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HORIZONS

Plankton digital twins—a new research tool

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Digital twins (DT) are simulation models that so closely replicate reality in their behaviour that experts may believe model output to be real. Plankton offer worthy yet tractable biological targets for digital twinning, due to their relatively simple physiology and significant role in ecology from theoretical studies through to planetary scale biogeochemistry. Construction of dynamic plankton DT (PDT), representing a supreme test of our understanding of plankton ecophysiology, would form the basis of education and training aids, provide platforms for hypothesis setting/testing, experiment design and interpretation, and support the construction and testing of large-scale ecosystem models and allied management tools. PDTs may be constructed using concepts from systems biology, with system dynamics, including feedback controls akin to biological (de)repression processes, to provide a robust approach to model plankton, with flexible core features enabling ready and meaningful configuration of phenotypic traits. Expert witness validation through Turing Tests would provide confidence in the end product. Through deployment of PDTs with appropriate input controls and output (visualization) tools, empiricists are more likely to engage with modelling, enhancing future science and increasing confidence in predictive operational and also in long-term climate simulations.

KEYWORDS: Simulation; digital twin; plankton; Turing Test

INTRODUCTION

Simulations provide a tool to test understanding and explore “what-if” scenarios. The ultimate simulation model would provide a digital twin (DT) of reality (Wright and Davidson, 2020). DTs are typically exploited in some form of decision support tool (DST), with various branches of science and business relying heavily on such approaches (Cimino et al., 2019; Erol et al., 2020; Liu et al., 2021; Phanden et al., 2021; Shao and Helu, 2020; Tao et al., 2019). For ecological and climate change science, simulation models are the only tools available (Bauer et al., 2021) but ecological applications of DTs (Nativi et al., 2021) remain a developing arena (Blair, 2021). Here, we consider digital twinning of plankton for research and management applications in freshwater and marine systems. To aid the reader, Table I provides definitions for technical terms.

Plankton research is a sprawling discipline involving a myriad of organisms, very few of which are understood in any detail, living and interacting in a complex 3D environment. Much effort is directed to identification of organisms, where they are and, critically, what they are doing. Molecular biology cannot provide detail on what they are doing (Liu et al., 2017; Strzepak et al., 2022); determining contributions of plankton to different processes (McLeod et al., 2021; Ozaki et al., 2019) requires knowledge of rate processes with numeric modelling to contextualize those rates. We need to bring information from biochemistry and ‘omics together with simulation modelling to progress, helping us interpret empirical data (Westerhoff et al., 2009; Figs 1 and 2). Digital twinning provides a focus for such developments.

While simulation models should by definition replicate reality, plankton models are typically extremely simplistic. Most conceptual cores date from the 1960’s to 1990’s (Droop, 1968; Shuter, 1979; Fasham et al., 1990; Evans and Garçon, 1997; see Anderson and Gentleman, 2019), with interactions between laboratory and field studies (Fig. 3). Most enhancements have been focussed on (Pahlow and Oeschlies, 2009; Smith et al., 2016), or dominated by (Cael et al., 2021; Follows et al., 2007; Lindemann et al., 2017), phytoplankton models. Piecemeal developments have carried risks of reuse of equations without verifying that they remain appropriate for the task at hand (Smith et al., 2014; e.g. coupling N and P ignoring associated physiological interactions—Flynn, 2008; Pahlow and Oeschlies, 2009; Sharma and Steuer, 2019). Grazers continue to be described using inappropriate approaches viewed through the lens of zooplankton ecophysiology (Everett et al., 2017; Flynn et al., 2021; Mitra et al., 2014). Descriptions of bacteria, viruses and mixoplankton are

conspicuous by their absence (Glibert and Mitra, 2022; Mateus, 2017).

An expert in empirical plankton science would have little trouble locating questionable aspects of a model output claimed to represent a particular planktonic system, which raises concerns as to the veracity of science stemming from those outputs. Plankton theoretical ecology also exploits models far removed from conforming to a DT; the extreme simplicity facilitates the establishment of analytical solutions, bifurcation and tipping points, etc. (Cuesta et al., 2018; Song et al., 2020). While not necessarily meaning that the emergent theory is flawed, if the concept had been explored using DTs, then it would be more robust set against real world expectations. Similar arguments run for ocean simulators; plankton sub-models, each individually that fail objective testing, do not necessarily mean that the ocean simulation fails, but if the components are questionable, then so must also be the product of those components. To become more credible, plankton models need to improve and strive to become DTs.

THE CORE OF THE PLANKTON DT

Organisms show great diversity but they are based on components sharing great commonality. A DT could exploit such modularity, enabling phenotypic features to be readily modified without requiring a radical rebuilding for each plankton model. This is akin to an engineering space-frame concept, where structures are easy to adapt with limited risk of critical failure. In contrast, most plankton models are akin to monocoques—lightweight efficient structures that are difficult to repurpose without radical redesign.

Systems biology concepts provide an obvious basis for developments, describing biological processes in a holistic (rather than a reductionist) fashion (Voit, 2013), from molecular biology through to whole organism physiology including models (Fig. 1). All systems biology applications have coarse-grain components (related to features such as stoichiometry; Inomura et al., 2020), with fine-grain detail only for explicit descriptions of individual processes, enzymes, metabolites, etc. (Sharma and Steuer, 2019). Interactions between physiological modules are achieved via feedback and feed-forward mechanisms akin to those mediated in reality by (de)repression processes (Flynn et al., 2015), which may be aligned with metabolomic signatures. Such signatures *in vivo* provide measured responses to stimuli providing robust models *in silico* (Fasham et al., 2006; Flynn et al., 1997; Mitra and Flynn, 2007). In contrast, most plankton models exploit passive equilibrium optimization controls

Table I: Definition of terms used in this work (terms in italics are defined elsewhere in the table)

Term	Explanation
Decision Support Tool (DST)	A framework, often supported by outputs from a computer programme, to optimize a management or other operational strategy. DSTs may be as simple as a look-up table or decision tree, or as complex as a <i>DT</i> enabling near-real-time analysis of options.
(de)repression	A biological control mechanism, usually involving feedback, through which physiological (biochemical, behavioural) processes are modulated by being gradually enabled (de-repressed) or disabled (repressed).
Digital Twin (DT)	An <i>in silico</i> representation of reality that may range from being static (e.g. geological structure) through to highly dynamic (aircraft in flight). Dynamic versions are often associated explicitly or implicitly with a <i>Decision Support Tool</i> to guide an intervention. DTs may be differentiated from a simulation model by the presence of an interface to enable a non-specialist to interact with the model and to explore features beyond the data originally used in model validation in a predictive or “what-if?” mode, perhaps in real time.
Dysfunctionality	Behavioural trait of a model that is contrary to expectation, as distinct from being absent through simplification (as per Flynn, 2005, 2010).
Dunning-Kruger effect	Cognitive bias that leads to an overestimation of one’s ability.
Empirical	Based on observation (e.g. field, laboratory) rather than through theory or logic. Empirical data may be subject to subsequent transformations or manipulations based upon theory or logic, but the data are not synthetic as generated by a model.
Expert Witness Validation (EWW)	A means to validate the performance of a numeric model by exploiting a form of <i>Turing Test</i> , asking of experts in the real world system “does this model output so-closely resemble reality that you could be fooled by it?” EWW minimizes the risks of <i>over-fitting</i> by explicitly considering the full breadth of phenomenological understanding.
Grain	Level of detail; fine grain for <i>systems biology</i> may describe individual biochemical processes, while coarse grain may refer to elemental stoichiometry.
Model	A simplification of reality, ranging from abstract to physical, static to dynamic, including mathematical constructs from statistical fits to <i>numeric models</i> that may be hypothetical, through to simulations and <i>DT</i> . Data generated by a mathematical model are synthetic rather than <i>empirical</i> .
Numeric model	A mathematical model that uses a complex series of equations, often involving differential calculus to described events changing over time as used in simulations.
‘omics	Molecular biological suffix (e.g. <i>genomics</i> , <i>transcriptomics</i> , <i>proteomics</i> , <i>metabolomics</i>) of terms for biological molecules that characterize organismal structures and functions.
Over-fitting	A consequence of fitting or <i>tuning</i> a model (especially a statistical model) that, because it describes a particular data set too closely, is then unable to reproduce the general case.
Simulation (model)	The output of a <i>numeric model</i> that provide an approximation of a real world process at least over the conditions under which it was validated (cf. <i>DT</i> , <i>validation</i>).
Systems biology	Computational analysis and modelling of complex biological interactions using a holistic approach (e.g. with explicit inclusion of <i>(de)repression</i> feedbacks), rather than the traditional reductionist approach of modelling in which simplification is a dominant feature.
System dynamics	A modelling approach characterized by feed-back, feed-forward interactions developed for simulating especially complex numeric data-poor situations.
Technology Readiness Level (TRL)	A grading of maturity in technology development, ranging from TRL1 (basic research), via TRL5 (technology development/demonstration) to TRL9 (mature and fully operational); see Fig. 4 for an example.
Tuning	Optimizing the fit of (minimizing differences between) model output and external (usually real world) data series by the modification of parameters or constants present in the model equations. cf. <i>validation</i> .
Turing Test	A test of a machine’s (computer programme’s) ability to exhibit a level of intelligent behaviour similar to, and thus indistinguishable from, that of a human (Turing, 1950). cf. <i>EWW</i> .
Validation	A means of determining the veracity of a model output against external (usually <i>empirical</i> numeric) data series independent from those data used for <i>tuning</i> or optimisation. Often there are very few data available once those used for <i>tuning</i> have been excluded. See also <i>EWW</i> .

(Armstrong, 1999; Geider et al., 1998; Grossowicz et al., 2017), which do not lend themselves readily to the control of multiple resources (Elrifi and Turpin, 1985; Harrison et al., 1976) and can cause problems in simulating the dynamics of those interactions (Flynn et al., 2001).

MODELING CHALLENGES

Inevitably, the extra fidelity of a DT incurs additional computational costs, while the increase in parameters ostensibly available for tuning may raise fears that model performance is compromised through over-fitting

(Hellweger, 2017). However, with care, the state variable count can be minimized and overfitting is not such an issue for systems biology models as responses are constrained by explicit feedbacks. Thus, in the light-N–Fe interaction, phytoplankton model of Fasham et al. (2006), a medium-coarse-grain, systems biology model contrasting strongly with traditional crude phytoplankton description typified by Fasham et al. (1990), very few of the parameters notionally available actually warranted tuning.

While a fundamental feature of real life is the individual, most models of plankton are biomass based

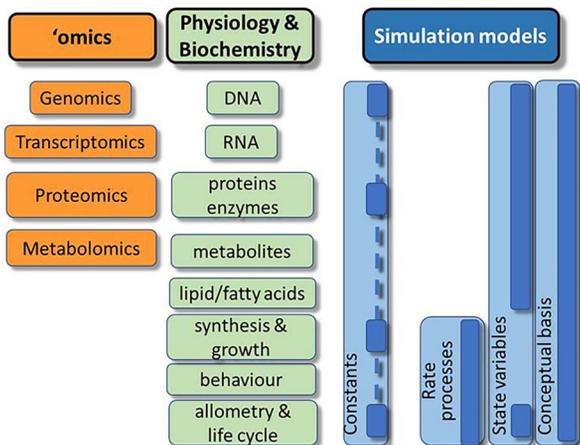


Fig. 1. Relationships between molecular biology ('omics), physiology and biochemistry, and simulation models. Alignments between these facets of biology are in the horizontal plane; thus, genomics aligns with DNA, which if included explicitly in models would constitute state variables (i.e. parameters with history). More often physiological features are controlled in models via constants encoding potential traits with fixed parameterization. Rates in models are calculated intermediaries. Note the lack of overlap between 'omics and the rate processes that dominate much of physiology (Liu et al., 2017; Strzepek et al., 2022) and that also align with features of simulation models. Systems biology provides an interface across these three approaches.

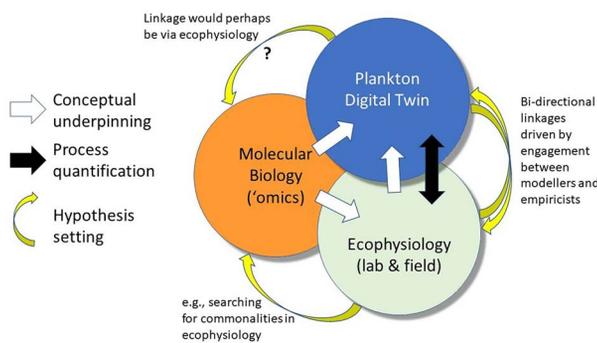


Fig. 2. Potential interactions between molecular biology, laboratory experimental and ecological ecophysiology, and the ultimate simulation model for plankton, the plankton DT. Ecology is an emergent function of biology and abiotic conditions. The linkage from 'omics to DT is most likely via ecophysiology, for support of the conceptual base of the twin; 'omics do not readily provide information on physiological rate processes' (Strzepek et al., 2022). See also Fig. 1 for interactions between these facets and Fig. 3 for placement in a historic context.

(Butenschön et al., 2016), with organism abundance calculated assuming a set biomass per individual. While studies of microbial cell–cell interactions could be studied in a digital laboratory with direct empirical insight from nanoSIMs technology (Pett-Ridge and Weber, 2021), pragmatically a routine use of individual based models (IBMs) describing millions of individual plankters L^{-1} may not be possible or necessary (cf, Lindemann et al., 2015). Agent-based model (ABM) formats, where

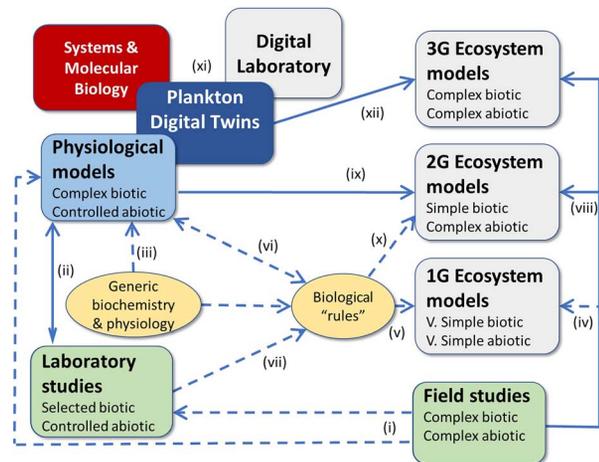


Fig. 3. Schematic for the development of ecosystem-facing plankton models. Conditions and biological composition at field sites inform field and laboratory studies (i). Information and data, from laboratory studies (ii), together with generic biochemical and physiological understanding (iii), enable the construction and testing of models describing the physiology (autecology) of organisms, and thence coupled models of simple trophic systems. Information flows (ii) from experimental to modeling research; *in silico* experiments may aid further rounds of laboratory studies. First-generation (1G) ecosystem models (typified by Fasham et al., 1990) contained much-simplified representations of the abiotic system (iv), together with very simple models of the biota configured from biological rules, (v) developed from general and theoretical principles, with some concepts developed from physiological models (vi), and data such as maximum growth rate estimates from laboratory studies (vii). Current, second-generation (2G), ecosystem models (viii) contain greatly enhanced abiotic descriptions, with some level of enhanced biotic description stemming from physiological models (ix) or from biological rules such as trait-trade-off assumptions (x). Development of DT (xi), exploiting systems biology approaches linked to molecular biology, tested in digital laboratories (which also provide a platform for theoretical biology and ecology science) provides the core plankton models for future (third-generation, or 3G) ecosystem models. Developed from Flynn and McGillicuddy (2018).

subpopulations of individuals are assumed to be in physiological and behavioural synchrony (Scheffer et al., 1995), are more plausible; these could still have explicit state variables for organism abundance ($N^{\circ} L^{-1}$) with allometry. For organisms with complex life cycles (including resting stages and diseased individuals), ABMs are more likely required to justify a credible DT label. Conceptually more challenging, can a DT be made of a Plankton Functional Type (PFT), an ecologically valid grouping (Gitay and Noble, 1997) of taxonomically disparate organisms? Pragmatically, large-scale simulators must operate using PFTs (Hashioka et al., 2013). A useful activity would be to run plankton DTs of multiple species/genus in a digital laboratory to generate high-resolution data (that could never be collected in the real world) against which we could test the consequences of groupings plankton species in different ways.

Introducing physiological detail for a DT may be considered a high-risk/low-reward exercise, and possibly as detrimental (Mitra et al., 2007); the inertia in continuing with what (sort of) works may be overpowering. The Dunning-Kruger effect may also operate with the subject arena dominated by researchers who, for whatever reason, fail to recognize that their models do not give appropriate descriptions of reality. Models have improved slowly. Well known as being incompatible with phytoplankton physiology (Geider and LaRoche, 2002) and trophic dynamics (Flynn, 2010; Sterner and Elser, 2002), the gradual rejection of Redfield ratios (Redfield, 1958) to an acceptance of variable stoichiometry in models has taken decades. Introducing plankton DTs may experience similar levels of resistance; the ultimate driver will be the demand for improved credibility by stakeholders.

THE ROLE OF THE EXPERT WITNESS

Determining how well a biological model performs is a major challenge (Brodland, 2015), a judgment call usually made by few anonymous scientists who are almost inevitably fellow modellers. An obvious challenge in building plankton DTs is the lack of suitable numeric data, and interpreting available data appropriately (Flynn et al., 2018). For organisms of biotechnological interest (Al-Hoqani et al., 2017; Butler et al., 2020), significant amounts of information may be available, although these organisms are often poor exemplars for plankton (Sabir et al., 2018). We need to engage the plankton scientists who are best placed to judge whether or not, for example, the “diatom” in an ecosystem model is indeed representative of any or all species of diatoms.

Much information is held at a phenomenological level by scientists we term, “expert witnesses.” Any attempt to produce a plankton DT requires buy-in from these expert witnesses. This commences with explaining the structure of models to that audience. Some form of code-of-conduct, standardization, in describing models may help, not just to support modelling (Grimm et al., 2006), but specifically to aid engagement with empiricists.

Exploitation of expert witness knowledge can proceed in two steps:

- 1) Detailed expectations can provide an initial check of model conceptual basis and behaviour, ensuring it conforms to a given plankton type without dysfunctions (Flynn, 2010).
- 2) Testing of the model by experts of the real-world system. This exploits an approach akin to the Turing Test (Turing, 1950), in which expert witnesses verify that the model behaves in a way that they find convincing.

For (i), as no DT could ever twin 100% with reality, some form of grading system may help, weighted for the importance of each characteristic in defining that organism’s ecophysiology. A level of objectivity and also subjectivity is required, acknowledging the variability in nature needs to be reflected in how models behave (Irigoiien, 2006) and that it is (to quote Keynes) “better to be roughly right than be precisely wrong”. The traditional notion of models only being used to answer the question posed at their inception (Yates et al., 2018) is far less likely to be applicable, or acceptable, with a DT.

Performing task (ii) requires a modelling platform with which the empiricist expert can readily interface, using some form of digital laboratory. Such an approach is not uncommon in hydrodynamic modelling, where known dynamical behaviours are tested against idealized scenarios (Penven et al., 2006; Debreu et al., 2012; Ilcak et al., 2012). A graphic user interface (GUI), needing no intimate understanding of computer coding nor direct access to specialized computing facilities, could make use of drop-down menus or sliders to select between parameter options. It would need to operate in units that an empiricist recognizes (invariably for plankton research, that includes numeric abundance).

The output display also needs consideration. Many plankton scientists never see clearly what they study; images of organisms below ca. 0.5 mm (most plankton are <0.05 mm) often lack well-defined physical features. Accordingly, plankton presence and activity are typically viewed in abstract form, via graphs. However, the greater realism of a DT likely demands a greater range of plots available from a user-friendly GUI. Gamification platforms could provide direct visualization of differences between plankton types and their interactions, recognizing the disproportionate importance in both biomass and productivity related to size (Finkel et al., 2010; Hansen et al., 1997). For example, diatoms are often placed in models as a single functional type (cf. Xu et al., 2020), despite their linear size range exceeding ca. 5–200 μm ; it is unlikely such an anomaly would be easily ignored if the graphic display was more in keeping with the data type (Steenbeek et al., 2021).

Given the ease with which computer graphics can persuasively misrepresent reality, perhaps we also need to make it clear when models are “inspired by true events,” rather than aspiring to a DT standard.

A ROAD MAP

The simplest applications of plankton dynamic DTs would describe a single microbe clone growing in a flask, replicating a classic wet laboratory setup, as a digital laboratory. Repeated and then combined for several

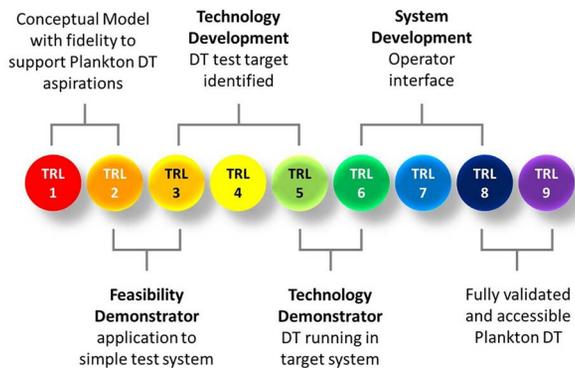


Fig. 4. Technology Readiness Level (TRL) schematic for DT development. For plankton DTs, expert witness validation, provided by those with empirical knowledge of the real system, is required throughout the process, ensuring the original concept design of the plankton model aligns with the deployment aspiration (TRL1/2), checking (validating) functionality at each development point, and contributing to design of the operator interface to produce the final product (TRL9). Progress from TRL1 to TRL6 may be restricted by a lack of appropriate data and understanding (see Fig. 2), which will become apparent only through attempting to develop the DT. This should not hinder initial efforts as the product will be subjected to revisions as science advances. Likewise TRL6–8 (operator interface) will undergo cycles of revision in response to user feedback, and will likely include instruction manuals and allied explanatory materials, disclaimers and caveats for deployment.

species, simple food-webs could be constructed in a digital mesocosm exploiting a suitable GUI. Plankton models individually accepted as DTs could then be operated together within more expansive physical descriptions, perhaps based on a representation of a cubic meter in a Lagrangian framework relatable to a limited geographic location, such as an oligotrophic gyre. Beyond that step, simulations would more likely operate using high-performance computers with more complex interfaces, but they would at least be conducted using descriptions of plankton that are themselves each considered (validated) as being well founded.

How far down the line are we with all of this? For biochemistry and physiology (autecology) of individual microalgae for commercial uses and allied DSTs (Flynn, 2021; Sharma and Steuer, 2019), we are perhaps at relatively high technology readiness levels (TRL, 5–9; Fig. 4). Building from these, at least for laboratory exemplars of plankton (e.g. *Dunaliella*, *Isochrysis*, *Oxyrrhis*), we could achieve TRL 4–7. The situation is rather different when we consider plankton DT applications within local, basin, or global scale models (TRL1,2?), and thence for management and planning (TRL1,2?). There are various barriers to overcome in implementing radical changes to Earth-system type of models, but this is where the real prize lays, and arguably for political and environmental reasons also where the application of plankton DTs is most important. Satisfying desires to better interface scientists with

policy makers and managers through exploiting models (Weiskopf et al., 2022) also requires modelling tools that are easily used and understood, and indeed also criticized.

CONCLUSIONS

We all need to have confidence in models used to guide management and the making of political decisions, as evidenced during the SARS-COV-2 pandemic (Eikenberry et al., 2020; James et al., 2021). The experience of the authors suggests that empirical plankton scientists may often not trust plankton models to represent reality in a useful way. Reasons for this situation are complex but building DTs by involving empiricists would improve that situation. A readily operable DT, in an appropriate technological or ecological setting, would represent a major breakthrough in plankton research, one that brings together knowledge (Figs 1–3) for emergent understanding, and one that highlights scope, and the need, for new research. Until ecology-facing funders are convinced of a need for DTs, progress is likely to be slow (noting, however, that the United Nations “Digital Twins of The Ocean” aspires significant progress during this decade—<https://ditto-oceandecade.org/>). However, as empiricists are required to actively engage with the building of plankton DTs, it is also likely that once started there will be a level of positive feedback across the science area to promote further development. We all learn much by mistakes, but we need first to see and recognize those mistakes; the bringing together of empiricists and modellers in dialogues that have long been recognized as lacking (Anderson, 2005; Everett et al., 2017; Flynn, 2005) in the attempt to build DT will at the least reinvigorate our science to the benefit of us all.

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