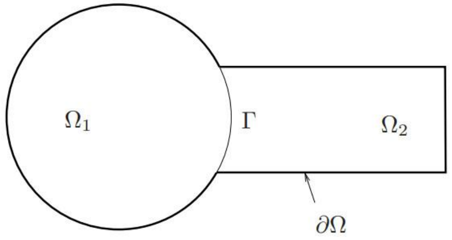
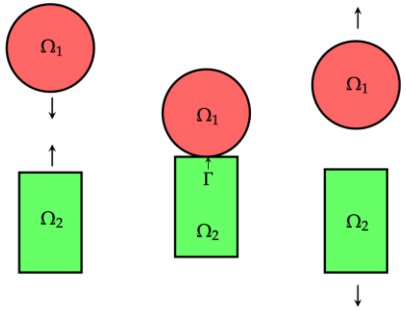
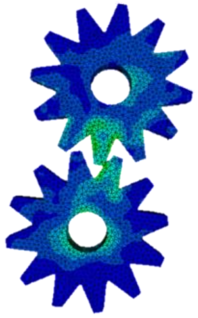
Sandia National Laboratories

The Schwarz Alternating Method for Multi-Scale Contact Mechanics







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

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

Congress on Numerical Methods in Engineering (CMN) 2022

Las Palmas de Gran Canaria, Spain September 12-14, 2022

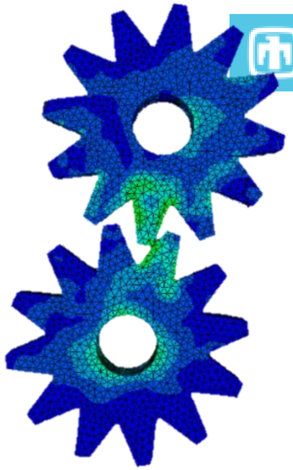
SAND2022-11528C

U.S. DEPARTMENT OF ENERGY NNSA

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

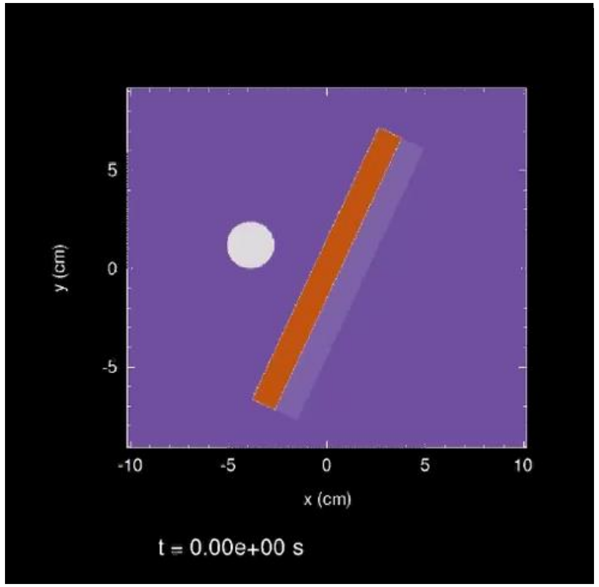
Motivation

- Stable, accurate and robust methods for simulating **mechanical contact** are extremely important in computational solid mechanics
  - ➢ *Example scenarios where contact arises*: touching surfaces, sliding, tightened bolts, impact, …



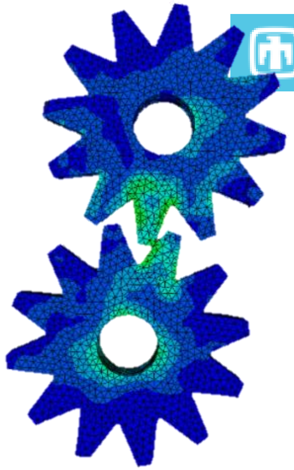
Above: gears in contact within MEMS device. From *sandia.gov/media*

Below: oblique cylinder impact simulated using Sandia's ALEGRA code.



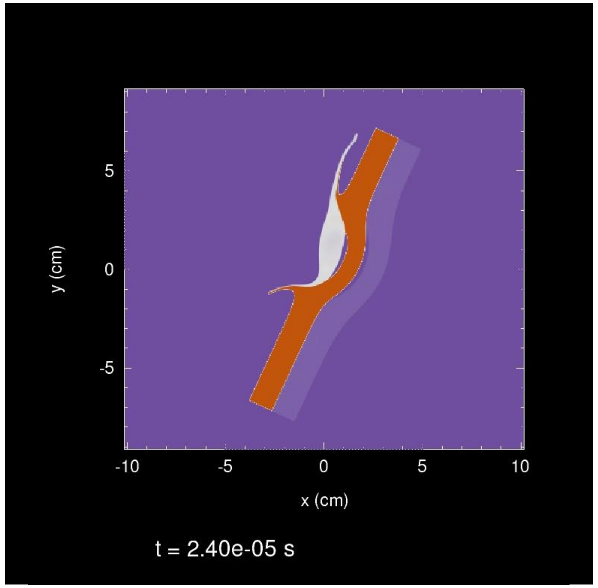
Motivation

- Stable, accurate and robust methods for simulating **mechanical contact** are extremely important in computational solid mechanics
    - ➢ *Example scenarios where contact arises*: touching surfaces, sliding, tightened bolts, impact, …



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

Below: oblique cylinder impact simulated using Sandia's ALEGRA code.



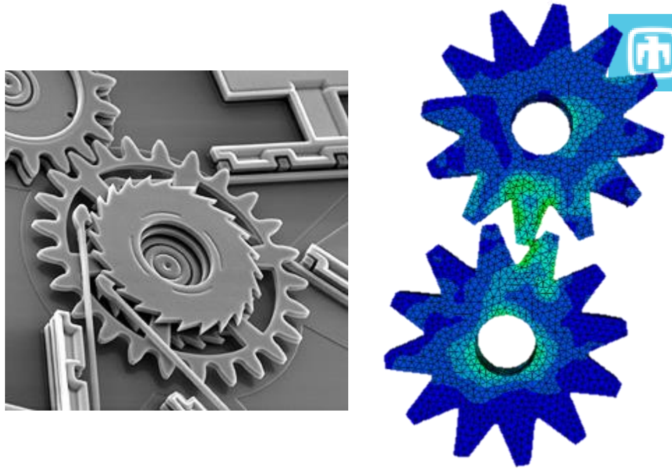
Two-step process to the computational simulation of contact:

1. **Proximity search**

2. **Contact enforcement step**

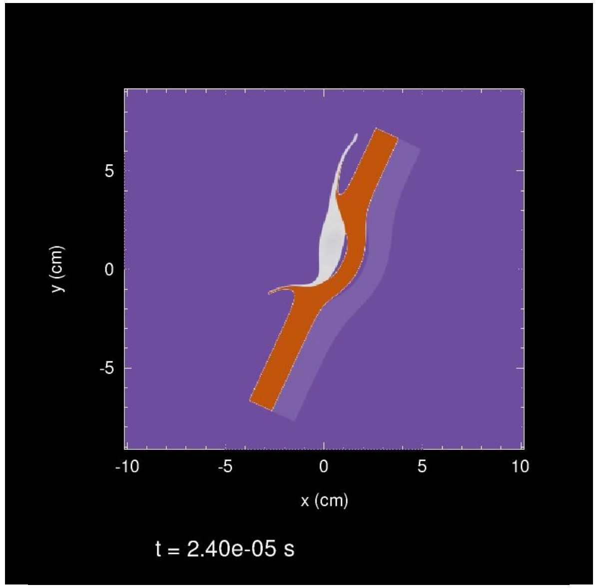
Motivation

- Stable, accurate and robust methods for simulating **mechanical contact** are extremely important in computational solid mechanics
  - *Example scenarios where contact arises*: touching surfaces, sliding, tightened bolts, impact, …



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

Below: oblique cylinder impact simulated using Sandia's ALEGRA code.



Two-step process to the computational simulation of contact:

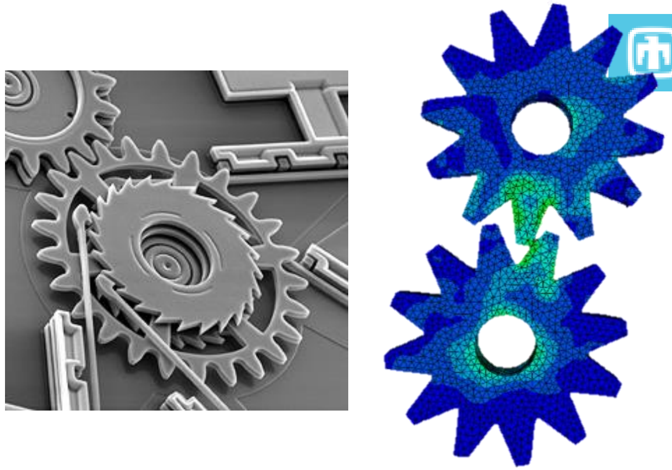
1. **Proximity search:** computer science problem, has received much attention due to importance in video game development ☺
2. **Contact enforcement step**

Motivation

- Stable, accurate and robust methods for simulating **mechanical contact** are extremely important in computational solid mechanics
  - *Example scenarios where contact arises*: touching surfaces, sliding, tightened bolts, impact, …

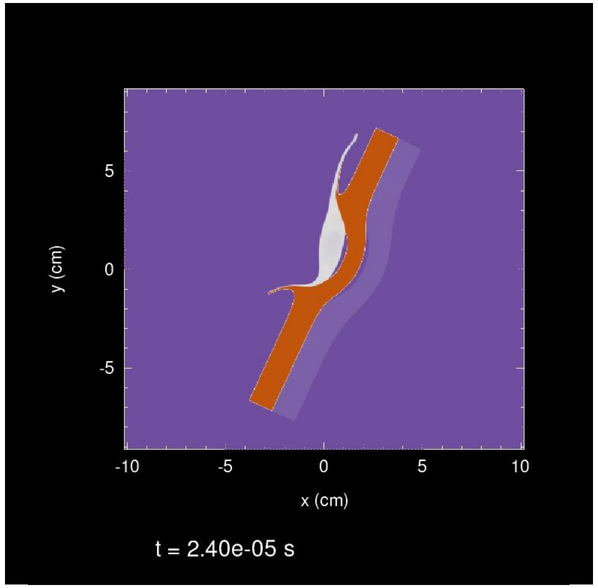
Two-step process to the computational simulation of contact:

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 ☹



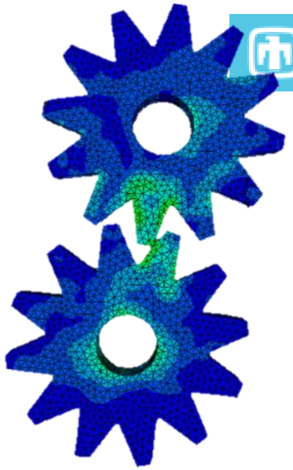
Above: gears in contact within MEMS device. From *sandia.gov/media*

Below: oblique cylinder impact simulated using Sandia's ALEGRA code.



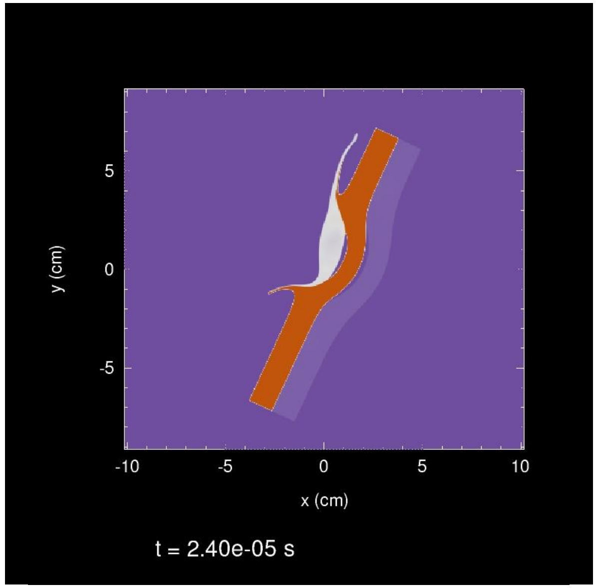
Motivation

- Stable, accurate and robust methods for simulating **mechanical contact** are extremely important in computational solid mechanics
  - ➢ *Example scenarios where contact arises*: touching surfaces, sliding, tightened bolts, impact, …



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

Below: oblique cylinder impact simulated using Sandia's ALEGRA code.

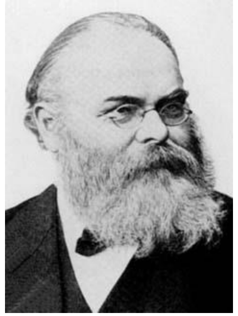


Two-step process to the computational simulation of contact:

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: new approach for simulating multi-scale mechanical contact using the **Schwarz alternating method.**

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

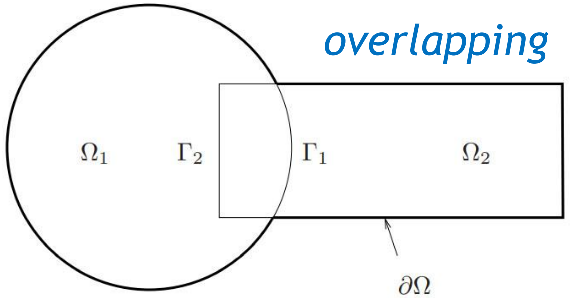
Initialize:

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

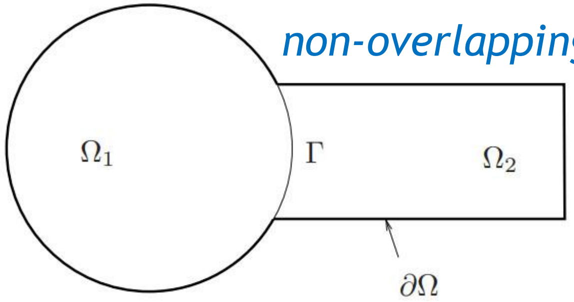
Iterate until convergence:

- Solve PDE by any method on Ω_2 w/ transmission BCs on Γ_2 based on values just obtained for Ω_1.
- Solve PDE by any method on Ω_1 w/ transmission BCs on Γ_1 based on values just obtained for Ω_2.

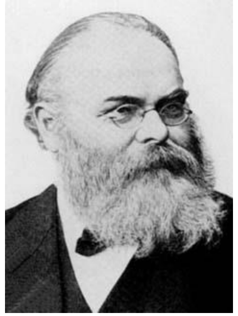
overlapping



non-overlapping



Schwarz Alternating Method for Domain Decomposition


H. Schwarz (1843–1921)

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

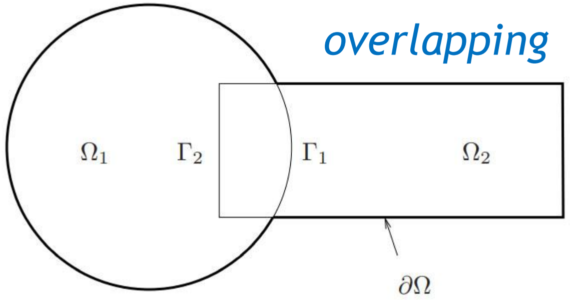
Crux of Method: if the solution is known in regularly shaped domains, use those as pieces to iteratively build a solution for the more complex domain.

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.
- Solve PDE by any method on Ω_1 w/ transmission BCs on Γ_1 based on values just obtained for Ω_2.

overlapping



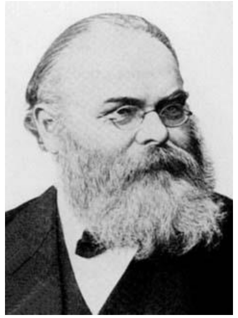
Overlapping Schwarz: convergent with all-Dirichlet transmission BCs[1] if $\Omega_1 \cap \Omega_2 \neq \emptyset$.

[1]Schwarz, 1870; Lions, 1988.

Schwarz Alternating Method for Domain Decomposition

- 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.



H. Schwarz (1843–1921)

Basic Schwarz Algorithm

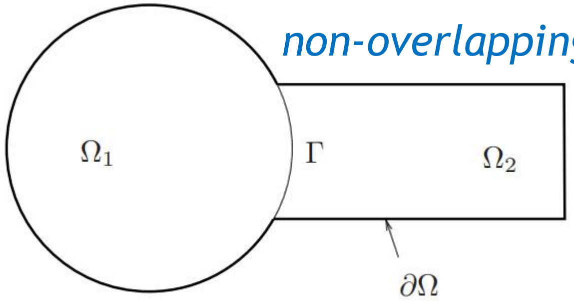
Initialize:

- 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.
- Solve PDE by any method on Ω_1 w/ transmission BCs on Γ_1 based on values just obtained for Ω_2.

non-overlapping

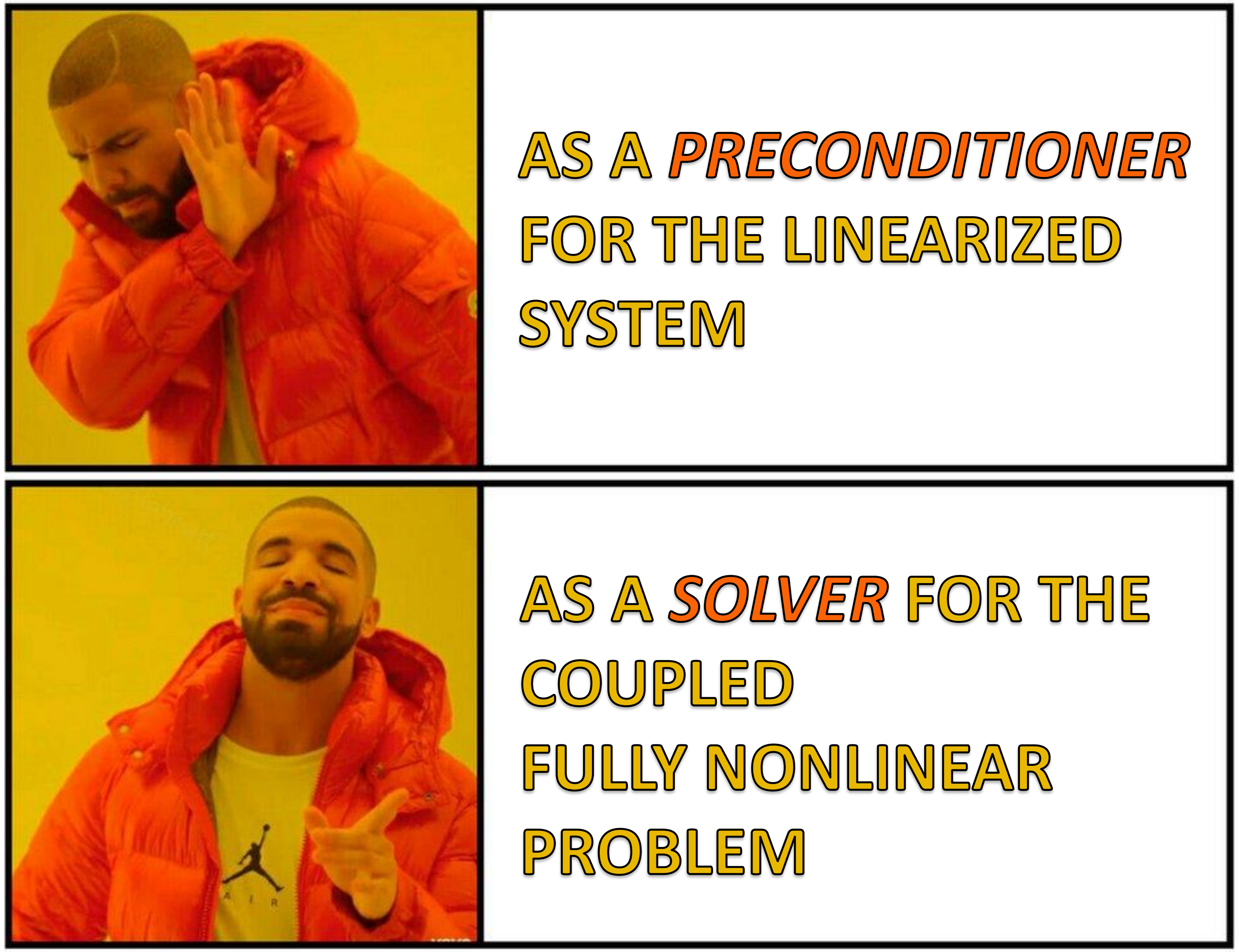


Overlapping Schwarz: convergent with all-Dirichlet transmission BCs[1] if $\Omega_1 \cap \Omega_2 \neq \emptyset$.

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

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

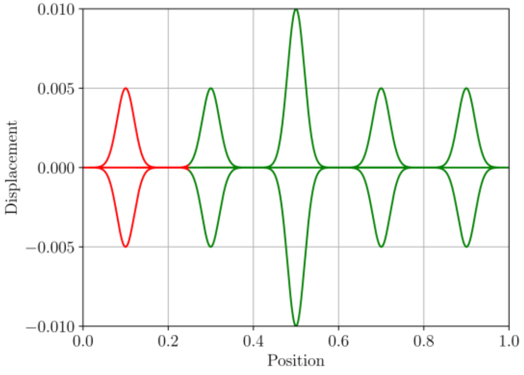
How We Use the Schwarz Alternating Method



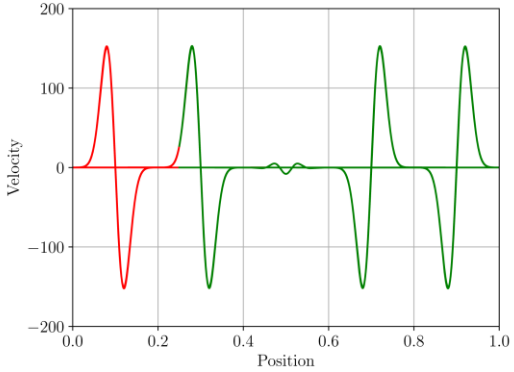
Overlapping Schwarz for Multi-Scale Coupling in Solid Mechanics

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

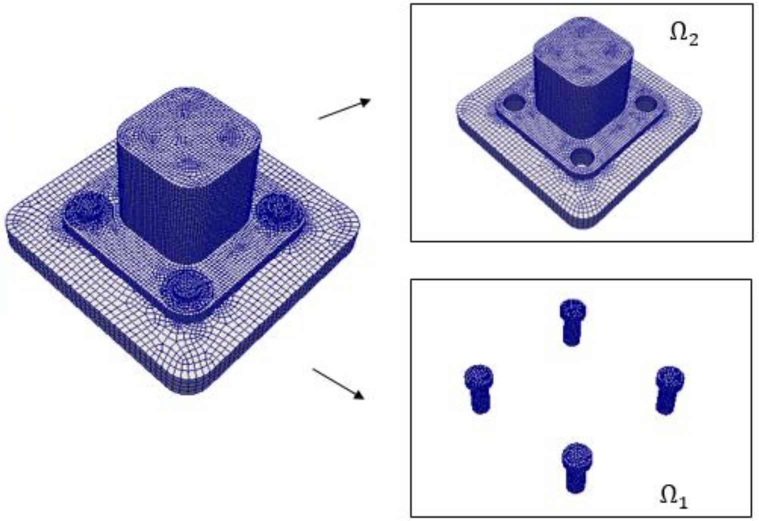
Displacement

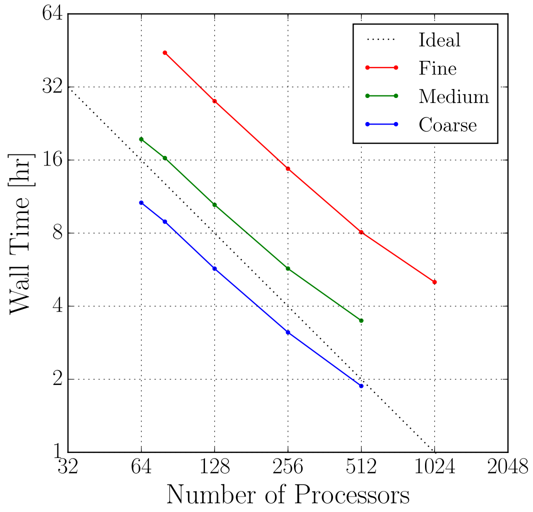


Velocity



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





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

[1]Mota *et al.*, 2017; Mota *et al.*, 2022.

*https://github.com/sandialabs/LCM

Solid Mechanics Problem Formulation

Kinetic Energy: $$T(\dot{\varphi}) := \frac{1}{2}\int_{\Omega} \rho_0 \dot{\varphi}\cdot\dot{\varphi}\ \mathrm{d}V,$$

Potential Energy: $$V(\varphi) := \int_{\Omega} A(\boldsymbol{F},\boldsymbol{Z})\ \mathrm{d}V - \int_{\Omega} \rho_0 \boldsymbol{B}\cdot\varphi\ \mathrm{d}V - \int_{\partial_{\boldsymbol{T}}\Omega} \boldsymbol{T}\cdot\varphi\ \mathrm{d}S,$$

Lagrangian: $$L(\varphi,\dot{\varphi}) := T(\dot{\varphi}) - V(\varphi),$$

Action Functional: $$S[\varphi] := \int_I L(\varphi,\dot{\varphi})\ \mathrm{d}t.$$

Euler-Lagrange Equations:

$$\begin{aligned}
\operatorname{Div}\boldsymbol{P} + \rho_0\boldsymbol{B} &= \rho_0\ddot{\varphi} \quad \text{in} \quad \Omega\times I,\\
\varphi(\boldsymbol{X},t_0) &= \boldsymbol{x}_0 \quad \text{in} \quad \Omega,\\
\dot{\varphi}(\boldsymbol{X},t_0) &= \boldsymbol{v}_0 \quad \text{in} \quad \Omega,\\
\varphi(\boldsymbol{X},t) &= \chi \quad \text{on} \quad \partial_{\varphi}\Omega\times I,\\
\boldsymbol{P}\boldsymbol{N} &= \boldsymbol{T} \quad \text{on} \quad \partial_{\boldsymbol{T}}\Omega\times I.
\end{aligned}$$

FEM →

Semi-Discrete Problem:

$$\begin{aligned}
\boldsymbol{M}\ddot{\boldsymbol{u}} + \boldsymbol{f}_{\text{int}}(\boldsymbol{u},\dot{\boldsymbol{u}}) &= \boldsymbol{f}_{\text{ext}}\\
\boldsymbol{u}(0) &= \boldsymbol{u}_0\\
\dot{\boldsymbol{u}}(0) &= \boldsymbol{v}_0
\end{aligned}$$

Traditional Solid Mechanics Contact Formulation

Kinetic Energy:

$$T(\dot{\varphi}) := \frac{1}{2}\int_{\Omega} \rho_0 \dot{\varphi} \cdot \dot{\varphi} \; \mathrm{d}V,$$

Potential Energy Augmented with Contact Constraint:

$$V(\varphi) := \int_{\Omega} A(\boldsymbol{F}, \boldsymbol{Z}) \; \mathrm{d}V - \int_{\Omega} \rho_0 \boldsymbol{B} \cdot \varphi \; \mathrm{d}V + \boxed{\int_{\Omega} I_{\mathcal{C}}(\varphi) \; \mathrm{d}V} - \int_{\partial_{\boldsymbol{T}}\Omega} \boldsymbol{T} \cdot \varphi \; \mathrm{d}S.$$

Lagrangian:

$$L(\varphi, \dot{\varphi}) := T(\dot{\varphi}) - V(\varphi),$$

Action Functional:

$$S[\varphi] := \int_{I} L(\varphi, \dot{\varphi}) \; \mathrm{d}t.$$

$\mathcal{C}$: The set of admissible configurations $\boldsymbol{\varphi}$ in which interpenetration does not occur

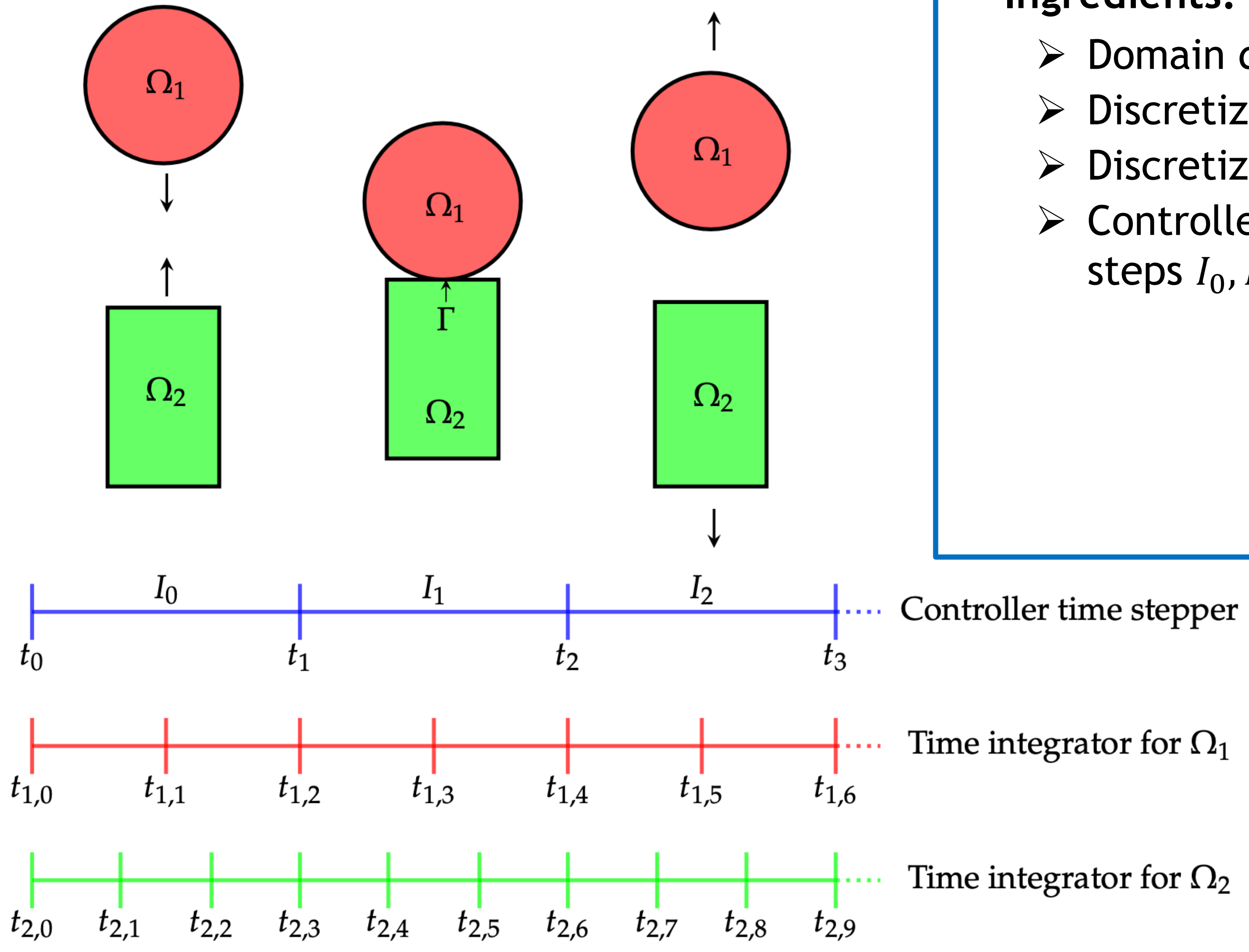
Indicator function for admissible set $\mathcal{C}$:

$$\boxed{I_{\mathcal{C}}(\varphi) := \begin{cases} 0, & \text{if } \varphi \in \mathcal{C}, \\ \infty, & \text{if } \varphi \notin \mathcal{C}, \end{cases}}$$

Contact constraint can be enforced strictly or approximately

- *Strict enforcement*: Lagrange multiplier methods
- *Approximate enforcement*: penalty methods

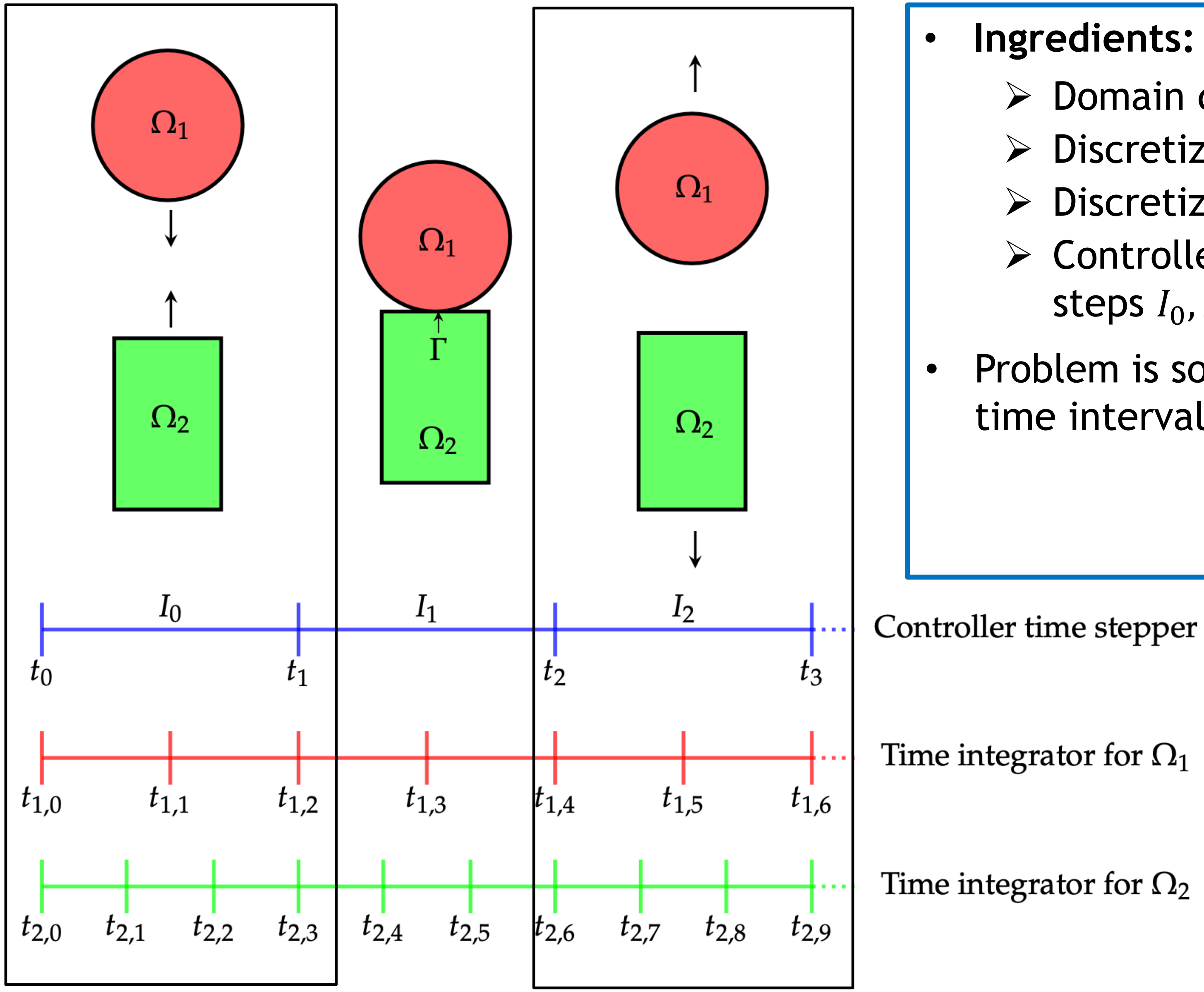
Non-Overlapping Schwarz Contact Formulation



- **Ingredients:**
  - Domain decomposition
  - Discretization and time-stepper in Ω_1 (red)
  - Discretization and time-stepper in Ω_2 (green)
  - Controller time-stepper (blue): defines global time-steps $I_0, I_1, \dots$ at which subdomains are synchronized

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

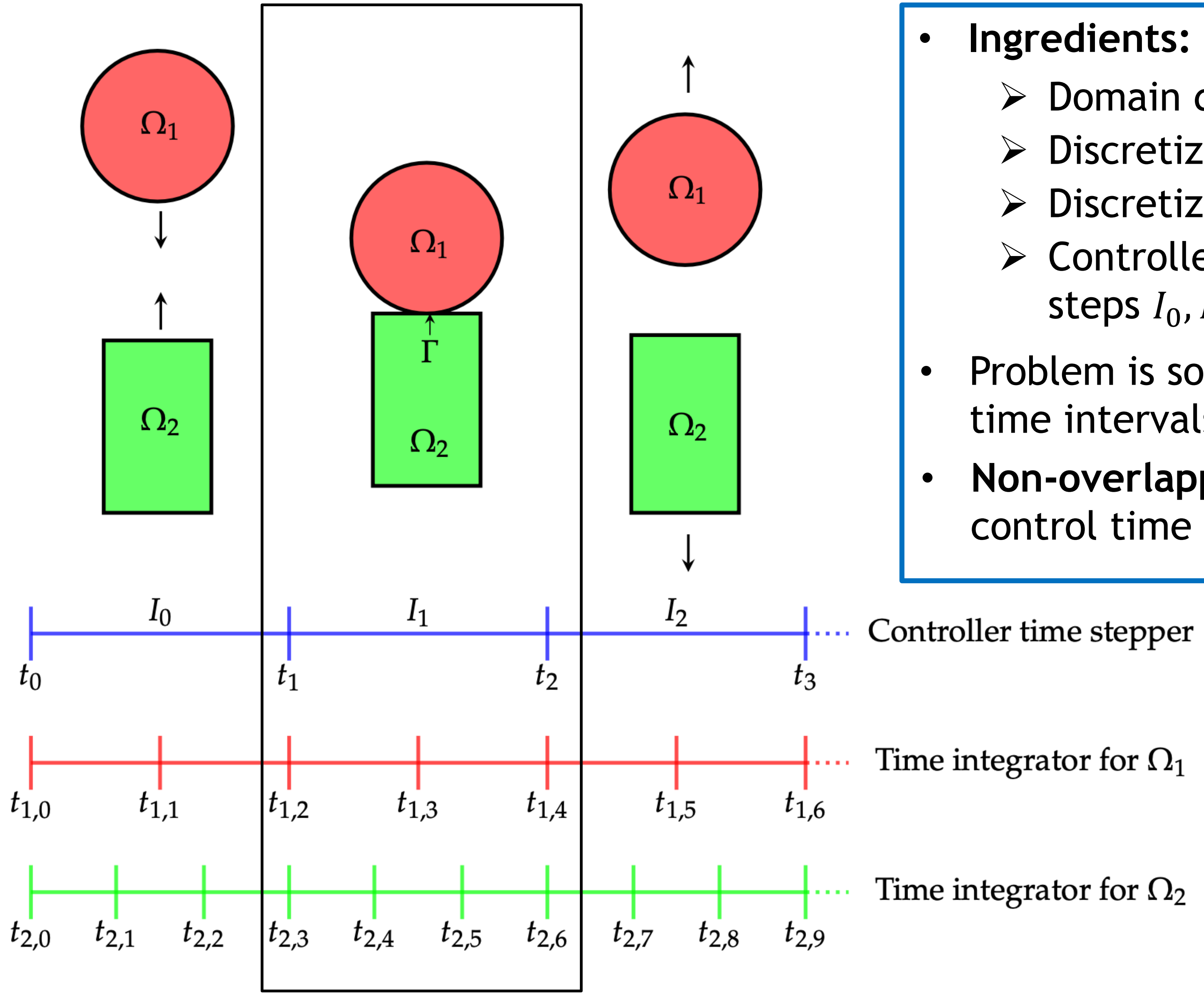
Non-Overlapping Schwarz Contact Formulation



- **Ingredients:**
  - Domain decomposition
  - Discretization and time-stepper in Ω_1 (red)
  - Discretization and time-stepper in Ω_2 (green)
  - Controller time-stepper (blue): defines global time-steps $I_0, I_1, \ldots$ at which subdomains are synchronized
- Problem is solved **without any Schwarz iteration** in time intervals I_0 and I_2, as there is no contact.

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

Non-Overlapping Schwarz Contact Formulation



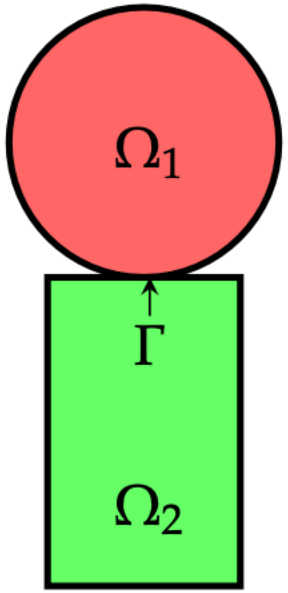
- **Ingredients:**
  - Domain decomposition
  - Discretization and time-stepper in Ω_1 (red)
  - Discretization and time-stepper in Ω_2 (green)
  - Controller time-stepper (blue): defines global time-steps $I_0, I_1, \dots$ at which subdomains are synchronized
- Problem is solved **without any Schwarz iteration** in time intervals I_0 and I_2, as there is no contact.
- **Non-overlapping Schwarz** algorithm **only applied** in control time interval I_1, when **contact is detected**.

Contact Criteria

- **Overlap:** interpenetration of subdomains
- **Compression:** positive normal traction
- **Persistence:** was in contact previous step

Non-Overlapping Schwarz Contact Formulation

- **Key idea:** a contact problem can be viewed as **coupled problem** while 2+ bodies are in contact
  - ➢ **Alternating** Dirichlet-Neumann (traction) **Schwarz iteration** is applied once interpenetration has been detected, to correct the **interpenetration**.



$$\begin{cases} \mathrm{Div}\,\boldsymbol{P}^{(n)} + \rho_0 \boldsymbol{B} = \rho_0 \ddot{\boldsymbol{\varphi}}^{(n)}, & \text{in } \Omega_1 \times I_k, \\ \boldsymbol{\varphi}^{(n)}(\boldsymbol{X}, t) = \boldsymbol{\chi}, & \text{on } \partial_{\boldsymbol{\varphi}}\Omega_1 \times I_k, \\ \boldsymbol{\varphi}^{(n)}(\boldsymbol{X}, t) = P_{\Omega_2 \to \Gamma}[\boldsymbol{\varphi}^{(n-1)}(\Omega_2, t_k)], & \text{on } \Gamma \times I_k, \\ \boldsymbol{P}^{(n)}\boldsymbol{N} = \boldsymbol{T}, & \text{on } [\partial_{\boldsymbol{T}}\Omega_1 \cup \Gamma] \times I_k, \end{cases}$$

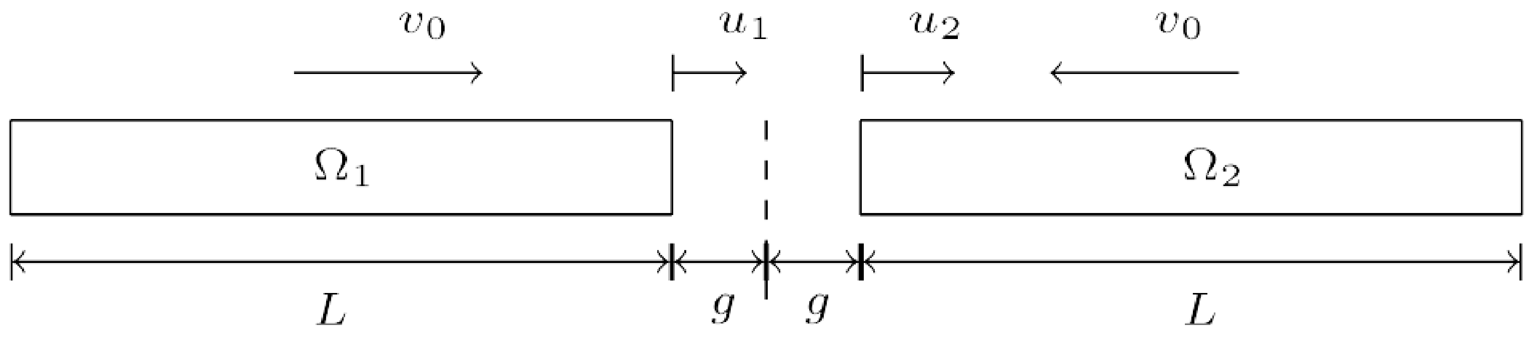
$$\begin{cases} \mathrm{Div}\,\boldsymbol{P}^{(n)} + \rho_0 \boldsymbol{B} = \rho_0 \ddot{\boldsymbol{\varphi}}^{(n)}, & \text{in } \Omega_2 \times I_k, \\ \boldsymbol{\varphi}^{(n)}(\boldsymbol{X}, t) = \boldsymbol{\chi}, & \text{on } [\partial_{\boldsymbol{\varphi}}\Omega_2 \cup \Gamma] \times I_k, \\ \boldsymbol{P}^{(n)}\boldsymbol{N} = \boldsymbol{T}, & \text{on } \partial_{\boldsymbol{T}}\Omega_2 \times I_k, \\ \boldsymbol{P}^{(n)}\boldsymbol{N} = P_{\Omega_1 \to \Gamma}[\boldsymbol{T}^{(n)}(\Omega_1, t_k)], & \text{on } \Gamma \times I_k, \end{cases}$$

There are no contact constraints!

Contact constraints replaced with **BCs** applied **iteratively** at contact boundaries.

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]

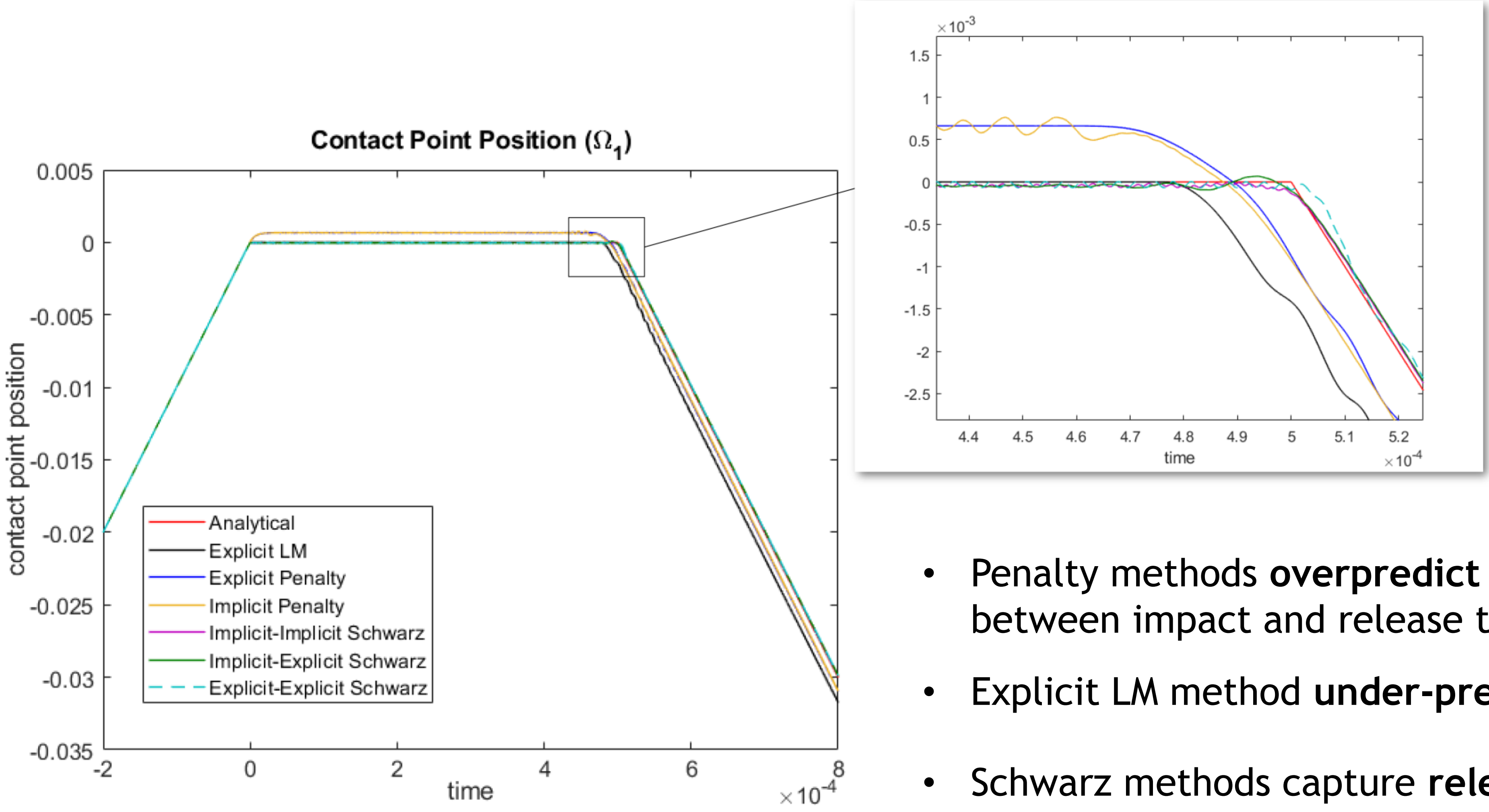


- Schwarz alternating method compared to **three conventional contact algorithms** with a **zero gap** contact constraint
  - ➢ **Implicit** and **explicit penalty method** with penalty parameter $\tau = 7.5 \times 10^4$
  - ➢ Forward increment (explicit) **Lagrange multiplier (LM)** method [Carpenter *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.*, 2022 (under review).

Numerical Results: 1D Impact Problem[1]

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

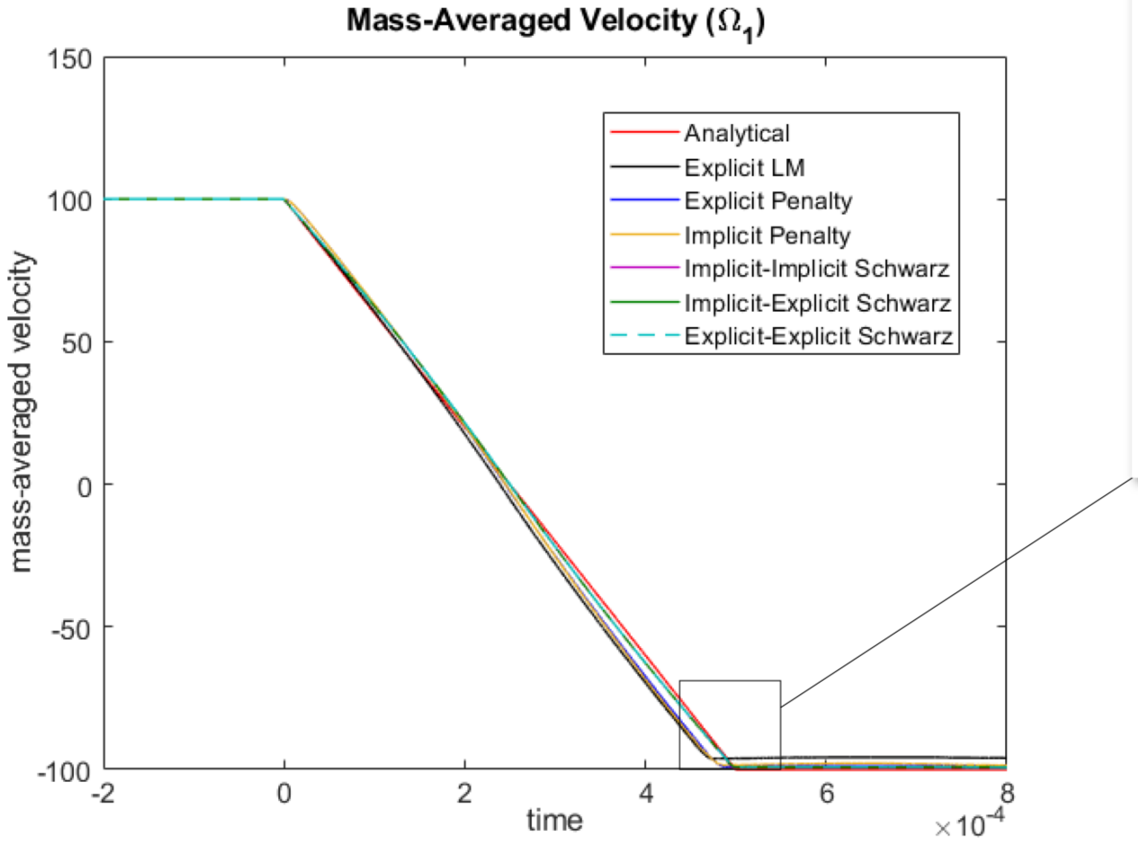


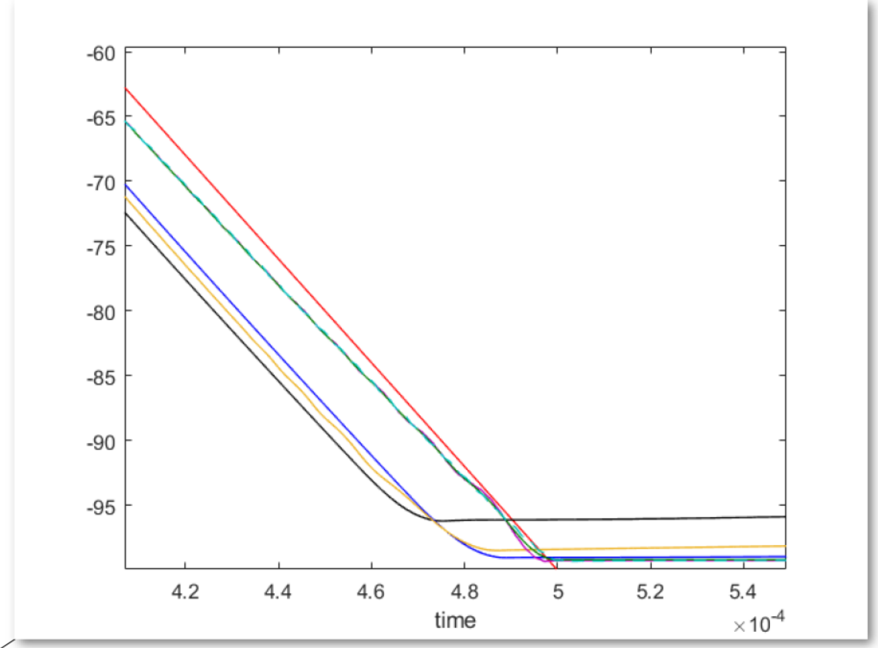
- Penalty methods **overpredict** contact point location between impact and release times
- Explicit LM method **under-predicts release time**
- Schwarz methods capture **release time** to an accuracy of $\approx 0.1\%$.

[1]Hoy *et al.*, 2021; Mota *et al.*, 2022 (under review).

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

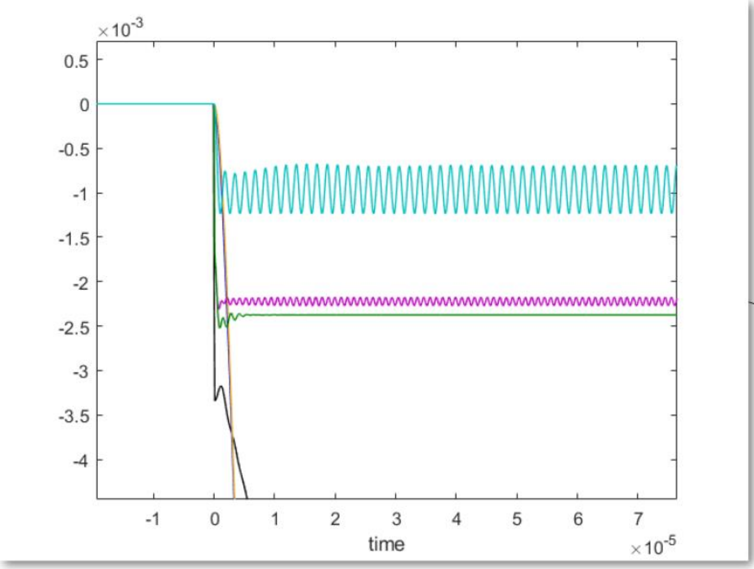
[1]Hoy *et al.*, 2021; Mota *et al.*, 2022 (under review).

Numerical Results: 1D Impact Problem[1]

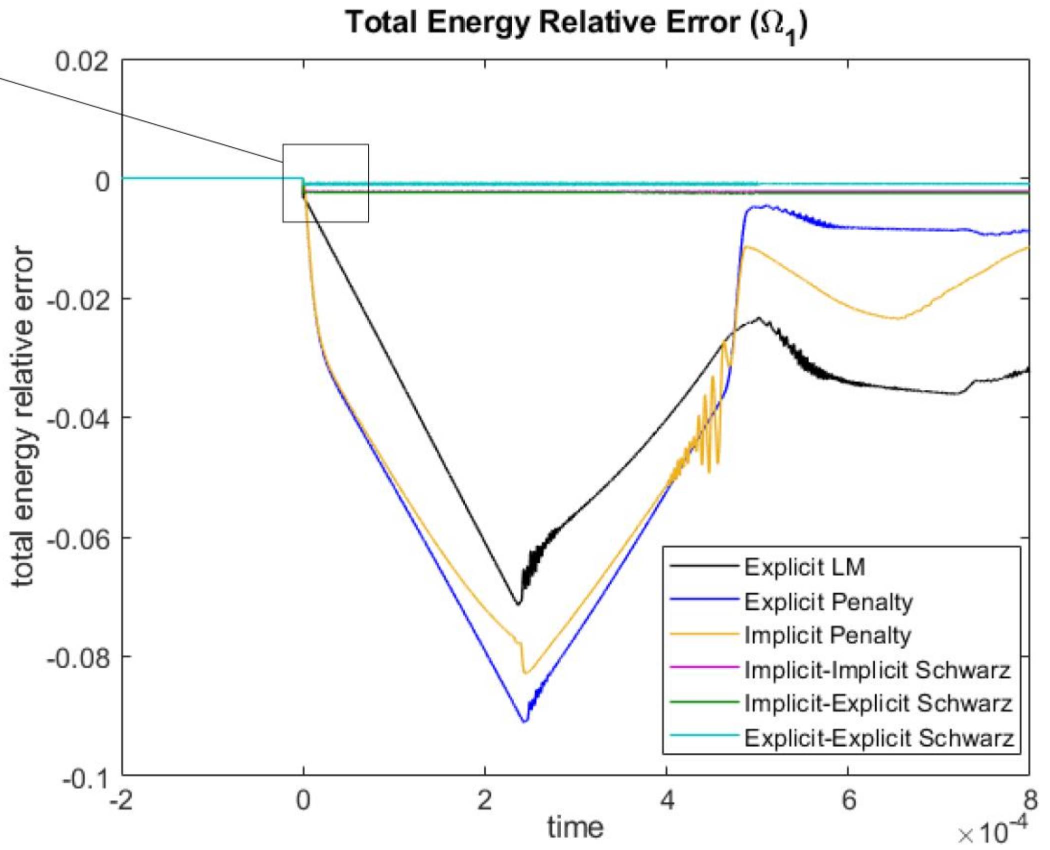
Total energy relative error: for the left bar (Ω_1) as a function of time

- 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



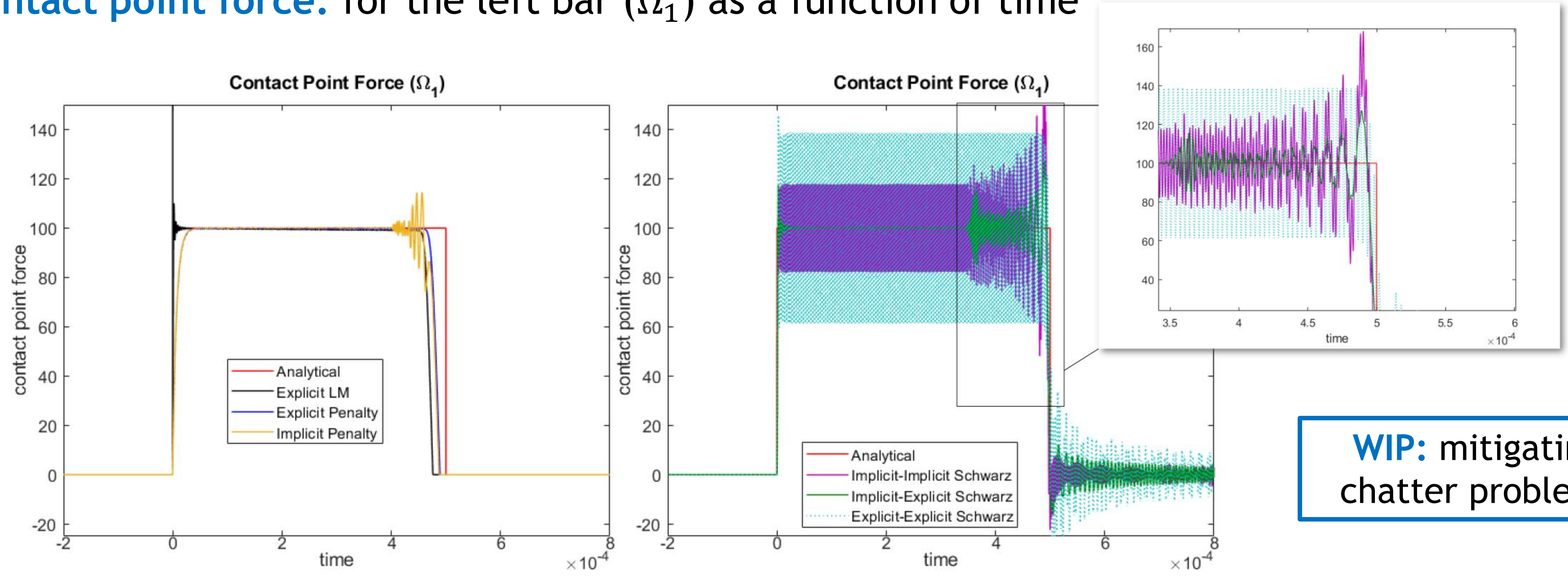
- Unlike conventional contact methods, **Schwarz** achieves an error of **at most 0.25%** in the total energy!
  - ➢ Explicit-Explicit Schwarz gives most accurate total energy, followed by Implicit-Implicit Schwarz and Implicit-Explicit Schwarz

[1]Hoy *et al.*, 2021; Mota *et al.*, 2022 (under review).

Numerical Results: 1D Impact Problem[1]

[1]Hoy *et al.*, 2021; Mota *et al.*, 2022 (under review).

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

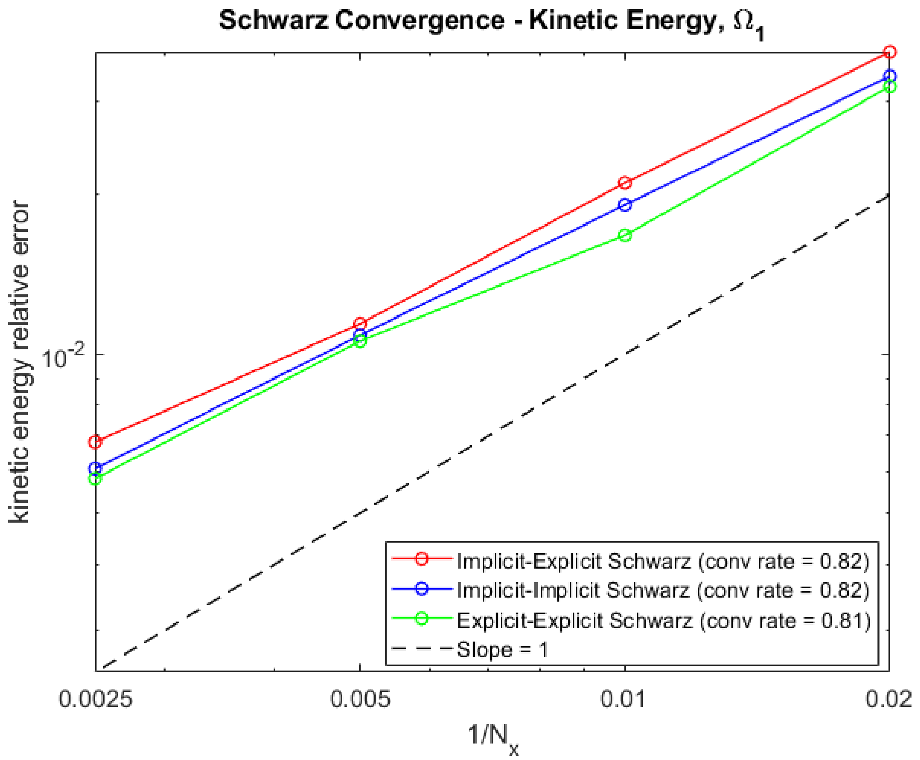


WIP: mitigating chatter problem.

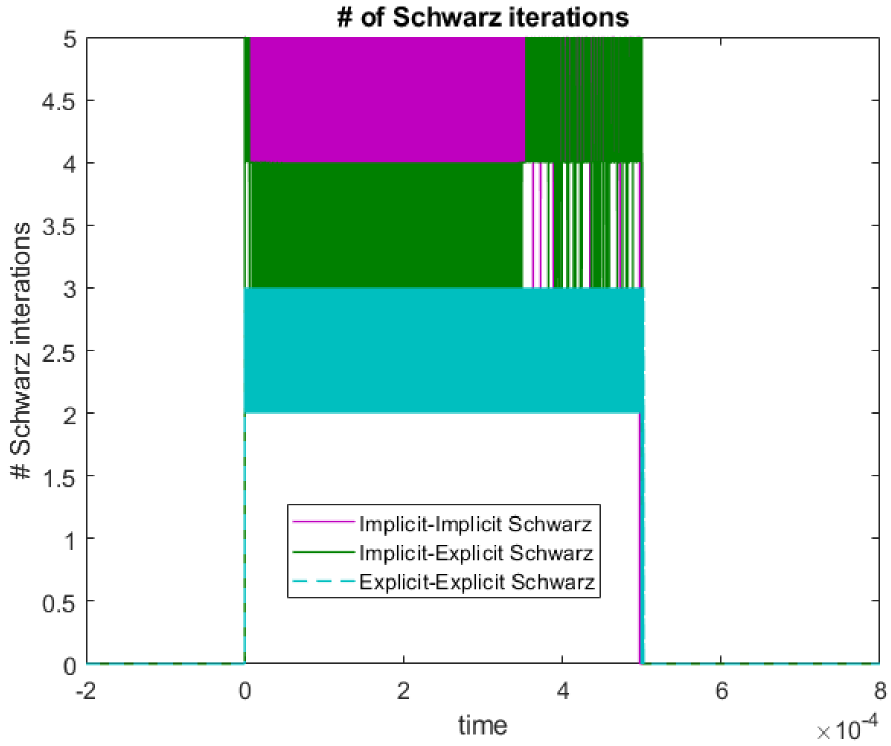
- Three conventional methods exhibit some **undesirable artifacts** in contact point force but deliver in general a **smooth solution**
- Schwarz solutions exhibit **oscillations** following instantiation of contact ⟶ **"chatter" problem**
  - ➢ Schwarz method with **largest total energy loss** (Implicit-Explicit) 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.*, 2021 (under review).

Summary & Future Work

Summary:

- 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.
- **Robin-Robin transmission condition** formulation of non-overlapping Schwarz → ***promising preliminary results!***
- Introduction of **additional** or **alternate contact conditions** into Schwarz formulation
- 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

References

- H. Schwarz, Uber einen Grenzubergang durch alternierendes verfahren, Vierteljahrsschriftder Naturforschenden Gesellschaft in Zurich, 15 (1870), pp. 272–286.
- P.L. Lions. “On the Schwarz alternating method I.” In: 1988, First International Symposium on Domain Decomposition methods for Partial Differential Equations, SIAM, Philadelphia.
- P. L. Lions, On the Schwarz alternating method III: A variant for nonoverlapping subdomains, in Third International Symposium on Domain Decomposition Methods for Partial Differential Equations, T. F. Chan, R. Glowinski, J. P´eriaux, and O. B. Widlund, eds., Society for Industrial and Applied Mathematics, 1990, pp. 202–223
- P. Zanolli, Domain decomposition algorithms for spectral methods, CALCOLO, 24 (1987), pp. 201–240.
- A. Mota, I. Tezaur, and C. Alleman, The Schwarz alternating method, Comput. Meth. Appl. Mech. Engng., 319 (2017), pp. 19–51.
- A. Mota, I. Tezaur, and G. Phlipot, The Schwarz alternating method for transient solid dynamics, Int. J. Numer. Meth. Engng. 1-35, 2022.
- N. J. Carpenter, R. L. Taylor, and M. G. Katona, Lagrange constraints for transient finite element surface contact, International journal for numerical methods in engineering, 32 (1991), pp. 103–128.
- J. Hoy, I. Tezaur, A. Mota. The Schwarz alternating method for multi-scale contact mechanics. CSRI Summer Proceedings, E. Galvan and D. Smith, eds., Technical Report SAND2021-9886C, Sandia National Laboratories, 2021.
- A. Mota, I. Tezaur, J. Hoy. The Schwarz alternating method for multi-scale contact mechanics. Mathematical & Computational Applications (MCA) (under review).
- J. M. Solberg and P. Papadopoulos, A finite element method for contact/impact, Finite Elements in Analysis and Design, 30 (1998), pp. 297–311.
- I. Tezaur, T. Voth, J. Niederhaus, J. Robbins, and J. Sanchez, An extended finite element method (XFEM) formulation for multi-material Eulerian solid mechanics in the Alegra code (in preparation).

Start of Backup Slides

Motivation

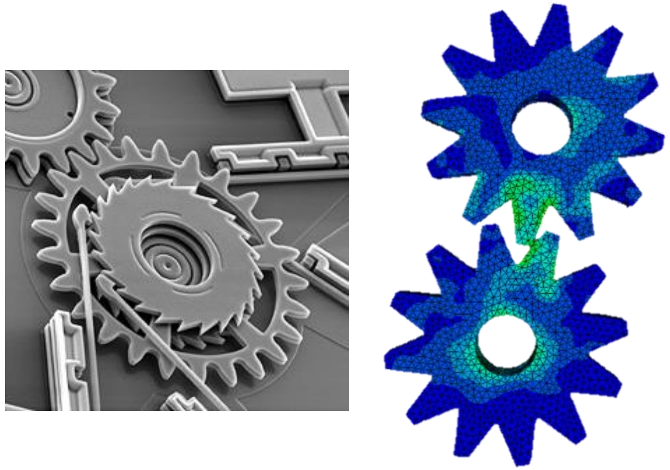
- **Large scale** structural **failure** frequently originates from **small scale** phenomena (e.g, defects, microcracks, inhomogeneities), which grow quickly in unstable manner
  - ➢ **Concurrent multiscale methods** are essential to capture correctly the multiscale behavior!
  - ➢ Stable, accurate 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:

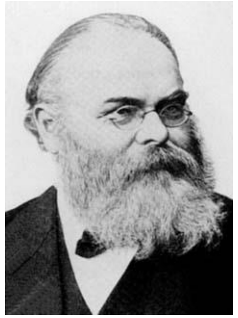
1. **Proximity search:** computer science problem, has received much attention due to importance in video game development ☺
2. **Contact enforcement step:** existing methods (penalty, Lagrange multiplier, augmented Lagrangian) suffer from poor performance ☹
   - ➢ Long simulation times ☹
   - ➢ Lack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

This talk.



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

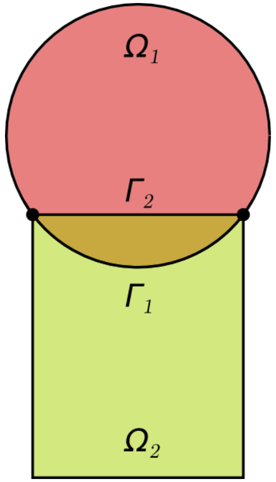
Schwarz Alternating Method for Domain Decomposition



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 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.

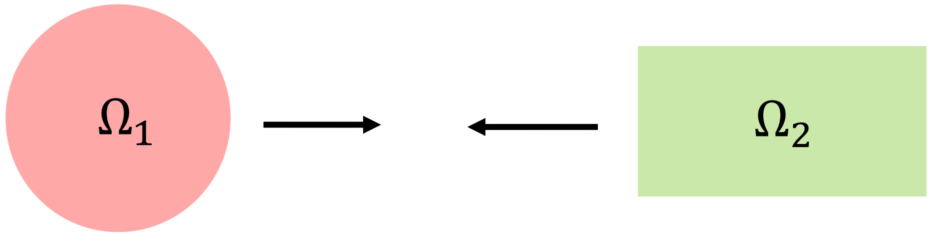
- Schwarz alternating method most commonly used as a ***preconditioner*** for Krylov iterative methods to solve linear algebraic equations.

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

Non-Overlapping Schwarz Contact Formulation

Non-Overlapping Schwarz Contact Formulation

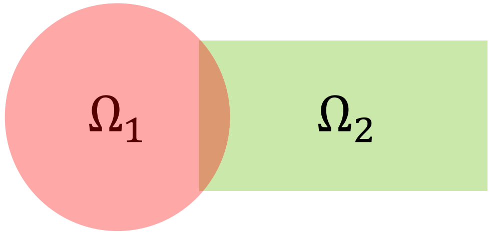
Before contact: simulation proceeds as usual



Key idea: a contact problem can be viewed as **coupled problem** while 2+ bodies are in contact

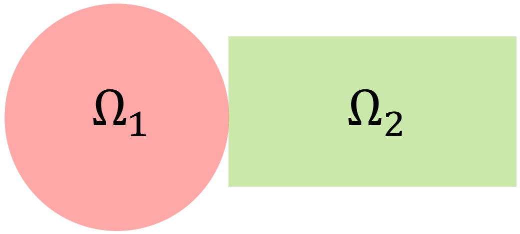
Detection of contact: proximity search and application of contact conditions to determine contact

- ***Overlap condition:*** triggered when two or more objects/domains have begun to overlap/penetrate each other
- ***Compression condition:*** positive normal traction
- ***Persistence condition:*** contact occurred in the previous step



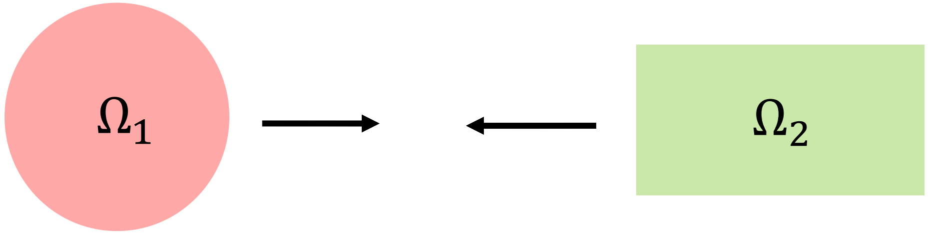
Enforcement of contact: alternating Schwarz iteration with Dirichlet-Neumann transmission BCs

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



Non-Overlapping Schwarz Contact Formulation

Before contact: simulation proceeds as usual

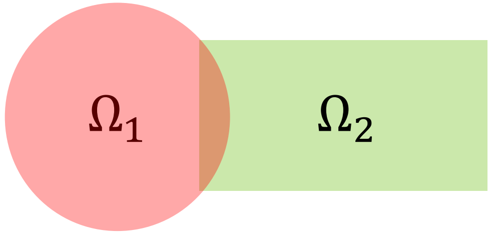


There are no contact constraints!

Contact constraints replaced with **BCs** applied **iteratively** at contact boundaries.

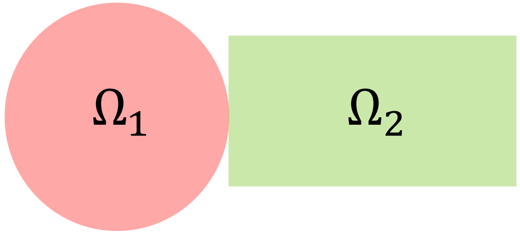
Detection of contact: proximity search and application of contact conditions to determine contact

- ***Overlap condition:*** triggered when two or more objects/domains have begun to overlap/penetrate each other
- ***Compression condition:*** positive normal traction
- ***Persistence condition:*** contact occurred in the previous step

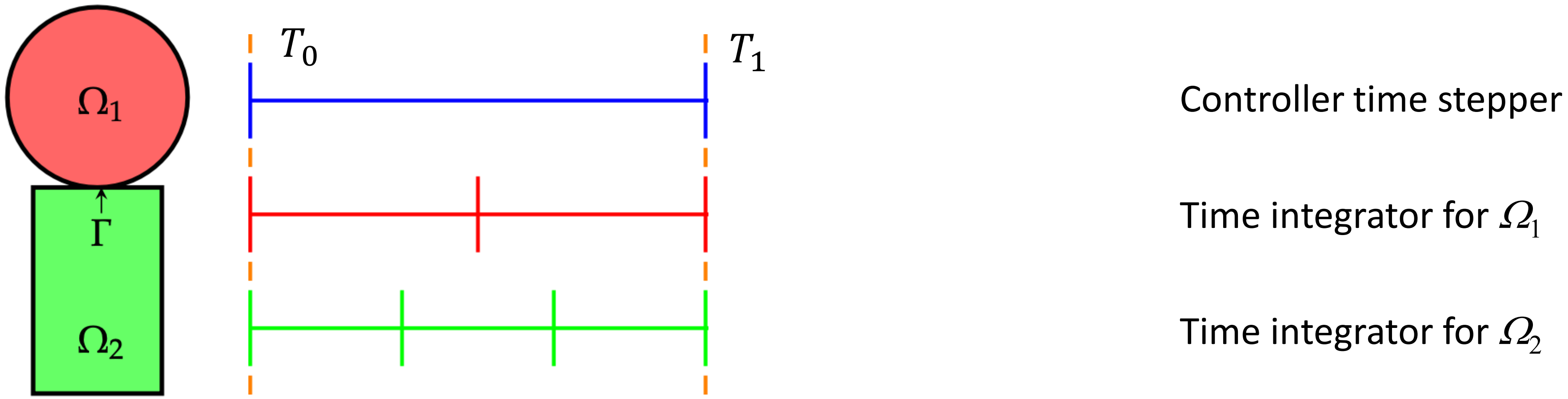


Enforcement of contact: alternating Schwarz iteration with Dirichlet-Neumann transmission BCs

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



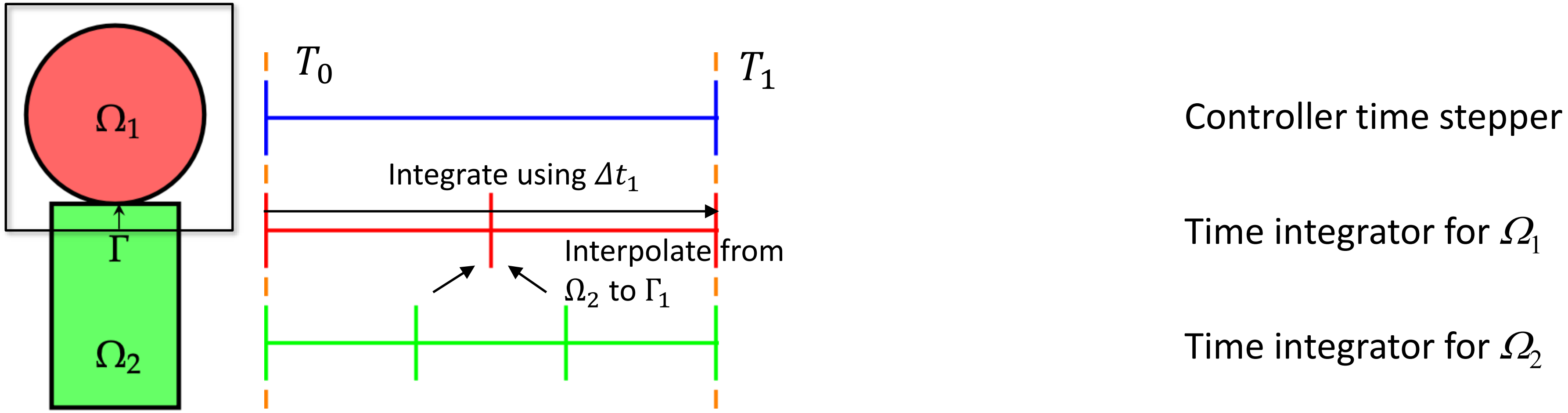
Enforcement of Contact via Alternating Schwarz



Key idea: a contact problem can be viewed as **coupled problem** while 2+ bodies are in contact

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

Enforcement of Contact via Alternating Schwarz

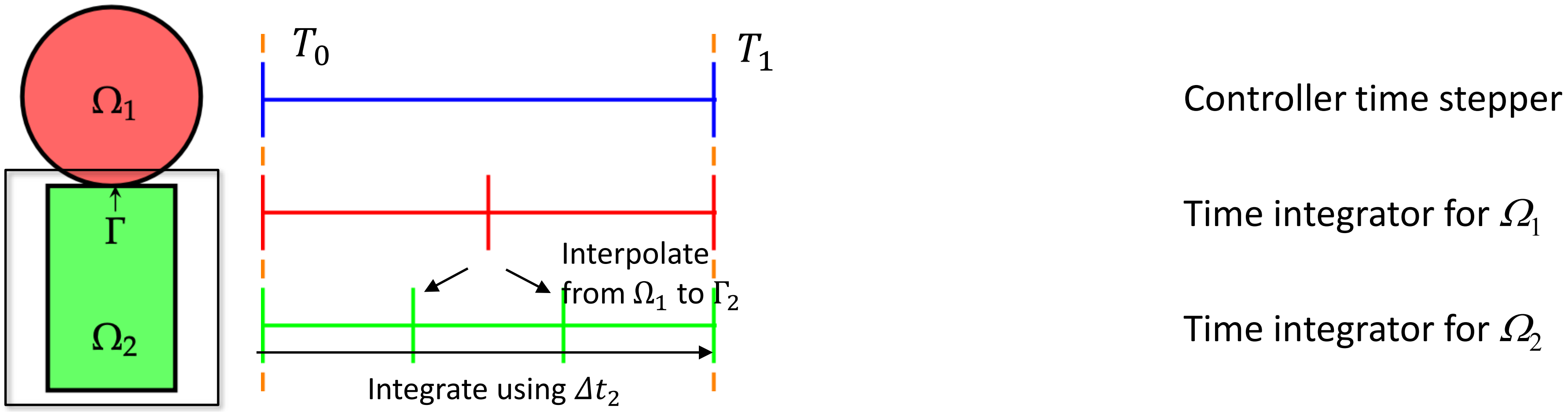


Key idea: a contact problem can be viewed as **coupled problem** while 2+ bodies are in contact

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

Step 1: Advance Ω_1 solution from time T_i to time T_{i+1} using time-stepper in Ω_1 with time-step Δt_1, using solution in Ω_2 interpolated to Γ at times $T_i + n\Delta t_1$ to apply Dirichlet BC.

Enforcement of Contact via Alternating Schwarz



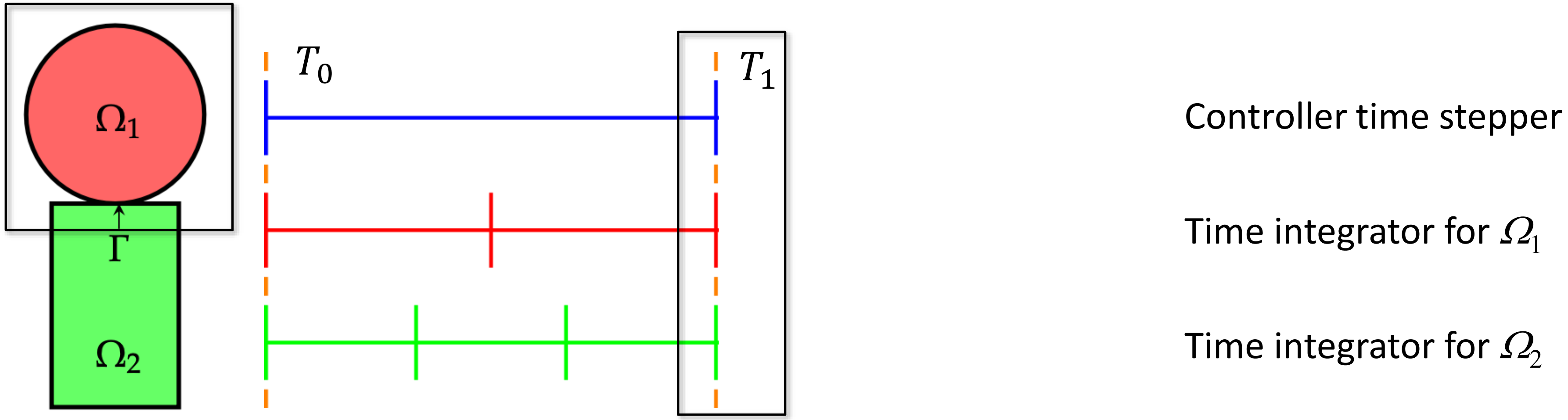
Key idea: a contact problem can be viewed as **coupled problem** while 2+ bodies are in contact

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

Step 1: Advance Ω_1 solution from time T_i to time T_{i+1} using time-stepper in Ω_1 with time-step Δt_1, using solution in Ω_2 interpolated to Γ at times $T_i + n\Delta t_1$ to apply Dirichlet BC.

Step 2: Advance Ω_2 solution from time T_i to time T_{i+1} using time-stepper in Ω_2 with time-step Δt_2, using solution in Ω_1 interpolated to Γ at times $T_i + n\Delta t_2$ to apply Neumann (traction) BC.

Enforcement of Contact via Alternating Schwarz



Key idea: a contact problem can be viewed as **coupled problem** while 2+ bodies are in contact

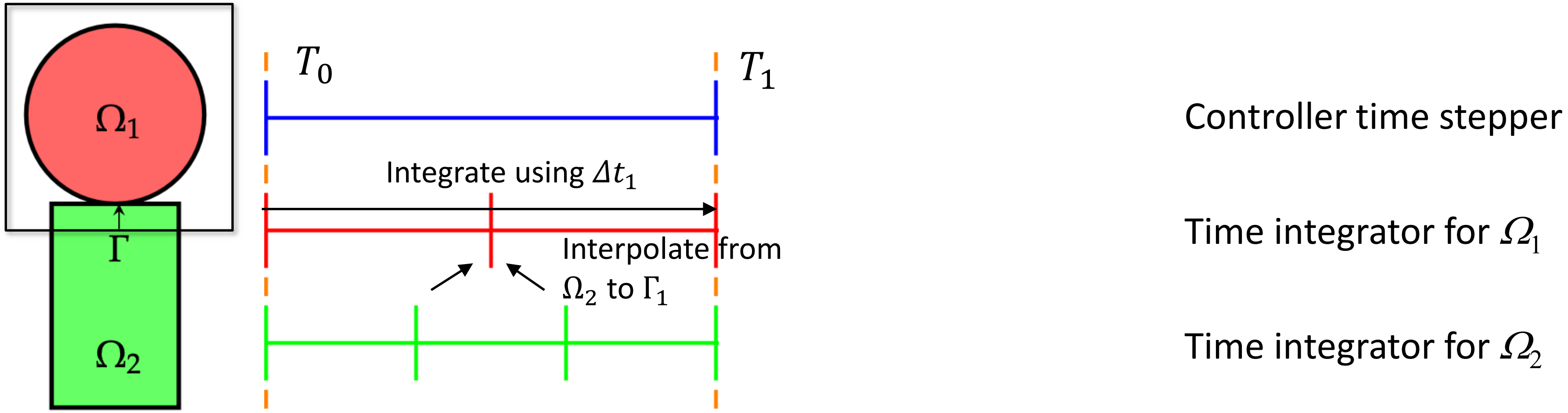
Step 0: Initialize $i = 0$ (controller time index).

Step 1: Advance Ω_1 solution from time T_i to time T_{i+1} using time-stepper in Ω_1 with time-step Δt_1, using solution in Ω_2 interpolated to Γ at times $T_i + n\Delta t_1$ to apply Dirichlet BC.

Step 2: Advance Ω_2 solution from time T_i to time T_{i+1} using time-stepper in Ω_2 with time-step Δt_2, using solution in Ω_1 interpolated to Γ at times $T_i + n\Delta t_2$ to apply Neumann (traction) BC.

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

Enforcement of Contact via Alternating Schwarz



Key idea: a contact problem can be viewed as **coupled problem** while 2+ bodies are in contact

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

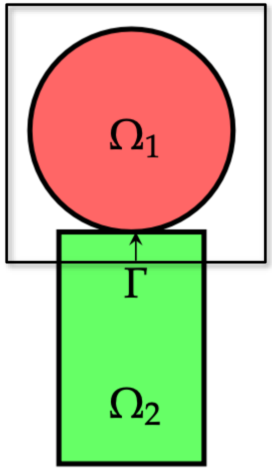
Step 1: Advance Ω_1 solution from time T_i to time T_{i+1} using time-stepper in Ω_1 with time-step Δt_1, using solution in Ω_2 interpolated to Γ at times $T_i + n\Delta t_1$ to apply Dirichlet BC.

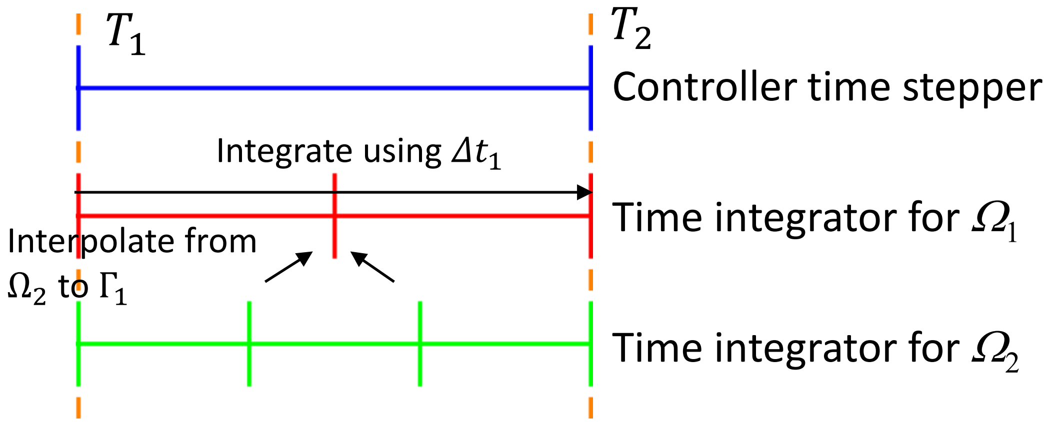
Step 2: Advance Ω_2 solution from time T_i to time T_{i+1} using time-stepper in Ω_2 with time-step Δt_2, using solution in Ω_1 interpolated to Γ at times $T_i + n\Delta t_2$ to apply Neumann (traction) BC.

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

- If unconverged, return to Step 1.

Enforcement of Contact via Alternating Schwarz





Key idea: a contact problem can be viewed as **coupled problem** while 2+ bodies are in contact

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

Step 1: Advance Ω_1 solution from time T_i to time T_{i+1} using time-stepper in Ω_1 with time-step Δt_1, using solution in Ω_2 interpolated to Γ at times $T_i + n\Delta t_1$ to apply Dirichlet BC.

Step 2: Advance Ω_2 solution from time T_i to time T_{i+1} using time-stepper in Ω_2 with time-step Δt_2, using solution in Ω_1 interpolated to Γ at times $T_i + n\Delta t_2$ to apply Neumann (traction) BC.

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.

Schwarz Algorithm for Contact

$k \leftarrow 0$
repeat ▷ controller time stepper
  Check contact criteria ▷ defined in Section 3.1
  if contact detected **then**
    $\varphi(\Omega, t_k) \leftarrow$ solution of Algorithm 2 in $\Omega \times I_k$ ▷ contact enforcement
  else
    $\varphi(\Omega, t_k) \leftarrow$ solution of (9) in $\Omega \times I_k$ ▷ no contact
  end if
  $k \leftarrow k + 1$
until $k = N$ ▷ N is the total number of steps

Algorithm 1: Full simulation workflow with Schwarz-based contact enforcement for the specific case of two subdomains.

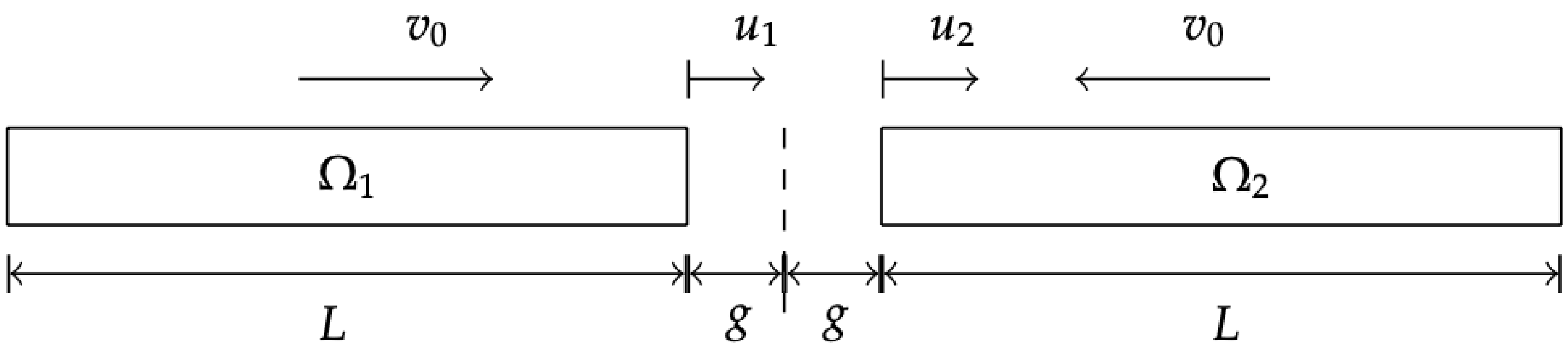
Contact criteria:

- **Overlap**: interpenetration of subdomains
- **Compression**: Positive normal traction
- **Persistence**: Was in contact previous step

$n \leftarrow 1$
repeat ▷ Schwarz loop
  for i from 1 to 2 **do** ▷ subdomain loop
    $\varphi^{(n)}(\Omega_i, t_k) \leftarrow \boldsymbol{x}_k^{(i)}$ ▷ position IC
    $\dot{\varphi}^{(n)}(\Omega_i, t_k) \leftarrow \boldsymbol{v}_k^{(i)}$ ▷ velocity IC
    if $i = 1$ **then** ▷ first subdomain
      $\varphi^{(n)}(\partial_{\varphi}\Omega_1, I_k) \leftarrow \boldsymbol{\chi}$ ▷ regular Dirichlet BC
      $\varphi^{(n)}(\Gamma, I_k) \leftarrow P_{\Omega_2 \to \Gamma}[\varphi^{(n-1)}(\Omega_1, I_k)]$ ▷ Schwarz Dirichlet BC
      $\boldsymbol{PN} \leftarrow \boldsymbol{T}$ on $[\partial_{\boldsymbol{T}}\Omega_1 \cup \Gamma] \times I_k$ ▷ regular traction BC
      $\varphi(\Omega_1, I_k) \leftarrow$ solution of (14) ▷ solve dynamic problem in $\Omega_1 \times I_k$
    else ▷ second subdomain
      $\varphi^{(n)}([\partial_{\varphi}\Omega_2 \cup \Gamma], I_k) \leftarrow \boldsymbol{\chi}$ ▷ regular Dirichlet BC
      $\boldsymbol{PN} \leftarrow \boldsymbol{T}$ on $\partial_{\boldsymbol{T}}\Omega_2 \times I_k$ ▷ regular traction BC
      $\boldsymbol{PN} \leftarrow P_{\Omega_1 \to \Gamma}[\boldsymbol{T}^{(n)}(\Omega_2, t_k)]$ ▷ Schwarz traction BC
      $\varphi(\Omega_2, I_k) \leftarrow$ solution of (15) ▷ solve dynamic problem in $\Omega_2 \times I_k$
    end if
  end for
  $n \leftarrow n + 1$
until converged

Algorithm 2: The Schwarz alternating method for contact enforcement during a controller time interval I_k for the specific case of two subdomains.

A Canonical 1D Problem – 2 Colliding Elastic Bars



Position and velocity of left contact point:

$$x(t) = \begin{cases} -g + v_0(t - t_0), & t < t_{\text{imp}}, \\ 0, & t_{\text{imp}} \le t \le t_{\text{rel}}, \\ -v_0(t - t_{\text{rel}}), & t > t_{\text{rel}}, \end{cases} \quad v(t) = \begin{cases} v_0, & t < t_{\text{imp}}, \\ 0, & t_{\text{imp}} \le t \le t_{\text{rel}}, \\ -v_0, & t > t_{\text{rel}}, \end{cases}$$

Impact & release times:

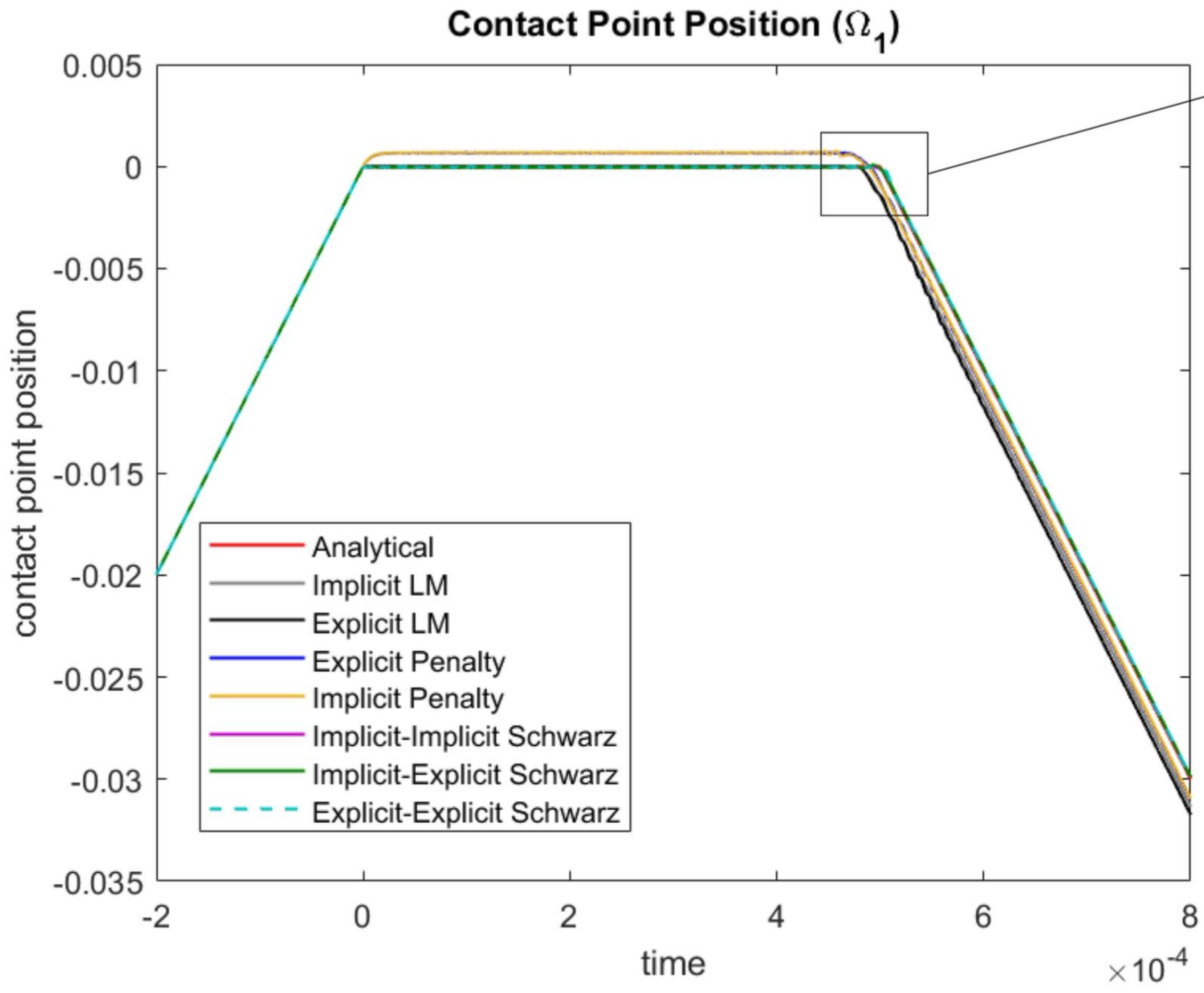
$$t_{\text{imp}} = t_0 + \frac{g}{v_0}, \quad t_{\text{rel}} = t_{\text{imp}} + 2L\sqrt{\frac{\rho}{E}},$$

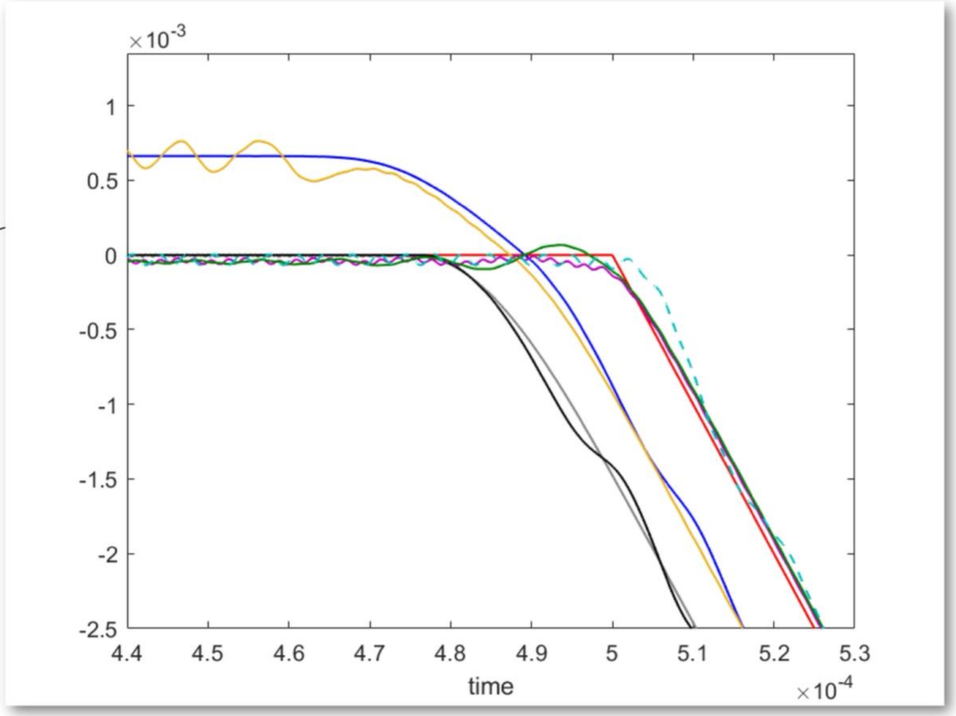
Contact force: $f_{\text{contact}} = v_0\sqrt{E\rho}A,$

Comparison of Results

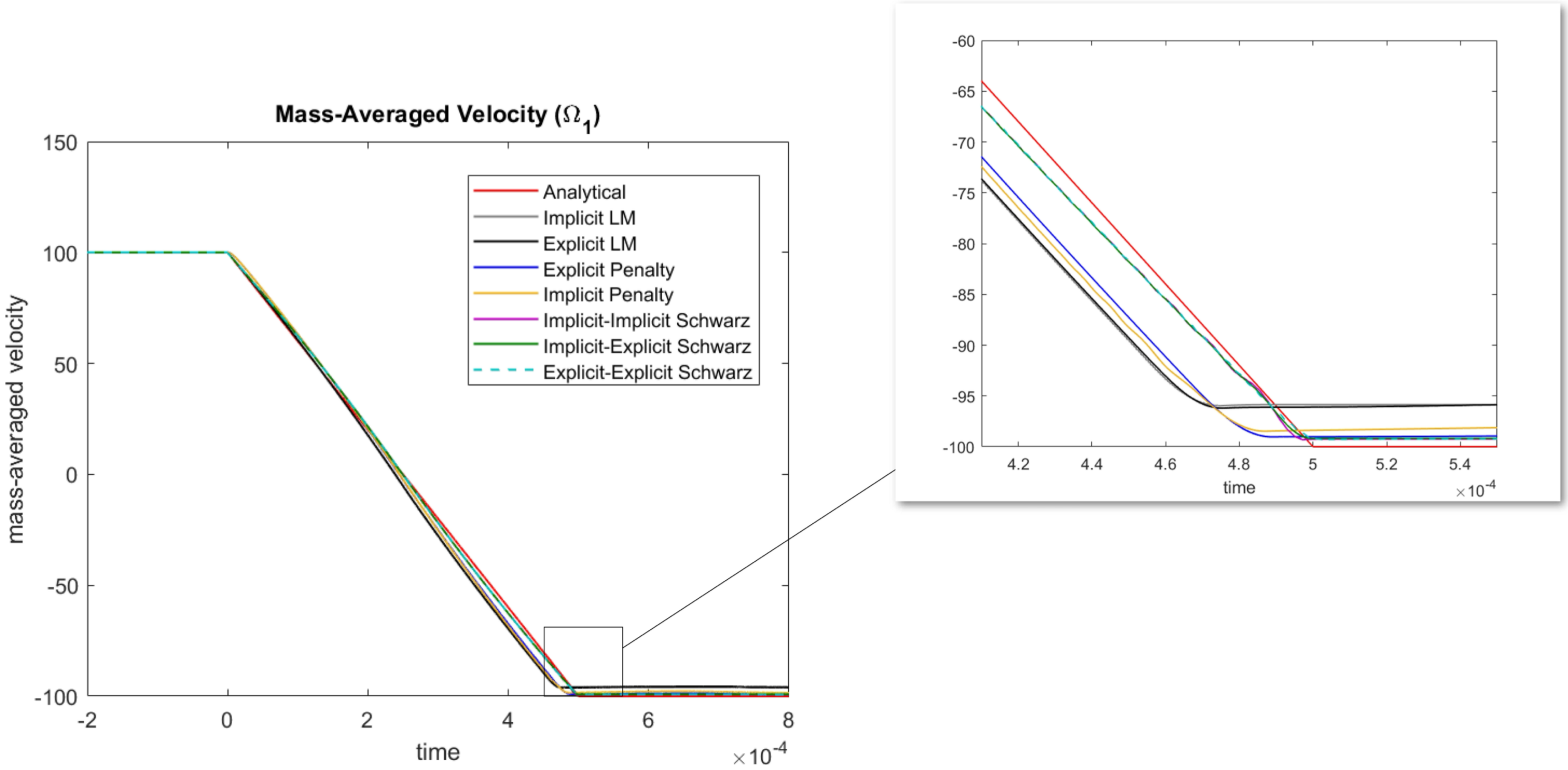
- Analytic solution
- Lagrange multiplier method with implicit time integration
- Lagrange multiplier method with explicit time integration
- Penalty method with implicit time integration
- Penalty method with explicit time integration
- Schwarz method with implicit-implicit integration
- Schwarz method with implicit-explicit time integration
- Schwarz method with explicit-explicit time integration

Contact Point Position

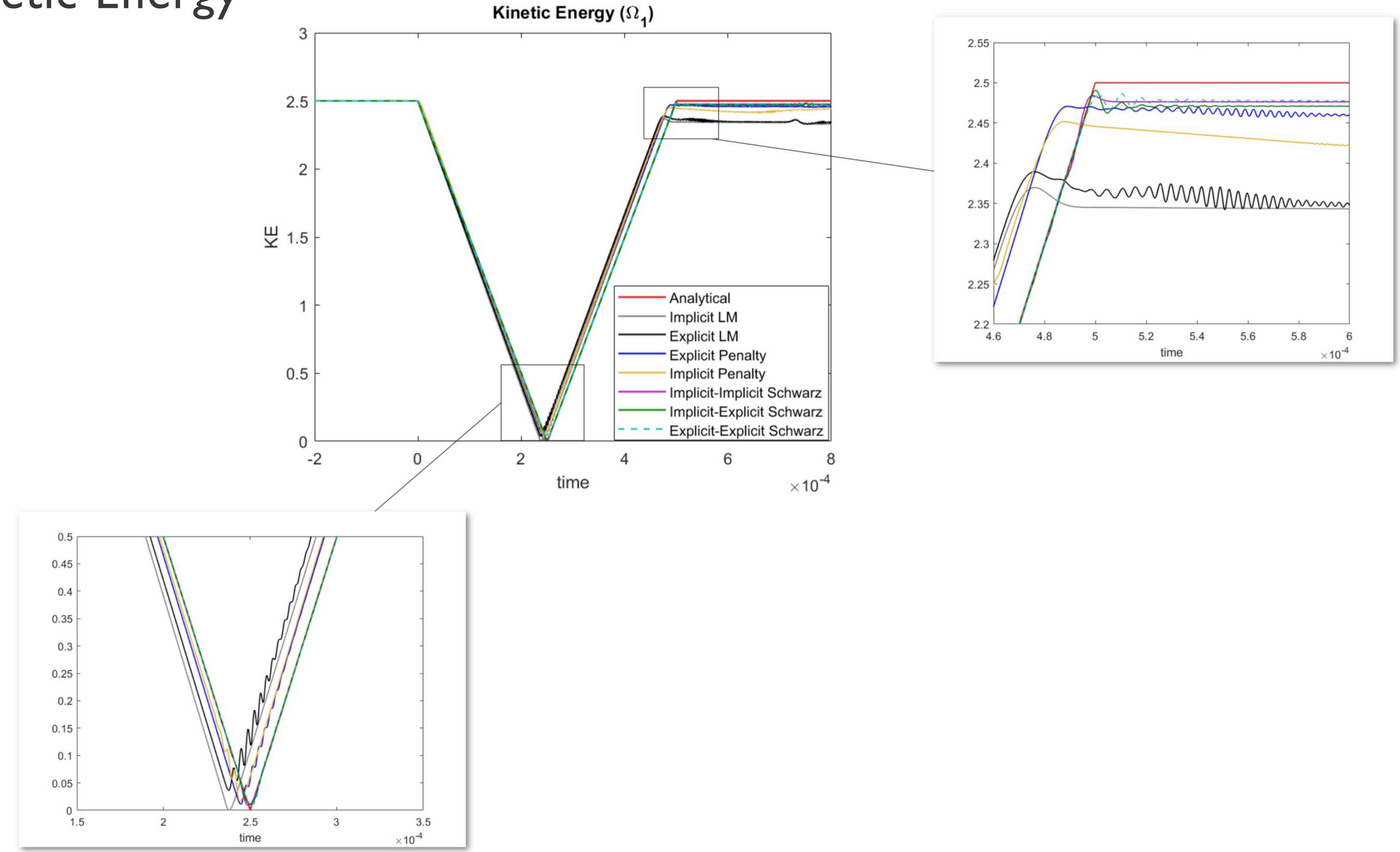




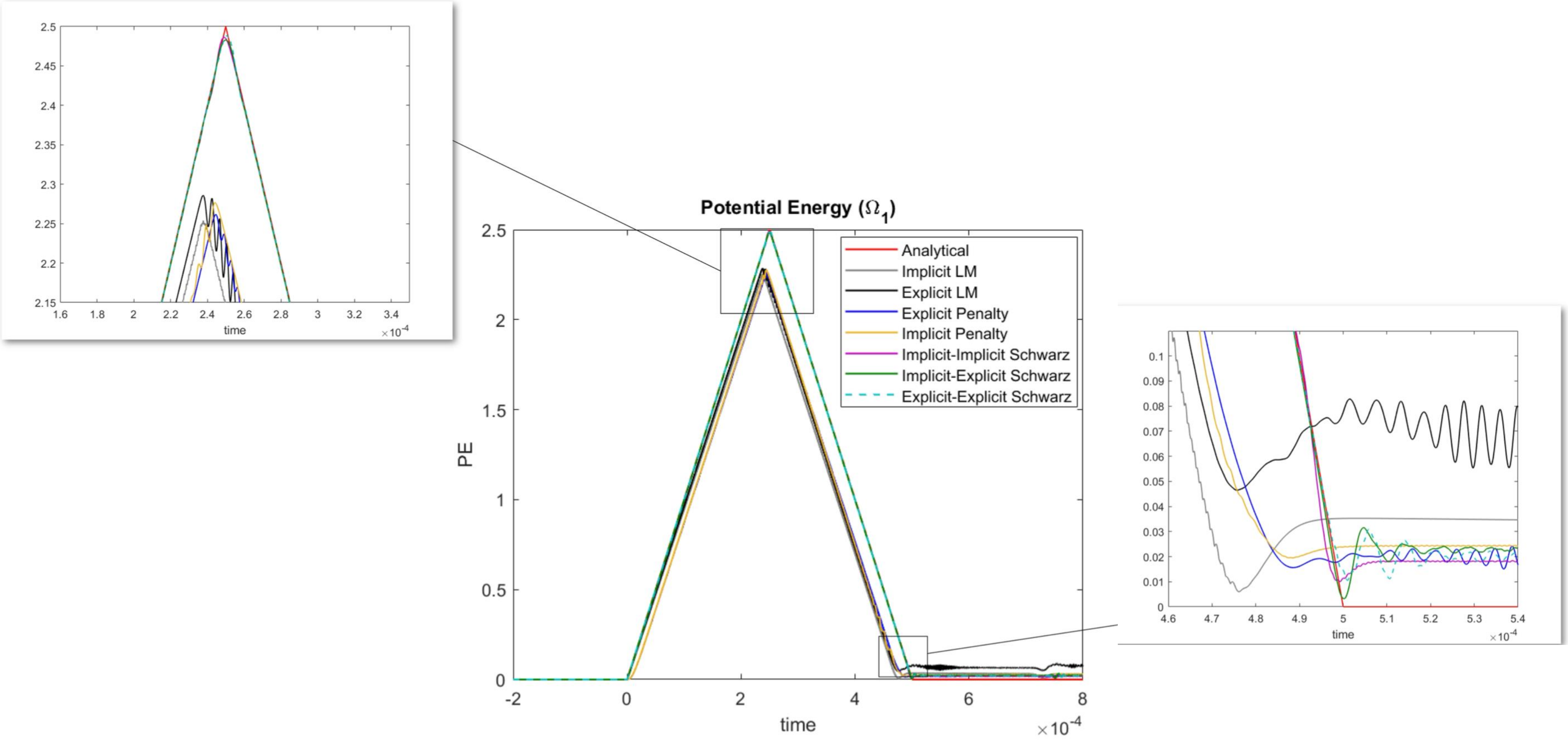
Mass-Averaged Velocity



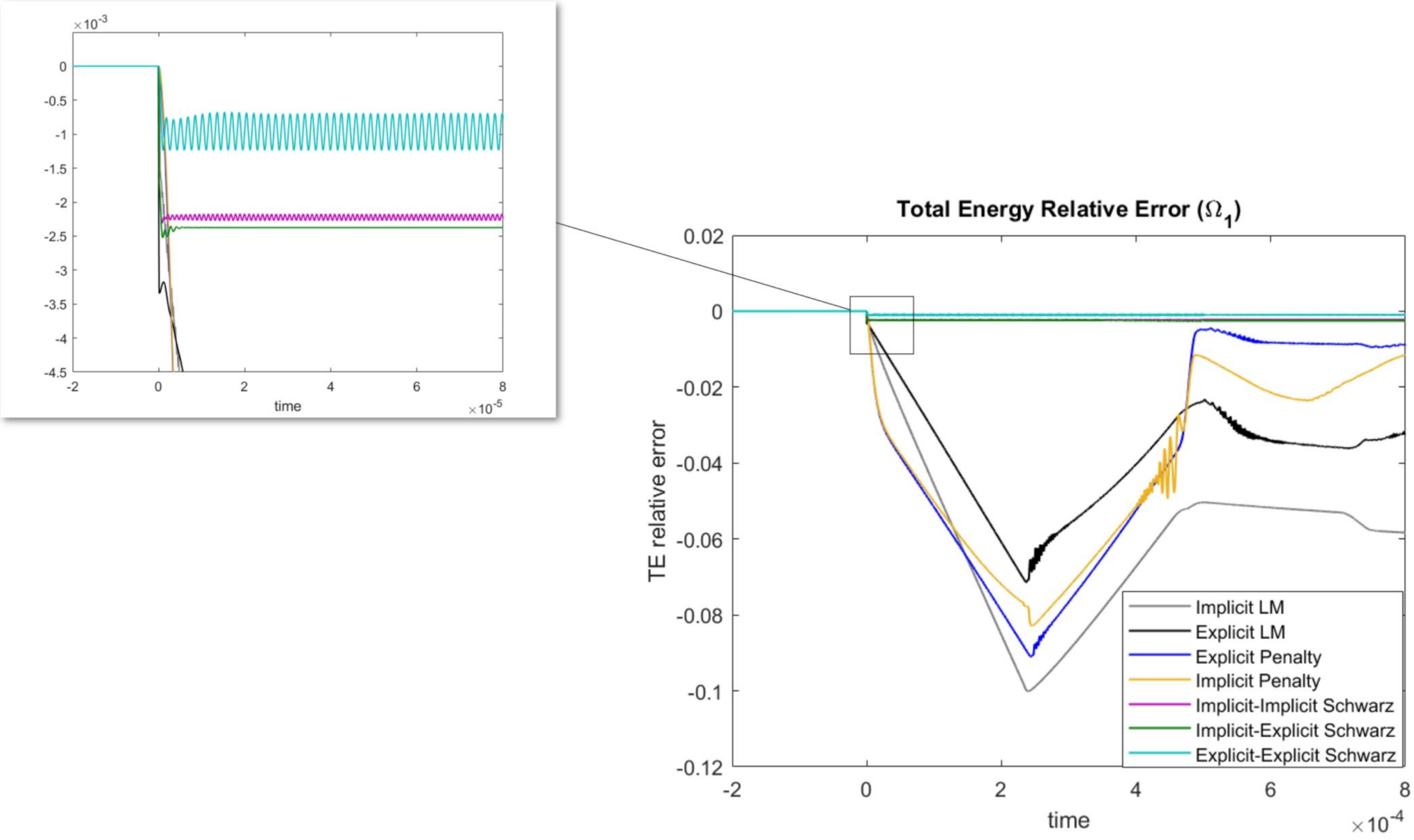
Kinetic Energy



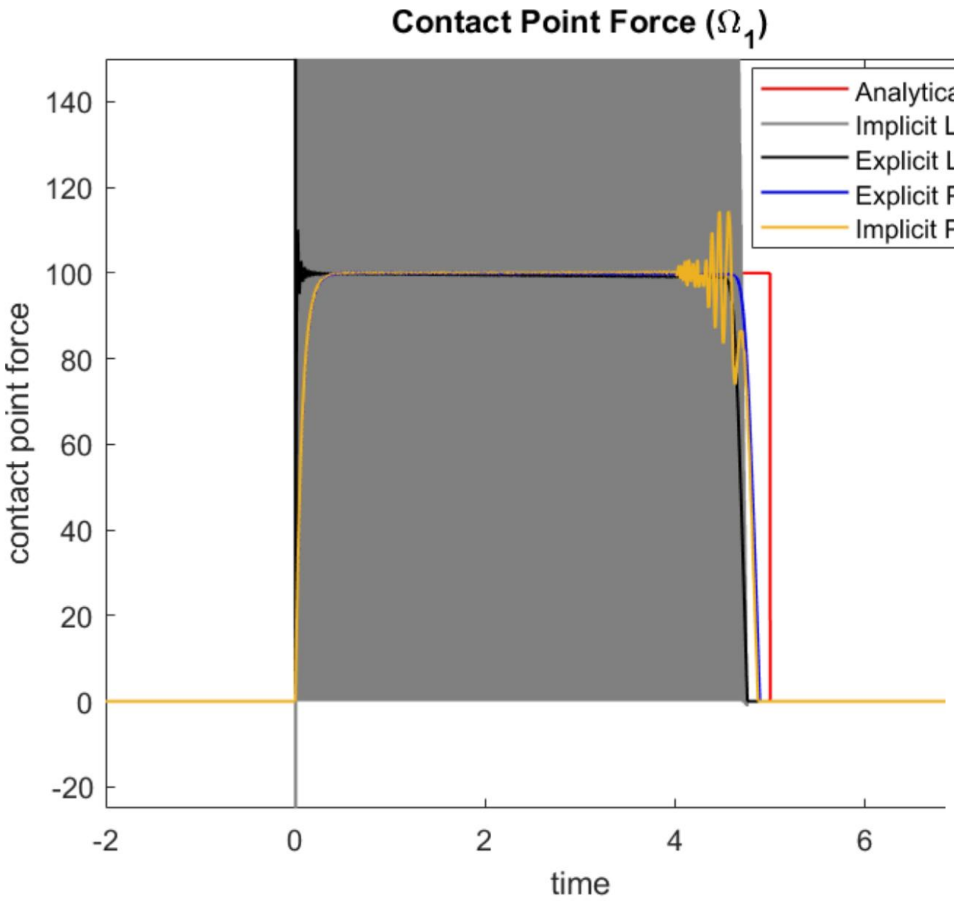
Potential Energy

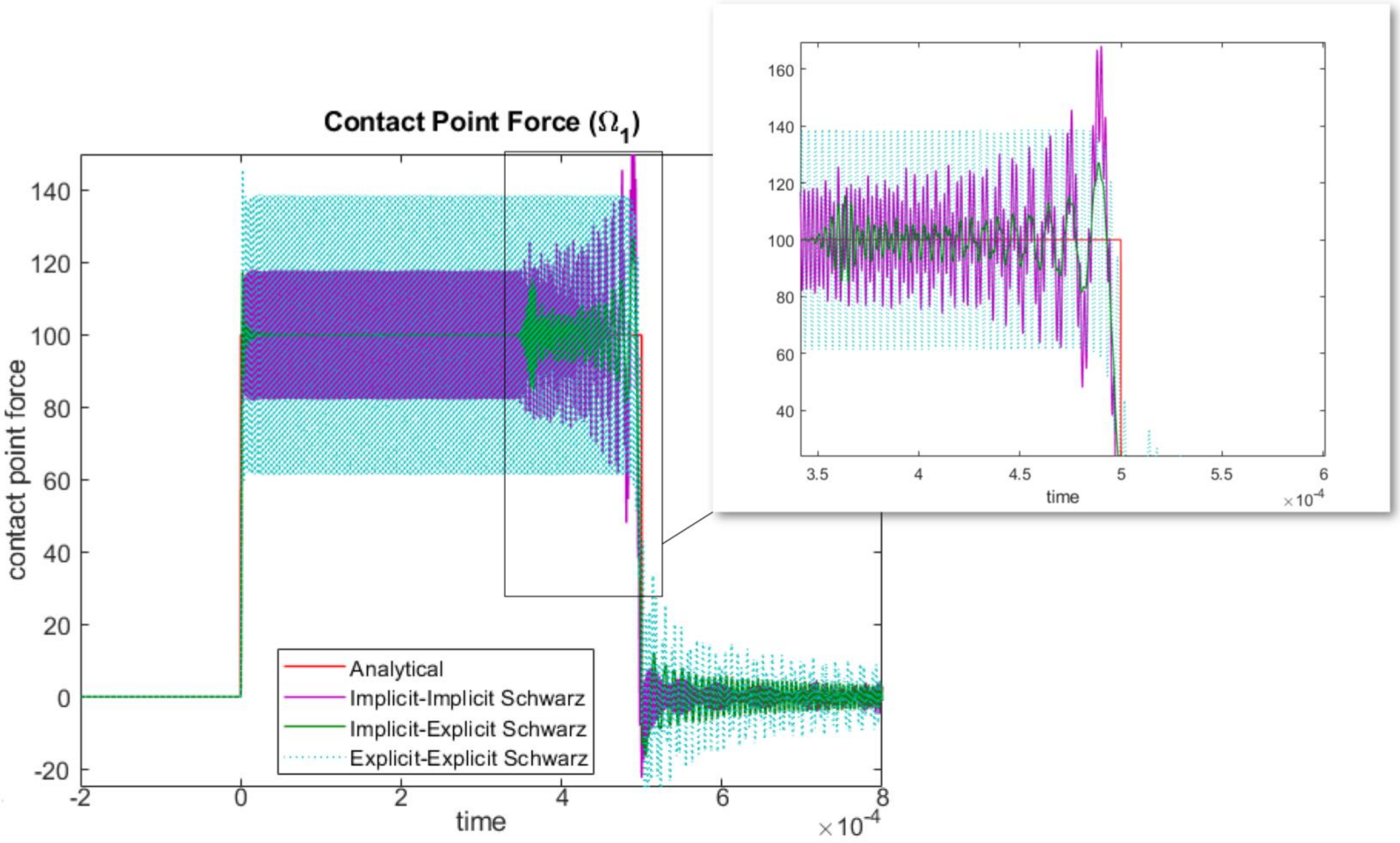


Total Energy



Contact Force





Contact Velocity