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Musings On The Question of First Principles-Based Prediction

Daniel J. Segalman and John R. Red-Horse

Sandia National Laboratories
P.O. Box 5800, MS0828
Albuquerque, NM, 87185 USA

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Outline

Topic Is Timely—Again

- Emergence of MP computing and supporting mathematics has pushed the boundaries of what we can analyze
- Issue of mesh convergence not as predominant in the mix of open issues
- Governmental and industrial strategies to rely increasingly on simulation and less on experiment

Assertions for Discussion

- All useful models contain some epistemological constituents
  - Based on prior information
  - Cannot be derived from First Principles
- Even at the quantum level:
  - Models include constitutive relationships
  - Constitutive relationships are epistemological
- Above the quantum level:
  - All models contain aggregated information embodying approximations
  - They also involve epistemological constituents
    - Constitutive models
    - External force models
    - Boundary and Initial Conditions models
    - Interface models

Assertions for Discussion

- The distinction between epistemic and aleatoric uncertainties is generally not possible;
  - Multiple sources of uncertainty difficult to untangle.
- First Principles alone insufficient to achieve solutions
  - Constitutive models are unavoidable
  - Math problem must be rendered well posed
  - Computational considerations include convergence and conditioning
- First Principles computing is a myth

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Starting with Quantum Level

- Note that the wave function of the Schrödinger equation

$$i\frac{\partial}{\partial t}\Psi(\mathbf{x},t) = -\frac{1}{2m}\nabla^2\Psi(\mathbf{x},t) + V(x)\Psi(\mathbf{x},t)$$

  contains a potential energy term, $V(\mathbf{x})$, whose form must be postulated; it cannot be derived from First Principles.
- Thus, even this basic model incorporates an inferential constituent and, thus, is not completely First Principles-based.

Scales Above Quantum Level

- Can we derive our models from the quantum level and retain that rigor?
  - No, all methods to work up from quantum level require their own approximations and elements that are based on prior information (e.g. mean field theory)
- Can we derive these higher length scale, e.g continuum, models from first principles?
  - No, First Principles are not enough. The rest of this talk examines this issue...

First Principles in Applied Mechanics

- First Principles in Applied Mechanics
  - Conservation of Mass
  - Conservation of Energy
  - Conservation of Momentum
  - Etc
- Must be complemented with something else
  - Generally constitutive assumptions and equations embodying those assumptions
- Examples Follow

Atomistic Mechanics

- Momentum Equation:

$$\frac{d\mathbf{p}}{dt} = \mathbf{F}$$

- Constitutive Equation:

$$\mathbf{F} = -\nabla V(\mathbf{x})$$

- Where does one get $V(\mathbf{x})$? It is postulated!
  - For example, Lennard-Jones 6-12:

$$V(\mathbf{r}) = 4\epsilon\left[\left(\frac{\sigma}{\mathbf{r}}\right)^{12} - \left(\frac{\sigma}{\mathbf{r}}\right)^{6}\right]$$

  - The "6" term is asymptotic for noble gases at large distance
  - The "12" term is for convenience

First Principles must be augmented by constitutive assumptions

An Observation about Entropy

The principle of non-negative entropy production can be seen as a constraint on constitutive models

- Example: Conductive Heat Transfer
- Postulate that heat flux is linear in temperature gradient: $\mathbf{q} = -\mathbf{K} \bullet \nabla T$
- Clausius-Duhem inequality: $-\mathbf{q} \bullet \nabla T \geq 0$
  - Second Law of Thermodynamics
- Conclude that the conductivity tensor is positive semi-definite: $\mathbf{K} \geq 0$

Incompressible Navier-Stokes Equation

- First Principles
  - Conservation of Mass
  - Conservation of Momentum
- Assumptions
  - Continuum Assumption
  - Incompressibility, a constitutive assumption
  - Newtonian shear viscosity, another constitutive assumption
- The Navier-Stokes equation is "First Principles" only in that first principles are among the ingredients in the derivation.

Observations

- First Principles must be augmented by epistemological assumptions
- Constitutive models are always approximate
  - Postulated
  - Evidence-based
- The relevant constitutive assumptions and models employ force and kinematic assumptions on the scale of the problem being addressed
  - Lennard-Jones in atomistics
  - Incompressibility of continuum in Navier-Stokes

The Issue of Uncertainty

- Evidence-based constitutive information often accommodated using uncertainty models
  - Epistemic
  - Aleatoric
- Uncertainty models require a change in analysis context; for example, for probabilistic modeling:
  - Must migrate analysis from context of deterministic functions, $f(x)$, to random fields, $f(x, \omega)$
  - Probability measures can be thought of as constitutive models in new context
- Analyses incorporating an uncertainty context are always imperfect: Models are still models, whatever the context.

Concluding Remarks

- In engineering analysis, one must always complement first principles with epistemological constituents
  - We cannot derive them from First Principles
  - Information based (Postulation, Observation, etc)
  - Often approximations of subscale effects
  - Examples: Constitutive models, External environments, Boundary conditions, Interfaces
- Uncertainty quantification (UQ) methods provide means to analyze systems with evidence-based constituents
  - Probability measures, e.g., can be thought of as constitutive relationships in a UQ analysis context
  - Provide a more explicit way to examine the effects of information
  - The distinction between epistemic and aleatoric uncertainties is often not possible (or necessary)

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Concluding Remarks

- One cannot describe a model on engineering length scales as predictive in an the sense of being exact
  - Epistemological constituents lead to inference, not pure prediction
  - The best we can hope for is to make a prediction that is consistent with available information
- Striking the proper balance is vital
  - Often it will be more productive overall to make incremental investments to improve estimates of boundary and initial conditions and constitutive properties than to perform more precise solutions to equations
- We must be content with defining engineering models as predictive when we can use them to make decisions

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