Uncertainty Quantification in Materials Modeling

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Outline

1. Uncertainty in materials modeling
2. Uncertainty quantification in materials modeling
3. Introduction to peridynamics
4. Uncertainty quantification in fracture simulations
5. Conclusions
Quantum Mechanics of Many-Electron Systems.

By P. A. M. Dirac, St. John’s College, Cambridge.

(Communicated by R. H. Fowler, F.R.S.—Received March 12, 1929.)

§1. Introduction.

The general theory of quantum mechanics is now almost complete, the imperfections that still remain being in connection with the exact fitting in of the theory with relativity ideas. These give rise to difficulties only when high-speed particles are involved, and are therefore of no importance in the consideration of atomic and molecular structure and ordinary chemical reactions, in which it is, indeed, usually sufficiently accurate if one neglects relativity variation of mass with velocity and assumes only Coulomb forces between the various electrons and atomic nuclei. The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble. It therefore becomes desirable that approximate practical methods of applying quantum mechanics should be developed, which can lead to an explanation of the main features of complex atomic systems without too much computation.

Uncertainty in materials modeling

2. Materials length scales

*Based on a figure at http://www.gpm2.inpg.fr/perso/chercheurs/dr_articles/multiscale.jpg.
Algorithm: Velocity Verlet

1: \( v_{i}^{n+1/2} = v_{i}^{n} + \frac{\Delta t}{2m} f_{i}^{n} \)

2: \( y_{i}^{n+1} = y_{i}^{n} + \Delta t \cdot v_{i}^{n+1/2} \)

3: \( v_{i}^{n} = v_{i}^{n+1/2} + \frac{\Delta t}{2m} f_{i}^{n+1} \)

Checking realistic systems

1 cm\(^3\) of material \( \approx 6.022 \cdot 10^{23} \) particles

\( \approx 10^{13} \) TB of storage (1TB = 10\(^{12}\) bytes)

We can only simulate “small” systems

Titan @ ORNL : 710 TB
4. The mesoscale

Mesoscale lies between **microscopic** world of atoms/molecules and **macroscopic** world of bulk materials

Mesoscale is characterized by

- Collective behaviors
- Interaction of disparate degrees of freedom
- Fluctuations and statistical variations

Mesoscopic models (incomplete list):

- Random Walk
- Brownian Dynamics
- Phase Field
- Lattice Gas
- Lattice Boltzmann
- Smoothed Particle Hydrodynamics
- Dissipative Particle Dynamics
- Coarse-Grained Potentials
- Higher-Order Gradient PDEs
- Nonlocal Continuum Models
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Uncertainty in materials modeling

5. Mesoscopic models

**Macromolecules**

Coarse-grained potentials

**Fluid flow in porous media**

Dissipative particle dynamics
Smoothed particle hydrodynamics

**Damage and failure**

**Grain Growth**

Nonlocal continuum models (Peridynamics)

Phase-field methods

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* http://compmech.lab.asu.edu/research.php
§ https://github.com/dealii/dealii/wiki/Gallery
Uncertainty quantification in materials modeling

1. General definition of uncertainty

**Uncertainty** is a state of limited knowledge where it is impossible to exactly describe an existing state or future outcomes.

Two types of uncertainty:

- **Aleatoric uncertainty** - caused by intrinsic randomness of a phenomenon
- **Epistemic uncertainty** - caused by missing information about a system

Uncertainty in materials modeling:

- Uncertainty in constitutive model
- Uncertainty in system geometry
- Uncertainty in loadings
- Uncertainty in material constants
- Uncertainty in material microstructure
Uncertainty quantification in materials modeling

2. UQ methods

**Uncertainty quantification (UQ)**

Uncertainty quantification is the science of **quantitative characterization** and **reduction of uncertainties** in both experiments and computer simulations.

Two types of UQ methods:

- **Forward uncertainty propagation**
  - quantification of variabilities in system output(s) due to uncertainties in inputs
    - Monte Carlo (MC) methods
    - Polynomial-based methods

- **Inverse uncertainty quantification**
  - estimation of model inputs based on experimental/computational data
    - Bayesian inference
Uncertainty quantification in materials modeling

3. UQ in multiscale simulations

- **Inverse UQ** for model validation
- **Inverse UQ** for model calibration
- **Forward UQ** for uncertainty propagation

- **Validation data**
  - Inverse UQ for model validation

- **Calibration data**
  - Inverse UQ for model calibration

- **Predictive simulation**
Introduction to peridynamics
1. Motivation: failure and damage in materials

Tacoma Narrows Bridge Collapse
November 7, 1940

SS Schenectady Hull Fracture
January 16, 1943

Cracked road after Burma’s earthquake
March 24, 2011

Aluminium perforation by projectile

https://upload.wikimedia.org/wikipedia/commons/thumb/4/47/TankerSchenectady.jpg/300px-TankerSchenectady.jpg
https://myburma.files.wordpress.com/2011/03/earthquake-myanmar-12.jpg
Classical continuum mechanics assumptions:

1. The medium is continuous;
2. Internal forces are contact forces;
3. Deformation twice continuously differentiable (relaxed in weak forms); and
4. Conservation laws of mechanics apply

However, based on Newton’s *Principia*,

1. All materials are discontinuous; and
2. All materials have internal forces across nonzero distances

Common challenging topics for classical continuum mechanics include:
defects, phase transformations, composites, fracture, dislocations, micromechanics, nanostructures, biological materials, colloids, large molecules, complex fluids, etc.

*Silling, in Handbook of peridynamic modeling. CRC Press, 2016.*
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2. Classical mechanics assumptions

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3. Nonlocal models

Objective of peridynamics

The objective of peridynamics is to unify the mechanics of discrete particles, continuous media, and continuous media with evolving discontinuities.

Two classes of nonlocal models

1. *Strongly Nonlocal*: based on integral formulations.
2. *Weakly Nonlocal*: based on higher-order gradients.

Both model classes introduce length scales in governing equations.

Peridynamic models are **strongly nonlocal**

“It can be said that all physical phenomena are nonlocal. Locality is a fiction invented by idealists.” A. Cemal Eringen
The peridynamic (PD) theory

Generalized continuum theory based on spatial integration, that employs a nonlocal model of force interaction.

State-based PD equation of motion

\[ \rho(x) \frac{\partial^2 u(x, t)}{\partial t^2} = \int_B \{ T(x, t) \langle x' - x \rangle - T(x', t) \langle x - x' \rangle \} dV_{x'} + b(x, t) \]

\( \rho \): material density, \( u \): displacement field, \( b \): body force density

Force vector state

\( T(x, t) \langle \cdot \rangle \): “bond” → force per volume squared

Neighborhood

\[ \mathcal{H}_x := \{ x' \in B : ||x' - x|| \leq \delta \} \]

\[ \Rightarrow T(x, t) \langle x' - x \rangle = 0, \text{ for } ||x' - x|| > \delta \]

PD horizon: \( \delta \) (length scale)

PD equation of motion

\[ \rho(x) \frac{\partial^2 u}{\partial t^2}(x, t) = \int_{H_x} \{ T[x, t] \langle x' - x \rangle - T[x', t] \langle x - x' \rangle \} dV_{x'} + b(x, t) \]

If: (a) \( y \) is twice continuously differentiable in space and time
(b) \( T \) is a continuously differentiable function of the deformation and \( x \),

\[ \rho(x) \frac{\partial^2 u}{\partial t^2}(x, t) = \nabla \cdot \nu(x, t) + b(x, t) \]

with the nonlocal stress tensor* 

\[ \nu(x, t) = \int_S \int_0^\delta \int_0^\delta (y + z)^2 T[x - zm, t] \langle (y + z)m \rangle \otimes m \, dz \, dy \, d\Omega_m \]

\[ \delta \to 0 \]

Piola-Kirchhoff stress tensor

Introduction to peridynamics
5. Meshfree method

Given the PD equation of motion

\[ \rho(x) \frac{\partial^2 u}{\partial t^2}(x, t) = \int_{\mathcal{H}_x} \{ T[x, t] \langle x' - x \rangle - T[x', t] \langle x - x' \rangle \} \text{d}V_{x'} + b(x, t) \]

we discretize the body \( \mathcal{B} \) into particles forming a cubic lattice

\[ \rho_i \frac{d^2 u_i}{dt^2} = \sum_{j \in \mathcal{F}_i} \{ T[x_i, t] \langle x_j - x_i \rangle - T[x_j, t] \langle x_i - x_j \rangle \} V_j + b_i \]

where \( \mathcal{F}_i = \{ j : \|x_j - x_i\| \leq \delta, j \neq i \} \)

Note: other discretization methods are possible, e.g., finite elements\(^\dagger\).

Introduction to peridynamics

6. Bond-breaking criterion

**Bond-based PD equation of motion**

\[
\rho(x) \frac{\partial^2 u(x, t)}{\partial t^2} = \int_{\mathcal{H}_x} \{ T[x, t] \langle x' - x \rangle - T[x', t] \langle x - x' \rangle \} dV_{x'} + b(x, t)
\]

**Pairwise force function** (elastic)

\[
T[x, t] \langle \xi \rangle = \frac{1}{2} c(\xi) s(\eta, \xi) \frac{\eta + \xi}{||\eta + \xi||}
\]

\(\xi := x' - x, \ \eta := u(x', t) - u(x, t), \ c: \) micromodulus function

**Stretch**

\[
s(\eta, \xi) = \frac{||\eta + \xi|| - ||\xi||}{||\xi||}
\]

**Bond breaking** (critical stretch criterion):

If \(s(\eta, \xi) > s_0\) for given \(\xi\) at \(\tilde{t} > 0\) \(\Rightarrow T[x, t] \langle \xi \rangle = 0\) \(\forall t > \tilde{t}\)

**Damage**

\[
\varphi(x) = 1 - \frac{\int_{\mathcal{H}_x} \mu(x', x, t) dV_{x'}}{\int_{\mathcal{H}_x} dV_{x'}} ; \ \mu(x', x, t) = \begin{cases} 1 & s(\eta, \xi) \leq s_0 \ \forall \tilde{t} \leq t \\ 0 & \text{otherwise} \end{cases}
\]

Introduction to peridynamics

7. Applications

(a) Projectile impact on brittle disk§ (with Michael Parks)

(b) Crack branching in soda lime glass* (with Yohan John)

(c) Microcrack propagation in polycrystal† (with Jeremy Trageser)

Notably appealing features of peridynamics for modeling fracture

1. **No external “crack growth law”:**
   Cracks simply follow the energetically-favorable paths for a given system;

2. **Natural complex crack dynamics:**
   Crack initiation, grows, branching, instability, and arrest, as well as related properties, such crack velocity and direction, are a natural consequence of the evolution equation and the material constitutive model, which incorporates damage at the bond level.

“In peridynamics, cracks are part of the solution, not part of the problem.” F. Bobaru
## Introduction to peridynamics

### 9. Validation

<table>
<thead>
<tr>
<th>Fracture in steel (Kalthoff-Winkler)</th>
<th>Crack branching in soda-lime glass</th>
<th>Taylor impact test with 6061-T6 aluminium</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image1.png" alt="Experiment" /></td>
<td><img src="image2.png" alt="Simulation" /></td>
<td><img src="image3.png" alt="Simulation" /></td>
</tr>
</tbody>
</table>

### References

State-based PD equation of motion with uncertainty

\[ \rho(x) \frac{\partial^2 u}{\partial t^2}(x, t) = \int_B \{ T[x, t] \langle x' - x \rangle - T[x', t] \langle x - x' \rangle \} dV_{x'} + b(x, t) \]
State-based PD equation of motion with uncertainty

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- Random vector \( y_1 \in \mathcal{U}_{d_1} \subset \mathbb{R}^{d_1} \) coming from the external loadings
Uncertainty quantification in fracture simulations

1. Peridynamic stochastic models

State-based PD equation of motion with uncertainty

\[ \rho(x, y_2) \frac{\partial^2 u}{\partial t^2}(x, t) = \int_B \{ T[x, t] \langle x' - x \rangle - \overline{T}[x', t] \langle x - x' \rangle \} dV_{x'} + b(x, t, y_1) \]

- Random vector \( y_1 \in \mathcal{U}_{d_1} \subset \mathbb{R}^{d_1} \) coming from the external loadings
- Random vector \( y_2 \in \mathcal{U}_{d_2} \subset \mathbb{R}^{d_2} \) coming from the mass distribution
Uncertainty quantification in fracture simulations
1. Peridynamic stochastic models

State-based PD equation of motion with uncertainty

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- Random vector \( y_1 \in \mathcal{U}_{d_1} \subset \mathbb{R}^{d_1} \) coming from the external loadings.
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Uncertainty quantification in fracture simulations
1. Peridynamic stochastic models

**State-based PD equation of motion with uncertainty**

$$\rho(x, y_2) \frac{\partial^2 u}{\partial t^2}(x, t) = \int_B \{T[x, t, y_3] \langle x' - x \rangle - T[x', t, y_3] \langle x - x' \rangle \} \, dV_{x'} + b(x, t, y_1)$$

- Random vector $y_1 \in \mathcal{U}_{d_1} \subset \mathbb{R}^{d_1}$ coming from the external loadings.
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- Random vector $y_3 \in \mathcal{U}_{d_3} \subset \mathbb{R}^{d_3}$ coming from the constitutive relation.
- We may have additional uncertainty in the initial and boundary conditions.
Uncertainty quantification in fracture simulations

1. Peridynamic stochastic models

**State-based PD equation of motion with uncertainty**

\[ \rho(x, y_2) \frac{\partial^2 u}{\partial t^2}(x, t) = \int_{B} \{ \mathbf{T}[x, t, y_3] \langle x' - x \rangle - \mathbf{T}[x', t, y_3] \langle x - x' \rangle \} dV_{x'} + \mathbf{b}(x, t, y_1) \]

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- Random vector \( y_3 \in \mathcal{U}_{d_3} \subset \mathbb{R}^{d_3} \) coming from the constitutive relation.
- We may have additional uncertainty in the initial and boundary conditions.

**Goal**

Given \( y \in \mathcal{U} = \mathcal{U}_{d_1} \times \mathcal{U}_{d_2} \times \ldots \times \mathcal{U}_{d_n} \subset \mathbb{R}^d \), quickly approximate the solution map \( y \rightarrow u(\cdot, y) \).
2. Example of uncertainty in impact direction

Example I: impact damage

Straight impact

Inclined impact (30° inclination)
Example II: crack branching

Medium traction ($\sigma = 2\text{MPa}$)

High traction ($\sigma = 4\text{MPa}$)
Example III: microcrack networks
Crack branching in soda-lime glass

<table>
<thead>
<tr>
<th>$\rho$</th>
<th>$E$</th>
<th>$G_0$</th>
<th>$\delta$</th>
<th>$\sigma$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2440 Kg / m$^3$</td>
<td>$70 \pm 7 \times 10^9$ Pa</td>
<td>3.8 J / m$^2$</td>
<td>0.001 m</td>
<td>$22.5 \pm 5 \times 10^5$ Pa</td>
</tr>
</tbody>
</table>

**Stochastic model:** We parametrize the Young’s modulus and traction as

$$E = (70 + 7y_1) \times 10^9, \quad \sigma = (22.5 + 5y_2) \times 10^5$$

; \quad y_1, y_2 \in [-1, 1]

- The displacement field $u(x, t; y)$ and bond-breaking indicator $\mu(x', x, t; y)$ depend on the parameter vector $y = (y_1, y_2)^T$ with $y_1, y_2 \in [-1, 1]$.
- Suppressing the dependence on $x$ and $t$, we consider the map $y \rightarrow u(y), \mu(y)$. 
Uncertainty quantification in fracture simulations

4. A surrogate modeling approach for cracks simulation

Given a parametric model, consider the input/output map

\[ y \rightarrow u(y) ; \quad y \in \Gamma \subset \mathbb{R}^d, u(y) \in H \]

Uncertainty quantification pertains to the statistics of \( u(y) \), but statistical analysis requires prohibitively large number of evaluations of \( u(y) \).

**Objective:** develop cheap method to evaluate surrogate model \( u(y) \approx \sum_{i=1}^{m} v_i \phi_i(y) \)

**Challenge:** develop techniques free from assumptions on regularity

- Irregular problems require dense \( H \), e.g., very dense mesh
- Irregular problems require irregular functions \( \phi_i(y) \), e.g., discontinuous basis
- Derive rigorous error bounds

\[ \left\| u(y) - \sum_{i=1}^{m} v_i \phi_i(y) \right\|_{L^2(\Gamma)} \]

- Provide robust algorithm applicable to black-box model
Uncertainty quantification in fracture simulations

4. A surrogate modeling approach for cracks simulation

Step I: reduced basis (RB) approximation

Theoretical background

Optimal low-dimensional approximation (Kolmogorov $n$-width)*

$$d_n = \inf_{\mathcal{V} \subset H: \dim(\mathcal{V}) = n} \sup_{y \in \Gamma} \inf_{w \in \mathcal{V}} \|u(y) - w\|_H$$

- Standard RB construction uses greedy search and Galerkin residual*, inapplicable to our context.
- We assume that for a moderate $n$, $d_n$ drops below some pre-defined tolerance $\epsilon$, and we seek a subspace $\mathcal{V}$ so that $\sup_{y \in \Gamma} \inf_{w \in \mathcal{V}} \|u(y) - w\|_H < \epsilon$.

Reduced basis algorithm

Let $\mathcal{V}_0 = \emptyset$, $n = 0$

for $s = 1, 2, \ldots, k$ do

- Select $y_s \in \Gamma$ (according to uniform distribution)
- Compute $u(y_s)$
- if $\inf_{w \in \mathcal{V}_n} \|u(y_s) - w\|_H > \epsilon$ then
  - $\mathcal{V}_{n+1} = \text{span}\{\mathcal{V}_n \cup \{u(y_s)\}\}$
  - $n = n + 1$
- end if

end for

return $\mathcal{V} = \mathcal{V}_n$

Uncertainty quantification in fracture simulations

4. A surrogate modeling approach for cracks simulation

Step I: reduced basis (RB) approximation

Error bounds

\[ E := \sup_{y \in \Gamma} \inf_{w \in V} \| u(y) - w \|_H \]

\[ \mathbb{E}_{\{y_s\}_{s=1}^k} [E] \leq \epsilon + \frac{M}{k - n} \]

\[ \mathbb{V}_{\{y_s\}_{s=1}^k} [E] \leq \frac{M^2}{(k - n)^2} \]

\( n = \text{dim}(V), \; k: \text{total number of samples}, \; M = \sup_{y \in \Gamma} \| u(y) \|_H \)

For a 2D 400 \times 160 grid, we have 128,000 unknowns for the displacement field.

For \( \epsilon = 10^{-4}, \; k = 2,500 \), we reduce \( \text{dim}(H) = 128000 \rightarrow \text{dim}(V) = 70 \)

Step II: a surrogate model based on sparse grids rules

We would like to approximate

$$u(y) \approx V \sum_{i=1}^{m} c_i \phi_i(y)$$

$V$: projection operator based on the RB functions.

Using the total number of samples, $k$, we solve an $\ell^2$ minimization

$$\min_{c_1,...,c_m} \frac{1}{2} \sum_{s=1}^{k} \left( \sum_{i=1}^{m} c_i \phi_i(y_s) - V^T u(y_s) \right)^2,$$

which, in matrix form, is given by

$$\begin{pmatrix}
\phi_1(y_1) & \cdots & \phi_m(y_1) \\
\vdots & \ddots & \vdots \\
\phi_1(y_k) & \cdots & \phi_m(y_k)
\end{pmatrix}
\begin{pmatrix}
c_1 \\
\vdots \\
c_m
\end{pmatrix}
= 
\begin{pmatrix}
V^T u(y_1) \\
\vdots \\
V^T u(y_k)
\end{pmatrix}$$
Step II: a surrogate model based on sparse grids rules

**Approach:** use $\ell^2$ projection on hierarchical piece-wise constant basis (reuse existing $k$ samples)
Uncertainty quantification in fracture simulations

5. Numerical results

<table>
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<tr>
<th>Full model</th>
<th>Surrogate model (34 RB functions)</th>
<th>Surrogate model (70 RB functions)</th>
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</tbody>
</table>
5. Numerical results

**Damage distribution (10,000 samples)**

\[
\varphi(x, t) = 1 - \frac{\int_{H_x} \mu(x', x, t) dV_{x'}}{\int_{H_x} dV_{x'}} ; \quad \bar{\varphi}(t) = \frac{1}{|B|} \int_{B} \varphi(x, t) dV_x
\]
5. Numerical results

**Damage distribution** (multi-branch)

![Graph showing the percentage of broken bonds over a range from 0.7 to 1.6](image-url)
Conclusions

- Uncertainty quantification (UQ) is fundamental for materials modeling
- In particular, UQ is critical for fracture problems
- Surrogate models allow to qualitatively capture fracture patterns
- Surrogate models can yield $10^{4-6}$ samples in feasible amount of time
- This enables the application of rigorous UQ techniques for uncertainty propagation, validation, and verification.

Reference:
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