Celebrating the Life and Work of J. Tinsley Oden: A Pioneer and a Mentor in Computational Mechanics

Predictive Science: A Quest for the Holy

Abani Patra, *Tufts University, Medford, MA 02155, USA*

Danial Faghihi, *University at Buffalo, Buffalo, NY 14051, USA*

Prashant K. Jha, *South Dakota School of Mines and Technology, Rapid City, SD 57701, USA*

Lianghao Cao, *California Institute of Technology, Pasadena, CA 91125, USA*

Kathryn A. Farrell-Maupin, *Sandia National Laboratories, Albuquerque, NM 87123, USA*

Abstract—The pioneering contributions of Dr. J. Tinsley Oden fundamentally redefined predictive computational science, transforming it into a rigorous discipline centered on making reliable predictions of complex physical systems. This article attempts to articulate Dr. Oden's vision and philosophy for scientific prediction, emphasizing the development of computational models that do not merely approximate some features but truly predict complex physical phenomena and systems, spanning applications from cancer treatment to the behavior of advanced nanomaterials. We highlight the core mathematical and statistical foundations he advanced, including Bayesian frameworks for uncertainty quantification, systematic methodologies for model validation, and adaptive strategies for controlling prediction error and balancing model complexity against predictive reliability. Finally, we discuss how Dr. Oden's legacy has established a new scientific paradigm of the science of prediction that continues to advance the frontier of computational science and engineering, guiding future generations toward the rigorous development of mathematical and computational models that span everyday technologies to high-consequence decision-making in critical systems.

Predictive computational science was defined by Dr. J. Tinsley Oden (JTO) as [15]:

> *The scientific discipline concerned with assessing the predictability of mathematical and computational models of events that occur in our physical universe in the presence of uncertainties in all the factors that determine the reliability and scientific significance of the prediction.*

In this short perspective article, we celebrate the arc of JTO's thinking about a central paradigm in science – computational prediction under uncertainty and limited information. In JTO's vision, true scientific prediction rested on integrating three pillars: observation (empirical data), theory (mathematical abstraction), and computational science. The last provides a pathway to knowledge through simulation when direct experimentation is infeasible or insufficient. JTO emphasized that computational predictions are only meaningful when model use is rigorously validated–an ethos now widely adopted across the validation, verification, and uncertainty quantification (VVUQ) community [14], [19]–ensuring that simulations are credible representations of physical systems rather than mere numerical mimicking of some features of it. Central to his philosophy was the recognition that "science is subject," that is, a model's validity must be context-dependent, reflecting both the problem's nature and the modeler's informed judgment about acceptable error and uncertainty to

XXXX-XXX © 2025 IEEE
Digital Object Identifier 10.1109/XXX.0000.0000000

This article has been accepted for publication in Computing in Science & Engineering. This is the author's version which has not been fully edited and content may change prior to final publication. Citation information: DOI 10.1109/MCSE.2025.3622975

deem a model to be *valid* for making predictions. JTO further advocated Bayesian inference as the only logically consistent foundation for predictive science, uniquely capable of unifying prior knowledge, empirical data, and model credibility into a systematic and principled framework for scientific reasoning under uncertainty.

Insight and Prediction, Models, Error and Uncertainty

Robust prediction is perhaps the oldest and most significant problem society poses to the science and engineering community, so we may plan and manage our lives, assets, and resources for the best outcomes. Let us attempt first a formal definition of prediction:

> *A prediction is a specification of a quantity of interest Q for unobserved system inputs using information from observed system behavior and relevant validated rules $\mathcal{E}$ applicable to the system.*

$\mathcal{E}$ is often expressed in the form of "mathematical constructs that describe a system and represent knowledge of the system in a usable form" [15] or, as is more popularly known, a mathematical model or governing equations representing our knowledge often stated as conservation laws, constitutive models, boundary conditions and closures. Lack of complete knowledge of the system and inherent randomness/stochasticity are intrinsic to most physical systems and are often characterized as the uncertainty associated with the model. Of course, the complexity of $\mathcal{E}$ implies that great effort must be expended in deriving satisfactory computational approximations $\mathcal{E}^h$. Generally, the process of prediction consists of the following steps:

$$\textit{Physical system} \rightarrow \textit{Model} \rightarrow \textit{Evaluation} \rightarrow \textit{Prediction}$$

where transitioning from 'Physical system' to 'Model' involves observation and the application of engineering principles, encoding key phenomena of interest into mathematical relations. The model introduces specific phenomenological parameters, which are assigned fixed values (deterministic) or probability distributions in the 'Evaluation' stage based on the available observation data. The model is also numerically approximated into a form that can be solved using computers. Finally, in the 'Prediction' stage, the calibrated model is utilized to make predictions about physical events while taking into account the model inadequacy, uncertainty in the observational data, and model parameters. While the steps appear to be linear and distinct, JTO was among the first to make them iterative, driven by mathematically rigorous estimates of error and uncertainty in the model and its evaluation [17].

The following two sections highlight some methodologies developed by, or inspired by, JTO that form the foundation of this transformative paradigm for modeling and prediction across a broad spectrum of complex physical systems and applications (see Figure 1 for illustrative examples). In the final section, we discuss how these fundamental principles continue to shape the future of computational science, even as modeling is undergoing a reinvention in the age of artificial intelligence (AI). In addition to these technical perspectives, we also include brief personal recollections from the authors (noted by initials), offering insight into JTO's philosophy and mentorship.

Bayesian frameworks: The foundation of predictive science

This section outlines the statistical foundations of predictive science, focusing on uncertainty quantification in computational models and observational data within a Bayesian framework for model validation and adaptive model selection. The presentation is largely adapted from the seminal works of JTO [16], [15].

To systematically address uncertainties, we define mathematical and computational models in an abstract form as

$$\mathcal{A}(\boldsymbol{\theta}, S; \boldsymbol{u}(\boldsymbol{\theta}, S)) = 0, \tag{1}$$

where $\mathcal{A}$ represents a set of operators, $\boldsymbol{\theta} \in \Theta$ is model parameter vector, and S denotes the scenario. The solution $\boldsymbol{u}(\boldsymbol{\theta}, S) \in U$ is the solution of the forward problem Equation 1, and the fundamental goal of solving this model is to use these solutions to compute specific quantities of interest (QoIs) $Q : U \rightarrow \mathbb{R}$; Figure 2 describes different levels of evaluation, with prediction being the ultimate goal.

Characterizing uncertainty in predictions

Scientific prediction inherently involves managing multiple sources of uncertainty throughout the prediction process, including:

1) $\mathcal{P}$ *uncertainty.* This systemic uncertainty pertains to selecting an appropriate mathematical framework for quantifying uncertainty in a logically consistent manner. It raises fundamental questions:

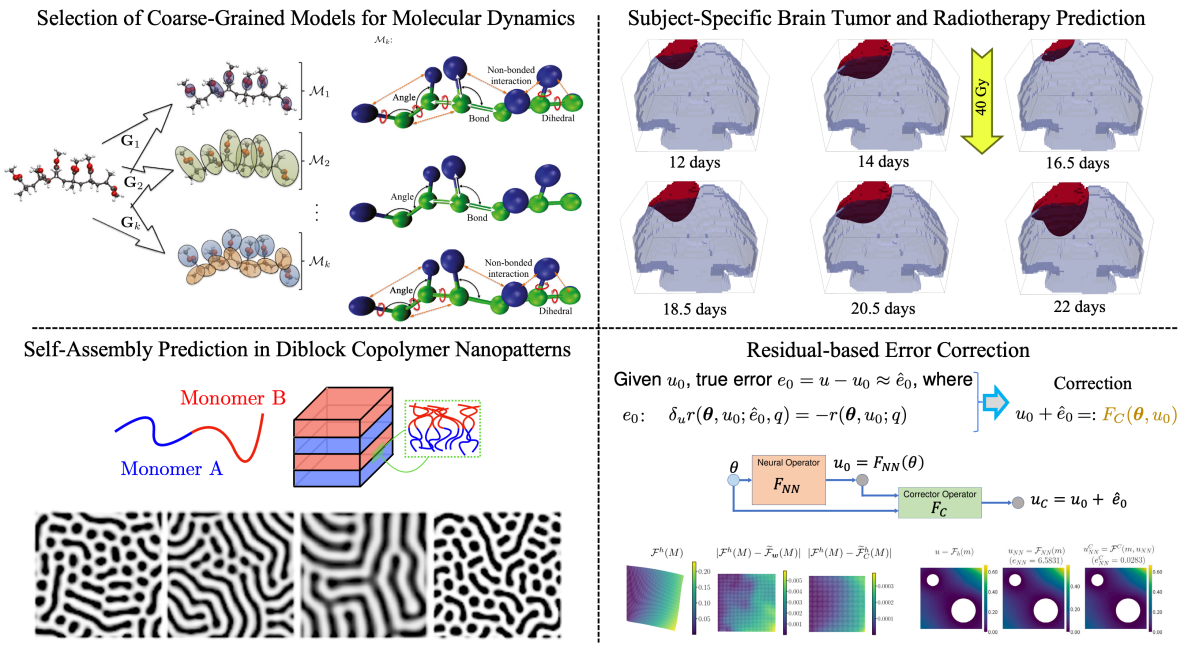

FIGURE 1. Illustrative applications of computational model validation, selection, and uncertainty quantification in complex physical systems. (Top left) Development of validated coarse-grained models for molecular dynamics simulations of polyethylene, requiring model selection across various coarse-graining maps and corresponding intermolecular force fields [5]. (Top right) 3D computational prediction of brain tumor (glioma) progression in a murine subject undergoing whole-brain radiotherapy of 40 Gy at t=14.5 days after tumor cell implantation. Data are obtained from longitudinal Magnetic Resonance Imaging (MRI) over approximately three weeks. The most predictive model is selected from 39 distinct continuum mixture models describing tumor growth and treatment response [10]. (Bottom left) Prediction of nano-pattern formation of self-assembled diblock copolymer materials using nonlocal Cahn-Hilliard phase field models and microscopy imaging data of the materials [4]. (Bottom right) Residual-based error correction for neural operators, based on the estimation of modeling error using the residual of the partial differential equation (PDE) [8].

Should predictions be formulated using probability theory (and if so, which variant?), possibility theory, fuzzy sets, Dempster–Shafer theory, or interval analysis? Which framework ensures internal consistency in uncertainty quantification? In [15], JTO argued that within the Cox-Jaynes probability framework, $\mathcal{P}$ uncertainty does not exist, as any logical extension of Aristotelian reasoning under uncertainty is inherently Bayesian.

2) $\mathcal{Y}$ *uncertainty.* Represents uncertainty in observational data, arising from experimental noise, spatiotemporal sparsity, and aleatoric variability in high-fidelity simulation data.
3) $\mathcal{M}$ *uncertainty.* Relates to model selection, an often overlooked yet critical source of uncertainty.
4) $\boldsymbol{\theta}$ *uncertainty.* Captures uncertainty in parameter values or parametric distributions, a fundamental factor in predictive modeling.
5) h *uncertainty.* Arises from numerical discretization (e.g., finite element, finite difference) in computational models. It pertains to model verification, involving solution verification (a-posteriori error estimation).

We now examine $\mathcal{Y}$ and $\boldsymbol{\theta}$ uncertainties in a Bayesian framework, address $\mathcal{M}$ uncertainty and h uncertainty in the next subsections. Given uncertain data (observations) $\boldsymbol{Y}$, Bayes' rule, expressed in terms of the probability distribution function (PDF) π, yields

$$\pi_{\text{post}}(\boldsymbol{\theta}|\boldsymbol{Y}, S) = \frac{\pi_{\text{like}}(\boldsymbol{Y}|\boldsymbol{\theta}, S)\pi_{\text{prior}}(\boldsymbol{\theta}|S)}{\pi_{\text{evid}}(\boldsymbol{Y}|S)}, \qquad (2)$$

where $\pi_{\text{prior}}(\boldsymbol{\theta}|S)$ is the prior PDF of model parameters, $\pi_{\text{like}}(\boldsymbol{Y}|\boldsymbol{\theta}, S)$ is the likelihood, $\pi_{\text{post}}(\boldsymbol{\theta}|\boldsymbol{Y}, S)$ is the posterior PDF, and $\pi_{\text{evid}}(\boldsymbol{Y}|S) = \int_{\Theta} \pi_{\text{like}}(\boldsymbol{Y}|\boldsymbol{\theta}, S)\pi_{\text{prior}}(\boldsymbol{\theta}|S)d\boldsymbol{\theta}$ is the evidence is the marginalization of the numerator to make sure $\int_{\Theta} \pi_{\text{post}}(\boldsymbol{\theta}|\boldsymbol{Y}, S)d\boldsymbol{\theta} = 1$.

This article has been accepted for publication in Computing in Science & Engineering. This is the author's version which has not been fully edited and content may change prior to final publication. Citation information: DOI 10.1109/MCSE.2025.3622975

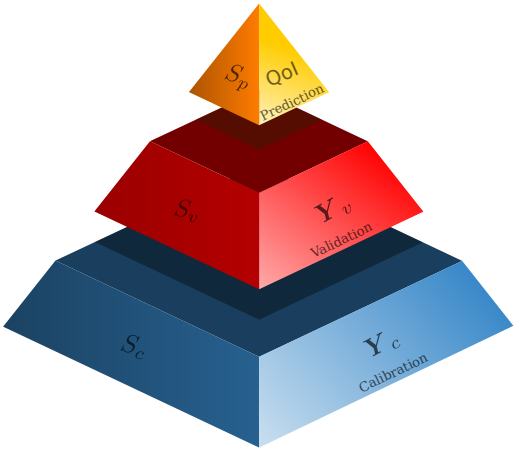

FIGURE 2. Bayesian prediction pyramid comprising three stages: calibration, validation, and prediction. The model is first calibrated using data $\boldsymbol{Y}_c$ collected under the calibration scenario S_c, which is designed to evaluate the model's subcomponents. It is then validated using data $\boldsymbol{Y}_v$ from the validation scenario S_v, which involves more complex conditions than calibration. Finally, the calibrated and validated model is used to predict quantities of interest under the prediction scenario S_p, where data collection is expensive or impossible [15].

Maximum entropy prior.
A rigorous approach for prior construction leverages Shannon's principle of maximum entropy, which provides a systematic framework when statistical information about parameters is available. This principle states that uncertainty can be encoded via entropy; for continuous variables one maximizes *relative* entropy $H(p \,\|\, m) = -\int p(\boldsymbol{x}) \log\big(p(\boldsymbol{x})/m(\boldsymbol{x})\big)\, d\boldsymbol{x}$ with respect to a chosen base measure m, subject to known constraints. Among a class of candidate densities, the most noncommittal distribution is the one that maximizes $H(p)$ while satisfying known constraints (e.g., specified moments such as mean and variance). Jaynes [6] introduced this concept for constructing meaningful priors.

Noise model for constructing likelihood.
Incorporating $\mathcal{Y}$ and $\boldsymbol{\theta}$ uncertainties in parameter inference depends on modeling data noise $\boldsymbol{\epsilon}$ with a probability distribution $p_{\text{data}}(\epsilon)$ and model inadequacy $\gamma(\boldsymbol{\theta}, S)$ with $p_{\text{model}}(\epsilon)$. Under an additive noise assumption, where the imperfect data and imperfect model are modeled as additive error to reality, it follows that (see [16] for details):

$$\boldsymbol{\epsilon} + \gamma(\boldsymbol{\theta}, S) = \boldsymbol{Y} - \boldsymbol{u}(\boldsymbol{\theta}, S). \tag{3}$$

Thus, the likelihood of observing data $\boldsymbol{Y}$ given $\boldsymbol{\theta}$ is

$$\pi_{\text{like}}(\boldsymbol{Y}|\boldsymbol{\theta}, S) = p_{\text{comp}}(\boldsymbol{Y} - \boldsymbol{u}(\boldsymbol{\theta}, S)), \tag{4}$$

where p_{comp} denotes the probability of total error, combining assumptions on data noise $p_{\text{data}}(\epsilon)$ (typically Gaussian) and model inadequacy $p_{\text{model}}(\epsilon)$ (see, e.g., [11] for various model inadequacy assumptions).

Scenario.
The term scenario refers to both the computational domain where the model is solved and the physical environment where experimental data are collected. For model validation, particularly when predicting *unobservable QoIs*, it is useful to establish a hierarchical structure as represented in the prediction pyramid in Figure 2:

- *Calibration Scenarios* (S_c): Initial parameter tuning using calibration data $\boldsymbol{Y}_c$;
- *Validation Scenarios* (S_v): Assessing the model's prediction ability and determining its validity using the validation data $\boldsymbol{Y}_v$; and
- *Prediction Scenarios* (S_p): Solving the forward problem Equation 1 to predict QoIs in the full system.

K.F.M. *recalls that JTO would sometimes refer to Figure 2 as a "prediction tetrahedron," noting that the back side, which cannot be seen, is the true value of QoI in each scenario.*

Occam Plausibility Algorithm: Adaptive selection and model validation

Addressing $\mathcal{M}$-uncertainty is one of the most challenging aspects of model validation and uncertainty quantification, and JTO's contributions in this area have had a lasting impact across diverse modeling problems. A key advancement was the Occam Plausibility Algorithm (OPAL), introduced in Farrell et al. [5]. OPAL provides a systematic, adaptive framework for model calibration and validation, integrating multiple uncertainty-quantification methodologies. Inspired by Occam's Razor, which favors the simplest model among those yielding equivalent predictions, OPAL defines the "best" predictive model as the simplest model that passes the model validation criteria.

K.F.M., *then a PhD student working on the selection and uncertainty*

quantification of coarse-grained atomistic models, and D.F.*, a postdoc at the time, recall the daily meetings JTO held to tackle the challenging problem of navigating numerous potential models (e.g., varying degrees of coarse-graining and choices of interatomic potentials). He met with them in a small conference room next to his office early each morning and sometimes again in the late afternoon, even during the ice storms that shut down Austin, TX, in January 2014. They remember his insistence on a deep understanding of the surrounding literature on coarse-graining, global sensitivity analysis, and model plausibility: he would buy books, print papers, and read and mark them overnight so that by the next morning he could drive the discussion further. Under his guidance, what began as an intractable attempt to examine every model gradually evolved into the adaptive strategy that became OPAL: eliminating implausible models while embedding validation under uncertainty as the criterion for predictive acceptance.* K.F.M. *notes that the discussions with JTO in developing OPAL shaped her core beliefs as a computational scientist and underlie all the work that she has done since.*

JTO later broadened OPAL's scope in a chapter of the *Encyclopedia of Computational Mechanics* [16], co-authored with Ivo Babuška and *D.F.*, extending its foundations to include both deterministic and Bayesian perspectives with examples in structural mechanics. He subsequently applied OPAL to identify valid models of tumor growth and radiotherapy in subject-specific glioma [10].

D.F. *recalls that in preparing the encyclopedia chapter, JTO's leadership was evident: he listened carefully to his co-authors' ideas but consistently steered decisions toward his core beliefs—for example, on objective versus subjective priors and measures of model complexity.*

Bayesian model plausibility. Various approaches exist for model comparison, but the gold standard relies on Bayesian posterior model plausibilities, which weigh the evidence PDF supporting each model. The revival of model plausibilities in the works of James L. Beck [1] drew JTO's attention, particularly for its implications in uncertainty quantification. The development of accurate sampling techniques for computing model evidence in complex computational models by Ernesto E. Prudencio [21], [22] further reinforced JTO's interest in this area. Notably, although JTO only later became aware of David J. C. MacKay's seminal work [12] on exploiting evidence PDF in Bayesian neural networks, the conceptual alignment between their approaches to model selection—despite JTO's focus on physics-based modeling and MacKey's on data-driven techniques—underscores a broader convergence in Bayesian inference methodologies.

This section outlines the fundamental concept of posterior model plausibilities, which form the systematic basis for model selection within the OPAL framework. Let $\mathcal{M} = \{\mathcal{P}_1(\boldsymbol{\theta}_1), \cdots, \mathcal{P}_m(\boldsymbol{\theta}_m)\}$ denote a set of m models $\mathcal{P}_j$ with parameters $\boldsymbol{\theta}_j$. The evidence PDF in Equation 2, representing the probability of observing data given the choice of model, is expressed as

$$\pi_{\text{evid}}(\boldsymbol{Y}|\mathcal{P}_j, \mathcal{M}, S) = \int_{\Theta} \pi_{\text{like}}(\boldsymbol{Y}|\boldsymbol{\theta}, \mathcal{P}_j, \mathcal{M}, S)\pi_{\text{prior}}(\boldsymbol{\theta}|\mathcal{P}_j, \mathcal{M}, S)d\boldsymbol{\theta}, \quad j = 1, \cdots, m. \tag{5}$$

This evidence serves as the likelihood in a second-level Bayesian inference, leading to the posterior model plausibilities:

$$\rho_j = \pi_{\text{post}}(\mathcal{P}_j|\boldsymbol{Y}, \mathcal{M}, S) = \frac{\pi_{\text{like}}(\boldsymbol{Y}|\mathcal{P}_j, \mathcal{M}, S)\pi_{\text{prior}}(\mathcal{P}_j|\mathcal{M}, S)}{\pi_{\text{evid}}(\boldsymbol{Y}|\mathcal{M}, S)}, \quad j = 1, \cdots, m. \tag{6}$$

The model (or models) in $\mathcal{M}$ with plausibilities ρ_j closest to unity ($\sum_j \rho_j = 1$) are considered the most plausible for given $\boldsymbol{Y}$ and S.

As JTO recognized, a model $\mathcal{P}_j$ may be the most plausible within $\mathcal{M}$ but still fail to meet validation criteria for reliable predictions, necessitating further validation tests using problem-specific metrics and tolerances. Moreover, evaluating model plausibilities and performing validation across a large model space is computationally prohibitive, except when $\mathcal{M}$ consists of only a few models. These challenges motivated the development of OPAL to navigate model selection and validation efficiently.

L.C. *recalls that JTO frequently expressed his reservations about Bayesian model averaging in physics-based models, an approach to handling $\mathcal{M}$-uncertainty by weighting predictions from multiple models. He regarded it as a misguided attempt to force consensus: "It's like making an important decision by a show of hands," he would say, "letting amateurs—models that might be completely off—drown out the one expert in the room who actually knows the right answer."*

Occam-Plausibility Algorithm (OPAL) strategy. OPAL utilizes plausibility to search through the model space efficiently and leverages a model validation test to validate (or refute) its predictive abilities. The key steps of OPAL, as shown in Figure 3, are as follows:

1) **Initialization.** Identify a set $\mathcal{M}$ of m possible models for predicting the QoI.
2) **Sensitivity Analysis.** Conduct a global sensitivity analysis (e.g., Sobol indices, elementary effect) for each model class to eliminate insensitive parameters, setting them to fixed values. This yields a reduced model set $\bar{\mathcal{M}}$.
3) **Occam Categories.** Partition $\bar{\mathcal{M}}$ based on model complexity measures (e.g., number of parameters), assigning the simplest models to Category 1, the next level of complexity to Category 2, and so on. This yields subsets $\bar{\mathcal{M}}_1, \bar{\mathcal{M}}_2, \cdots, \bar{\mathcal{M}}_N$.
4) **Calibration.** Statistically calibrate all models in Category 1 ($\bar{\mathcal{M}}_1$) using a designated calibration scenario S_c. This results in a set of calibrated models: $\bar{\mathcal{M}}_1^* \sim \{\mathcal{P}_1^*(\boldsymbol{\theta}_1^*), \mathcal{P}_2^*(\boldsymbol{\theta}_2^*), \cdots, \mathcal{P}_k^*(\boldsymbol{\theta}_k^*)\}, \quad k < l$.
5) **Plausibility.** Compute Bayesian posterior plausibilities ρ_j^* for the calibrated models in $\bar{\mathcal{M}}_1^*$. The most plausible model(s), denoted $\mathcal{P}_i^*(\boldsymbol{\theta}_i^*)$, is the one with the highest plausibility: $\rho_i^* \geq \rho_j^*$, $1 \leq j \leq k$.
6) **Validation.** Having identified the most plausible model in Category 1, the next step is to assess its validity. This is done by transitioning to the validation scenario, where the model's calibrated parameters are updated using Bayesian statistical inversion. The forward problem is then solved in S_v to generate model predictions for comparison with experimental validation data $\boldsymbol{Y}_v$. To determine whether the model is valid, we evaluate the agreement between model predictions and validation data based on a predefined metric and tolerance threshold. Let $q_v(\mathbf{y})$ represent the probability density of the validation data, and let $\pi_v(\mathbf{y}, \boldsymbol{\theta}^{**})$ denote the model-generated density approximating $q_v(\mathbf{y})$, obtained using the updated posterior distributions in S_v. Given an appropriate distance measure $d(\cdot,\cdot)$ and a validation tolerance γ_{tol}, the model is deemed valid if
$$d\left(q_v, \pi_v(\mathbf{y}, \boldsymbol{\theta}^{**})\right) \leq \gamma_{\text{tol}}. \tag{7}$$
7) **Iteration or Solution.** If the model satisfies the validation criterion (7), the parameters $\boldsymbol{\theta}^{**}$ are used in the forward problem for the prediction scenario S_p to compute the solution $(u(\boldsymbol{\theta}^{**}, S))$ and predict the QoI. If none of the Category 1 models is valid, the process returns to Step 3, setting $\mathcal{M} = \bar{\mathcal{M}}_2$, and the procedure is repeated until a valid model is identified. The process terminates upon identifying a model that meets the validation criterion, even if other untested models could yield lower error. If none of the models in the original set $\mathcal{M}$ are valid, the candidate model space must be expanded until a valid model is found, if possible.

We note that while Bayesian calibration and model selection have been explored in computational mechanics [2], [9], JTO's program is distinguished by embedding validation under uncertainty within a hierarchy of scenarios and using model plausibility to guide adaptive, complexity-ordered searches across large model spaces, aiming at the particularly difficult problem of extrapolative prediction of unobservable QoIs. Tan et al. [24] later extended OPAL by introducing a method for designing model-specific validation scenarios S_v (Step 6 of OPAL), specifically for predicting unobservable QoIs. They proposed that for a model to reliably extrapolate to a QoI, its validation data must effectively inform the parameters critical for that prediction while ensuring experimental feasibility. Their approach computes global sensitivity in the prediction scenario S_p with respect to the QoI and compares it to the sensitivity of validation parameters to observables in S_v. A validation experiment is deemed effective when the sensitivity profiles for prediction and validation align. Paquette et al. [20] further refined this idea by using influence matrices from active subspace methods to identify validation settings best aligned with S_p. Nevertheless, while the OPAL strategy and validation under uncertainty provide a principled foundation for predicting unobservable QoIs, their implementation

This article has been accepted for publication in Computing in Science & Engineering. This is the author's version which has not been fully edited and content may change prior to final publication. Citation information: DOI 10.1109/MCSE.2025.3622975

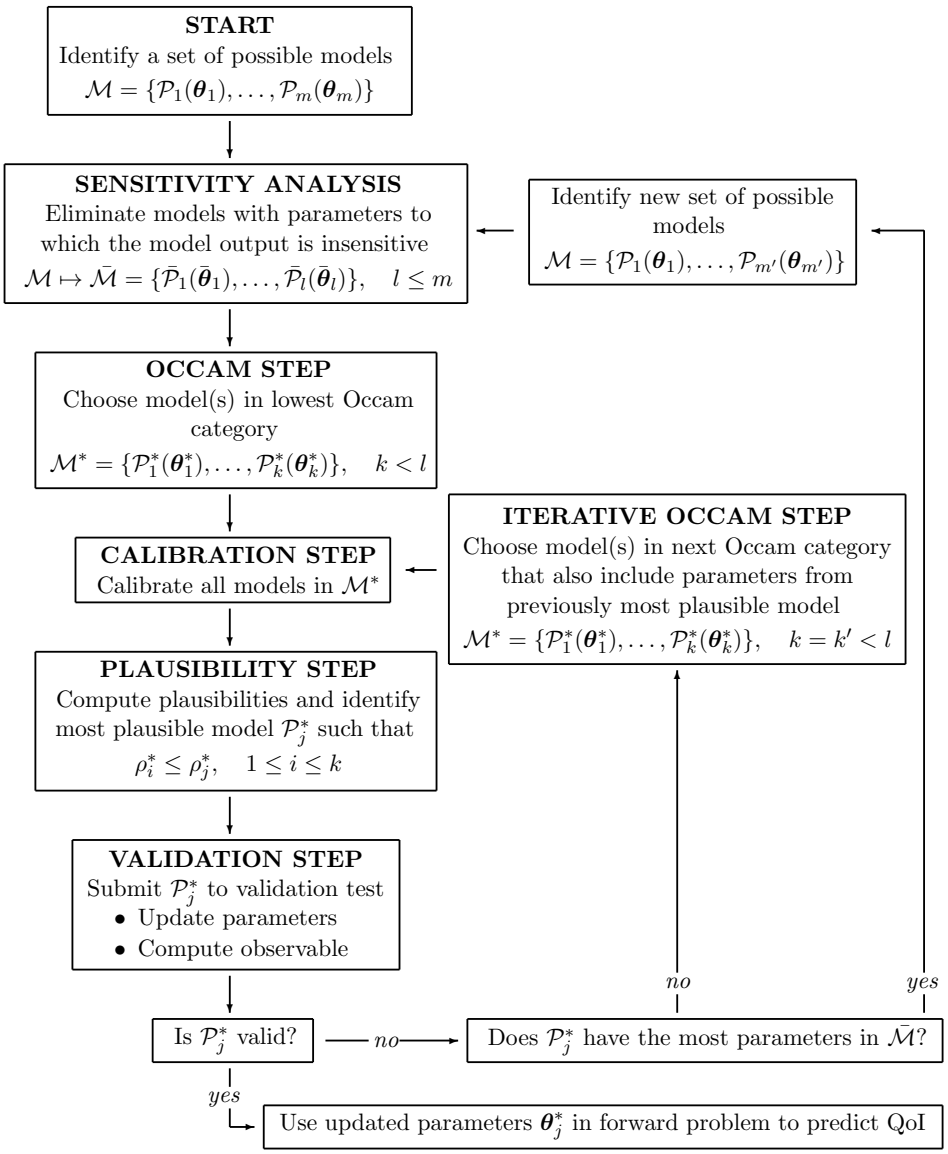

FIGURE 3. Flowchart for the Occam-Plausibility Algorithm (OPAL) [5].

can be computationally intensive. Depending on the prediction purposes, this challenge can be mitigated through frequentist methods or the use of surrogate models.

h-Uncertainty and modeling error

One of the fundamental sources of uncertainty briefly introduced in the previous section is the *h*-uncertainty that arises from the numerical approximation of the mathematical models. In JTO's framework for validation and uncertainty quantification, *h*-uncertainty is not a peripheral concern, but a critical and quantifiable component of the broader landscape of model-based prediction. As he emphasized in his theoretical and applied work, a-posteriori error estimation is a rigorous and necessary means to measure and control this discretization-induced uncertainty [15].

Within the broader VVUQ framework, *h*-uncertainty plays a central role in the verification step: the process by which we ensure that the numerical solution approximates the mathematical model correctly. For

a family of discretized operators $\mathcal{A}_h$, where h represents mesh size, h-uncertainty quantifies the deviation from the idealized continuous operator $\mathcal{A}$. This modeling perspective treats discretizations themselves as a family of computational models. Accordingly, h-uncertainty is an expression of modeling error given by $\Xi := Q(\boldsymbol{u}) - Q(\boldsymbol{u}_0)$, where $\boldsymbol{u}$ and $\boldsymbol{u}_0$ are solutions of two different models (or discretized models for two different meshes). Estimates of Ξ can be useful in determining the optimal mesh that meets the specified accuracy and involves strategically refining regions based on QoI error estimates. This typically results in a refined mesh that achieves the target QoI accuracy at a lower computational cost compared to uniform mesh refinement. JTO saw great potential in this area and played a crucial and leading role in the development of goal-oriented a-posteriori error estimates for designing efficient finite element discretization of PDE-based models. These contributions span solid mechanics, fluid mechanics, phase-field models for tumor growth, and multiscale methods. Going beyond, JTO and Prudhomme in [18] realized the framework of goal-oriented a-posteriori error estimates can also be extended to a much broader class of problems – comparing models of different fidelities, which then leads to multiple possibilities, including model selection based on modeling error, model misfit of a lower fidelity model based on a higher fidelity model, calibration of models with respect to a "true" model [8], and more recently building correction to surrogate models (e.g., correcting neural operator predictions) [3].

To make the ideas precise, suppose $\mathcal{A}(\boldsymbol{\theta}, S; \boldsymbol{u}(\boldsymbol{\theta})) = 0$ represents the higher-fidelity problem and $\mathcal{A}_0(\boldsymbol{\theta}_0, S; \boldsymbol{u}_0(\boldsymbol{\theta}_0)) = 0$ represents the lower-fidelity problem, possibly with different parameters (i.e., $\boldsymbol{\theta} \neq \boldsymbol{\theta}_0$), with $\boldsymbol{u}$ and $\boldsymbol{u}_0$ approximating the same state. We also suppose that $\mathcal{R}(\boldsymbol{\theta}, \boldsymbol{u}; \boldsymbol{v}) = 0$ is the weak form associated with $\mathcal{A}$, where $\mathcal{R}$ is the residual, possibly nonlinear in the first two arguments, and $\boldsymbol{u} \in U$ and $\boldsymbol{v} \in V$ are trial and test functions in appropriate function spaces, respectively. The goal-oriented a-posteriori error estimates of Ξ takes the form, [18],

$$\begin{aligned} \Xi &= \mathcal{R}(\boldsymbol{\theta}, \boldsymbol{u}_0; \boldsymbol{p}_0) + \mathcal{R}(\boldsymbol{\theta}, \boldsymbol{u}_0; \varepsilon_0) + r \\ &\approx \mathcal{R}(\boldsymbol{\theta}, \boldsymbol{u}_0; \boldsymbol{p}_0) + \mathcal{R}(\boldsymbol{\theta}, \boldsymbol{u}_0; \varepsilon_0)\,, \end{aligned} \tag{8}$$

where r is the remainder term involving higher-order Gâteaux derivatives of $\mathcal{A}$ and QoI functional Q, $\boldsymbol{p}_0$ is the so-called dual/adjoint variable that solves the following dual/adjoint problem associated with the $\mathcal{A}_0(\boldsymbol{\theta}_0, S; \boldsymbol{u}_0) = 0$, and $\varepsilon_0 = \boldsymbol{p} - \boldsymbol{p}_0$ is the error between adjoint solutions of higher and lower fidelity models. We also let $\boldsymbol{e}_0 = \boldsymbol{u} - \boldsymbol{u}_0$. The difficulty with the above estimate and other versions of estimates in [18] is the dependence on errors $\boldsymbol{e}_0$ and ε_0, which require the knowledge of higher-fidelity solutions $(\boldsymbol{u}_0, \boldsymbol{p}_0)$. To remedy this, [18] computes estimators $(\hat{\boldsymbol{e}}_0, \hat{\varepsilon}_0)$ of errors $(\boldsymbol{e}_0 = \boldsymbol{u} - \boldsymbol{u}_0, \varepsilon_0 = \boldsymbol{p} - \boldsymbol{p}_0)$ using the two linear variational boundary value problems:

$$\text{Find } \hat{\boldsymbol{e}}_0 \text{ s.t. } -\delta_u \mathcal{R}(\boldsymbol{u}_0; \hat{\boldsymbol{e}}_0, \boldsymbol{v}) = \mathcal{R}(\boldsymbol{u}_0; \boldsymbol{v}),\ \forall \boldsymbol{v} \in V \tag{9}$$

and

$$\begin{aligned} \text{Find } \hat{\varepsilon}_0 \text{ s.t. } &-\delta_u \mathcal{R}(\boldsymbol{u}_0; \boldsymbol{v}, \hat{\varepsilon}_0) = \delta_u Q(\boldsymbol{u}_0; \boldsymbol{v}_0) \\ &+ \delta_u \mathcal{R}(\boldsymbol{u}_0; \boldsymbol{v}, \boldsymbol{p}_0),\ \forall \boldsymbol{v} \in V\,, \end{aligned} \tag{10}$$

where

$$\begin{aligned} \delta_u \mathcal{R}_0(\boldsymbol{u}_0; \boldsymbol{w}_0, \boldsymbol{p}_0) &= \lim_{\eta \to 0} \eta^{-1} \left[\mathcal{R}_0(\boldsymbol{u}_0 + \eta \boldsymbol{w}_0; \boldsymbol{p}_0) \right. \\ &\qquad \left. - \mathcal{R}_0(\boldsymbol{u}_0; \boldsymbol{p}_0)\right] \\ \delta_u Q(\boldsymbol{u}_0; \boldsymbol{w}_0) &= \lim_{\eta \to 0} \eta^{-1} \left[Q(\boldsymbol{u}_0 + \eta \boldsymbol{w}_0) - Q(\boldsymbol{u}_0)\right] \end{aligned}$$

are the Gâteuax derivatives. In the above, we suppress the dependence of residual $\mathcal{R}$ on model parameters $\boldsymbol{\theta}$. Combining, one can use the estimates of error, $(\hat{\boldsymbol{e}}_0, \hat{\varepsilon}_0)$, obtained by solving the linear problems in Equation 9 and Equation 10, together with the approximation of Ξ in Equation 8 to compute the estimates of the goal-oriented error.

In [18], such an estimation technique was applied to (i) comparing heterogeneous and homogenized elastic materials and (ii) comparing versions of incompressible Navier-Stokes and Stokes equations. Recently, [8] applied the above model misfit approach to calibrate the higher-fidelity model given the knowledge of the lower-fidelity model. Further extension of the work discussed in the next section includes correcting neural operator surrogates of PDE-based forward operators [3].

A.P. *has great memories of working with JTO and several other students/postdocs in the '90s K. Bey, W. Wu, M. Ainsworth and others where the notion of a posteriori error estimates for finite element models and their use in a dynamic strategy to deliver "Optimal numerical approximations" led to the current thinking on delivering certifiable models. The language was often salty but the rigor of thinking and writing incredible and indelible in our minds. As others like Ivo Babuska joined this conversation it became clear that much more than better finite element models were needed – an early stage in the evolution of ideas that*

later shaped the conversations recounted by D.F. *and* K.F.M..

Future Impacts and New Directions Inspired by JTO

The fundamental principles of predictive science advanced by JTO—rigorous model adaptivity, goal-oriented error estimation, model validation for purpose, and uncertainty quantification—have evolved from best practices into indispensable pillars of modern predictive computational science. Remarkably, the methodologies he began advancing as early as the 1990s are now widely embraced across the computational science community. As digital twins and AI models increasingly drive high-consequence decisions across healthcare, climate, energy, manufacturing, and autonomy, the demand for reliable computational predictions is now critical. Forward-looking strategic national reports, including *Foundational Research Gaps and Future Directions for Digital Twins* [13] and the *AI for Science, Energy, and Security Report* [25] explicitly emphasize the need to integrate robust validation, uncertainty quantification, and adaptive modeling into next-generation computational frameworks. In this evolving landscape, JTO's early vision and rigorous methodologies offer not just historical significance but a critical foundation for developing trustworthy computational models that support rational decision-making in complex and often life-critical environments. These principles have been broadly taken up across various engineering disciplines, informing today's common VVUQ practice.

JTO was among the first to conceptualize patient-specific cancer treatment as a digital twin, integrating biomechanical tumor growth models with clinical imaging to optimize individualized therapy planning, e.g., [10]. He later emphasized that predictive and personalized digital twins must be grounded in validated physics-based models with quantified uncertainties, establishing a rigorous framework for dynamic model selection and adaptive UQ in real-time monitoring of physical systems [21]. These foundational contributions continue to guide the development of next-generation digital twins for safety-critical applications, ranging from regulatory science in evaluating medical devices to real-time decision support in autonomous systems.

On the other hand, the rapid integration of AI into scientific discovery and technological innovation has exposed a critical gap: the lack of built-in mechanisms for error control and systematic frameworks for quantifying uncertainty and assessing the reliability of model predictions. In this context, JTO's foundational contributions offer an indispensable scientific approach for constructing trustworthy AI models. Particularly, his legacy in goal-oriented a-posteriori error estimation is poised to reshape how we assess the inadequacy and improve predictive ability in AI models. The recent extension of error estimation to neural operator surrogate models [3], [7], demonstrating that residual-based corrector frameworks can enhance accuracy and reliability through variational analysis of the governing PDEs. When coupled with infinite-dimensional Bayesian inference, these techniques further reduce approximation bias [3]. Equally transformative is the extension of JTO's methodologies to uncertainty quantification and model validation for AI models, in the same way they guide physics-based model selection. For example, OPAL has been recently extended to discover Bayesian neural network models that explicitly confront multifaceted sources of uncertainty, including data sparsity, aleatoric variability, numerical convergence errors, and architecture selection [23].

P.K.J. *learned topics in uncertainty quantification, model error, and goal-oriented a posteriori error estimates from JTO, who also encouraged him to explore their connections to emerging AI and machine learning methods. His intellectual curiosity was extraordinary; he was always eager to explore new areas.* P.K.J. *vividly recalls JTO preparing handwritten notes on deep learning, starting from the fundamentals of feed-forward neural networks and backpropagation. At the same time, JTO maintained a healthy skepticism toward the way machine learning was often applied in engineering contexts. He felt that much of the research lacked a rigorous foundation and was, at times, ad hoc. His approach was always to ground new methods in solid mathematical and physical principles. While working together on multiphysics modeling of tumor growth,* P.K.J. *gained a new perspective from JTO on balancing model complexity with the practical challenges of calibration and validation. JTO often*

emphasized that a model too simple to capture essential physics has limited predictive value, whereas an overly complex model with numerous parameters can be challenging to calibrate and validate, leading to significant predictive uncertainties. His philosophy was to find a thoughtful balance: adapt models based on physical understanding, rigorously account for model error, and focus on systematic calibration and validation. P.K.J. *learned immensely from working closely with JTO between 2019 and 2023 and feels deeply fortunate to have had such a formative experience.*

JTO's vision continues to define the trajectory of predictive science, bridging the rigor of classical computational science with the transformative potential of modern data-driven modeling and simulations. His legacy endures in the foundational principles that now guide the development of robust, trustworthy models for high-consequence applications, from scientific discovery to clinical diagnostics.

ACKNOWLEDGMENTS

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525. This paper describes objective technical results and analysis. Any subjective views or opinions that might be expressed in the paper do not necessarily represent the views of the U.S. Department of Energy or the United States Government.

REFERENCES

1. J. L. Beck. Bayesian system identification based on probability logic. *Structural Control and Health Monitoring*, 17(7):825–847, 2010.
2. J. L. Beck and K.-V. Yuen. Model selection using response measurements: Bayesian probabilistic approach. *Journal of Engineering Mechanics*, 130(2):192–203, 2004.
3. L. Cao, T. O'Leary-Roseberry, P. K. Jha, J. T. Oden, and O. Ghattas. Residual-based error correction for neural operator accelerated infinite-dimensional bayesian inverse problems. *Journal of Computational Physics*, page 112104, 2023.
4. L. Cao, K. Wu, J. T. Oden, P. Chen, and O. Ghattas. Bayesian model calibration for diblock copolymer thin film self-assembly using power spectrum of microscopy data and machine learning surrogate. *Computer Methods in Applied Mechanics and Engineering*, 417:116349, 2023. A Special Issue in Honor of the Lifetime Achievements of T. J. R. Hughes.
5. K. Farrell, J. T. Oden, and D. Faghihi. A bayesian framework for adaptive selection, calibration, and validation of coarse-grained models of atomistic systems. *Journal of Computational Physics*, 295:189–208, 2015.
6. E. T. Jaynes. *Probability theory: The logic of science*. Cambridge university press, 2003.
7. P. K. Jha. Residual-based error corrector operator to enhance accuracy and reliability of neural operator surrogates of nonlinear variational boundary-value problems. *Computer Methods in Applied Mechanics and Engineering*, 419:116595, 2024.
8. P. K. Jha and J. T. Oden. Goal-oriented a-posteriori estimation of model error as an aid to parameter estimation. *arXiv preprint arXiv:2205.15131*, 2022.
9. M. C. Kennedy and A. O'Hagan. Bayesian calibration of computer models. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, 63(3):425–464, 2001.
10. E. Lima, J. T. Oden, B. Wohlmuth, A. Shahmoradi, D. Hormuth II, T. Yankeelov, L. Scarabosio, and T. Horger. Selection and validation of predictive models of radiation effects on tumor growth based on noninvasive imaging data. *Computer methods in applied mechanics and engineering*, 327:277–305, 2017.
11. Y. Ling, J. Mullins, and S. Mahadevan. Selection of model discrepancy priors in bayesian calibration. *Journal of Computational Physics*, 276:665–680, 2014.
12. D. J. MacKay. Probable networks and plausible predictions-a review of practical bayesian methods for supervised neural networks. *Network: computation in neural systems*, 6(3):469, 1995.
13. National Academies of Sciences, Engineering, and Medicine. *Foundational Research Gaps and Future Directions for Digital Twins*. The National Academies Press, Washington, DC, 2023.
14. W. L. Oberkampf and C. J. Roy. *Verification and validation in scientific computing*. Cambridge university press, 2010.
15. J. T. Oden. Adaptive multiscale predictive modelling. *Acta Numerica*, 27:353–450, 2018.

16. J. T. Oden, I. Babuška, and D. Faghihi. Predictive computational science: Computer predictions in the presence of uncertainty. *Encyclopedia of Computational Mechanics Second Edition*, pages 1–26, 2017.
17. J. T. Oden and A. Patra. A parallel adaptive strategy for hp finite element computations. *Computer Methods in Applied Mechanics and Engineering*, 121(1):449–470, 1995.
18. J. T. Oden and S. Prudhomme. Estimation of modeling error in computational mechanics. *Journal of Computational Physics*, 182(2):496–515, 2002.
19. T. A. Oliver, G. Terejanu, C. S. Simmons, and R. D. Moser. Validating predictions of unobserved quantities. *Computer Methods in Applied Mechanics and Engineering*, 283:1310–1335, 2015.
20. A. Paquette-Rufiange, S. Prudhomme, and M. Laforest. Optimal design of validation experiments for the prediction of quantities of interest. *Computer Methods in Applied Mechanics and Engineering*, 414:116182, 2023.
21. E. Prudencio, P. Bauman, D. Faghihi, K. Ravi-Chandar, and J. Oden. A computational framework for dynamic data-driven material damage control, based on bayesian inference and model selection. *International Journal for Numerical Methods in Engineering*, 102(3-4):379–403, 2015.
22. E. E. Prudencio and K. W. Schulz. The parallel C++ statistical library 'QUESO': Quantification of uncertainty for estimation, simulation and optimization. In *European Conference on Parallel Processing*, pages 398–407. Springer, 2011.
23. P. K. Singh, K. A. Farrell-Maupin, and D. Faghihi. A framework for strategic discovery of credible neural network surrogate models under uncertainty. *Computer Methods in Applied Mechanics and Engineering*, 427:117061, 2024.
24. J. Tan, B. Liang, P. K. Singh, K. A. Farrell-Maupin, and D. Faghihi. Toward selecting optimal predictive multiscale models. *Computer Methods in Applied Mechanics and Engineering*, 402:115517, 2022.
25. U.S. Department of Energy, Office of Science. AI for Science, Energy, and Security Report 2023. Technical report, 2023.