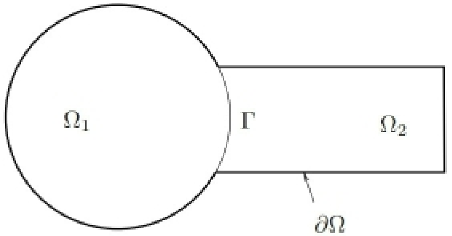
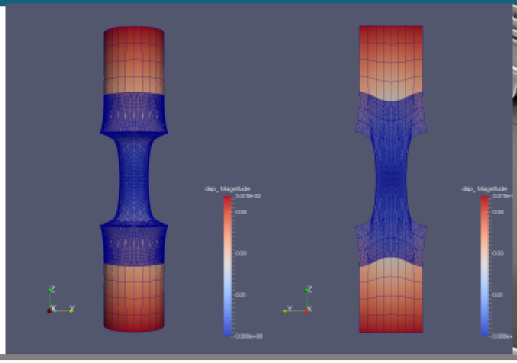
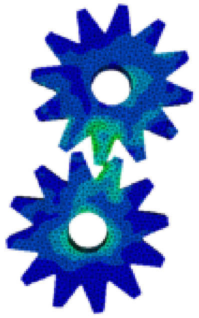
SAND2021-12680C

Sandia National Laboratories

The Schwarz Alternating Method for Multi-Scale Coupling and Contact in Solid Mechanics







Alejandro Mota[1], **Irina Tezaur**[1], Jonathan Hoy[2]

[1]Sandia National Laboratories, [2]University of Southern California

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U.S. DEPARTMENT OF ENERGY · NNSA

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Motivation

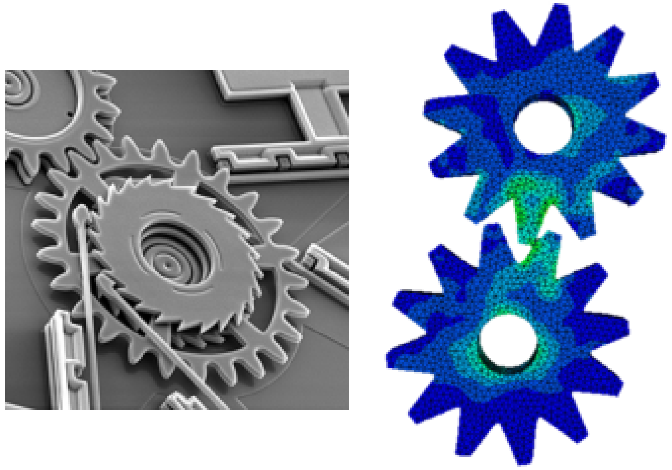
- **Large scale** structural **failure** frequently originates from **small scale** phenomena (e.g, defects, microcracks, inhomogeneities), which grow quickly in unstable manner
  - ➢ **Concurrent multiscale methods** are essential to capture correctly the multiscale behavior!
  - ➢ Stable, accurate and robust methods for simulating **mechanical contact** (touching surfaces, sliding, tightened bolts, impact) are equally important!

Above: roof failure of Boeing 737 aircraft due to fatigue cracks. From *imechanica.org*

Two-step process to the computational simulation of contact:

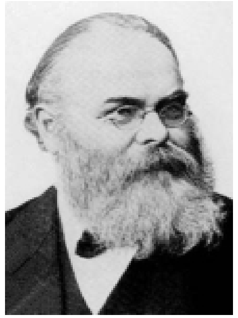
1. **Proximity search:** computer science problem, has received much attention due to importance in video game development ☺
2. **Contact enforcement step:** existing methods (penalty, Lagrange multiplier, augmented Lagrangian) suffer from poor performance ☹
   - ➢ Long simulation times ☹
   - ➢ Lack of accuracy ☹
   - ➢ Lack of robustness ☹

This talk.



Above: gears in contact within MEMS device. From *sandia.gov/media*

Schwarz Alternating Method for Domain Decomposition



H. Schwarz (1843–1921)

- Proposed in 1870 by H. Schwarz for solving Laplace PDE on irregular domains.

Crux of Method: if the solution is known in regularly shaped domains, use those as pieces to iteratively build a solution for the more complex domain.

Basic Schwarz Algorithm

Initialize:

- Solve PDE by any method on Ω_1 w/ initial guess for transmission BCs on Γ_1.

Iterate until convergence:

- Solve PDE by any method on Ω_2 w/ transmission BCs on Γ_2 based on values just obtained for Ω_1.
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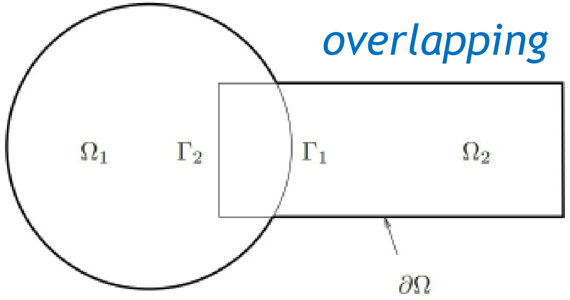

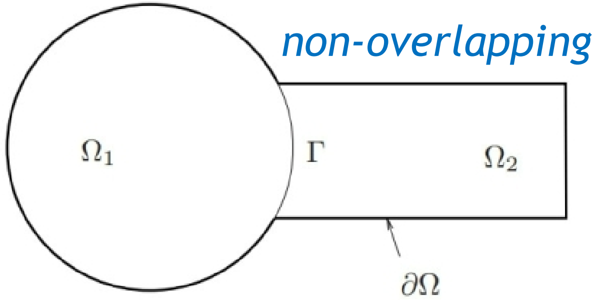

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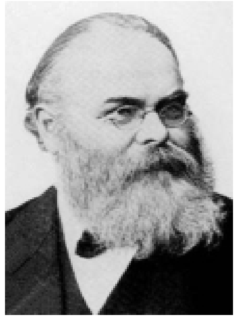

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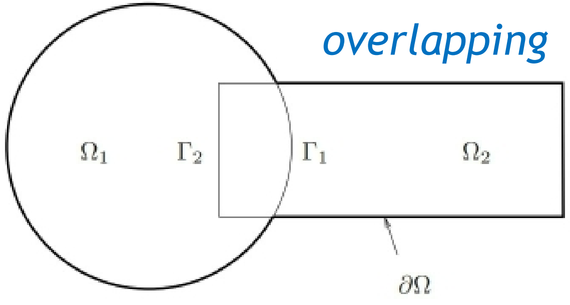

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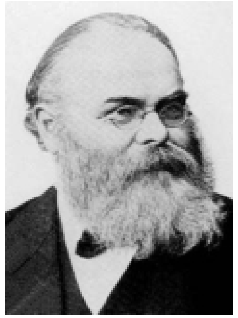
Overlapping Schwarz: convergent with all-Dirichlet transmission BCs[1] if $\Omega_1 \cap \Omega_2 \neq \emptyset$.

[1]Schwarz, 1870; Lions, 1988.

Schwarz Alternating Method for Domain Decomposition



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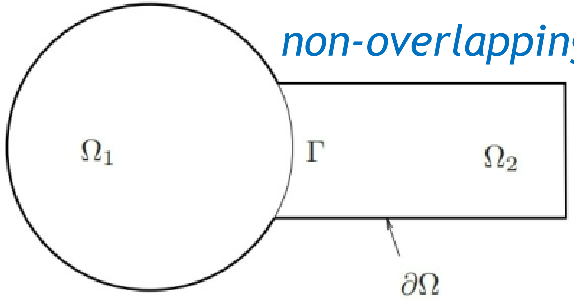
non-overlapping

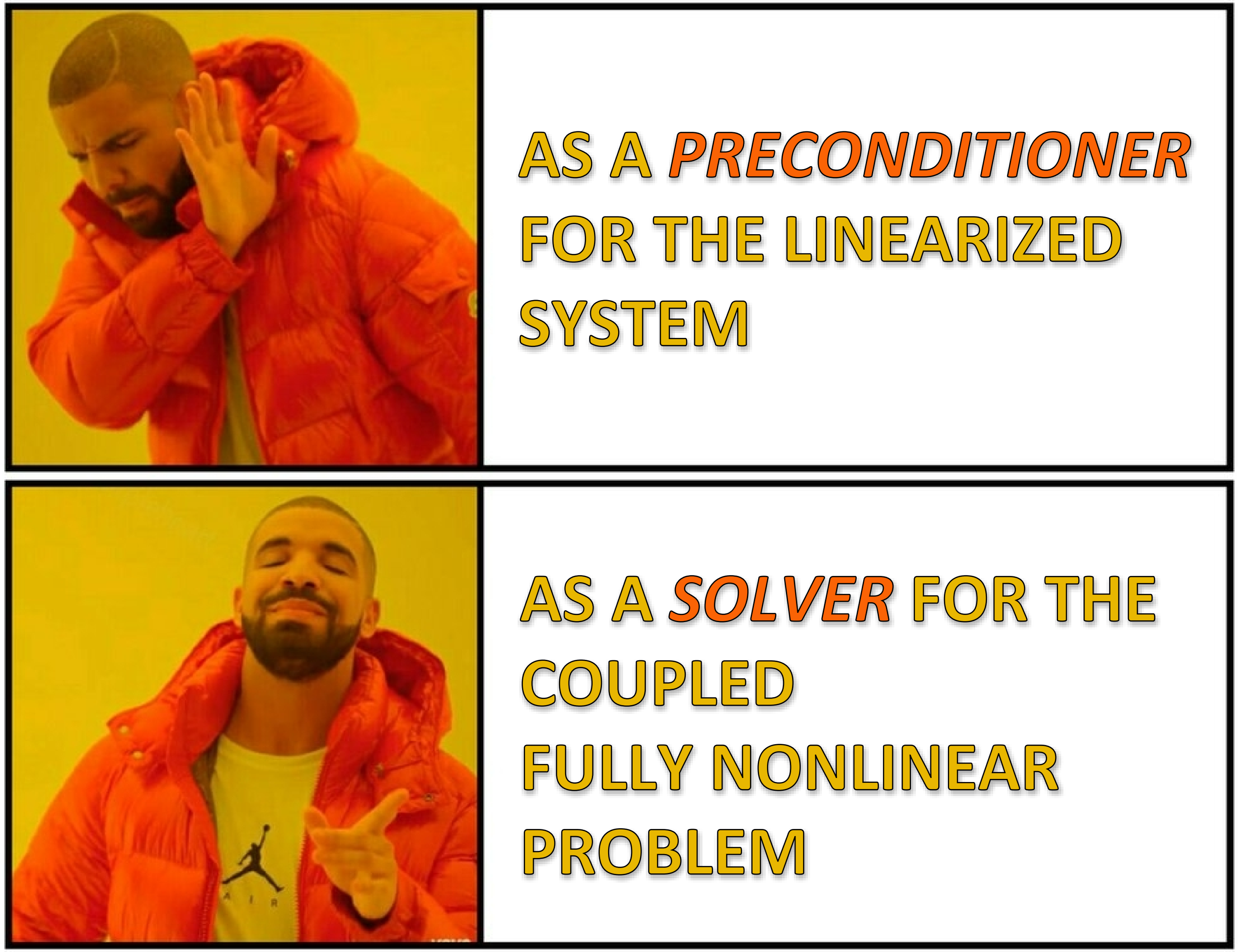


Overlapping Schwarz: convergent with all-Dirichlet transmission BCs[1] if $\Omega_1 \cap \Omega_2 \neq \emptyset$.

Non-overlapping Schwarz: convergent with Robin-Robin[2] or alternating Neumann-Dirichlet[3] transmission BCs.

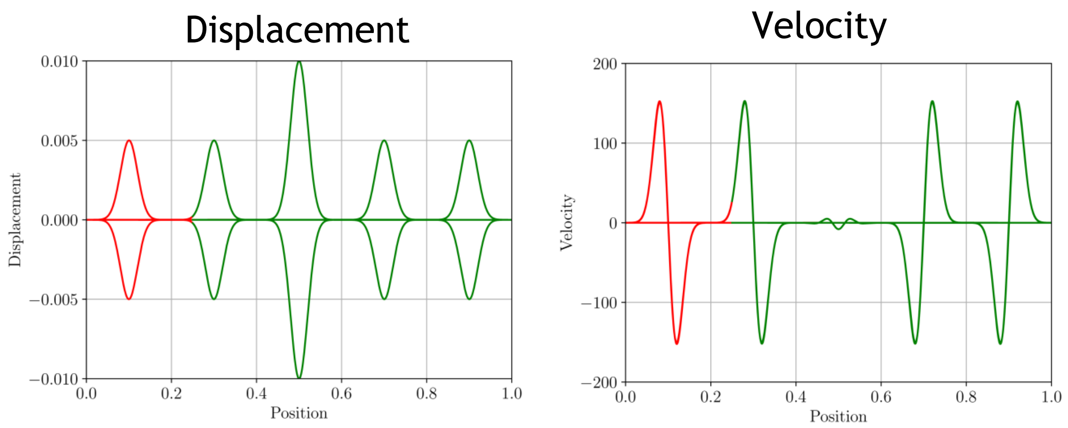
[1]Schwarz, 1870; Lions, 1988. [2]Lions, 1990. [3]Zanolli *et al.*, 1987.

How We Use the Schwarz Alternating Method

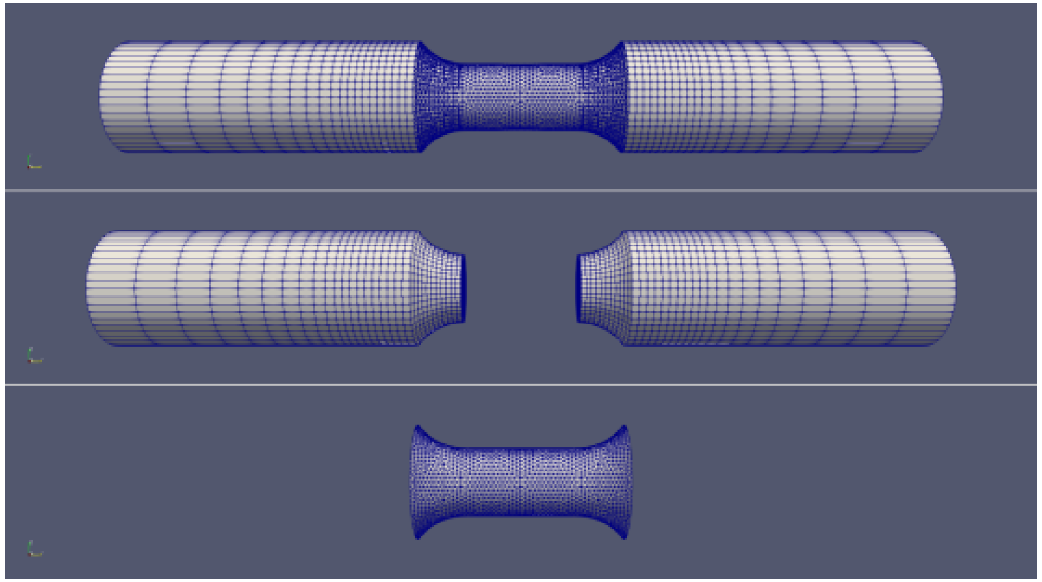


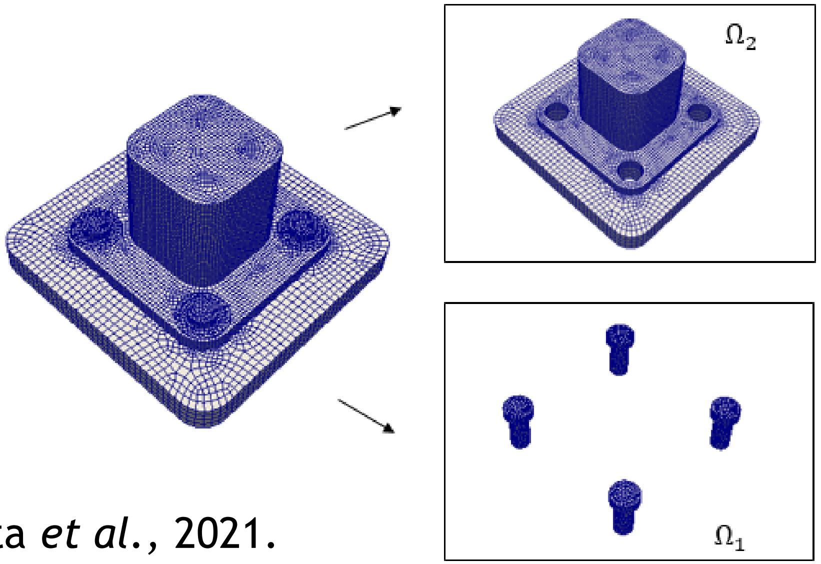
Overlapping Schwarz for Multiscale Coupling in Solid Mechanics

The **Schwarz alternating method** has been developed/implemented for **concurrent multiscale quasistatic & dynamic modeling** in Sandia's *Albany/LCM* and *Sierra/SM* codes.



- Coupling is **concurrent** (two-way)
- **No nonphysical artifacts** and theoretical **convergence properties**[1]
- **"Plug-and-play" framework**: couples different meshes, element types, solvers, integrators



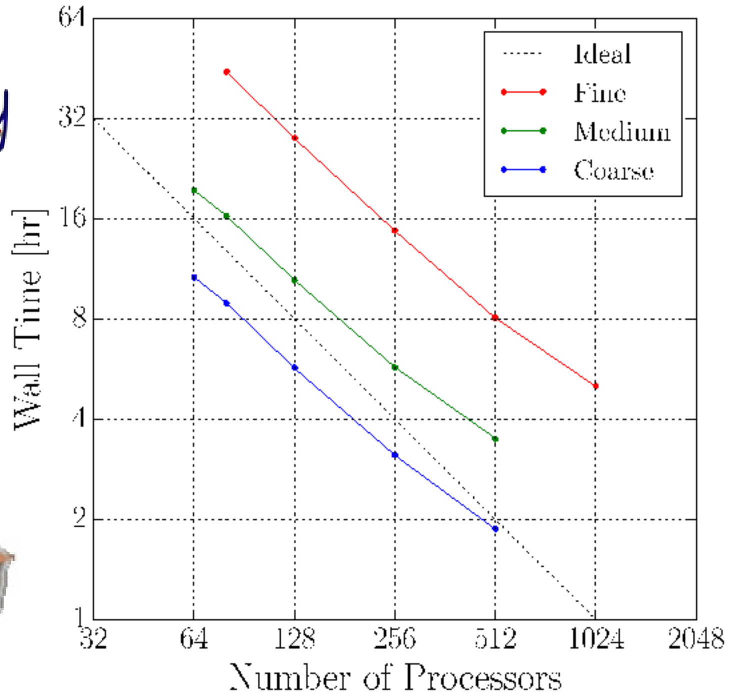


[1]Mota *et al.*, 2017; Mota *et al.*, 2021.

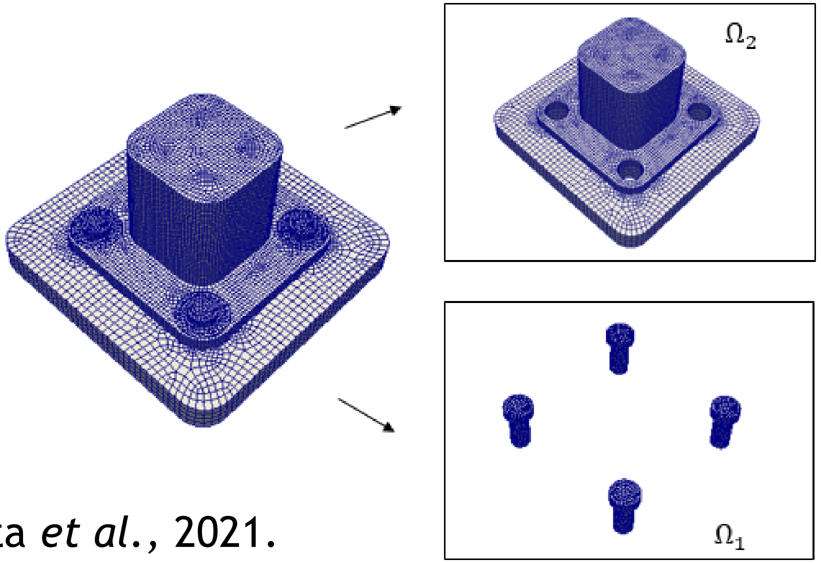
Overlapping Schwarz for Multiscale Coupling in Solid

The **Schwarz alternating method** has been developed/implemented for **concurrent multiscale quasistatic & dynamic modeling** in Sandia's *Albany/LCM* and *Sierra/SM* codes.

	CPU times	# Schwarz iters
Single Ω	3h 34m	–
Schwar	2h 42m	3.22



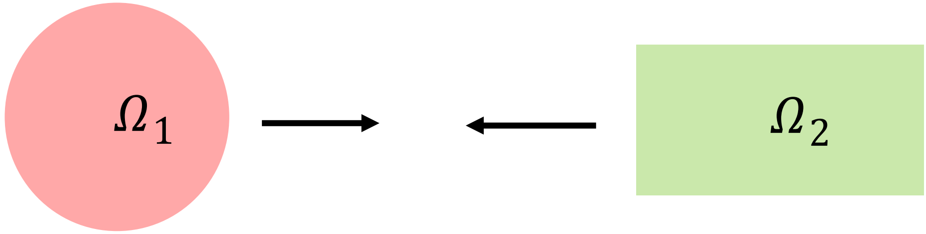
- Coupling is **concurrent** (two-way)
- **No nonphysical artifacts** and theoretical **convergence properties**[1]
- **"Plug-and-play" framework**: couples different meshes, element types, solvers, integrators
- **Easy to implement** in existing HPC codes, and **scalable, fast, robust**



[1]Mota *et al.*, 2017; Mota *et al.*, 2021.

Non-Overlapping Schwarz Formulation for Contact Mechanics

Before contact: simulation proceeds as usual

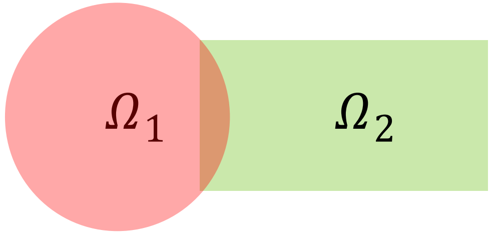


There are no contact constraints!

Contact constraints replaced w/ **BCs** applied **iteratively** at contact boundaries.

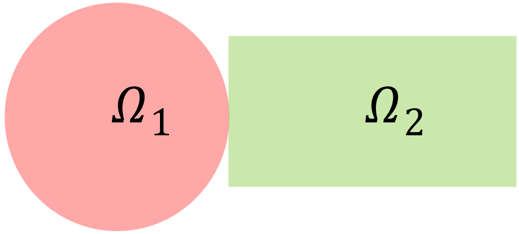
Detection of contact: proximity search and application of contact conditions to determine contact

- ***Overlap condition:*** triggered when two or more objects/domains have begun to overlap/penetrate each other
- ***Push condition:*** triggered when both of the following properties hold
  - ***Compression:*** the tractions at the interface are compressive
  - ***Sustainability:*** there was contact in the previous controller time step

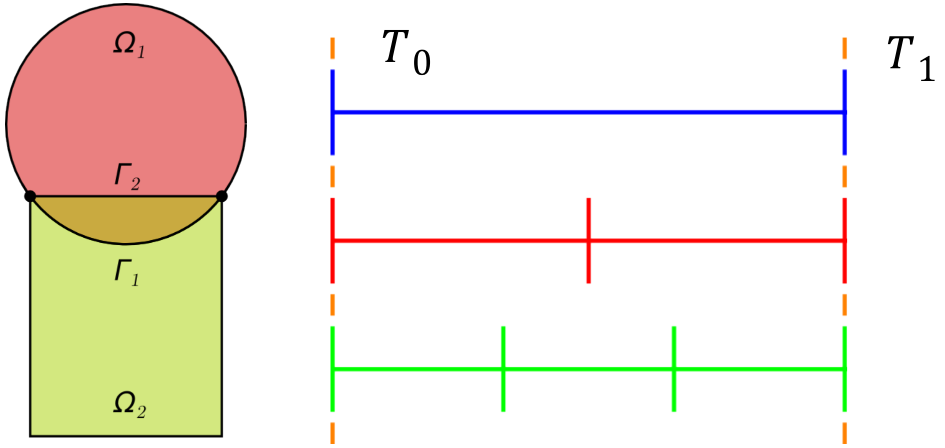


Enforcement of contact: alternating Schwarz iteration with Dirichlet-Neumann transmission BCs

$$\begin{cases} \boldsymbol{M}_1 \ddot{\boldsymbol{u}}_1^{n+1} + \boldsymbol{f}_1^{\text{int;n+1}} = \boldsymbol{f}_1^{\text{ext;n+1}} \\ \boldsymbol{\varphi}_1^{n+1} = \boldsymbol{\chi}, \text{ on } \partial_{\varphi}\Omega_1 \backslash \Gamma, \\ \boldsymbol{\varphi}_1^{n+1} = \boldsymbol{\varphi}_2^{n}, \text{ on } \Gamma, \end{cases} \qquad \begin{cases} \boldsymbol{M}_2 \ddot{\boldsymbol{u}}_2^{n+1} + \boldsymbol{f}_2^{\text{int;n+1}} = \boldsymbol{f}_2^{\text{ext;n+1}} \\ \boldsymbol{\varphi}_2^{n+1} = \boldsymbol{\chi}, \text{ on } \partial_{\varphi}\Omega_2 \backslash \Gamma, \\ \boldsymbol{T}_2^{n+1} = \boldsymbol{T}_1^{n+1}, \text{ on } \Gamma \end{cases}$$



Non-Overlapping Schwarz Formulation for Contact Mechanics



Controller time stepper

Time integrator for Ω_1

Time integrator for Ω_2

Controller time stepper: defines global ΔTs at which subdomains are synchronized

Step 0: Initialize $i = 0$ (controller time index).

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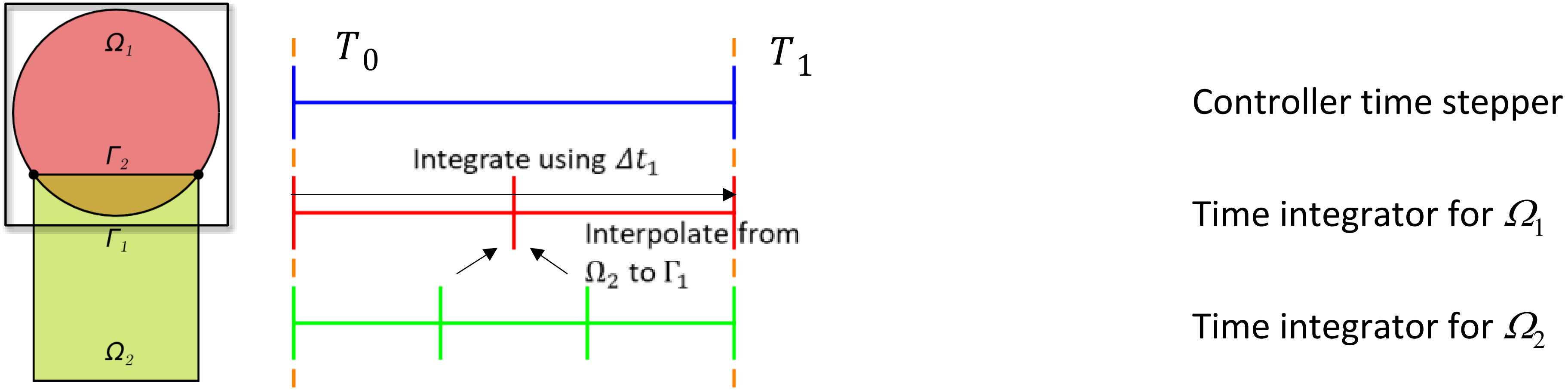

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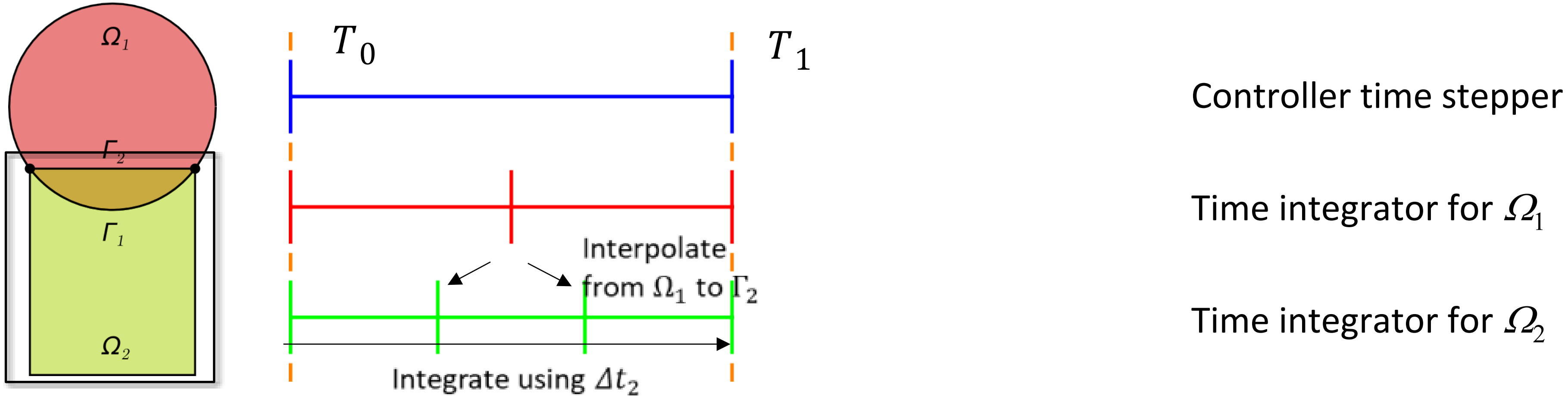

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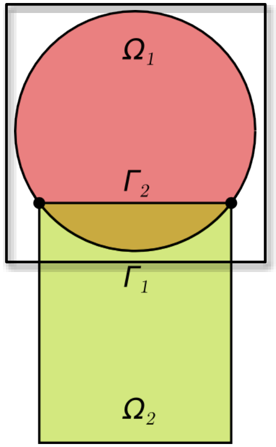

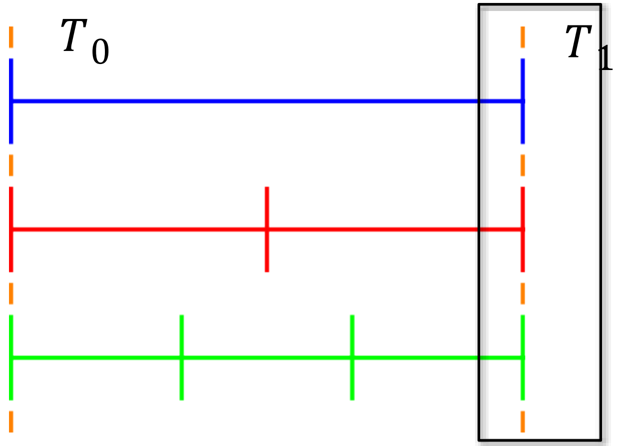

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Step 3: Check for convergence at time T_{i+1}.

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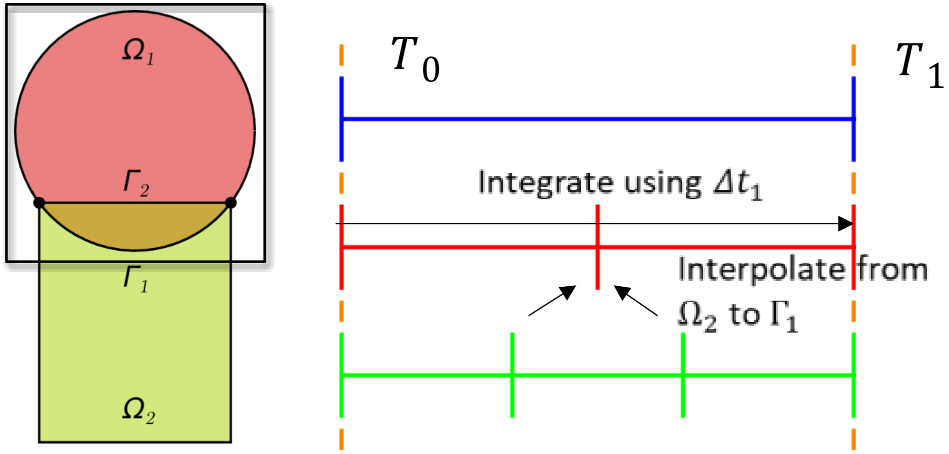

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- If unconverged, return to Step 1.

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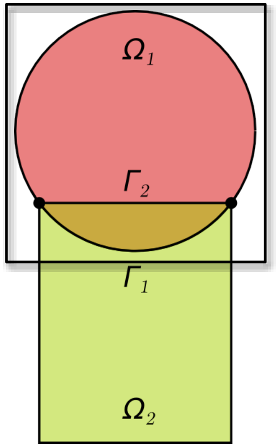

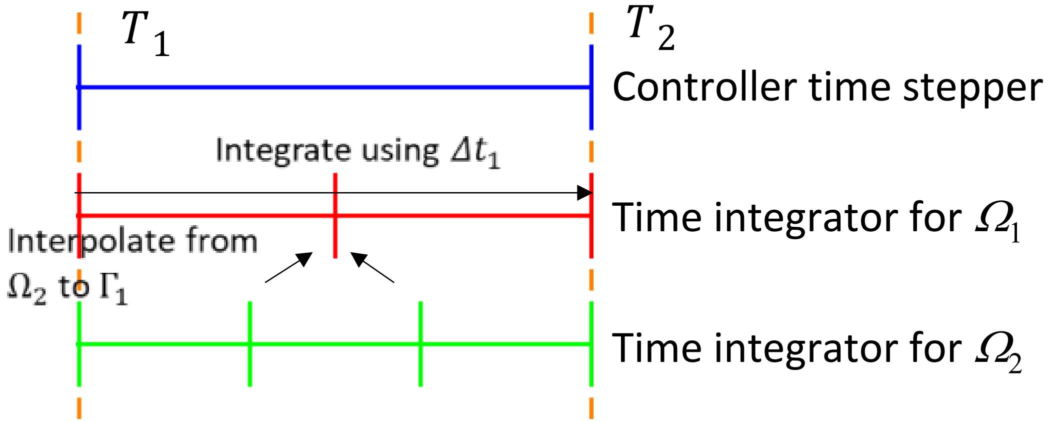

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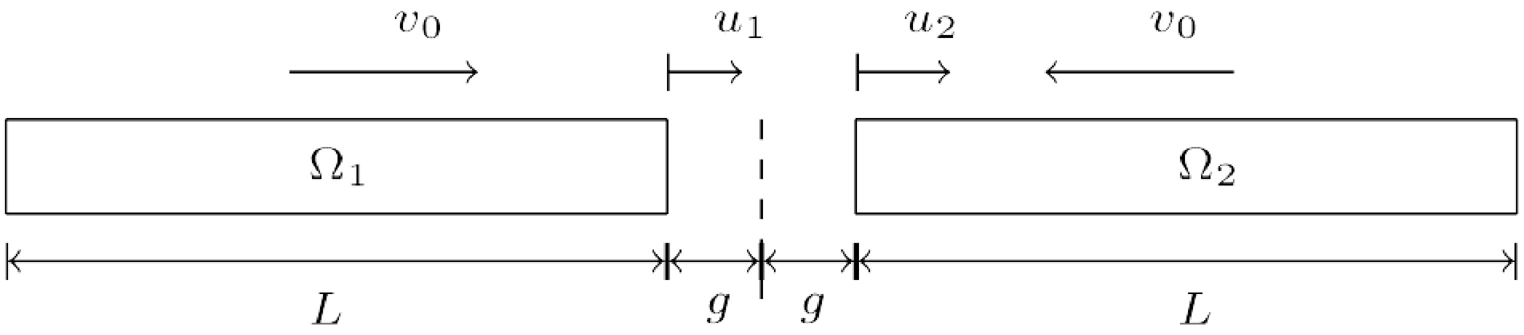
Step 3: Check for convergence at time T_{i+1}.
- If unconverged, return to Step 1.
- If converged, set $i = i + 1$ and return to Step 1.

Can use ***different integrators*** with ***different time steps*** within each domain!

Numerical Results: 1D Impact Problem[1]

- **Impact** of two **1D identical linear elastic prismatic rods** discretized using $N_x = 200$ linear elements with exact analytic solution [Carpenter *et al.*, 1991]

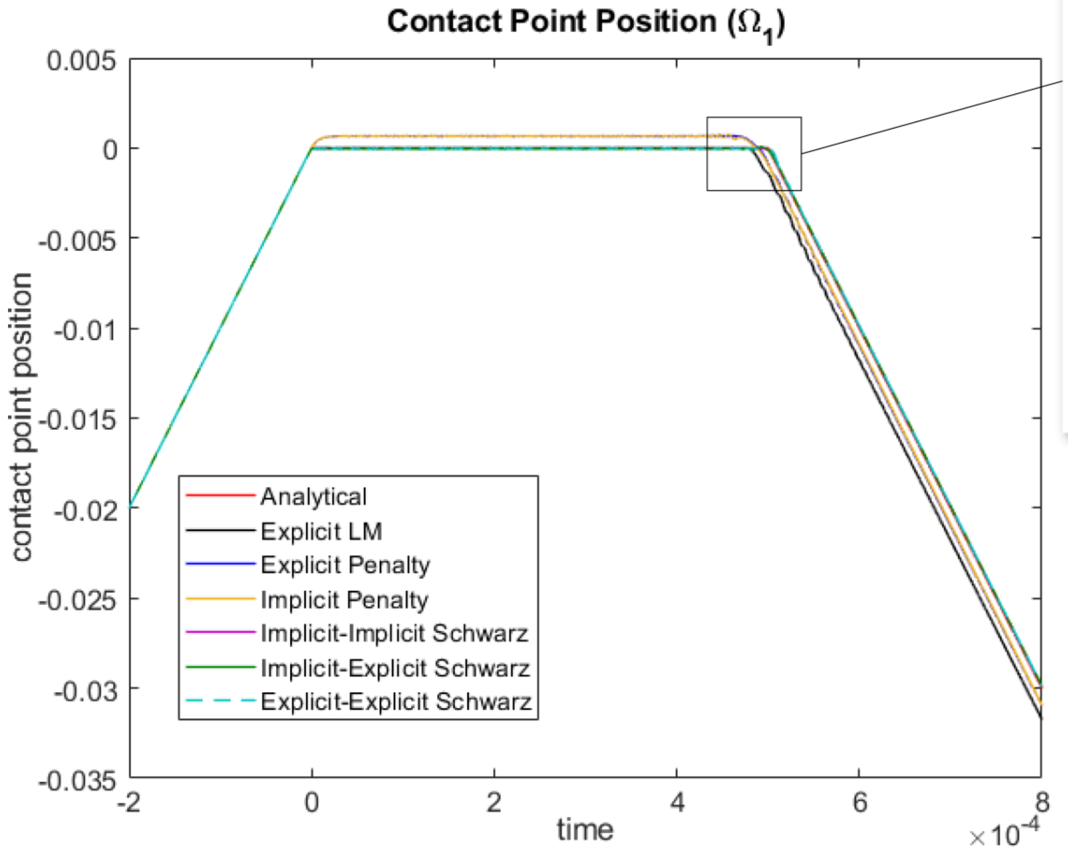


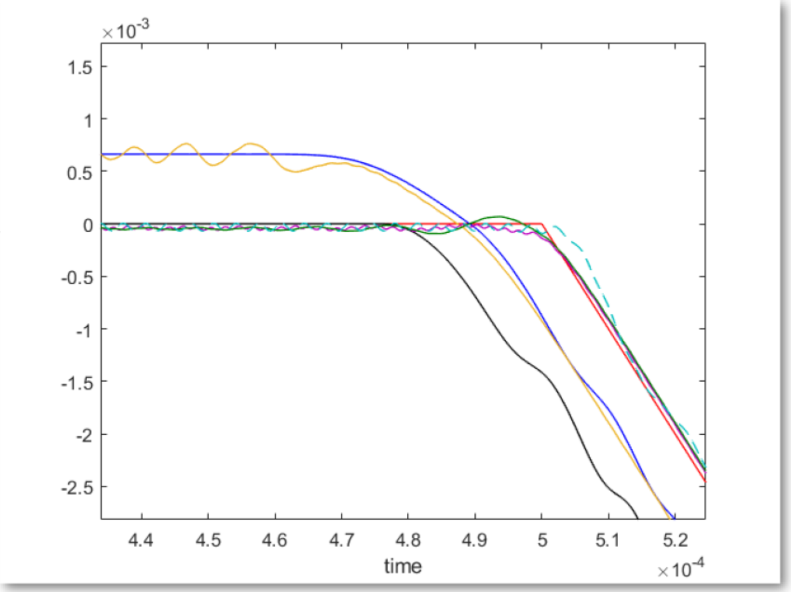
- Schwarz alternating method compared to **two conventional contact algorithms** with a **zero gap** contact constraint
  - ➢ Implicit and explicit **penalty method** with penalty parameter $\tau = 7.5 \times 10^4$
  - ➢ Forward increment (explicit) **Lagrange multiplier (LM)** method [Carpenter *et al.*, 1991]
- **Time stepper:** Newmark-beta
  - ➢ Schwarz couplings included Explicit-Explicit, Implicit-Explicit and Implicit-Implicit
  - ➢ $\Delta t = 1.0 \times 10^{-7}$ used for all methods except Implicit-Explicit Schwarz, which uses $\Delta t = 1.0 \times 10^{-8}$ in explicit domain.

[1]Hoy *et al.*, 2021; Mota *et al.* (in prep), 2021.

Numerical Results: 1D Impact Problem[1]

Contact point position: of the right-most node of left bar (Ω_1) as a function of time



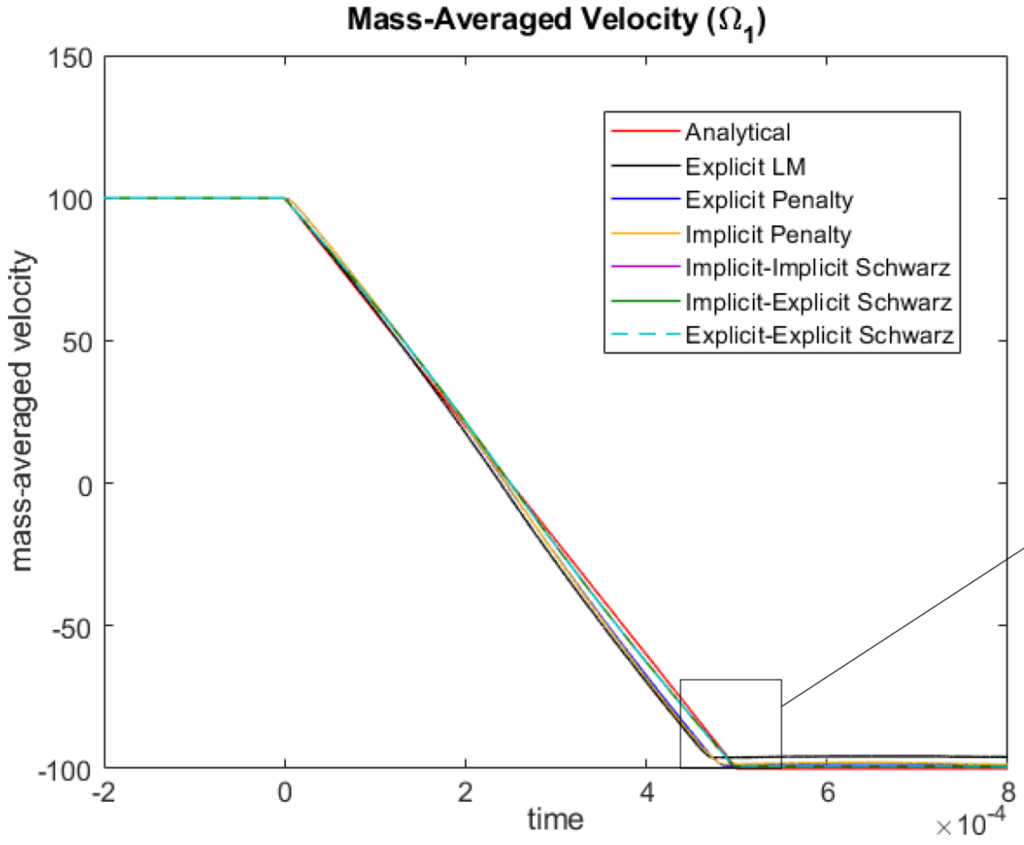


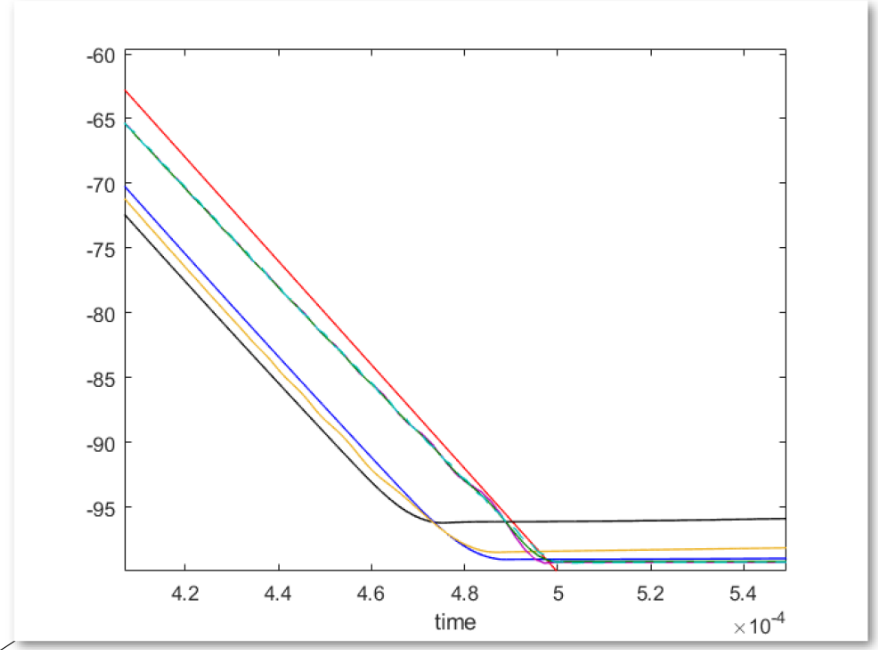
- Penalty methods **overpredict** contact point location between impact and release times
- Schwarz methods capture **release time** to an accuracy of ≈0.1%.

[1]Hoy *et al.*, 2021; Mota *et al.* (in prep), 2021.

Numerical Results: 1D Impact Problem[1]

Mass-averaged velocity: of the left bar (Ω_1) as a function of time





- **Similar conclusions** can be drawn from mass-averaged velocity
- Schwarz variants calculate mass-averaged velocity to a **sufficiently greater accuracy** than any of the conventional methods, especially near the time of release

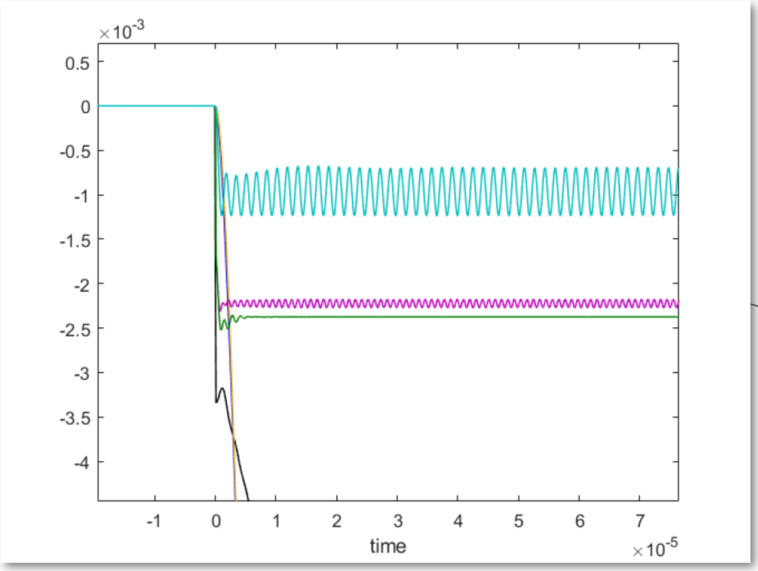
[1]Hoy *et al.*, 2021; Mota *et al.* (in prep), 2021.

Numerical Results: 1D Impact Problem[1]

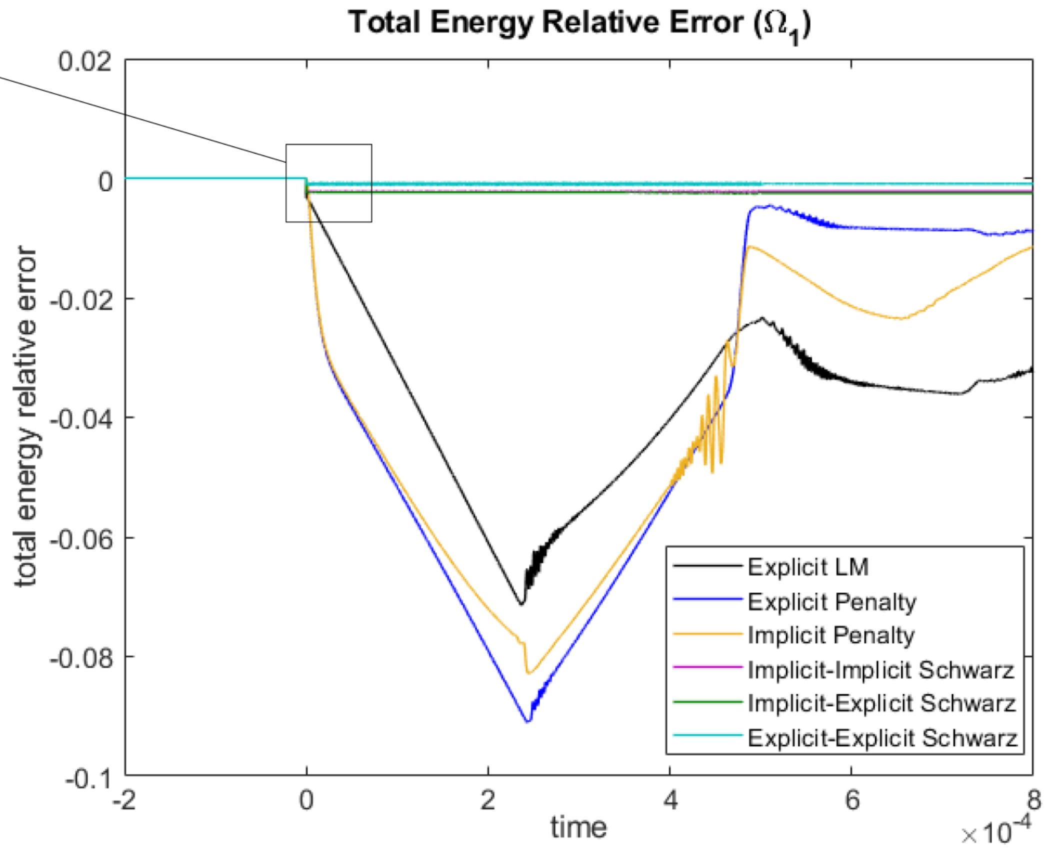
Total energy relative error: for the left bar (Ω_1) as a function of time

- Total energy error is **negative** for all 6 methods $\Longrightarrow$ all methods are **stable.**

- All three conventional methods exhibit **total energy loss** of up to 9% following contact.



Total energy should be **conserved** for this problem

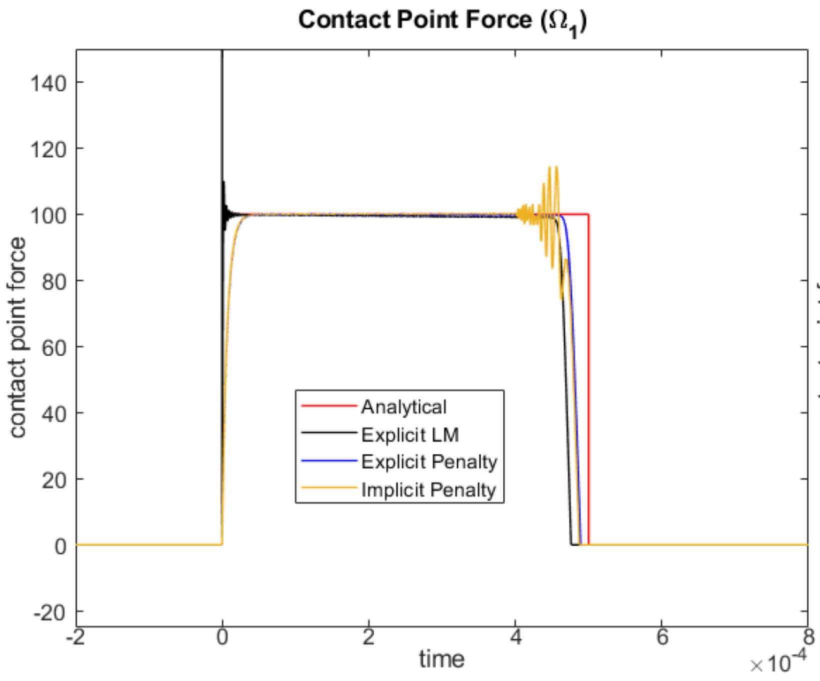


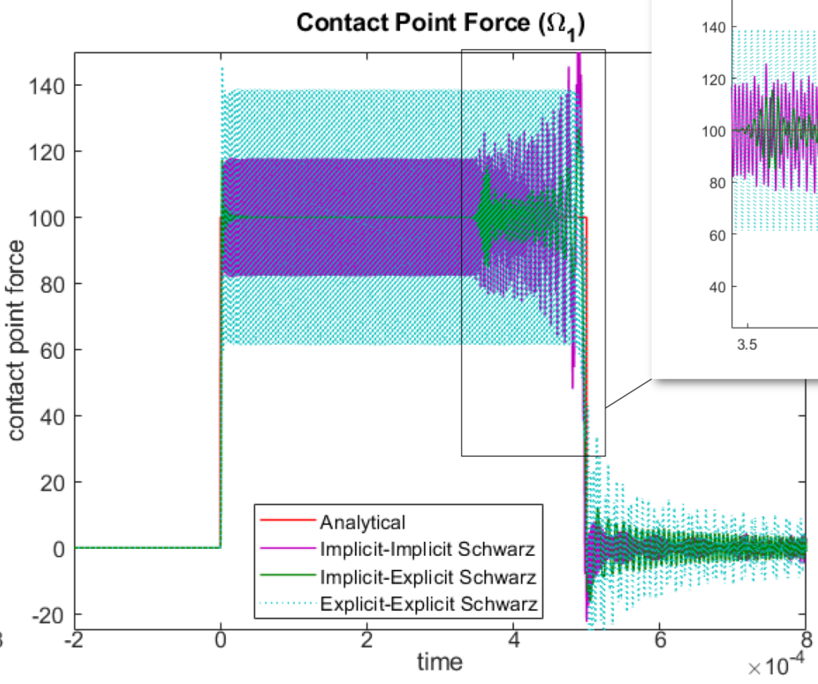
- Unlike conventional contact methods, **Schwarz** achieves an error of **at most 0.25%** in the total energy!
  - ➢ Explicit-Explicit Schwarz gives most accurate total energy, followed by Implicit-Implicit Schwarz and Implicit-Explicit Schwarz

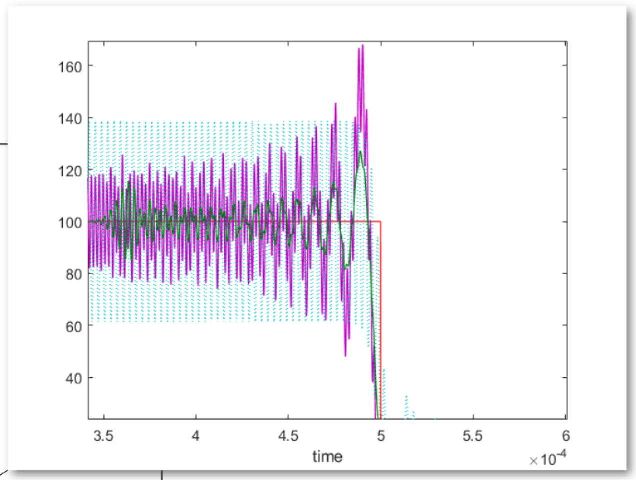
[1]Hoy *et al.*, 2021; Mota *et al.* (in prep), 2021.

Numerical Results: 1D Impact Problem[1]

Contact point force: for the left bar (Ω_1) as a function of time





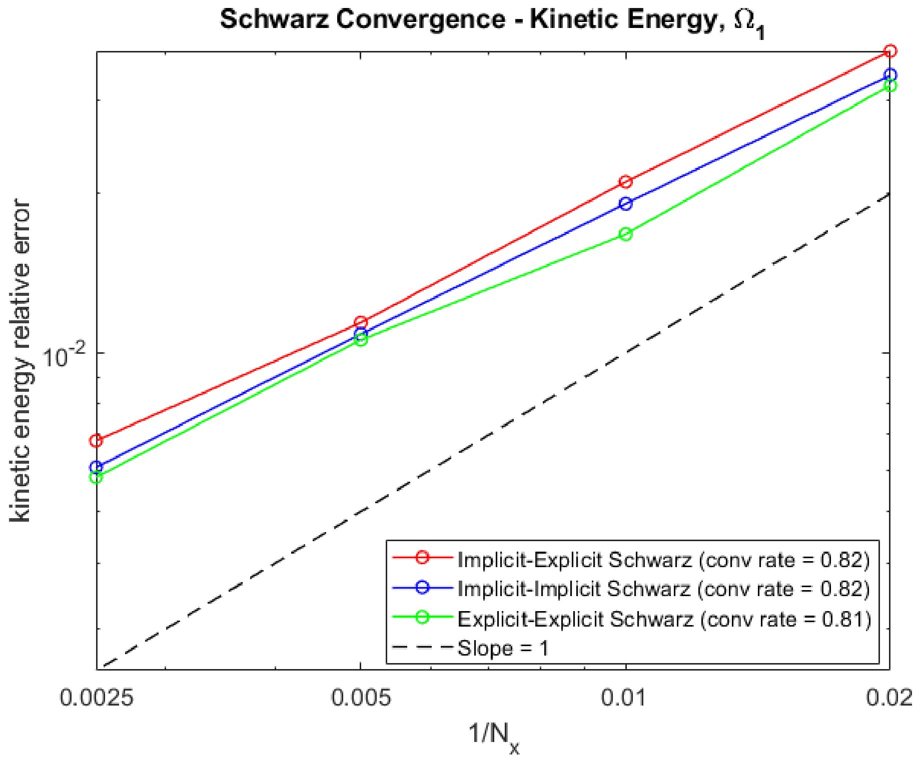


[1]Hoy *et al.*, 2021;
Mota *et al.* (in prep), 2021.

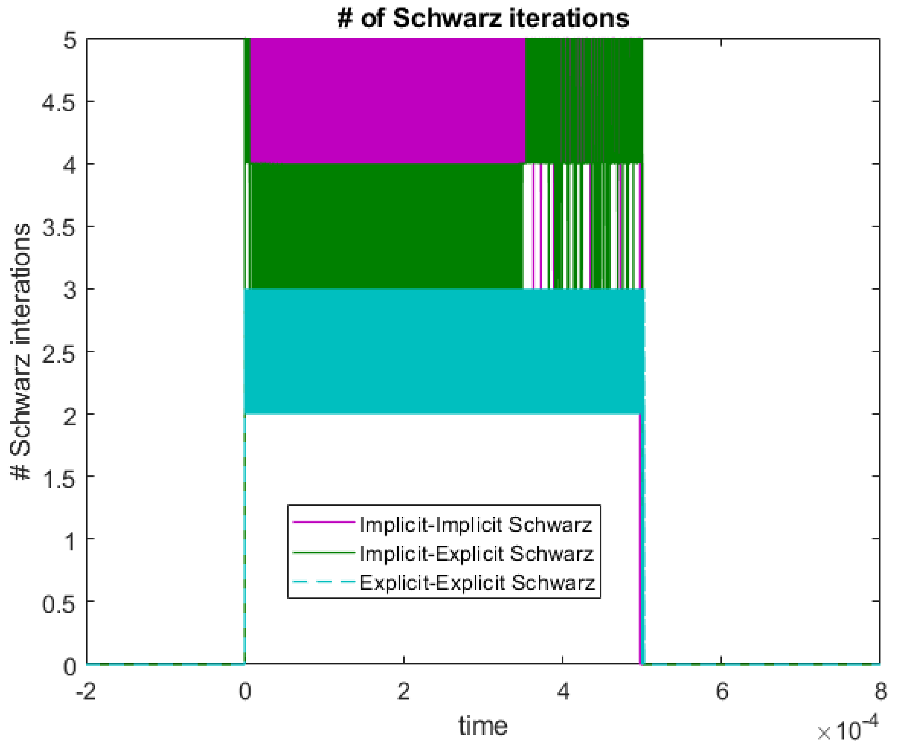
- Three conventional methods exhibit some **undesirable artifacts** in contact point force but deliver in general a **smooth solution**
- Schwarz solutions exhibit **oscillations** following instantiation of contact ⟶ **"chatter" problem**
  - ➢ Schwarz method with **largest total energy loss** (Implicit-Explicit) exhibits **least amount of chatter**
  - ➢ **Energy dissipation** is necessary for establishment of persistent contact [Solberg *et al.*, 1998]
    - ➢ Chatter problem can likely be mitigated through addition of **numerical dissipation**

Numerical Results: 1D Impact Problem[1]

Convergence of Schwarz methods



Mesh convergence of kinetic energy for left bar (Ω_1) when $\Delta t = 1.0 \times 10^{-8}$



Schwarz iterations required for convergence (N_x =200, $\Delta t = 1.0 \times 10^{-7}$)

- Convergence rates are comparable to published results [Tezaur *et al.*, 2021]
- At most 5 Schwarz iterations are needed for convergence
  - Explicit-Explicit Schwarz variant requires fewest # iterations for convergence

[1]Hoy *et al.*, 2021; Mota *et al.* (in prep), 2021.

Summary & Future Work

Summary:

- The Schwarz alternating method was shown to be an effective **multi-scale coupling** method in solid mechanics
- The Schwarz alternating method has shown promise as a **novel technique** for simulating **multi-scale mechanical contact**
  - ➢ Contact constraints are replaced with **transmission BCs** applied iteratively on contact boundaries
  - ➢ Schwarz method delivers **substantially more accurate solution** than conventional contact approaches in contact point displacement, mass-averaged velocity, impact time, release time, and kinetic, potential total energies
  - ➢ An unfortunate consequence of the method's ability to **conserve energy so well** appears to be the introduction of **chatter** in contact point velocity and force.

Ongoing/future work:

- Introduction of **dissipation** and/or **numerical relaxation** to mitigate chatter problem
- Introduction of **additional** or **alternate contact constraints** into Schwarz formulation
- Comparison to conventional contact formulations with **zero gap rate constraint**
- Implementation/evaluation of the Schwarz alternating method in **multi-D**
  - ➢ Requires the development of operators for **consistent transfer** of contact traction BCs using concept of prolongation/restriction

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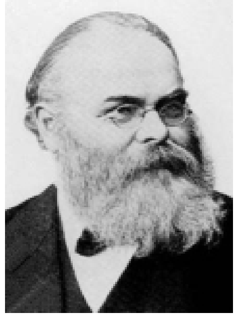
Start of Backup Slides

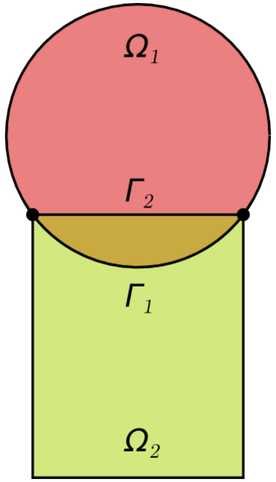
Schwarz Alternating Method for Domain Decomposition



H. Schwarz (1843 – 1921)

- Proposed in 1870 by H. Schwarz for solving Laplace PDE on irregular domains.

Crux of Method: if the solution is known in regularly shaped domains, use those as pieces to iteratively build a solution for the more complex domain.



Basic Schwarz Algorithm

Initialize:

- Solve PDE by any method on Ω_1 w/ initial guess for Dirichlet BCs on Γ_1.

Iterate until convergence:

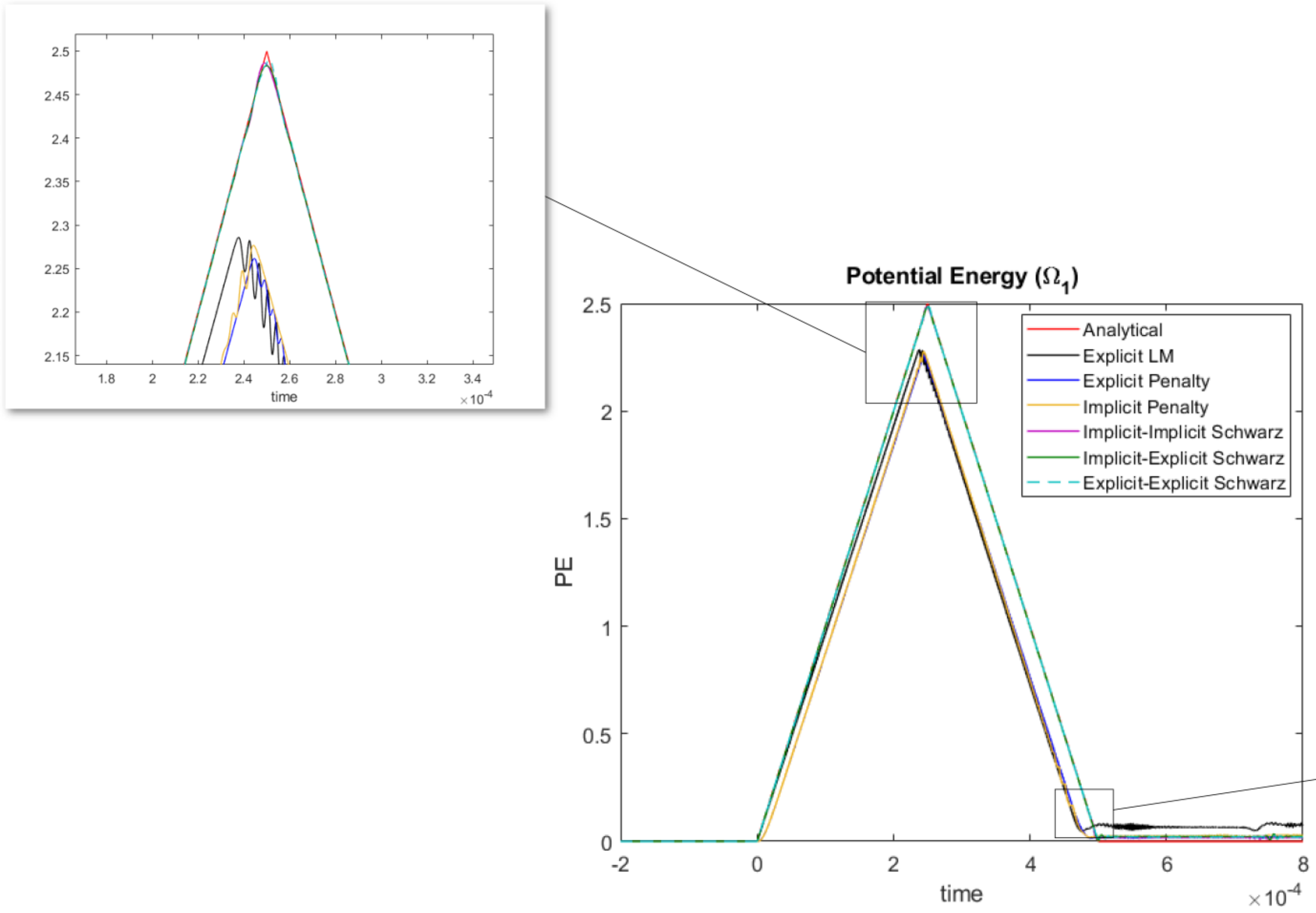
- Solve PDE by any method (can be different than for Ω_1) on Ω_2 w/ transmission BCs on Γ_2 that are the values just obtained for Ω_1.
- Solve PDE by any method (can be different than for Ω_2) on Ω_1 w/ transmission BCs on Γ_1 that are the values just obtained for Ω_2.

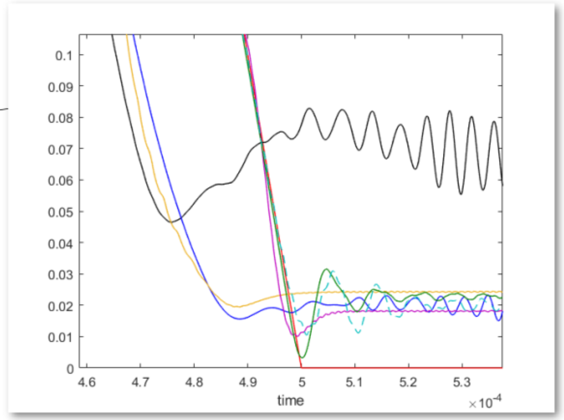
- Schwarz alternating method most commonly used as a ***preconditioner*** for Krylov iterative methods to solve linear algebraic equations.

Novel idea: using the Schwarz alternating as a ***discretization method*** for solving multiscale partial differential equations (PDEs).

Numerical Results: 1D Impact Problem[1]

Potential energy: for the left bar (Ω_1) as a function of time





- **Similar conclusions** can be drawn from potential energy plots.
- All three conventional methods **underpredict peak potential energy** by $\approx$10%.
- Schwarz solutions **capture peak potential energy** with relative error <0.1%

[1]Hoy *et al.*, 2021; Mota *et al.* (in prep), 2021.

Numerical Results: 1D Impact Problem[1]

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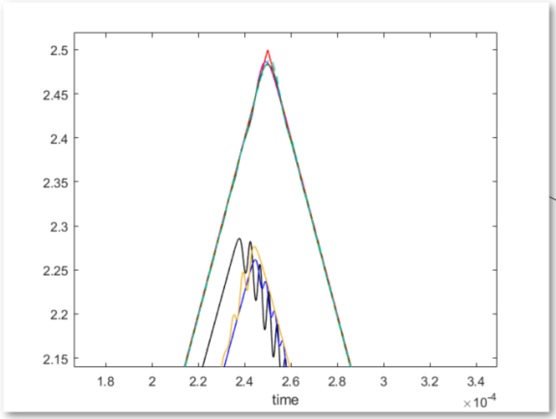
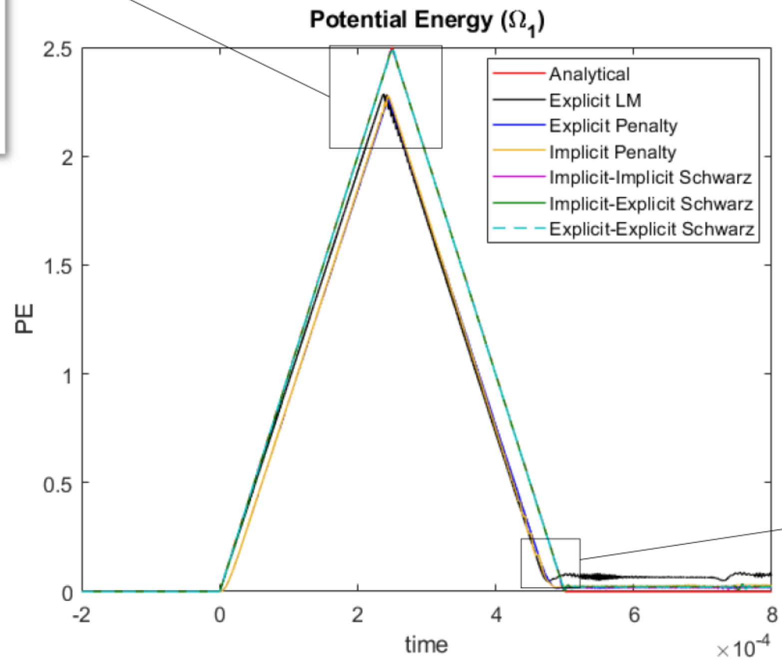
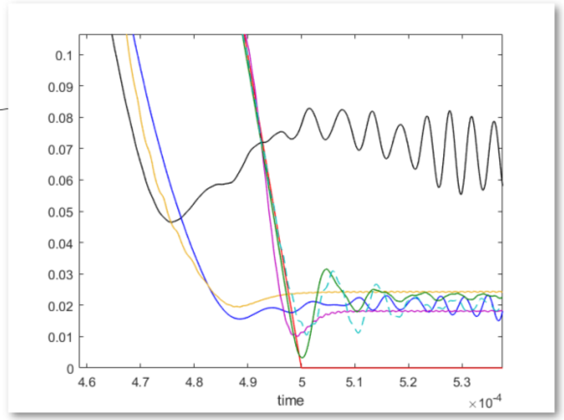




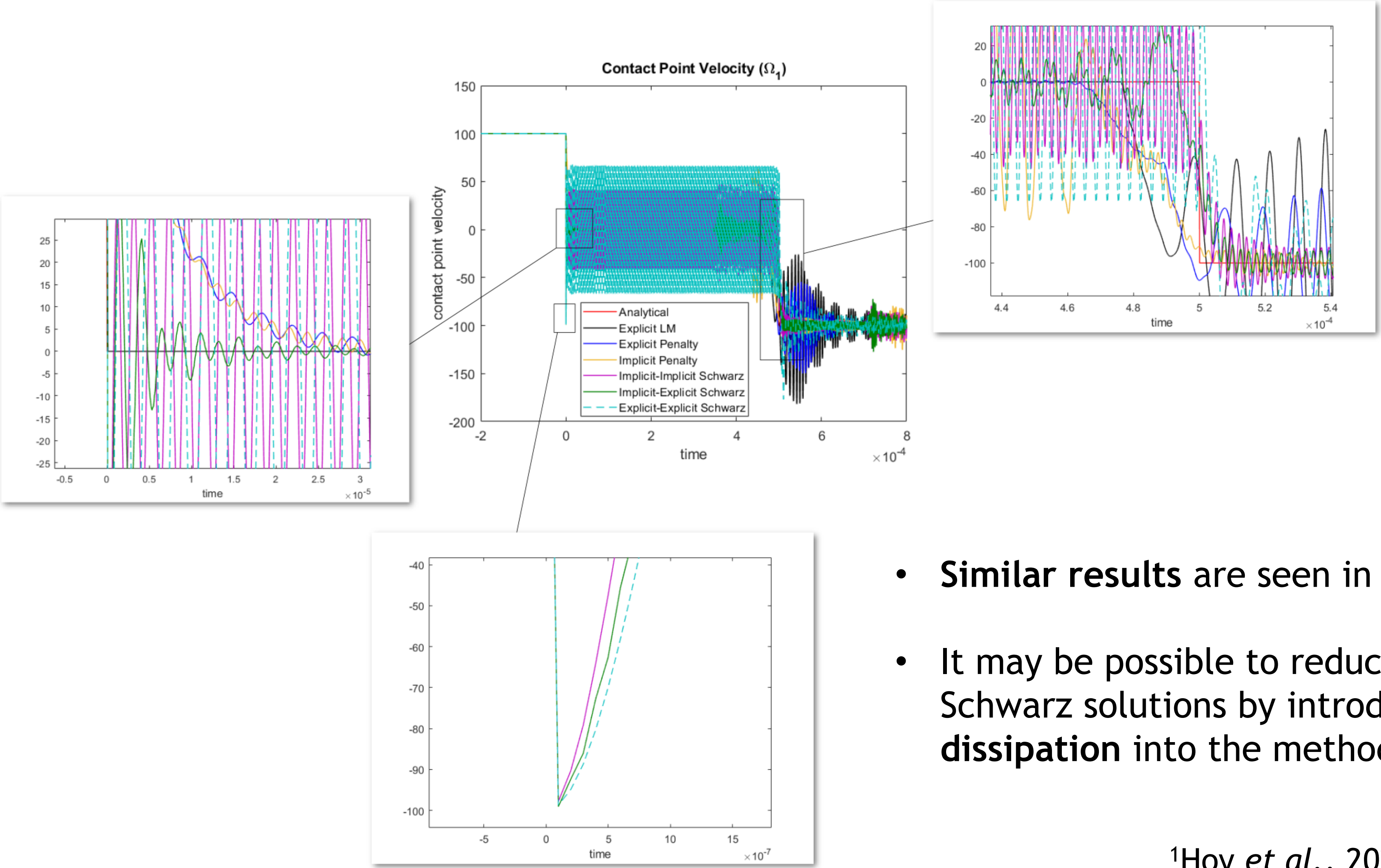


- **Similar conclusions** can be drawn from potential energy plots.
- All three conventional methods **underpredict peak potential energy** by ≈10%.
- Schwarz solutions **capture peak potential energy** with relative error <0.1%

[1]Hoy *et al.*, 2021; Mota *et al.* (in prep), 2021.

Numerical Results: 1D Impact Problem[1]

Contact point velocity: for the left bar (Ω_1) as a function of time



- **Similar results** are seen in the contact point velocity
- It may be possible to reduce amount of chatter in Schwarz solutions by introducing **numerical dissipation** into the method.

[1]Hoy *et al.*, 2021; Mota *et al.* (in prep), 2021.