: Factor w/ 4 levels "?","aff","cf",..: 1 2 3 4 1 2 3 4
 $ Freq : int  9 7 14 379 5 7 9 172
 $ GROUP: Factor w/ 2 levels "COUNTRY","Canada": 1 1 1 1 2 2 2 2
```

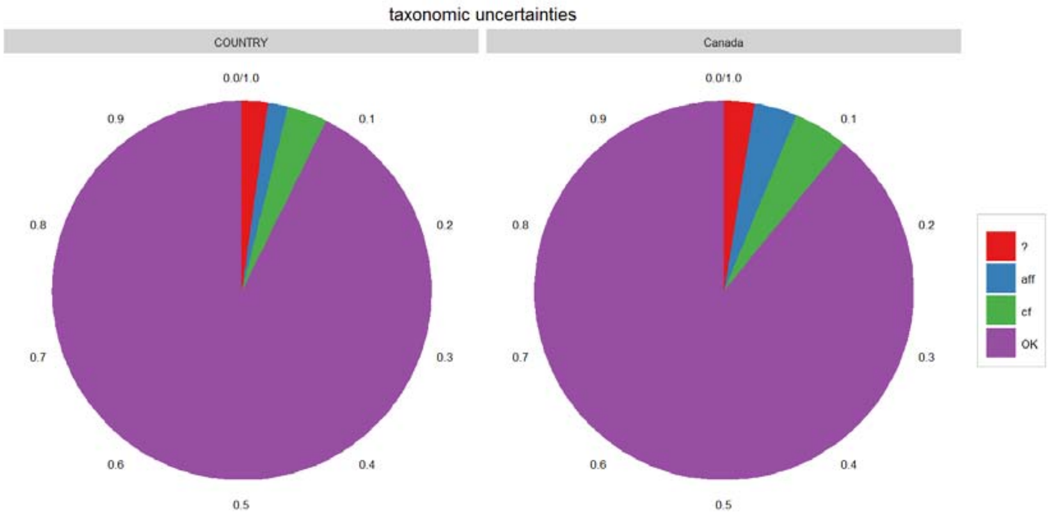


FIGURE : Pie chart of taxonomic uncertainties.

8 End of Session and Citation

REFERENCES.- This report displays the results of data analyses computed with the **R scientific computing language (http://www.r-project.org/)** version **3.3.0** (R Core Team 2016). When you use R for data analysis, you need to cite using the base package and the additional packages in the publications where you report the results of the data analysis. For this vignette, the general computation is based on the package **'epaleo'** version **0.4.27** (Monnet 2016), and most figures are constructed using the package **'ggplot2'** version **2.1.0** (Wickham 2009).

- R Core Team (2016) R: A language and environment for statistical computing. R Foundation for Statistical Computing, Vienna, Austria http://www.R-project.org/ (http://www.R-project.org/)
- Monnet C (2016) epaleo: an R package for paleontological data analysis. University of Lille, France (unpublished)
- Wickham H (2009) ggplot2: elegant graphics for data analysis. Springer-Verlag, New York. ISBN 978-0-387-98140-6

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Save figures in a multi-page PDF file
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Fri Sep 09 17:21:18 2016
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    EPALEO version 0.4.27
    GGPLOT2 version 2.1.0
Variables in memory : AG, CST, DFS, DFT, DFW, do, ds, dt, dv, EV, f, FG, k, lt, mx, n, p, s, sl, st, STATE, sx, sy
, t, tk, ts
```

Prospects

Taxonomy and morphometrics

Devonian of Algeria

With regard to alpha taxonomy, I am currently supervising (PhD: Ninon Allaire) the preparation and taxonomic description of Devonian ammonoids from several areas in Algeria (the Bechar Basin and Saoura Valley).

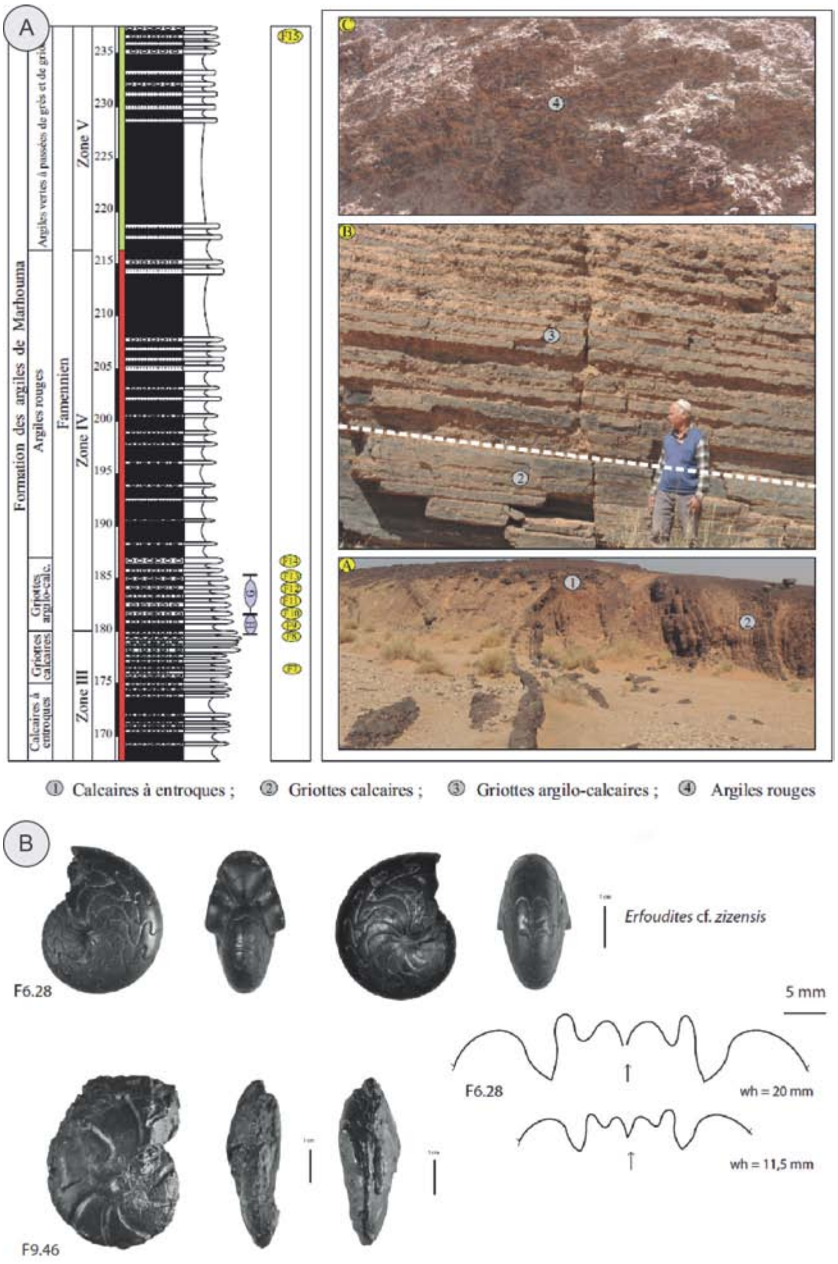

***Figure –** One studied Devonian section from Algeria (**A**) with illustration of one species from this section (**B**).*

Geometric morphometrics 3D

With regard to morphometrics, I am currently supervising studies with the acquisition of 3D scans of ammonoids that will be then modeled and analyzed by means of geometric morphometrics with the following goals (among others): comparing the efficiency of 2D and 3D in quantifying shell and suture shapes, in discriminating taxa, and in investigating macroevolution in the context of morphospaces.

Figure – *The 3D blue light scanner of the lab (**A**) with illustration of two ammonoid reconstruction (**B**).*

Databases: Devonian and Triassic

In order to prepare thorough studies in macroevolution, I am currently filling several databases (the worldwide collaborative Paleobiology Database, and personal databases) at the individual level with necessary information of space, time, and morphometry.

Quantitative biochronology

With regard to quantitative biochronology, I have two projects in mind. The first concerns the efficiency of quantitative methods in reconstructing biozonations. As seen in a previous chapter, there exist several competing quantitative methods to reconstruct biozonations by altering ranges of taxa in different ways. However, the actual efficiency, precision and robustness of all these methods is completely unknown; only their relative performance on real datasets is known, mainly because the true solution of these datasets cannot be known (incomplete fossil record). Therefore, I am developing a project to investigate this topic by means of computer-simulated fossil records and controlling various biasing factors such as amount/eveness of completeness/sampling, geographic cover, and uneven/abrupt evolutionary rates and lifespan of fossils. Also, it will enable evaluating the actual part of the original signal which is recovered and if it is correlated to the amount of biostratigraphic contradictions. Incidentally, such a project will help evaluating the impact of the options and critical steps of each method on the efficiency/precision of the reconstructed biozonation. Eventually, recommendation on the best options (if any) and corrections to the algorithms of each method could be proposed. Also, the sensitivity of the methods with regards to "errors" (e.g. taxonomic mis-identification, reworkings) can be evaluated.

Because most biodiversity analyses rely on the biochronostratigraphic scales available, the second project will focus on evaluating the impact of reconstructed biozonations by these quantitative methods on the correctness of biodiversity curves derived from these biozonations, also by means of computer-simulated fossil records and by applying the diversity of biodiversity indices. Again, several parameters will be used to identify for instance the ability of a method to account for extinction or biodiversification events.

Macroevolution

Evolutionary trends in morphospaces

With regard to macroevolution, I will continue to investigate evolutionary trends of ammonoids, but based on the complete database/record during one period (e.g. Triassic), and not a single family at a time as currently done. In order to gain better insights into the interpretation of these trends, I will use the Pareto approach to evaluate the existence of adaptive peaks. Also, I will use machine learning approaches to automatically detect patterns, and not just focusing on expected ones such as increase in size. In addition, I will use time series analyses to detect possible links/impacts with environmental proxies. Finally, I will investigate and compare the biodiversities of taxonomic richness and of morphological disparity.

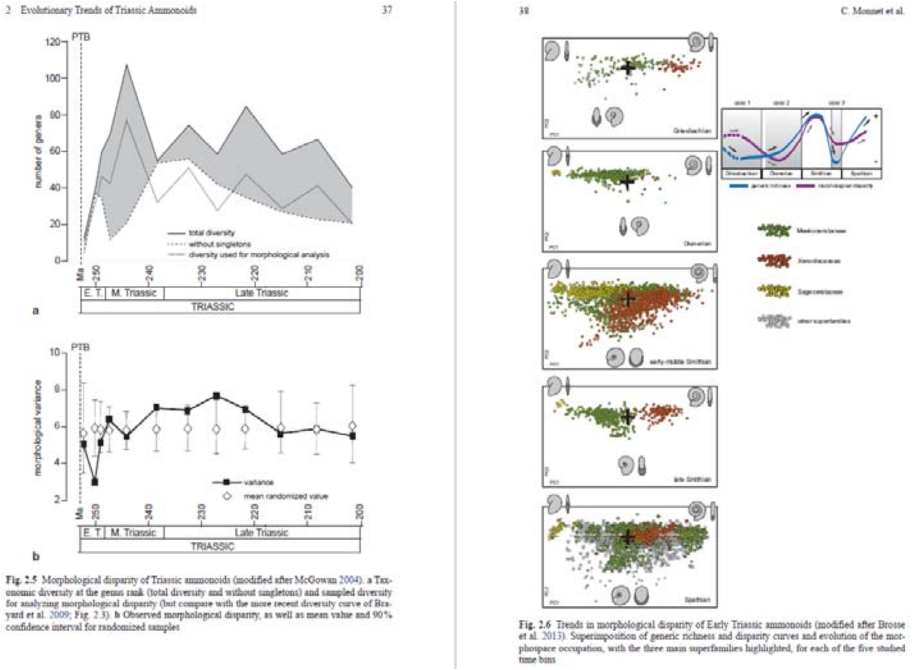
2 Evolutionary Trends of Triassic Ammonoids 37

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Fig. 2.5 Morphological disparity of Triassic ammonoids (modified after McGowan 2004). **a** Taxonomic diversity at the genus rank (total diversity and without singletons) and sampled diversity for analyzing morphological disparity (but compare with the more recent diversity curve of Brayard et al. 2009; Fig. 2.3). **b** Observed morphological disparity, as well as mean value and 90 % confidence interval for randomized samples

Fig. 2.6 Trends in morphological disparity of Early Triassic ammonoids (modified after Brosse et al. 2013). Superimposition of generic richness and disparity curves and evolution of the morphospace occupation, with the three main superfamilies highlighted, for each of the five studied time bins

Figure – *Much remain to be done on evolutionary trends of Triassic ammonoids as highlighted by my recent review (Monnet et al 2015d).*

Phylogeny of ammonoids

In the context of macroevolution, my research is currently always framed by the chronostratigraphic context of the studied data. However, there are nowadays many powerful methods to analyse character states along evolutionary trees and that are able to provide important insights into macroevolution (of ammonoids). Therefore, one major goal of my next research will be to reconstruct ammonoid phylogeny by means of modern, standard phylogenetic methods (cladistics). I am currently collaborating with Malagasy colleagues on reconstructing the phylogeny of some major Late Cretaceous ammonoids, and I am currently mounting another project for Devonian and Triassic ammonoids.

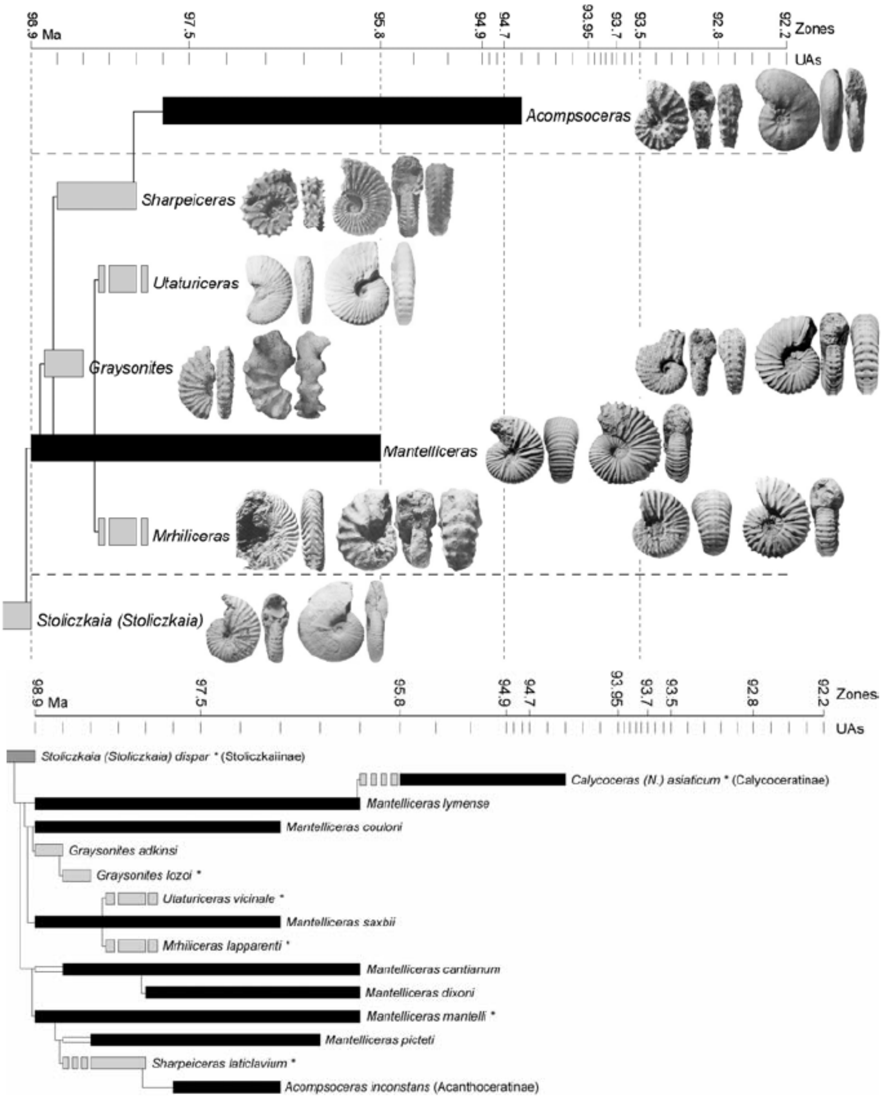

Figure – *Phylogeny of Cenomanian (Late Cretaceous) Mantelliceratinae by means of parsimony cladistic (unpublished).*

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