Uncertainty Quantification in Materials Modeling

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Quantification of Uncertainty: Improving Efficiency and Technology
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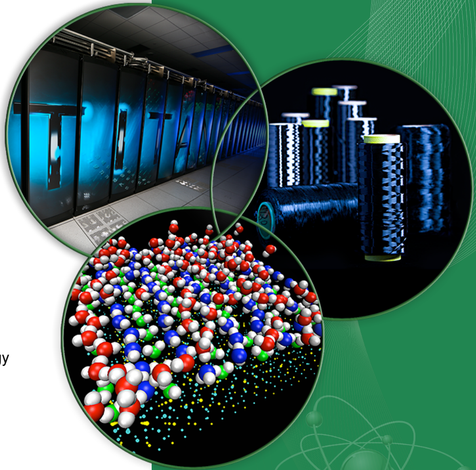

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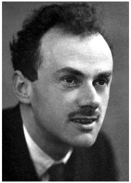
Outline

1. Uncertainty in materials modeling
2. Uncertainty quantification in materials modeling
3. Introduction to peridynamics
4. Uncertainty quantification in fracture simulations
5. Conclusions



Paul A. M. Dirac
(1902-1984)

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.)

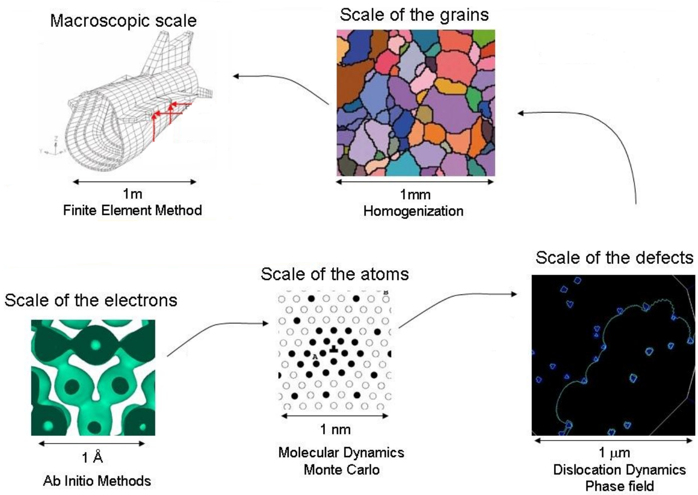
§ 1. *Introduction.*

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.

* Dirac, *Proc. R. Soc. Lond. A* 123 (1929): 714–733.

Uncertainty in materials modeling

2. Materials length scales



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

Uncertainty in materials modeling

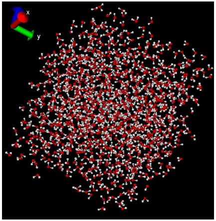
3. Computational complexity

Algorithm: Velocity Verlet

1: $\mathbf{v}_i^{n+1/2} = \mathbf{v}_i^n + \frac{\Delta t}{2m}\mathbf{f}_i^n$

2: $\mathbf{y}_i^{n+1} = \mathbf{y}_i^n + \Delta t\, \mathbf{v}_i^{n+1/2}$

3: $\mathbf{v}_i^n = \mathbf{v}_i^{n+1/2} + \frac{\Delta t}{2m}\mathbf{f}_i^{n+1}$



Checking realistic systems

1cm^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

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Uncertainty in materials modeling

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

Uncertainty in materials modeling

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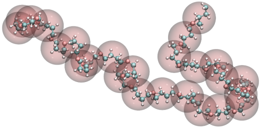
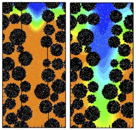
Macromolecules



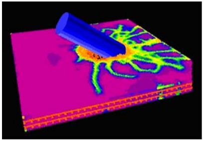
*Coarse-grained potentials**

Fluid flow in porous media



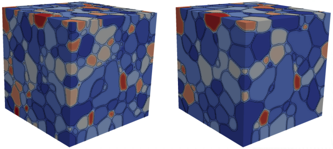
Dissipative particle dynamics
Smoothed particle hydrodynamics†

Damage and failure



Nonlocal continuum models (Peridynamics)‡

Grain Growth



Phase-field methods§

* http://compmech.lab.asu.edu/research.php
† Tartakovsky, Meakin, *Advances in Water Resources* 29 (2006): 1464–1478.
‡ http://www.sandia.gov/~sasilli/ses-silling-2014.pdf
§ https://github.com/dealii/dealii/wiki/Gallery

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 (UQ)

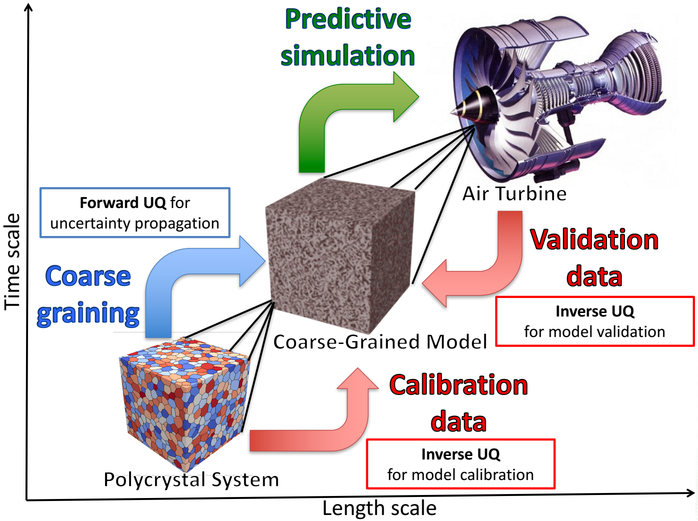
Uncertainty quantification is the science of **quantitative characterization** and **reduction of uncertainties** in both experiments and computer simulations.

Two types of UQ methods:

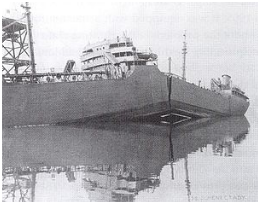
- **Forward uncertainty propagation**
  - quantification of variabilities in system output(s) due to uncertainties in inputs
    - Monte Carlo (MC) methods
    - Polynomial-based methods
- **Inverse uncertainty quantification**
  - estimation of model inputs based on experimental/computational data
    - Bayesian inference

Uncertainty quantification in materials modeling

3. UQ in multiscale simulations

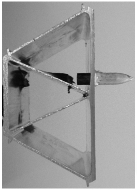


Tacoma Narrows Bridge Collapse
November 7, 1940



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/4/4a/Tacoma-narrows-bridge-collapse.jpg/200px-Tacoma-narrows-bridge-collapse.jpg
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
Børvik, Clausen, Eriksson, Berstad, Hopperstad, Langseth, *Int. J. Impact Eng.* 32 (2005): 35–64.

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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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

* Silling, in Handbook of peridynamic modeling. CRC Press, 2016.

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

$$\rho(\mathbf{x})\frac{\partial^2\mathbf{u}}{\partial t^2}(\mathbf{x},t) = \int_{\mathcal{B}} \left\{\underline{\mathbf{T}}\left[\mathbf{x},t\right]\langle\mathbf{x}'-\mathbf{x}\rangle - \underline{\mathbf{T}}\left[\mathbf{x}',t\right]\langle\mathbf{x}-\mathbf{x}'\rangle\right\} dV_{\mathbf{x}'} + \mathbf{b}(\mathbf{x},t)$$

ρ: material density, $\mathbf{u}$: displacement field, $\mathbf{b}$: body force density

Force vector state

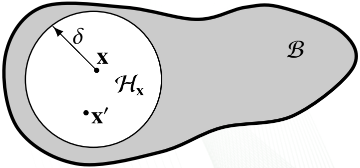
$\underline{\mathbf{T}}\left[\mathbf{x},t\right]\langle\cdot\rangle$: “bond” → force per volume squared

Neighborhood

$\mathcal{H}_{\mathbf{x}} := \{\mathbf{x}' \in \mathcal{B} : ||\mathbf{x}'-\mathbf{x}|| \leq \delta\}$

$\Rightarrow \underline{\mathbf{T}}\left[\mathbf{x},t\right]\langle\mathbf{x}'-\mathbf{x}\rangle = \mathbf{0}$, for $||\mathbf{x}'-\mathbf{x}|| > \delta$

PD horizon: δ (length scale)



* Silling, Epton, Weckner, Xu, Askari, *J. Elast.* 88 (2007): 151–184.

PD equation of motion

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

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

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

with the **nonlocal stress tensor***

$$\boldsymbol{\nu}(\mathbf{x},t) = \int_{\mathcal{S}}\int_0^\delta\int_0^\delta (y+z)^2\underline{\mathbf{T}}[\mathbf{x}-z\mathbf{m},t]\langle (y+z)\mathbf{m}\rangle\otimes\mathbf{m}\, dz\,dy\,d\Omega_{\mathbf{m}}$$

$\delta \to 0$

Piola-Kirchhoff stress tensor

* Silling, Lehoucq, *J. Elast.* 93 (2008): 13–37.

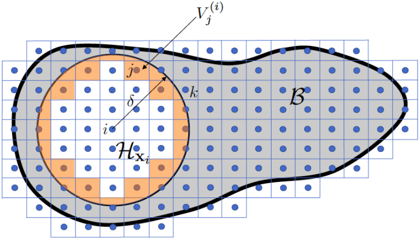
Introduction to peridynamics

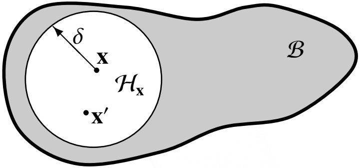
5. Meshfree method

Given the PD equation of motion

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

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





to get

$$\rho_i\frac{d^2\mathbf{u}_i}{dt^2} = \sum_{j\in\mathcal{F}_i} \left\{ \underline{\mathbf{T}}\left[\mathbf{x}_i,t\right]\left\langle\mathbf{x}_j-\mathbf{x}_i\right\rangle - \underline{\mathbf{T}}\left[\mathbf{x}_j,t\right]\left\langle\mathbf{x}_i-\mathbf{x}_j\right\rangle \right\} V_j + \mathbf{b}_i$$

$$\mathcal{F}_i = \{ j \ : \ \|\mathbf{x}_j - \mathbf{x}_i\| \le \delta, \ j \ne i \}$$

Note: other discretization methods are possible, e.g., finite elements[†].

[*] Silling, Askari, *Computers & Structures* 83 (2005): 1526–1535.
[†] Chen, Gunzburger, *Comput. Methods Appl. Mech. Engrg.* 200 (2011): 1237–1250.

Introduction to peridynamics

6. Bond-breaking criterion

Bond-based PD equation of motion

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

Pairwise force function (elastic)

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

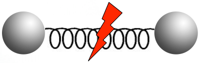
$\boldsymbol{\xi} := \mathbf{x}'-\mathbf{x}$, $\boldsymbol{\eta} := \mathbf{u}(\mathbf{x}',t)-\mathbf{u}(\mathbf{x},t)$, c: micromodulus function

Stretch

$$s(\boldsymbol{\eta},\boldsymbol{\xi}) = \frac{\|\boldsymbol{\eta}+\boldsymbol{\xi}\| - \|\boldsymbol{\xi}\|}{\|\boldsymbol{\xi}\|}$$

Bond breaking (critical stretch criterion):

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



Damage

$$\varphi(\mathbf{x}) = 1 - \frac{\int_{\mathcal{H}_\mathbf{x}} \mu(\mathbf{x}',\mathbf{x},t)\,dV_{\mathbf{x}'}}{\int_{\mathcal{H}_\mathbf{x}} dV_{\mathbf{x}'}} \quad ; \quad \mu(\mathbf{x}',\mathbf{x},t) = \begin{cases} 1 & s(\boldsymbol{\eta},\boldsymbol{\xi}) \le s_0 \;\forall \tilde{t} \le t \\ 0 & \text{otherwise} \end{cases}$$

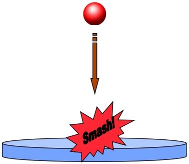
* Silling, Askari, *Computers & Structures* 83 (2005): 1526–1535.

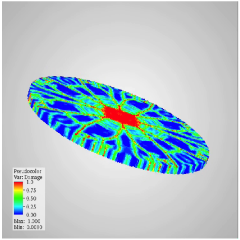
Introduction to peridynamics

7. Applications

(a) Projectile impact on brittle disk[§]

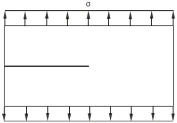
(with Michael Parks)

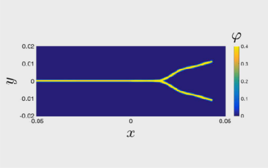


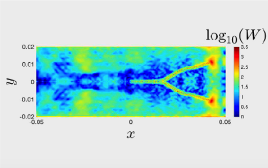


(b) Crack branching in soda lime glass[*]

(with Yohan John)

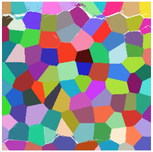


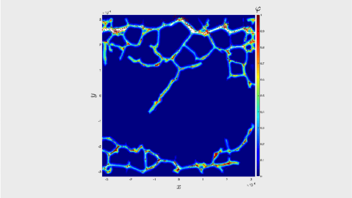




(c) Microcrack propagation in polycrystal[†]

(with Jeremy Trageser)





[§] Silling, Askari, *Comput. Struct.* 83 (2005): 1526–1535.
[*] Bobaru, Zhang, *Int. J. Fract.* 196 (2015):59–98.
[†] Ghajari, Iannucci, Curtis, *Comput. Methods Appl. Mech. Engrg.* 276 (2014): 431–452.

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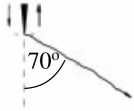
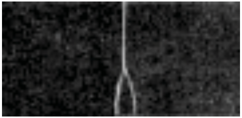
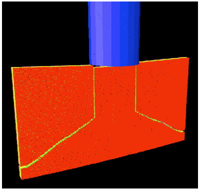
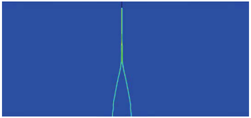
Notably appealing features of peridynamics for modeling fracture

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

	Fracture in steel (Kalthoff-Winkler)	Crack branching in soda-lime glass	Taylor impact test with 6061-T6 aluminium
Experiment			
Simulation			
	Simulation in EMU	**Simulation in PD-LAMMPS**	**Simulation in EMU**

* Bowden, Brunton, Field, Heyes, *Nature* 216 (1967), pp. 38–42.
Anderson, Nicholls, Chocron, Ryckman, *AIP Conf. Proc.*, vol. 845, Melville, N.Y. (2006), pp. 1367–1370.
Silling, in Computational Fluid and Solid Mechanics 2003, K.J. Bathe, ed., pp. 641–644.
Foster, Silling, Chen, *Int. J. Numer. Meth. Engng.* 81 (2010), pp. 1242–1258.

State-based PD equation of motion with uncertainty

$$\rho(\mathbf{x}) \frac{\partial^2 \mathbf{u}}{\partial t^2}(\mathbf{x}, t) = \int_{\mathcal{B}} \left\{ \underline{\mathbf{T}}\left[\mathbf{x}, t\right] \langle \mathbf{x}' - \mathbf{x} \rangle - \underline{\mathbf{T}}\left[\mathbf{x}', t\right] \langle \mathbf{x} - \mathbf{x}' \rangle \right\} dV_{\mathbf{x}'} + \mathbf{b}(\mathbf{x}, t)$$

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- Random vector $\boldsymbol{y}_1 \in \mathcal{U}_{d_1} \subset \mathbb{R}^{d_1}$ coming from the external loadings

State-based PD equation of motion with uncertainty

$$\rho(\mathbf{x}, \boldsymbol{y}_2)\frac{\partial^2 \mathbf{u}}{\partial t^2}(\mathbf{x}, t) = \int_{\mathcal{B}} \{\underline{\mathbf{T}}[\mathbf{x}, t]\langle \mathbf{x}' - \mathbf{x}\rangle - \underline{\mathbf{T}}[\mathbf{x}', t]\langle \mathbf{x} - \mathbf{x}'\rangle\} \, dV_{\mathbf{x}'} + \mathbf{b}(\mathbf{x}, t, \boldsymbol{y}_1)$$

- Random vector $\boldsymbol{y}_1 \in \mathcal{U}_{d_1} \subset \mathbb{R}^{d_1}$ coming from the external loadings
- Random vector $\boldsymbol{y}_2 \in \mathcal{U}_{d_2} \subset \mathbb{R}^{d_2}$ coming from the mass distribution

State-based PD equation of motion with uncertainty

$$\rho(\mathbf{x}, \boldsymbol{y}_2) \frac{\partial^2 \mathbf{u}}{\partial t^2}(\mathbf{x}, t) = \int_{\mathcal{B}} \{\underline{\mathbf{T}}[\mathbf{x}, t, \boldsymbol{y}_3]\langle \mathbf{x}' - \mathbf{x} \rangle - \underline{\mathbf{T}}[\mathbf{x}', t, \boldsymbol{y}_3]\langle \mathbf{x} - \mathbf{x}' \rangle\} dV_{\mathbf{x}'} + \mathbf{b}(\mathbf{x}, t, \boldsymbol{y}_1)$$

- Random vector $\boldsymbol{y}_1 \in \mathcal{U}_{d_1} \subset \mathbb{R}^{d_1}$ coming from the external loadings.
- Random vector $\boldsymbol{y}_2 \in \mathcal{U}_{d_2} \subset \mathbb{R}^{d_2}$ coming from the mass distribution.
- Random vector $\boldsymbol{y}_3 \in \mathcal{U}_{d_3} \subset \mathbb{R}^{d_3}$ coming from the constitutive relation.

State-based PD equation of motion with uncertainty

$$\rho(\mathbf{x}, \boldsymbol{y}_2)\frac{\partial^2 \mathbf{u}}{\partial t^2}(\mathbf{x}, t) = \int_{\mathcal{B}} \{\underline{\mathbf{T}}[\mathbf{x}, t, \boldsymbol{y}_3]\langle \mathbf{x}' - \mathbf{x}\rangle - \underline{\mathbf{T}}[\mathbf{x}', t, \boldsymbol{y}_3]\langle \mathbf{x} - \mathbf{x}'\rangle\} \, dV_{\mathbf{x}'} + \mathbf{b}(\mathbf{x}, t, \boldsymbol{y}_1)$$

- Random vector $\boldsymbol{y}_1 \in \mathcal{U}_{d_1} \subset \mathbb{R}^{d_1}$ coming from the external loadings.
- Random vector $\boldsymbol{y}_2 \in \mathcal{U}_{d_2} \subset \mathbb{R}^{d_2}$ coming from the mass distribution.
- Random vector $\boldsymbol{y}_3 \in \mathcal{U}_{d_3} \subset \mathbb{R}^{d_3}$ coming from the constitutive relation.
- We may have additional uncertainty in the initial and boundary conditions.

State-based PD equation of motion with uncertainty

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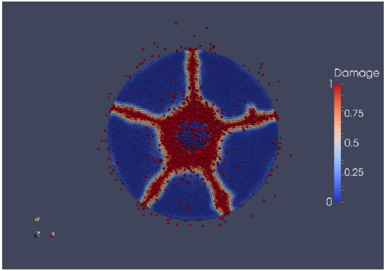
- Random vector $\boldsymbol{y}_3 \in \mathcal{U}_{d_3} \subset \mathbb{R}^{d_3}$ coming from the constitutive relation.
- We may have additional uncertainty in the initial and boundary conditions.

Goal

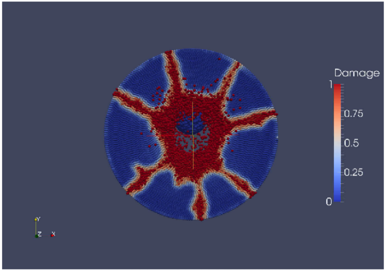
Given $\boldsymbol{y} \in \mathcal{U} = \mathcal{U}_{d_1} \times \mathcal{U}_{d_2} \times \ldots \times \mathcal{U}_{d_n} \subset \mathbb{R}^d$, quickly approximate the solution map $\boldsymbol{y} \to \mathbf{u}(\cdot, \boldsymbol{y})$.

Example I: impact damage

Straight impact

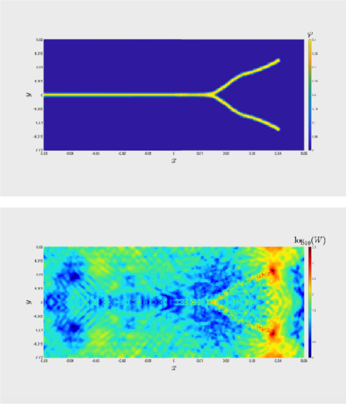


Inclined impact (30^o inclination)

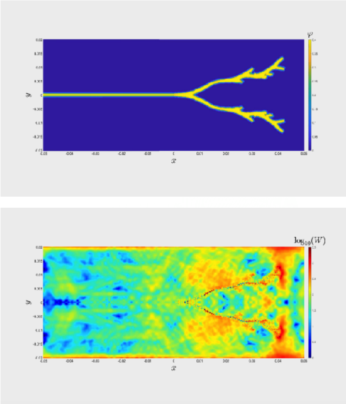


Example II: crack branching

Medium traction ($\sigma = 2$MPa)



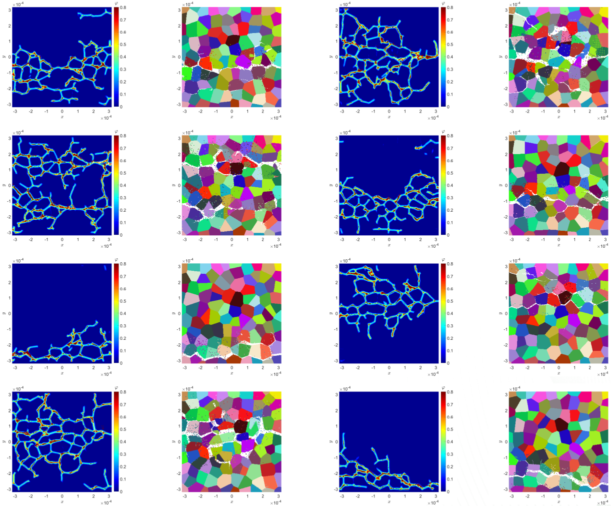
High traction ($\sigma = 4$MPa)



Uncertainty quantification in fracture simulations

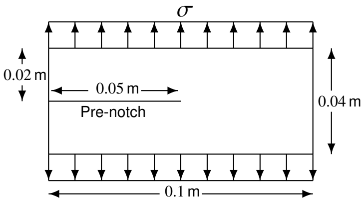
4. Example of uncertainty in microstructure

Example III: microcrack networks



Crack branching in soda-lime glass

ρ	E	G_0	δ	σ
2440 Kg / m^3	$70 \pm 7 \times 10^9$ Pa	3.8 J / m^2	0.001 m	$22.5 \pm 5 \times 10^5$ Pa



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

$$E = (70 + 7y_1) \times 10^9, \qquad \sigma = (22.5 + 5y_2) \times 10^5 \qquad ; \qquad y_1, y_2 \in [-1, 1]$$

- The displacement field $\mathbf{u}(\mathbf{x}, t; \boldsymbol{y})$ and bond-breaking indicator $\mu(\mathbf{x}', \mathbf{x}, t; \boldsymbol{y})$ depend on the parameter vector $\boldsymbol{y} = (y_1, y_2)^T$
- Suppressing the dependence on $\mathbf{x}$ and t, we consider the map $\boldsymbol{y} \to \mathbf{u}(\boldsymbol{y}), \mu(\boldsymbol{y})$

Given a parametric model, consider the input/output map

$$\boldsymbol{y} \to \mathbf{u}(\boldsymbol{y}) \qquad ; \qquad \boldsymbol{y} \in \Gamma \subset \mathbb{R}^d, \mathbf{u}(\boldsymbol{y}) \in H$$

Uncertainty quantification pertains to the statistics of $\mathbf{u}(\boldsymbol{y})$, but statistical analysis requires prohibitively large number of evaluations of $\mathbf{u}(\boldsymbol{y})$

Objective: develop cheap method to evaluate surrogate model $\mathbf{u}(\boldsymbol{y}) \approx \sum_{i=1}^m \mathbf{v}_i \phi_i(\boldsymbol{y})$

Challenge: develop techniques free from assumptions on regularity

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

$$\left\| \mathbf{u}(\boldsymbol{y}) - \sum_{i=1}^{m} \mathbf{v}_i \phi_i(\boldsymbol{y}) \right\|_{L^2(\Gamma)}$$

- Provide robust algorithm applicable to black-box model

Step I: reduced basis (RB) approximation

Theoretical background

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

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

- 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 ϵ, and we seek a subspace $\mathcal{V}$ so that $\sup_{\boldsymbol{y}\in\Gamma} \inf_{\mathbf{w}\in\mathcal{V}} \|\mathbf{u}(\boldsymbol{y}) - \mathbf{w}\|_H < \epsilon$.

Reduced basis algorithm

Let $\mathcal{V}_0 = \emptyset$, $n = 0$
for $s = 1, 2, \ldots, k$ **do**
  Select $\boldsymbol{y}_s \in \Gamma$ (according to uniform distribution)
  Compute $\mathbf{u}(\boldsymbol{y}_s)$
  if $\inf_{\mathbf{w}\in\mathcal{V}_n} \|\mathbf{u}(\boldsymbol{y}_s) - \mathbf{w}\|_H > \epsilon$ **then**
    $\mathcal{V}_{n+1} = span\{\mathcal{V}_n \bigcup \{\mathbf{u}(\boldsymbol{y}_s)\}\}$
    $n = n + 1$
  end if
end for
return $\mathcal{V} = \mathcal{V}_n$

*Binev, Cohen, Dahmen, DeVore, Petrova, Wojtaszczyk, *SIAM J. Math. Anal.* 43(3) (2011): 1457–1472.
†Stoyanov, Webster, *Int. J. Uncertain Quantif.* 5 (2015): 49–72.

Step I: reduced basis (RB) approximation

Error bounds*

$$E := \sup_{\boldsymbol{y}\in\Gamma} \inf_{\mathbf{w}\in\mathcal{V}} \|\mathbf{u}(\boldsymbol{y}) - \mathbf{w}\|_H$$

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

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

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

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

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

*Stoyanov, Webster, *Int. J. Uncertain Quantif.* 5 (2015): 49–72.

Step II: a surrogate model based on sparse grids rules

We would like to approximate

$$\mathbf{u}(\boldsymbol{y}) \approx V \sum_{i=1}^{m} \mathbf{c}_i \phi_i(\boldsymbol{y})$$

V: projection operator based on the RB functions.

Using the total number of samples, k, we solve an ℓ^2 minimization

$$\min_{\mathbf{c}_1,\ldots,\mathbf{c}_m} \frac{1}{2} \sum_{s=1}^{k} \left(\sum_{i=1}^{m} \mathbf{c}_i \phi_i(\boldsymbol{y}_s) - V^T \mathbf{u}(\boldsymbol{y}_s) \right)^2 ,$$

which, in matrix form, is given by

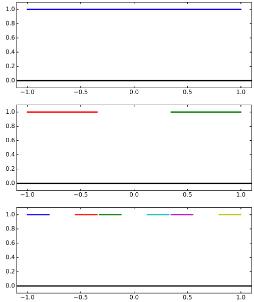
$$\begin{pmatrix} \phi_1(\boldsymbol{y}_1) & \cdots & \phi_m(\boldsymbol{y}_1) \\ \vdots & \ddots & \vdots \\ \phi_1(\boldsymbol{y}_k) & \cdots & \phi_m(\boldsymbol{y}_k) \end{pmatrix} \begin{pmatrix} \mathbf{c}_1 \\ \vdots \\ \mathbf{c}_m \end{pmatrix} = \begin{pmatrix} V^T \mathbf{u}(\boldsymbol{y}_1) \\ \vdots \\ V^T \mathbf{u}(\boldsymbol{y}_k) \end{pmatrix}$$

Uncertainty quantification in fracture simulations

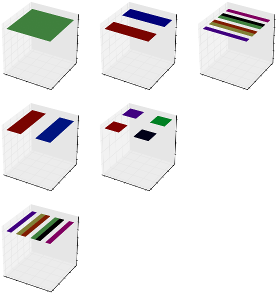
4. A surrogate modeling approach for cracks simulation

Step II: a surrogate model based on sparse grids rules

Approach: use ℓ^2 projection on hierarchical piece-wise constant basis
(reuse existing k samples)



1-D piece-wise constant hierarchy of basis functions



2-D functions constructed from sparse tensorization

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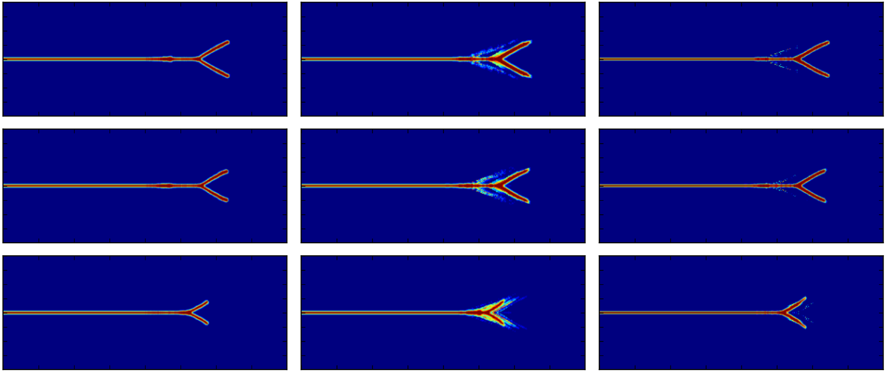
Uncertainty quantification in fracture simulations

5. Numerical results

Full model | **Surrogate model** (34 RB functions) | **Surrogate model** (70 RB functions)



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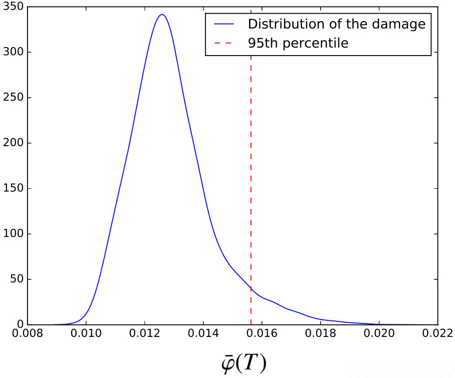
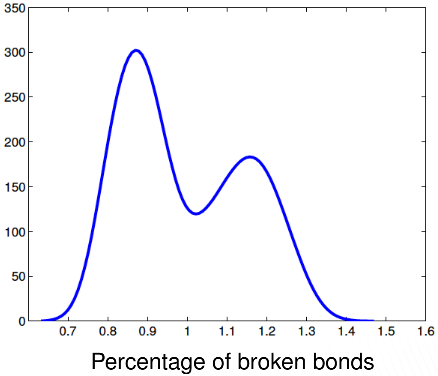
Damage distribution (10,000 samples)

$$\varphi(\mathbf{x},t) = 1 - \frac{\int_{\mathcal{H}_\mathbf{x}} \mu(\mathbf{x}',\mathbf{x},t)dV_{\mathbf{x}'}}{\int_{\mathcal{H}_\mathbf{x}} dV_{\mathbf{x}'}} \quad ; \quad \bar{\varphi}(t) = \frac{1}{|\mathcal{B}|}\int_{\mathcal{B}} \varphi(\mathbf{x},t)dV_\mathbf{x}$$



Damage distribution (multi-branch)



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:

M. Stoyanov, P. Seleson, and C. Webster, A surrogate modeling approach for crack pattern prediction in peridynamics, *19th AIAA Non-Deterministic Approaches Conference*, AIAA SciTech Forum, (AIAA 2017-1326).

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