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A Multi-Time-Step Method for Partitioned Time Integration of Peridynamics

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Outline

- ❑ **Peridynamics Review**
- ❑ Motivating Multi-Time-Stepping
- ❑ Nonlocal Multi-Time-Stepping
- ❑ Numerical Example

What is Peridynamics?

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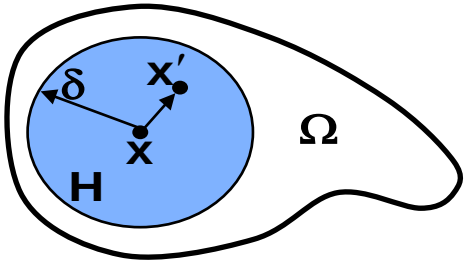
- Peridynamics is a nonlocal extension of classical solid mechanics that permits discontinuous solutions

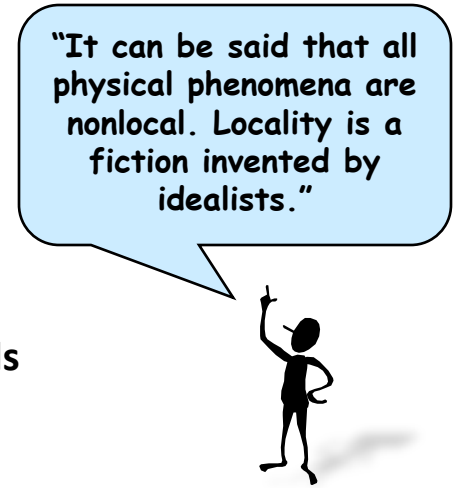


Point x interacts directly with all points x' within H

- Peridynamic equation of motion (integral, nonlocal)

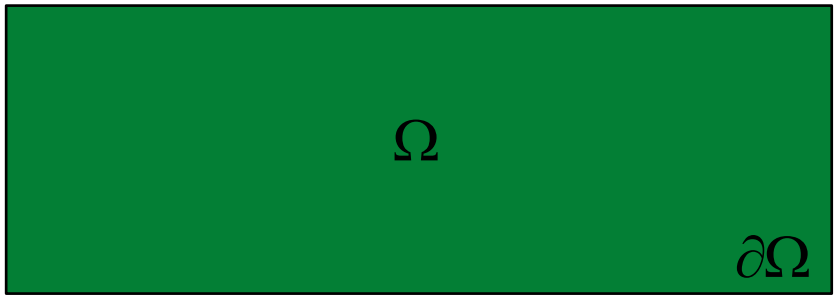
$$\rho\ddot{u}(x,t) = \int_H \left(T[x,t]\langle x'-x\rangle - T[x',t]\langle x'-x\rangle \right) dV_{x'} + b(x,t)$$

  - Replace PDEs with integral equations
  - Utilize same equation everywhere; nothing "special" about cracks
  - No assumption of differentiable fields (admits fracture)
  - Damage incurred when deformation criteria satisfied (critical stretch, etc.)
  - No obstacle to integrating nonsmooth functions
  - Integrand is "force" function; contains constitutive model
  - Integrand = 0 for points x,x' more than δ apart (like cutoff radius in MD!)
  - PD is "continuum form of molecular dynamics"
- Impact
  - Nonlocality
  - Larger solution space than corresponding classical PDE-based models (fracture)
  - Account for material behavior at small & large length scales (multiscale material model)

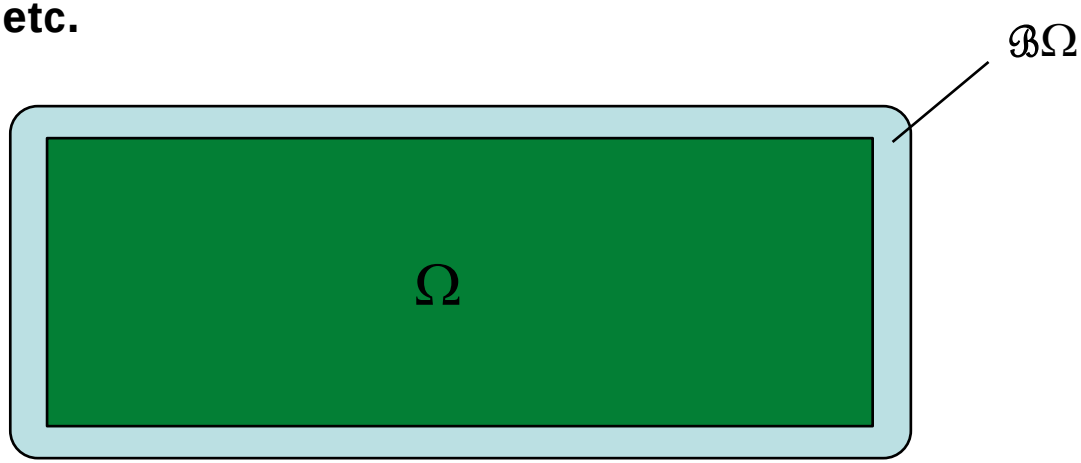


Nonlocal Boundary Conditions

- For local models (for example, PDE-based models), we apply boundary conditions on … the boundary.

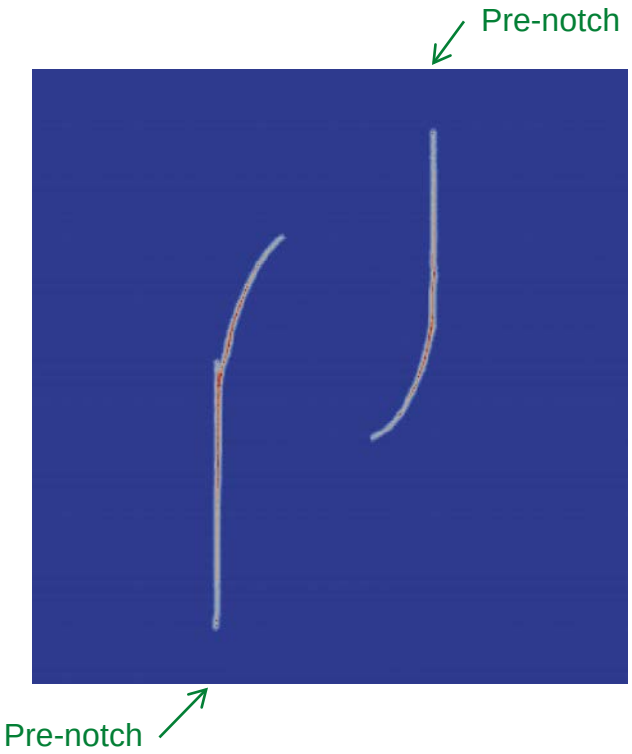


- A Peridynamic "boundary" becomes a volumetric region, sometimes called a "nonlocal boundary", "collar", etc.
- Boundary conditions are called "nonlocal boundary conditions", "volume constraints", etc.

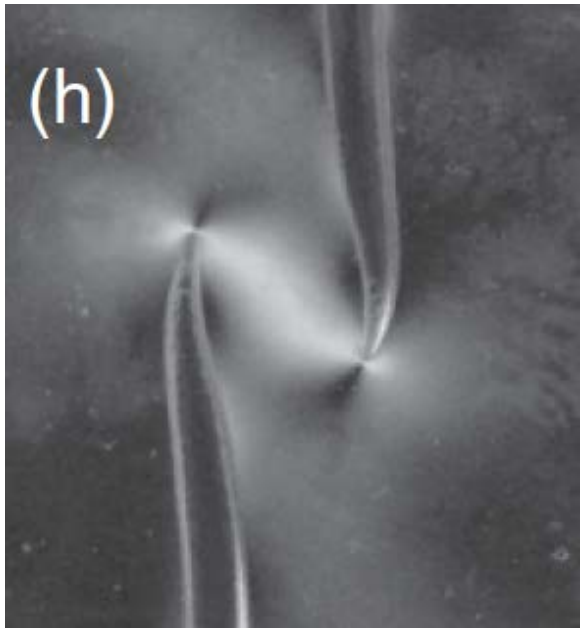


Two Interacting Cracks

- Offset notches thin rectangular elastic plate
- Uniaxial strain applied from sides
- Approaching cracks produce “en passant” crack pattern



Peridynamics



Physical Experiment*

* M. Fender, F. Lechenault, and K. Daniels, Universal Shapes Formed by Two Interacting Cracks, Phys. Rev. Lett. 105, 125505 (2010) .

Fracture in Glass Plate

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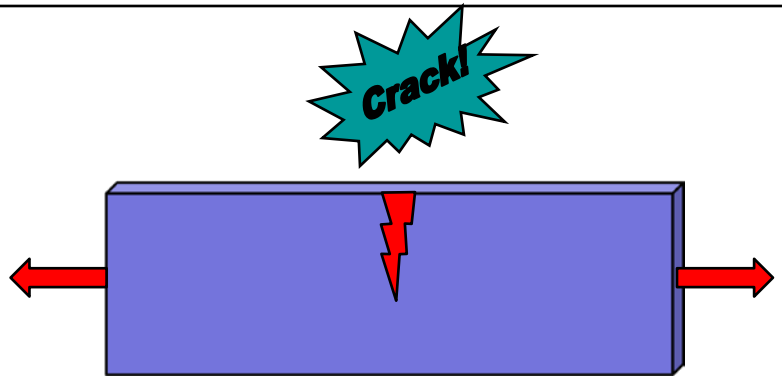
- With Florin Bobaru (Nebraska), Youn-Doh Ha, & Stewart Silling (Sandia)

- Soda-lime glass plate (microscope slide)
  - Dimensions: 3” x 1” x 0.05”
  - Density: 2.44 g/cm3
  - Elastic Modulus: 79.0 Gpa

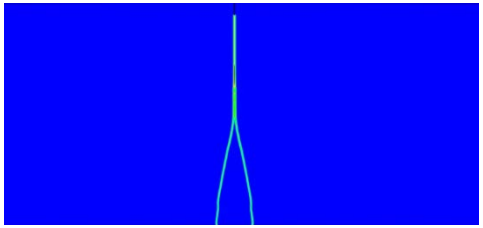
- Dawn (LLNL): IBM BG/P (500 TF; 147,456 cores)
  - Mesh spacing: 35 microns
  - Approx. 82 million particles
  - Time: 50 microseconds (20k timesteps)
  - 6 hours on 65k cores

Setup

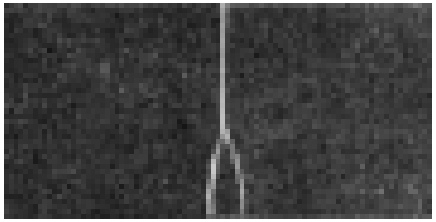
- Glass microscope slide
- Dimensions: 3” x 1” x 0.05”
- Notch at top, pull on ends



Results



Peridynamics



Physical Experiment*

Strain Energy Density

*S F. Bowden, J. Brunton, J. Field, and A. Heyes, *Controlled fracture of brittle solids and interruption of electrical current*, Nature, 216, 42, pp.38-42, 1967.

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- ❑ **Motivating Multi-Time-Stepping**
- ❑ Nonlocal Multi-Time-Stepping
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Motivating Multi-Time-Stepping

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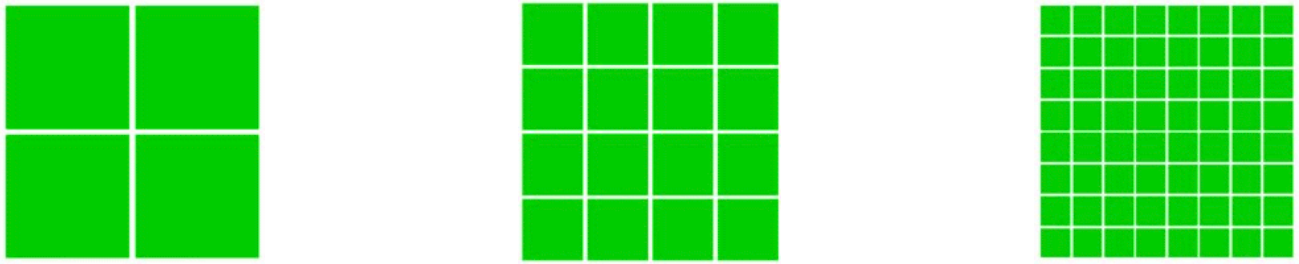
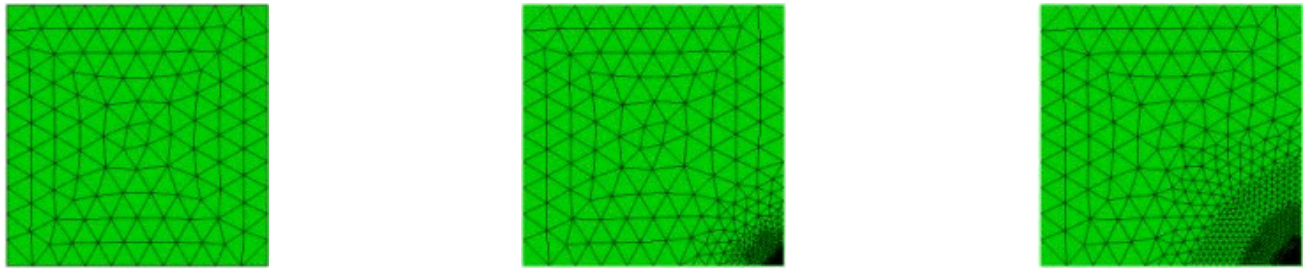
- Mesh refinement increases resolution and accuracy of computed solution.



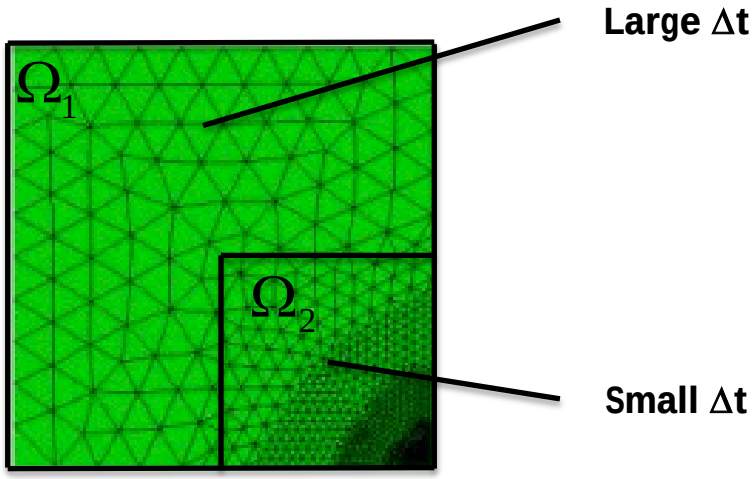
- Local mesh refinement puts more mesh only where needed.



- We need to refine our temporal discretization, too.
- In dynamics, frequently use same timestep everywhere.
  - This means timestep refinement must be uniform.
- Like uniform mesh refinement, uniform timestep refinement can generate unnecessary work. May not need a small timestep everywhere!
- Making matters worse for uniform timestep refinement, to satisfy CFL, timestep usually dictated by the smallest element size. May have really small timestep *everywhere*.

Motivating Multi-Time-Stepping

- Use small timesteps only where needed; Larger timesteps everywhere else.
- Cut up our domain and choose a timestep for each subdomain.



- This process is known as multi-time-stepping (sometimes called subcycling).
- Cutting up our domain is easy…
  - … but we'll need to tie it all back together again!

- We need to leverage ideas from domain decomposition.

Domain Decomposition (DD)

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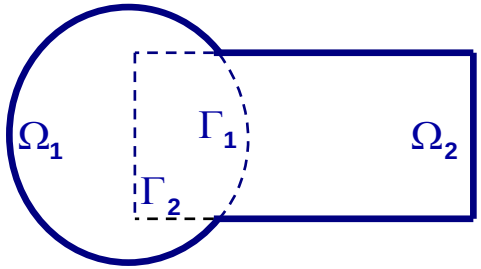
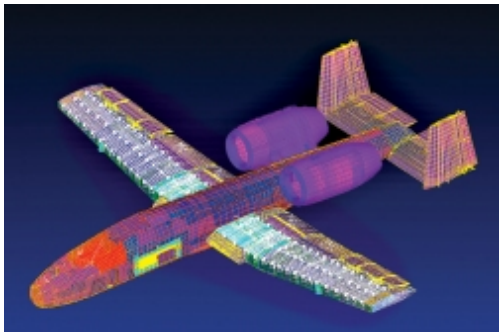
- Original DD method (overlapping method) dates back to Schwarz (1870).



H. A. Schwarz

- Nonoverlapping DD (substructuring) used by engineers for decades. Original motivation was that entire model wouldn't fit into computer memory.

- By cutting model into substructures and solving for unknowns along interfaces, can decouple domains and solve each independently.



$$\begin{bmatrix} K_{11} & 0 & K_{1\Gamma} \\ 0 & K_{22} & K_{22} \\ K_{\Gamma 1} & K_{\Gamma 2} & K_{\Gamma\Gamma} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_\Gamma \end{bmatrix} = \begin{bmatrix} f_1 \\ f_2 \\ f_\Gamma \end{bmatrix}$$

$$\left(K_{\Gamma\Gamma} - K_{\Gamma 2}K_{22}^{-1}K_{22} - K_{\Gamma 1}K_{11}^{-1}K_{11}\right)x_\Gamma = f_\Gamma - K_{\Gamma 2}K_{22}^{-1}f_2 - K_{\Gamma 1}K_{11}^{-1}f_1$$

- We recognize this as taking a Schur complement with respect to the interface.

Domain Decomposition (DD)

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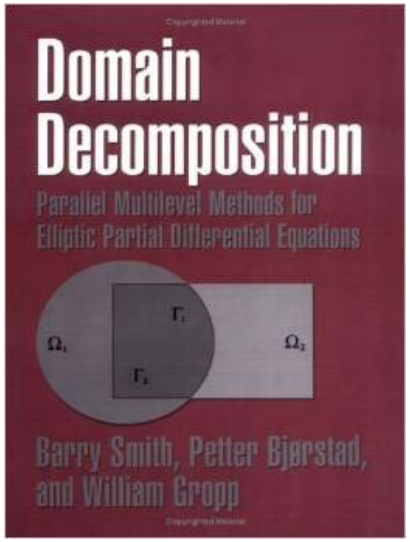
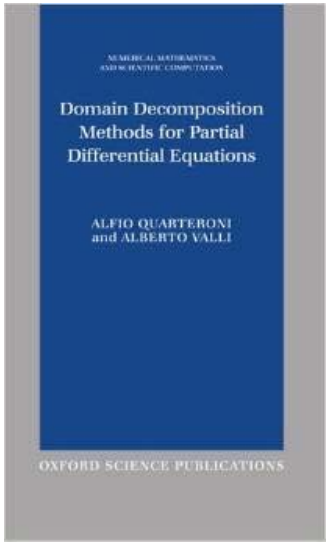
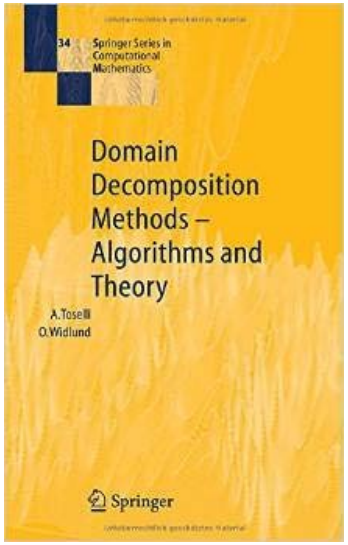
- DD is the mathematical and computational technology allowing us to map our problems onto parallel computers. Cut problem into pieces, assign each to a node.
- Subdomains communicate only though their interfaces.
- Primal Schur complement methods (substructuring) isolate subdomains by solving for displacements along an interfacial boundary. Dual Schur complement methods (FETI-type methods) isolate subdomains by solving for forces along an interfacial boundary.
- This lead to highly successful computational approaches and some really elegant mathematical analysis.
- The details can be found in some fantastic texts.

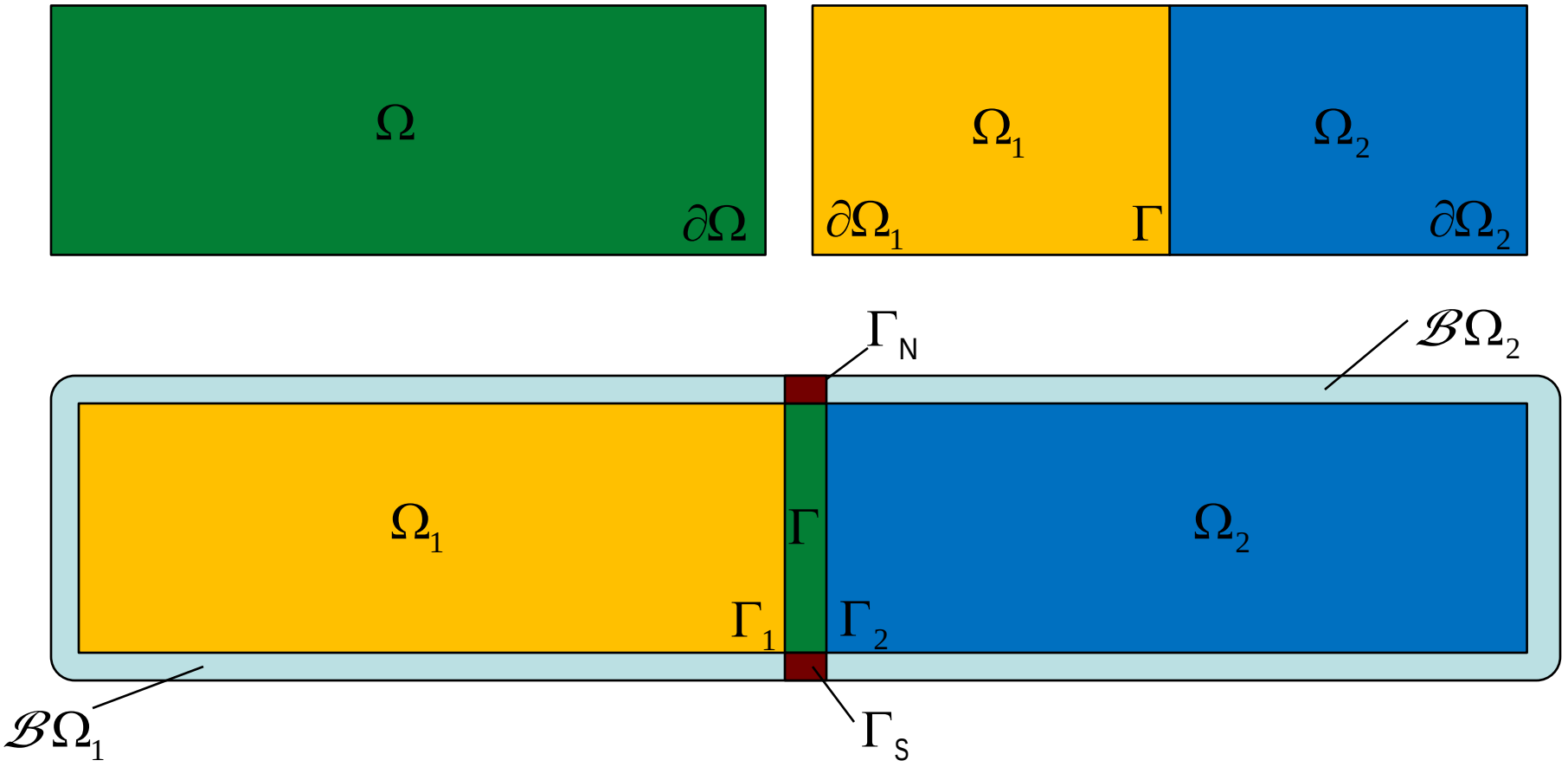






Nonlocal Domain Decomposition (NLDD)

- For nonlocal models, we can extend some of the classical results.*
- Interfaces and boundaries for nonlocal models are volumetric.



*B. Aksoylu and M.L. Parks, *Variational Theory and Domain Decomposition for Nonlocal Problems*, Applied Mathematics and Computation, 217, pp. 6498-6515, 2011.

Time Integration

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- Consider one-domain problem with equation of motion

$$\mathbf{M}\ddot{\mathbf{U}}(t) + \mathbf{K}\mathbf{U}(t) = \mathbf{F}(t)$$
$$\mathbf{U}(0) = \mathbf{U}_0$$
$$\mathbf{U}(t) = \mathbf{U}_{B\Omega}$$

- Discretize with Newmark-Beta:

$$\dot{\mathbf{U}}_{n+1} = \dot{\mathbf{U}}_n + \Delta t(1-\gamma)\ddot{\mathbf{U}}_n + \gamma\Delta t\ddot{\mathbf{U}}_{n+1}$$
$$\mathbf{U}_{n+1} = \mathbf{U}_n + \Delta t\dot{\mathbf{U}}_n + \left(\tfrac{1}{2}-\beta\right)\Delta t^2\ddot{\mathbf{U}}_n$$

- Second order iff $\gamma = 1/2$.
- Unconditionally stable if $\beta \geq \gamma/2 \geq 1/4$.

Time Integration

- We can write a step of Newmark-Beta as

$$\mathbb{M}\mathbb{U}_{n+1} = \mathbb{F}_{n+1} - \mathbb{N}\mathbb{U}_n$$

where

$$\mathbb{M} = \begin{bmatrix} \mathbf{M} & \mathbf{0} & \mathbf{K} \\ -\gamma\Delta t\mathbf{I} & \mathbf{I} & \mathbf{0} \\ -\beta\Delta t^2\mathbf{I} & \mathbf{0} & \mathbf{I} \end{bmatrix} \quad \mathbb{N} = \begin{bmatrix} \mathbf{0} & \mathbf{0} & \mathbf{0} \\ -\Delta t(1-\gamma)\mathbf{I} & -\mathbf{I} & \mathbf{0} \\ -\Delta t^2\left(\frac{1}{2}-\beta\right)\mathbf{I} & -\Delta t\mathbf{I} & -\mathbf{I} \end{bmatrix} \quad \mathbb{U}_n = \begin{bmatrix} \ddot{\mathbf{U}}_n \\ \dot{\mathbf{U}}_n \\ \mathbf{U}_n \end{bmatrix} \quad \mathbb{F}_{n+1} = \begin{bmatrix} \mathbf{F}_{n+1} \\ \mathbf{0} \\ \mathbf{0} \end{bmatrix}$$

- By analogy, we can write m steps of Newmark-Beta as

$$\begin{bmatrix} \mathbb{M} & & & \\ \mathbb{N} & \mathbb{M} & & \\ & \ddots & \ddots & \\ & & \mathbb{N} & \mathbb{M} \end{bmatrix} \begin{bmatrix} \mathbb{U}_{n+1} \\ \mathbb{U}_{n+1} \\ \vdots \\ \mathbb{U}_{n+m} \end{bmatrix} = \begin{bmatrix} \mathbb{F}_{n+1} - \mathbb{N}\mathbb{U}_n \\ \mathbb{F}_{n+1} \\ \vdots \\ \mathbb{F}_{n+m} \end{bmatrix}$$

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Nonlocal Multi-Time-Stepping (MTS)

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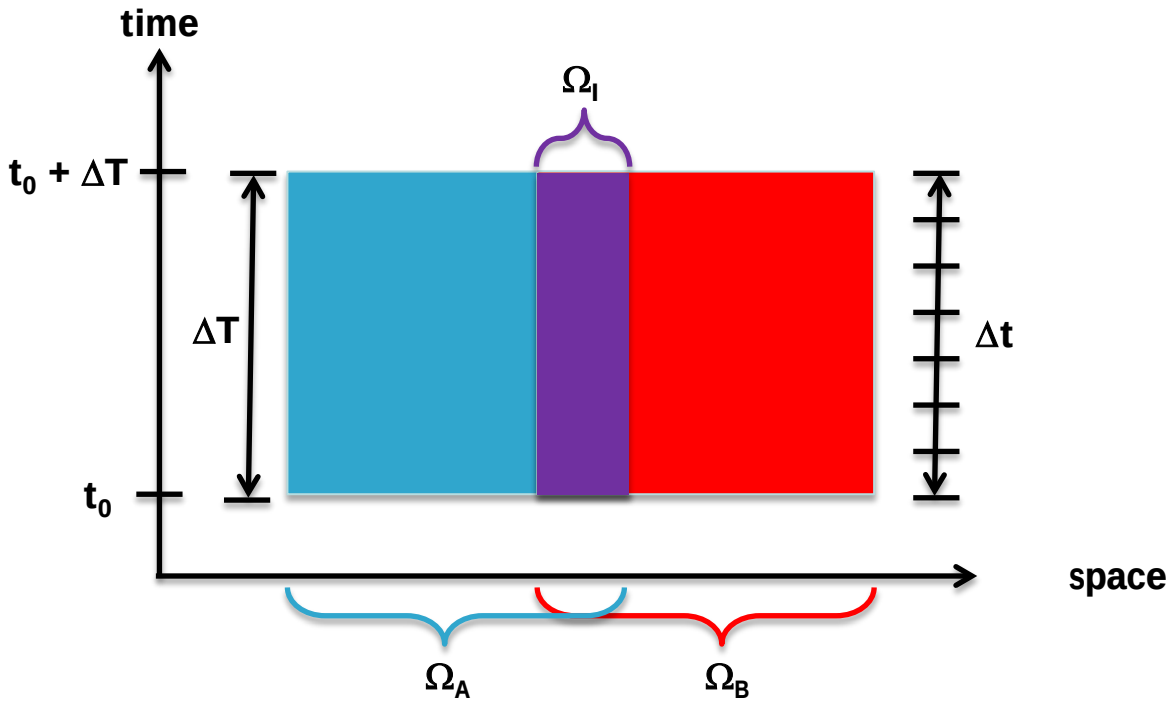
- With this notation, let's couple subdomains with different time steps (MTS).



- Let $\Delta T = m\,\Delta t$ for some positive integer m.
- We will impose transmission conditions between the two subdomains.
- In this work, we adapt the MTS method of Prakash & Hjelmstad*

*A. Prakash and K. Hjelmstad, *A FETI-based multi-time-stepping coupling method for Newmark schemes in structural dynamics*, IJNME, 61:2183-2204, 2004.

Nonlocal Multi-Time-Stepping (MTS)

- We will choose to couple interface with Lagrange multipliers, and enforce constraint that velocity at interface is consistent across boundary.

$$\mathbf{M}^k\ddot{\mathbf{U}}^k + \mathbf{K}^k\mathbf{U}^k + \left(\mathbf{C}^k\right)^T\boldsymbol{\Lambda} = \mathbf{F}^k \qquad k = 1,\ldots,s$$

$$\sum_{k=1}^{s}\mathbf{C}^k\dot{\mathbf{U}}^k = \mathbf{0}$$

where C is a boolean matrix that extracts interfacial DOFs to form an interface vector.

- Fully discretized equations for subdomain A at time t_m are

$$\mathbb{M}^A\mathbb{U}_m^A + \mathbb{C}^A\boldsymbol{\Lambda}_m = \mathbb{F}_m^A - \mathbb{N}^A\mathbb{U}_0^A$$

- Similarly, discretized equations for subdomain B at time t_j (j = 1,…,m) are

$$\mathbb{M}^B\mathbb{U}_j^B + \mathbb{C}^B\boldsymbol{\Lambda}_j = \mathbb{F}_j^B - \mathbb{N}^B\mathbb{U}_{j-1}^B$$

- We enforce continuity of velocity only at time t_m*

$$\mathbf{C}^A\dot{\mathbf{U}}_m^A + \mathbf{C}^B\dot{\mathbf{U}}_m^B = \mathbf{0}$$

* A. Combescure & A. Garavouil, A numerical scheme to couple subdomains with different time-steps for predominantly linear transient analysis. CMAME, 191:1129—1157, 2002.

Nonlocal Multi-Time-Stepping (MTS)

- To solve equations for subdomains A and B and satisfy the constraint equation, split equation for subdomain A into two parts:

$$\mathbb{M}^{A}\mathbb{U}_{m}^{A}+\mathbb{C}^{A}\,\Lambda_{m}=\mathbb{F}_{m}^{A}-\mathbb{N}^{A}\mathbb{U}_{0}^{A}$$

$$\downarrow$$

$$\mathbb{U}_{m}^{A}=\mathbb{V}_{m}^{A}+\mathbb{W}_{m}^{A}$$

$$\mathbb{M}^{A}\mathbb{V}_{m}^{A}=\mathbb{F}_{m}^{A}-\mathbb{N}^{A}\mathbb{U}_{0}^{A}$$

$$\mathbb{V}_{m}^{A}=\begin{bmatrix}\ddot{\mathbf{V}}_{m}^{A}\\ \dot{\mathbf{V}}_{m}^{A}\\ \mathbf{V}_{m}^{A}\end{bmatrix}$$

Free Problem

$$\mathbb{M}^{A}\mathbb{W}_{m}^{A}=-\mathbb{C}^{A}\,\Lambda_{m}$$

$$\mathbb{W}_{m}^{A}=\begin{bmatrix}\ddot{\mathbf{W}}_{m}^{A}\\ \dot{\mathbf{W}}_{m}^{A}\\ \mathbf{W}_{m}^{A}\end{bmatrix}$$

Interface Problem

Nonlocal Multi-Time-Stepping (MTS)

- After solving the free problem, can compute the state variables for subdomain A at intermediate times t_j through linear interpolation between t_0 and t_m.

$$\mathbb{V}_j^A = \left(1 - \frac{j}{m}\right)\mathbb{U}_0^A + \left(\frac{j}{m}\right)\mathbb{V}_m^A$$

- Knowing free state at t_j, can compute unbalanced free interface reaction at t_j (amount subdomain A is out of equilibrium due to external forces only) as

$$\mathbf{S}_j = \mathbf{C}^A\left(\mathbf{F}_j^A - \mathbf{M}^A\ddot{\mathbf{V}}_j^A - \mathbf{K}^A\mathbf{V}_j^A\right)$$

- After much derivation, we can rewrite the equation of motion for subdomain B as

$$\mathbb{M}^B\mathbb{U}_j^B + \left(\frac{j}{m}\right)\mathbb{C}^B\,\mathbf{\Lambda}_m = \mathbb{F}_j^B - \mathbb{N}^B\mathbb{U}_{j-1}^B - \mathbb{C}^B\,\mathbf{S}_j$$

where we have replaced Λ_j in favor of Λ_m.

Nonlocal Multi-Time-Stepping (MTS)

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- We can now write the complete set of equations to be solved:

$$
\left[\begin{array}{ccccc|c|c}
\mathbb{M}^B & & & & & & \frac{1}{m}\mathbb{C}^B \\
\mathbb{N}^B & \mathbb{M}^B & & & & & \frac{2}{m}\mathbb{C}^B \\
 & \ddots & \ddots & & & & \vdots \\
 & & \mathbb{N}^B & \mathbb{M}^B & & & \frac{m}{m}\mathbb{C}^B \\
\hline
 & & & & \mathbb{M}^A & \mathbb{C}^A & \\
\hline
 & & & \mathbb{B}^A & \mathbb{B}^B & \mathbf{0} &
\end{array}\right]
\left[\begin{array}{c}
\mathbb{U}_1^B \\ \mathbb{U}_2^B \\ \vdots \\ \mathbb{U}_m^B \\ \hline \mathbb{U}_m^A \\ \hline \Lambda_m
\end{array}\right]
=
\left[\begin{array}{c}
\mathbb{F}_1^B - \mathbb{N}^B\mathbb{U}_0^B - \mathbb{C}^B\mathbf{S}_1 \\
\mathbb{F}_2^B - \mathbb{C}^B\mathbf{S}_2 \\
\vdots \\
\mathbb{F}_m^B - \mathbb{C}^B\mathbf{S}_m \\ \hline
\mathbb{F}_m^A - \mathbb{N}^A\mathbb{U}_0^A \\ \hline
\mathbf{0}
\end{array}\right]
$$

where $\mathbb{B}^A = \begin{bmatrix}\mathbf{0} & \mathbf{C}^A & \mathbf{0}\end{bmatrix}$ $\mathbb{B}^B = \begin{bmatrix}\mathbf{0} & \mathbf{C}^B & \mathbf{0}\end{bmatrix}$

Nonlocal Multi-Time-Stepping (MTS)

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- We can re-write as

$$\begin{bmatrix} M & C \\ B & 0 \end{bmatrix} \begin{bmatrix} U \\ \Lambda_m \end{bmatrix} = \begin{bmatrix} P \\ 0 \end{bmatrix}$$

where U = V+W, and solve as a multistep process:

1) Compute $\mathbb{V}^A$ (free system)
2) Compute reaction forces S_j.
3) Compute $\mathbb{V}^B$.
4) Solve for Λ_m (interface reaction force at time t_m), then determine Λ_j
5) Using Λ_j, compute $\mathbb{W}^A$, $\mathbb{W}^B$.
6) Update solution $\mathbb{U}^A$, $\mathbb{U}^B$.

- Tedious, but straightforward!

Numerical Properties

- We can write the change in energy of the coupled system from time t_0 to t_m as

$$\Delta\mathcal{E} = -\left(\gamma_A - \tfrac{1}{2}\right)\left(\ddot{\mathbf{U}}^A_m - \ddot{\mathbf{U}}^A_0\right)^T\left[\mathbf{M}^A + \Delta T^2\left(\beta_A - \tfrac{\gamma_A}{2}\right)\mathbf{K}^A\right]\left(\ddot{\mathbf{U}}^A_m - \ddot{\mathbf{U}}^A_0\right)$$

$$-\left(\gamma_B - \tfrac{1}{2}\right)\sum_{j=1}^{m}\left(\ddot{\mathbf{U}}^B_j - \ddot{\mathbf{U}}^B_{j-1}\right)^T\left[\mathbf{M}^B + \Delta t^2\left(\beta_B - \tfrac{\gamma_B}{2}\right)\mathbf{K}^B\right]\left(\ddot{\mathbf{U}}^B_j - \ddot{\mathbf{U}}^B_{j-1}\right)$$

$$+ E_\Lambda$$

- If $\Delta\mathcal{E} \le 0$, we assert our method is stable.
- If M^A, K^A, M^B, K^B, are SPD and we choose β_A, γ_A, β_B, γ_B, for unconditional stability, then $E_\Lambda \le 0$ is sufficient to guarantee stability. After much derivation, can show that

$$E_\Lambda \propto \mathbf{C}^A\left(\dot{\mathbf{U}}^A_m - \dot{\mathbf{U}}^A_0\right) + \mathbf{C}^B\left(\dot{\mathbf{U}}^B_m - \dot{\mathbf{U}}^B_0\right) = \mathbf{0}$$

- Thus, coupling method neither adds nor removes energy from coupled system, hence:

1) Coupling method is stable (if the Newmark-Beta integrators for Ω_A, Ω_B are stable).
2) Coupling method does not introduce any additional dissipation.

Truncation Error

- For a two node problem, can eliminate acceleration variables and rewrite as

$$\mathbf{y}_1 = \mathbf{A}\mathbf{y}_0 + \mathbf{c}_0$$

where y_1 is vector of numerical solutions at next full timestep.

- Truncation error is

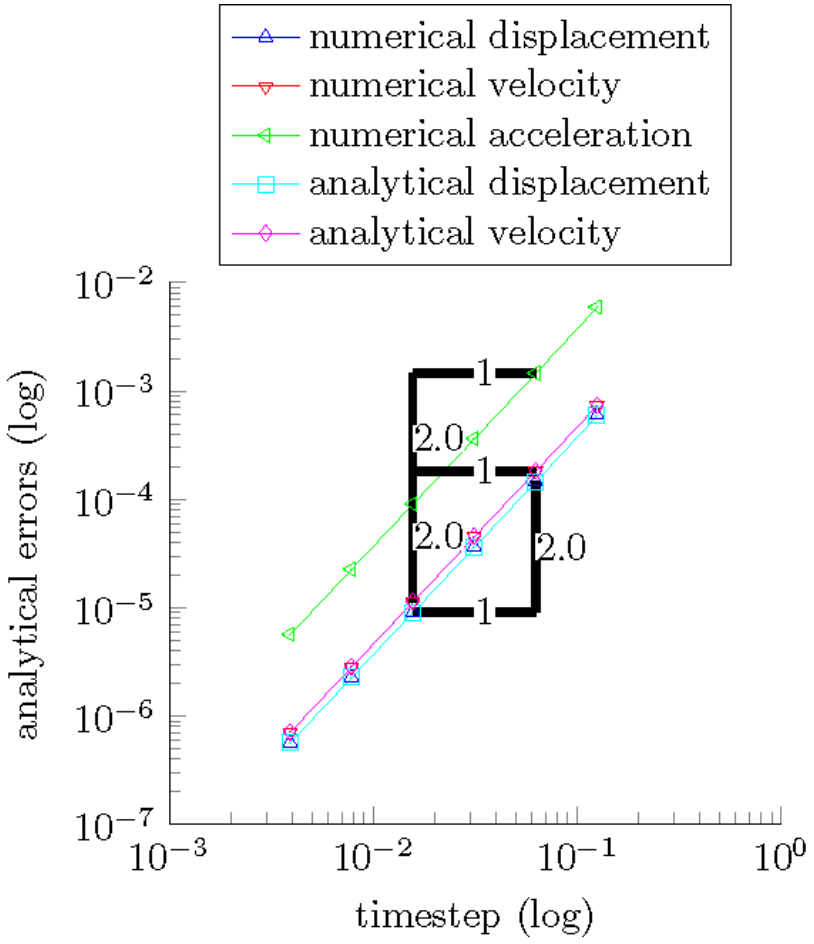
$$\boldsymbol{\tau}(t_0) = \mathbf{y}(t_1) - \mathbf{y}_1 = \mathbf{y}(t_1) - \mathbf{A}\mathbf{y}(t_0) - \mathbf{c}(t_0)$$

where $y(t_1)$ is vector of exact kinematic values. Using Taylor series, get

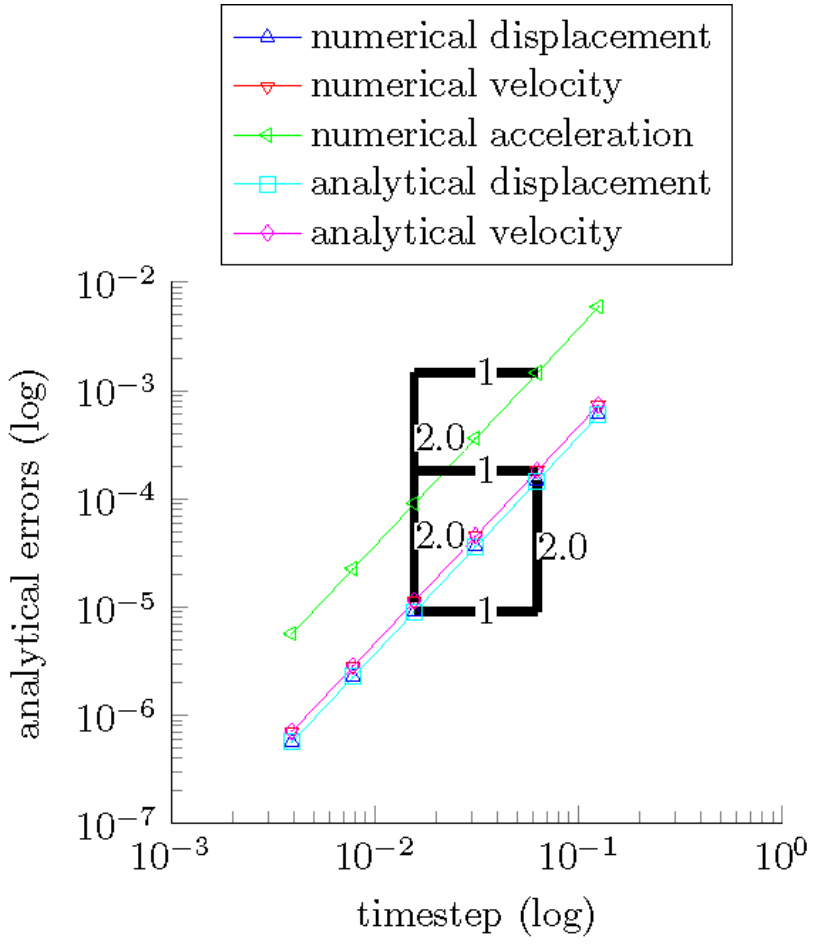
$$\boldsymbol{\tau}(t_0) = \begin{bmatrix} \tau_{u_{1,1}}(t_0) \\ \tau_{u_{1,2}}(t_0) \\ \tau_{u_{2,2}}(t_0) \\ \tau_{\dot{u}_{1,1}}(t_0) \\ \tau_{\dot{u}_{1,2}}(t_0) \\ \tau_{\dot{u}_{2,2}}(t_0) \\ \tau_{\Lambda}(t_0) \end{bmatrix} = \begin{bmatrix} O(\Delta t^2) \\ O(\Delta t^2) \\ O(\Delta t^2) \\ -\dfrac{(2\gamma-1)\Delta t\left(CV_2\left(\dot{u}_2(t_0) - \dot{u}_1(t_0)\right) + \dot{f}(t_0)\right)}{2\rho} + O(\Delta t^2) \\ -\dfrac{(2\gamma-1)\Delta t\left(CV_1\left(\dot{u}_2(t_0) - \dot{u}_1(t_0)\right) + \dot{f}(t_0)\right)}{2\rho} + O(\Delta t^2) \\ -\dfrac{(2\gamma-1)\Delta t\left(CV_1\left(\dot{u}_2(t_0) - \dot{u}_1(t_0)\right) + \dot{f}(t_0)\right)}{2\rho} + O(\Delta t^2) \\ O(\Delta t^2) \end{bmatrix}$$

Truncation Error

- Direct numerical simulation of two node system



$\gamma = 1/2, \beta = 0$



$\gamma = 1/2, \beta = 1/4$

Rough Cost Estimate

- Suppose there are n_A elements in domain $\Omega_A \backslash \Omega_B$, n_B elements in domain $\Omega_B \backslash \Omega_A$, and n_I elements in $A \cap B$.
- Let $n = n_A + n_B + n_I$.
- Further suppose each element has n_b bonds.
  (Ignore that the number of bounds near a boundary is not n_b.)

- If we use a uniform timestep and take m steps, computational work ~ nn_bm.
- For the MTS scheme, computational work ~ $n_b (n_A + n_I + m(n_I + n_b))$.

- MTS scheme becomes advantageous if $(m-1)n_A > n_I$.

- For example, if n_B is 10% of overall domain size, m=2,` then

$$\frac{\text{Computational Work for Uniform Timestep}}{\text{Computational Work for MTS Timestep}} \approx 1.8$$

Outline

- ❑ Peridynamics Review
- ❑ Motivating Multi-Time-Stepping
- ❑ Nonlocal Multi-Time-Stepping
- ❑ **Numerical Example**

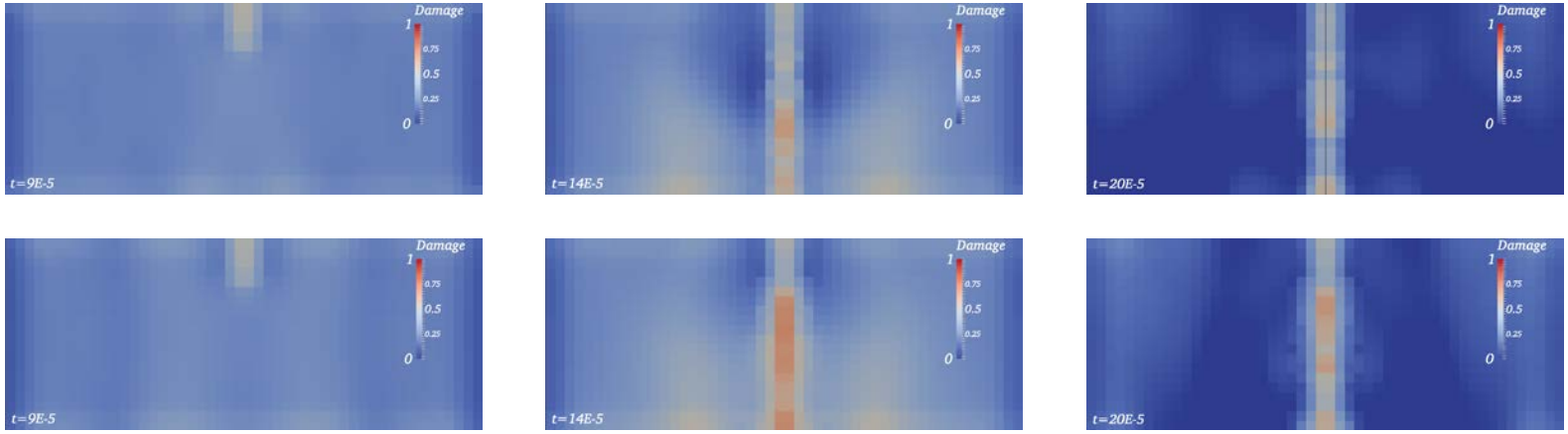
Numerical Example – Cracked Plate

- Dimensions: 20 mm x 10 mm x 0.1 mm plate; h = 0.1 mm.
- ρ = 2235 kg/m^3, E = 13.5 MPa; G_0 = 204 J/m^2.
- Gamma = 1/2; beta = 1/4.
- For MTS, $\Delta t = 1\times10^{-8}$; $\Delta T = m\Delta t$. Fast timestep region was middle 20% of plate.

- Execution ~ 10× faster than uniform fine timestep, but with improved accuracy in middle of plate (crack).

PD

MTS-PD, m=10



time = t_A time = t_B time = t_C

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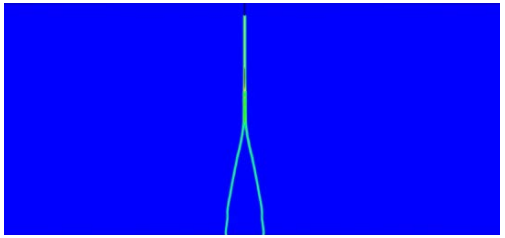
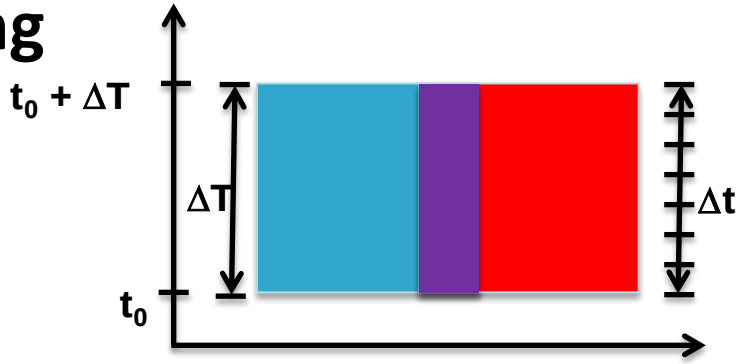
Method	Time t_A	Time t_B	Time t_C
PD, $\Delta t = 10\times10^{-8}$	1.86×10^{-6}	3.26×10^{-6}	3.27×10^{-5}
MTS-PD, m=10	1.76×10^{-6}	2.95×10^{-6}	1.59×10^{-5}

- Error (avg. rel. error over all cells) was computed with respect to one-domain PD solution with $\Delta t = 1\times10^{-8}$.

Summary

- ❑ Peridynamics Review
- ❑ Motivating Multi-Time-Stepping
- ❑ Domain Decomposition
- ❑ Nonlocal Multi-Time-Stepping
- ❑ Numerical Properties
- ❑ Numerical Example
- ❑ Questions?





$$\begin{bmatrix} \mathbb{M}^B & & & & \frac{1}{m}\mathbb{C}^B & \mathbb{U}_1^B \\ \mathbb{N}^B & \mathbb{M}^B & & & \frac{2}{m}\mathbb{C}^B & \mathbb{U}_2^B \\ & \ddots & \ddots & & \vdots & \vdots \\ & & \mathbb{N}^B & \mathbb{M}^B & \frac{m}{m}\mathbb{C}^B & \mathbb{U}_m^B \\ \hline & & & \mathbb{M}^A & \mathbb{C}^A & \mathbb{U}_m^A \\ \hline & & & \mathbb{B}^A & \mathbb{B}^B & 0 & \Lambda_m \end{bmatrix} = \begin{bmatrix} \mathbb{F}_1^B - \mathbb{N}^B\mathbb{U}_0^B - \mathbb{C}^B\mathbb{S}_1 \\ \mathbb{F}_2^B - \mathbb{C}^B\mathbb{S}_2 \\ \vdots \\ \mathbb{F}_m^B - \mathbb{C}^B\mathbb{S}_m \\ \hline \mathbb{F}_m^A - \mathbb{N}^A\mathbb{U}_0^A \\ \hline 0 \end{bmatrix}$$