

Stochastic Peridynamics and local Thermostats

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Molecular Dynamics

For a solid to which we apply some force, we consider the equation for motion of each individual molecule.

$$m_i \ddot{y}_i(t) = -\frac{\partial U(y)}{\partial y_i} + B_i^{MD}, \quad (1)$$

where

- m_i is the mass of the i -th particle,
- $y_i(t)$ is the position,
- $U(y)$ is the potential energy,
- B_i^{MD} is the external force.

$$m_i \ddot{y}_i = \sum_{j=0, j \neq i}^N F(y_i, y_j) + B_i^{MD}. \quad (2)$$

Continuum Mechanics

Starting with

$$m_i \ddot{y}_i(t) = -\frac{\partial U(y)}{\partial y_i} + B_i^{MD}, \quad (3)$$

Continuum Mechanics replaces the discrete $y_i(t)$ with a continuous function $y(t, x)$, then the model is transformed into:

$$\rho(x) \ddot{y}(t, x) = y_{xx}(t, x) + y_{yy}(t, x) + y_{zz}(t, x) + B^{CM}(x), \quad (4)$$

where $\rho(x)$ is the mass density of the material and B^{CM} is the external force measured in the appropriate units.

Peridynamics

Starting with

$$m_i \ddot{y}_i = \sum_{j=0, j \neq i}^N F(y_i, y_j) + B_i^{MD}, \quad (5)$$

Peridynamics models combine the best of both worlds. Let $u(t, x)$ be the displacement field for the "particles" and $y(t, x) = x + u(t, x)$, then

$$\rho(x) \ddot{u}(t, x) = \int_{H_x} f(u(t, x') - u(t, x), x' - x) dx' + B^{PD}(x). \quad (6)$$

$$\rho(x)\ddot{u}(t, x) = \int_{H_x} f(u(t, x') - u(t, x), x' - x)dx' + B^{PD}(x), \quad (7)$$

where

- $\rho(x)$ is the mass density of the material,
- $f(\cdot, \cdot)$ is a force density kernel,
- H_x is a neighborhood of interaction around x ,
- the region H_x is usually a sphere centered at x with some fixed radius δ .

This is non-local model since "particles" separated by finite distance are allowed to interact through the kernel.

Crack Dynamics

We rewrite the Peridynamics model as

$$\rho(x)\ddot{u}(t, x) = \int_{H_x} \mu(u(t, x'), u(t, x), x', x) f(u(t, x') - u(t, x), x' - x) dx',$$

where the function $\mu(u', u, x', x)$ gives values of 0 and 1 as

$$\mu(u', u, x', x) = \begin{cases} 1, & \text{if } x' \text{ and } x \text{ are "connected",} \\ 0, & \text{if } x' \text{ and } x \text{ are "disconnected".} \end{cases} \quad (8)$$

We can further make $\mu(\cdot)$ history dependent, that means once cracks form, we don't let them "heal".

Stochastic Thermostat for Molecular Dynamics

$$m_i \ddot{y}_i = -\frac{\partial U(y)}{\partial y_i} + B_i^{MD} - \Gamma m_i \dot{y}_i + \sqrt{2m_i \kappa_B T \Gamma} dW_i(t), \quad (9)$$

where

- T is the temperature,
- Γ is a friction coefficient,
- κ_B is the Boltzmann's constant,
- dW_i is independent normalized Weiner noise.

We wish to upscale this to the Peridynamics model:

$$\rho(x)\ddot{u}(t, x) = \int_{H_x} f(u(t, x') - u(t, x), x' - x) dx' + B^{PD}(x) - \Gamma \rho(x) \dot{u}(t, x) + \sqrt{2\rho(x)\kappa_B T \Gamma} d\hat{W}(t, x). \quad (10)$$

The discrete Weiner noise transforms into white noise $d\hat{W}(t, x)$ throughout the domain, with units of square root of volume time inverse (i.e. $m^{-\frac{3}{2}} s^{-\frac{1}{2}}$).

Project Goals

- current Peridynamics models for cracks are mainly deterministic with respect to all of the material properties,
- we wish to add stochastic perturbation to both $f(\cdot, \cdot)$ and the additive stochastic thermostat, this will create more realistic and more interesting behavior for cracks formation and growth as well as the general displacement field,
- energy criteria for formation of cracks may also need revision.

Thank you!

For details please, see my poster.