Challenges for DEB modeling of organismal responses of organisms exposed to ”forever chemicals”

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Abstract

Per- and polyfluoroalkyl substances (PFAS), - ”forever chemicals” - pose risks to human and environmental health. We report progress in the DEB component of a study on toxicity of complex PFAS mixtures. The goal is to develop a testing framework that will evaluate mixture toxicity by connecting macromolecular and sub-organismal response to impacts on whole animals. We follow an approach advocated by Murphy et al. (2018: DOI: 10.1002/ieam.4063) that was previously implemented in experiments on *Daphnia magna* (DM) exposed to coalash, a mixture of approximately 30 metals (poster in this symposium). Our data set includes experiments measuring the lethal and sublethal impacts of a single compound (PFOS) and a PFAS mixture across the full DM life cycle. Individuals were sacrificed throughout at important developmental time points to measure gene expression. Parallel bioaccumulation studies are in progress. The presentation focuses on the challenges faced by DEB modelers. ”DEBtox” modeling involves linked modules describing: (i) energy and material flows within an organism (DEB): (ii) uptake, transformation and excretion of toxicant (TK); (iii) a characterization of the toxicant action (TD). For PFOS, we first fit a DEB model to our control data plus literature data. When data become available, we will choose a TK module and estimate its parameters. The TD module will initially use a single ”damage” variable that potentially affects all DEB processes. The biggest challenge for the DEB modeling is determining the level of detail to include, an issue highlighted recently by Romoli et al (2024: DOI: 10.1002/etc.5795) who concluded that ecological risk assessment cannot be based solely on goodness-of-fit or on the precision of model predictions. This finding has immediate implications beyond ecotoxicity and supports our emphasis on the value of molecular data.

*Speaker

Keywords: DEBtox, PFAS, Daphnia, gene expression

High Throughput Adaptation of Standardized Ecotoxicological Exposure Tests in Daphnia magna and Other Invertebrates

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Abstract

Modern mechanistic modelling can create extrapolations of chemical toxicity across multiple organisms; however, it tends to require large amounts of measurements. New technology and equipment have introduced the opportunity of using high-throughput testing techniques to facilitate the collection and automated processing of high volumes of experimental data. This study demonstrates the adaptation of *Daphnia magna* chronic OECD standard procedures to a High Throughput setting using a Cell imager and well plates. The method was extended to other invertebrates used in similar ecotoxicological tests, such as *Moina macrocopa and Heterocypris incongruens*. In the experiment, *D. magna* was cultured closely following OECD guidelines, adapting them to culturing in well plates. The experiment comprised ten individuals per replicate for each of five concentrations for eight chemicals. A further 80 individuals were established in the medium without any chemical addition to serve as controls. This required twenty-four 24-well plates with 480 wells used in total in the experiment.

D. magna lengths ranged between 1.8 and 3.0 cm after 14 days, with little mortality ($< 20\%$). A dose-response effect for sublethal endpoints (growth and reproduction) was found for all eight chemicals tested.

We aimed to standardize high throughput methods by exposing the organisms to a range of different chemicals, measure chronic toxicity responses and use Dynamic Energy Budget Theory (DEB) Toxicokinetic – Toxicodynamic (TKTD) modelling to test fits and derive relevant parameters. Results indicate that this technique can greatly improve cost efficiency of ecotoxicological tests to complement mechanistic modelling needs.

Keywords: Standardized, Ecotoxicology, Daphnia, OECD, High, Throughput

*Speaker

Modelling domoic acid retention in Argopecten purpuratus and Pecten maximus: comparison of dynamics in fast and slow depurators.

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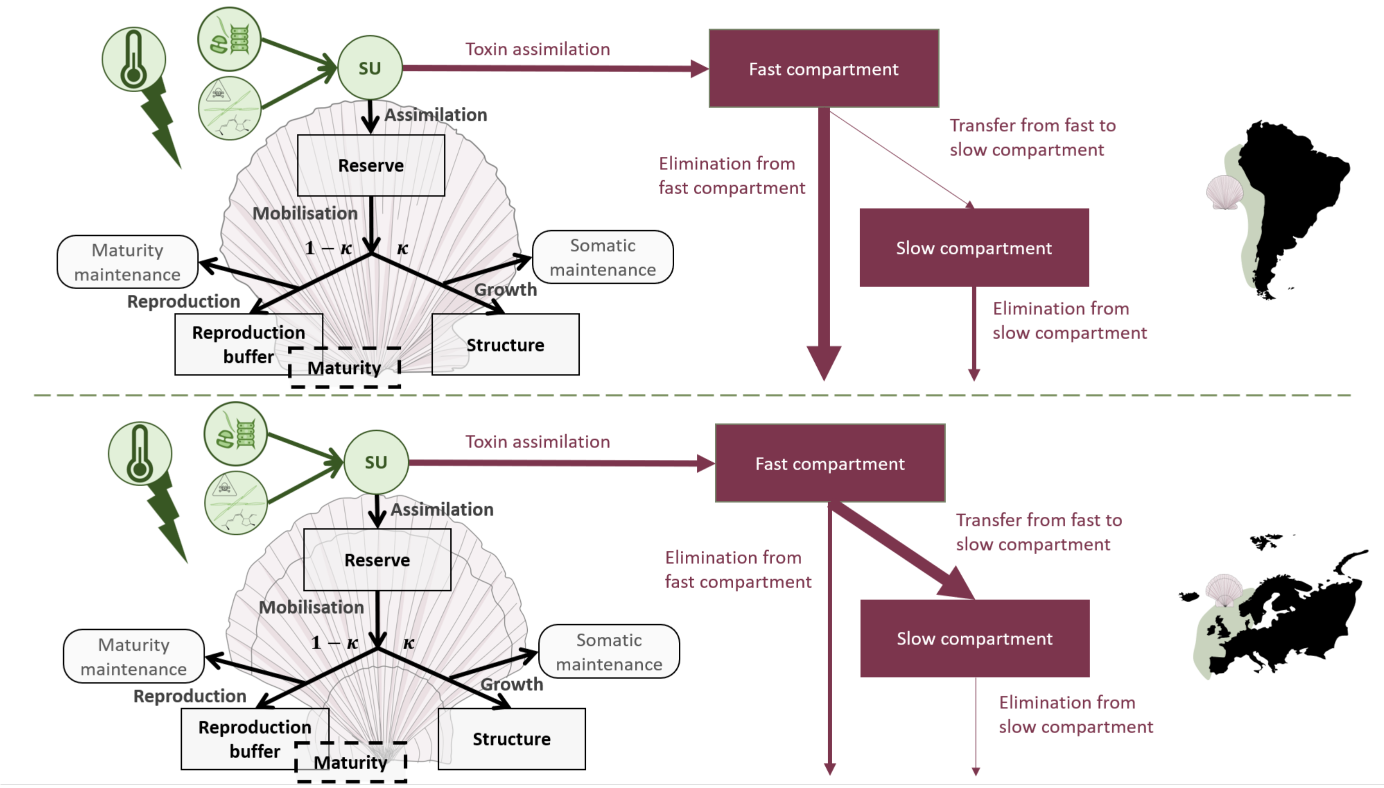
Abstract

As filter feeders, bivalves of the Pectinidae family are exposed to domoic acid (DA), the Amnesic Shellfish Toxin (AST) produced by species of the genus *Pseudo-nitzschia*. Pectinids can accumulate the toxin and transfer it to higher trophic levels, representing a significant socio-economic concern due to their high economic value. The DA retention is species-specific, some species, such as king scallops, retain the toxin for extended periods, while others, such as Chilean scallops, exhibit faster depuration rates. The physiological mechanisms explaining these differences are not fully understood yet. This study aims to develop a bioenergetic model based on Dynamic Energy Budget (DEB) theory integrated with a toxin kinetic module to describe DA retention. The model assumes that DA does not impact individual physiology and integrates two compartments: (1) a rapidly depurating compartment where the assimilated toxin is initially stored, and (2) a secondary compartment where a fraction of the toxin is transferred and eliminated more slowly. Initially, the DEB-DA model was calibrated and validated on the Chilean scallop using data from laboratory and field experiments following natural bloom of toxic *Pseudo-nitzschia* sp. Secondly, the model was applied to the king scallops based on data from field monitoring and experimental decontamination monitoring also following a natural bloom of *Pseudo-nitzschia*. The parameters of the toxin kinetic module were calibrated for each species and correspond to the hypotheses of physiological structures that trap DA in tissues present in king scallops, called autophagosome-like vesicles. This study provides new insights into species specific DA retention dynamics.

Keywords: Amnesic Shellfish Poisoning, toxin kinetics, pectinids, species comparison, DEB model

*Speaker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Toxin assimilation
Fast compartment
Assimilation
Transfer from fast to slow compartment
Reserve
Elimination from fast compartment
Slow compartment
Mobilisation
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Maturity maintenance
Somatic maintenance
Growth
Reproduction
Elimination from slow compartment
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Maturity maintenance
Somatic maintenance
Growth
Reproduction
Elimination from slow compartment
Reproduction buffer
Structure
Maturity

Modeling the Spatiotemporal Impacts of Ocean Warming and Acidification on the U.S. Atlantic Sea Scallop to Guide Adaptive Fisheries Management

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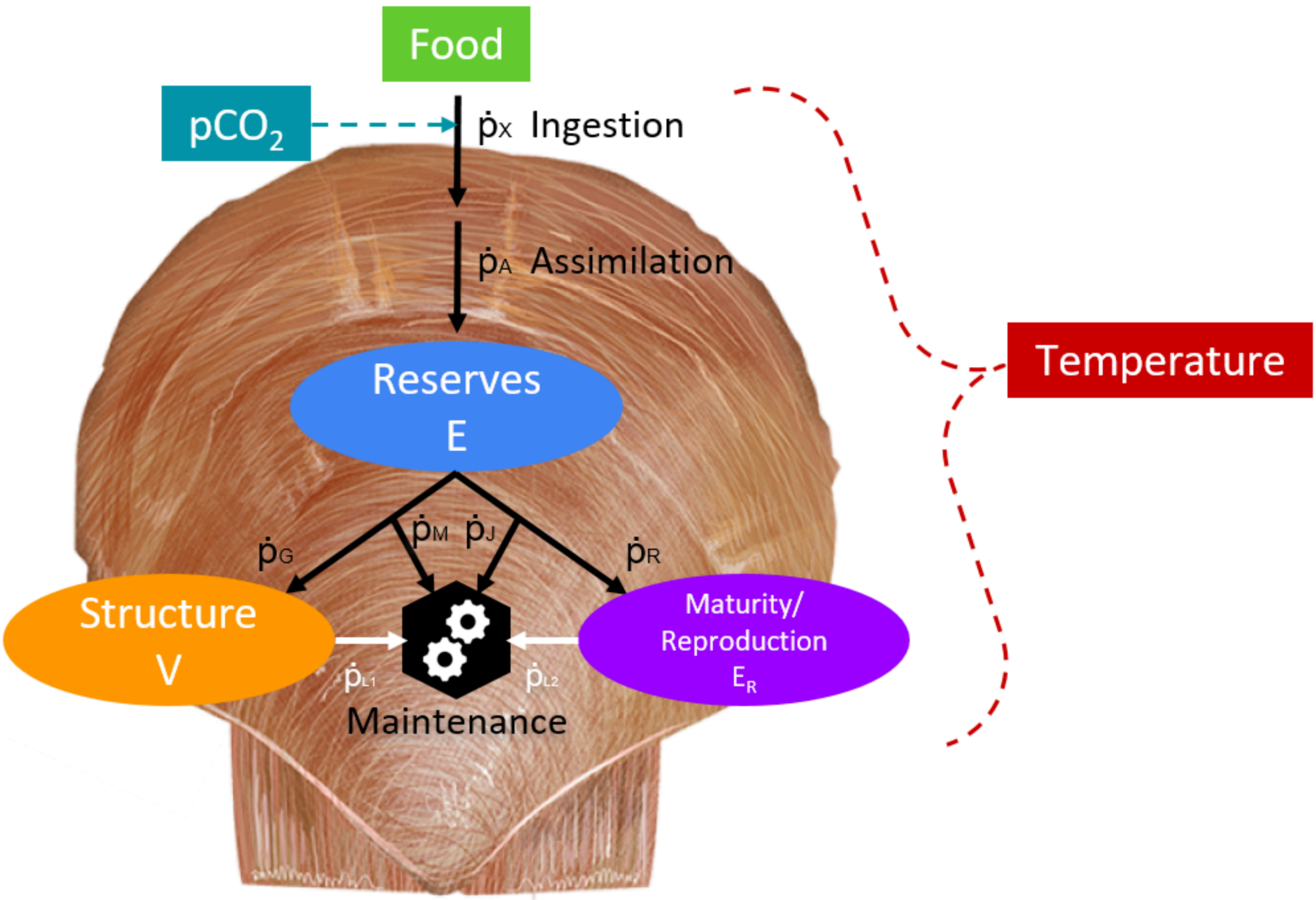
Abstract

The Atlantic sea scallop (Placopecten magellanicus) fishery is one of the most valuable fisheries in the U.S. However, changing ocean conditions driven by climate change and ocean acidification (OA) may cause declines in scallop availability, harvest, and revenue. Scallop habitats in the Northeast and Mid-Atlantic already experience suboptimal temperature and carbonate chemistry conditions episodically. Regional oceanographic models predict that these conditions will continue and worsen in the future under the most severe emissions scenario, projecting that most scallop habitats will experience chronic stressful conditions by 2100. Here, we project the effects of OA and warming on sea scallop growth historically and over the next century using a dynamic energy budget (DEB) model coupled to a regional ocean model. The model was able to simulate observed patterns in scallop growth based solely on temperature, food, and pCO2 conditions. Under combined end-of-century OA and warming, scallops grew slightly faster but reached smaller maximum shell heights in most areas, with mortality largely confined to the southern Mid-Atlantic. While OA contributed to sublethal impacts on growth uniformly across the region, warming had a more variable effect, ranging from positive in the north to lethal in the south. Notably, the cold pool area and deep Gulf of Maine emerged as thermal refugia and simulated scallops there did not experience net negative impacts on growth despite OA, making these areas potential candidates for rotational management. Altogether, our findings demonstrate the utility of the spatially coupled DEB model as a tool to inform adaptive fisheries management.

Keywords: Bivalve, climate change, multiple stressors, future projections, fisheries management

*Speaker



Food
pCO2
ṗX Ingestion
ṗA Assimilation
Reserves
E
Temperature
ṗG
ṗM
ṗJ
ṗR
Structure
V
Maturity/
Reproduction
ER
ṗL1
ṗL2
Maintenance

Refuges lost? Searching for refuges from disease and climate change for the critically endangered golden frog, Atelopus zeteki/varius

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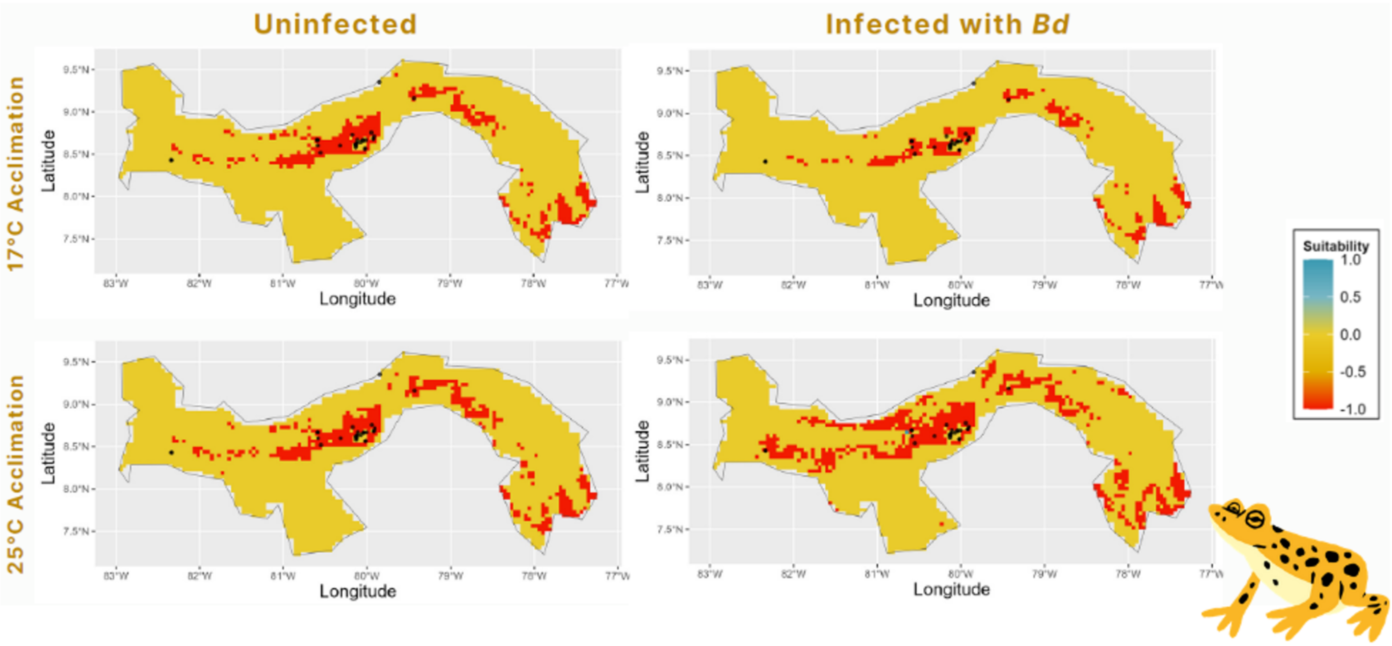
Abstract

Harlequin toads have experienced dramatic population declines, primarily driven by infections caused by the fungal pathogen *Batrachochytrium dendrobatidis* (Bd). The fungus has led to near extinction in the wild of the Panamanian golden frog, *Atelopus zeteki/varius*. Climate change exacerbates these threats by altering environmental conditions that influence host susceptibility and pathogen dynamics, further jeopardizing the survival of remaining populations. In this study, we integrate the Dynamic Energy Budget (DEB) theory to assess how Bd infection interacts with climate to shape the thermal ecology and potential spatial distribution of *Atelopus spp.* We combine previously collected data on how Bd infection affects thermal preferences with experimentally obtained measures of critical thermal limits (CTmin, CTmax) and locomotor performance in infected and uninfected frogs to determine activity restriction across space using field-collected body temperature (Tb) data, Bd infection status, and environmental temperature data from HOBO loggers. By coupling these physiological responses with DEB-based and ecological niche models (ENMs), we explore how infection-induced energetic constraints alter individual survival and environmental suitability under future climate scenarios. Our findings highlight the importance of DEB modeling in understanding the bioenergetic consequences of disease in amphibians, offering a mechanistic approach to predicting species responses to multiple stressors. This study contributes to advancing DEB applications in conservation physiology and provides insights into the persistence of one of the most imperiled amphibian groups in the Neotropics.

Keywords: Atelopus zetekii, DEB model, ecophysiology, Bd, conservation

*Speaker


Uninfected
Infected with *Bd*
17°C Acclimation
25°C Acclimation
Latitude
Longitude
9.5°N
9.0°N
8.5°N
8.0°N
7.5°N
83°W
82°W
81°W
80°W
79°W
78°W
77°W
Suitability
1.0
0.5
0.0
-0.5
-1.0

Modelling the Impact of Climate Change on Mountain Pine Beetle (*Dendroctonus ponderosae*) Cryoprotection Energy Allocation

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Abstract

Ectothermic insects depend on external temperatures to regulate their metabolism and energy use. Historically in temperate ecosystems, cold winters have naturally kept insect pest populations in check by causing increased mortality rates. However, with temperatures predicted to increase on average, climate change causes winters to warm faster than summers, thus increasing pest overwinter survival. Climate change has significantly contributed to the spread of the Mountain Pine Beetle (MPB) (*Dendroctonus ponderosae*), a native-invasive forest pest from Western North America. Warmer temperatures have facilitated its expansion eastwards into the boreal forest and across Canada. Recent outbreaks in the 2000s have killed approximately 54% of the merchantable pine in British Columbia. The cold-intolerant MPB successfully overwinters by accumulating cryoprotectants, such as glycerol, which lower its freezing point as temperature decreases in winter. This cryoprotectant synthesis is assumed to be an extra energetic cost for the beetle included in somatic maintenance. As winter temperatures increase and thus cold-related mortality decreases, we hypothesize that the cost of cryoprotection diminishes, and the beetle allocates previous cryoprotection energy allocation to growth, with impacts in other fluxes such as reproduction. To test this hypothesis, we formulated the first hex Dynamic Energy Budget model to estimate the MPB metabolic costs of maintenance, growth, and reproduction. This approach aims to enhance our understanding of how energy allocation strategies may evolve in response to climate change and their potential impact on MPB populations and future outbreaks.

Keywords: Cryoprotection, Cold tolerance, Climate change, Mountain Pine Beetle, Dynamic Energy Budget theory

*Speaker

Determining the population implications of the sublethal impacts of sea lamprey parasitism on two coexisting lake trout morphotypes using a DEB-IBM

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Abstract

Lake trout (*Salvelinus namaycush*) are a vital ecological and economic species in the Great Lakes, but their populations were severely depleted in the early 20th century due to overfishing and parasitism by invasive sea lamprey (*Petromyzon marinus*). Management efforts have focused on suppressing sea lamprey, primarily considering lethal impacts, while overlooking sublethal effects that may influence lake trout dynamics. Additionally, lake trout exhibit morphotypic variation, with leans prioritizing reproduction over survival following sea lamprey attacks, whereas siscowets sacrifice reproduction to recover.

To evaluate how sublethal effects and morphotype differences influence lake trout populations, we developed a Dynamic Energy Budget–Individual-Based Model (DEB-IBM). This model simulates pools of young lake trout, sea lamprey, and individual juvenile and adult lake trout of both morphotypes. Daily growth, starvation, maturation, and reproduction are determined using DEB dynamics, while fishing mortality and attack probabilities are externally defined. DEB parameters were derived from laboratory and literature-based data, with sublethal effects of parasitism incorporated as stressors on volume-specific maintenance and maturity maintenance parameters using data from a common environment experiment documenting changes in reproduction and lipid storage as a result of parasitism.

Our DEB-IBM framework allows us to assess: (1) the impact of sublethal sea lamprey effects on lake trout abundance and (2) whether morphotypic differences facilitate sea lamprey persistence when one morphotype is suppressed. By integrating physiological responses to parasitism, this model provides a more comprehensive understanding of lake trout–sea lamprey dynamics in Lake Superior, offering insights for more effective conservation and management strategies.

Keywords: Parasitic stress, IBM, ABM, lake trout, sea lamprey

*Speaker

Sea lamprey wounding and mortality

Energy restrictions cancel the effect of temperature on the common sole (Solea solea) in the Gironde estuary

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[3]UR EABX – Institut national de recherche pour l'agriculture, l'alimentation et l'environnement (INRAE) – France
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Abstract

Estuarine and coastal ecosystems are key nursery habitats for the development and growth of many juveniles of marine fish species. Human-induced environmental changes, to which coastal and estuarine areas are particularly sensitive, will largely impact juveniles' life history traits and consequently, the whole population at sea. Increase of water temperature is the best described and predicted environmental change related to climate change, and will certainly affect the nursery function of estuarine areas. Yet, our capacity to estimate consequences are limited and lack mechanistic models applied at the population level. As a major estuary of Western Europe, the Gironde estuary is a relevant case study to evaluate the effects of rising temperature on fish populations.
To study the specific impact of temperature on life history traits of juvenile common soles (*Solea solea*) in the Gironde estuary, we used a bioenergetic model based on DEB theory. Since the estuary is supposed to have reached its maximum carrying capacity, effects were also estimated in a context of limited energy availability, with forecast scenario based on IPCC previsions.
As soles in the Gironde estuary are below their thermal optimum, growth and development are expected to accelerate with increased temperature when food is not a limiting factor. Consequently, soles reach maturity sooner and grow larger. However, when we consider a restriction in available energy, linked to limited carrying capacity of the estuary, the effect of temperature is cancelled and changes in life history traits are negligible. However, a reduced energy in the reserve is estimated, which might alter the response to other environmental changes.

Keywords: Estuary, temperature, stress, energy restriction, juvenile fish

*Speaker


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Closing lecture, with remarkable AmP entries and a short outlook

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Abstract

My lecture has 3 chapters. I start with some evaluation remarks about what I heard during the symposium, underscoring some highlights.

Then, we now have 6000 entries in the AmP collection, 2000 more than in 2023, with a median Mean Relative Error of 0.04 for some 90000 data sets. I will discuss some problems, propose partial solutions and explain for a small selection of entries why they are remarkable from a biological or methodological point of view. This will be not that easy to detect when one skims rapidly through the collection. Examples are

a) ovoviviparous sharks incubate 1 or 2 yrs longer than data suggest, based on postnatal development.

Illustrating to need of theory to interpret data

b) why quite a few abj-entries have E_Hj very close to E_Hb as estimates, but this is not realistic and the result of absence of data on early growth.

Illustrating the need to detailed data to estimate parameters

c) slow growth can only be captured with a low somatic maintenance, with the need to make sure that the maintenance ratio remains smaller than one.

Finaly I make some remarks on possible future developments in DEB theory, linking levels of organisation and linking parameter values to eco-physiological properties.
Coral reefs, for instance, vary little in conditions over the seasons, which makes it likely that the inhabiting species have a low growth rate and so a low somatic maintenance.
By contrast, the growing season shortens towards the poles, which might relate to high maintenance on the basis of the waste-to-hurry principle.
A kind of inter-species variant of the Bergmann rule, where the intra-species variant is based on food density.
I expect new developments in the eco-evolutionary controls of the position of species in the altricial-precocial spectrum to supplements our earlier findings that
the cumulated total weight of neonates more or less equals the ultimate mother weight.
Altricial neonates tend to be relatively small and many with links to population dynamics

*Speaker

and trophic position, so to MacArthur's r/K-selection.
The aim is to build on the structure of meta-theory, by not only finding patterns in parameter values, but also patterns in these patterns
to improve our understanding of underlying evolutionary processes..

Keywords: AmP, meta theory, patterns in parameter values