



Exceptional service in the national interest

The Dirichlet-Neumann Schwarz alternating method for contact problems in elastodynamics

Techniques for reducing artificial oscillations

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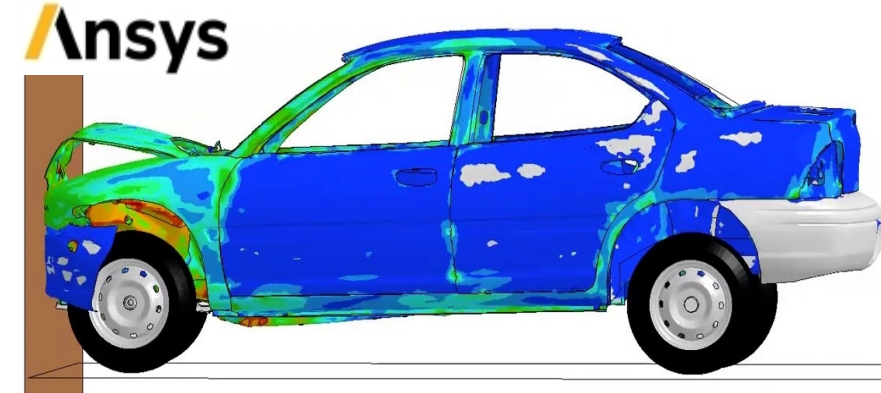
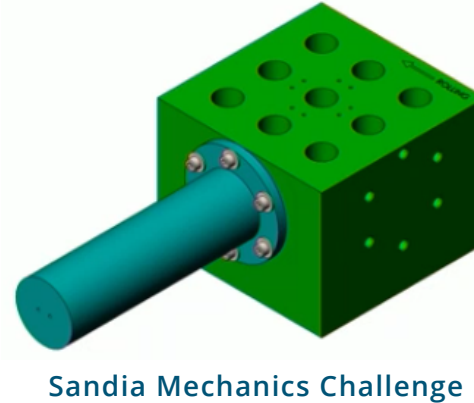
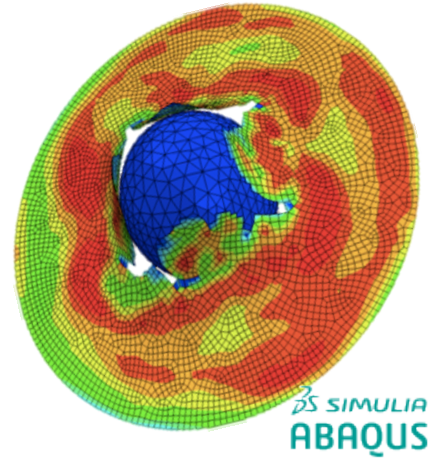
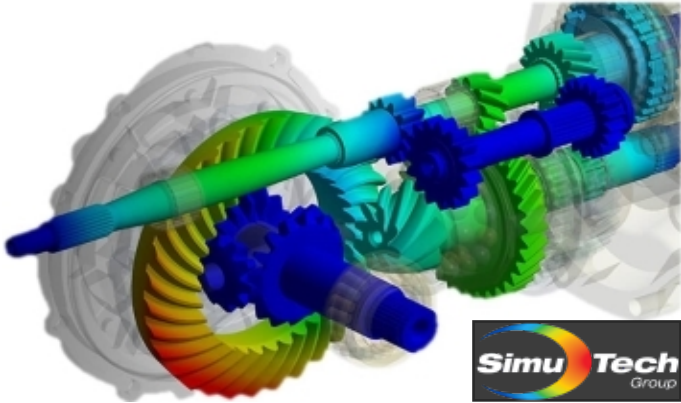
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Albuquerque, New Mexico, July 23-27, 2023

Context and motivations



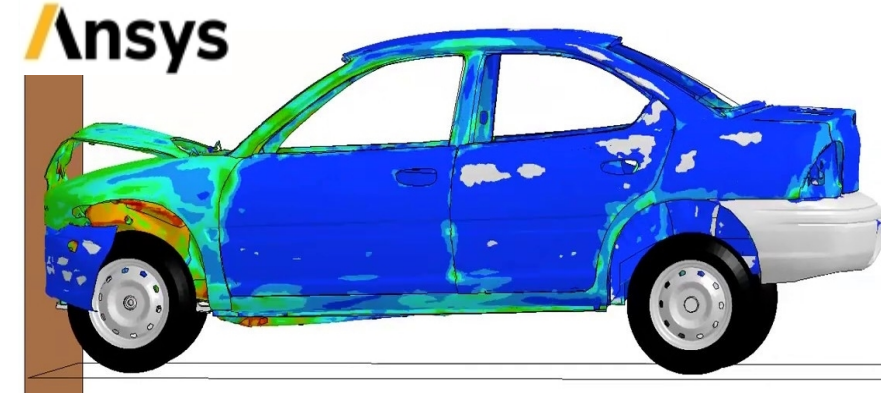
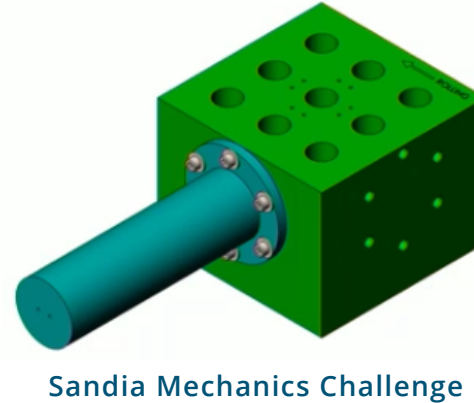
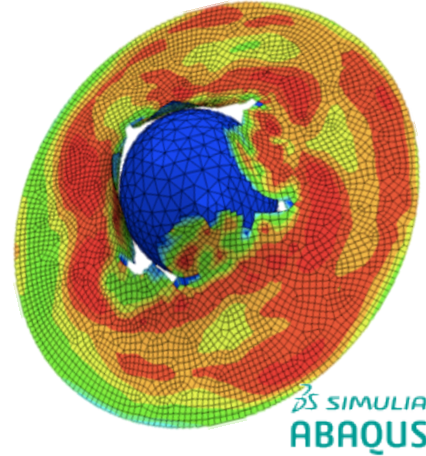
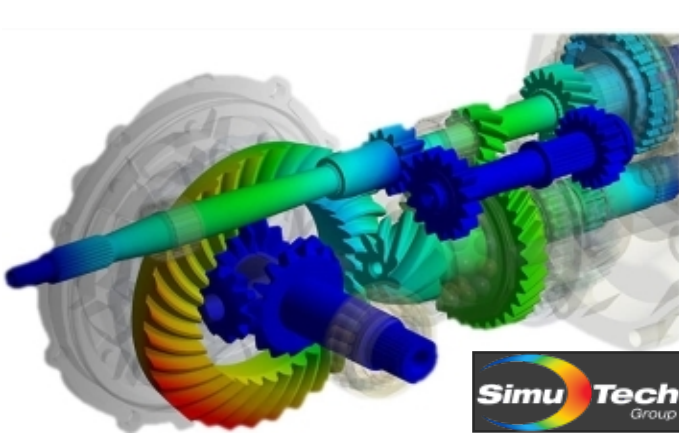
Numerical simulation of challenging mechanical contact problems

Localized contact, impact, touching surfaces, sliding, bolted/fastener joint, ...
→ presence of nonlinearities and lack of smoothness



Numerical simulation of challenging mechanical contact problems

Localized contact, impact, touching surfaces, sliding, bolted/fastener joint, ...
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→ Need a robust, stable and accurate method for mechanical contact

- accurate prediction of quantities of interest (velocities, contact forces, energies, ...)
- multiscale & multiphysics context (different time integrators, solvers, meshes, material models for different bodies)
- numerical efficiency and robustness
- non-intrusive implementation in existent legacy solvers (e.g. Sierra/Solid Mechanics (Sierra/SM), Albany, ...)

Numerical simulation of challenging multiscale contact problems

Conventional contact methods

- introduce **contact constraints** into the variational form
- solve all bodies involved in contact as a "coupled" system

Penalty method – amount of interpenetration $\sim$ contact pressure

[G. L. Goudreau et al. (1982) | T. Belytschko et al. (1991)]

Lagrange Multipliers method – additional Lagrange constraints

[T. J. R. Hushes. (1976) | K. J. Bathe et al. (1956)]

Perturbed and Augmented Lagrangian methods – constrained optimization theory, hybrid penalty/LM approach

[J. C. Simo et al. (1985, 1992) | R. Glowinski et al. (1989)]

Nitsche method – optimization problem with contact constraints

[F. Chouly et al. (2016) | P. Wriggers et al. (2008)]

- + well-established (proven convergence, ...)
- accuracy and stability often affected by problem-dependent parameters
- all bodies are coupled and solved simultaneously
- intrusive implementation

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Schwarz alternating method

- treats each body separately (as non-overlapping subdomains)
- prevents interpenetration through an **alternating Dirichlet-Neumann iterative process**

Domain Decomposition context – solving PDEs on irregular domains by splitting them into domains of regular shape, overlapping and non-overlapping approaches [H. Schwarz (1870) | P. I. Lions (1990)]

Multiscale coupling – overlapping approach [A. Mota et al. (2017, 2021)]

Contact/impact dynamics – non-overlapping approach [A. Mota et al. (2023)*]

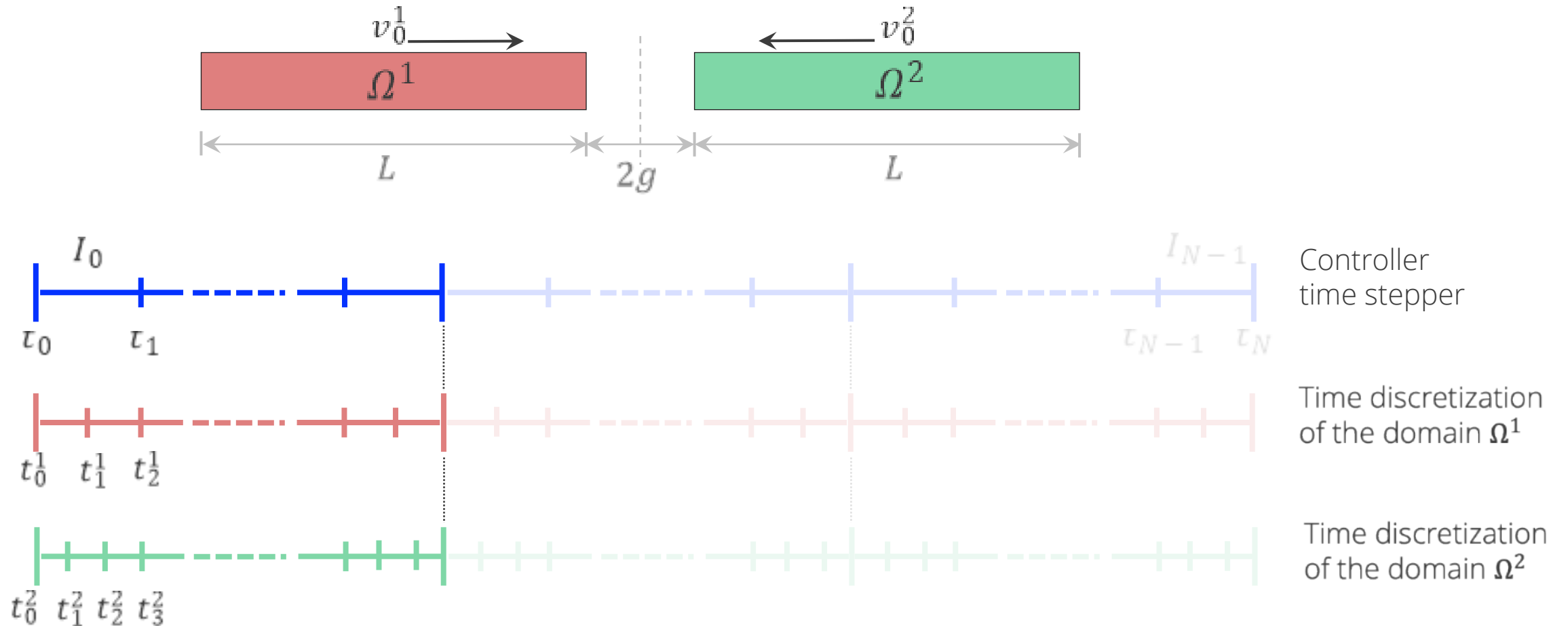
- + strong theoretical basis (domain decomposition context)
- + flexible (different time integration schemes, solvers, meshes, material models for different bodies)
- + non-intrusive implementation
- iterative process and transfer operators

Schwarz alternating method for contact problems

Schwarz alternating method for contact problems

Before the contact phase:

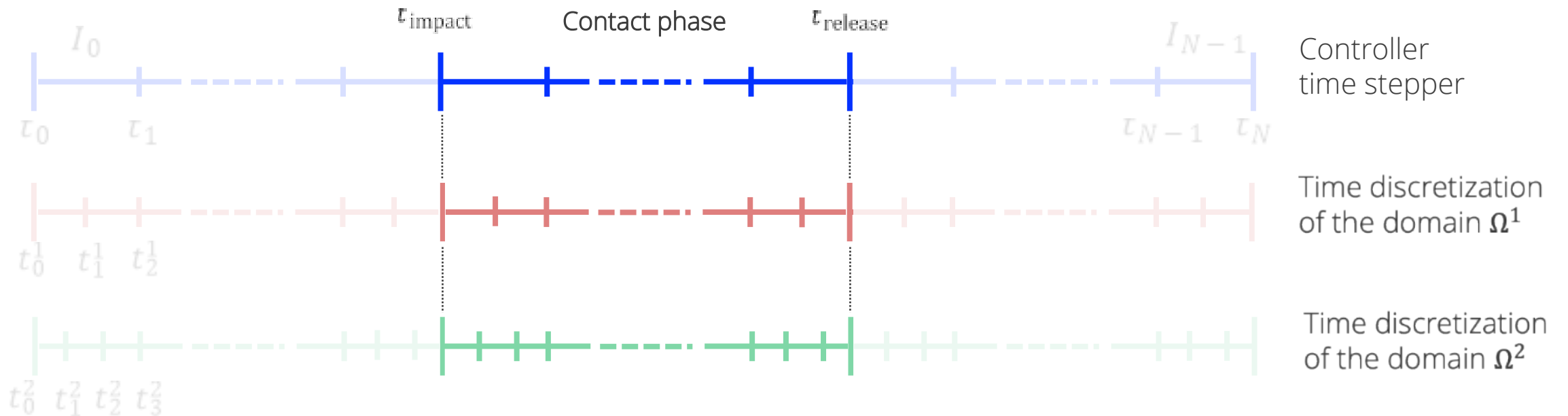
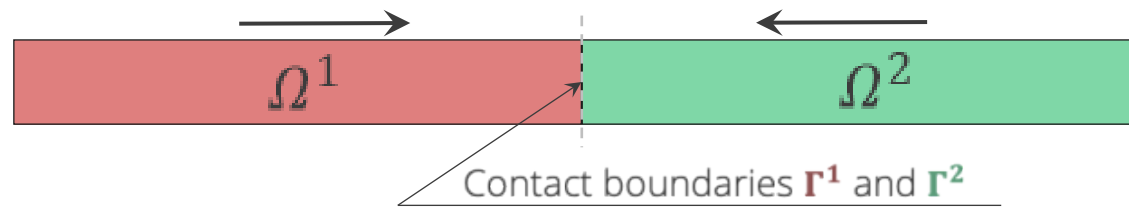
- solve PDEs in each body separately (different solvers, discretization techniques, time integrators, ...)
- check contact criteria at each controller time step (overlap/distance conditions, compression condition, ...)



Schwarz alternating method for contact problems

During the contact phase:

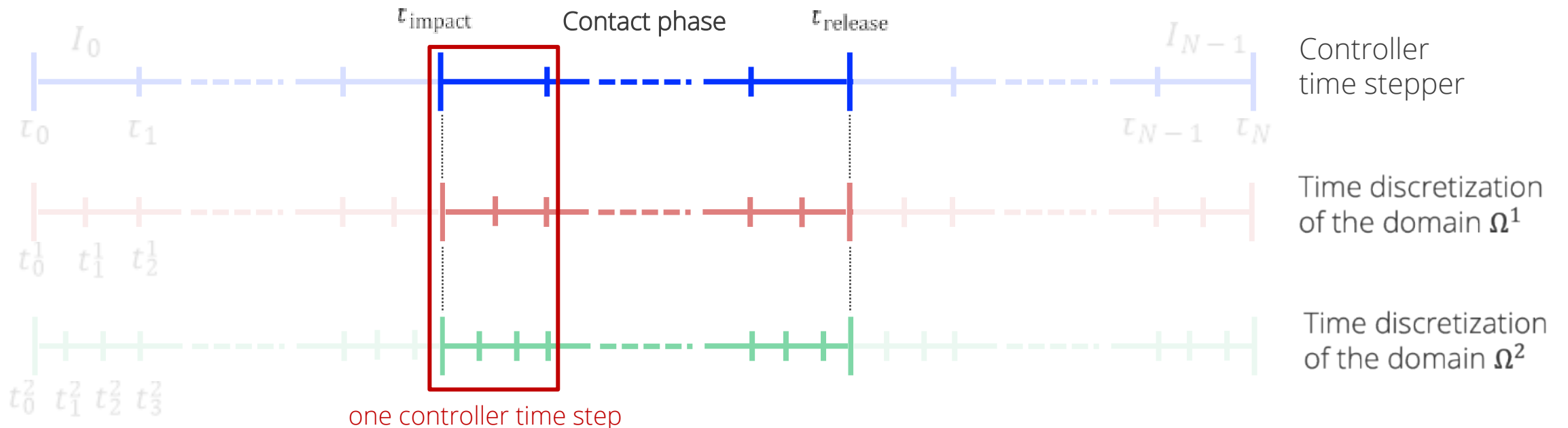
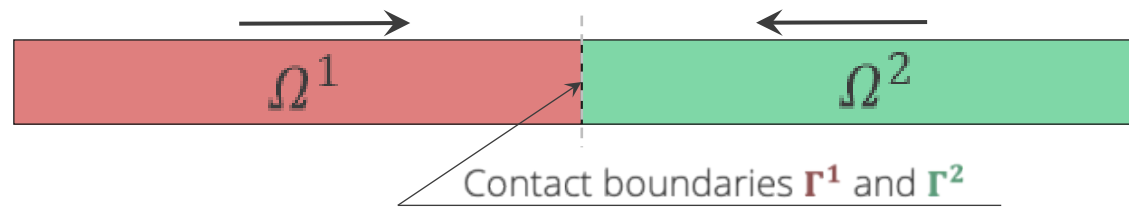
- solve PDEs in each body separately (different solvers, discretization techniques, time integrators, ...)
- prevent interpenetration through an iterative process based on the **Dirichlet-Neumann contact boundary conditions**
- check contact criteria at each controller time step (overlap/distance conditions, compression condition, ...)



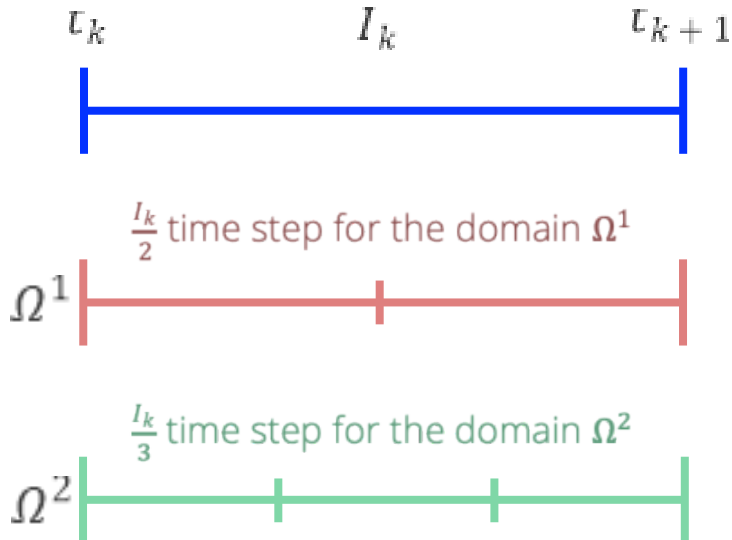
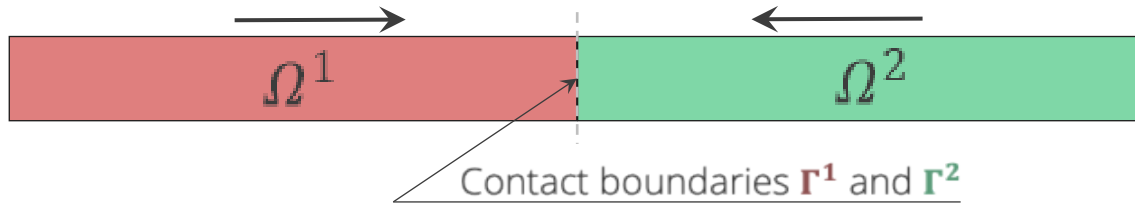
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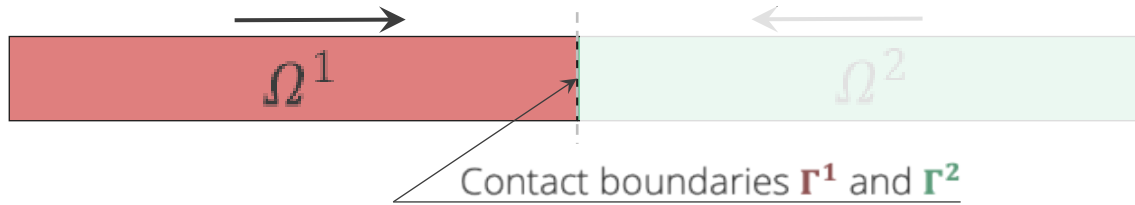


$$\Omega^1 \begin{cases} \operatorname{div} \mathbf{P}^n + \rho \mathbf{B} = \rho \ddot{\boldsymbol{\varphi}}^n & \text{in } \Omega^1 \times I_k & \text{Dynamic problem} \\ \boldsymbol{\varphi}^n(\mathbf{x}, t) = \chi & \text{on } \partial_{\varphi} \Omega^1 \times I_k & \text{Regular Dirichlet BCs} \\ \mathbf{P}^n \mathbf{N} = \mathbf{T} & \text{on } \partial_T \Omega^1 \times I_k & \text{Regular Neumann BCs} \\ \boldsymbol{\varphi}^n(\mathbf{x}, t) = \mathcal{P}_{(\Gamma^2 \rightarrow \Gamma^1) \times I_k}^{\varphi} \boldsymbol{\varphi}^{n-1}(\Omega^2, t) & \text{on } \Gamma^1 \times I_k & \text{Contact Dirichlet BCs} \end{cases}$$

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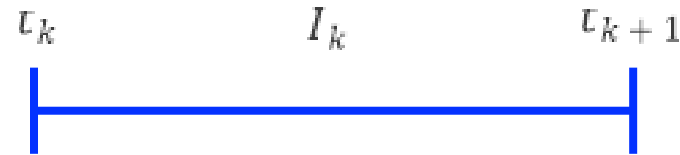
Iterate until Schwarz convergence criteria are satisfied

Schwarz alternating method for contact problems

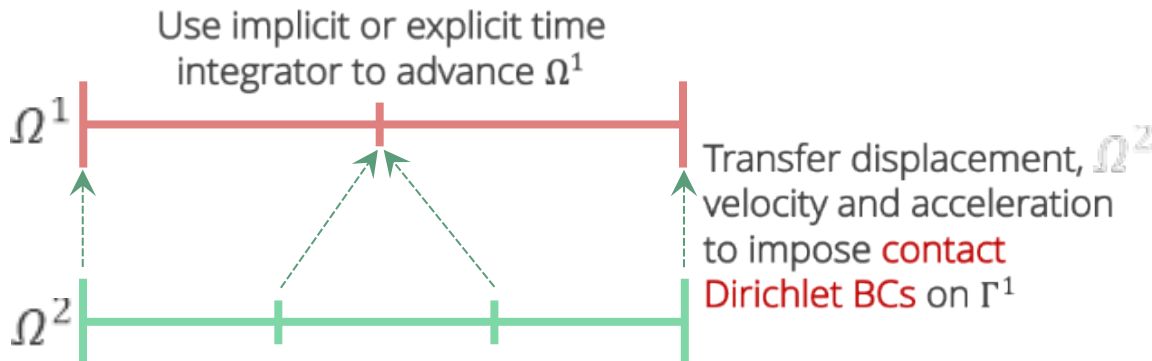


Notations

displacement	φ	mass density	ρ
acceleration	$\ddot{\varphi}$	body force	$\rho \mathbf{B}$
Piola-Kirchoff stress	$\mathbf{P}$	traction	$\mathbf{T}$



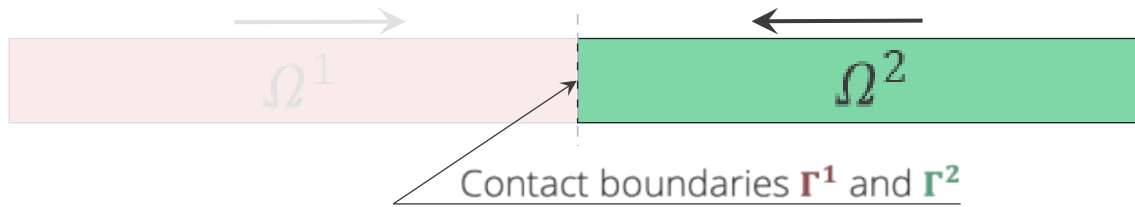
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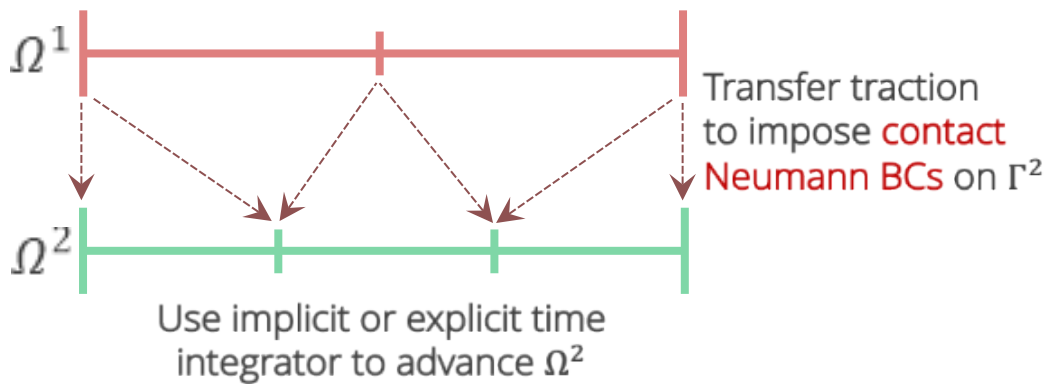
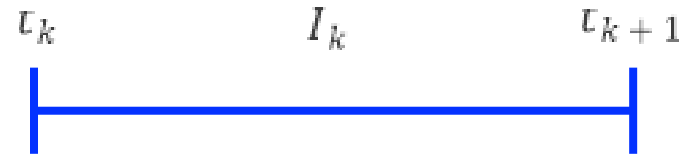
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Schwarz alternating method for contact problems



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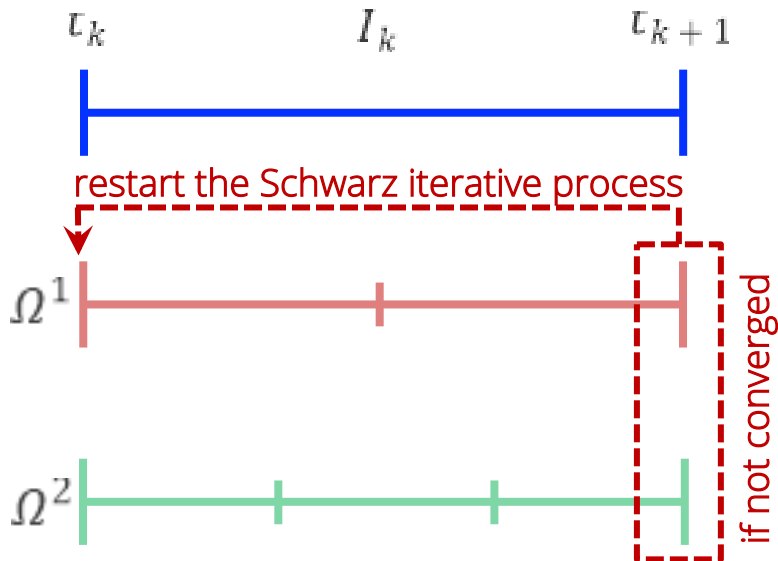
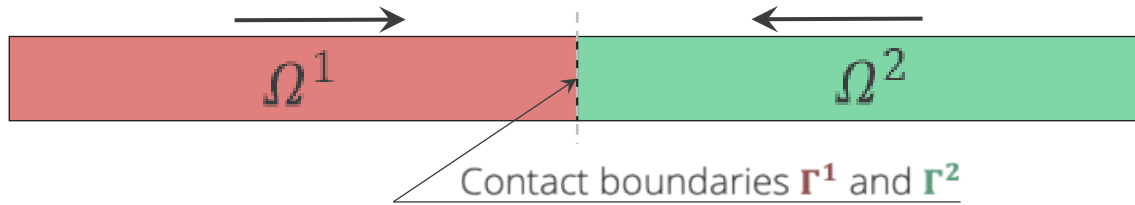


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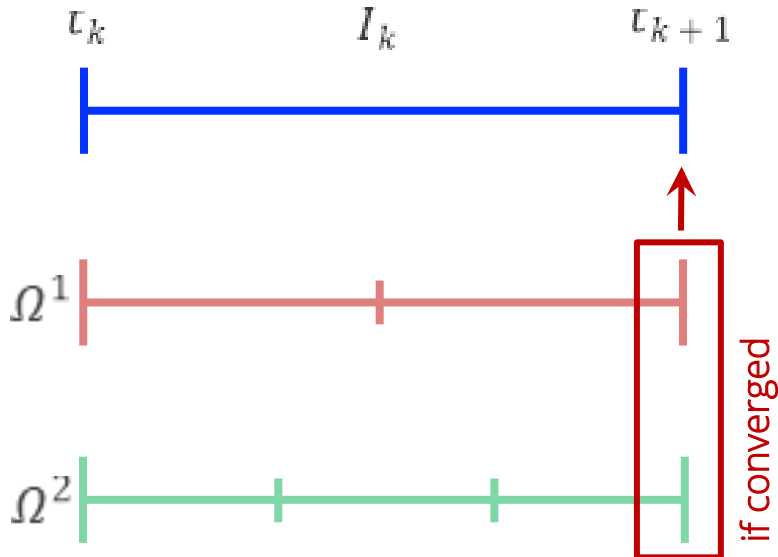
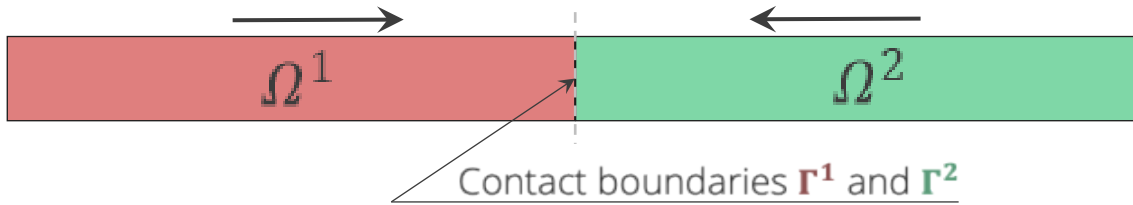


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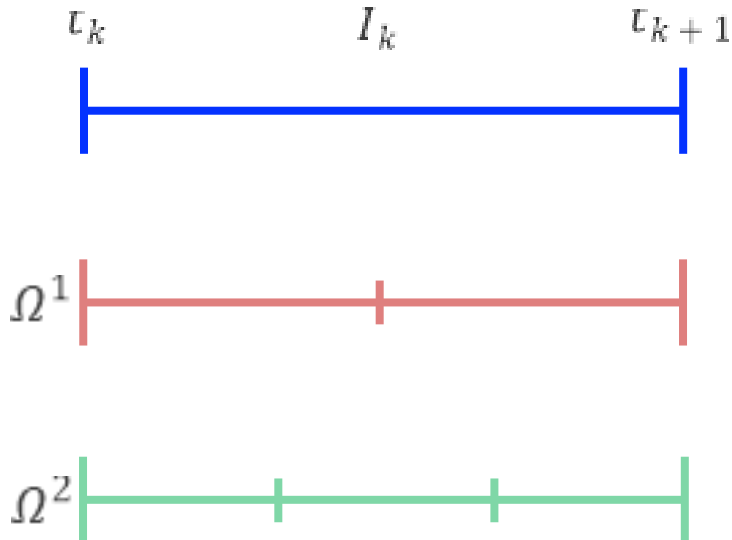
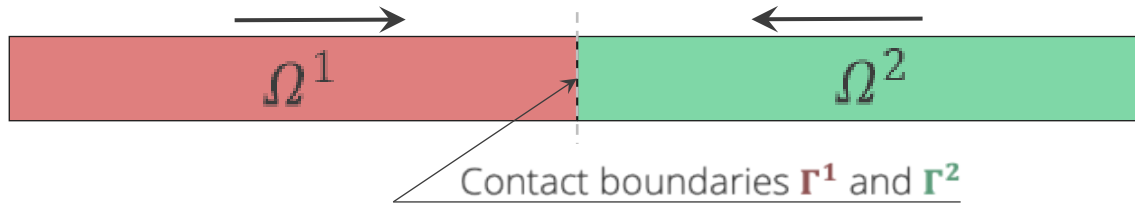


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Schwarz alternating method for contact problems



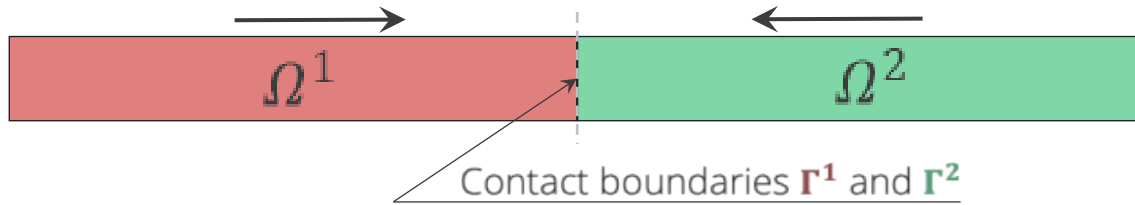
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- Dirichlet-Neumann BCs can be swapped
- Can be easily coupled with different time integrators – implicit, explicit Newmark- β , ... schemes

• $\mathcal{P}$ and $\mathcal{P}^T$ are transfer operators for displacement and traction

Schwarz alternating method for contact problems

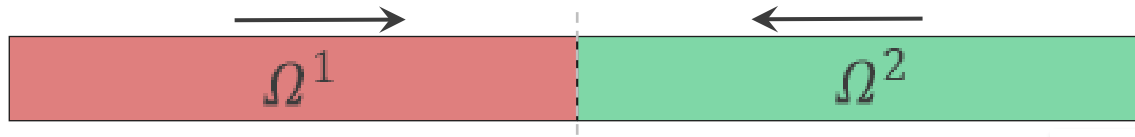


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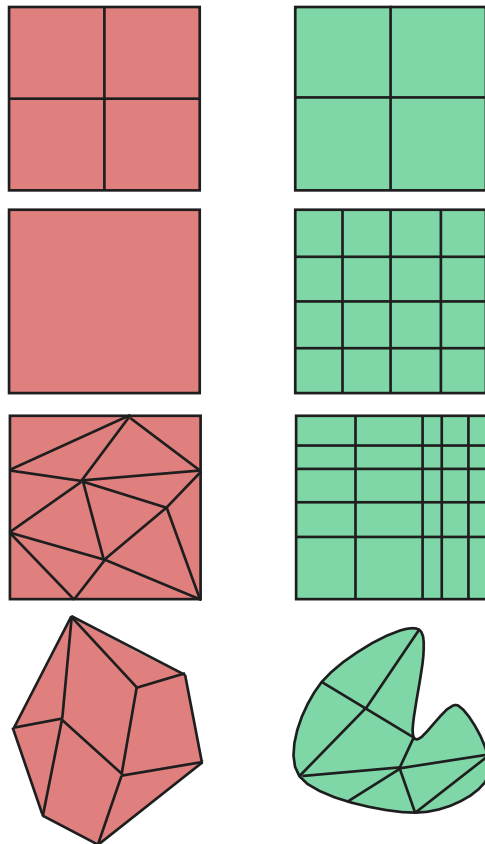
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- Dirichlet-Neumann BCs can be swapped
- Can be easily coupled with different time integrators – implicit, explicit Newmark- β , ... schemes
- **Challenge:** appropriate transfer operators for displacement and traction

Schwarz alternating method for contact problems



Contact boundaries Γ^{src} and Γ^{dst}



- Displacement transfer operator from Γ^{src} to Γ^{dst}

$$\mathcal{P}^{\varphi} = \left[\int_{\Gamma^{\text{dst}}} \mathcal{N}^{\text{dst}} (\mathcal{N}^{\text{dst}})^{\text{T}} \text{d}S \right]^{-1} \left[\int_{\Gamma^{\text{dst}}} \mathcal{N}^{\text{dst}} (\mathcal{N}^{\text{src}})^{\text{T}} \text{d}S \right]$$

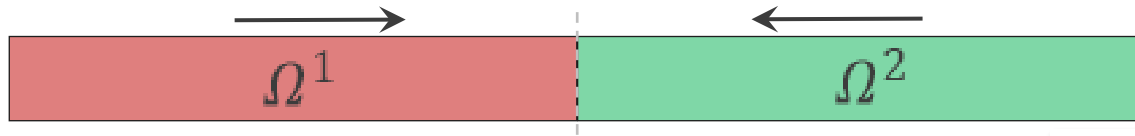
- Traction transfer operator from Γ^{src} to Γ^{dst}

$$\mathcal{P}^T = \left[\int_{\Gamma^{\text{dst}}} \mathcal{N}^{\text{dst}} (\mathcal{N}^{\text{src}})^{\text{T}} \text{d}S \right] \left[\int_{\Gamma^{\text{src}}} \mathcal{N}^{\text{src}} (\mathcal{N}^{\text{src}})^{\text{T}} \text{d}S \right]^{-1}$$

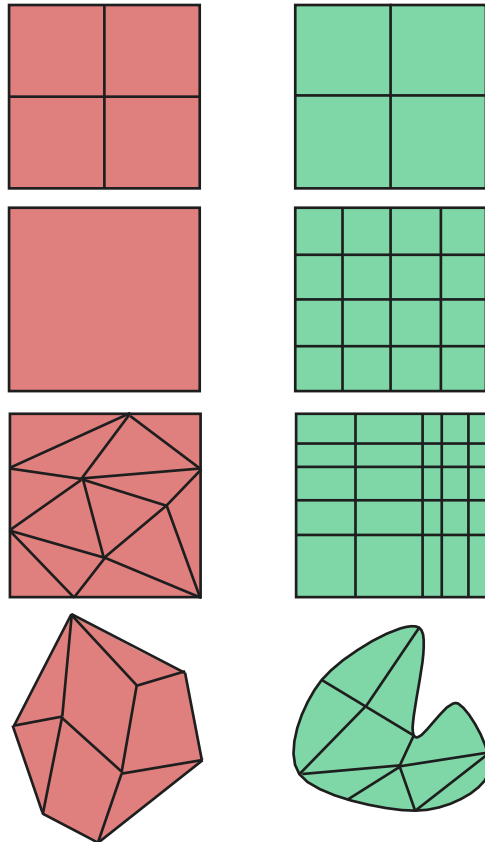
$\mathcal{N}^{\text{src}}$ and $\mathcal{N}^{\text{dst}}$ - finite elements interpolation functions defined on Γ^{src} and Γ^{dst}

- Generic (appropriate for different type of geometries, mesh types and sizes, ...)
- Same operator used for all Schwarz iterations within one controller time step

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- Displacement transfer operator from Γ^{src} to Γ^{dst}

$$\mathcal{P}^{\varphi} = \left[\int_{\Gamma^{\text{dst}}} \mathcal{N}^{\text{dst}} (\mathcal{N}^{\text{dst}})^{\text{T}} \text{d}S \right]^{-1} \left[\int_{\Gamma^{\text{dst}}} \mathcal{N}^{\text{dst}} (\mathcal{N}^{\text{src}})^{\text{T}} \text{d}S \right]$$

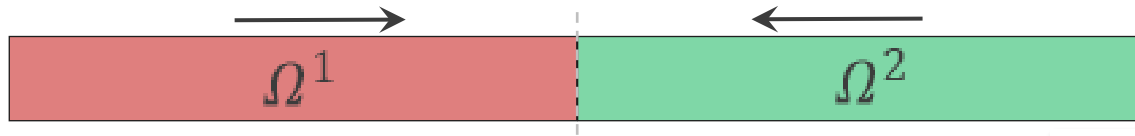
- Traction transfer operator from Γ^{src} to Γ^{dst}

$$\mathcal{P}^{\text{T}} = \left[\int_{\Gamma^{\text{dst}}} \mathcal{N}^{\text{dst}} (\mathcal{N}^{\text{src}})^{\text{T}} \text{d}S \right] \left[\int_{\Gamma^{\text{src}}} \mathcal{N}^{\text{src}} (\mathcal{N}^{\text{src}})^{\text{T}} \text{d}S \right]^{-1}$$

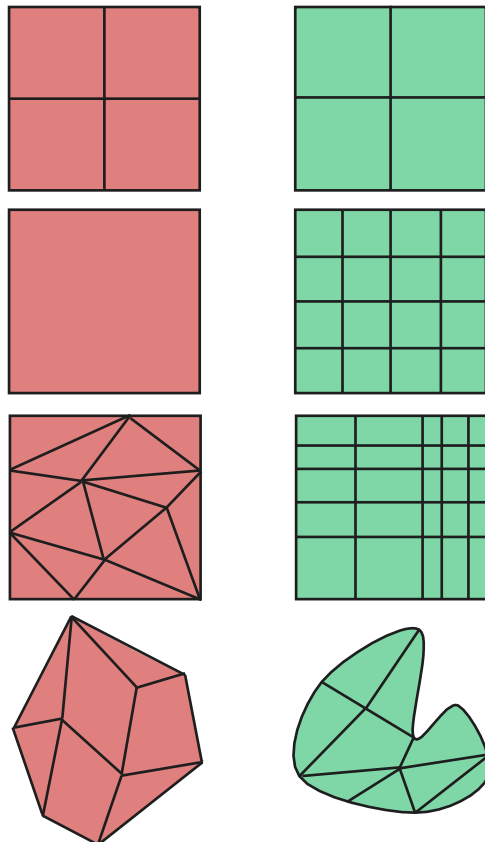
$\mathcal{N}^{\text{src}}$ and $\mathcal{N}^{\text{dst}}$ - finite elements interpolation functions defined on Γ^{src} and Γ^{dst}

- Generic (appropriate for different type of geometries, mesh types and sizes, ...)
- Same operator used for all Schwarz iterations within one controller time step

Schwarz alternating method for contact problems



Contact boundaries Γ^{src} and Γ^{dst}



- Displacement transfer operator from Γ^{src} to Γ^{dst}

$$\mathcal{P}^{\varphi} = \left[\int_{\Gamma^{\text{dst}}} \mathcal{N}^{\text{dst}} (\mathcal{N}^{\text{dst}})^{\text{T}} \text{d}S \right]^{-1} \left[\int_{\Gamma^{\text{dst}}} \mathcal{N}^{\text{dst}} (\mathcal{N}^{\text{src}})^{\text{T}} \text{d}S \right]$$

- Traction transfer operator from Γ^{src} to Γ^{dst}

$$\mathcal{P}^{\text{T}} = \left[\int_{\Gamma^{\text{dst}}} \mathcal{N}^{\text{dst}} (\mathcal{N}^{\text{src}})^{\text{T}} \text{d}S \right] \left[\int_{\Gamma^{\text{src}}} \mathcal{N}^{\text{src}} (\mathcal{N}^{\text{src}})^{\text{T}} \text{d}S \right]^{-1}$$

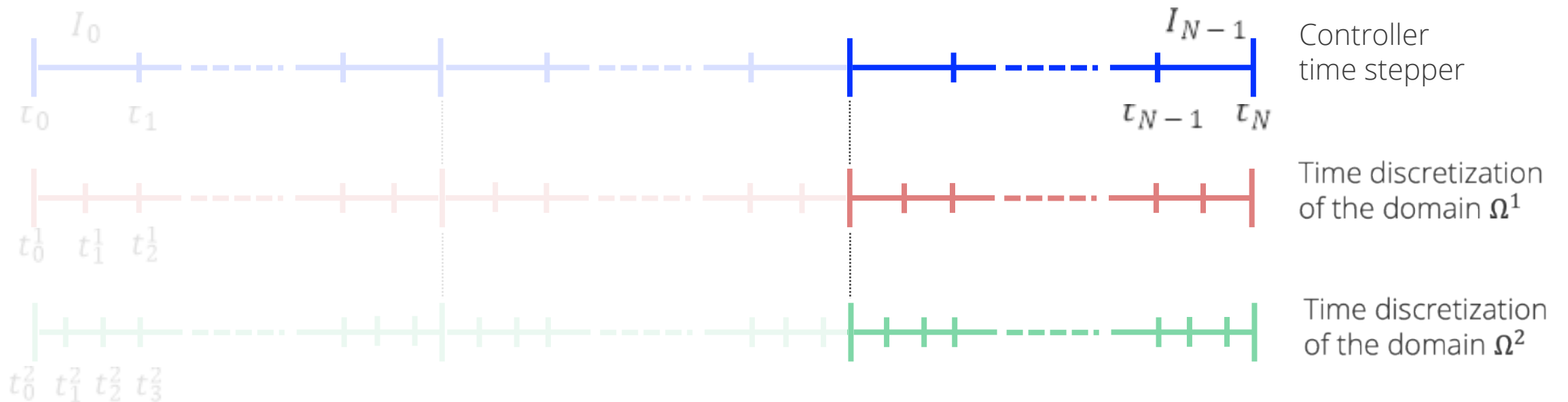
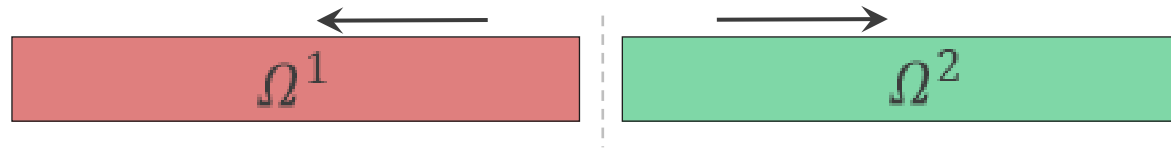
$\mathcal{N}^{\text{src}}$ and $\mathcal{N}^{\text{dst}}$ - finite elements interpolation functions defined on Γ^{src} and Γ^{dst}

- Generic (appropriate for different type of geometries, mesh types and sizes, ...)
- Same operator used for all Schwarz iterations within one controller time step

Schwarz alternating method for contact problems

After the contact phase:

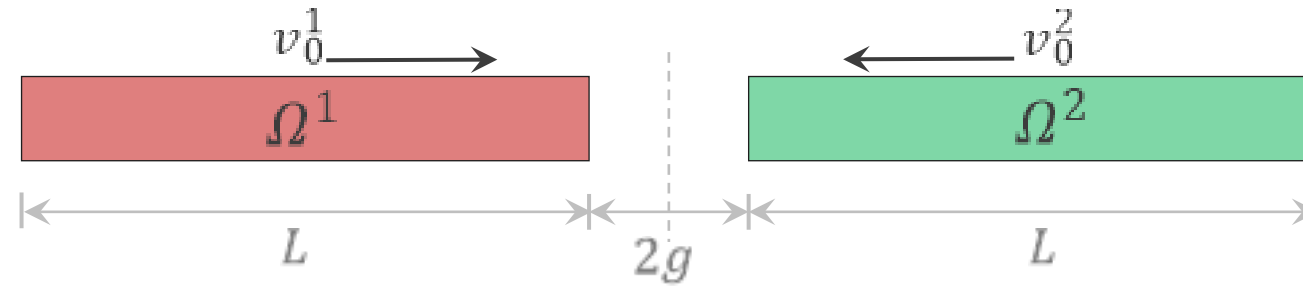
- solve PDEs in each body separately (different solvers, discretization techniques, time integrators, ...)
- prevent interpenetration through an iterative process based on the **Dirichlet-Neumann contact boundary conditions**
- check contact criteria at each controller time step (overlap/distance conditions, compression condition, ...)



Academic benchmark

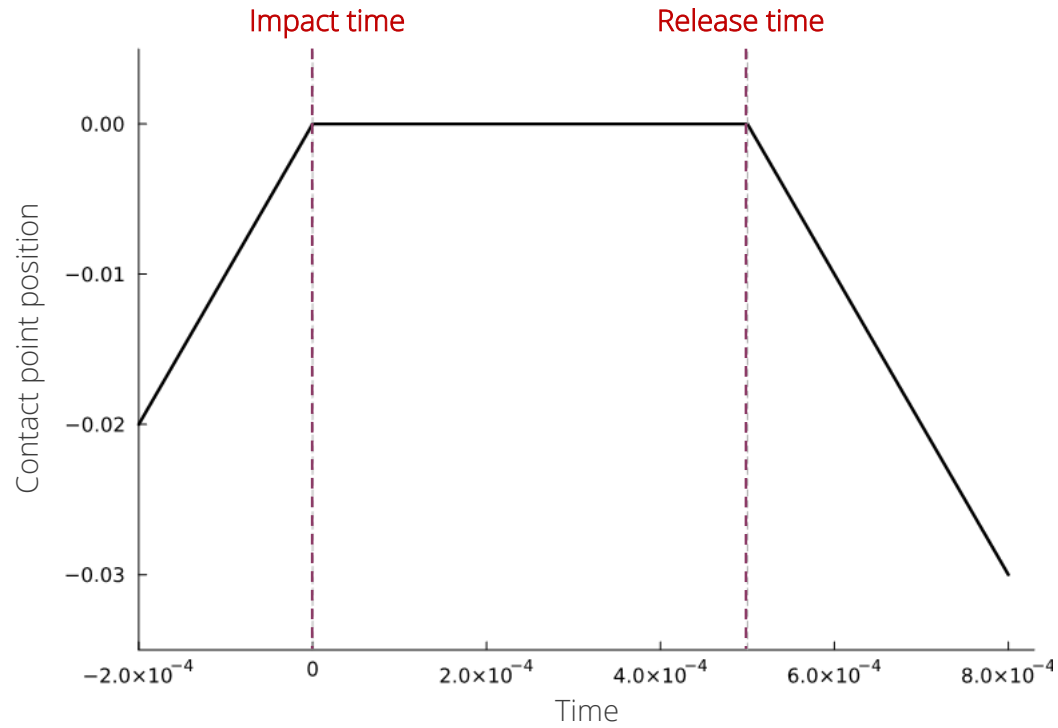
Schwarz contact method vs conventional methods

Impact of two 1D linear elastic prismatic rods



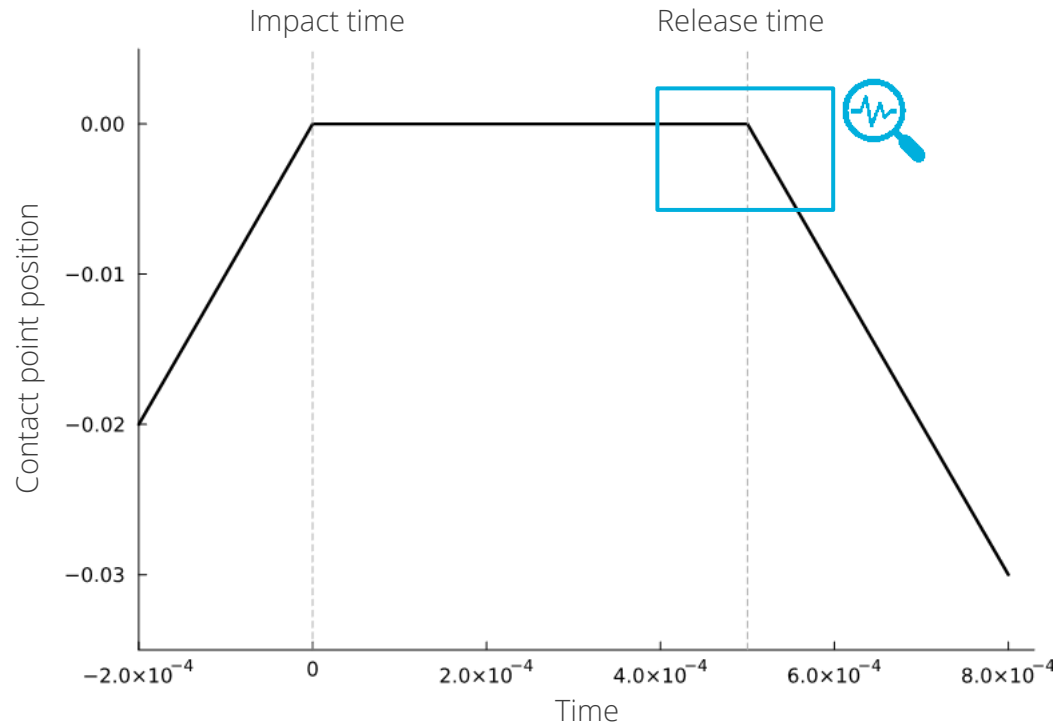
- Analytical solution available in *[Carpenter et al., 1991]*
- Newmark- β time integrator
- Numerical comparison: Schwarz method vs conventional contact methods
 - implicit and explicit Lagrange multiplier methods
 - implicit and explicit penalty methods
 - explicit-explicit, implicit-implicit, implicit-explicit Schwarz methods

Contact point position



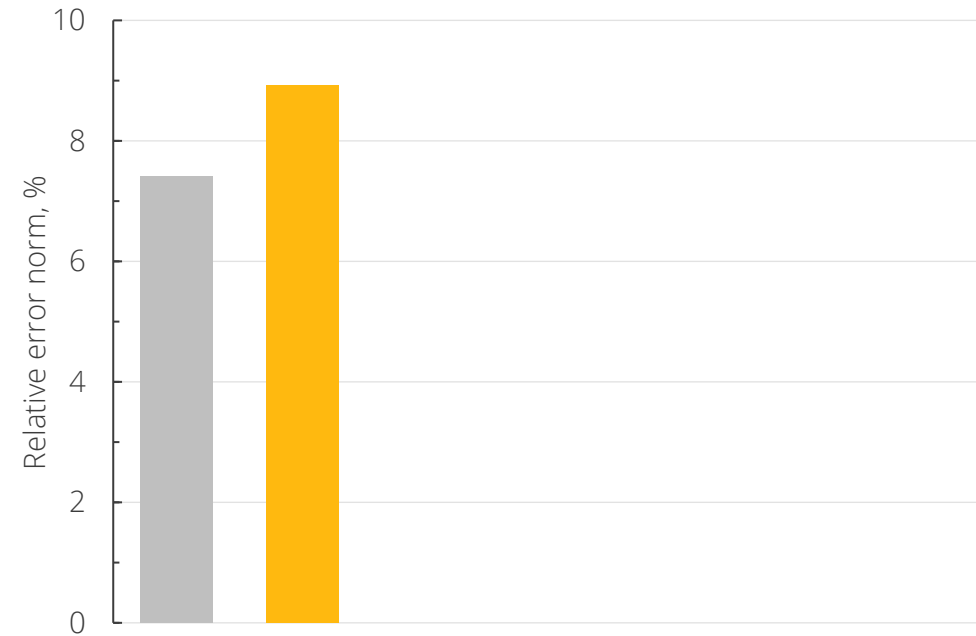
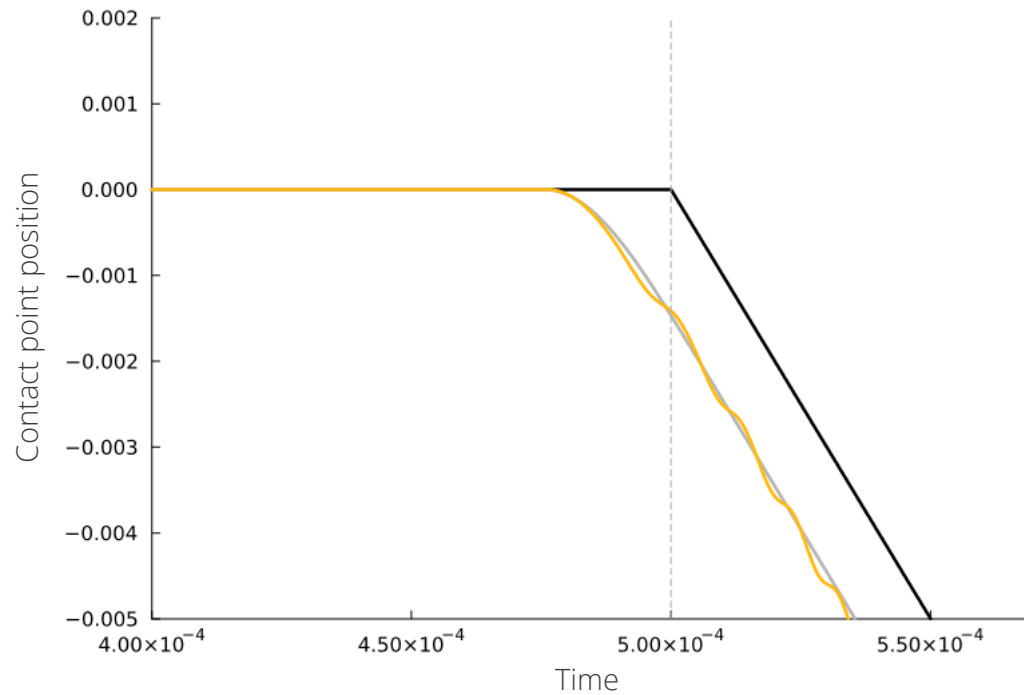
■ Analytical solution

Contact point position



■ Analytical solution

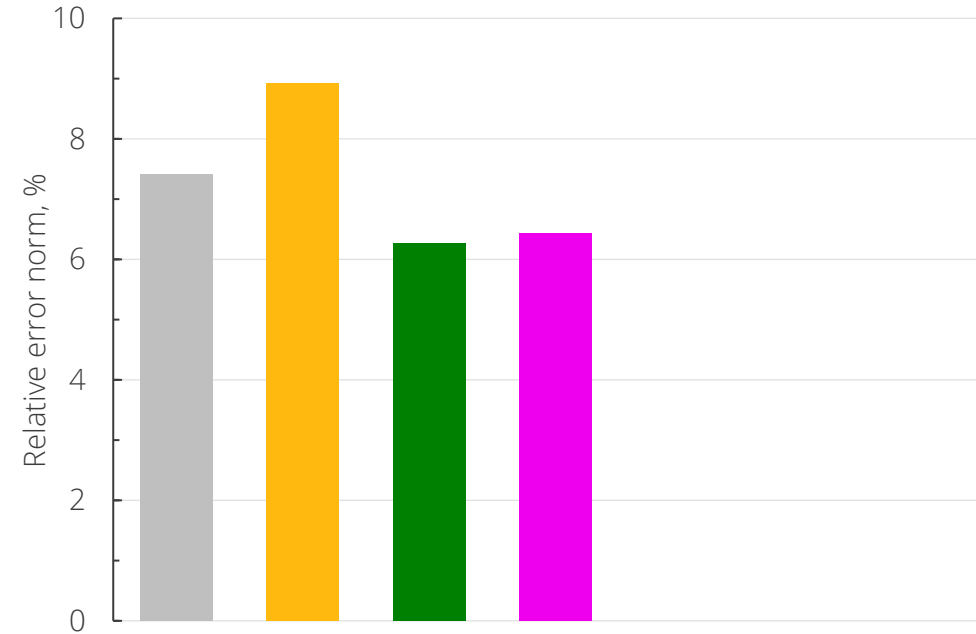
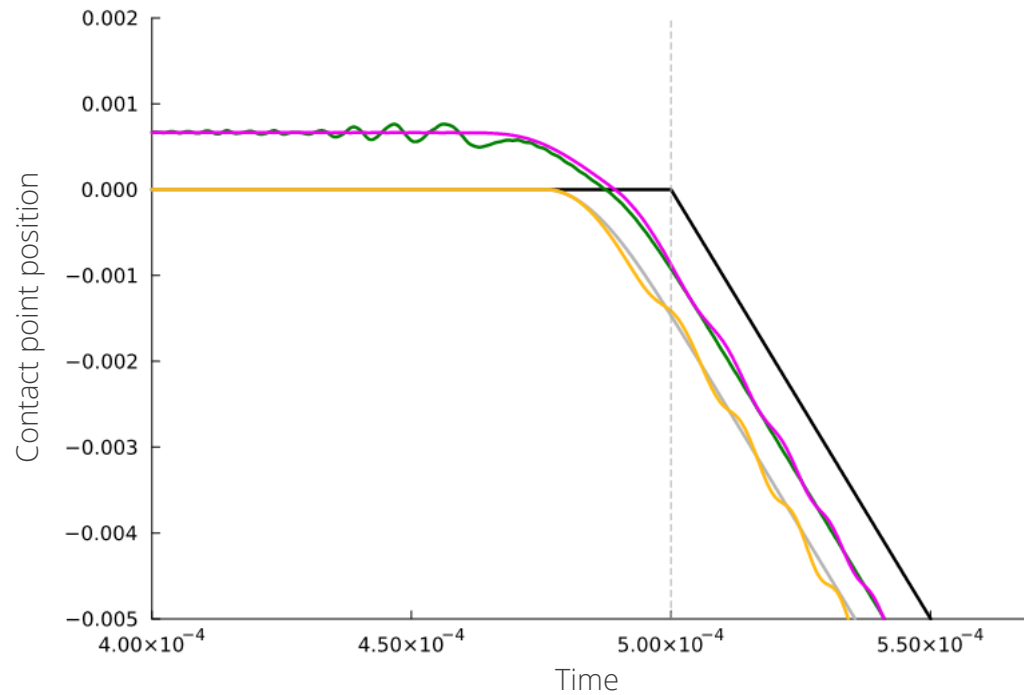
Contact point position



- Analytical solution
- Implicit LM
- Explicit LM

- Lagrange Multiplier methods: under-predict the release time

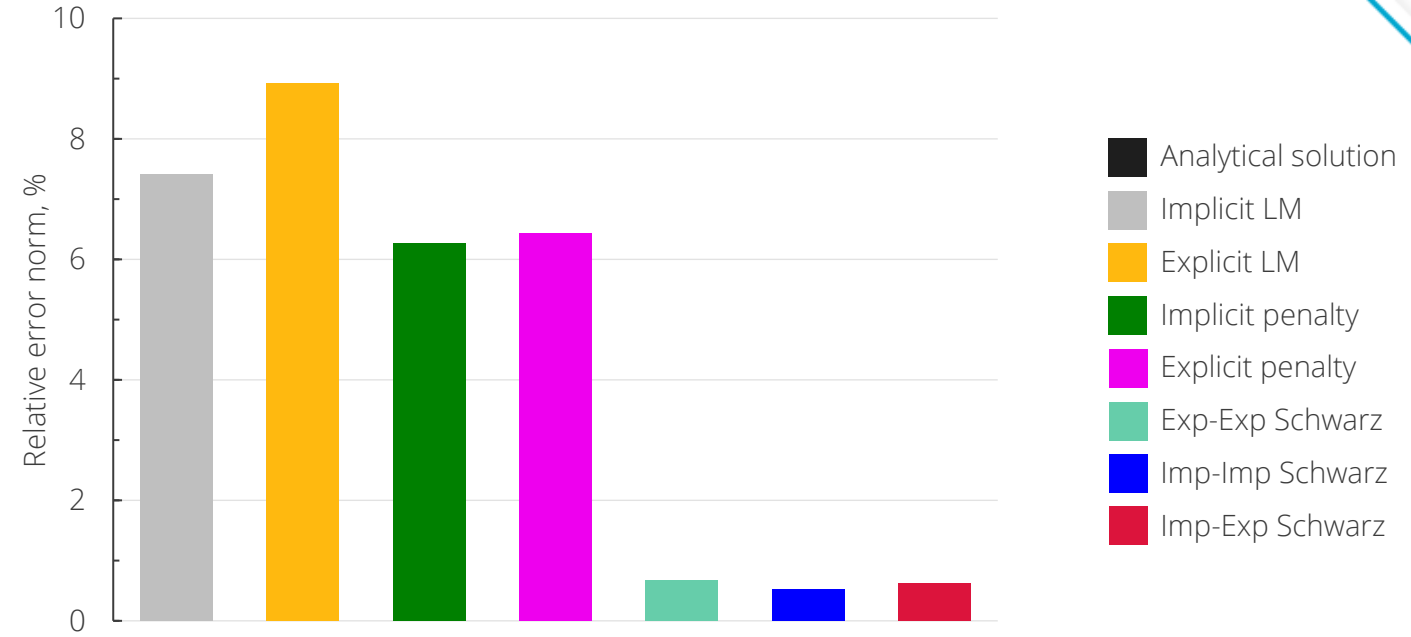
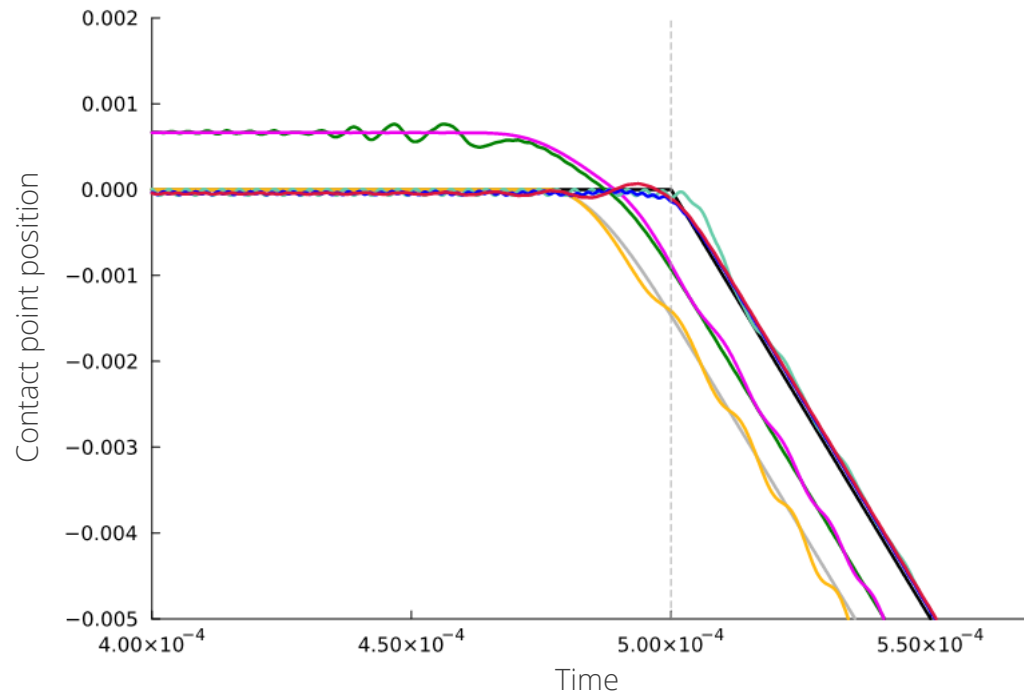
Contact point position



- Analytical solution
- Implicit LM
- Explicit LM
- Implicit penalty
- Explicit penalty

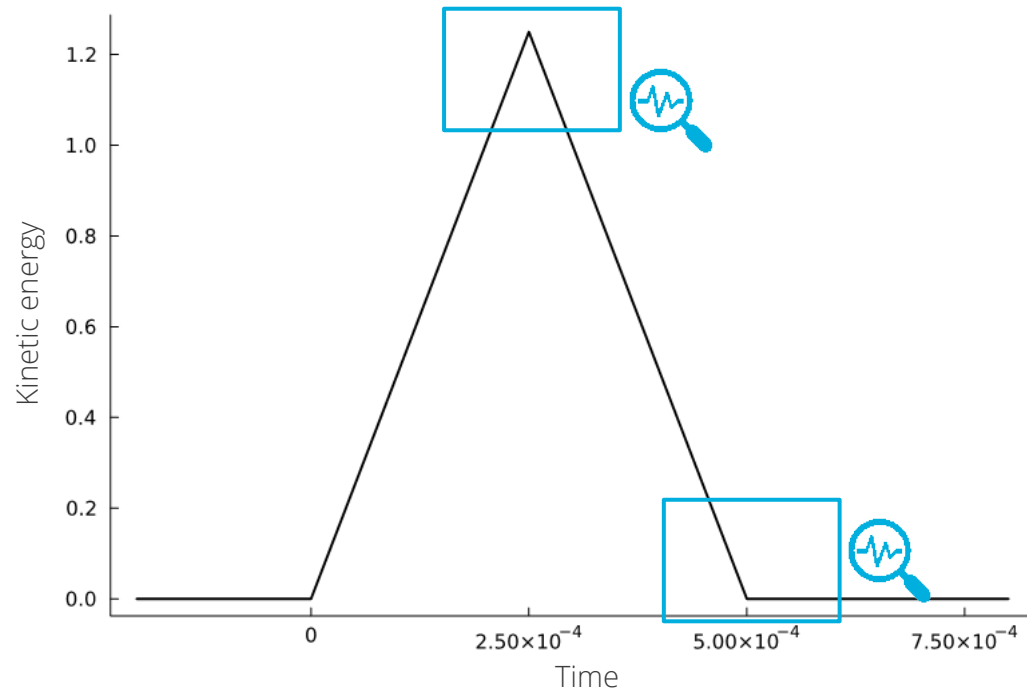
- **Lagrange Multiplier methods:** under-predict the release time
- **Penalty methods:** over-predict the contact point position and under-predict the release time

Contact point position



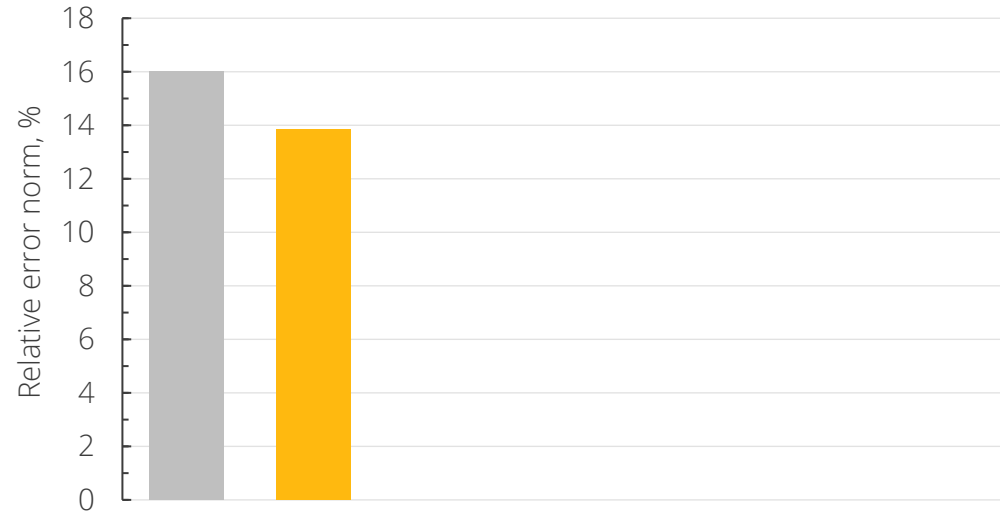
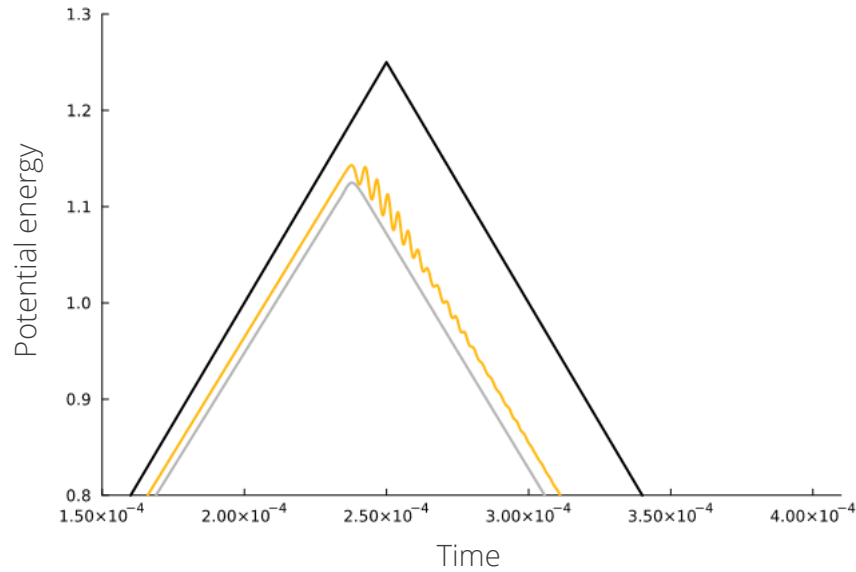
- **Lagrange Multiplier methods:** under-predict the release time
- **Penalty methods:** over-predict the contact point position and under-predict the release time
- **Schwarz methods:** accurately predict the contact point position and release time

Potential energy

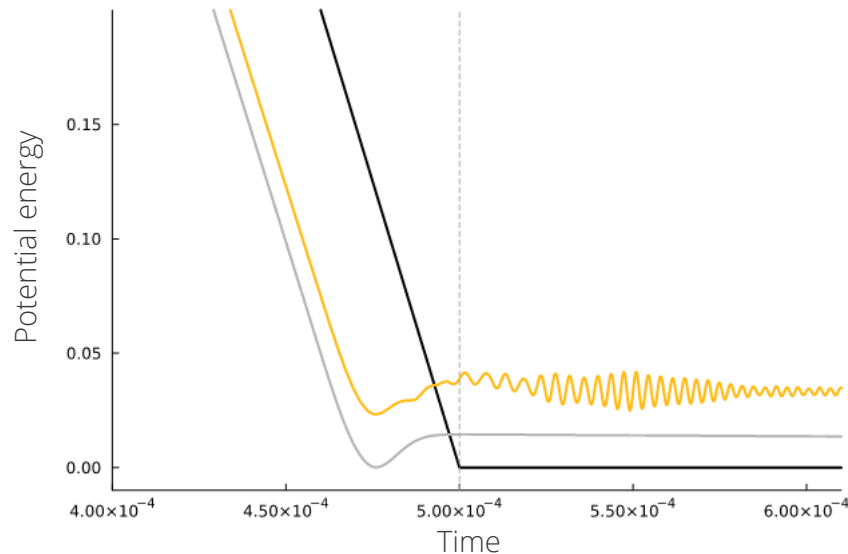


■ Analytical solution

Potential energy

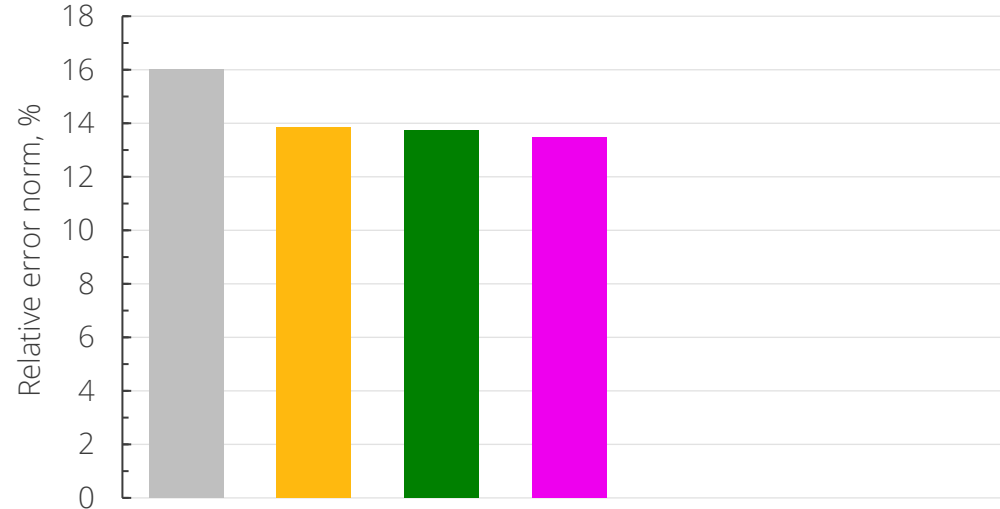
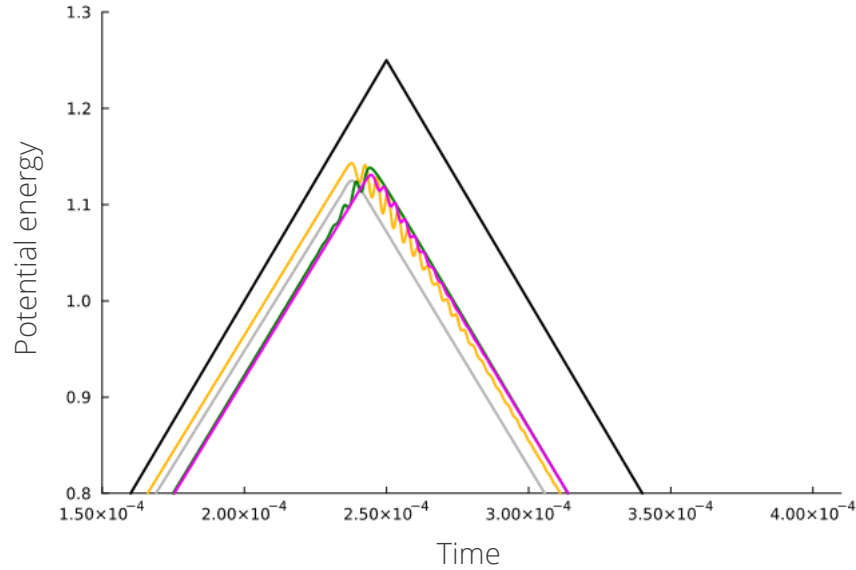


■ Analytical solution
■ Implicit LM
■ Explicit LM

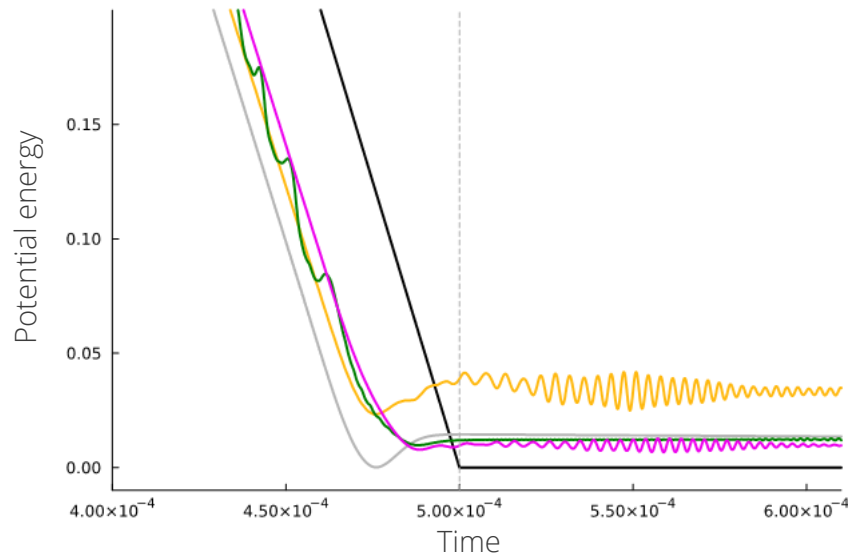


- **Lagrange Multiplier methods:** under-predict the maximum potential energy peak and over-predicts the energy after release

Potential energy

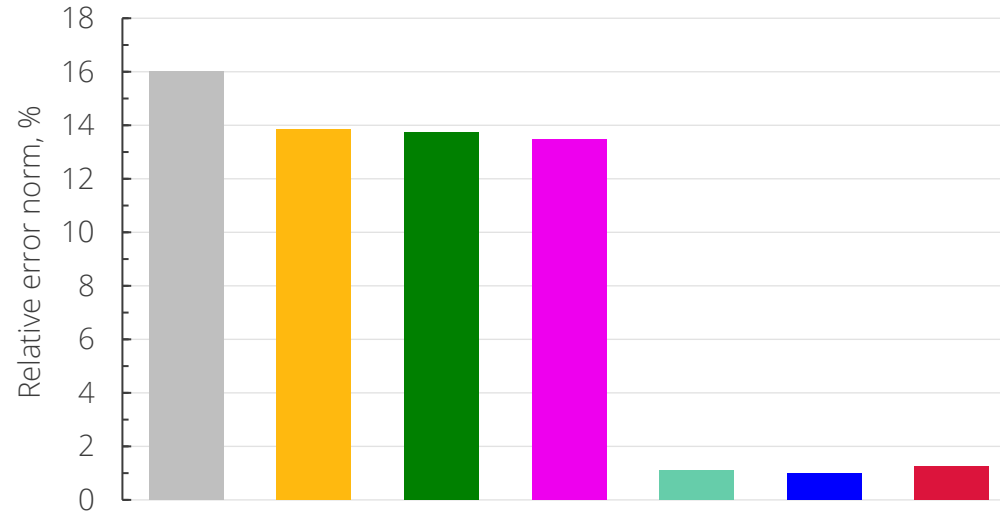
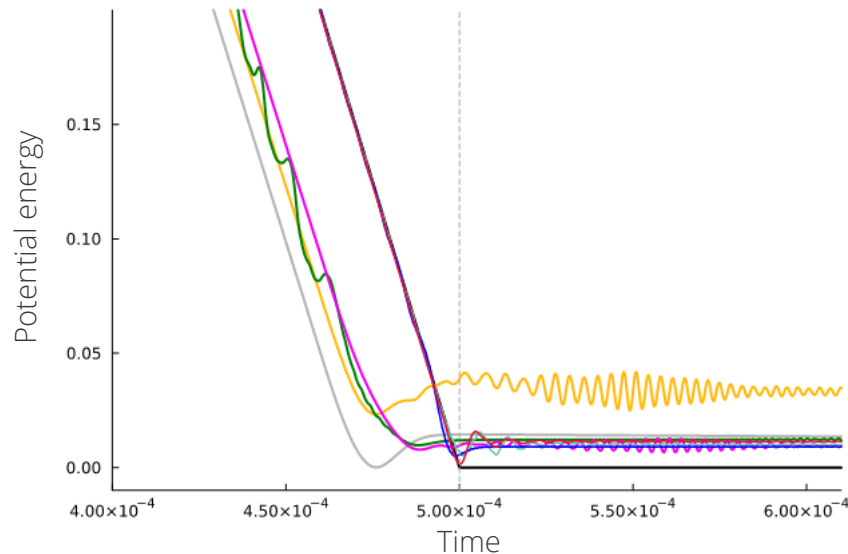
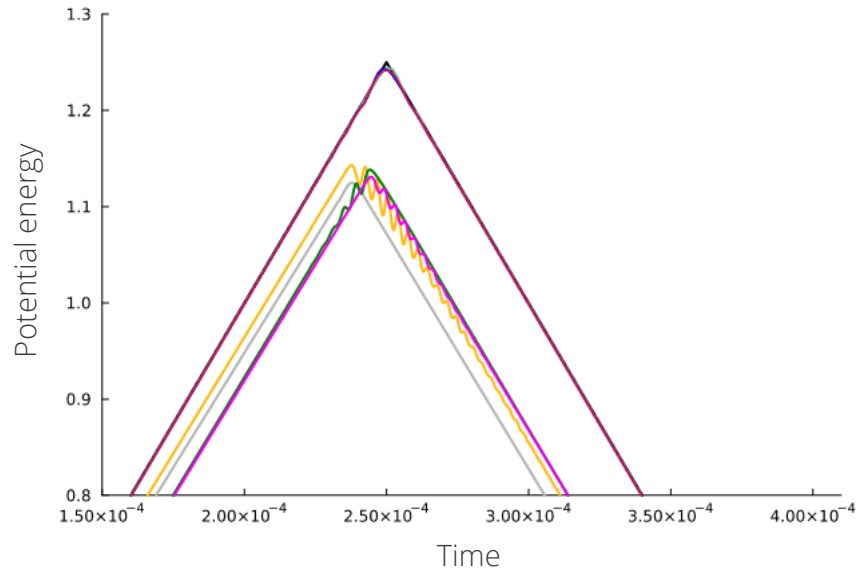


- Analytical solution
- Implicit LM
- Explicit LM
- Implicit penalty
- Explicit penalty



- **Lagrange Multiplier methods:** under-predict the maximum potential energy peak and over-predicts the energy after release
- **Penalty methods:** similar behavior as LM methods

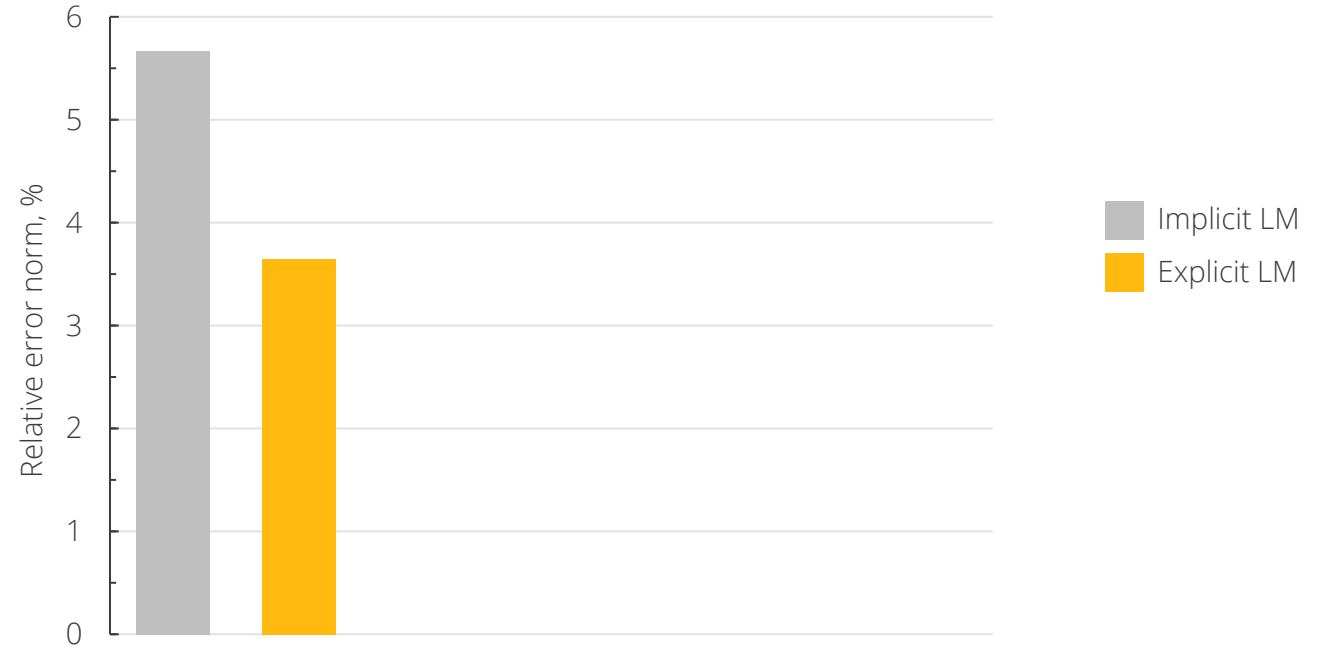
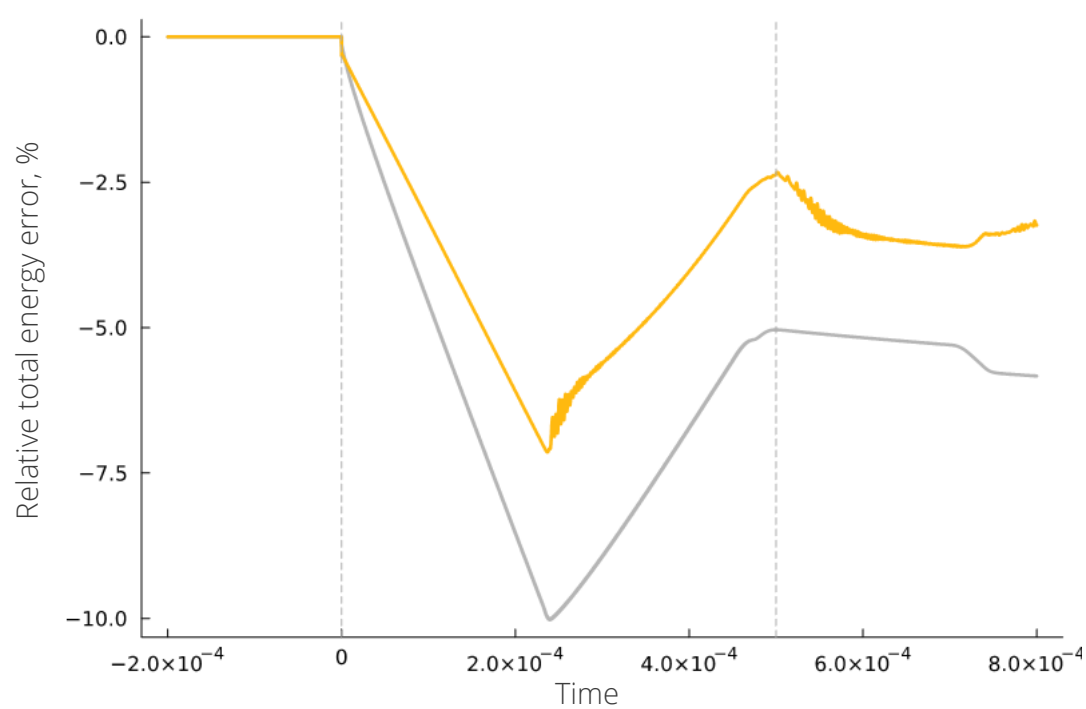
Potential energy



- Analytical solution
- Implicit LM
- Explicit LM
- Implicit penalty
- Explicit penalty
- Exp-Exp Schwarz
- Imp-Imp Schwarz
- Imp-Exp Schwarz

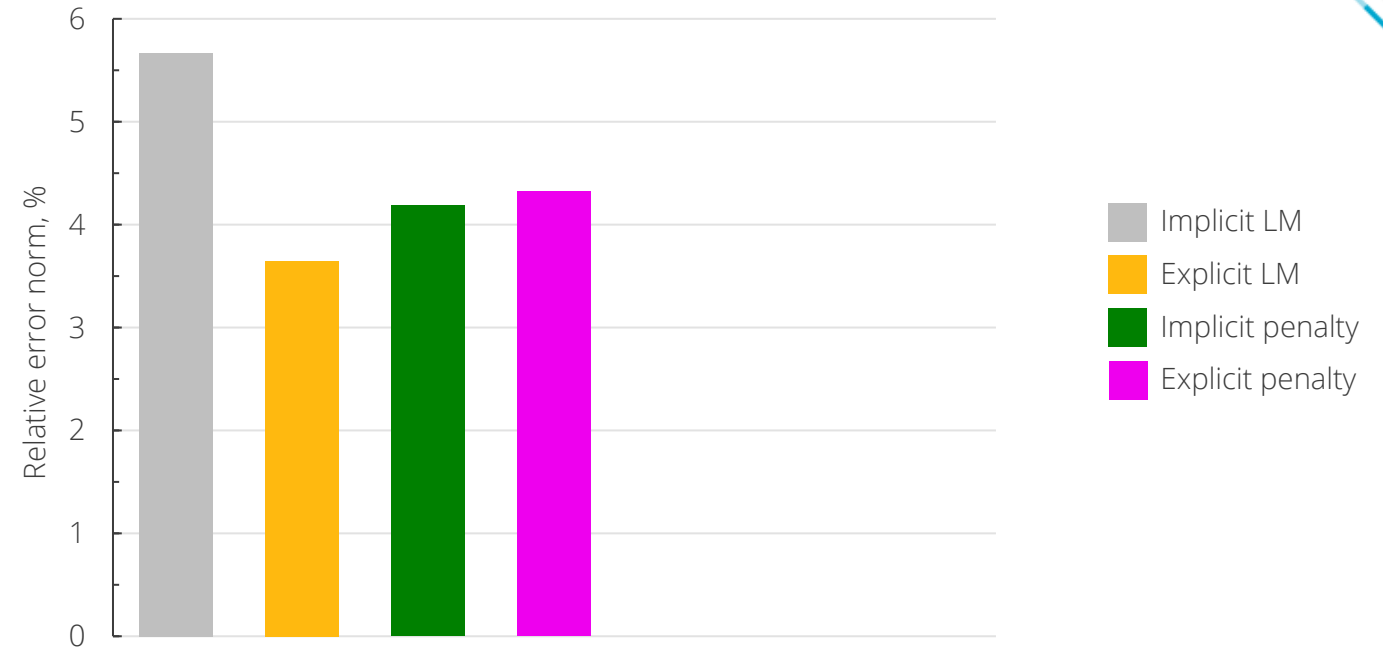
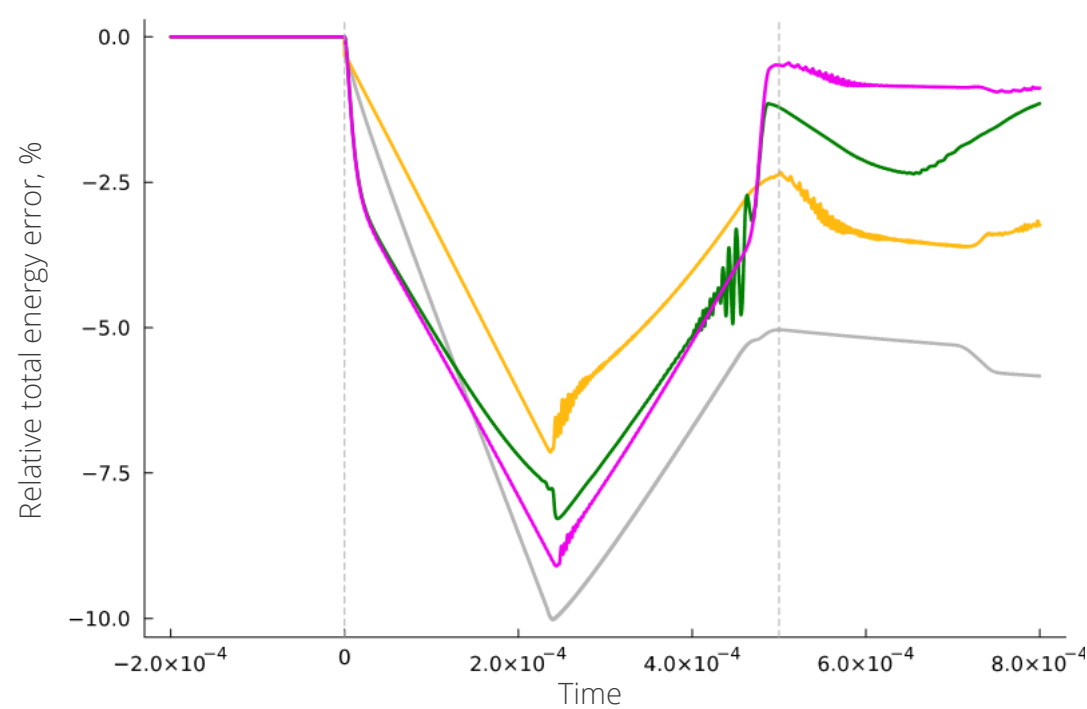
- **Lagrange Multiplier methods:** under-predict the maximum potential energy peak and over-predicts the energy after release
- **Penalty methods:** similar behavior as LM methods
- **Schwarz methods:** accurately predicts the maximum energy peak and better capture the energy after release

Total energy conservation



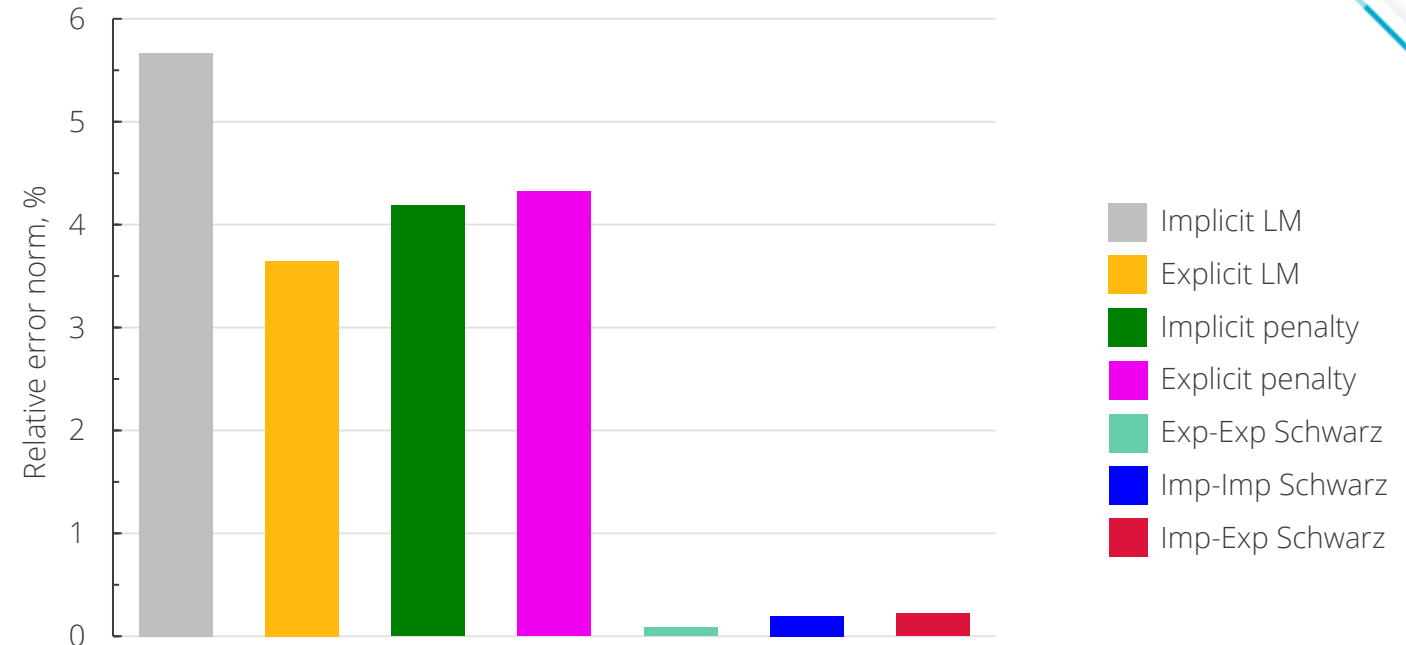
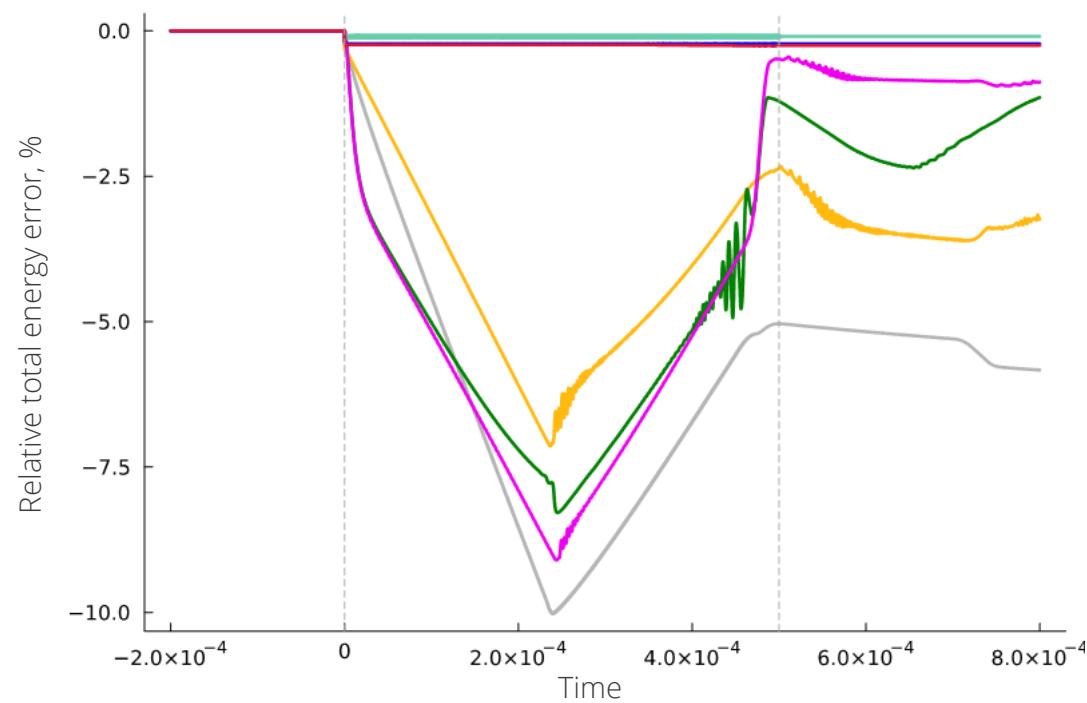
- **Lagrange Multiplier methods:** important energy loss up to 7% (explicit) and 10% (implicit)

Total energy conservation



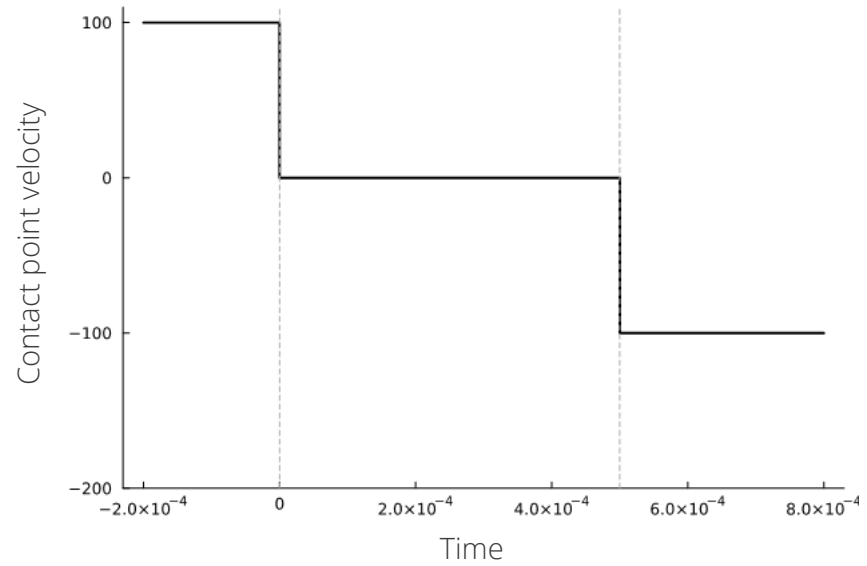
- **Lagrange Multiplier methods:** important energy loss up to 7% (explicit) and 10% (implicit)
- **Penalty methods:** important energy loss up to 8% (implicit) and 9% (implicit)

Total energy conservation



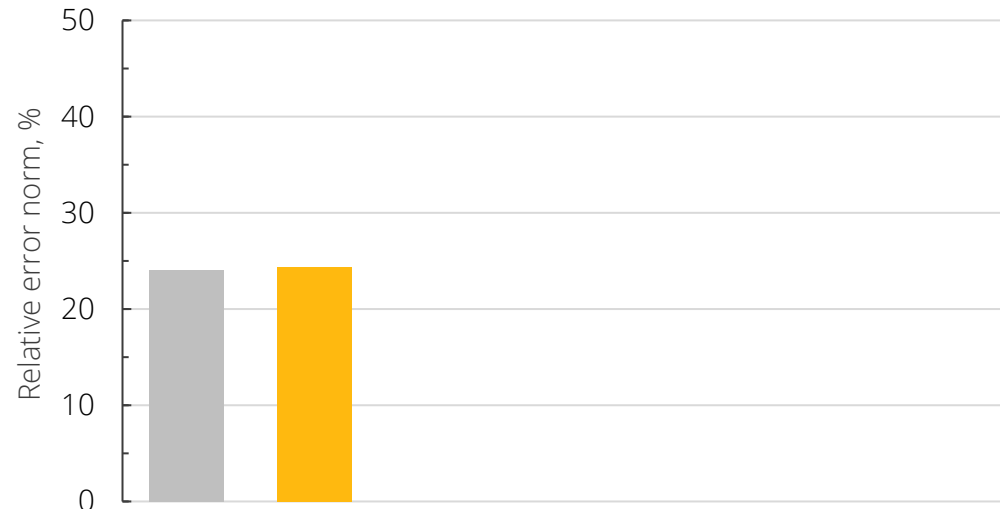
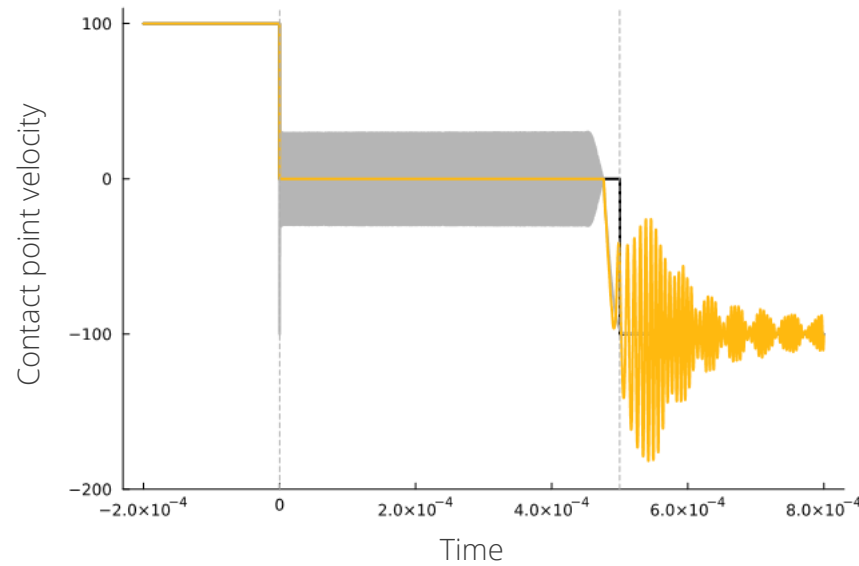
- **Lagrange Multiplier methods:** important energy loss up to 7% (explicit) and 10% (implicit)
- **Penalty methods:** important energy loss up to 8% (implicit) and 9% (implicit)
- **Schwarz methods:** remarkable energy conservation properties – energy loss less than 0.3%

Contact point velocity



■ Analytical solution

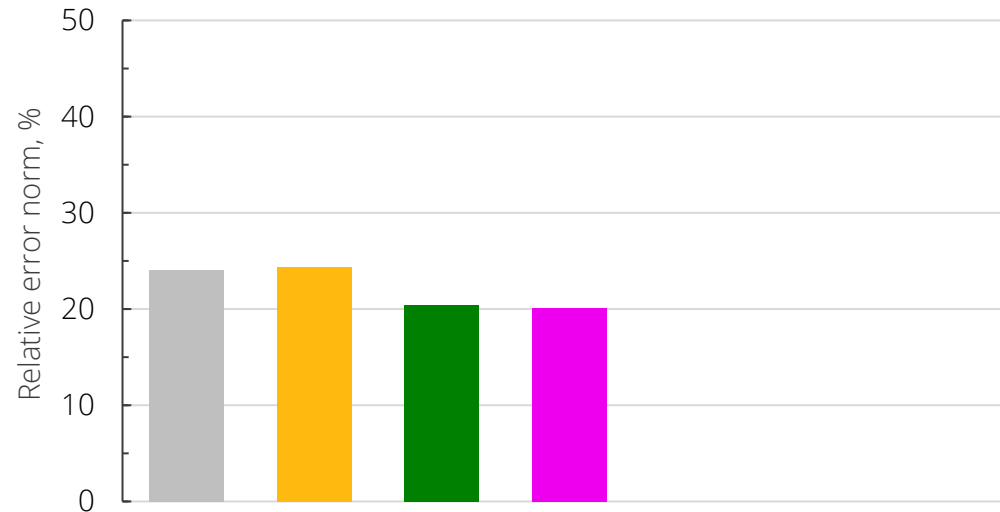
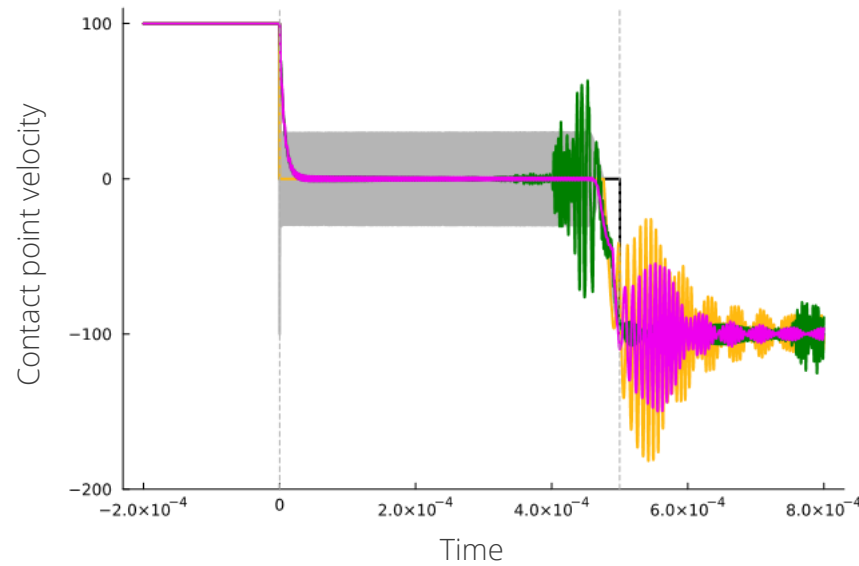
Contact point velocity



■ Analytical solution
■ Implicit LM
■ Explicit LM

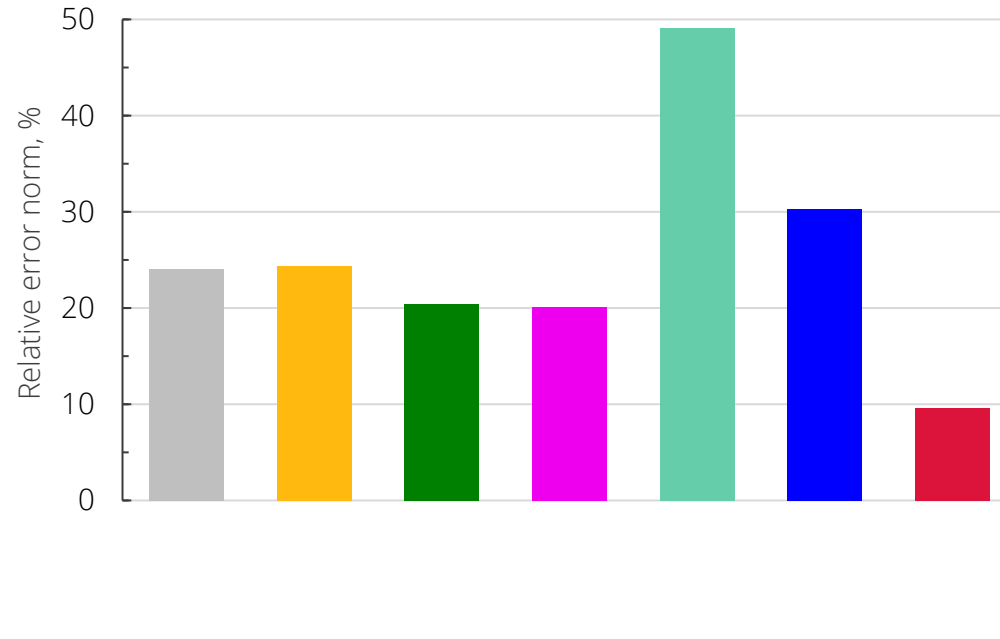
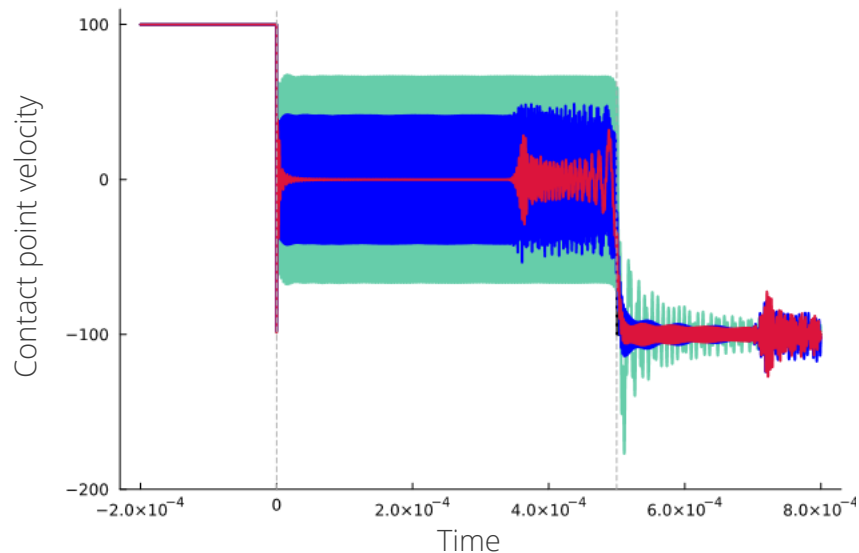
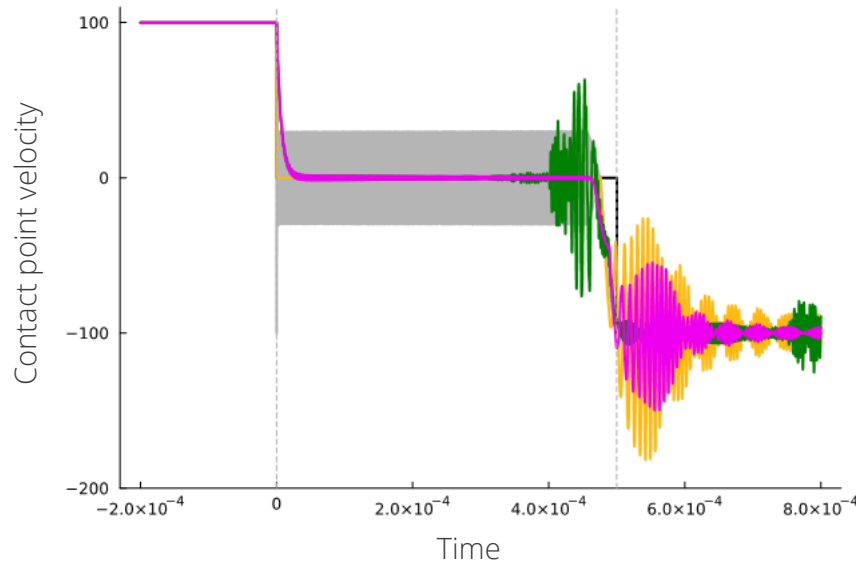
- **Lagrange Multiplier methods:** artificial oscillations during the contact phase and after the release

Contact point velocity



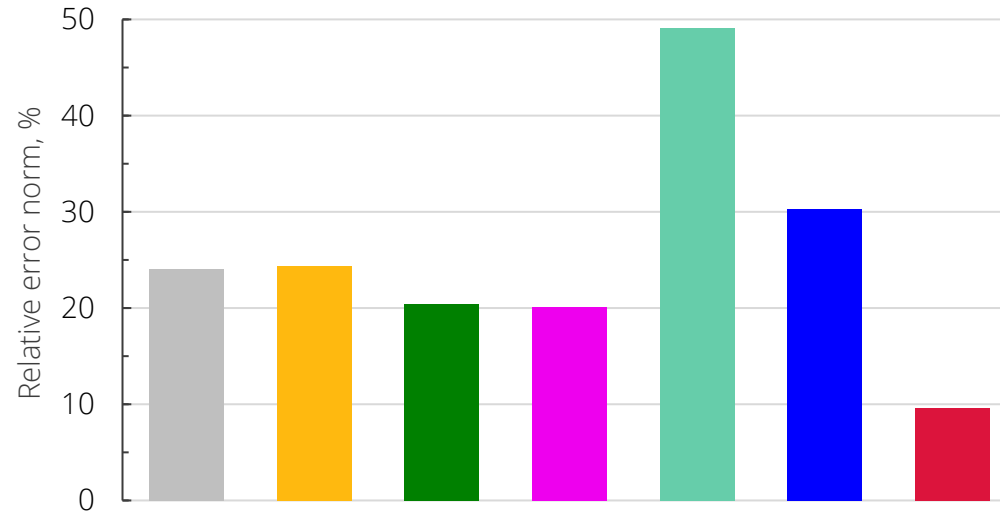
- **Lagrange Multiplier methods:** artificial oscillations during the contact phase and after the release
- **Penalty methods:** artificial oscillations during the contact phase and after the release

Contact point velocity

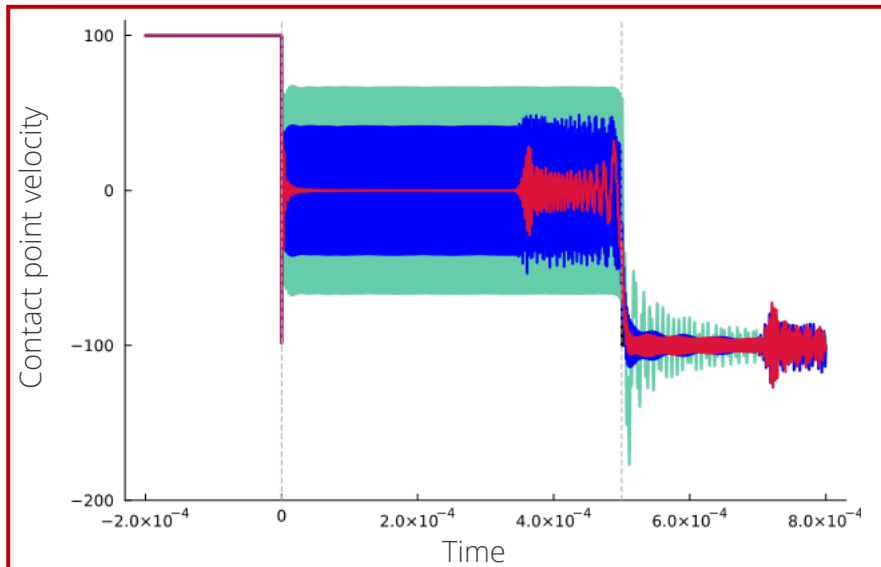


- **Lagrange Multiplier methods:** artificial oscillations during the contact phase and after the release
- **Penalty methods:** artificial oscillations during the contact phase and after the release
- **Schwarz methods:** artificial oscillations during the contact phase and after the release

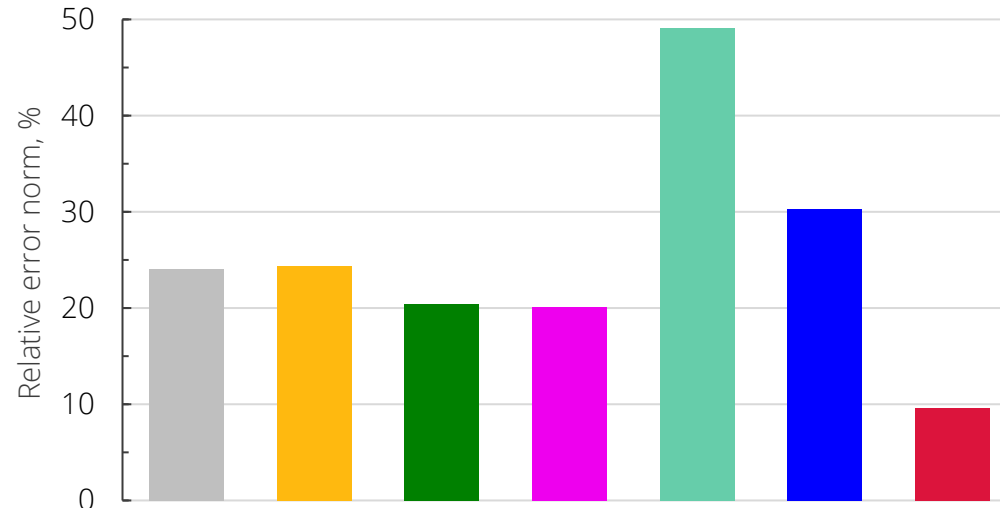
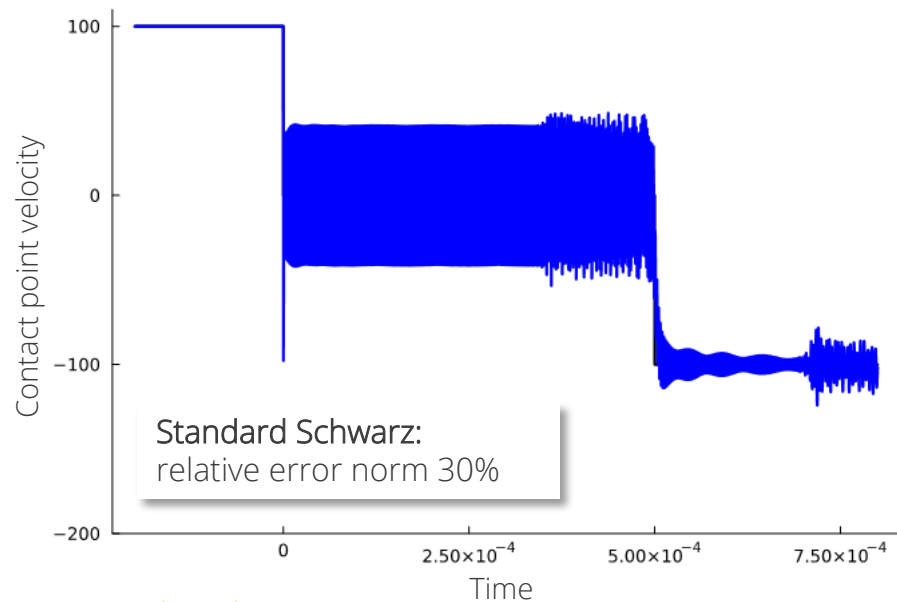
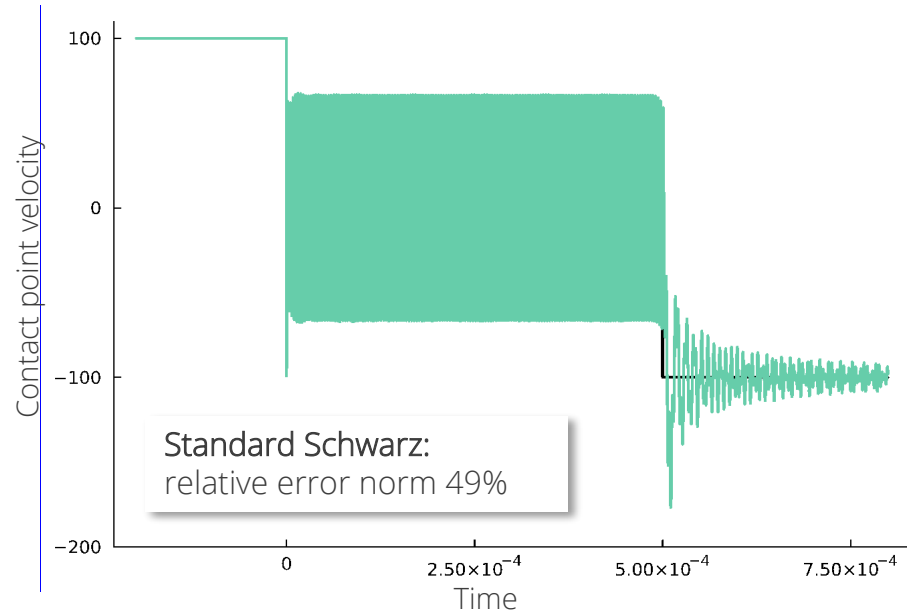
Techniques for reducing artificial oscillations



- Analytical solution
- Implicit LM
- Explicit LM
- Implicit penalty
- Explicit penalty
- Exp-Exp Schwarz
- Imp-Imp Schwarz
- Imp-Exp Schwarz

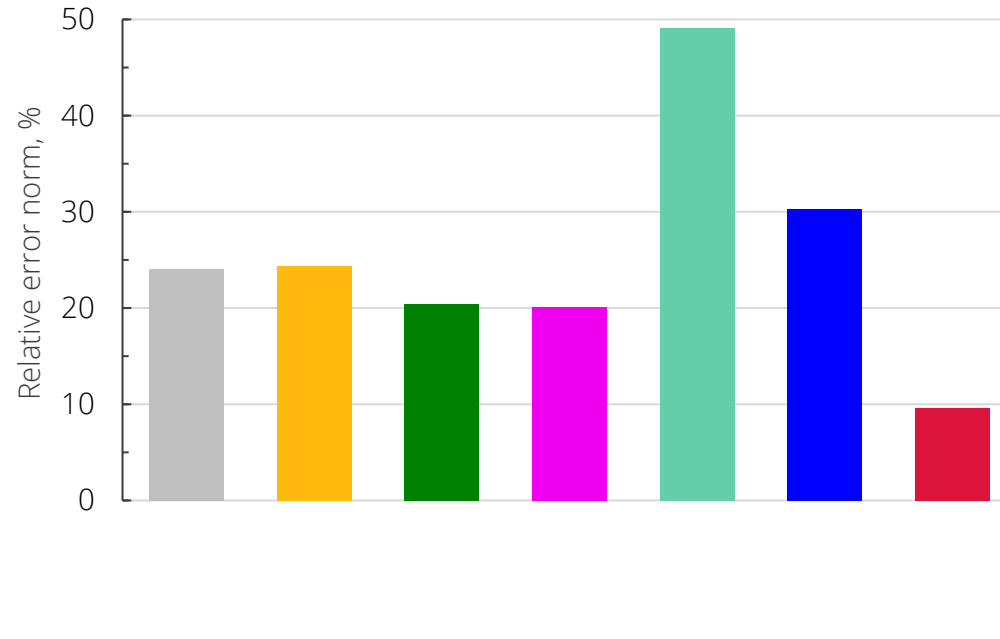
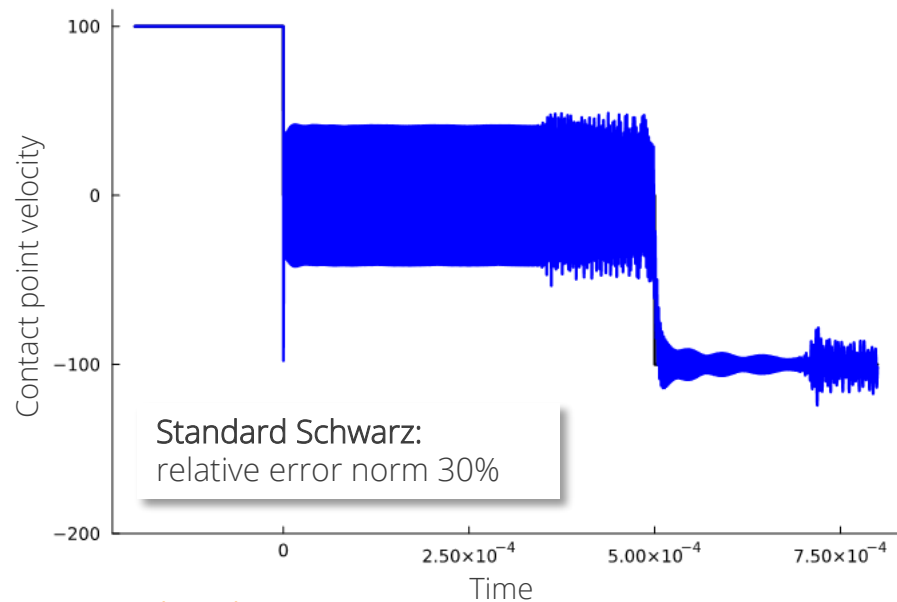
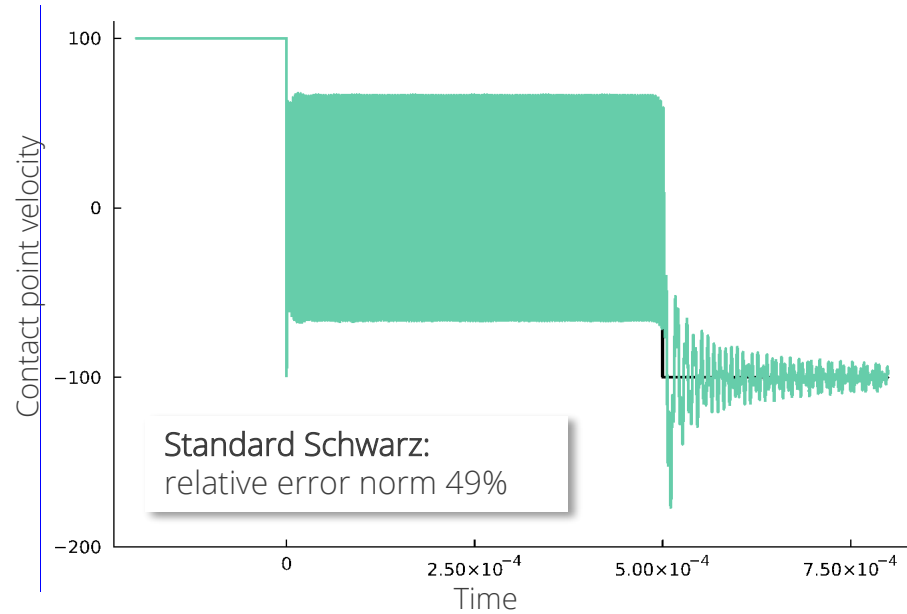


Techniques for reducing artificial oscillations



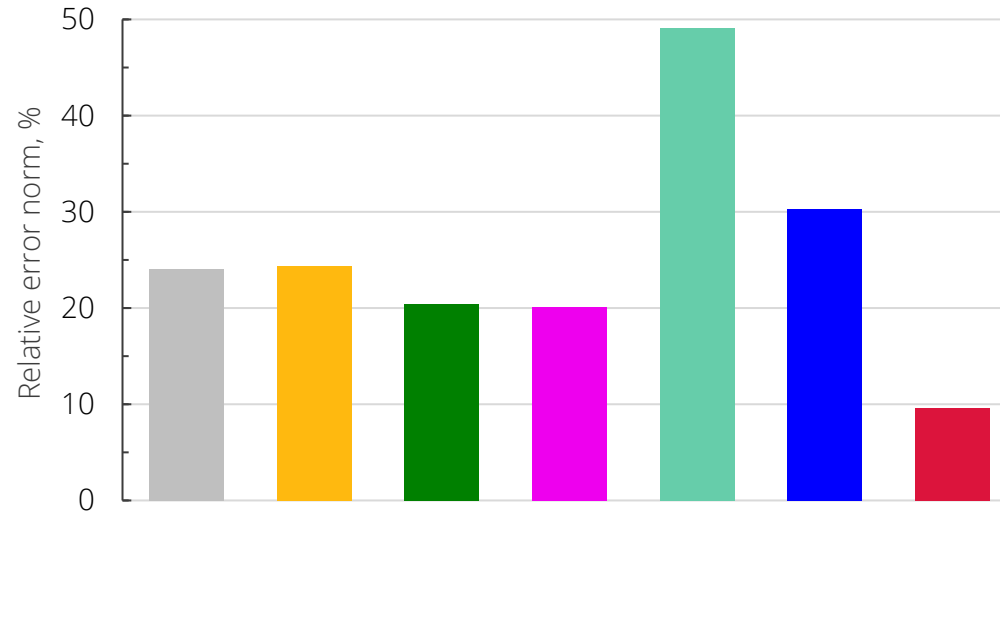
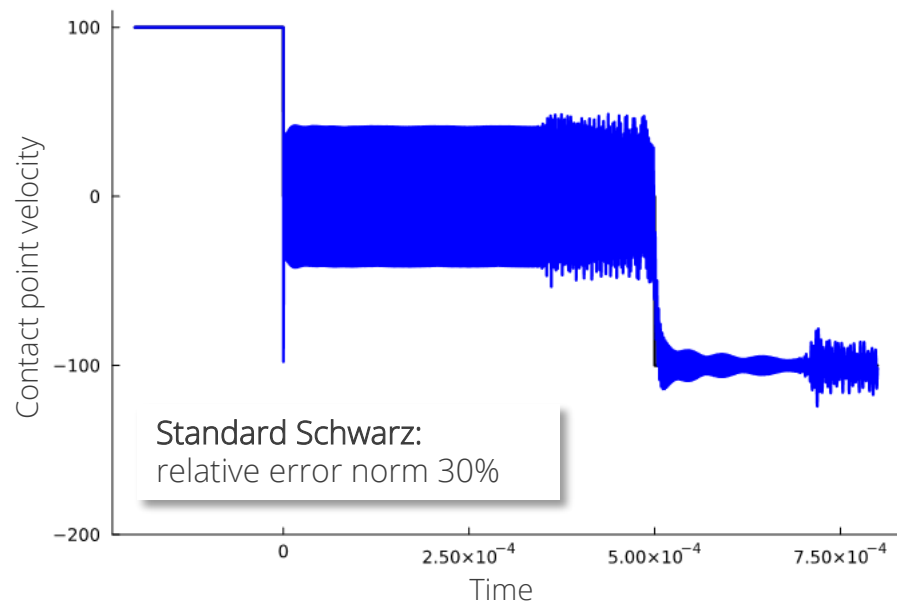
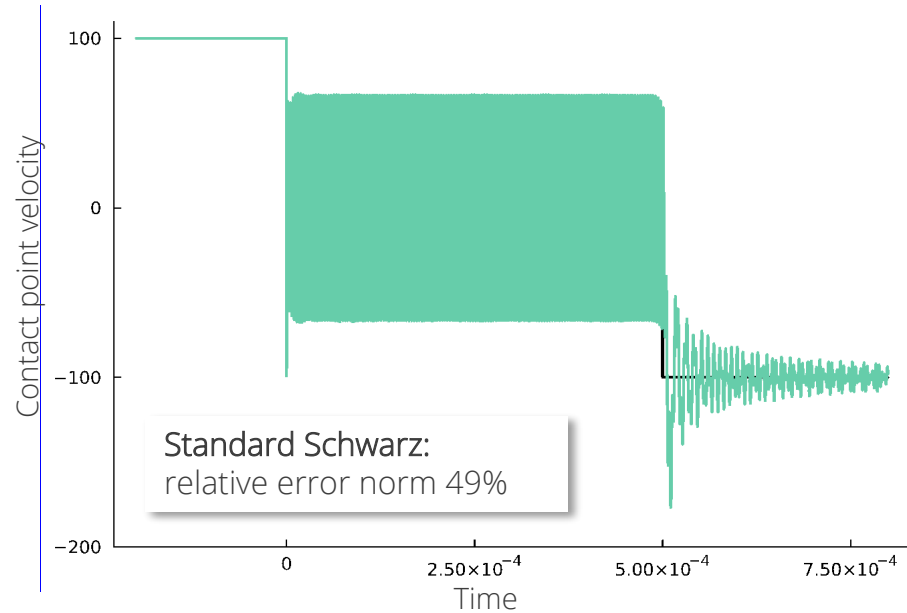
- Analytical solution
- Implicit LM
- Explicit LM
- Implicit penalty
- Explicit penalty
- Exp-Exp Schwarz
- Imp-Imp Schwarz
- Imp-Exp Schwarz

Techniques for reducing artificial oscillations



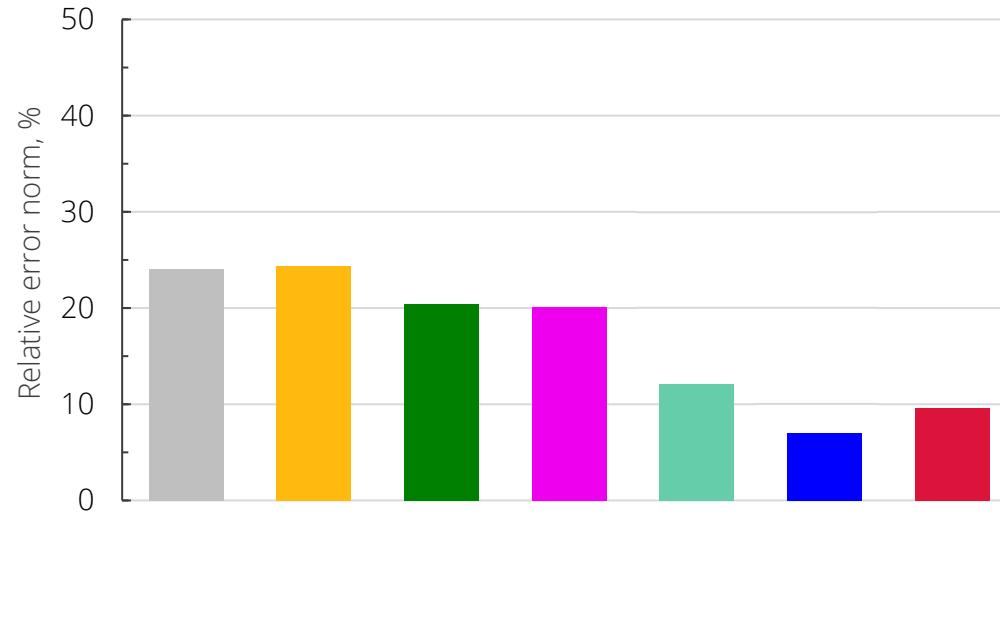
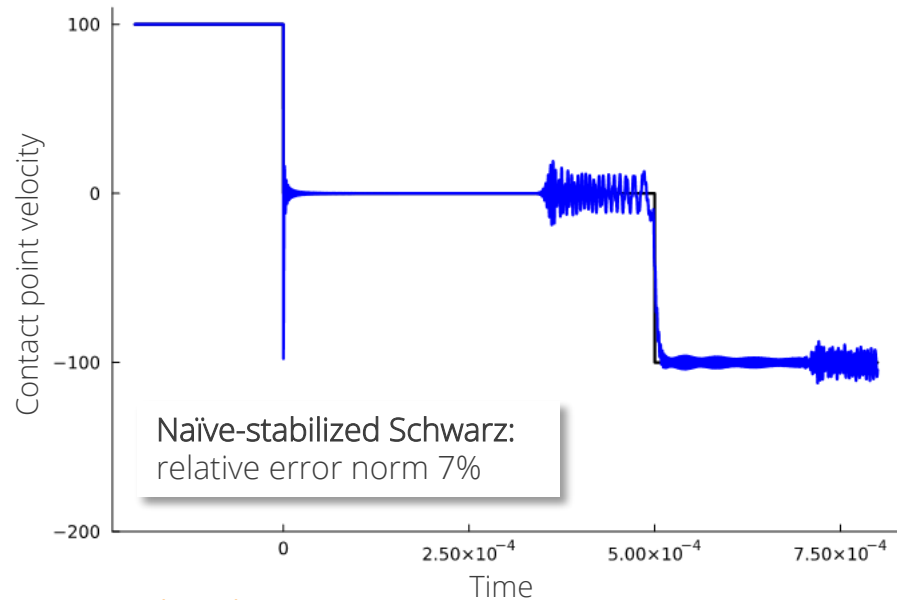
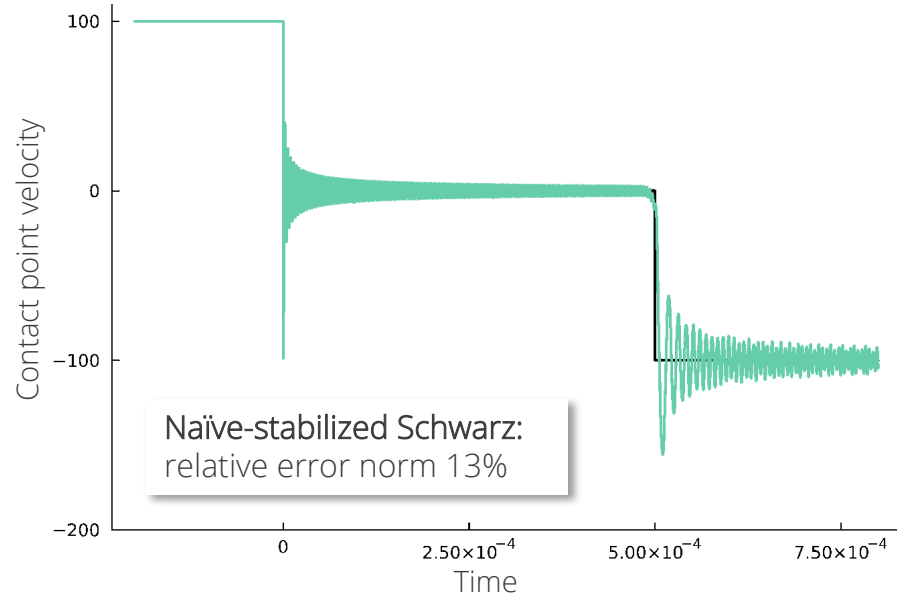
- **Contact enforcement methods:** contact laws in terms of the velocity [*M. Jean (1999)* | *J.J. Moreau. (1999)*] or position [*L. Paoli et al. (2001, 2002)*]
- **Mass redistribution methods:** reconstruct the mass matrix with zero mass assigned to nodes on the contact boundaries, keep unchanged the invariants of original mass matrix [*H. Khenous et al. (2008)* | *C. Hager et al. (2008)*]
- **Time integrators introducing numerical dissipation:** modified variants of the Newmark-beta scheme [*A. Chaudhary et al. (1986)* | *J. Chung et al. (1994)* | *B. Tchamwa et al. (1999)* | *T. C. Fung et al. (2003)*]
- **Stabilization methods:** make the inertia on the contact boundary vanish [*C. Kane et al. (1999)* | *P. Deuffhard et al. (2008)* | *D. Doyen et al. (2009)*]

Techniques for reducing artificial oscillations

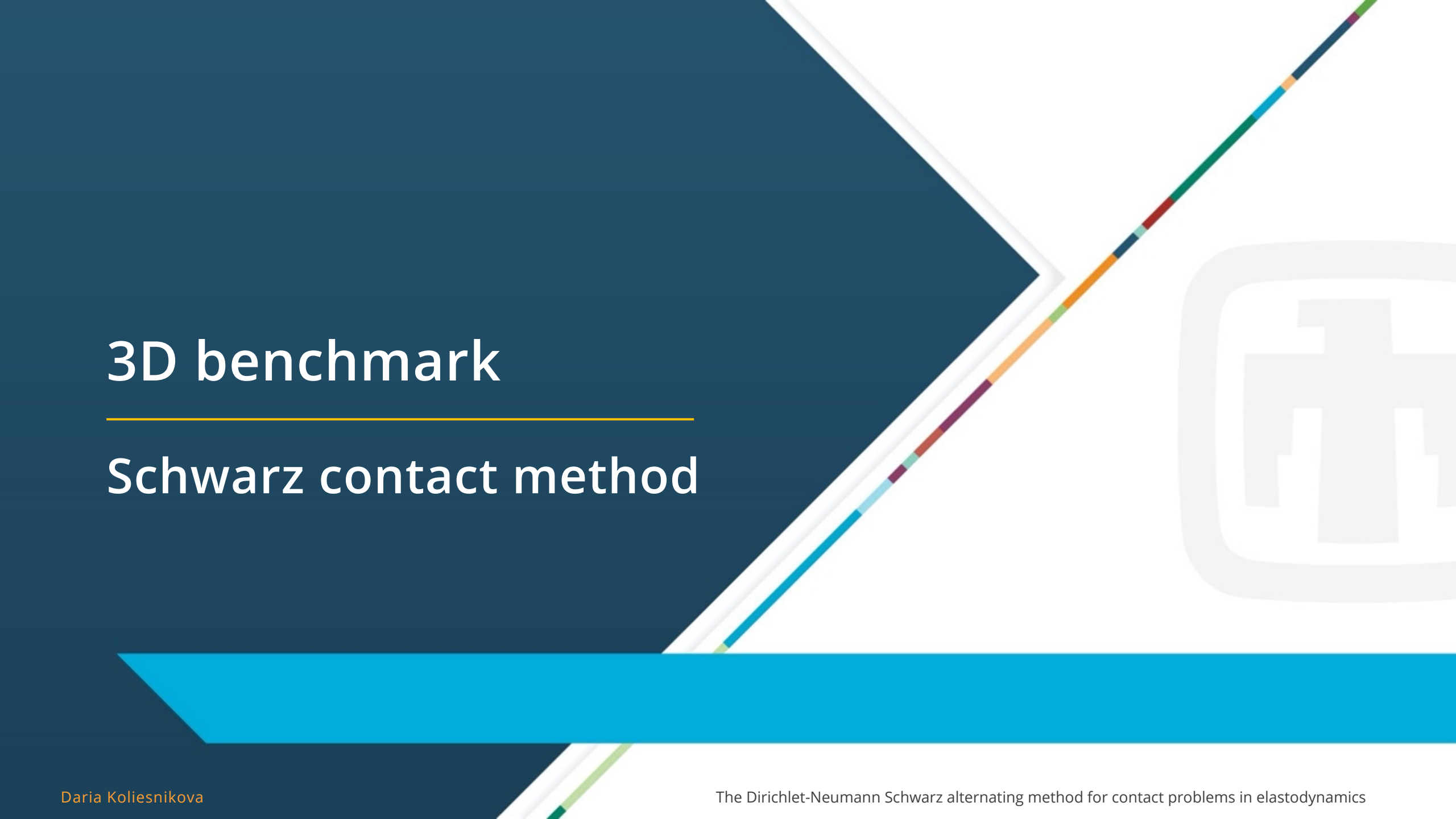


- **Contact enforcement methods:** contact laws in terms of the velocity [*M. Jean (1999)* | *J.J. Moreau. (1999)*] or position [*L. Paoli et al. (2001, 2002)*]
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- **Stabilization methods:** make the inertia on the contact boundary vanish [*C. Kane et al. (1999)* | *P. Deuffhard et al. (2008)* | *D. Doyen et al. (2009)*]
 ➤ naïve-stabilized approach: setting the contact accelerations to zero

Techniques for reducing artificial oscillations



- Significant reduction of artificial oscillations
- Global relative error smaller compared to the conventional methods
- Original Schwarz method's accuracy and energy conservation properties preserved

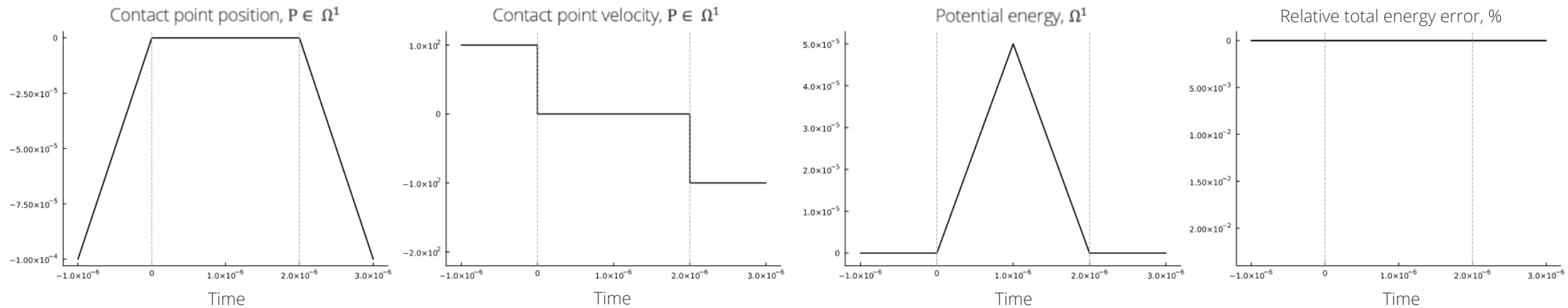


3D benchmark

Schwarz contact method

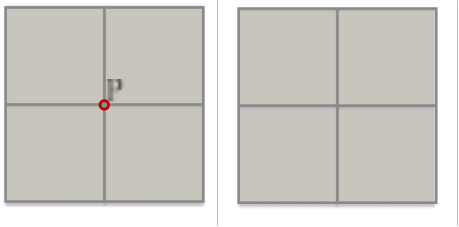
3D benchmark

Analytical solution



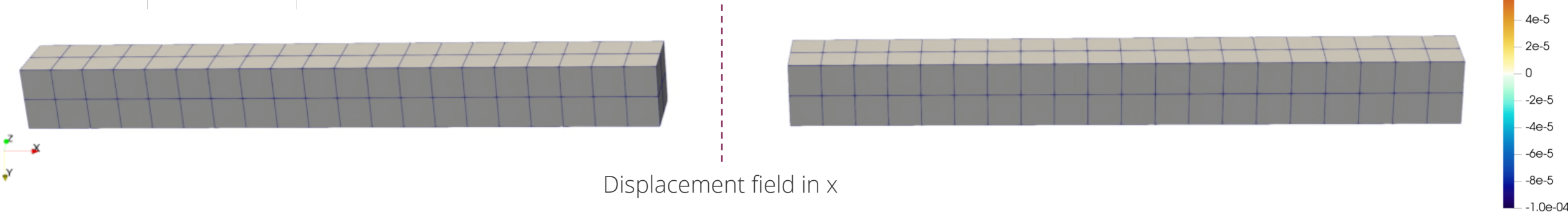
3D benchmark

Contact boundaries Γ^1 and Γ^2

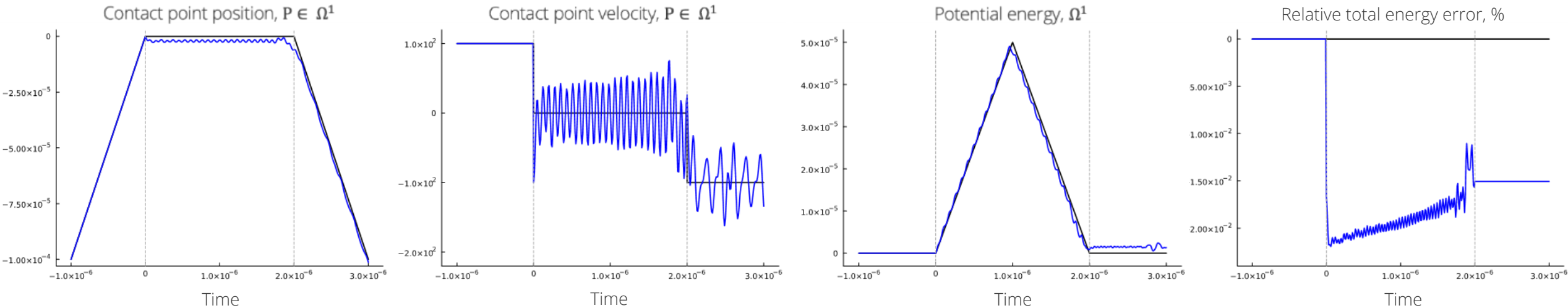


Analytical solution

	Elements type		Mesh size		Number of nodes		Time step		Average number of Schwarz iterations
	Ω^1	Ω^2	Ω^1	Ω^2	Ω^1	Ω^2	Ω^1	Ω^2	
Imp-Imp Schwarz	HEX8	HEX8	$1/2 \cdot 10^{-4}$		189		$1 \cdot 10^{-10}$		7

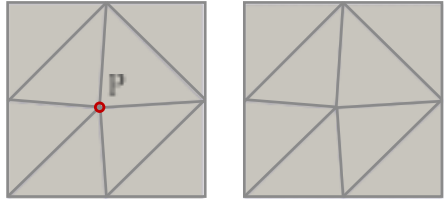


Displacement field in x



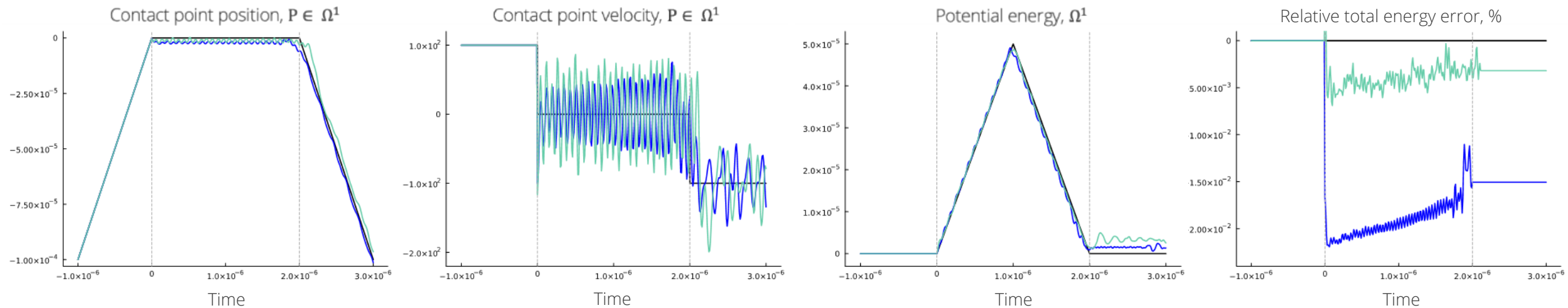
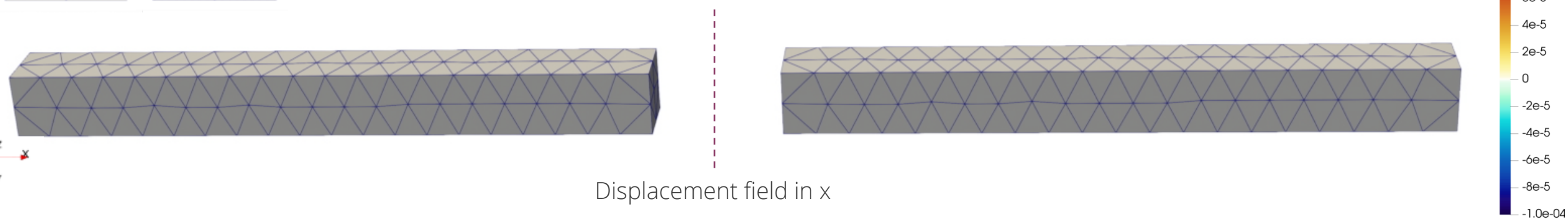
3D benchmark

Contact boundaries Γ^1 and Γ^2



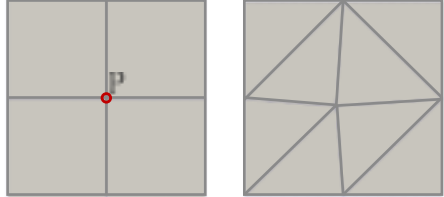
Analytical solution

	Elements type		Mesh size		Number of nodes		Time step		Average number of Schwarz iterations
	Ω^1	Ω^2	Ω^1	Ω^2	Ω^1	Ω^2	Ω^1	Ω^2	
Imp-Imp Schwarz	HEX8	HEX8	$1/2 \cdot 10^{-4}$		189		$1 \cdot 10^{-9}$		7
Exp-Exp Schwarz	TETRA4	TETRA4	$1/2 \cdot 10^{-4}$		199		$1 \cdot 10^{-9}$		6



3D benchmark

Contact boundaries Γ^1 and Γ^2



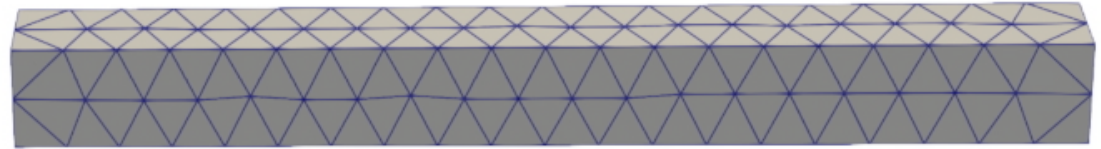
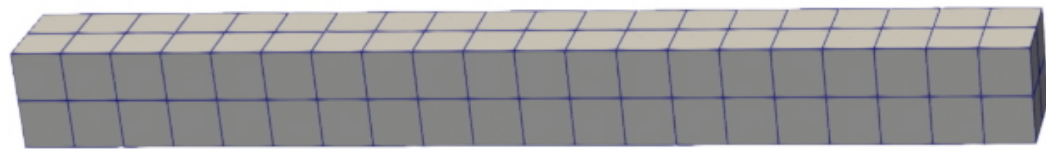
Analytical solution

Imp-Imp Schwarz

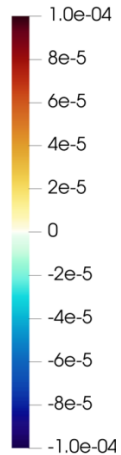
Exp-Exp Schwarz

Imp-Exp Schwarz

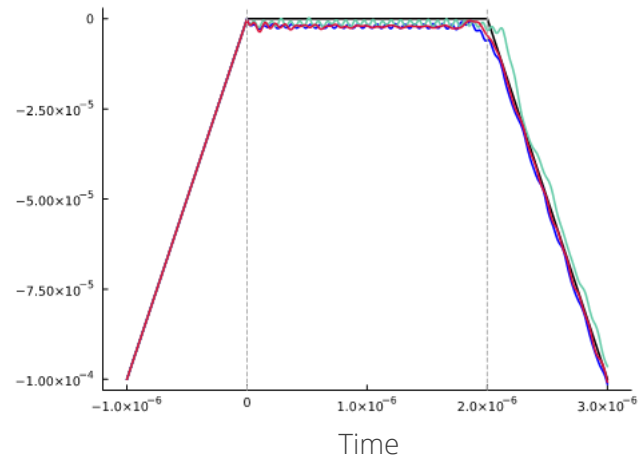
	Elements type		Mesh size		Number of nodes		Time step		Average number of Schwarz iterations
	Ω^1	Ω^2	Ω^1	Ω^2	Ω^1	Ω^2	Ω^1	Ω^2	
Imp-Imp Schwarz	HEX8	HEX8	$1/2 \cdot 10^{-4}$		189		$1 \cdot 10^{-8}$		7
Exp-Exp Schwarz	TETRA4	TETRA4	$1/2 \cdot 10^{-4}$		199		$1 \cdot 10^{-9}$		6
Imp-Exp Schwarz	HEX8	TETRA4	$1/2 \cdot 10^{-4}$		189	199	$1/2 \cdot 10^{-8}$	$1 \cdot 10^{-9}$	6



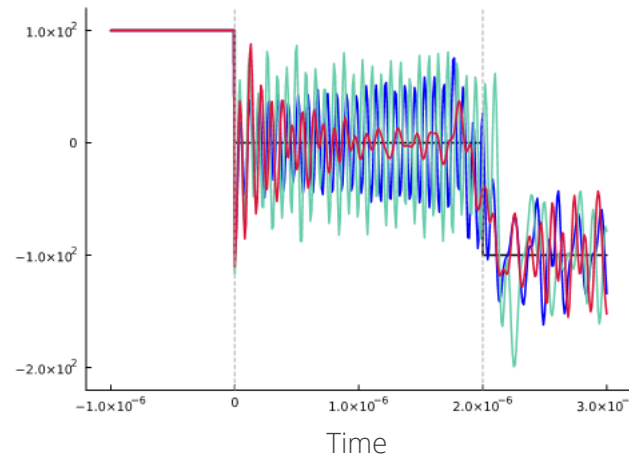
Displacement field in x



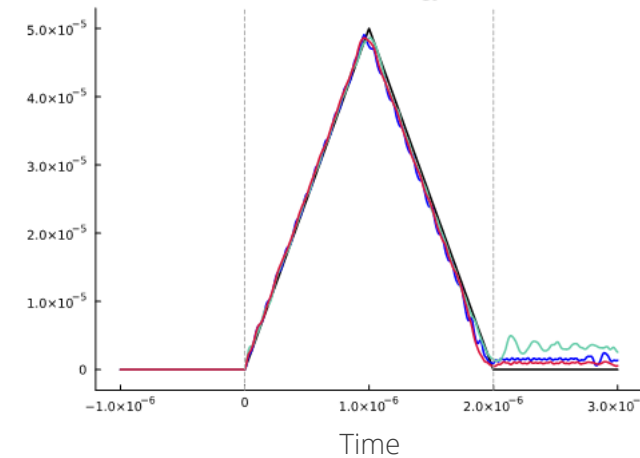
Contact point position, $P \in \Omega^1$



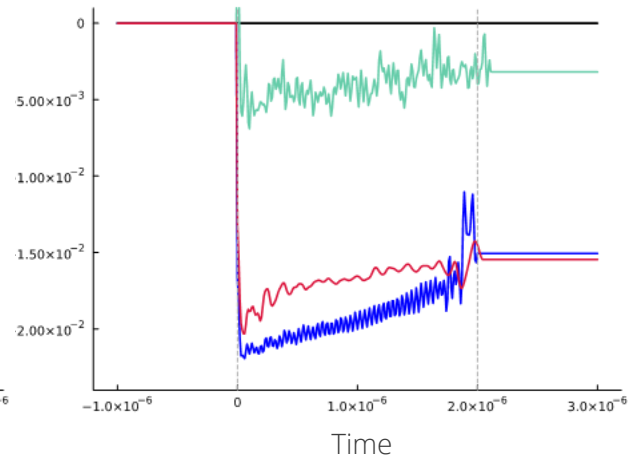
Contact point velocity, $P \in \Omega^1$



Potential energy, Ω^1

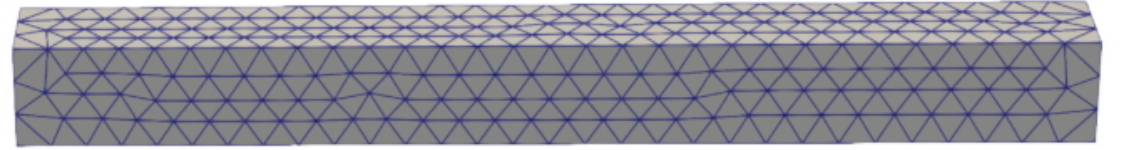
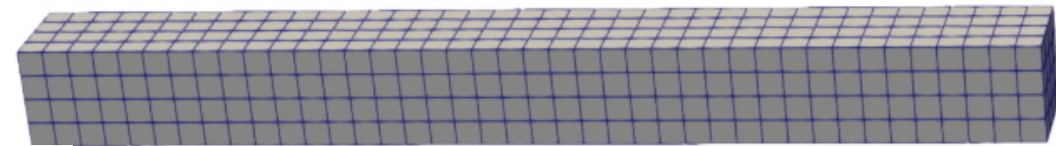
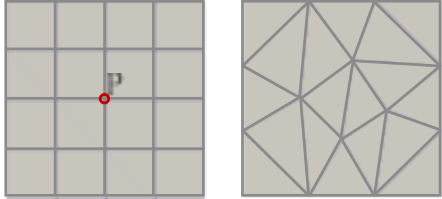


Relative total energy error, %



3D benchmark

Contact boundaries Γ^1 and Γ^2

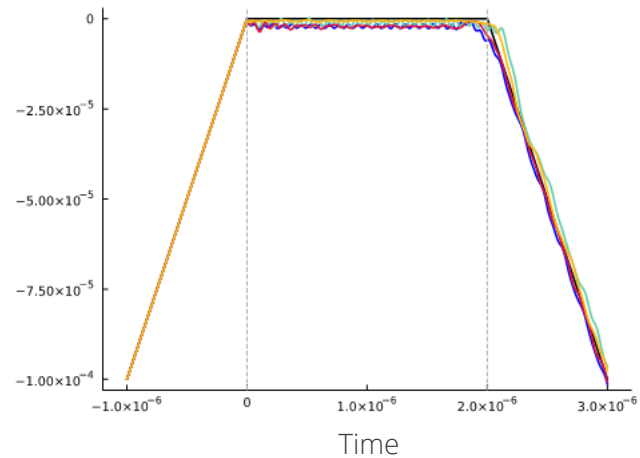


Displacement field in x

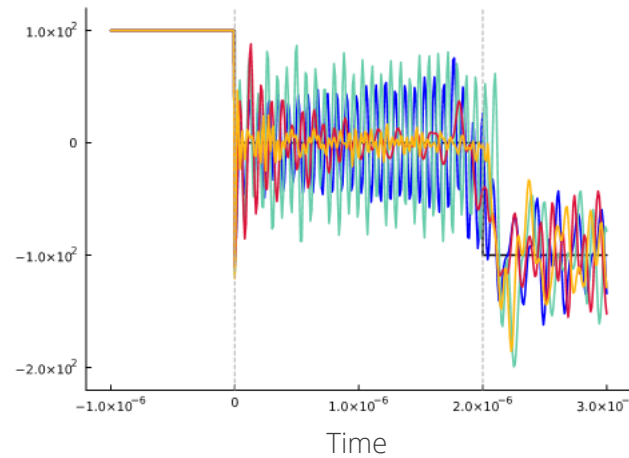
Analytical solution

	Elements type		Mesh size		Number of nodes		Time step		Average number of Schwarz iterations
	Ω^1	Ω^2	Ω^1	Ω^2	Ω^1	Ω^2	Ω^1	Ω^2	
Imp-Imp Schwarz	HEX8	HEX8	$1/2 \cdot 10^{-4}$		189		$1 \cdot 10^{-8}$		7
Exp-Exp Schwarz	TETRA4	TETRA4	$1/2 \cdot 10^{-4}$		199		$1 \cdot 10^{-9}$		6
Imp-Exp Schwarz	HEX8	TETRA4	$1/2 \cdot 10^{-4}$		189	199	$1/2 \cdot 10^{-8}$	$1 \cdot 10^{-9}$	6
Exp-Imp Schwarz	HEX8	TETRA4	$1/4 \cdot 10^{-4}$	$1/3 \cdot 10^{-4}$	1025	745	$1 \cdot 10^{-9}$	$1/2 \cdot 10^{-8}$	8

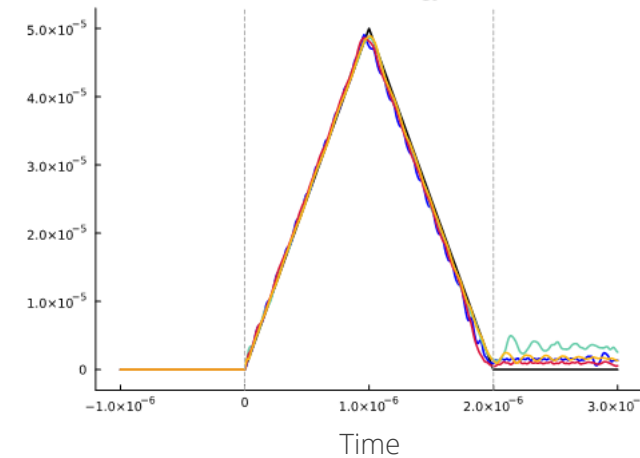
Contact point position, $P \in \Omega^1$



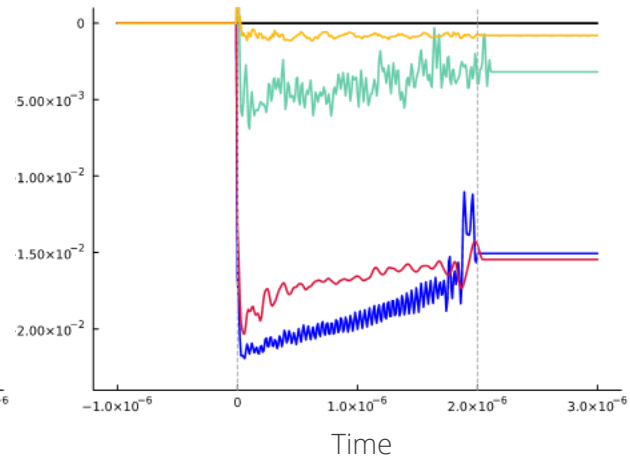
Contact point velocity, $P \in \Omega^1$



Potential energy, Ω^1



Relative total energy error, %

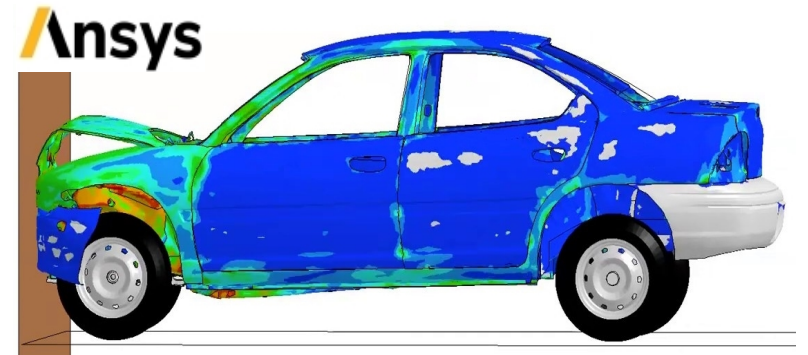
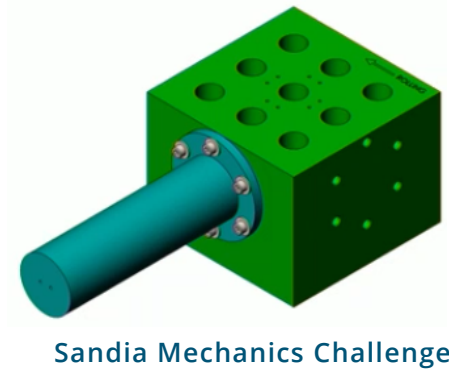
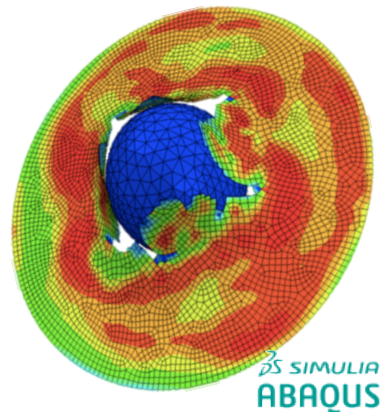
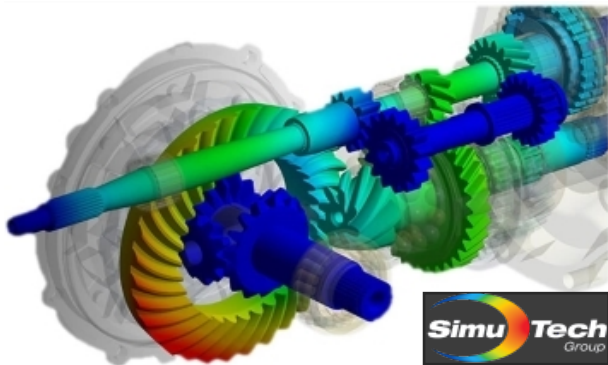


Summary and perspectives



Summary

- Schwarz contact method: a promising alternative to conventional contact methods
 - Accurate predictions of quantities of interest
 - Remarkable energy conservation
 - Different integrators, times steps, mesh resolutions and mesh types !

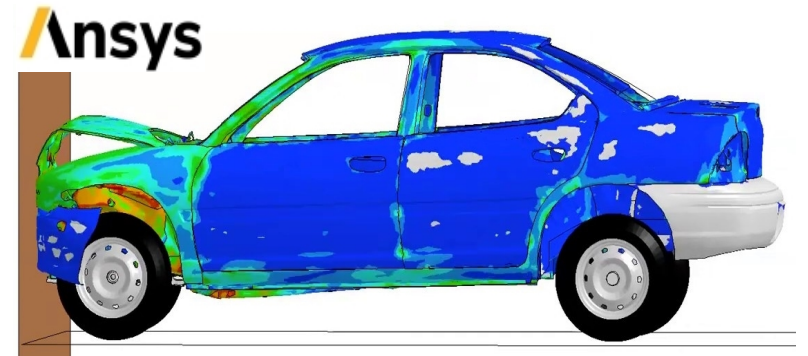
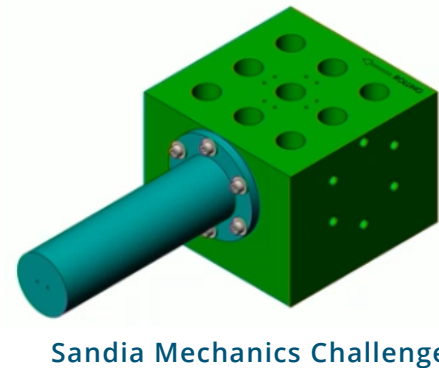
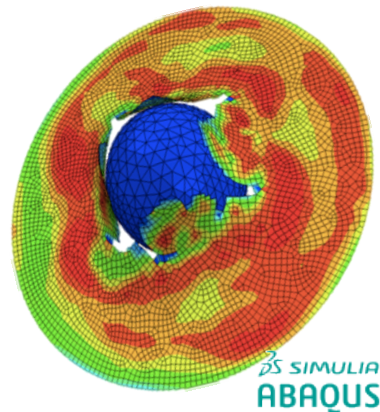
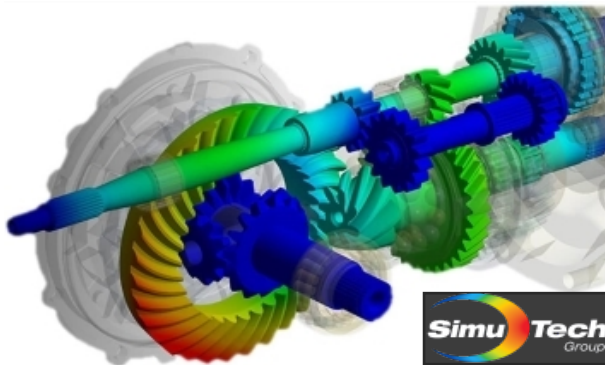


Summary

- Schwarz contact method: a promising alternative to conventional contact methods
 - Accurate predictions of quantities of interest
 - Remarkable energy conservation
 - Different integrators, times steps, mesh resolutions and mesh types !

Ongoing/future work

- Julia prototype for multidimensional Schwarz methods: <https://github.com/lxmota/norma>
 - Schwarz-based contact method
 - Schwarz-based coupling/multiphysics algorithm (overlapping and non-overlapping approaches)
- Adding friction, rolling, sliding conditions, ...
- Implementation in the Sandia's production codes (Sierra/SM, Albany)





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Thank you for your attention!



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