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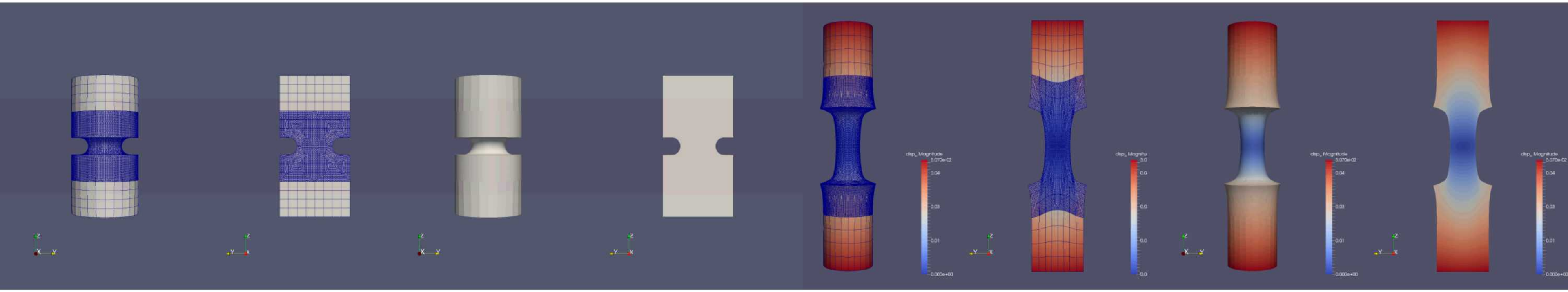

The Schwarz Alternating Method for Concurrent Multiscale in Finite Deformation Solid Mechanics

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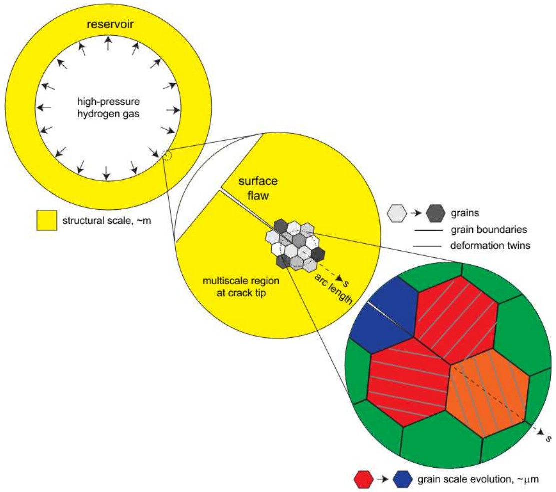
Concurrent Multiscale Coupling

- Large scale structural failure frequently originates from small scale phenomena such as defects, microcracks, inhomogeneites and more.
- Failure occurs due to tightly coupled interaction between small scale (stress concentrations, material instabilities, cracks, etc.) and large scale (vibration, impact, high loads and other perturbations).
- Concurrent multiscale methods are essential for understanding and prediction of behavior of engineering systems when a small scale failure determines the performance of the entire system.

Roof failure of Boeing 737 aircraft due to fatigue cracks. From *imechanica.org*



Surface flaw in pressure vessel by J. Foulk.

Previous Efforts on Concurrent Multiscale Coupling

Comput Mech (2014) 54:803–820
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ORIGINAL PAPER

A multiscale overlapped coupling formulation for large-deformation strain localization

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Abstract We generalize the multiscale overlapped domain framework to couple multiple rate-independent standard dissipative material models in the finite deformation regime across different length scales. We show that a fully coupled multiscale incremental boundary-value problem can be recast as the stationary point that optimizes the partitioned incremental work of a three-field energy functional. We also establish inf-sup tests to examine the numerical stability issues that arise from enforcing weak compatibility in the three-field formulation. We also devise a new block solver for the domain coupling problem and demonstrate the performance of the formulation with one-dimensional numerical examples. These simulations indicate that it is sufficient to introduce a localization limiter in a confined region of interest to regularize the partial differential equation if loss of ellipticity occurs.

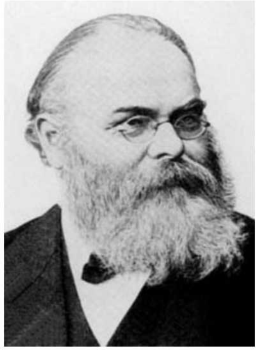
strain localization may lead to the eventual failure of materials, this phenomenon is of significant importance to modern engineering applications.

The objective of this work is to introduce concurrent coupling between sub-scale and macro-scale simulations for inelastic materials that are prone to strain localization. Since it is not feasible to conduct sub-scale simulations on macroscopic problems, we use the domain coupling method such that computational resources can be efficiently allocated to regions of interest [14,23,24,30]. To the best of our knowledge, this is the first work focusing on utilizing the domain coupling method to model strain localization in inelastic materials undergoing large deformation.

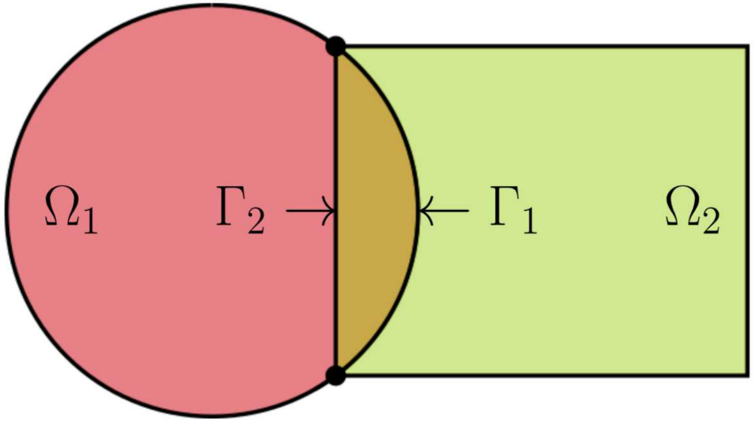
Nevertheless, modeling strain localization with the conventional finite element method may lead to spurious mesh-dependent results due to the loss of ellipticity at the onset of strain localization [31]. To circumvent the loss of mate-

Schwarz Alternating Method for Domain Decomposition

- First developed in 1870 for solving Laplace's equation in irregularly shaped domains.
- Simple idea: if the solution is known in regularly shaped domains, use those as pieces to iteratively build a solution for the more complex domain.



Karl Hermann Amandus Schwarz (1843 – 1921). Source: *bibmath.net*



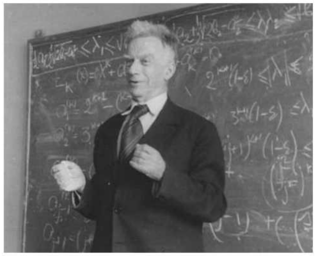
- Initialize:
  - Solve PDE by any method on Ω_1 using an initial guess for Dirichlet BCs on Γ_1.
- Iterate until convergence:
  - Solve PDE by any method (can be different than for Ω_1) on Ω_2 using Dirichlet BCs on Γ_2 that are the values just obtained for Ω_1.
  - Solve PDE by any method (can be different than for Ω_2) on Ω_1 using Dirichlet BCs on Γ_1 that are the values just obtained for Ω_2.

The Schwarz Alternating Method after Schwarz

- S. L. Sobolev posed the Schwarz method for linear elasticity in variational form and proved convergence of the method for linear elasticity in 1936 by proposing a convergent sequence of energy functionals.
- Convergence for general linear elliptic partial differential equations was not proved until much later by S. G. Mikhlin (1951) and I. Babuška (1956).
- We have adapted the alternating Schwarz for the finite deformation, nonlinear PDE and determined that the it converges geometrically for the finite deformation problem. *Computer Methods in Applied Mechanics and Engineering (2017)*.

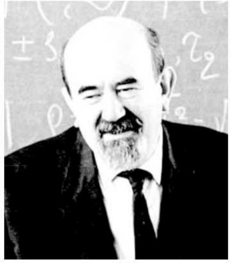
$$\Phi[\boldsymbol{\varphi}] = \int_B W(\boldsymbol{F}, \boldsymbol{Z}, T)\, dV - \int_B \boldsymbol{B} \cdot \boldsymbol{\varphi}\, dV - \int_{\partial_T B} \bar{\boldsymbol{T}} \cdot \boldsymbol{\varphi}\, dS$$

$$\mathrm{Div}\, \boldsymbol{P} + \boldsymbol{B} = \boldsymbol{0}$$



Sergei Lvovich Sobolev (1908 – 1989).

Source: *www.math.nsc.ru*



Solomon Grigoryevich Mikhlin (1908 – 1990). Source: *www-history.mcs.st-andrews.ac.uk*

Ivo Babuška

(1926). Source: *www-history.mcs.st-andrews.ac.uk*

Schwarz Alternating Method for Multiscale Coupling in Quasistatics

$\boldsymbol{\varphi}^{(0)} \leftarrow \mathrm{id}_{\boldsymbol{X}}$ in Ω_2 ▷ initialize to zero displacement or a better guess in Ω_2

$n \leftarrow 1$

repeat ▷ Schwarz loop

  $\boldsymbol{\varphi}^{(n)} \leftarrow \boldsymbol{\chi}$ on $\partial_{\boldsymbol{\varphi}}\Omega_i$ ▷ Dirichlet BC for Ω_i

  $\boldsymbol{\varphi}^{(n)} \leftarrow P_{\Omega_j \to \Gamma_i}[\boldsymbol{\varphi}^{(n-1)}]$ on Γ_i ▷ Schwarz BC for Ω_i

  $\boldsymbol{\varphi}^{(n)} \leftarrow \arg\min_{\boldsymbol{\varphi} \in \mathcal{S}_i} \Phi_i[\boldsymbol{\varphi}]$ in Ω_i ▷ solve in Ω_i

  $n \leftarrow n + 1$

until converged

- It allows the coupling of regions with different meshes, different element types, levels of refinement, and non-conforming.
- Information is exchanged among two or more regions, thus the coupling is concurrent.
- Different solvers can be used for the different regions.
- Different material models can be coupled provided that they are compatible in the overlap region.
- Conceptually very simple.

Four Variants of the Schwarz Alternating Method

$\boldsymbol{x}_B^{(1)} \leftarrow \boldsymbol{X}_B^{(1)}$ in Ω_1, $\boldsymbol{x}_b^{(1)} \leftarrow \chi(\boldsymbol{X}_b^{(1)})$ on $\partial_\varphi\Omega_1$, $\boldsymbol{x}_\beta^{(1)} \leftarrow \boldsymbol{X}_\beta^{(1)}$ on Γ_1 ▷ initialize for Ω_1
$\boldsymbol{x}_B^{(2)} \leftarrow \boldsymbol{X}_B^{(2)}$ in Ω_2, $\boldsymbol{x}_b^{(2)} \leftarrow \chi(\boldsymbol{X}_b^{(2)})$ on $\partial_\varphi\Omega_2$, $\boldsymbol{x}_\beta^{(2)} \leftarrow \boldsymbol{X}_\beta^{(2)}$ on Γ_2 ▷ initialize for Ω_2
repeat ▷ Schwarz loop
    $\boldsymbol{y}^{(1)} \leftarrow \boldsymbol{x}_B^{(1)}$ ▷ for convergence check
    $\boldsymbol{x}_\beta^{(1)} \leftarrow \boldsymbol{P}_{12}\boldsymbol{x}_B^{(2)} + \boldsymbol{Q}_{12}\boldsymbol{x}_b^{(2)} + \boldsymbol{G}_{12}\boldsymbol{x}_\beta^{(2)}$ ▷ project from Ω_2 to Γ_1
    repeat ▷ Newton loop for Ω_1
        $\Delta\boldsymbol{x}_B^{(1)} \leftarrow -\boldsymbol{K}_{AB}^{(1)}(\boldsymbol{x}_B^{(1)};\boldsymbol{x}_b^{(1)};\boldsymbol{x}_\beta^{(1)})\backslash\boldsymbol{R}_A^{(1)}(\boldsymbol{x}_B^{(1)};\boldsymbol{x}_b^{(1)};\boldsymbol{x}_\beta^{(1)})$ ▷ linear system
        $\boldsymbol{x}_B^{(1)} \leftarrow \boldsymbol{x}_B^{(1)} + \Delta\boldsymbol{x}_B^{(1)}$
    until $||\Delta\boldsymbol{x}_B^{(1)}||/||\boldsymbol{x}_B^{(1)}|| \leq \epsilon_{\text{machine}}$ ▷ tight tolerance
    $\boldsymbol{y}^{(2)} \leftarrow \boldsymbol{x}_B^{(2)}$ ▷ for convergence check
    $\boldsymbol{x}_\beta^{(2)} \leftarrow \boldsymbol{P}_{21}\boldsymbol{x}_B^{(1)} + \boldsymbol{Q}_{21}\boldsymbol{x}_b^{(1)} + \boldsymbol{G}_{21}\boldsymbol{x}_\beta^{(1)}$ ▷ project from Ω_1 to Γ_2
    repeat ▷ Newton loop for Ω_2
        $\Delta\boldsymbol{x}_B^{(2)} \leftarrow -\boldsymbol{K}_{AB}^{(2)}(\boldsymbol{x}_B^{(2)};\boldsymbol{x}_b^{(2)};\boldsymbol{x}_\beta^{(2)})\backslash\boldsymbol{R}_A^{(2)}(\boldsymbol{x}_B^{(2)};\boldsymbol{x}_b^{(2)};\boldsymbol{x}_\beta^{(2)})$ ▷ linear system
        $\boldsymbol{x}_B^{(2)} \leftarrow \boldsymbol{x}_B^{(2)} + \Delta\boldsymbol{x}_B^{(2)}$
    until $||\Delta\boldsymbol{x}_B^{(2)}||/||\boldsymbol{x}_B^{(2)}|| \leq \epsilon_{\text{machine}}$ ▷ tight tolerance
until $\left[\left(||\boldsymbol{y}^{(1)} - \boldsymbol{x}_B^{(1)}||/||\boldsymbol{x}_B^{(1)}||\right)^2 + \left(||\boldsymbol{y}^{(2)} - \boldsymbol{x}_B^{(2)}||/||\boldsymbol{x}_B^{(2)}||\right)^2\right]^{1/2} \leq \epsilon_{\text{machine}}$ ▷ tight tolerance

Full Schwarz

$\boldsymbol{x}_B^{(1)} \leftarrow \boldsymbol{X}_B^{(1)}$ in Ω_1, $\boldsymbol{x}_b^{(1)} \leftarrow \chi(\boldsymbol{X}_b^{(1)})$ on $\partial_\varphi\Omega_1$, $\boldsymbol{x}_\beta^{(1)} \leftarrow \boldsymbol{X}_\beta^{(1)}$ on Γ_1 ▷ initialize for Ω_1
$\boldsymbol{x}_B^{(2)} \leftarrow \boldsymbol{X}_B^{(2)}$ in Ω_2, $\boldsymbol{x}_b^{(2)} \leftarrow \chi(\boldsymbol{X}_b^{(2)})$ on $\partial_\varphi\Omega_2$, $\boldsymbol{x}_\beta^{(2)} \leftarrow \boldsymbol{X}_\beta^{(2)}$ on Γ_2 ▷ initialize for Ω_2
repeat ▷ Newton-Schwarz loop
    $\boldsymbol{x}_\beta^{(1)} \leftarrow \boldsymbol{P}_{12}\boldsymbol{x}_B^{(2)} + \boldsymbol{Q}_{12}\boldsymbol{x}_b^{(2)} + \boldsymbol{G}_{12}\boldsymbol{x}_\beta^{(2)}$ ▷ project from Ω_2 to Γ_1
    $\Delta\boldsymbol{x}_B^{(1)} \leftarrow -\boldsymbol{K}_{AB}^{(1)}(\boldsymbol{x}_B^{(1)};\boldsymbol{x}_b^{(1)};\boldsymbol{x}_\beta^{(1)})\backslash\boldsymbol{R}_A^{(1)}(\boldsymbol{x}_B^{(1)};\boldsymbol{x}_b^{(1)};\boldsymbol{x}_\beta^{(1)})$ ▷ linear system
    $\boldsymbol{x}_B^{(1)} \leftarrow \boldsymbol{x}_B^{(1)} + \Delta\boldsymbol{x}_B^{(1)}$
    $\boldsymbol{x}_\beta^{(2)} \leftarrow \boldsymbol{P}_{21}\boldsymbol{x}_B^{(1)} + \boldsymbol{Q}_{21}\boldsymbol{x}_b^{(1)} + \boldsymbol{G}_{21}\boldsymbol{x}_\beta^{(1)}$ ▷ project from Ω_1 to Γ_2
    $\Delta\boldsymbol{x}_B^{(2)} \leftarrow -\boldsymbol{K}_{AB}^{(2)}(\boldsymbol{x}_B^{(2)};\boldsymbol{x}_b^{(2)};\boldsymbol{x}_\beta^{(2)})\backslash\boldsymbol{R}_A^{(2)}(\boldsymbol{x}_B^{(2)};\boldsymbol{x}_b^{(2)};\boldsymbol{x}_\beta^{(2)})$ ▷ linear system
    $\boldsymbol{x}_B^{(2)} \leftarrow \boldsymbol{x}_B^{(2)} + \Delta\boldsymbol{x}_B^{(2)}$
until $\left[\left(||\Delta\boldsymbol{x}_B^{(1)}||/||\boldsymbol{x}_B^{(1)}||\right)^2 + \left(||\Delta\boldsymbol{x}_B^{(2)}||/||\boldsymbol{x}_B^{(2)}||\right)^2\right]^{1/2} \leq \epsilon_{\text{machine}}$ ▷ tight tolerance

Modified Schwarz

$\boldsymbol{x}_B^{(1)} \leftarrow \boldsymbol{X}_B^{(1)}$ in Ω_1, $\boldsymbol{x}_b^{(1)} \leftarrow \chi(\boldsymbol{X}_b^{(1)})$ on $\partial_\varphi\Omega_1$, $\boldsymbol{x}_\beta^{(1)} \leftarrow \boldsymbol{X}_\beta^{(1)}$ on Γ_1 ▷ initialize for Ω_1
$\boldsymbol{x}_B^{(2)} \leftarrow \boldsymbol{X}_B^{(2)}$ in Ω_2, $\boldsymbol{x}_b^{(2)} \leftarrow \chi(\boldsymbol{X}_b^{(2)})$ on $\partial_\varphi\Omega_2$, $\boldsymbol{x}_\beta^{(2)} \leftarrow \boldsymbol{X}_\beta^{(2)}$ on Γ_2 ▷ initialize for Ω_2
repeat ▷ Schwarz loop
    $\boldsymbol{y}^{(1)} \leftarrow \boldsymbol{x}_B^{(1)}$ ▷ for convergence check
    $\boldsymbol{x}_\beta^{(1)} \leftarrow \boldsymbol{P}_{12}\boldsymbol{x}_B^{(2)} + \boldsymbol{Q}_{12}\boldsymbol{x}_b^{(2)} + \boldsymbol{G}_{12}\boldsymbol{x}_\beta^{(2)}$ ▷ project from Ω_2 to Γ_1
    repeat ▷ Newton loop for Ω_1
        $\Delta\boldsymbol{x}_B^{(1)} \leftarrow -\boldsymbol{K}_{AB}^{(1)}(\boldsymbol{x}_B^{(1)};\boldsymbol{x}_b^{(1)};\boldsymbol{x}_\beta^{(1)})\backslash\boldsymbol{R}_A^{(1)}(\boldsymbol{x}_B^{(1)};\boldsymbol{x}_b^{(1)};\boldsymbol{x}_\beta^{(1)})$ ▷ linear system
        $\boldsymbol{x}_B^{(1)} \leftarrow \boldsymbol{x}_B^{(1)} + \Delta\boldsymbol{x}_B^{(1)}$
    until $||\Delta\boldsymbol{x}_B^{(1)}||/||\boldsymbol{x}_B^{(1)}|| \leq \epsilon$ ▷ loose tolerance, e.g. $\epsilon \in [10^{-4}, 10^{-1}]$
    $\boldsymbol{y}^{(2)} \leftarrow \boldsymbol{x}_B^{(2)}$ ▷ for convergence check
    $\boldsymbol{x}_\beta^{(2)} \leftarrow \boldsymbol{P}_{21}\boldsymbol{x}_B^{(1)} + \boldsymbol{Q}_{21}\boldsymbol{x}_b^{(1)} + \boldsymbol{G}_{21}\boldsymbol{x}_\beta^{(1)}$ ▷ project from Ω_1 to Γ_2
    repeat ▷ Newton loop for Ω_2
        $\Delta\boldsymbol{x}_B^{(2)} \leftarrow -\boldsymbol{K}_{AB}^{(2)}(\boldsymbol{x}_B^{(2)};\boldsymbol{x}_b^{(2)};\boldsymbol{x}_\beta^{(2)})\backslash\boldsymbol{R}_A^{(2)}(\boldsymbol{x}_B^{(2)};\boldsymbol{x}_b^{(2)};\boldsymbol{x}_\beta^{(2)})$ ▷ solve linear system
        $\boldsymbol{x}_B^{(2)} \leftarrow \boldsymbol{x}_B^{(2)} + \Delta\boldsymbol{x}_B^{(2)}$
    until $||\Delta\boldsymbol{x}_B^{(2)}||/||\boldsymbol{x}_B^{(2)}|| \leq \epsilon$ ▷ loose tolerance, e.g. $\epsilon \in [10^{-4}, 10^{-1}]$
until $\left[\left(||\boldsymbol{y}^{(1)} - \boldsymbol{x}_B^{(1)}||/||\boldsymbol{x}_B^{(1)}||\right)^2 + \left(||\boldsymbol{y}^{(2)} - \boldsymbol{x}_B^{(2)}||/||\boldsymbol{x}_B^{(2)}||\right)^2\right]^{1/2} \leq \epsilon_{\text{machine}}$ ▷ tight tolerance

Inexact Schwarz

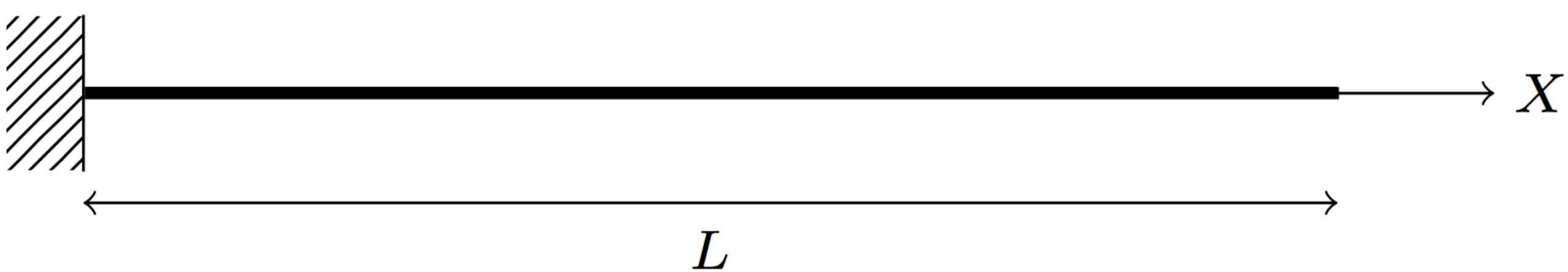
$\boldsymbol{x}_B^{(1)} \leftarrow \boldsymbol{X}_B^{(1)}$ in Ω_1, $\boldsymbol{x}_b^{(1)} \leftarrow \chi(\boldsymbol{X}_b^{(1)})$ on $\partial_\varphi\Omega_1$, ▷ initialize for Ω_1
$\boldsymbol{x}_B^{(2)} \leftarrow \boldsymbol{X}_B^{(2)}$ in Ω_2, $\boldsymbol{x}_b^{(2)} \leftarrow \chi(\boldsymbol{X}_b^{(2)})$ on $\partial_\varphi\Omega_2$, ▷ initialize for Ω_2
repeat ▷ Newton-Schwarz loop
    $\begin{Bmatrix}\Delta\boldsymbol{x}_B^{(1)} \\ \Delta\boldsymbol{x}_B^{(2)}\end{Bmatrix} \leftarrow \begin{pmatrix}\boldsymbol{K}_{AB}^{(1)} + \boldsymbol{K}_{A\beta}^{(1)}\boldsymbol{H}_{11} & \boldsymbol{K}_{A\beta}^{(1)}\boldsymbol{H}_{12} \\ \boldsymbol{K}_{A\beta}^{(2)}\boldsymbol{H}_{21} & \boldsymbol{K}_{AB}^{(2)} + \boldsymbol{K}_{A\beta}^{(2)}\boldsymbol{H}_{22}\end{pmatrix} \backslash \begin{Bmatrix}-\boldsymbol{R}_A^{(1)} \\ -\boldsymbol{R}_A^{(2)}\end{Bmatrix}$ ▷ linear system
    $\boldsymbol{x}_B^{(1)} \leftarrow \boldsymbol{x}_B^{(1)} + \Delta\boldsymbol{x}_B^{(1)}$
    $\boldsymbol{x}_B^{(2)} \leftarrow \boldsymbol{x}_B^{(2)} + \Delta\boldsymbol{x}_B^{(2)}$
until $\left[\left(||\Delta\boldsymbol{x}_B^{(1)}||/||\boldsymbol{x}_B^{(1)}||\right)^2 + \left(||\Delta\boldsymbol{x}_B^{(2)}||/||\boldsymbol{x}_B^{(2)}||\right)^2\right]^{1/2} \leq \epsilon_{\text{machine}}$ ▷ tight tolerance

Monolithic Schwarz

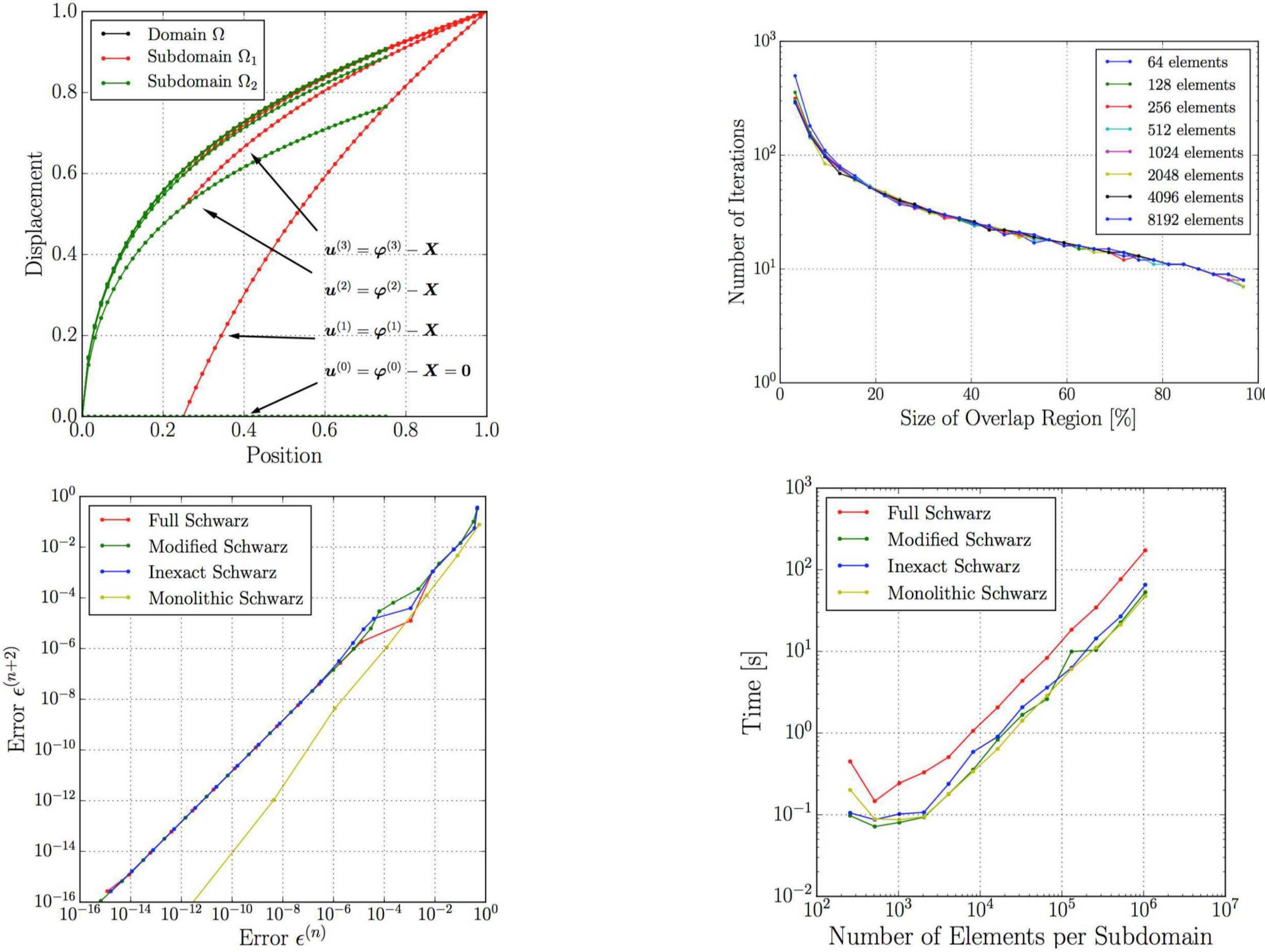
Foulk's Singular Bar

- 1D Proof of concept problem.
- Explore viability of method.
- Test convergence and compare with literature (Evans, 1986).
- Expect faster convergence in fewer iterations with increased overlap.
- Area proportional to square root of length.
- Strong singularity on left end of bar.
- Simple hyperelastic model with damage.
- Four Schwarz variants implemented in Matlab.

$u(0) = 0$ $\quad$ $A(X) = A_0\sqrt{X/L}$ $\quad$ $u(L) = \Delta$



Singular Bar and Schwarz Variants

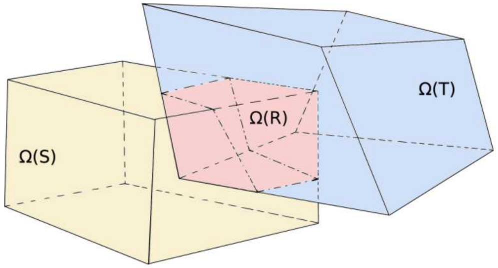


Schwarz Alternating Method in Albany

- Modified Schwarz version implemented in Sandia's open-source Albany code within the LCM project.
- Use of components in code design for rapid development of capabilities.
- Extensive use of libraries from the open-source TRILINOS project.
- Use of the TRILINOS PHALANX package to decompose complex problem into simpler problems with managed dependencies.
- Use of the TRILINOS SACADO package for automatic differentiation. The stiffness is neither derived nor implemented explicitly.
- Use of TRILINOS TEKO package for block preconditioning.
- Parallel implementation uses the Data Transfer Kit (DTK).
- All software available on GitHub.

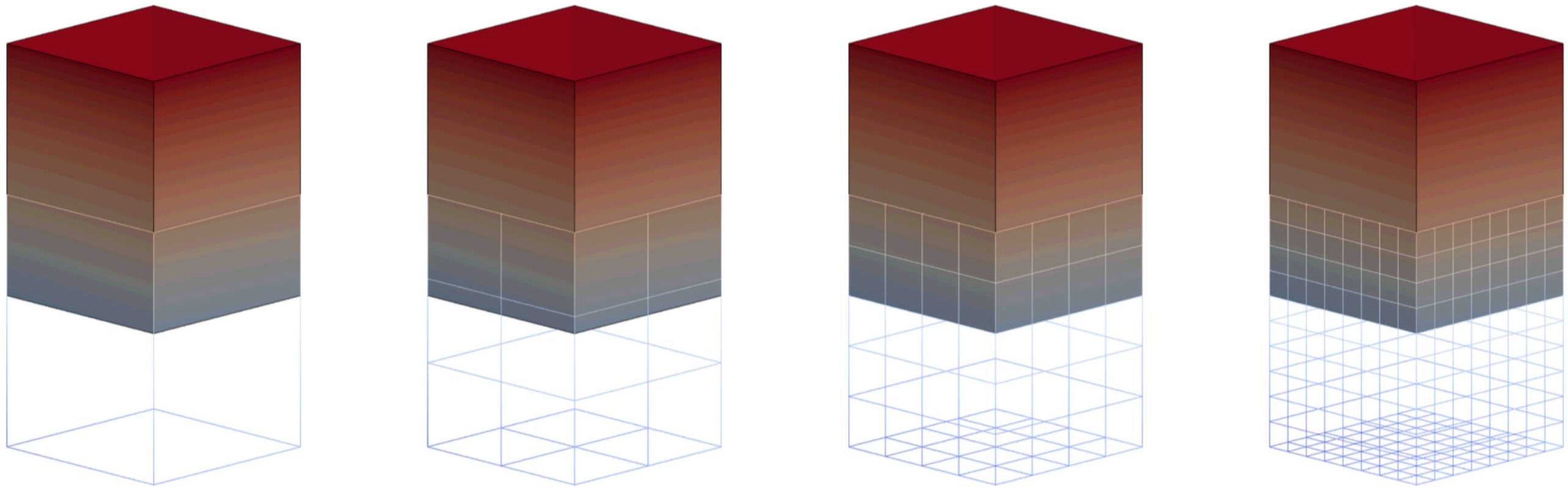
https://github.com/trilinos/trilinos

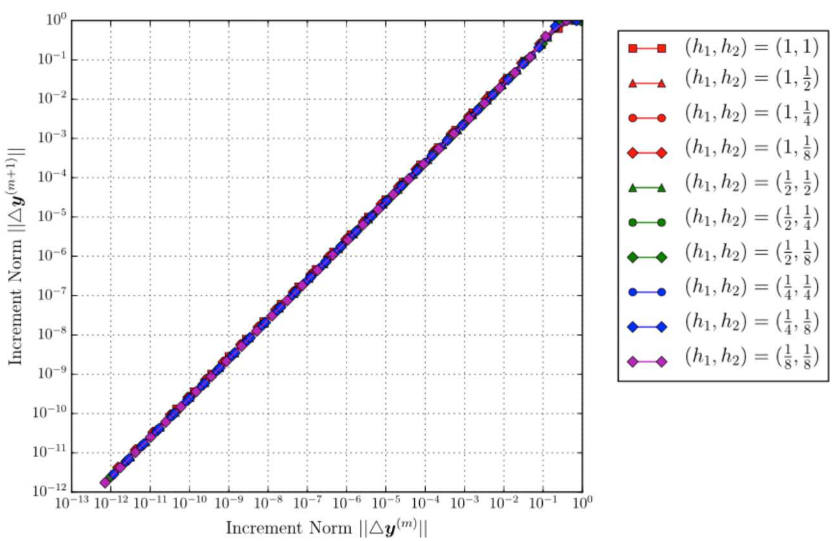
https://github.com/gahansen/Albany

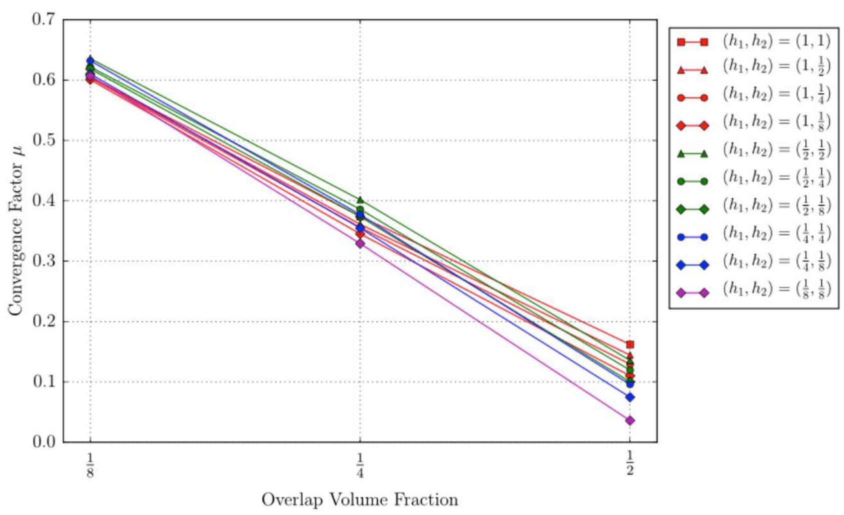


https://github.com/ORNL-CEES/DataTransferKit

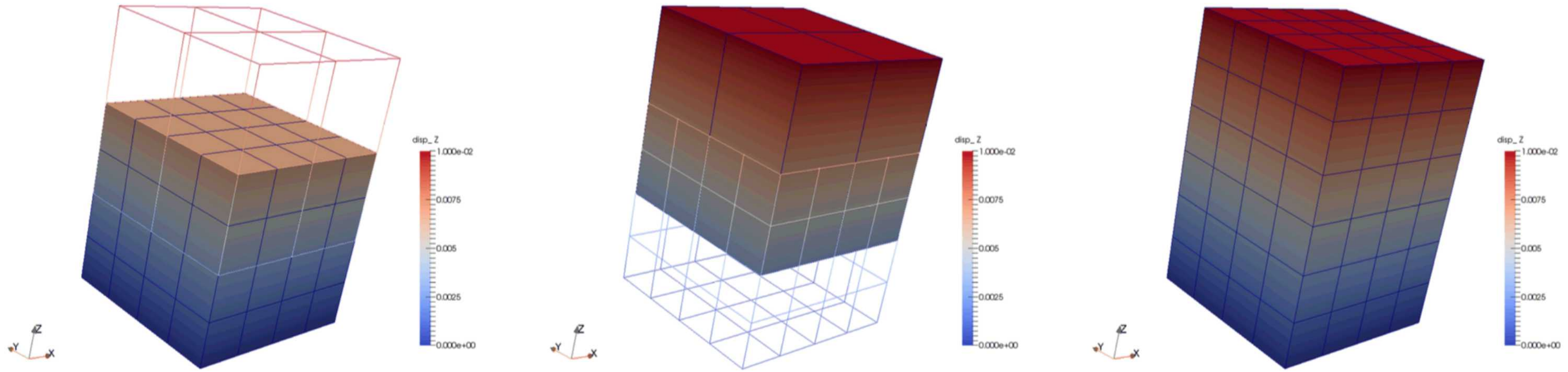
Hyperleastic Cuboid, Convergence with Overlap and Mesh Size





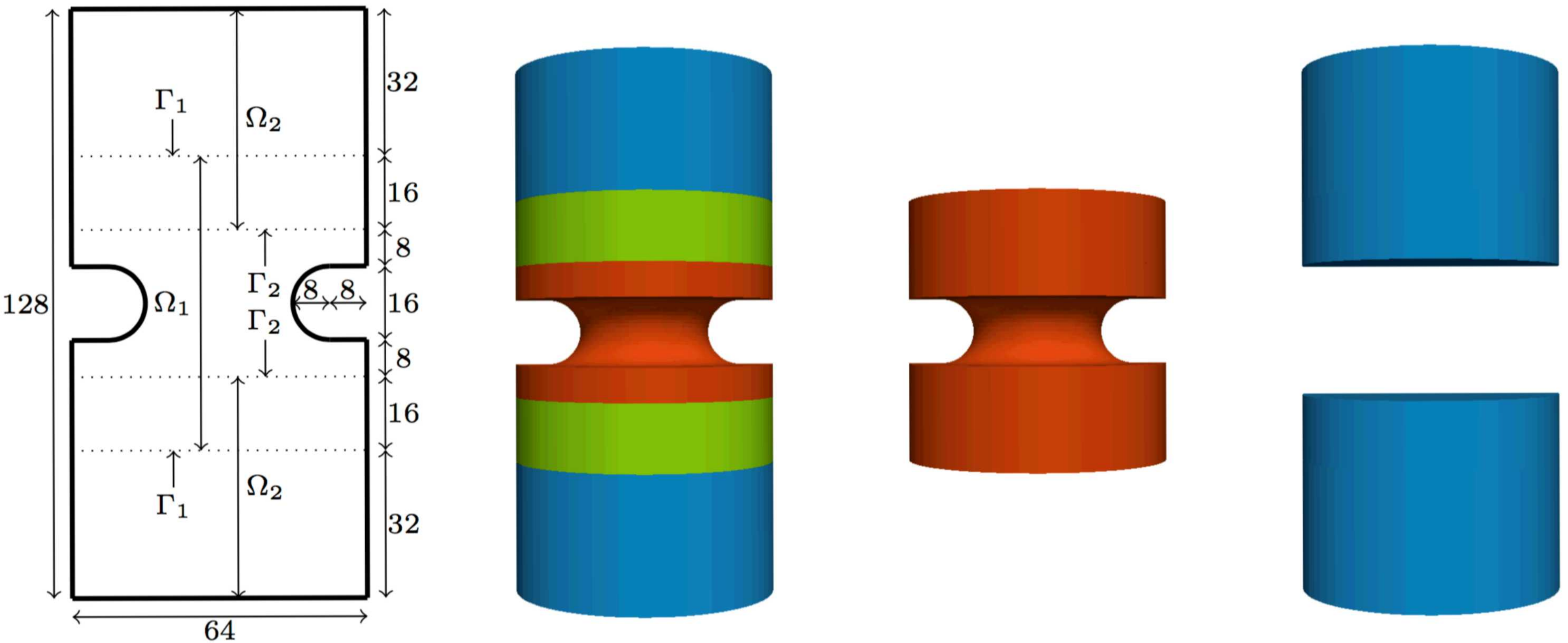


Cuboid: Schwarz Error



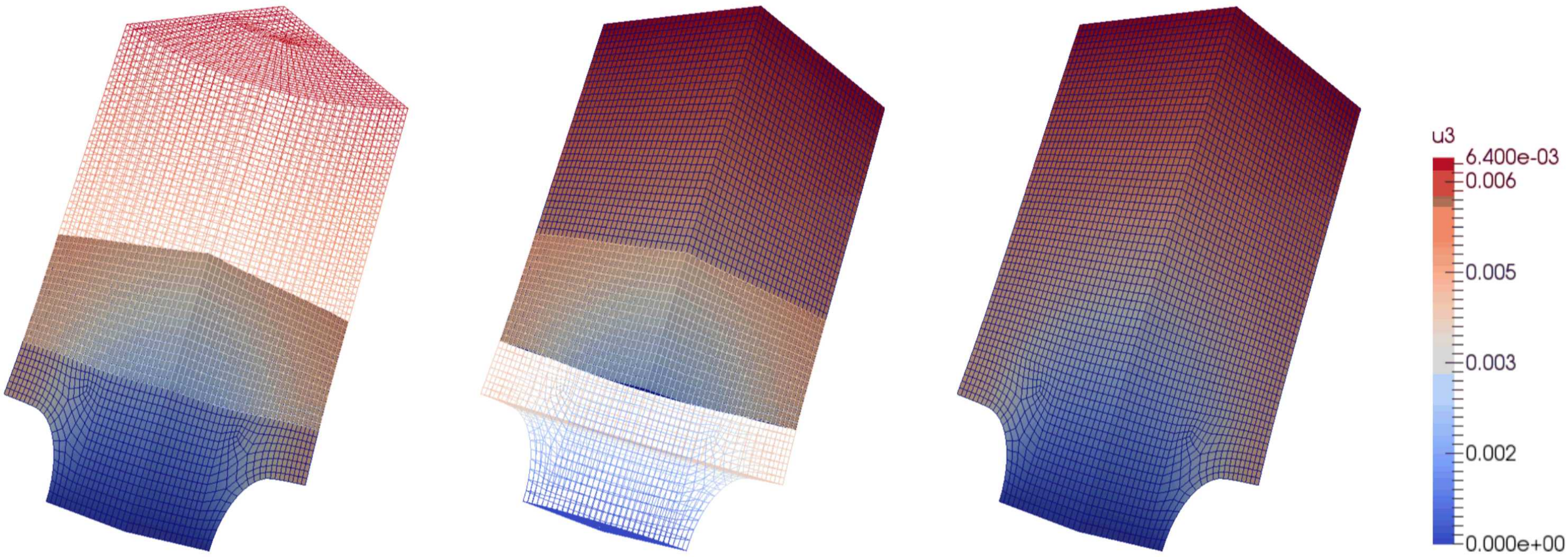
Subdomain	u_3 relative error	σ_{33} relative error
Ω_1	1.24×10^{-14}	2.31×10^{-13}
Ω_2	7.30×10^{-15}	3.06×10^{-13}

Hyperleastic Notched Cylinder



(a) Schematic **(b)** Entire Domain Ω **(c)** Fine Region Ω_1 **(d)** Coarse Region Ω_2

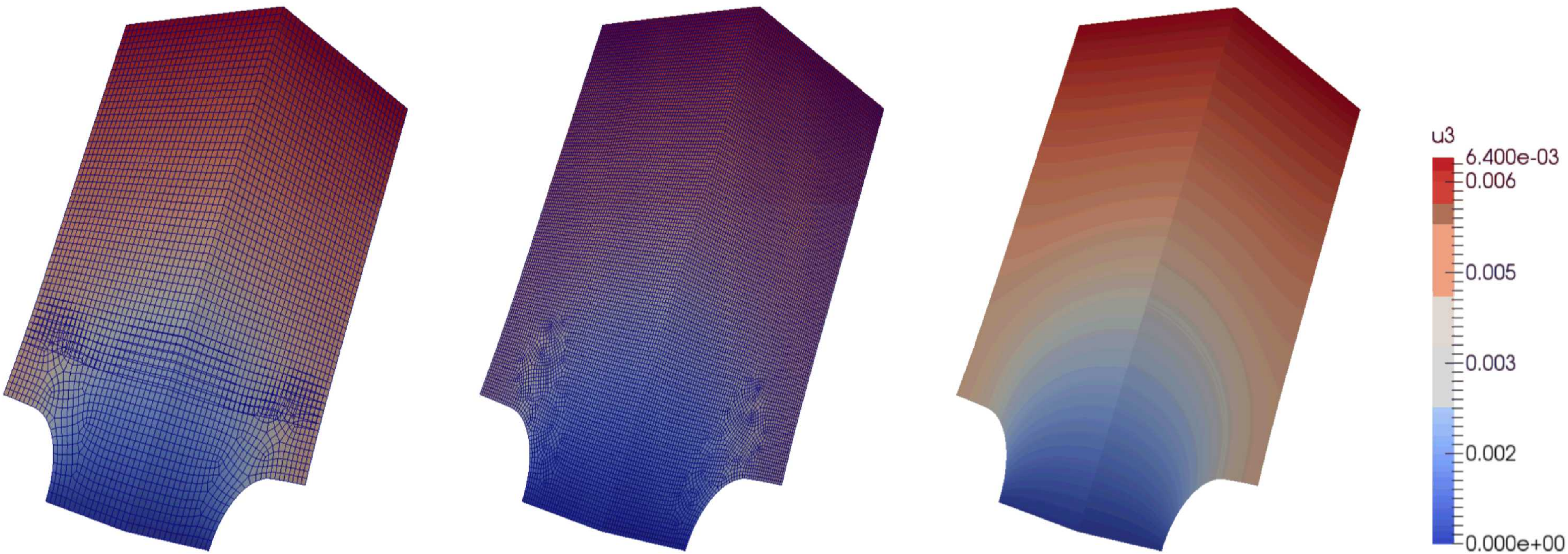
Notched Cylinder: Conformal HEX-HEX Coupling



(a) Ω_1 (b) Ω_2 (c) Ω_{ref}

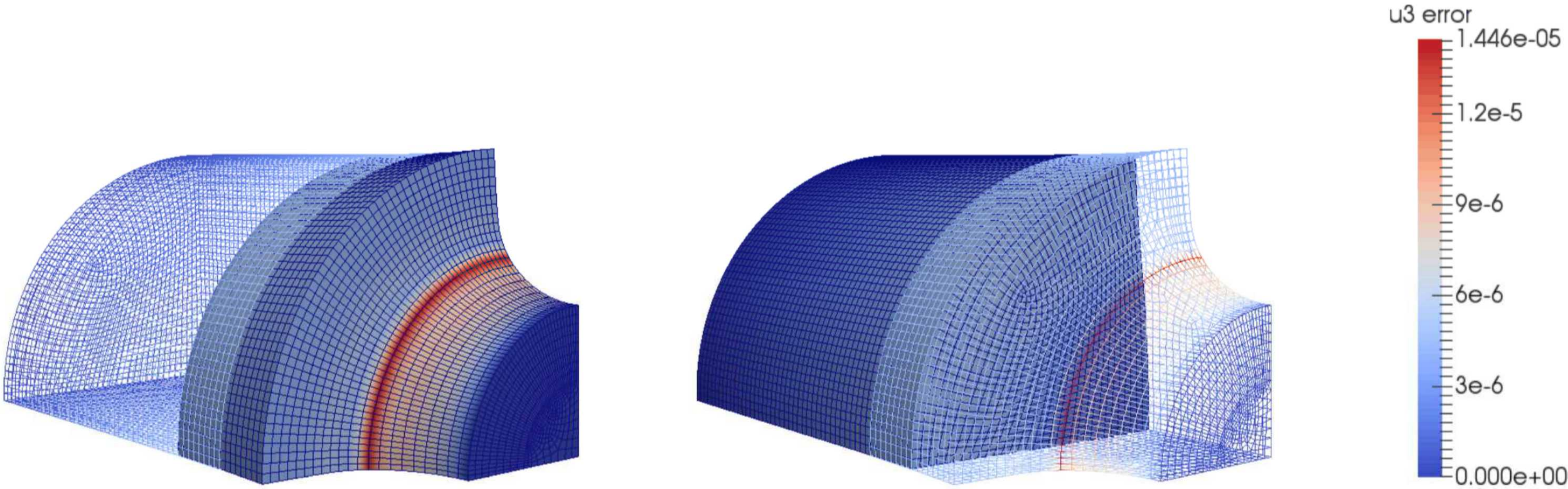
	u_3 relative error	
Absolute residual tolerance	Ω_1	Ω_2
1.0×10^{-4}	7.60×10^{-3}	3.20×10^{-3}
1.0×10^{-8}	3.10×10^{-5}	1.71×10^{-5}
1.0×10^{-12}	1.34×10^{-9}	5.10×10^{-10}
1.0×10^{-14}	1.23×10^{-11}	4.69×10^{-12}
2.5×10^{-16}	1.14×10^{-13}	8.37×10^{-14}

Notched Cylinder: Non-Conformal HEX-HEX Coupling



(a) Ω_1 and Ω_2 **(b)** Ω_{ref} mesh **(c)** Ω_{ref} solution

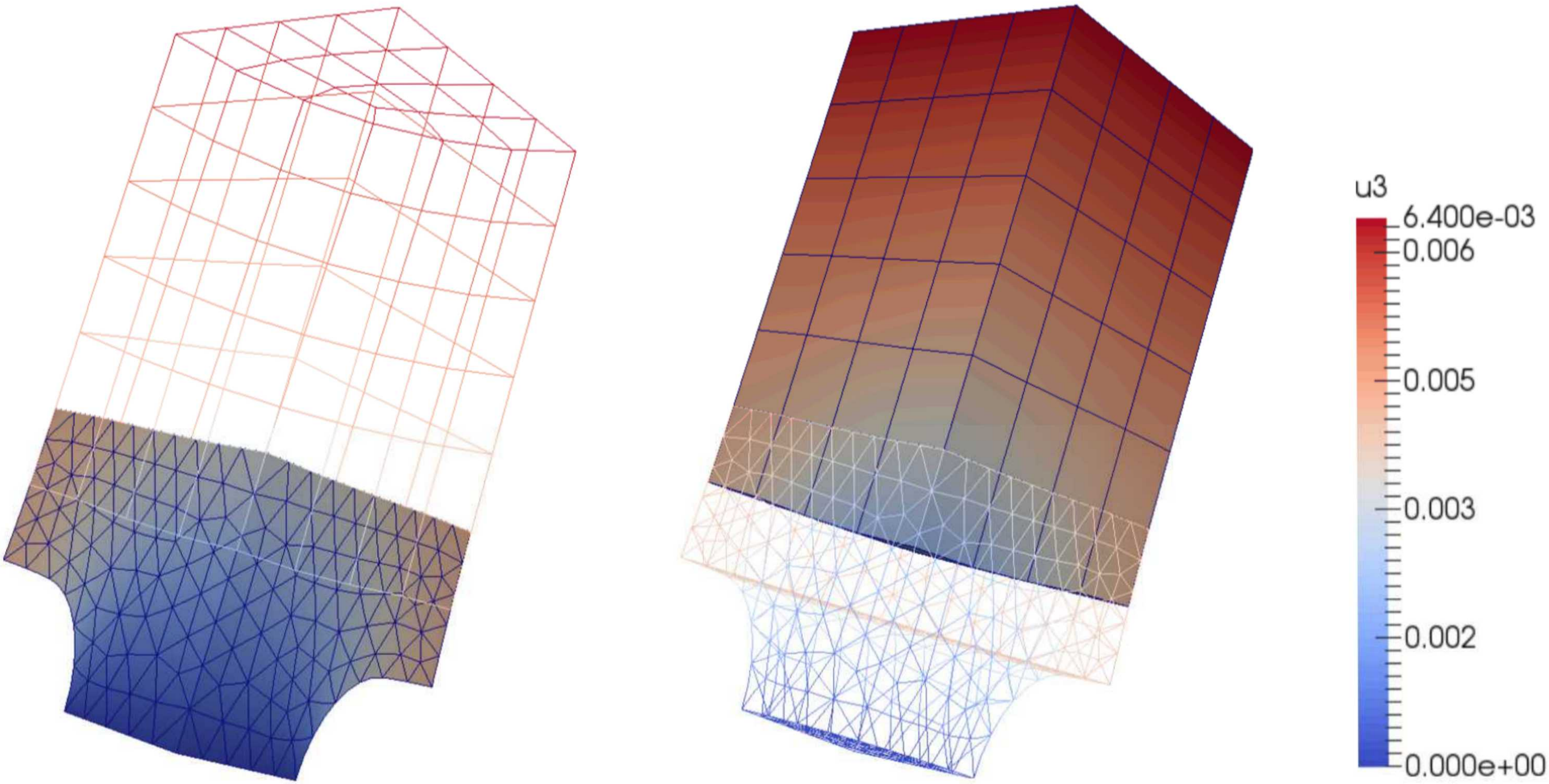
Notched Cylinder: Non-Conformal HEX-HEX Coupling



(a) Ω_1 (b) Ω_2

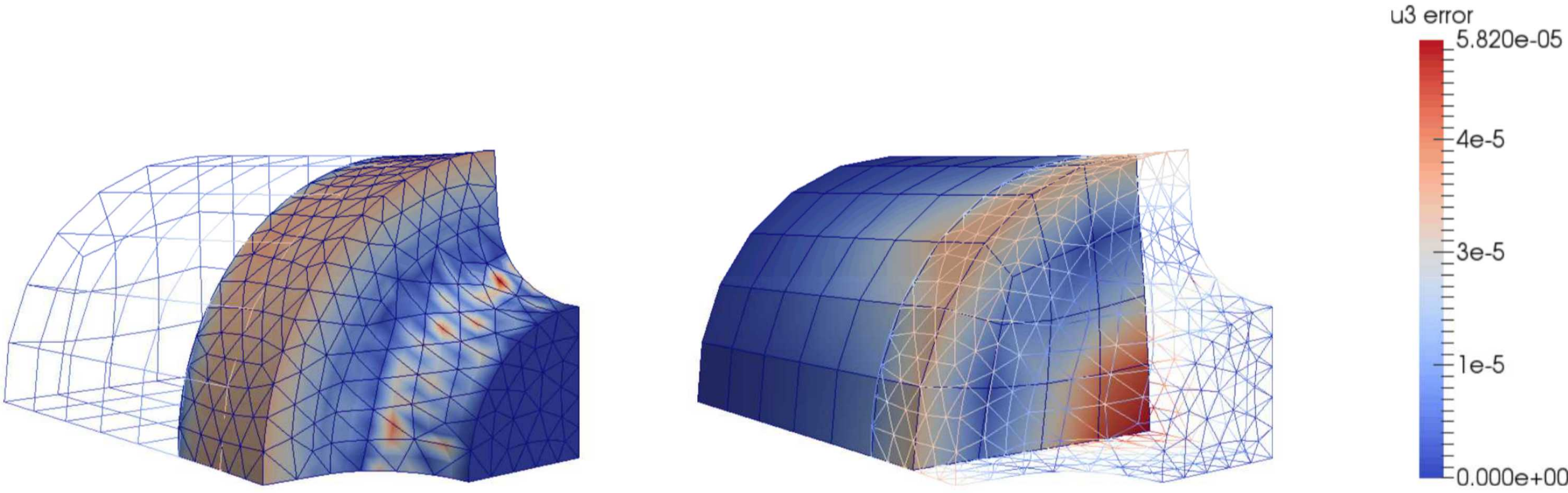
Absolute residual tolerance	u_3 relative error Ω_1	Ω_2
1.0×10^{-8}	1.31×10^{-3}	4.45×10^{-4}
1.0×10^{-12}	1.30×10^{-3}	4.43×10^{-4}
1.0×10^{-14}	1.30×10^{-3}	4.43×10^{-4}
2.5×10^{-16}	1.30×10^{-3}	4.43×10^{-4}

Notched Cylinder: TET-HEX Coupling



(a) Ω_1 (b) Ω_2

Notched Cylinder: TET-HEX Coupling

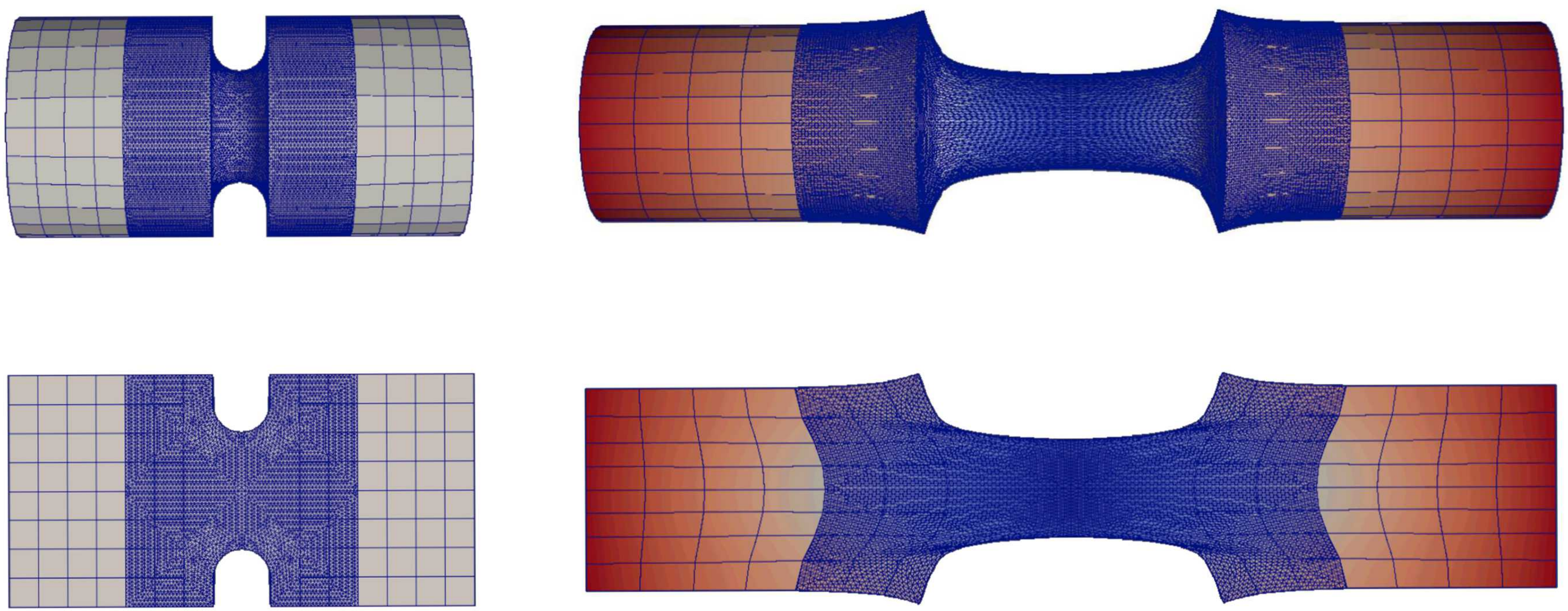


(a) Ω_1 **(b)** Ω_2

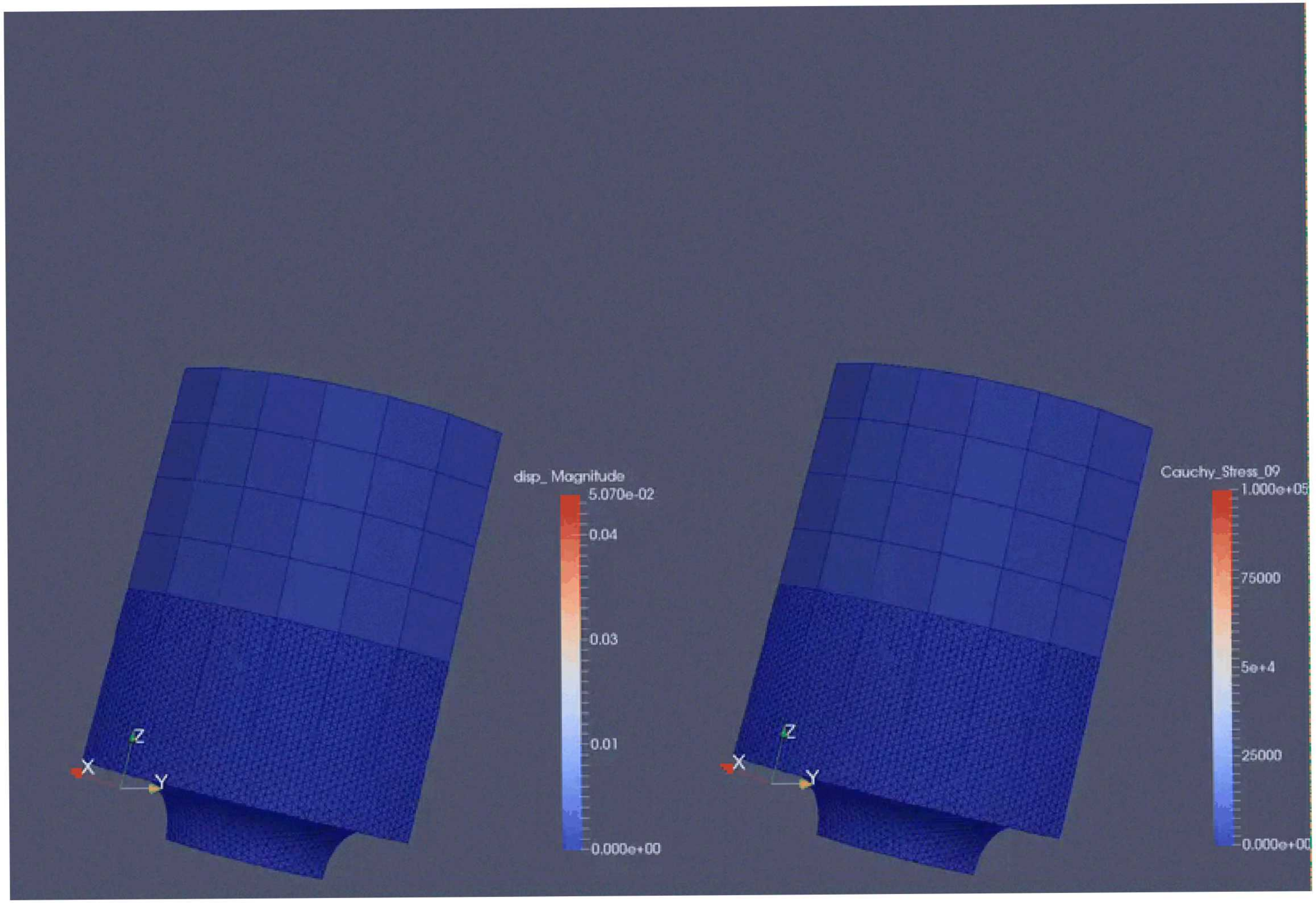
Absolute residual tolerance	u_3 relative error Ω_1	Ω_2
1.0×10^{-14}	9.27×10^{-3}	3.70×10^{-3}

Notched Cylinder: TET-HEX Coupling

- The method is capable of coupling different mesh topologies.
- The notched region, where stress concentrations are expected, is finely meshed with tetrahedral elements.
- The top and bottom regions, presumably of less interest, are meshed with coarser hexahedral elements.



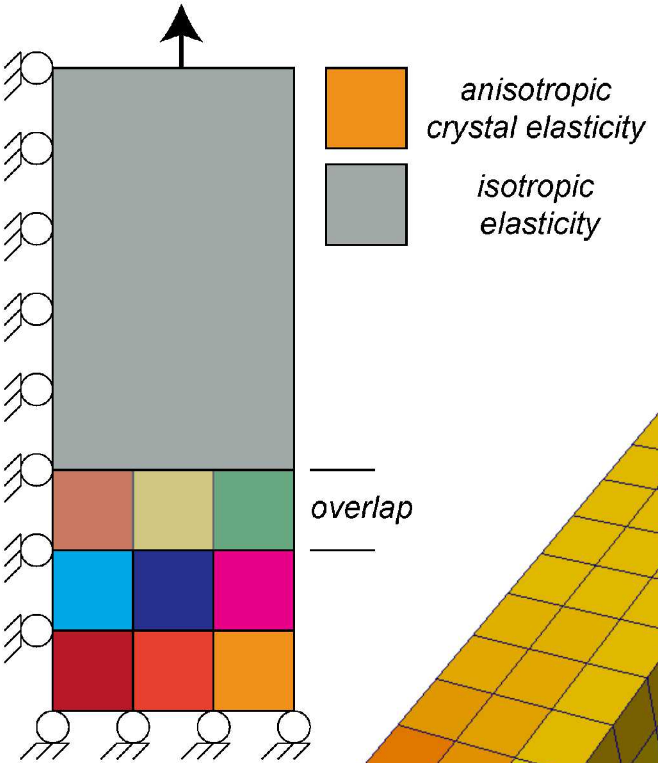
Notched Cylinder: TET-HEX Coupling

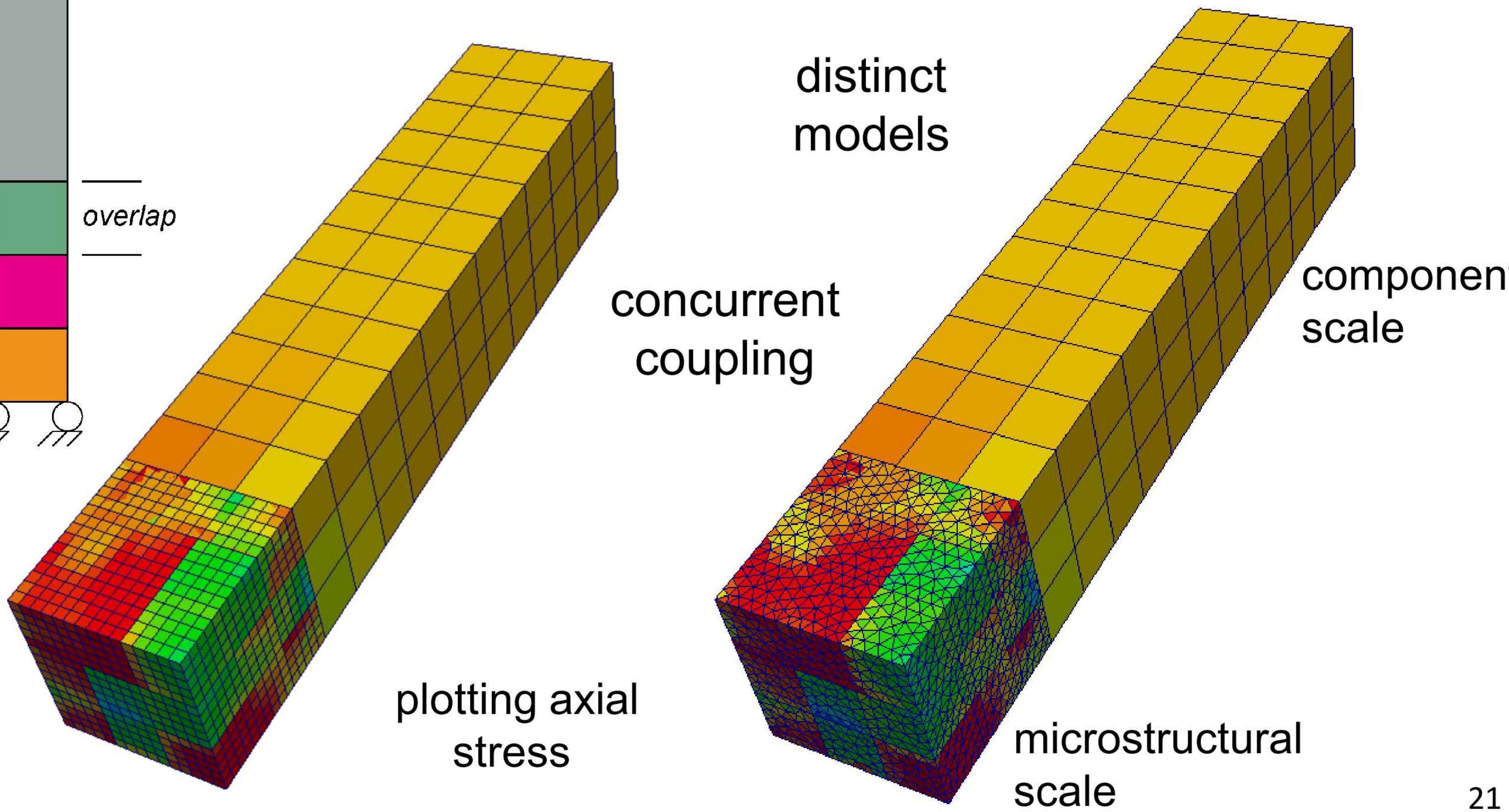


Coupling Isotropic and Crystal Hyperelasticity

Two distinct bodies, the component scale and the microstructural scale, are coupled iteratively with alternating Schwarz

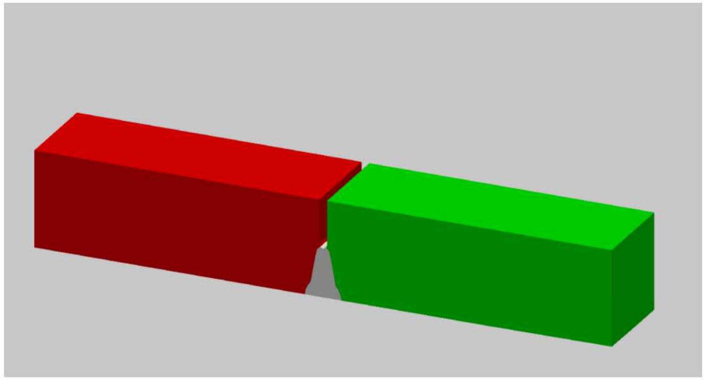
Work by J. Foulk, D. Littlewood, C. Battaile, H. Lim

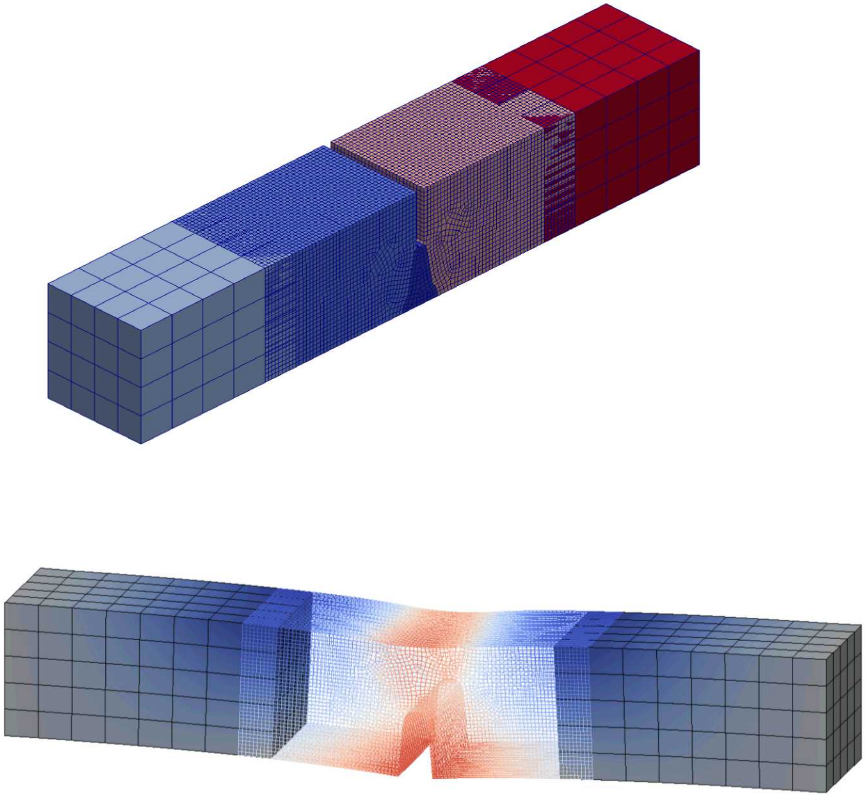


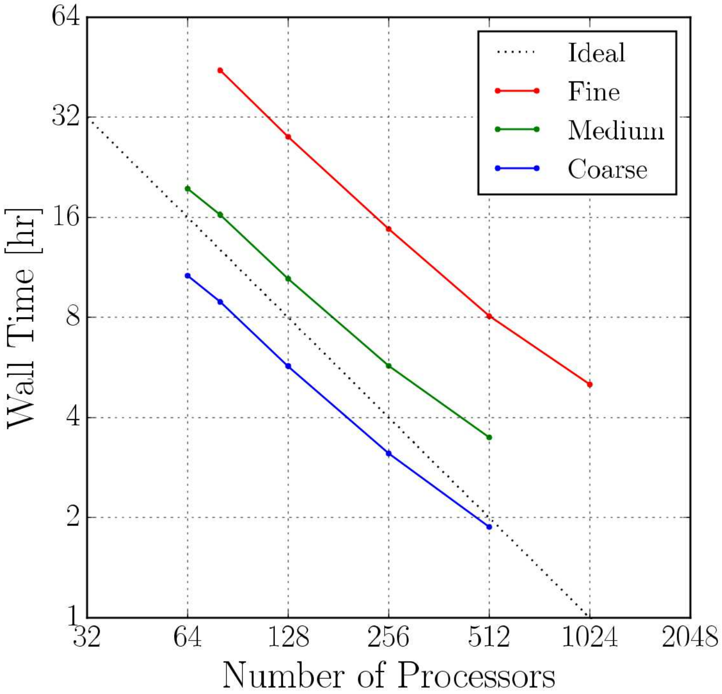


Laser Weld: Strong Scalability of Parallel Schwarz with DTK

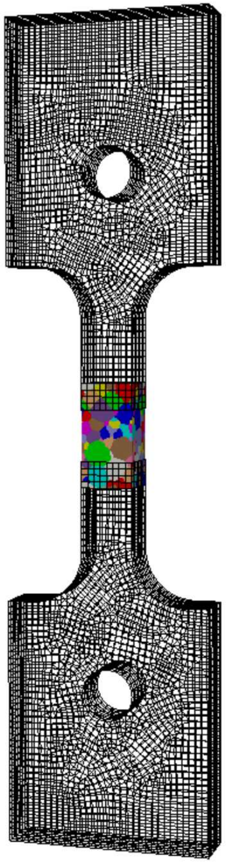
- Isotropic elasticity
- J2 plasticity
- Identical parameters for weld and base materials for proof of concept, to become independent models
- ~200,000 DOFs





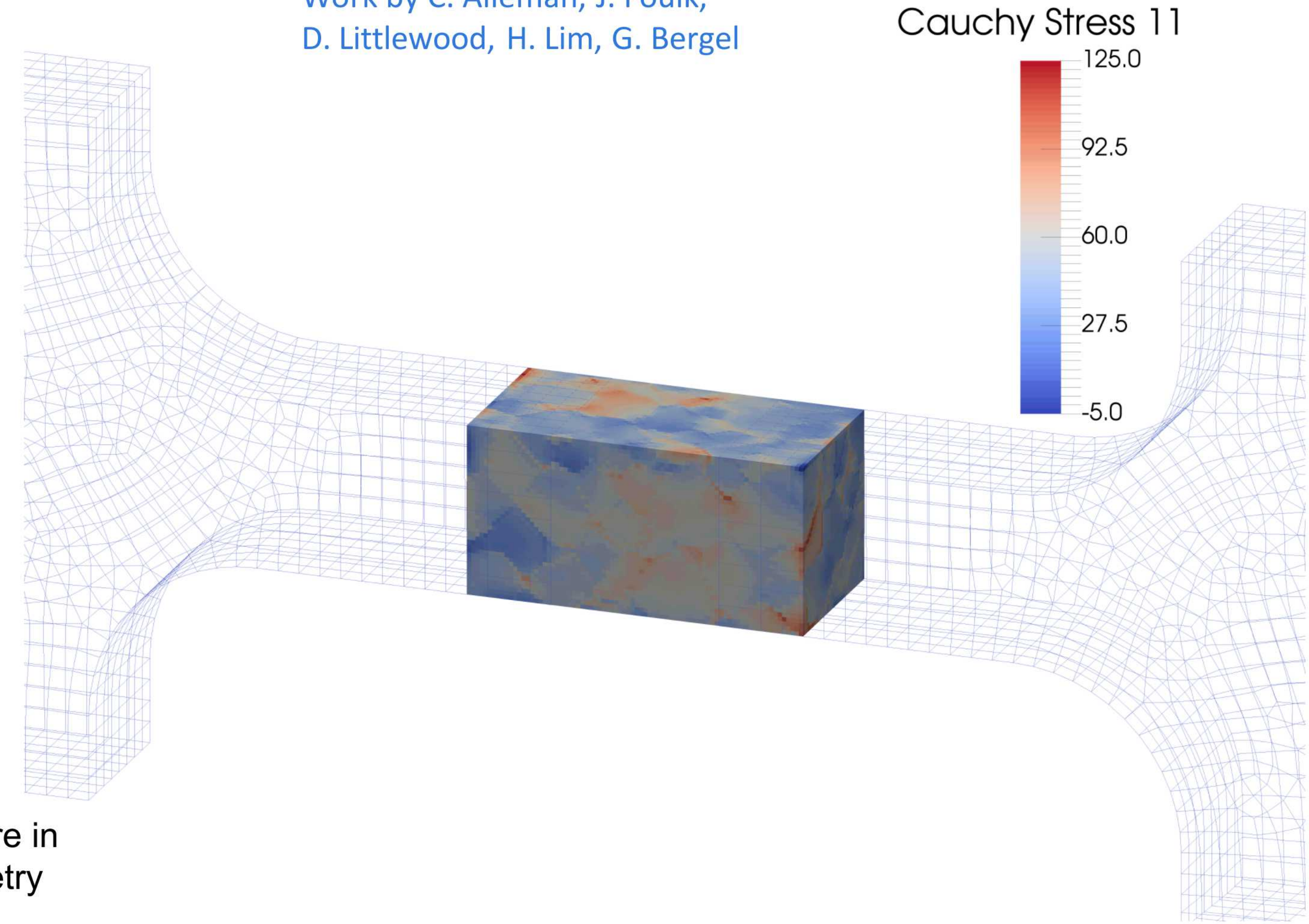


Numerical Example: Tensile Bar



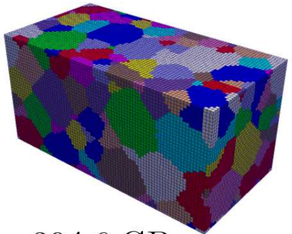
Embed microstructure in ASTM tensile geometry

Work by C. Alleman, J. Foulk, D. Littlewood, H. Lim, G. Bergel



Tensile Bar: Meso-Macroscale Coupling

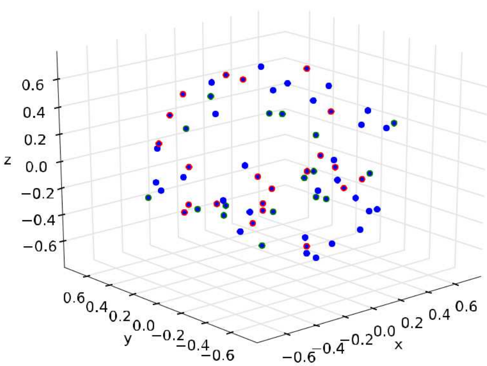
Mesoscale



SPARKS-genereated microstructure (F. Abdeljawad)

$$\text{cubic elastic constant} : C_{11} = 204.6 \text{ GPa}$$
$$\text{cubic elastic constant} : C_{12} = 137.7 \text{ GPa}$$
$$\text{cubic elastic constant} : C_{44} = 126.2 \text{ GPa}$$
$$\text{reference shear rate} : \dot{\gamma}_0 = 1.0 \text{ 1/s}$$
$$\text{rate sensitivity factor} : m = 20$$
$$\text{hardening rate parameter} : \dot{g}_0 = 2.0 \times 10^4 \text{ 1/s}$$
$$\text{initial hardness} : g_0 = 90 \text{ MPa}$$
$$\text{saturation hardness} : g_s = 202 \text{ MPa}$$
$$\text{saturation exponent} : \omega = 0.01$$

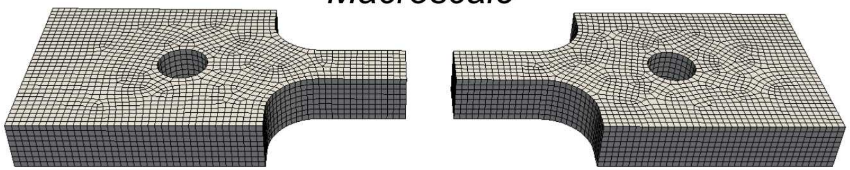
Fix microstructure, investigate ensembles



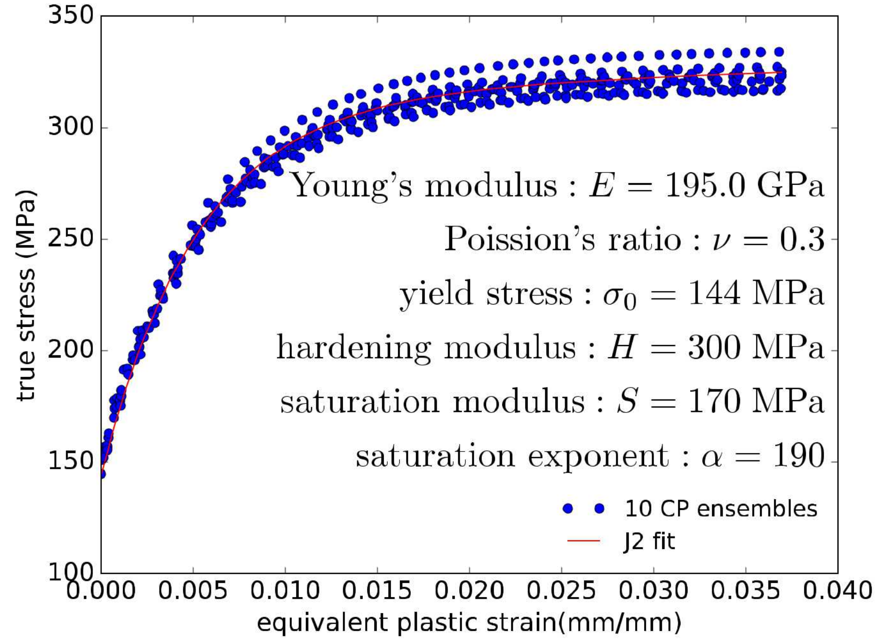
151 axial vectors from 3 of the 10 ensembles of random rotations (blue, green, red)

\+

Macroscale



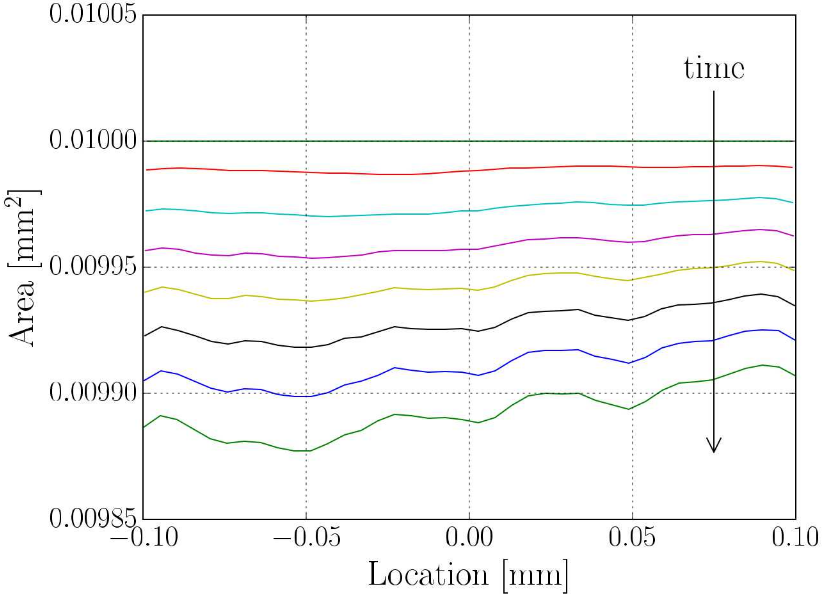
- Load microstructural ensembles in uniaxial stress
- Fit flow curves with a macroscale J_2 plasticity model

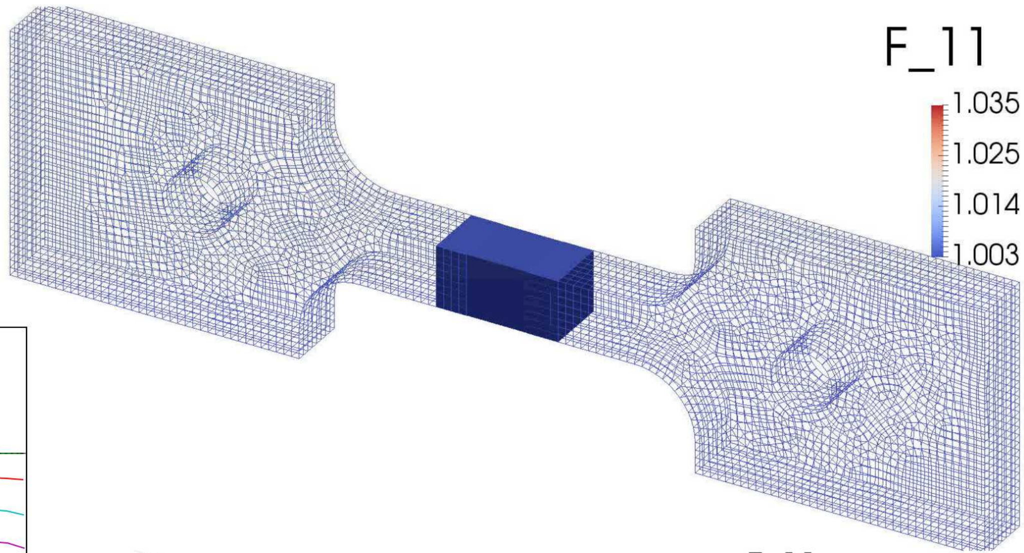


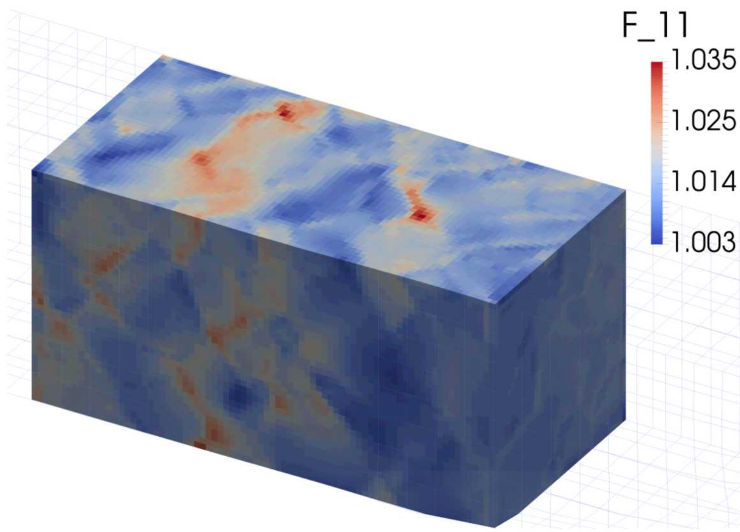
$$\sigma_y = \sigma_0 + H\epsilon_p + S(1 - e^{-\alpha\epsilon_p})$$

Tensile Bar: Results

Reduction in cross-sectional area over time







Schwarz Alternating Method: Summary of Findings

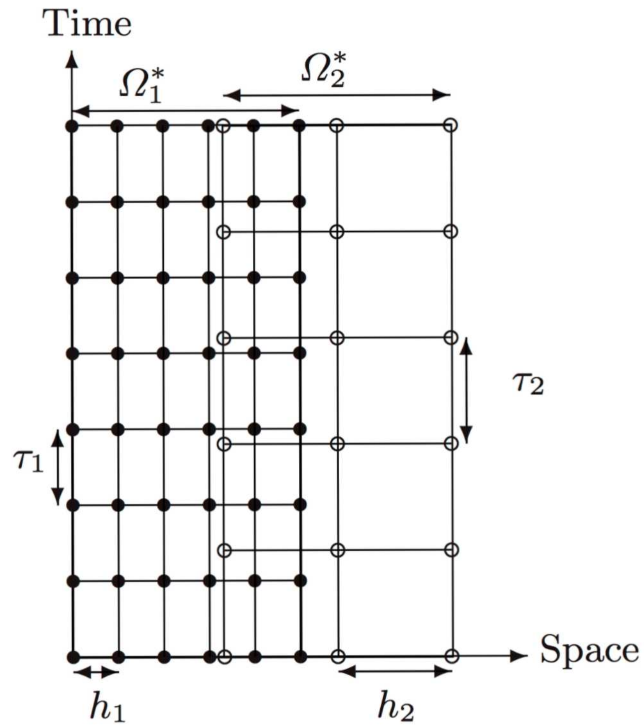
- Adopt the original method developed by Schwarz for the finite-deformation solid mechanics problem. The method is formulated by recourse to a variational setting.
- The development and introduction of four variants of the Schwarz alternating method and explicit algorithms for their implementation. The choice of one variant over another depends on the existing infrastructure of a computer implementation.
- Demonstration by means of numerical examples that the convergence of the Schwarz method in its four variants is for the most part linear. The numerical examples revealed that the Modified Schwarz method occasionally displays non-monotonic behavior.
- Demonstration of coupling of conformal meshes, non-conformal meshes, meshes with different levels of refinement, meshes with different element topologies, and more than two subdomains.
- Demonstration that the error in the coupling can be decreased up to numerical precision provided that no other sources of error (such as geometric mismatch) exist.
- The development of a parallel implementation of the Schwarz method in the ALBANY code and demonstration that the strong scalability of our implementation is close to ideal.

Schwarz Alternating Method: Future Work

- Extension of the methods presented herein to transient dynamics problems with the ability to use different time steps and time integrators for each subdomain.
- Development of a multi-physics coupling framework based on variational formulations and the Schwarz alternating method.

Schwarz Alternating Method in Dynamics

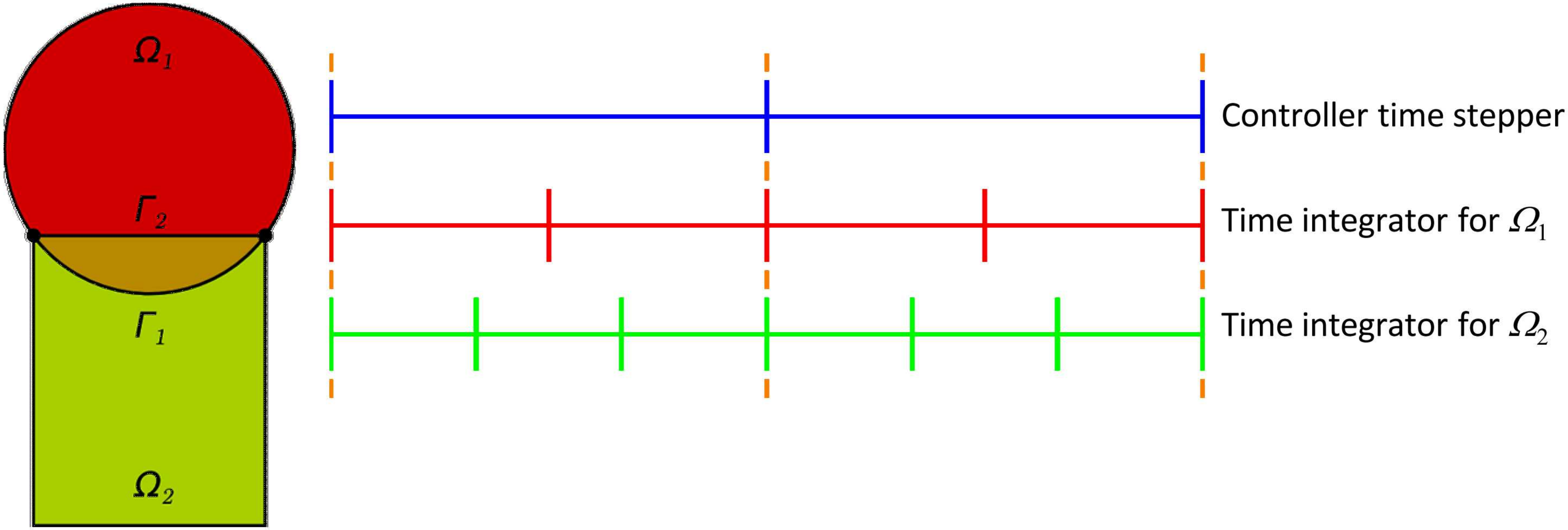
- In the literature the Schwarz method is applied to dynamics by using space-time discretizations.
- This was deemed unfeasible given the design of our current codes and size of simulations.



Overlapping non-matching meshes and time steps in dynamics.

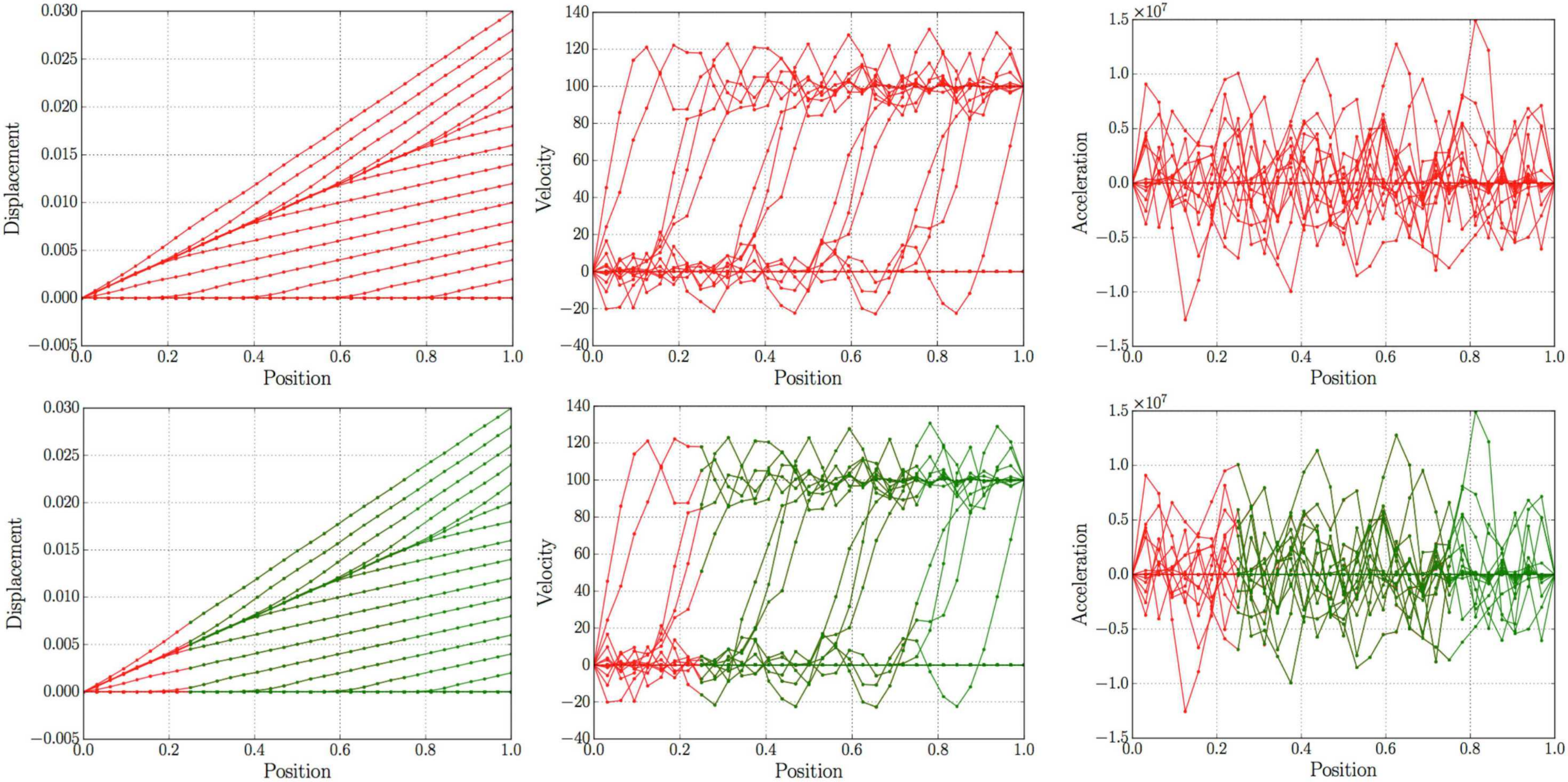
A Schwarz-like Time Integrator.

- We developed an extension to Schwarz coupling to dynamics using a governing time stepping algorithm that controls time integrators within each domain.
- Can use different integrators with different time steps within each domain.
- 1D results show smooth coupling without numerical artifacts such as spurious wave reflections at boundaries of coupled domains.



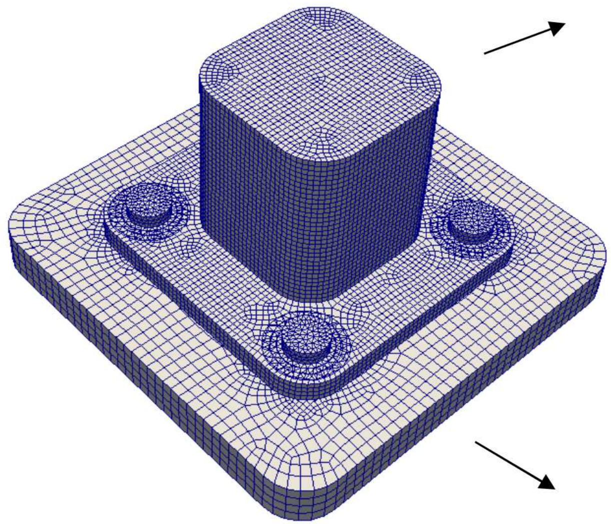
Dynamic Singular Bar

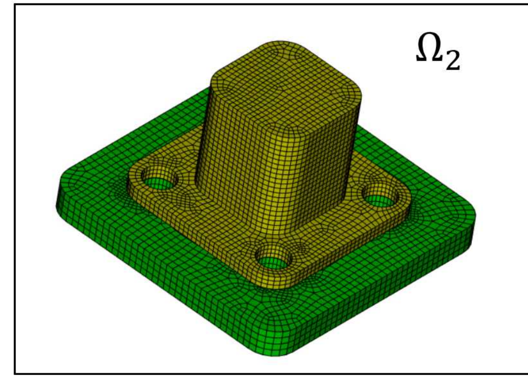
- Inelasticity masks problems by introducing energy dissipation.
- Schwarz does not introduce numerical artifacts.
- Can couple domains with different time integration schemes (Explicit-Implicit below).



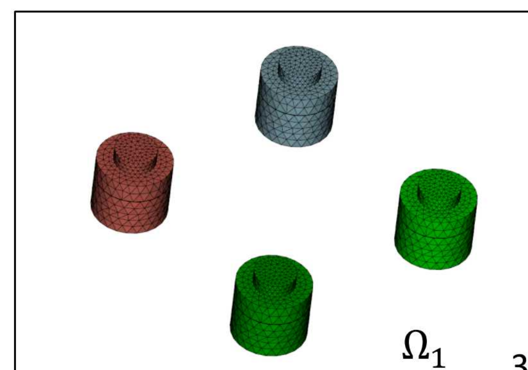
Schwarz Domain Decomposition for Bolted Joint Problem

- Schwarz solution compared to single-domain solution on composite tet 10 mesh.



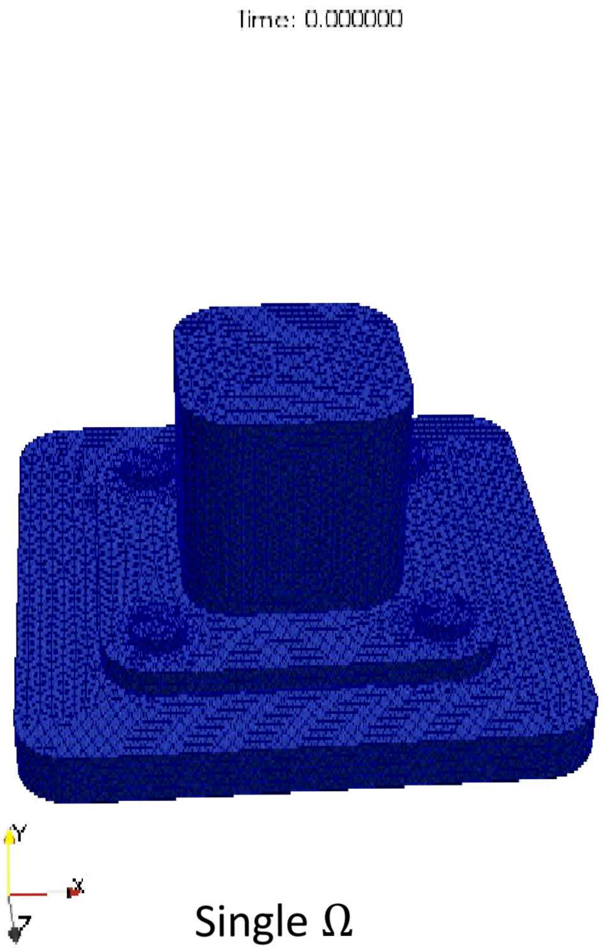


- BC: x-disp = 0.02 at T = 1.0e-3 on top of parts.
- Run till T = 5.0e-4 w/ dt = 1e-5 + implicit Newmark with analytic mass matrix for composite tet10s.



- Ω_1 = bolts (composite tet 10), Ω_2 = parts (hex 8).
- ***Inelastic J2 material model*** in both subdomains.
  - Ω_1: steel
  - Ω_2: steel component, aluminum (bottom) plate

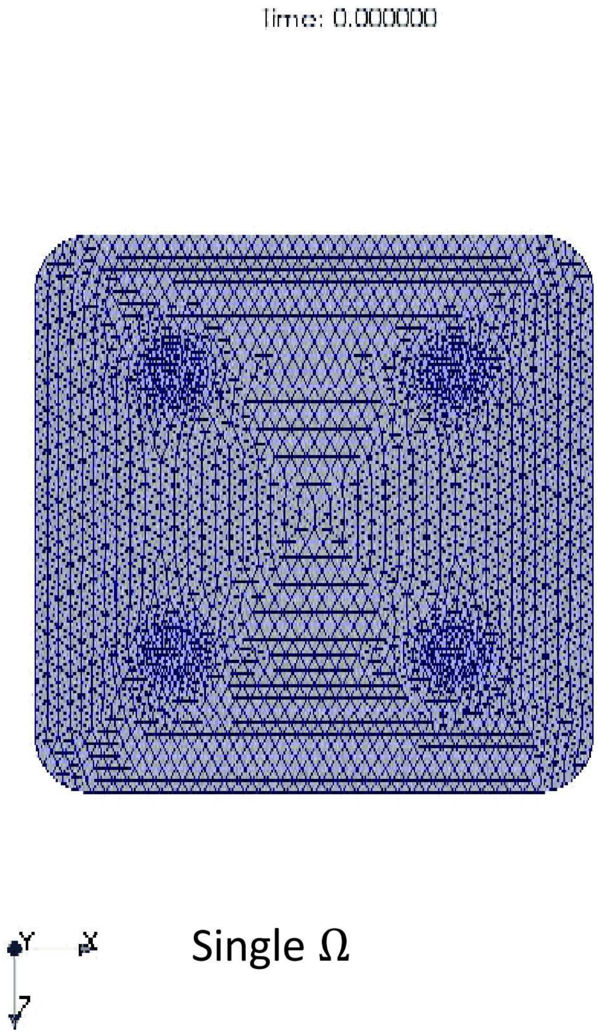
Bolted Joint Problem: x-displacement



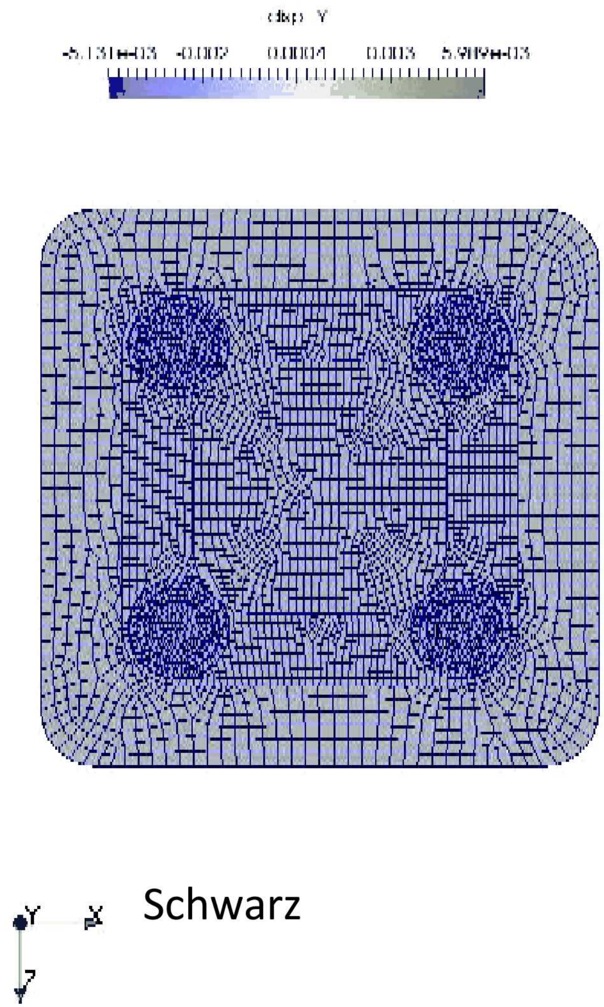
Single Ω

Schwarz

Bolted Joint Problem: y-displacement

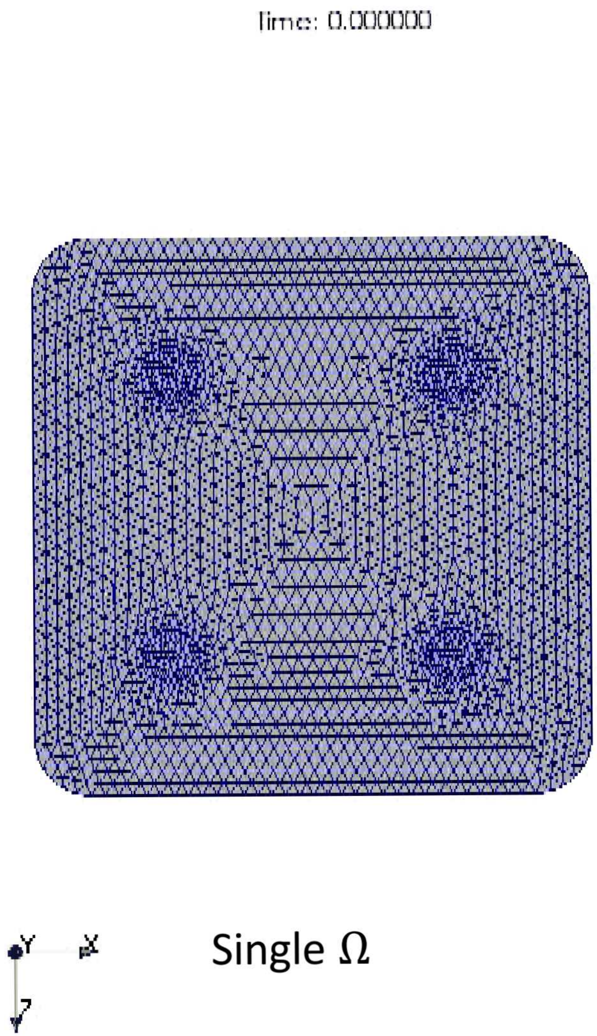


Single Ω

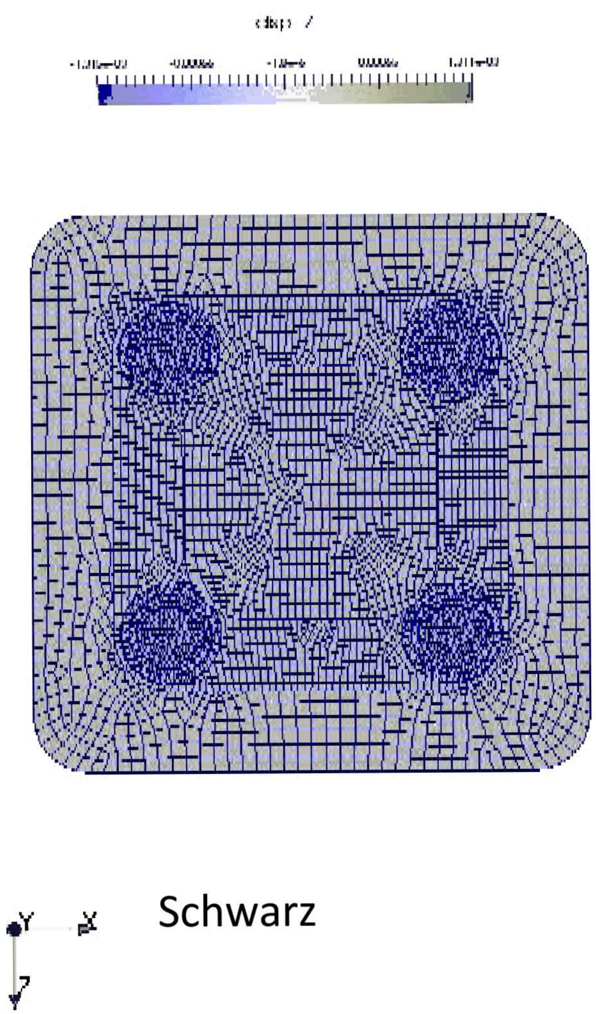


Schwarz

Bolted Joint Problem: z-displacement

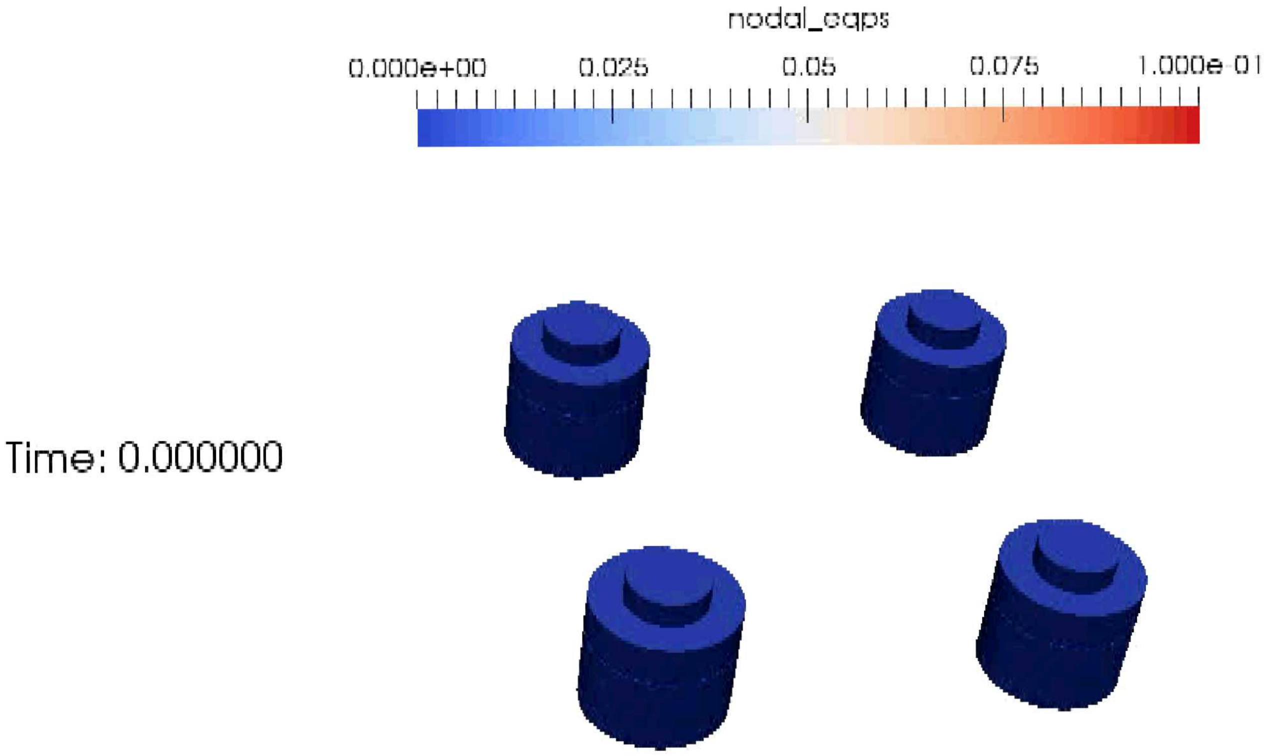


Single Ω

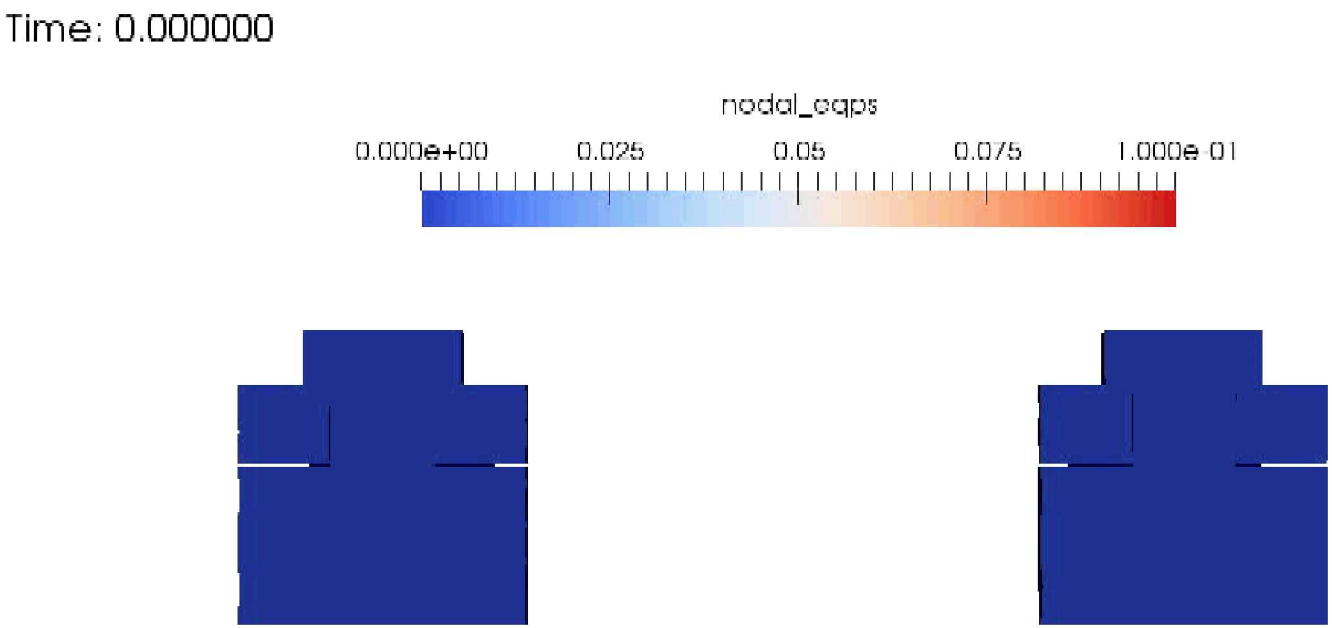


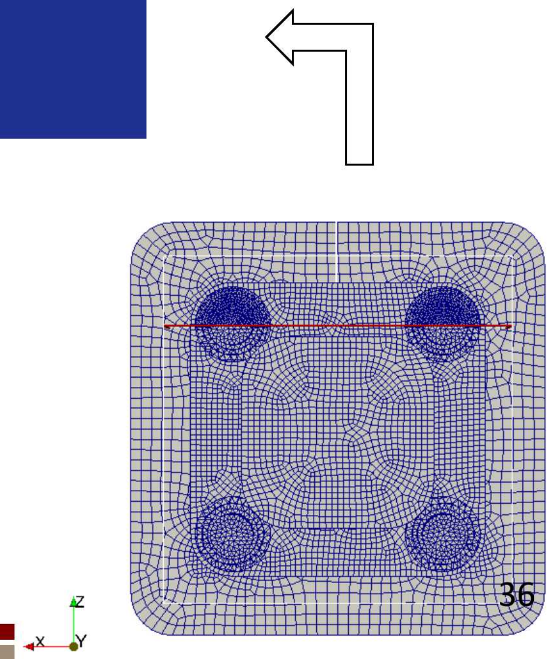
Schwarz

Bolted Joint Problem: nodal eqps



Bolted Joint Problem: nodal eqps



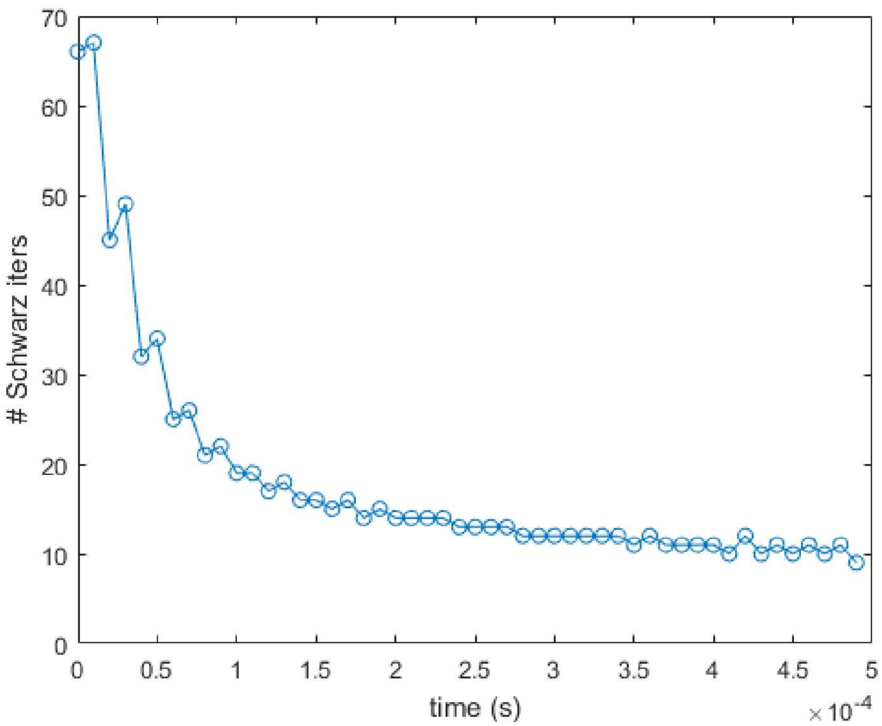


Cross-section of bolts obtained via clip (right)

Bolted Joint Problem: Some Schwarz Performance Results

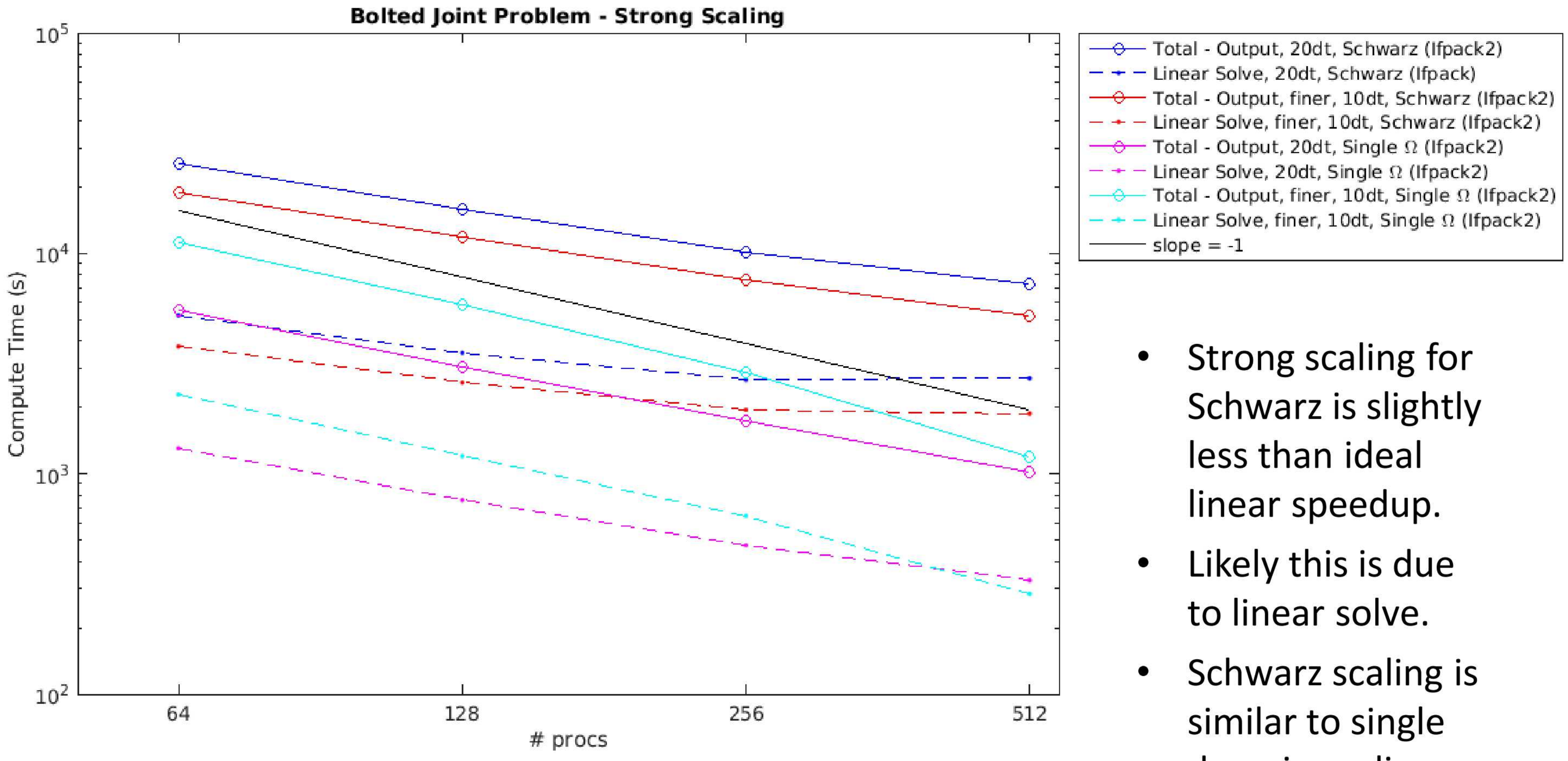
Schwarz / solver settings

- Relatively loose Schwarz tolerances were used:
  - Relative Tolerance: 1.0e-03.
  - Absolute Tolerance: 1.0e-04.
- Newton tolerance on NormF: 1e-8
- Linear solver tolerance: 1e-5
- MueLu preconditioner



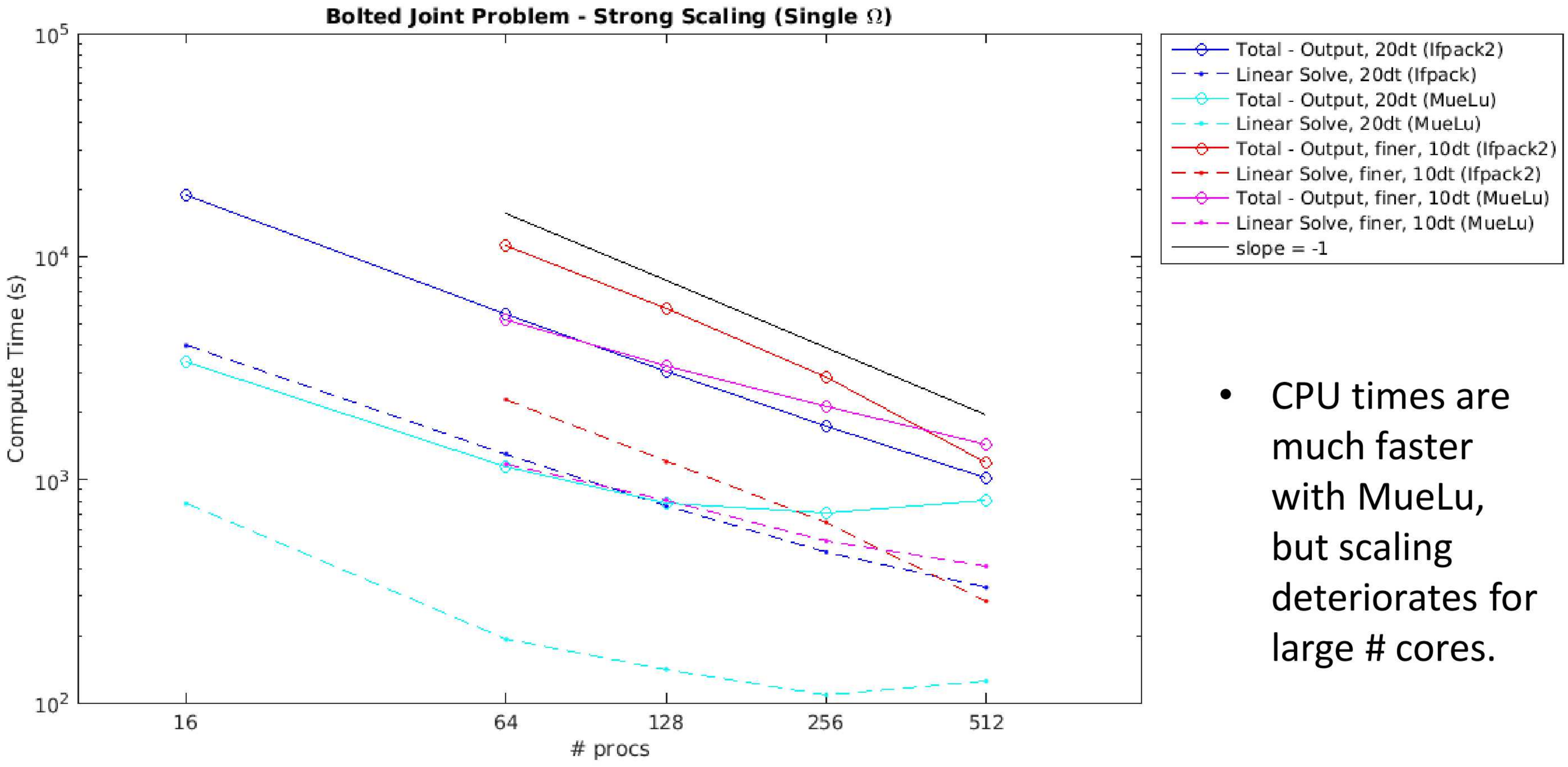
- *Top right plot:* # Schwarz iterations for each time step.
  - After start-up, # Schwarz iterations / time step is ~9-10 – this is not bad given how small is the size of the overlap region for this problem.

Bolted Joint Strong Scaling on Skybridge: Schwarz vs. Single Domain with Ifpack2



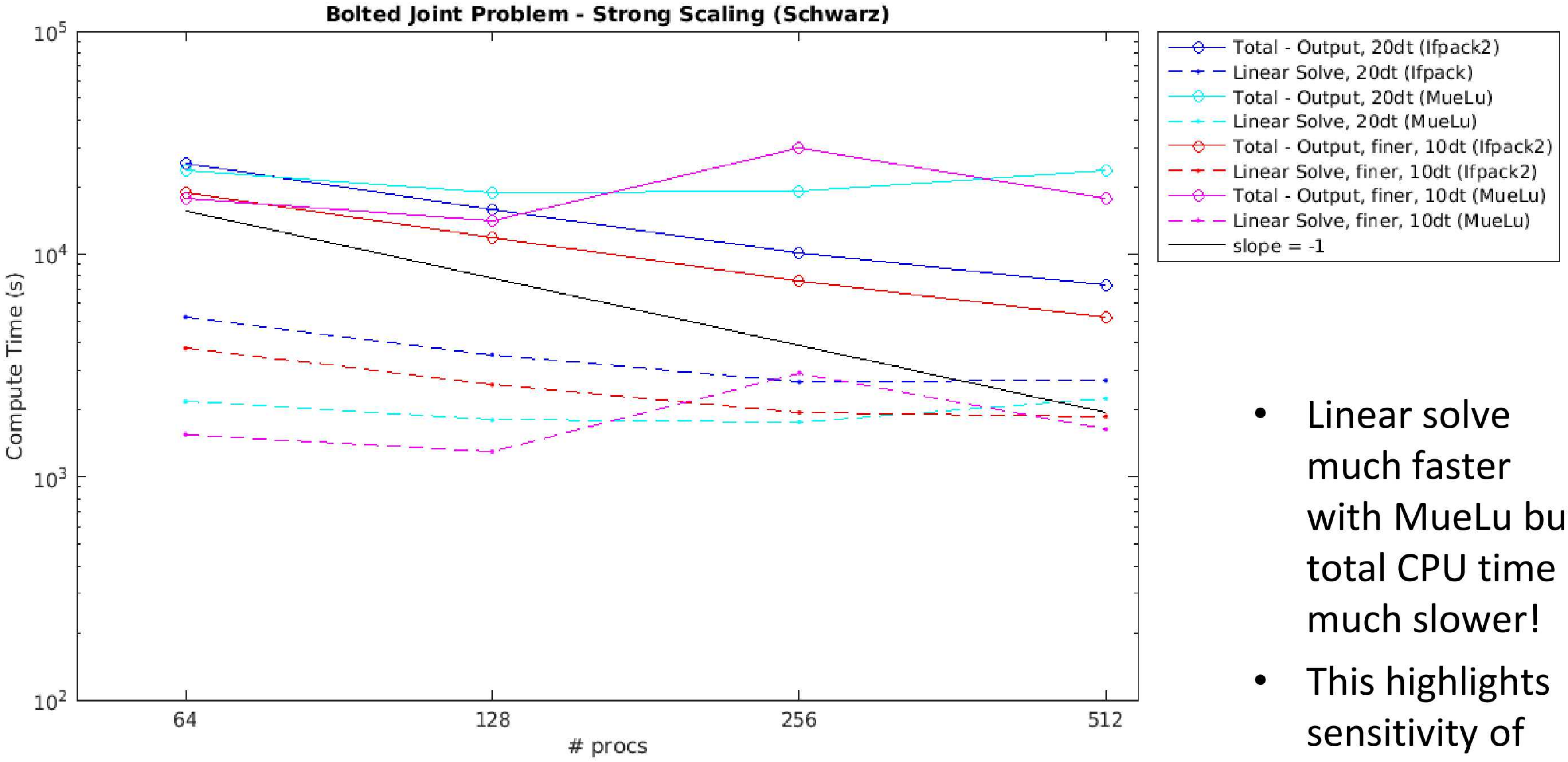
- Strong scaling for Schwarz is slightly less than ideal linear speedup.
- Likely this is due to linear solve.
- Schwarz scaling is similar to single domain scaling.

Bolted Joint Strong Scaling on Skybridge: Single Domain, Ifpack2 vs. MueLu



- CPU times are much faster with MueLu, but scaling deteriorates for large # cores.

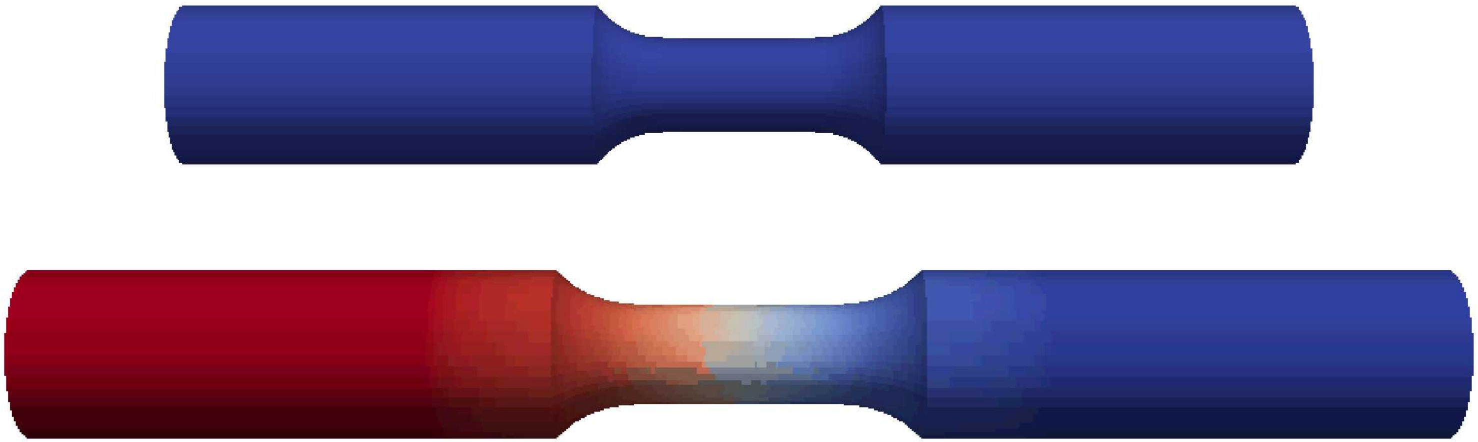
Bolted Joint Strong Scaling on Skybridge: Schwarz, Ifpack2 vs. MueLu



- Linear solve much faster with MueLu but total CPU time much slower!
- This highlights sensitivity of nonlinear solver trajectory.

Tension Specimen Problem

- Specimen is pulled from top (upper_grip) and bottom (lower_grip) simultaneously such that displacement of 0.01 is attained at time T = 1e-3.
- Zero velocity and displacement initial condition.
- Problem is run using implicit Newmark-Beta.
- J2 material model is employed with properties of aluminum.
- Figure below shows initial and final configurations.

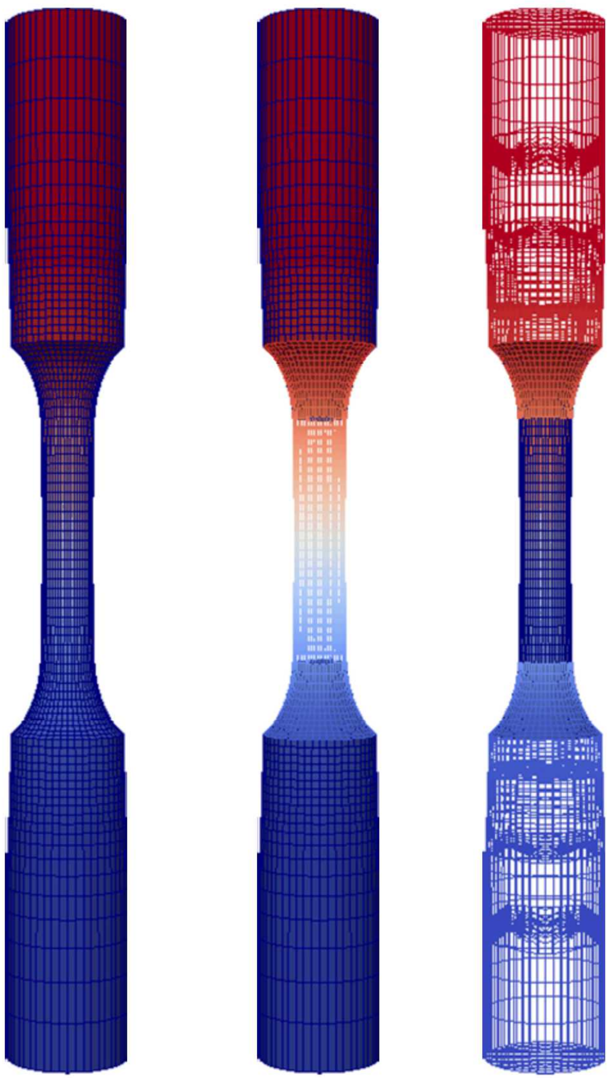


Initial y-disp

Final y-disp

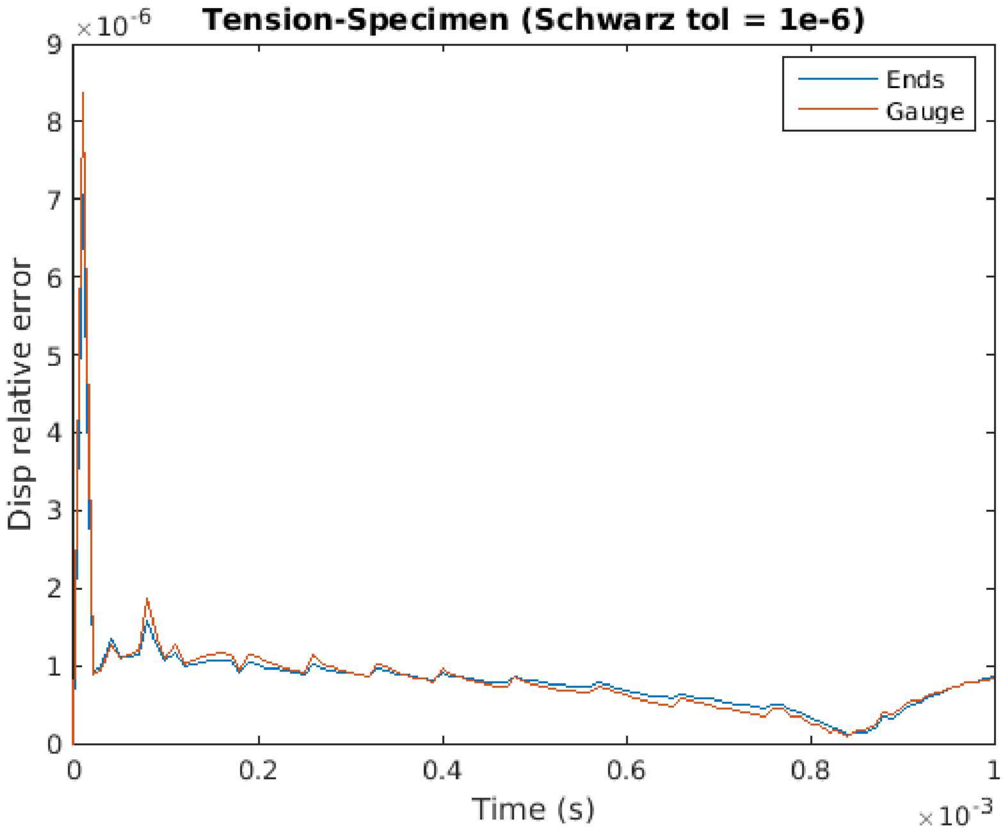
Tension Specimen Problem: Conformal Hex-Hex Schwarz Coupling

- Domain is decomposed into 2 subdomains for Schwarz, discretized with conformal hexahedral meshes.
- Schwarz solution is compared with single-domain solution computed on a hex mesh conformal with the Schwarz meshes.
- Implicit Newmark-Beta is employed with dt = 1e-5.
- Schwarz relative and absolute tolerances = 1e-6.
- QoIs: displacement, nodal_eqps, nodal_Cauchy_Stress_5.



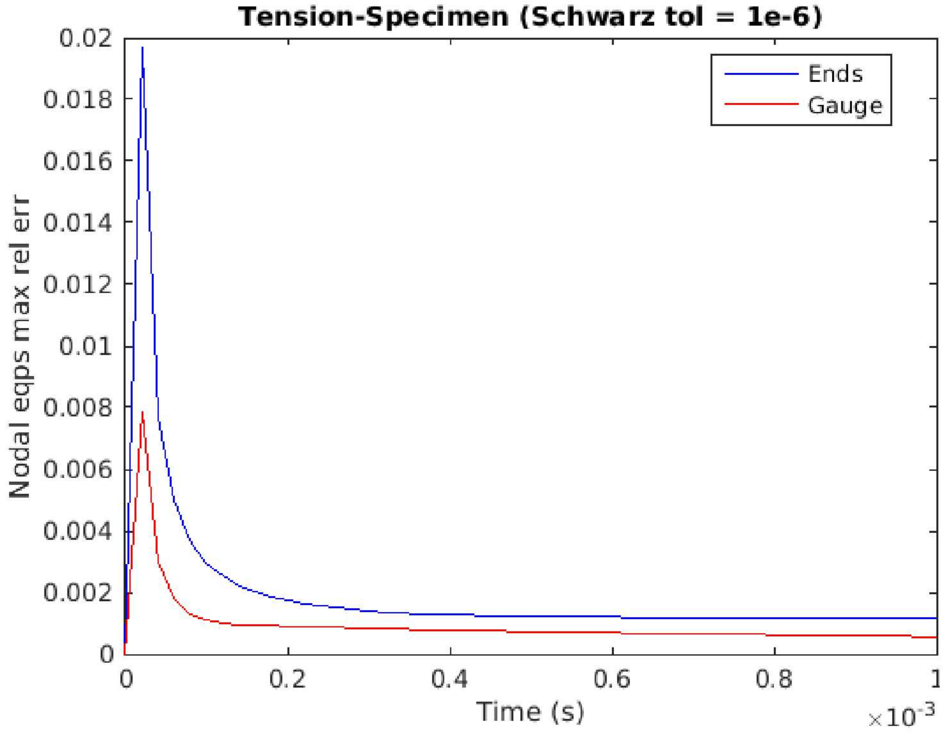
Ω_{ref} Ω_1 Ω_2

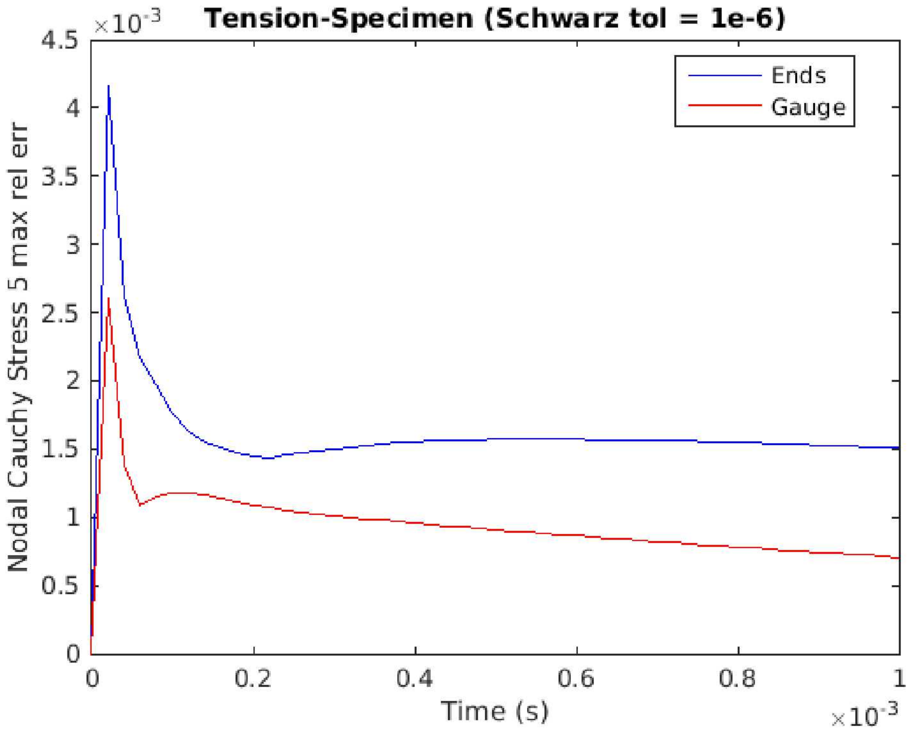
Tension Specimen Problem: Conformal Hex-Hex Schwarz Coupling



- Displacement relative errors in Schwarz solution is of O(1e-6), same as Schwarz tolerance (as expected!).
- Errors do not grow in time.

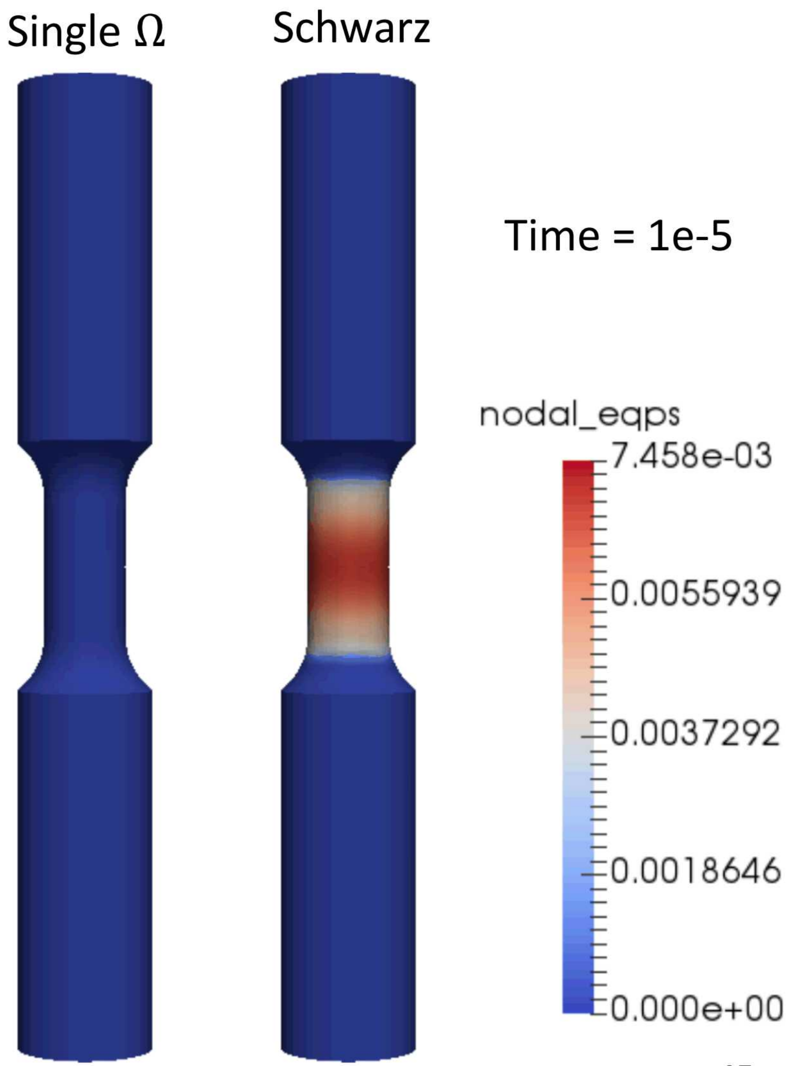
Tension Specimen Problem: Conformal Hex-Hex Schwarz Coupling





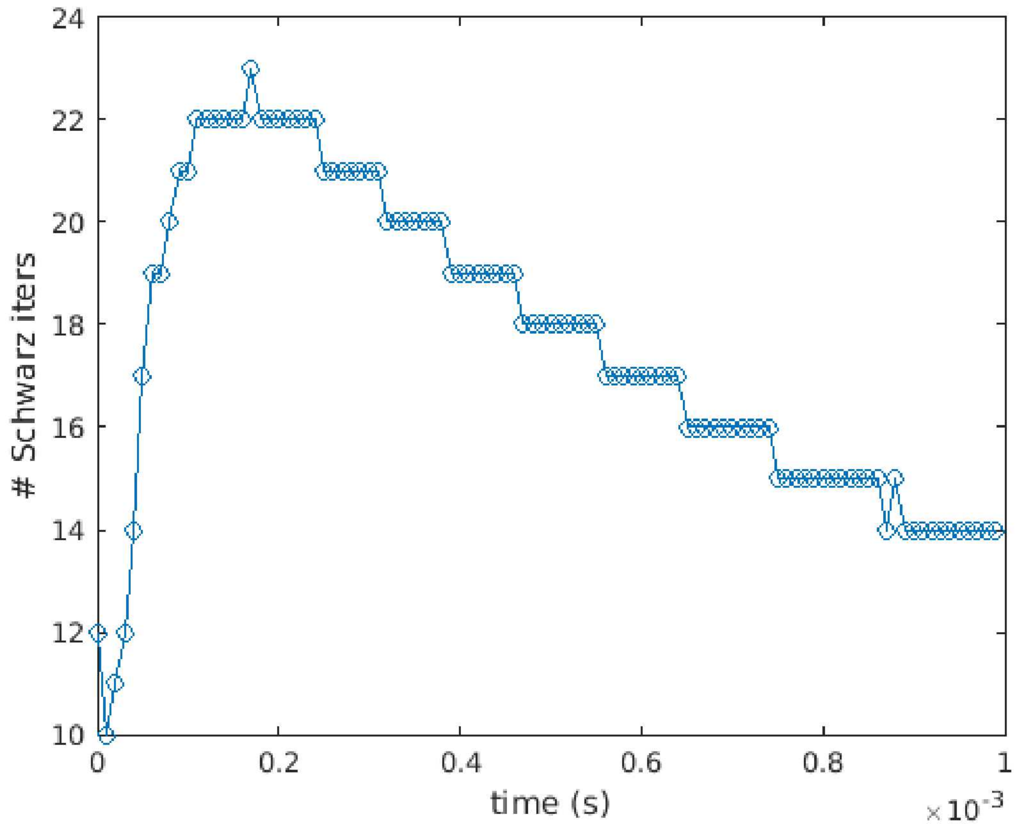
- Above plots show maximum relative error in nodal eqps (left) and 5th component of nodal Cauchy Stress (right). Errors are O(1e-3).

Tension Specimen Problem: Conformal Hex-Hex Schwarz Coupling



- Note that there is a bug in computing the nodal_epqs and nodal_Cauchy_ Stress fields in the single domain run – these fields are 0 in 1st time-step for reference (single domain) solution if “Exodus Write Interval” = 1.
  - The same thing happens for bolted joint problem.
  - Non-nodal eqps and Cauchy_Stress fields are non-zero in 1st time step.
  - Problem does not occur when Exodus Write Interval > 1.

Tension Specimen Problem: Schwarz Convergence for Conformal Hex-Hex Coupling

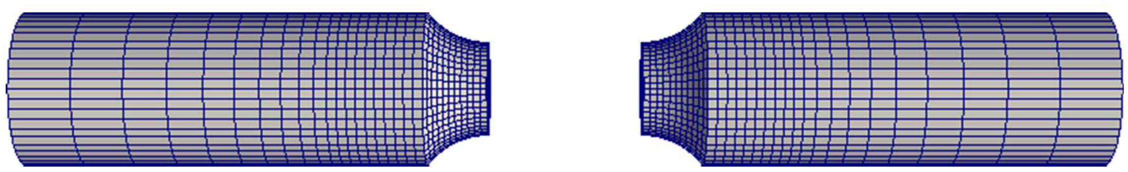


- *Above plot:* # Schwarz iterations for each time step.
  - # Schwarz iters declines during transient runs.
  - Schwarz tolerance is pretty small (1e-6) even though overlap is large.

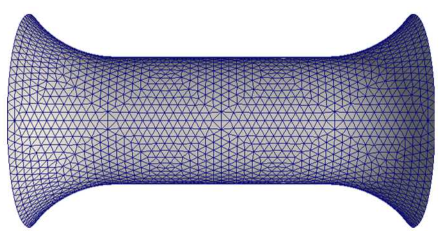
Tension Specimen Problem: Hex-Composite Tet Coupling

- I tried to run this with ends hex meshed and the gauge composite tet 10 meshed, but linear solver in composite tet 10 mesh failed (Ifpack2 and MueLu).
- Same thing happened with all composite tet 10 single domain mesh obtained by splitting original hex mesh into tets.
- Need to try again with "good" all composite tet 10 mesh.
- Thoughts? Run quasi-statically? Talk to MueLu guys about settings?

Ω_1



Ω_2



Tension Specimen Problem with Faster Loading

- Same problem as before except we apply a faster loading to run explicitly.
- Specimen is pulled from top (upper_grip) and bottom (lower_grip) simultaneously such that displacement of 0.01 is attained at time T = 1e-6.
- Zero velocity and displacement initial condition.
- Problem is to be run using explicit Newmark-Beta (or explicit-implicit coupling using Schwarz).
  - Need to discuss issue with running explicitly – solution is incorrect.
- J2 material model is employed with properties of aluminum.