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Position Paper

Making spatial-temporal marine ecosystem modelling better – A perspective

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ABSTRACT

Marine Ecosystem Models (MEMs) provide a deeper understanding of marine ecosystem dynamics. The United Nations Decade of Ocean Science for Sustainable Development has highlighted the need to deploy these complex mechanistic spatial-temporal models to engage policy makers and society into dialogues towards sustainably managed oceans. From our shared perspective, MEMs remain underutilized because they still lack formal validation, calibration, and uncertainty quantifications that undermines their credibility and uptake in policy arenas.

We explore why these shortcomings exist and how to enable the global modelling community to increase MEMs' usefulness. We identify a clear gap between proposed solutions to assess model skills, uncertainty, and confidence and their actual systematic deployment. We attribute this gap to an underlying factor that the ecosystem modelling literature largely ignores: technical issues. We conclude by proposing a conceptual solution that is cost-effective, scalable and simple, because complex spatial-temporal marine ecosystem modelling is already complicated enough.

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1. Introduction

Marine biodiversity is the foundation for marine ecosystem function and processes, providing goods and services and bringing substantial health, social and economic benefits to coastal communities and beyond. Worldwide, increasing direct and indirect human pressures on marine biodiversity threaten a sustainable future for coupled human-nature systems (e.g., Halpern et al., 2019). A stronger action is needed as marine and coastal ecosystem biodiversity loss is exacerbated by climate change (Arneth et al., 2020; e.g., Smale et al., 2019). With the simultaneous declarations of 2021–2030 as the Decade of Ocean Science for Sustainable Development and the Decade for Ecosystem Restoration, the United Nations has given the ocean science community a unique opportunity and imperative to work towards sustainable future oceans (Heymans et al., 2020; Ryabinin et al., 2019). This includes a more extensive use of spatial-temporal marine ecosystem modelling, a discipline increasingly recognized as an indispensable asset to aid natural resource assessments and marine ecosystem management (Brotons et al., 2016; Christensen and Maclean, 2011; IPCC, 2019; Link et al., 2011).

Marine ecosystem models help improve our understanding of the impacts of human activities, natural phenomena, and climate change on marine food webs (Heymans et al., 2020; Stow et al., 2009). Offering the most comprehensive platforms to unify ecological processes with statistical insights and data-driven approaches (Ellis et al., 2020), complex, mechanistic ecosystem models are increasingly applied in ecological research, management advice, policy exploration, and environmental impact analysis under climate change scenarios (Borja et al., 2020; Fulton et al., 2015; Kytinou et al., 2020; Link et al., 2011; Peck et al., 2018; Serpetti et al., 2017). Ecosystem modelling integrates a wide range of disciplines (Fulton, 2010), including physical oceanography, biochemistry, food-web dynamics, risk analysis, decision making, economics and the social sciences (Fig. 1). For proper understanding of the interplay between species, habitats, natural phenomena, anthropogenic stressors and management actions, models are required that are inherently dynamical and spatially explicit, across temporal and spatial scales that can span several orders of magnitude (Hyder et al., 2015).

There is an urgent need for ecosystem models to rise to the Ocean Decade challenges (Heymans et al., 2020) by: i) making ecosystem modelling more accessible to decision makers and ocean managers; ii) bridging disciplines to meaningfully communicate marine ecosystem modelling sciences to the audiences that need it; and iii) ensuring that marine ecosystem models are co-created and co-designed with stakeholders to enhance their application. From our perspectives across various scientific disciplines, collected during an EuroMarine Foresight Workshop held in Barcelona in 2019, we argue that most modellers do not utilize their models to their full capacity. Consequently, in this paper we explore a fourth challenge: iv) solving the long-standing technical problems that prevent robust use of spatial-temporally explicit marine ecosystem models, and making their outcomes more credible.

While aspects of this discussion could apply to many of the complex modelling in different scientific fields, we focus on marine ecosystem models. These models span a broad range of model types and modelling philosophies. Nevertheless, they face common challenges. Consequently, for the sake of brevity, and unless explicitly stated, all modelling henceforth will refer to the use of complex, mechanistic, spatially and temporally explicit models that concern the dynamics of marine life and the influence of drivers of change. The models themselves will be referred to by their common acronym, MEM (Marine Ecosystem Model, Lotze et al., 2019). This class of models explicitly represent food web and spatial distribution processes that are driven by habitat and other environmental or anthropogenic factors.

Whereas non-spatial marine ecosystem models, and complex and computationally demanding global circulation models and hydrodynamic models have a long history of model benchmarking (Christensen and Maclean 2011), spatially-temporally explicit MEMs that represent complex energetic pathways have not made significant advances in this realm (e.g., Oliveros-Ramos et al., 2017; Pethybridge et al., 2019). Regarding prediction capabilities, the quantification of uncertainties and errors in MEM output is essential to identify model strengths and limitations, which provides the transparency needed to interpret, communicate, and apply model results (Bennett et al., 2013; Hyder et al., 2015; Stelzenmüller et al., 2018; Uusitalo et al., 2016). This topic

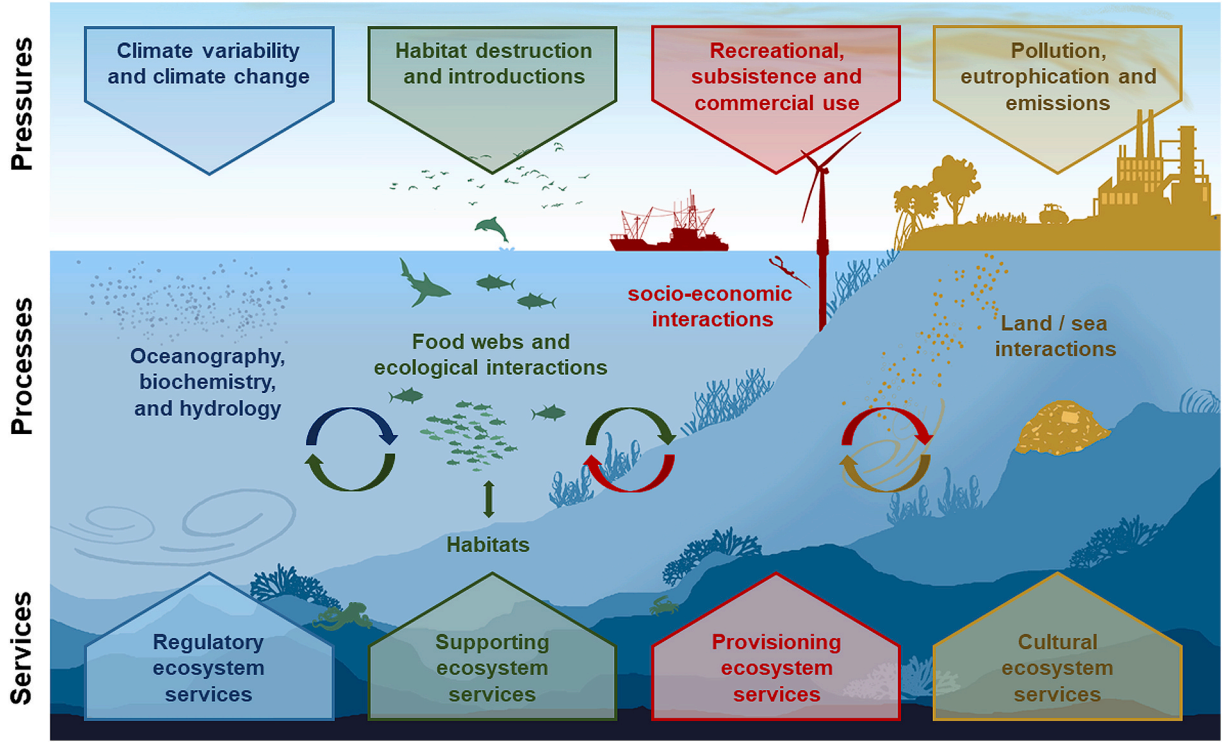

Fig. 1. The range of interconnected pressures, processes and ecosystem services that complex spatial-temporal marine ecosystem models may consider.

is a recurring and persistent concern, despite a discussion extending back to the early 1980s (Hamel and Bryant, 2017; Pennekamp et al., 2017; Rounsevell et al., 2021).

Even though there is a wide array of suggested methodologies and potential frameworks to improve the use of MEMs (Hipsey et al., 2020; e.g., Robson et al., 2018), their applications is rarely described in the literature (Pethybridge et al., 2019) despite the number of papers calling for comprehensive model validations, assessment of the various types of uncertainty, and calibration (Fulton, 2011; Grüss et al., 2017; Hipsey et al., 2020; Rose et al., 2010; Schuwirth et al., 2019; Stelzenmüller et al., 2018; Stow et al., 2009). Only recently have efforts started appearing to ensure MEMs are ecologically realistic and can replicate observed spatial and temporal patterns (Link et al., 2020; Moullec et al., 2019; e.g., Oliveros-Ramos et al., 2017; Petrik et al., 2020; Püts et al., 2020).

What would be the needed steps to execute systematic assessments such as calibration and validation of a spatial-temporal marine ecosystem model, and why has it proven so hard to implement widely? From our shared perspective, we contend that to improve the outcomes and confidence of MEMs, we must address one of the most basic issues that confront marine ecosystem modellers: technical limitations that prohibit the systematic mass-execution of MEMs to perform these assessments (Fig. 2).

We review the required steps highlighted and occasionally applied in the literature to perform robust ecosystem simulations. We explore the technical challenges that complicate the implementation of robust simulations. We conclude by proposing a conceptual solution that is cost-effective, scalable and – most importantly – simple to facilitate global uptake.

2. Review

2.1. Skill assessments

First, one needs to be able to quantify how well a MEM reproduces relevant historical ecological and socio-economic trends using available data. This analysis is captured broadly under the term "skill assessments", where MEM skill is appraised by comparing the residuals between model output and observations using quantitative metrics (Stow et al., 2009).

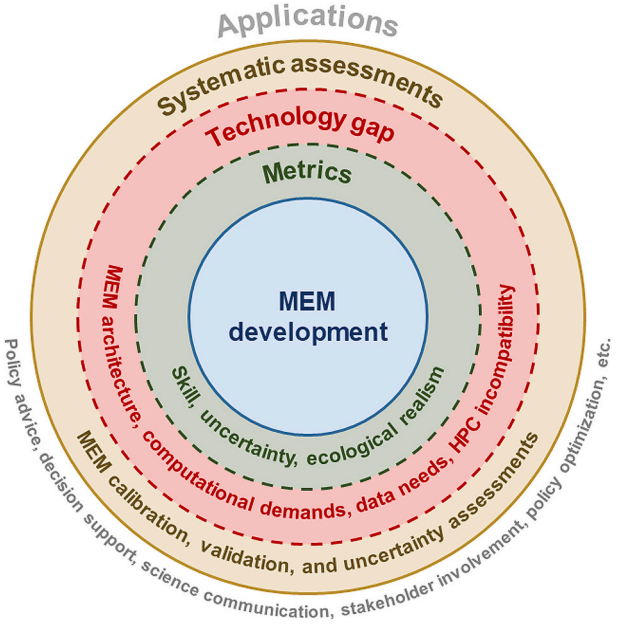

Fig. 2. The state of mechanistic, spatial-temporal explicit ecosystem modelling in a nutshell. The literature offers many metrics to assess ecosystem models, but due to a technology gap, the Marine Ecosystem Modelling (MEM) community is largely unable to perform systematic assessments. These are needed to contribute model output with confidence to real-world applications. The acronym HPC stands for High Performance Computing.

The literature provides many suggestions for metrics and their application to assess the skill of models to reproduce observations, as reviewed by Bennett et al. (2013) and Hipsey et al. (2020). Traditional skill metrics encompass univariate and multivariate statistical approaches (Diele and Marangi, 2020; Matott et al., 2009; Stow et al., 2009), but their focus on quantifying adherence to observations makes statistical approaches less useful to explain ecological behaviour (Olsen et al., 2016; Pennekamp et al., 2017). Therefore, to obtain deeper insights into the ecological patterns and processes within MEM output, system-wide metrics should be included which assess emergent properties such as ecological patterns in marine food webs, network structures (Fath et al., 2019), and commonly accepted ecological indicators (Coll and Steenbeek, 2017; Olsen et al., 2016).

Assemblies of skill metrics (Gupta et al., 2012; Olsen et al., 2016; Stow et al., 2009), or multi-level skill metrics (Hipsey et al., 2020) unify several approaches into information-rich skill assessment frameworks. The choice of skill metrics is highly dependent on model structure, available data, ecological understanding, the spatial and temporal scales over which modelled processes play out (Fulton et al., 2009), and the purpose for which a given model was built (Bennett et al., 2013; Olsen et al., 2016; Uusitalo et al., 2016).

In the realm of marine ecosystem modelling, skill metrics are extensively used in model validation and time series fitting exercises for non-spatial MEMs. In contrast, comprehensive skill assessments for spatially explicit MEMs are mostly absent from the literature.

2.2. Uncertainty

Second, there is the issue of uncertainty, which propagates through the non-linear processes and feedbacks in complex models and may overwhelm significant trends in model output (Fulton et al., 2003; Link et al., 2012). As such, uncertainty warrants comprehensive identification, quantification, and communication for interpreting results and assessing MEM skill (Uusitalo et al., 2016). There are four main types of uncertainty in complex deterministic models (Payne et al., 2016) as laid out below in the order of model development and execution. These have not been addressed equally, with much of the modelling literature focused on parametric uncertainty until fairly recently (Wang and Grant, 2019):

1. Structural uncertainty – or model uncertainty - derives from the equations used to construct a model and the implicit hypotheses they represent. MEMs are inherently subject to structural uncertainty due to their simplification of complex ecosystem dynamics (Collie et al., 2016) and parameterizations (e.g., Anderson et al., 2010). Insights into the impact of structural uncertainty can be garnered through ensemble modelling approaches (Lewis et al., 2021; Lotze et al., 2019), flexibility in the coupling between biophysical forcing and ecosystem models (Tittensor et al., 2018), and flexibility in the inclusion of ecological mechanisms within complex models (Audzijonyte et al., 2019; Coll et al., 2020). Hybrid models that adaptively switch the mathematical representations of sub-models to best suit the state of an ecosystem (Gray and Wotherspoon, 2015), are a promising yet underexplored approach for addressing structural uncertainty.
2. Initialization and internal variability (IIV) uncertainty relates to the uncertainty in adequately representing the initial conditions, temporal variabilities, and numerical sensitivities within complex models that may lead to "deterministic chaos" (Anderson et al., 2010). Promising approaches include adopting a modular design to model construction that allows for bypassing internal computations with the advice from dedicated expert models (Christensen et al.,

2014; Coll et al., 2020; Steenbeek et al., 2016). Climate models quantify IIV uncertainty by starting models at different times with different realizations (e.g., Nadiga et al., 2019), which is hard to achieve for marine ecosystem models that have much more complex starting states to represent the living components in the system (e.g., Skogen et al., 2021). This difficulty is exacerbated by the much sparser nature of ecological data, which has yet to achieve the precision and coverage of physiochemical ocean properties. As such, beyond the use of burn-in or spin-up periods to address the impact of initialization uncertainty, lack of explicit discussion in the literature leads us to believe that IIV uncertainty is a largely under-explored area in marine ecosystem modelling (e.g., Woodworth-Jefcoats et al., 2019).

3. Parametric uncertainty refers to how perturbations in input parameters - or in abstract parameters (also called tuning parameters or hyperparameters) that bear no direct ecological relevance - can influence model outcomes. For input parameters, this type of uncertainty is commonly explored by varying these parameters according to pre-defined plausible ranges and shapes based on *in-situ* measurements and observations, or on ecological theory such as species' functional responses to environmental drivers (Austin, 2007), while state-space models offer potential to calibrate abstract parameters (Spence et al., 2021). Full parametric uncertainty assessments are impossible for complex ecosystem models (Gaichas et al., 2012), but comprehensive assessments, such as Management Strategy Evaluation (MSE) where the impact of parameters that reflect ecologically viable ecosystem states are explored (e.g, Mackinson et al., 2017) are mostly confined to non-spatial models. For more complex models, adaptive parameter sensitivity screening (Pantus, 2007) may serve to greatly reduce the number of needed parametric uncertainty iterations. Uncertainties in observations (Skogen et al., 2021) and driver data (Coll et al., 2020) can be considered as parametric uncertainty too, and should be treated as such in uncertainty assessments.
4. Scenario uncertainty relates to the inability to accurately define future contexts within which the dynamic conditions captured within a MEM play out. This type of uncertainty can be addressed by conducting scenario analysis, i.e. exploring alternative paths along which the future might unfold (Van der Heijden, 2005), and running models for ranges of possible futures. This allows for exploration of upper and lower bounds to assumptions regarding socio-economic pathways and climate change, thus obtaining a bandwidth of predictions for possible futures (de Mutsert et al., 2021; Hamon et al., 2021; Lotze et al., 2019; Maury et al., 2017). Closely related is the uncertainty in making ecosystem predictions for future conditions, based on present and past conditions. It is widely acknowledged that a MEM's ability to replicate the past (explanatory prediction) is by no means a guarantee that it can accurately predict the future (anticipatory prediction) under combinations of parameter values that have not yet been encountered (Olsen et al., 2016; Pennekamp et al., 2017). In ecosystem modelling, this challenge is typically addressed by partitioning observational data into a historical part for training and forecast portion for testing. However, Pennekamp et al. (2017) argue against this approach, stating that training data and test data should be independent, and that the "gold standard" of prediction is a transferrable model that can genuinely predict a novel state of a system. MEMs such as Atlantis (Audzijonyte et al., 2019), OSMOSE (Shin and Cury, 2004), and Ecopath with Ecosim (Christensen and Walters, 2004) strike a balance, offering transferrable equations and ecological assumptions to describe generic ecological processes (Cuddington et al., 2013), but requiring location and time-specific empirical data to parameterize for a specific ecosystem.

MEM ensemble modelling, where multiple MEMs, each with their strengths and weaknesses, are forced under shared drivers of change, is seen as another "gold standard" for projecting the magnitude and distribution of the impacts of changing environments and anthropogenic activities. Ensemble modelling is increasingly applied (Lotze et al., 2019; Piroddi et al., 2021; e.g., Tittensor et al., 2018) and aims to side-step uncertainty related issues by obtaining average projections across a range of different ecosystem models – an approach that commonly outperforms any single model (Rougier, 2016). However, Spence et al. (2018) argue that using multiple model averages is not a guarantee to provide the best prediction, as discrepancies in each of the models are not independent. They demonstrate that statistical meta-modelling allows focussing on individual models strengths in an ensemble approach, drawing benefit from fundamental differences in underlying structures in each of the models, with the potential to reduce the impact of structural and parameter uncertainty.

2.3. Ecological realism

Third, it must be possible to quantify whether an ecosystem model produces results that are based on ecologically plausible parameter sets, as correlation between model output and observations does not guarantee a model will adhere to natural processes (Anderson et al., 2010) – i.e. that it is correct for the right reasons. These emergent properties of MEMs are equally important for model credibility as comparing predicted and observed values. Thus, models should adhere to basic expectations about their input parameterization, such as mass-balancing constraints (Heymans et al., 2016), expectations of the spread of biomasses and vital ratios across trophic levels (Link, 2010) and reproduction of a myriad of observed "meta-patterns" with ecosystems (Monbet, 1992; Schwinghamer, 1981; e.g., Sheldon et al., 1972). More generically, multi-level skill metrics can quantify the ability of a model to capture relevant processes at the population, food web, and ecosystem level (Hipsey et al., 2020; Lewis et al., 2021), with potential applications for Machine Learning approaches (Williams et al., 2014).

Assessing ecological realism of state variables within a running MEM is much trickier, and leaves open the debate whether a model's ability to reproduce observed trends is ecologically realistic, or a merely numerical artefact (Arhonditsis and Brett, 2004), exacerbated by the general equifinal (Hipsey et al., 2020) and underdetermined (Anderson et al., 2010) nature of ecosystem models. Safeguarding internal ecological realism can be improved through careful selection of the geometric numerical integrations used within a MEM (Diele and Marangi, 2020). For MEMs that are open to code modifications, internal state variables (for instance, related to consumption, displacement, recruitment, niches, mortalities, etc.) can be added to the list of model outputs, thus enabling independent validation of the internal state of a model while a MEM executes.

Ecological validation of spatial-temporal models greatly increases data demands. Bounds for processes for which no empirical data are available can be estimated from literature (Hamel and Bryant, 2017) or can be approximated through "simpler" sub-models such as models of intermediate complexity (MICE, Plaganyí, 2007), non-deterministic models (Mullon et al., 2009; Planque et al., 2014) that focus on specific processes, or complex models that focus on sub-regional dynamics (e.g., de Mutsert et al., 2017).

2.4. Model calibration

Last, there is the crucial issue of how to improve the calibration of a MEM. Calibrating is the process of adjusting input parameters to obtain the best fit between model output and observed values (Arhonditsis and Brett, 2004). Whereas simple or non-spatial ecological models are analysed and optimized regularly with automated tools, complex process-based spatial-temporal ecosystem model calibration is largely a manual effort guided by intuition (Anderson et al., 2010), expert opinion (Krueger et al., 2012), and limited, ad-hoc analysis (Anderson et al., 2010; Pethybridge et al., 2019) or brute-force Monte Carlo approaches. Spence et al. (2021) demonstrate that fitting a model to more or longer time series of observations will reduce the uncertainty in abstract

parameters, but cannot counter the uncertainty in input parameters, thus indicating that abstract parameters such as the vulnerability parameter in Ecopath with Ecosim (Christensen and Walters, 2004) may be more suitable targets for model calibration than input parameters. Adaptive screening (Pantus, 2007) and press-perturbations (Hipsey et al., 2020) are comparatively less demanding approaches to identify the most sensitive parameters, after which sensitivity tests and ecological realism tests can further identify candidate variables for improving a model fit. Multivariate comparison methods (Hipsey et al., 2020) and machine learning techniques (Williams et al., 2014) can reveal emergent patterns that may provide further clues to refining a models' behaviour.

3. Challenges

Naturally, assessing spatial-temporal models depends on the availability of large amounts of data that may be hard to come by. This is a legitimate and often acknowledged modelling challenge. However, experienced modellers can point to multiple cases where systematic validation does not occur even when more comprehensive datasets exist. This experience confirms that data (or the lack thereof) is not the sole (perhaps not even the main) bottleneck to the implementation of frameworks that systematically assess, validate, and improve outputs of MEMs. We rather highlight what is possibly the main hurdle to improving the parameterization of complex MEMs: prohibitive computational cost. Looking across the literature, only a few papers touch on the topic (e.g., Fer et al., 2018; Pethybridge et al., 2019). Whereas some of the most computationally demanding models, such as oceanographic physical-biogeochemical models, are validated in a systematic way, MEMs are not, suggesting that there are additional bottlenecks that prohibit MEMs from making similar advances. Here we identify the main technical bottlenecks.

3.1. Model architecture

The ability to access internal state variables, flexibility in the use of model assumptions, and flexibility in a model's scope are all rooted in how a model software is designed and implemented, with implications for the level of control modellers have to assess and improve their model's behaviour (Steenbeek et al., 2016). Despite a growing trend of specialization (Robson, 2014), marine ecosystem models are often being initiated by ecologists or mathematicians rather than computer scientists or software engineers. MEMs are mostly slowly developing emergent products of a research team's progressive work on addressing specific research questions. With some notable exceptions (Audzijonyte et al., 2019; Purves et al., 2013; Steenbeek et al., 2016), the choice of analytical framework, programming language, operating system and other implementation decisions tend to be dictated by the experiences within a research group. Consequently, MEMs are still rarely developed according to modern software engineering practices.

Publications that detail marine ecosystem model capabilities focus on equations, but rarely mention the design of the underlying software architecture and design principles that can provide invaluable insights in the true potential of a model. The lack of transparency is exacerbated by the fact that most MEMs do not provide access to their source code, limiting the ability to evaluate the inner workings and thus to systematically recalibrate such a model (Jardim et al., 2021; e.g., Steenbeek et al., 2016).

It must be noted that even where significant effort has gone into discussing the implications of particular design decisions, the capacity to revisit those decisions over the course of decades is often hampered by academic funding schemes. These look to new tools and novel applications, and expressly do not support code revision and large-scale overhauls of the kind, typical in commercial software products. Moreover, the open access motivation of scientific programmers means there is no licencing funds to draw on for such revision work either. While some of the global MEMs may be drawn into earth system modelling stables with support through funding arrangements oriented toward supporting global programs such as IPCC and IPBES, it is likely that regional models will remain in this funding scheme for the foreseeable future.

3.2. Computational costs

A major prohibiting factor to executing MEMs is computational complexity. MEMs incorporate a wide range of deterministic and stochastic approaches to represent discrete and continuous processes which can play out at vastly different temporal and spatial scales. This calls for use of a wide range of mathematical approaches that must interlink while a model iterates over time, especially when considering the ubiquitous presence of non-linear species interdependencies with feedbacks across the food web over space and time. While the implementation of individual mathematical solutions can be highly optimized in computer code, the need to connect different processes through non-linear interactions between species, changing environmental conditions and fisheries within a MEM means that the computational runtime of most MEMs can be reduced only to a degree.

When integrating climate hind- and forecasts, a running MEM requires access to many types of spatial-temporal explicit data that describes the relevant environmental changes over time. The volumes of required data can be ingested from pre-computed time series of maps or through one-way or bi-directional linkages with expert models. In return, MEMs produce volumes of spatial-temporal estimates related to species presence, densities, and inter-species interactions that require storage for further analysis. File access is one of the slowest aspects of high-performance computing (Harrington et al., 2017), which means that a MEM can appear computationally slow when, in fact, access to data storage is the limiting factor. This issue can be remedied in several ways, but it can be as simple as using different storage devices for reading and writing data, or by making technical provisions within a model's code.

High Performance Computing (HPC) is the *de-facto* standard to run complex models on dedicated hardware, but from the summary above it is obvious that unless a MEM is specifically designed to utilize the benefits of a specific cluster, high-performance hardware can only offer partial reprieve. Deploying model software on clusters can be complicated and may require technical assistance, and academic institutional access to HPC infrastructures is still limited, especially in the developing world (Moses Mwasaga and Joy, 2020). Most commercial HPC facilities allow only execution of software that is written to strict Application Programming Interfaces (APIs) to enforce security and prevent misuse, and use pricing models that are beyond academic budgets. Public scientific distributed computing efforts, including volunteer computing frameworks (Agliamzanov et al., 2019; e.g., Anderson et al., 2002), scientific clusters such as Galileo (Galileo, 2021), and open-source projects such as Ray (Moritz et al., 2018), allow scientific code to run in their original form but only cater to lightweight processes. Scalable distributed computing platforms that allow original code to run by packaging them in containers (e.g., Ahmed and Pierre, 2018) are equally suitable only for low processing needs and data volumes, while requiring considerable skill and some funding to operate.

4. Recommendations

We thus contend that although HPC offers significant benefits in processing power for running MEM validation and fitting frameworks, limited availability to academia means that they cannot be the focal platform for hosting a generic solution to solve the immediate challenges that the global MEM community faces. We pose that the global MEM community needs a technical remote execution framework that supports the simultaneous execution of multiple MEM simulations, where a desktop workflow is simply scaled up to be performed many times on available computers (Fig. 3), with minimal reliance on funding, programming skills, and HPC access, to facilitate global uptake and MEM

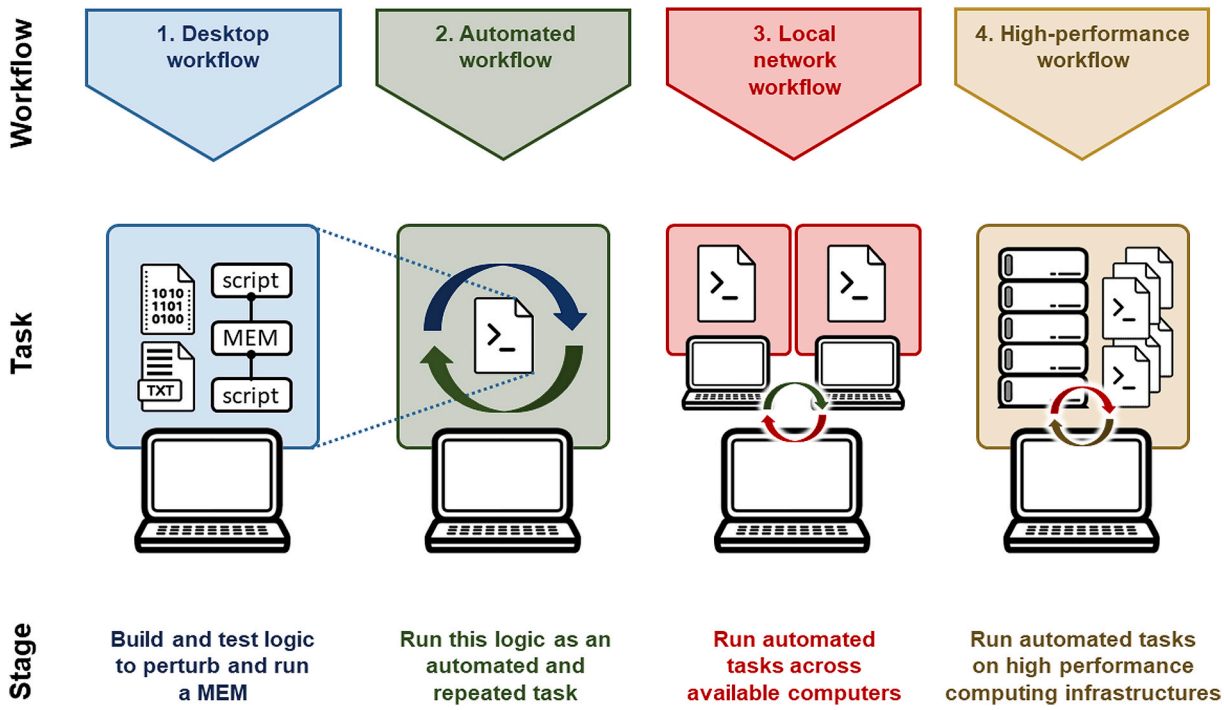

Fig. 3. A conceptual overview of a framework needed by ecological modellers to run demanding MEMs, where desktop workflows that involve the scripted running of a MEM (1) can be integrated into an automated assessment (2), which can be deployed over a local network of available computers (3) or even high-performance computing infrastructures.

capacity building.

We suggest that a remote execution framework should have a number of specific characteristics to enable simultaneous perturbation, execution and analysis of resource-heavy MEMs and their results. These characteristics include:

- **Generic**: a framework should support the execution of any scientific software, and should not be tied to any specific MEM or analytical software in order to facilitate the broadest possible uptake among the scientific community;
- **Simple**: a framework must be able to run models and statistical tools as they are (i.e. in their legacy form without substantial adjustment or redevelopment), as executed on a single desktop or workstation, just scaled up across a larger computing infrastructure and executed simultaneously. It is crucial that executed tasks retain their original form to focus on solving scientific problems, and do not have to be rewritten to meet specific demands of computing hardware architectures and their code frameworks;
- **Cross-platform**: a framework must be able to run on, and collaborate across, different operating systems;
- **Distributed**: a framework must be able to dispatch tasks, designed on a single computer, to multiple computers, processors or cluster nodes for simultaneous execution, with straightforward means of tracking progress of those tasks;
- **Self-sufficient**: a framework should be able to synchronize run instructions, possibly large amounts of driver data, skill assessment diagnostics, and model output without any manual intervention. It would be sensible to focus on incremental data exchange protocols to distribute run data across participating hardware; whether executables should be synchronized with the data needs to careful consideration as this could imply security risks and potential malicious use;
- **Fast**: models should run in close proximity to data storages to minimize file access delays, and potential bottlenecks (like file access latency) should be considered in the design of a framework;
- **Scalable**: a framework must be flexible to utilize changes in hardware availability;
- **Modular**: a framework should be built with unknown future uses in mind, adopting an modular architecture that will allow expanding its workings;
- **Open source**: the framework should be built on open-source software and should be 100% open source itself to provide transparency to its inner workings, to facilitate uptake, and to facilitate community development;
- **Low-tech:** in order to simplify its use, as little as possible knowledge about computer networking should be required to deploy and run a framework, beyond the knowledge required to run the required modelling tasks;
- **Cost-effective**: it is imperative that a framework can be deployed on any available hardware with minimal specifications to account for the uneven distribution of MEM capacity around the globe (Heymans et al., 2020).
- **Collaborative**: Ideally, the framework construction should also learn from the physical sciences and their large-scale collaborations to leverage the enthusiasm and resources of the MEM community rather than seeing individual research groups necessarily "go at it alone".

To our best knowledge, such a framework does not exist.

With a physical separation between a remote execution framework and available hardware and scientific applications (Fig. 4), a remote execution framework could be deployed to perform MEM validation, calibration and uncertainty assessments as follows:

4.1. Calibration

A MEM calibration exercise is a centrally controlled, iterative process. At the framework server, given a particular parameterization of a MEM, informed and optimized parameter perturbations lead to dispatched MEM executions across available remote computing capacity. On the remote computers, perturbed MEMs are executed and their

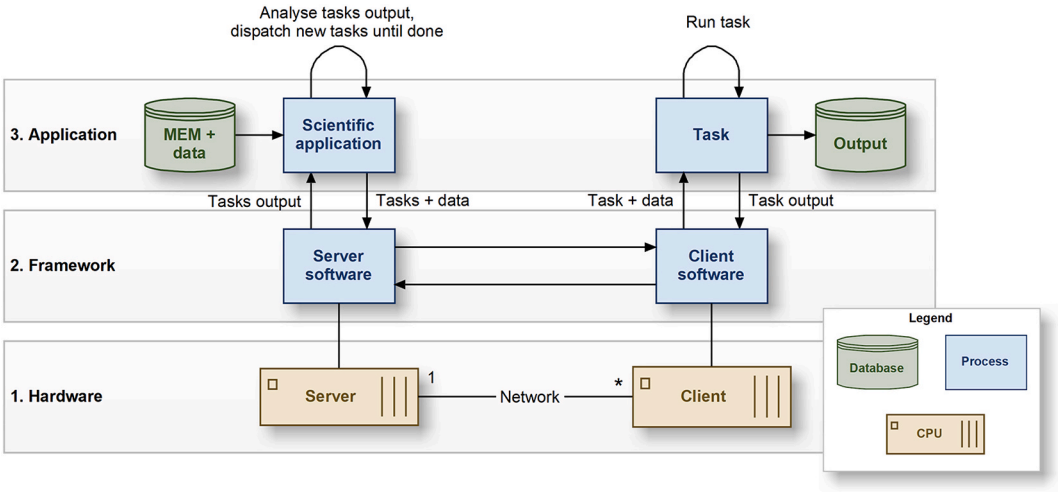

Fig. 4. Schematic overview of the physical separation of remote execution framework, the hardware that it is deployed on, and the scientific applications that use the framework. One server node connects to multiple clients. CPU stands for "Central Processing Unit", the core processing units in computers that execute software.

model skill to replicate observations is assessed under the new set of parameters. Better fits, for the correct reasons, are retained by the server, which keeps iterating until the calibration process has satisfactory converged. A calibration report should be available for the modeller to verify the process (Fig. 5).

4.2. Validation

A MEM validation exercise could benefit from available remote computing capacity to execute a MEM and assess its skill to replicate independent validation data while adhering to ecological realism. A validation summary should be available on the central server for the benefit of the modeller (Fig. 6).

4.3. Uncertainty assessments

In this work, we reviewed various types of uncertainty. Here, we hypothesise how the remote execution framework could be used to perform a limited structural uncertainty assessment. In this particular example, the aim is to find the combination of ecological hypotheses and environmental driver data to best approximate validation data. The outcome of this iterative process should be captured in a calibration report for modeller scrutiny (Fig. 7).

5. Conclusions

The field of ecosystem modelling is now making inroads in policy and decision-making arenas, but the success of ecosystem modelling efforts will ultimately depend on the quality of the models. Robust understanding of model strengths and weaknesses, and rigorous assessments and handling of error are needed in order to communicate and interpret model results with more confidence. As we outline in this work, the various building blocks to execute the needed assessments to obtain this robustness are readily available. However, the marine ecosystem modelling community is still lacking the foundation to systematically obtain these robust insights. For this, we need technical solutions to mass-execute resource-heavy ecosystem models across available computing hardware to provide the capacity to leverage new methods (such as machine learning) or methods from other fields and make the process of modelling better.

A generic framework catered to the execution of resource-hungry software, such as spatial-temporal marine ecosystem models, will

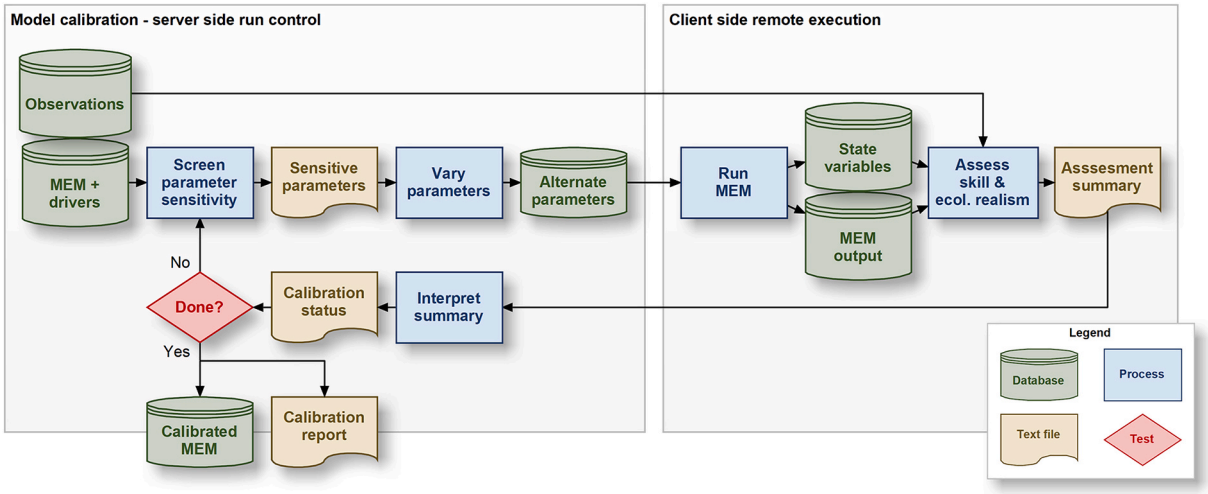

Fig. 5. Conceptual diagram how a model calibration exercise could be deployed via the remote execution framework. At a central server, parameters are screened for sensitivity, and alternate parameters are chosen. Remove clients execute the model with alternate parameters, and assess the model skill and ecological realism. Assessment summaries are sent back to the server where they are interpreted for next iterations until the calibration process has converged satisfactory.

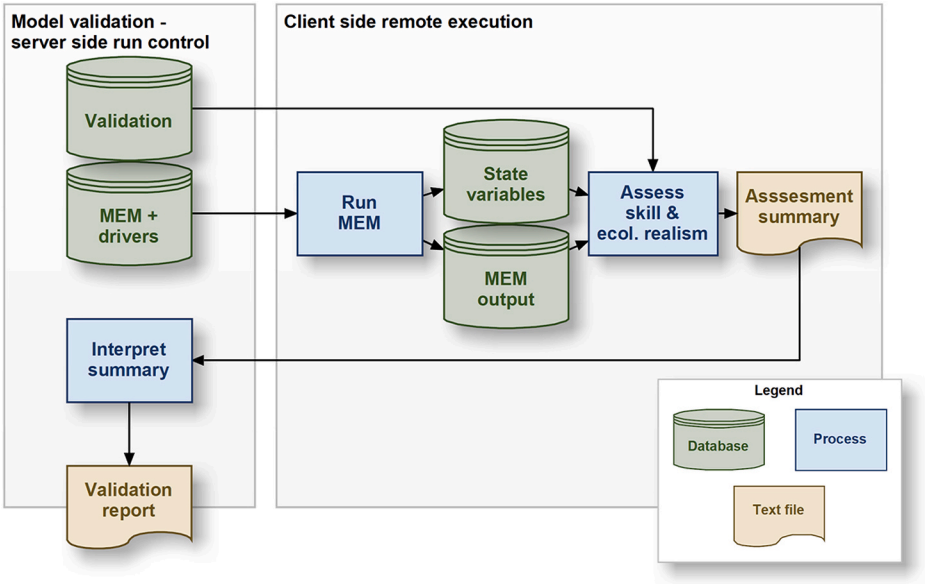

Fig. 6. Conceptual diagram how MEM validation could be deployed via the remote execution framework.

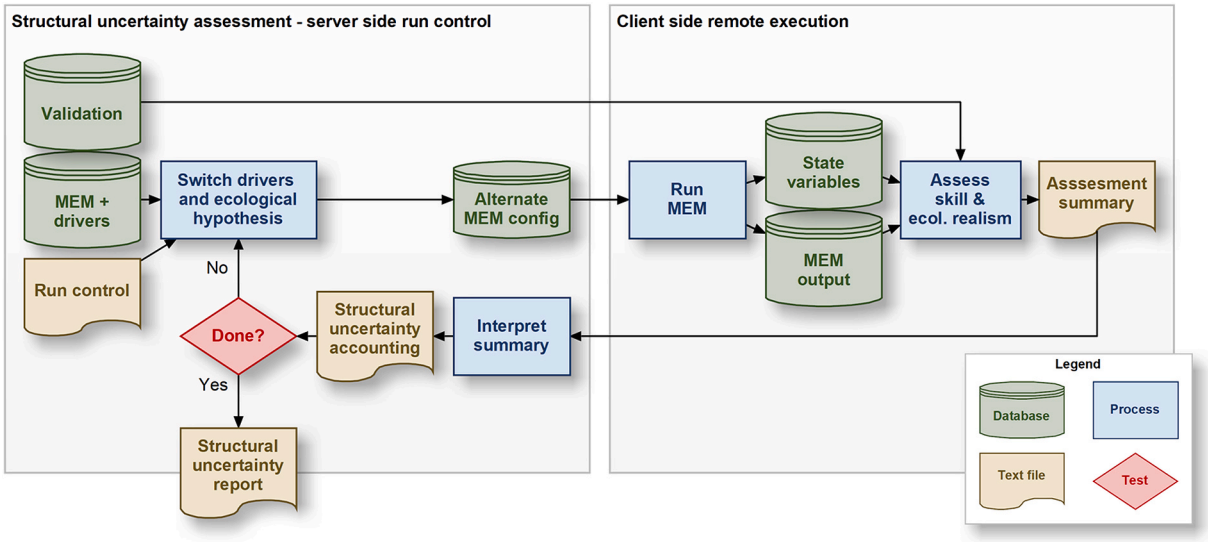

Fig. 7. Conceptual diagram how a limited structural uncertainty assessment could be deployed via the remote execution framework. At a central server, combinations of different climate change drivers and ecological hypotheses internal to the MEM are explored to find the combination that best fits validation data. The task of selecting combinations of drivers is performed by the server, and remote client computing capacity is used to execute the perturbed MEMs and to assess the model skill. Assessment summaries are collected at the server. The process should repeat until all most logical combinations have been tried.

prove highly useful to the modelling community (and potentially other resource-hungry processing), and can become the foundation to allow ecosystem models to fully live up to the challenges raised by the declaration of the Ocean Decade (Heymans et al., 2020). With the increasing need to apply ecosystem modelling in Digital Twins of the Oceans (Nativi et al., 2020) and scenario building (e.g., Ferrier et al., 2016), and the emergent potential for integrating big data, artificial intelligence and machine learning approaches into mechanistic ecosystem assessments (e.g., Guidi et al., 2020), a generic capacity to use MEMs with more confidence is paramount.

We contend that this framework must scale up workflows that scientists are familiar with to make using the framework simple, and the framework must work with any existing hardware to reduce costs. Last, to lower the technical thresholds to adopting such a framework and to facilitate capacity building in the use of MEMs around the world, the framework should be built on simple technologies that scientists are already familiar with, because complex spatial-temporal marine ecosystem modelling is already complicated enough.

Accessible information is key to good evidence-based decision making. While the framework proposed here would not automatically address communication and interpretation, it would directly address the need for reliable information sources that (i) do not require prohibitive resources to generate; (ii) meaningfully bridge disciplines and span socioecological systems; and (iii) allow for participatory modelling and coproduction of ocean solutions (Steenbeek et al., 2021, 2020).

While it may sound like a fanciful wish list, we believe it is possible given the success of GitHub, OpenStack, Apache Spark and a range of other distributed frameworks comprised of predominantly open-source approaches that would have been thought impossible until in place. We do not doubt the framework will not spring into being full-formed, but will need to evolve through incremental applications. It may well be that expectations and requirements will have to be adjusted

throughout iterations of development. Nonetheless, we feel it is important to share our full vision and begin working towards it in order to give MEMs the critical mass and credibility needed to help deliver the solutions required in addressing the many challenges already facing the world's marine ecosystems.

We challenge the ecosystem modelling community to construct this framework, which will empower the community with the foundation for building the tools to make better use of the outcomes of spatial-temporally explicit marine ecosystem models. In turn, this will see modelling more fully realise its capacity to help communities, regional and national bodies to take ownership of their ocean resources, and realise the transformational solutions needed to achieve sustainable and equitable ocean-based futures.

Author contributions

JS conceived and lead the study and wrote the MS. All other authors participated in the EuroMarine Foresight Workshop, added perspectives from their respective disciplines and contributed to crafting the final paper.

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Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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