Peridynamic Structures Simulated on the GPU

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1. Introduction

Peridynamics [2] is a recently developed non-local theory of continuum mechanics that is useful in simulating multi-scale phenomena. Its formulation is based upon an integral equation of motion so that discontinuities may spontaneously form and propagate without special treatment, thus it is naturally well-suited to modeling fracture, dislocations, and phase boundaries.

The governing equations of peridynamics permit a "mesh-free" solution method [3] that has the same computational structure as a molecular dynamics simulation. Molecular dynamics [1] and other similar particle-based simulations have been seen large speedups and linear scaling when implemented on graphics processing units (GPUs), which excel at such data-parallel computational tasks.

In this work, we review a particle-based solution method for the governing equations of peridynamics, and detail our efforts to extend this method to the GPU using NVIDIA's CUDA parallel computing architecture.

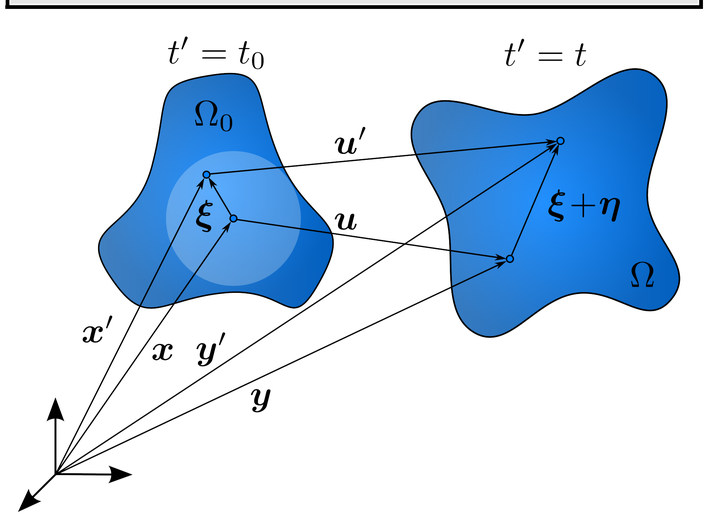


Figure 1: *Kinematic quantities that describe a peridynamic continuum body in its reference (Ω_0) and current (Ω) configurations.*

2. Peridynamic Model

Peridynamic theory is a reformulation of continuum mechanics that employs a non-local force model to account for long-range material interactions. It is governed by an integro-differential equation of motion that avoids spatial derivatives. In this way, the same description of motion is valid over the entire material body, regardless of the presence of defects.

$$\rho \frac{\partial^2 \boldsymbol{u}}{\partial t^2}(\boldsymbol{x},t) = \int_{\mathscr{H}_{\boldsymbol{x}}} \boldsymbol{f}(\boldsymbol{u}'-\boldsymbol{u}, \boldsymbol{x}'-\boldsymbol{x})\, dV_{\boldsymbol{x}'} + \boldsymbol{b}(\boldsymbol{x},t) \tag{1}$$

From here on, the relative position between particles in the reference configuration is denoted by $\boldsymbol{\xi}$ and in the current configuration by $\boldsymbol{\xi}+\boldsymbol{\eta}$, where $\boldsymbol{\eta}$ is the relative displacement. The pairwise internal force function $\boldsymbol{f}(\boldsymbol{\eta},\boldsymbol{\xi})$ contains all of a material body's constitutive information and the force term $\boldsymbol{b}(\boldsymbol{x},t)$ accounts for all external forces acting upon the body.

Although a specific functional form for the internal force density $\boldsymbol{f}(\boldsymbol{\eta},\boldsymbol{\xi})$ depends on the system begin modeled, it must exhibit certain properties to satisfy momentum conservation principles. To conserve linear momentum, it is required that particle force interactions are symmetric,

$$\boldsymbol{f}(-\boldsymbol{\eta},-\boldsymbol{\xi}) = -\boldsymbol{f}(\boldsymbol{\eta},\boldsymbol{\xi}). \tag{2}$$

Similarly, angular momentum is conserved when,

$$(\boldsymbol{\eta}+\boldsymbol{\xi}) \times \boldsymbol{f}(\boldsymbol{\eta},\boldsymbol{\xi}) = \boldsymbol{0}, \tag{3}$$

that is, the force interaction between any two particles acts parallel to the line that connects them in the current configuration.

In the general *state-based* theory of peridynamics, the non-local forces acting on a particle $\boldsymbol{x}$ are determined by the collective deformation of all the material within its neighborhood $\mathscr{H}_{\boldsymbol{x}}$. In this work, we focus solely on the simplified *bond-based* theory, where it is assumed that the collection of bonds associated with a particle do not interact with each other. Furthermore, we restrict our study to micro-elastic materials, in which the pairwise force function is conservative, so $\boldsymbol{f}(\boldsymbol{\eta},\boldsymbol{\xi})$ can be written as the gradient of a scalar micro-potential.

$$\boldsymbol{f}(\boldsymbol{\eta},\boldsymbol{\xi}) = \frac{\partial w}{\partial \boldsymbol{\eta}}(\boldsymbol{\eta},\boldsymbol{\xi}) \tag{4}$$

The total energy density of a micro-elastic particle can be separated into its internal and external components,

$$\text{Potential:} \quad E_{\text{pot}}(\boldsymbol{x},t) = \frac{1}{2}\int_{\mathscr{H}_{\boldsymbol{x}}} w(\boldsymbol{\eta},\boldsymbol{\xi})\, dV_{\xi}, \tag{5}$$

$$\text{Kinetic:} \quad E_{\text{kin}}(\boldsymbol{x},t) = \frac{\rho}{2}\frac{\partial \boldsymbol{u}}{\partial t}(\boldsymbol{x},t)\cdot\frac{\partial \boldsymbol{u}}{\partial t}(\boldsymbol{x},t), \tag{6}$$

$$\text{External:} \quad E_{\text{ext}}(\boldsymbol{x},t) = -\frac{1}{2}\boldsymbol{b}(\boldsymbol{x},t)\cdot\boldsymbol{u}(\boldsymbol{x},t). \tag{7}$$

Above, the internal energy is comprised of the elastic potential energy and kinetic contributions, and the external energy accounts for all externally applied forces.

3. Prototype Micro-elastic Brittle (PMB) Material

Two particles in a PMB material are initially bonded if they are positioned within some neighborhood $\|\boldsymbol{\xi}\| \leq \delta$ in the reference configuration. Bonded particles exert a bond force on each other that is analogous to that of an elastic spring.

$$w = \frac{1}{2}\frac{c}{\|\boldsymbol{\xi}\|}\left(\|\boldsymbol{\eta}+\boldsymbol{\xi}\| - \|\boldsymbol{\xi}\|\right)^2 \tag{8}$$

$$\boldsymbol{f} = \frac{c}{\|\boldsymbol{\xi}\|}\left(\|\boldsymbol{\eta}+\boldsymbol{\xi}\| - \|\boldsymbol{\xi}\|\right)\frac{\boldsymbol{\eta}+\boldsymbol{\xi}}{\|\boldsymbol{\eta}+\boldsymbol{\xi}\|} \tag{9}$$

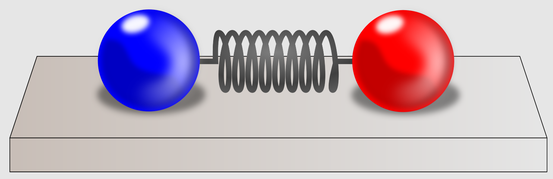


Figure 2: *In a PMB material, bonded continuum particles attract and repel in a spring-mass system until their bond is broken.*

The stretch of a bond is defined as the relative difference of the particle's relative separation distance in the reference and current configuration,

$$s = \frac{\|\boldsymbol{\eta}+\boldsymbol{\xi}\| - \|\boldsymbol{\xi}\|}{\|\boldsymbol{\xi}\|}. \tag{10}$$

In a brittle damage model, bonds stretched beyond a certain critical stretch value are broken irreversibly so that the involved particles no longer interact. This effect is tracked through a history-dependent boolean function

$$\mu(t,\xi) = \begin{cases} 1 & s(t',\xi) < s_0(t')\ \forall\ t' \in (0,t) \\ 0 & \text{otherwise} \end{cases}. \tag{11}$$

This allows us to define a scalar damage measure.

$$\varphi(\boldsymbol{x},t) = 1 - \frac{\int_{\mathscr{H}_{\boldsymbol{x}}} \mu(t,\xi)\, dV_{\xi}}{\int_{\mathscr{H}_{\boldsymbol{x}}} dV_{\xi}} \tag{12}$$

4. Short-Range Forces

Short-range forces are introduced in the current configuration to prevent the overlap of moving material. Thus, for each particle pair such that $\|\boldsymbol{\eta}+\boldsymbol{\xi}\| \leq d^s$, we include an additional term in the expressions for the micro-potential and internal forces.

$$w^s = \frac{1}{2}\frac{c^s}{\delta}\left(\|\boldsymbol{\eta}+\boldsymbol{\xi}\| - d^s\right)^2 \tag{13}$$

$$\boldsymbol{f}^s = \frac{c^s}{\delta}\left(\|\boldsymbol{\eta}+\boldsymbol{\xi}\| - d^s\right)\frac{\boldsymbol{\eta}+\boldsymbol{\xi}}{\|\boldsymbol{\eta}+\boldsymbol{\xi}\|} \tag{14}$$

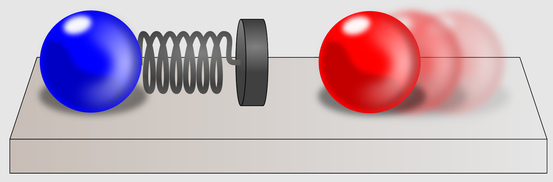


Figure 3: *Short range forces are necessary to prevent the overlap of nearby continuum particles in the current configuration.*

5. Discretization

Various numerical integration techniques have been useful in approximating the peridynamic equation of motion, including Gaussian quadrature, finite elements, and spectral methods. Our solution scheme uses the so-called mesh-free "EMU" method [3] which discretizes spatial quantities using the composite midpoint rule,

$$\rho\frac{\partial^2 \boldsymbol{u}_i^n}{\partial t^2} = \sum_p \boldsymbol{f}\left(\boldsymbol{u}_p^n - \boldsymbol{u}_i^n, \boldsymbol{x}_p - \boldsymbol{x}_i\right) V_p + \boldsymbol{b}_i^n, \tag{15}$$

and temporal quantities using an explicit central difference (Verlet) recurrence relation,

$$\frac{\partial^2 \boldsymbol{u}_i^n}{\partial t^2} \approx \frac{\boldsymbol{u}_i^{n+1} - 2\boldsymbol{u}_i^n + \boldsymbol{u}_i^{n-1}}{(\Delta t)^2}, \tag{16}$$

in which a we choose a constant time step no larger than

$$\Delta t < \sqrt{\frac{2\rho}{\sum_p \left\|\frac{\partial \boldsymbol{f}}{\partial \boldsymbol{\eta}}(\boldsymbol{0},\boldsymbol{\xi})\right\| V_p}}, \tag{17}$$

as suggested by von Neumann stability analysis [3]. In the above equations, superscripts indicate the time step number during which a quantity is evaluated, and subscripts represent the node number. Using this method, a volume is attributed to each continuum particle. The quantity V_p represents the portion of that particle volume that is contained within the neighborhood of $\boldsymbol{x}$ for which the pairwise force function is non-zero.

6. Algorithm

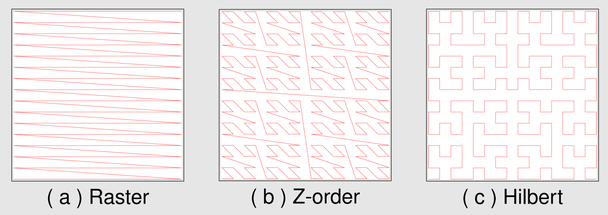
Graphics Processing Units (GPUs) are powerful data-parallel computation engines already installed in many computer workstations. Recent advances in GPU hardware and software support their use in accelerating general purpose computations. The "EMU" discretization of peridynamics models lends itself naturally to such a computational architecture because it is both FLOPS-intensive and data-parallel. Adapting computer programs designed for CPUs to a GPU architecture is non-trivial and requires traditional algorithms and data structures to be rethought. Here we outline our solution algorithm for solving the peridynamic equations of motion in parallel, entirely on the GPU.

For each time-step:

1. Update positions and half-step velocities of all particles
2. Update computation of bond forces
3. Reduce axis-aligned bounding box for particle cloud
4. Determine cell index for each particle, interleave bits to obtain Z-value
5. Sort positions based on location on Z-order curve
6. Compute short range forces; neighbor query can be terminated early due to structure of Z-order curve
7. Finish velocity update of all particles
8. When needed, reduce energy and scalar damage of each particle.

7. Space-Filling Curves

Space-filling curves are an essential ingredient to enabling parallelism and scalability of this algorithm.



(a) Raster (b) Z-order (c) Hilbert

Figure 4: *Examples of space-filling curves in two dimensions (order=4).*

A space-filling curve is as a continuous function that maps points in n-dimensional space to the unit interval $[0,1]$. Certain properties of space-filling curves (e.g. choice of endpoints, locality, & symmetry) lead to many useful applications.

(a) order = 1 (b) order = 2 (c) order = 3

Figure 5: *Z-order curves of various orders in three-dimensions.*

In this code, we employ the z-order space filling curve because it has improved spatial locality over the common raster order and is relatively simple to implement by interleaving bits. This enables a sparse data structure for storing the history of inter-particle bonds, and an efficient algorithm for ball neighbor queries.

8. Summary and Future Work

- The theory described here has been implemented in a C++ code using NVIDIA's CUDA parallel computing architecture and the Thrust library.
- The neighbor query incurred in introducing the short-range forces has been reduced in complexity by using space-filling curves. Additional work is planned to further prune these search ranges.
- The scaling of this code is currently limited by the storage requirements for the bond histories. We are currently looking for a more efficient data structure that can record the past states of bonds.
- After code testing is complete, we plan to apply our method to studying the failure of composite structures.

References

[1] J. A. Anderson, C. D. Lorenz, and A. Travesset. General purpose molecular dynamics simulations fully implemented on graphics processing units. *J. Comput. Phys.*, 227:5342–5359, 2008.

[2] S. A. Silling. Reformulation of elasticity theory for discontinuities and long-range forces. *J. Mech. Phys. Solids*, 48:175–209, 2000.

[3] S. A. Silling and E. Askari. A meshfree method based on the peridynamic model of solid mechanics. *Comput. Struct.*, 83:1526–1535, 2005.