Calling for a National Model Benchmarking Facility

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Abstract

The modern world uses predictive computer models for many important purposes, including weather predictions, epidemic management, flood forecasting and warnings, and economic policymaking. We need to know how much we can trust the projections of these models, not only to achieve more accurate projections for systems, but also to undertake scientific learning about systems by incrementally testing hypotheses using models. But we routinely fail to adequately benchmark the performance of our complicated models of systems due to the cost and complexity of the task and owing to social and institutional barriers. Decades of lessons learned from Model Intercomparison Projects (MIPs) and similar community modeling efforts have yielded understanding of both the challenge and the opportunity facing 21st century model benchmarking efforts. To implement this understanding at scale, we call for the establishment of a major national research facility for scientific computer model benchmarking. Such a facility would institutionalize and properly resource the technically challenging and laborious work of computer model benchmarking, thereby establishing a firm foundation for 21st century science and prediction. This facility would advance basic science, overcome many of the social barriers to benchmarking, and would improve projections and decisions.

Keywords

Model benchmarking, research infrastructure, systems science, data science, model intercomparison, community science

Plain Language Summary

This opinion argues for the establishment of a National Model Benchmarking Facility (NMBF), a major research instrumentation that will advance systems science and computer modeling of systems by facilitating rigorous model standardization, publication, and benchmarking.

Key Points

Computer models of systems have become dauntingly complex, which is a barrier to scientific learning about systems.

Advances in model benchmarking and intercomparison demonstrate our technical capability to solve the problem.

A National Model Benchmarking Facility will accelerate systems science by institutionalizing computer model benchmarking.

Main Text

Challenges and Opportunities in Model Benchmarking

The modern world uses models of systems—especially predictive computer models—for many important purposes, including the earth science applications like natural resource management, weather predictions, climate change analysis, epidemic management, flood forecasting and warnings, and economic policymaking. Evaluation of model performance is an integral part of how we improve understanding and develop trust in model forecasts. However, models are developed for many different purposes, posing a challenge for evaluating and communicating what we commonly call "model trust". Model trust is built on communication, socialization, iteratively posing and testing hypothesis, and the scientific consensus formed around the results of well-documented and tested hypotheses (Chinn et al., 2018; Chabbi et al., 2017). However, as computer models have become more complex, voluminous, and interdisciplinary over the past 40 years, it has become increasingly difficult to apply the scientific method to test and compare alternative models of systems. Two high-level multidisciplinary and multiagency reports have detailed these serious challenges in the context of environmental modeling (Table 1, Beck et al., 2008; IHTM, 2020). These challenges and the potential solution hold true for all kinds of systems modeling.

Table 1: Challenges for environmental modeling summarized from Beck et al. (2008) and IHTM (2020)

GRAND CHALLENGES
How do we scientifically learn using models?
What cyberinfrastructure support is needed for widespread experimentation with model structure?
How do we robustly represent, report, and review model uncertainty?
How do we organize communities for model development?

TECHNICAL CHALLENGES
Standardization of data and models
Development of shared testbed problems
Model-data integration workflows

ORGANIZATIONAL CHALLENGES
Minimize duplication of effort
Reward systems acknowledging data and code sharing
A culture of interagency cooperation and open science
Collaboration of agency and academic scientists
Sharing resources across agencies
Adopting standards across agencies

There are good reasons why model builders increasingly struggle to rigorously and scientifically evaluate their computer models of complex systems.

1. First, model builders are usually disciplinary scientists and not experts at the theory or methods of scientific model evaluation.
2. Second, the complexity and opaqueness of models makes rigorous peer-review of large computer models far too expensive for volunteer reviewers.
3. Third, intercomparisons of model results among different models often reveal more about how well the models agree with each other than how the models correspond to reality (Huntzinger et al., 2013).
4. Fourth, employing the “deluge” of observational data to evaluate models is increasingly expensive and technically challenging (Schwalm et al., 2013).
5. Fifth, computer model evaluation tends to lag multiple development cycles behind model building (Dietze et al., 2018; Loescher et al., 2017).
6. Sixth, the intended function of the models may be different from their actual function in ways that are hard for the model builders to perceive (Clark et al., 2016; Tang and Riley 2018; Bisht et al. 2019).
7. Seventh, the complexity of models has made it difficult to isolate the contribution of an individual model component to the final model output and thereby test the constitutive hypotheses that comprise a model (Luo et al., 2015; Luo et al., 2012).
8. Eighth, model calibration using inadequate datasets and constraints results in equifinality and posterior uncertainty (Luo et al. 2017, 2019; Tang and Riley 2020).

A solution to many of these challenges is to formally apply model benchmarking through an expertly administered and fully resourced model benchmarking process. Benchmarking is the broad set of methods that support systematic comparison of a model’s inputs, outputs, algorithms, numerical solutions, functional responses, architecture, statistical uncertainties, predictions, and projections against both theoretical and applied model quality standards such as error, robustness, and parsimony. Benchmarking includes both “apples to apples” comparisons of the operational performance of multiple models, and rigorous testing of alternative scientific hypotheses embedded in each of the models (Bisht and Riley, 2019; Huang et al., 2018; Clark et al., 2015; Bellocchi et al., 2011; Anand and Kodali, 2008; Kirchner 2006; Kirchner et al., 1996; Holm et al., 2020). Rigorous benchmarking of scientific models would go a long way toward clarifying how much—and in what specific ways—we can trust each model’s predictions.

Fortunately, the science of model benchmarking has come a long way in the past two decades. In the past, models were commonly benchmarked by comparing their mean outputs with observations (Krause et al., 2005). However, researchers are now advancing model validation benchmarks through a wider variety of sophisticated strategies emphasizing statistical error distributions, sensitivity analysis, functional response, internal process connectivity, information content, constraints, parsimony, and equifinality (Nearing et al., 2020; Weijs and Ruddell, 2020; Cox 2019; Cox et al., 2018; Nearing et al., 2018; Ruddell et al., 2019; Collier et al. 2018; Haughton et al., 2016; Best et al., 2015; Maxwell et al., 2014; Gong et al., 2013; Reed et al., 2013; Luo et al., 2012; Matott et al., 2012; McMillan et al., 2012; Moges et al., 2022; Randerson et al., 2009). Researchers are also developing methods for evaluation of the numerical accuracy and software architecture integrity of the model (Bisht and Riley 2019, Kennedy et al. 2017). Machine learning models are no different from process-based models in their need for benchmarking, but may be especially useful as comparative benchmarks for process-based models (Nearing et al., 2020, Reichstein et al., 2019, Weijs and Ruddell, 2020). Examination of error, uncertainty, functional responses, and internal processes address the challenge of ensuring a model “right for the right reasons” (Kirchner, 2006). Towards this end for example, Kumar et al. (2006) suggested a benchmarking approach for NASA's Land Information System, to provide a robust assessment of (1) internal model-consistency (e.g., numerical, code, documentation, stability, support); (2) modeled vs. observed fluxes, states, and parameter estimates (including error analysis); (3) relationships between fluxes and states (e.g., internal processes, feedback mechanisms, and model architecture); and (4) uncertainty and equifinality (e.g., standardizing the approaches to estimate model uncertainty, sensitivity analysis, and model intercomparisons). We have built up a body of knowledge thousands of publications deep on how to benchmark models properly and are now prepared to deploy that knowledge more systematically.

Scientific communities have organized themselves via Model Intercomparison Projects (MIPs) to put this experience to work on their own disciplinary models. (Tijerina et al., 2021, Collier et al., 2018; Kollet et al., 2017; Müller et al., 2017; Donatelli et al. 2016; Eyring et al., 2016; Haughton et al., 2016; Holzworth et al., 2015; Best et al., 2015; Dankers et al., 2014; Maxwell et al., 2014; Warszawski et al., 2014; Wang et al., 2014; Huntzinger et al., 2013; Young et al., 2013; Lawrence et al., 2011; Kravitz et al., 2011; Confalonieri et al., 2009; Oleson et al., 2008; Kumar et al. 2006; Reed et al., 2004; Meehl et al., 2000; Gates et al., 1999; Gates et al., 1992). This MIP literature began with benchmarking best practices, emphasizing model skill at generating operationally useful outputs, and analysis of model sensitivity to variations in input data and parameter values. More recent MIPs emphasize internal model diagnostics of key physical processes combined with more formal community review processes. Individual scientific communities have developed best practices for community model benchmarking (Table S1), and that expertise is ready to be deployed more systematically via a thoroughly resourced and institutionalized process.

The 21st century "data deluge" fueled by the recent emergence of many environmental research infrastructures has not made the scientific method obsolete (contrary to Anderson, 2008). Instead, the data deluge creates the opportunity for much more rigorous model benchmarking than was possible in the past (Roberti et al. 2018; Csavina et al., 2017; Baatz et al., 2018; Bell et al., 2009; Loescher et al., 2017, Schwalm et al., 2013; Hey et al. 2009). The value of the data deluge is greatest for modelers that deal with irreducibly complex real-world systems that are inaccessible to controlled experimentation, such as earth systems (Brown et al. 2005, Granger 1969; Glymour et al., 1987; Pearl 1995; Reichstein et al., 2019; Goodwell et al. 2020; Kirchner et al. 1996; Nearing et al. 2020). The data deluge provides a 21st century 'macroscope' (De Rosnay, 1979) that systems modelers can use to test system-level hypotheses (Chabbi et al. 2107). Unfortunately, the data deluge has transformed model evaluation from the simple disciplinary task of benchmarking a model's average predictions into the laborious computer science task of building data pipelines, processing metadata, building data models, and implementing high performance computing and visualization methods. To exploit the data deluge for model benchmarking, we must first systematically deploy the computer science capabilities necessary to make use of the big data.

At present, our scientific agencies and science funding programs are not taking full advantage of the opportunity to transform the impact and scientific validity of their work through systematic model benchmarking. Because we now know exactly how to benchmark models (as argued above), this missed opportunity has roots in our scientific institutions and processes, rather than in our scientific knowledge. People generally manage what they measure (Drucker, 1995), and this tendency is especially strong in governmental and scientific organizations (Hicks et al., 2015). For example, the US federal government evaluates an agency's performance against the agency's stated mission (NRC, 2005), as required by the

Government Performance and Results Act of 1993. For agencies with scientific, forecasting, or planning missions, one could argue that the performance of the "models of record" funded or employed by the agency should be part of the agency's annual performance evaluation. One could also argue that peer-review of scientific models should require systematic benchmarking before publication. But, at present, this benchmarking is not required or funded at the same level as model development or other parts of the mission. The lack of agency prioritization and funding for model benchmarking is the big barrier to its implementation (Williams et al., 2012; IHTM, 2020). If agency processes, priorities, and funding are the problem, then institutionalized process, priority, and funds could be the solution.

Calling for a National Model Benchmarking Facility

We call for the multi-agency design and subsequent permanently funded establishment of a national model benchmarking facility (NMBF). The NMBF would initially focus on computer models of earth systems but could later be expanded to broader categories of models. This facility and its community partners would provide the capabilities, resources, and credibility for benchmarking and improving scientific computer models, thereby establishing a firmer foundation for 21st century modeling science and prediction. This facility will raise professional standards for computer modeling, incentivize measurable improvement in model performance, increase public trust in scientific agencies, and make the most out of public investments in scientific modeling and scientific data collection. Through its strong example this facility will set a much-needed de facto standard for rigor for the plethora of computer models originating from the far corners of the world. Other practical benefits of a central facility include significant cost reductions to individual modeling projects through efficiency gains, improved data and model accessibility, and advances in shared modeling tools.

How should we begin to establish the facility? The facility will begin by leading a collaborative effort by multiple agencies and the scientific community to design a process for model benchmarking. The objectives of this design effort are to identify the necessary incentives for model developer participation, scope the appropriate level of funding for the facility, specify the necessary specialized cyberinfrastructure and tools, agree on a model review and certification standard, pave a career pathway for model benchmarking specialists, synthesize existing technical frameworks for model benchmarking, and secure the necessary institutional support from agency leaders, policymakers, and funders. Once designed and funded, the NMBF will bring together full-time modelers, computer scientists, software engineers, statisticians, data scientists, leading-edge high-performance computing (HPC) power, modeling cyberinfrastructure, data visualization systems, archival publication capacity, and a new process for peer review of models. This facility will systematically deploy the model benchmarking best practices developed in recent decades by formally institutionalizing and fully resourcing those best practices. As with other significant research infrastructures developed in the past, we expect that the details of the NMBF's design will take time and negotiation for the community to get right, so it makes sense to get started now.

The logistics of the facility are to be determined. A variety of funding and governance structures could be imagined for the NMBF, including as a type of major research instrumentation. Regardless of funding source or authorization, the NMBF must be guaranteed a type of "academic freedom" and independence so that the benchmarking process is transparently free from political influence. The facility should be accessible by a wide range of agencies and academic scientists and should be scoped to handle the fullest possible range of model benchmarking requirements. The facility's data scientists should partner with federal agencies and with the private technology sector to build and exploit "big data" pipelines that make robust observational data readily accessible to fuel model development and model benchmarking. The facility will partner with existing high-performance computing networks, scientific modeling workspaces (e.g., CyVerse, GeoCODES, CSDMS), scientific funding programs, agency-supported data networks (e.g., ESS-DIVE, EarthCube), and high-performance computing networks (e.g. NSF XSEDE, DOE NERSC and ESnet, or USGS Denali). To increase access and equity, the facility may need funding to award its own model benchmarking grants to support participation by independent researchers who lack access to agency support for their modeling work.

We propose a preliminary outline for the NMBF's benchmarking process itself (Figure 1). The facility's operations and culture would revolve around a model benchmarking process that formalizes recent lessons learned and recent advances in benchmarking methods, grounded in the processes, tools, and best practices of the existing intercomparison projects and communities. We propose a process with three model certification levels: Compliant, Basic, and Advanced. The ten individual steps in the process are loosely analogous to Technology Readiness Levels (TRLs) wherein level ten corresponds to an operationally mature and reliable technology (Table S2). Compliant models demonstrate a correct implementation of the facility's standards for computational structure, parallel architecture, modularity, and documentation (e.g., Peckham et al., 2013; Castranova et al., 2013; Gregersen et al., 2007; Argent et al., 2004; Fila et al., 2003). Basic models have completed the facility's standard benchmarking process and the model's benchmarked performance scores, code, documentation, and data are subsequently published by the facility, possibly following an embargo period. Advanced models have completed a supplemental benchmarking process specific to the priorities and applied performance standards of the discipline or client of the model (e.g., predicting wind speed for tropical storms with sufficient accuracy to use in warning and evacuation decisions). The Advanced certification recognizes that models exist for different purposes and attempts to contextualize benchmarking methods accordingly, without replacing the more universal Basic certification. This process will be refined to support a formal model benchmarking standard.

Participation in the facility's benchmarking process will provide many advantages to model developers and their supporting agencies. These benefits include access to data pipelines and specialized computing resources, access to model benchmarking specialists, an enhanced career path for model benchmarking specialists, archival publication and citation services for models, improved model and dataset inter-comparability and understandability between different agencies and scientific communities, and attainment of a rigorous peer-reviewed certification for high quality models. The facility might also take on model ensemble generation and reanalysis tasks for community modeling efforts (IPCC, 2013; Hagedorn et al, 2005; Palmer et al. 2004; Lambert and Boer, 2001). The NMBF could provide very strong data management plans and support services as a part of modeling teams seeking agency funding. The basic certification could satisfy an academic journal's requirements for code and data publication and could add rigor and speed to journal peer review of modeling work. The attainment of an Advanced certification would be especially beneficial to build public trust in operational "models of record" of national importance. These benefits motivate a significant investment in a shared National Model Benchmarking Facility (NMBF).

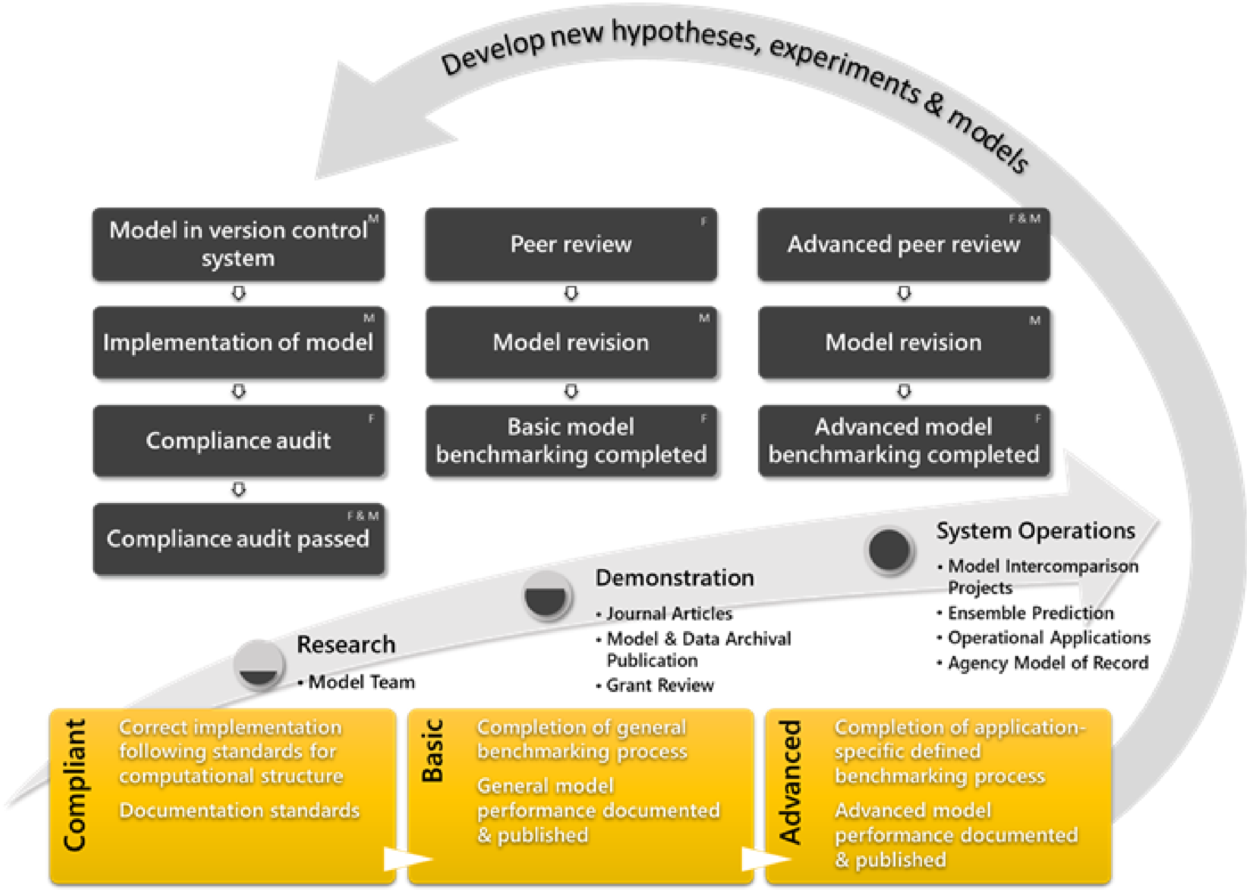

Figure 1: Graphical summary of the National Model Benchmarking Facility's process. Some process steps are led by modelers and some by the facility (M and F in Process Table S2). There are ten steps contributing toward three certification milestones; the Compliant Certification is most useful for modeling teams to verify the documentation and architecture of the model; the Basic Certification applies generic performance benchmarks used for publications and funding opportunities; and the Advanced Certification is used by agencies and advanced model intercomparison teams for application-specific performance benchmarking and for documenting the performance of their "models of record" used for policy and decision making.

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Table S1: Summary of best practices identified by recent Model Intercomparison Projects (MIPs), community efforts, and the model benchmarking literature. Many best practices remain elusive in practice.

Benchmarking	Standardization	Community
• Information content • Dynamics • Means • Performance/skill statistics • Domain-specific phenomena of interest • Numerical implementation • Input data • Parameters • Validation data • Tradeoffs between complexity, cost, detail, and performance • Sensitivity analysis • Out of sample vs. in sample testing • Multiple input datasets • Multiple validation datasets • Extreme events • Likely scenarios • Limiting Cases • Analytically solved special cases • Internal process performance • Predictive output performance • Statistical and machine learning benchmarks • Understandability by and communicability to people • Stability	• Forcings, inputs, and boundary conditions • Time and space reference and(or) resolution • Calibration methods • Ensembles • Methods and frequencies for data assimilation • Documentation, metadata, and architecture • Standard models of record • Standard data models, ontologies, and definitions • Interoperable, formal, modular architecture • Multiphysics/swappable architecture • Capable of varying model complexity • Visualization of model output and performance • Scientific workflows • Verifiable data sources • Standard performance metrics • Comparability of internal processes, not just outputs	• Shared and adequate computing infrastructure • Funding specifically for the benchmarking effort • Independent peer review • Incentives for participation • Exact reproducibility • Strict rules and processes for participation • Cyberinfrastructure bridging research infrastructures • Periodic competition and intercomparison efforts • Published, open, and archival model code, data, and results • Implementation of benchmarking best practices (to left) • Implementation of standardization best practices (to left)

Table S2: Three levels (in ten sub-steps) of a model benchmarking facility's formal model certification and publication process: Compliant, Basic, and Advanced. Each level is led by the (F)acility and (or) (M)odeler.

1. (M) Versioned model creation and formal "push" by the modeler; this is already routinely completed by modelers as a best practice.
2. (M) Initial implementation of the model using the facility's computer science standards (input/output data models, HPC architectures, modular code architecture, etc.) is completed by the modeler, with free training and consultation provided by facility staff. If funding is available, facility staff could provide extensive assistance to the modelers for this implementation.
3. (F) Auditing against the facility's computer science standards for computational optimality, stability, architectural compliance, and documentation by facility staff, yielding a private review containing also limited consulting on how to best address the issues raised. If funding is available, facility staff could provide extensive assistance to the modelers to address issues raised in the review.
4. **Compliant Certification** (M+F) Implementation of requested changes to computational optimality, stability, architectural compliance, and documentation by the modeler, yielding certification at the Compliant level once the model passes a second audit by facility staff. The Compliant certification does *not* mean the model is the best available for a purpose, but rather that it is compliant with a set of purpose-agnostic computer science quality criteria. A Compliant model is not necessarily made public or published.
5. (F) Completion of a basic set of model performance tests using the facility's infrastructure, yielding an open (to the community) peer review comment period beginning with a basic benchmarking review report by facility staff; the basic report reviews model output performance (e.g. state variables and fluxes) along with a generic set of internal process diagnostics (e.g. couplings and feedbacks between state variables), sensitivity and uncertainty analysis, and computational size and cost, with all benchmarks presented in comparison with "null" models (e.g. statistical reference models) and other related models certified by the facility.
6. (M) Completion of revision of the model to address the basic review, with facility staff who did not help with the compliance steps serving as editors of the review.
7. **Basic Certification** (F) Certification of the revised model at the Compliant level followed by archival open access publication including a DOI, a reproducible model workflow, the as-revised benchmarking performance report, model outputs, and a visualization of model performance and outputs using the facility's software systems. Basic certification yields an archival quality peer reviewed model publication, optionally embargoed for a time. The Basic certification does *not* mean the model is the best available for a purpose, but rather that its structure and performance has been thoroughly and transparently documented, benchmarked, and published according to a set of generic criteria that are universal to all kinds of models and model applications addressed by the NMBF.
8. (M+F) Submission by modeling teams holding the Basic certification to the facility for Advanced certification, which repeats steps 5-7 with a collaboratively developed set of custom benchmarks and standards specific to the community, client, and purpose served by the model (e.g. different benchmarks and standards for hydrology vs. ecosystem or scientific vs. operational models). The facility may need funding from the model's agency supporters to complete this step. Step eight yields an open (to the community) peer review including advanced custom benchmarking results, mirroring step five.

9. (M) Completion of revision of the model to address the advanced review, with facility staff who did not help with the compliance steps serving as editors of the review.
10. **Advanced Certification** (F) Certification and publication of the revised model at the Advanced level, mirroring the Basic level but using context-specific benchmarking criteria. The Advanced certification does *not* mean the model is the best available for a purpose, but rather that its structure and performance has been thoroughly and transparently documented, benchmarked, and published using additional criteria that are required or preferred by the specific type of client and community that this model serves.