Meshfree Methods for PDEs

Galerkin Methods & Generalized Finite Elements

Marc Alexander Schweitzer

Institut für Numerische Simulation
Rheinische Friedrich-Wilhelms-Universität Bonn

Fraunhofer-Institut für Algorithmen und Wissenschaftliches Rechnen (SCAI)

September 15, 2017

Meshfree Methods: Galerkin Methods

$$\begin{aligned} \nabla \cdot \sigma(u) + b &= 0 && \text{in } \Omega \\ \sigma(u) \cdot n &= h && \text{on } \Gamma_N \subset \partial\Omega \\ u &= g && \text{on } \partial\Omega \setminus \Gamma_N =: \Gamma_D \end{aligned}$$

with e.g. $\sigma(u) = C\epsilon(u) = \frac{1}{2}C(\nabla u + (\nabla u)^T)$ or $\kappa \nabla u$.

Galerkin Discretization

$$\begin{aligned} \langle \nabla \cdot \sigma(u) + b, v \rangle &= 0 && \text{for all } v \in V \cap \Omega \\ \sigma(u) \cdot n &= h && \text{on } \Gamma_N \subset \partial\Omega \\ u &= g && \text{on } \partial\Omega \setminus \Gamma_N = \Gamma_D \end{aligned}$$

- Which V? $V \subset H^1$? $V \subset H^1_{\Gamma_D,0}$?
- Implementation essential boundary conditions
- Integration by parts, appropriate domain & surface integration
- Properties of resulting linear system

schweitzer@scai.fraunhofer.de

Meshfree Methods: Essential Boundary Conditions

Issue

Meshfree trial and test functions in general do not satisfy respective boundary conditions.

- Lagrange multipliers:
  - Saddle point structure
  - Selection of multiplier space with LBB
  - Conditioning
- Penalty methods:
  - Consistency error
  - Conditioning
- Nitsche's method
- Conforming treatment

schweitzer@scai.fraunhofer.de

Essential Boundary Conditions: Conforming Treatment

Simple approach:

$$V_{\Gamma_D,g} = \text{span}\{v \in V | \, \text{supp}(v) \cap \Gamma_D = \emptyset\}$$

Global approach:

$$V_{\Gamma_D,g} = \text{span}\{v \in V | \gamma(v)|_{\Gamma_D} = 0\}$$

- Identification of the kernel of the trace operator.
- Discretization of the trace operator.
- Global direct solver for surface problem.
- Weak form of PDE identical to FEM.
- How to set non-vanishing boundary conditions?

Essential Boundary Conditions: Nitsche's Method

$$
\begin{aligned}
-\operatorname{div}\boldsymbol{\sigma}(u) &= f && \text{in } \Omega \subset \mathbb{R}^D, \\
\boldsymbol{\sigma}(u)\cdot n &= g_N && \text{on } \Gamma_N \subset \partial\Omega, \\
u \cdot n &= g_{D,n} && \text{on } \Gamma_D = \partial\Omega \setminus \Gamma_N, \\
(\boldsymbol{\sigma}(u)\cdot n)\cdot t &= 0 && \text{on } \Gamma_D = \partial\Omega \setminus \Gamma_N,
\end{aligned}
\tag{1}
$$

where $\boldsymbol{\sigma}(u)$ denotes the symmetric stress tensor and $\epsilon(u)$ the symmetric strain tensor.
Integrating by parts and utilizing the symmetry of $\boldsymbol{\sigma}(u)$, we obtain

$$
-\int_\Omega \operatorname{div}\boldsymbol{\sigma}(u)\cdot v \, dx = \int_\Omega \boldsymbol{\sigma}(u) : \epsilon(v) - \int_{\partial\Omega} \boldsymbol{\sigma}(u) n \cdot v \, ds = \int_\Omega fv \, dx.
$$

Decomposing the boundary $\partial\Omega$ into the Neumann Γ_N and Dirichlet parts $\Gamma_D = \partial\Omega \setminus \Gamma_N$ we can bring the Neumann boundary conditions to the right-hand side. On the left hand side only the *consistency* term on the Dirichlet boundary Γ_D remains.

$$
\int_\Omega \boldsymbol{\sigma}(u) : \epsilon(v) \, dx - \int_{\Gamma_D} \boldsymbol{\sigma}(u) n \cdot v \, ds = \int_\Omega fv \, dx + \int_{\Gamma_N} g_N v \, ds
$$

Essential Boundary Conditions: Nitsche's Method

On Γ_D we have essential boundary conditions in normal direction but vanishing natural boundary conditions in tangential direction. Therefore, we split the integrand of the consistency term on the left hand side into normal and tangential parts.

$$\int_{\Gamma_D} \boldsymbol{\sigma}(u)n \cdot v \; ds = \int_{\Gamma_D} \big((n \cdot \boldsymbol{\sigma}(u)n)n + (t \cdot \boldsymbol{\sigma}(u)n)t\big) \cdot v \; ds$$

With (**??**) we obtain

$$\int_{\Omega} \boldsymbol{\sigma}(u) : \boldsymbol{\epsilon}(v) \; dx - \int_{\Gamma_D} (n \cdot \boldsymbol{\sigma}(u)n)n \cdot v \; ds = \int_{\Omega} fv \; dx + \int_{\Gamma_N} g_N v \; ds$$

Now we are in a position to symmetrize the bilinear form consistently using available boundary values only.

$$\int_{\Omega} \boldsymbol{\sigma}(u) : \boldsymbol{\epsilon}(v) \; dx - \int_{\Gamma_D} \big((n \cdot \boldsymbol{\sigma}(u)n)n \cdot v + (n \cdot \boldsymbol{\sigma}(v)n)n \cdot u\big) \; ds$$
$$= \int_{\Omega} fv \; dx + \int_{\Gamma_N} g_N v \; ds - \int_{\Gamma_D} g_{D,n}(n \cdot \boldsymbol{\sigma}(v)n) \; ds$$

schweitzer@scai.fraunhofer.de

Essential Boundary Conditions: Nitsche's Method

Finally, we introduce the regularization term which again may only involve available boundary information. Hence, the regularization for this model problem employs information in normal direction only, e.g.

$$a_\beta(u,v) := \int_\Omega \boldsymbol{\sigma}(u) : \boldsymbol{\epsilon}(v)\, dx - \int_{\Gamma_D} \left((n\cdot\boldsymbol{\sigma}(u)n)n\cdot v + (n\cdot\boldsymbol{\sigma}(v)n)n\cdot u\right) ds + \beta \int_{\Gamma_D} u\cdot n v\cdot n\, ds$$

and

$$\langle l_\beta, v\rangle := \int_\Omega fv\ dx + \int_{\Gamma_N} g_N v\ ds - \int_{\Gamma_D} g_{D,n}(n\cdot\boldsymbol{\sigma}(v)n) + \beta \int_{\Gamma_D} g_{D,n} v\cdot n\ ds.$$

Essential Boundary Conditions: Nitsche's Method

Coercivity on V can be shown can be shown under the assumption of an inverse inequality

$$\begin{aligned} \|(n \cdot \boldsymbol{\sigma}(u)n)\|^2_{L^2(\partial\Omega,\mathbb{R}^D)} &\leq C^2_{\text{inv}} \int_\Omega \boldsymbol{\sigma}(u) : \epsilon(v)\, dx \\ &= C^2_{\text{inv}} a(u,u) \\ &\leq C^2_{\text{inv}} C_{\text{cont}} \|\epsilon(u)\|^2_{L^2(\Omega,\mathbb{R}^D)} \end{aligned} \tag{2}$$

holds for all $u \in V$ and the choice of the regularization parameter $\beta > C^2_{\text{inv}}$.

Optimal convergence rates can be shown under the assumption that $C_{\text{inv}} \asymp h^{-1/2}$ where $h \asymp \operatorname{diam}\operatorname{supp}(\phi)$.

How to obtain $\beta > C^2_{\text{inv}}$ for a particular space V, domain Ω and boundary segment Γ_D?

Essential Boundary Conditions: Nitsche's Method

Mathematical approach

Impose many restrictions on space V, domain Ω and boundary segment Γ_D and prove the inverse estimate with explicit constants.

Good luck!

$$\begin{aligned} \|(n \cdot \boldsymbol{\sigma}(u)n)\|^2_{L^2(\Gamma_D,\mathbb{R}^D)} &\leq C^2_{\text{inv}} \int_\Omega \boldsymbol{\sigma}(u) : \boldsymbol{\epsilon}(v)\, dx \\ &= C^2_{\text{inv}} a(u,u) \end{aligned}$$

Pragmatic approach

Directly compute C^2_{inv} for the particular discrete configuration at hand.

Generalized eigenvalue problem!

schweitzer@scai.fraunhofer.de

Meshfree Methods: Domain Integration

- Meshfree shape functions are in general piecewise rational functions.
- Global regularity is “limited” by employed weight/kernel (but higher than in FE).
- Evaluation of meshfree shape functions rather expensive.

Early Approaches

- Gauß integration on (independent) background mesh.
- Naive nodal integration.

Encountered Issues

- Very expensive and convergence rates maybe affected.
- Stability, support size, ...

schweitzer@scai.fraunhofer.de

Meshfree Methods: Fixing Numerical Integration

Most Simple Situation: Poisson Problem

$$\int_\Omega \nabla\phi_i(x)\nabla\phi_j(x)\,dx =: K_{ij}, \quad \mathcal{I}_\Omega \nabla\phi_i(x)\nabla\phi_j(x)\,dx =: \hat{K}_{ij}$$

- All meshfree basis functions satisfy

$$\sum_{i=0}^{N} \phi_i \equiv 1, \qquad \nabla \sum_{i=0}^{N} \phi_i = \sum_{i=0}^{N} \nabla\phi_i \equiv 0$$

- Any discrete integration scheme should yield

$$\sum_{j=0}^{N} \hat{K}_{ij} = \sum_{j=0}^{N} \mathcal{I}_\Omega \nabla\phi_i(x)\nabla\phi_j(x)\,dx = 0$$

schweitzer@scai.fraunhofer.de

Meshfree Methods: Fixing Nodal Integration

Integration Constraint / Divergence Constraint

$$\mathcal{I}_\omega \nabla \phi_i(x)\, dx = \mathcal{I}_{\partial\omega} \phi_i(x) \cdot n(x)\, ds$$

- Number of approaches to enforce this constraint.
- Changing the basis functions.
- Changing the definition of the gradient.

Stabilized Conforming Nodal Integration

$$\tilde{\nabla}\phi_i(x_j) := \frac{1}{W_j} \int_{\omega_j} \nabla \phi_i(x)\, dx = \frac{1}{W_j} \int_{\omega_j} \phi_i(x) \cdot n(x)\, ds$$

schweitzer@scai.fraunhofer.de

Meshfree Methods: Fixing Nodal Integration

Smoothed Gradients

$$\tilde{\nabla}\phi_i(x_j) := \frac{1}{W_j}\int_{\omega_j} \nabla\phi_i(x)\, dx = \frac{1}{W_j}\int_{\omega_j} \phi_i(x)\cdot n(x)\, ds$$

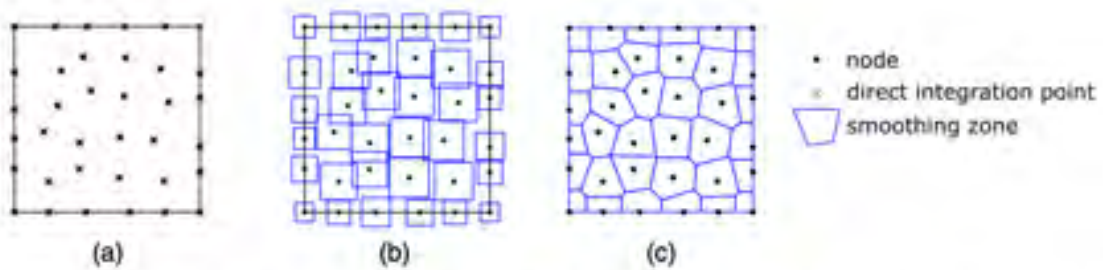


Fig. 13. Nodal integration schemes in meshfree methods: (a) direct nodal integration; (b) stabilized nonconforming nodal integration; (c) stabilized conforming nodal integration

- Yields optimal convergence for linearly exact meshfree basis functions.
- Generalization to other fields/equations e.g. strain smoothing.
- Generalization to “variationally consistent integration” framework.

schweitzer@scai.fraunhofer.de

Meshfree Methods: Fixing Nodal Integration

Variationally Consistent Integration

Generalization of condition

$$\mathcal{I}_\omega \nabla \phi_i(x)\, dx = \mathcal{I}_{\partial\omega} \phi_i(x) \cdot n(x)\, ds$$

to integration by parts when testing with monomials of order $\leq n$

$$\mathcal{I}_\omega \nabla \phi_i(x) \cdot p_\alpha\, dx = -\mathcal{I}_\omega \phi_i(x) \cdot \nabla p_\alpha\, dx + \mathcal{I}_{\partial\omega} \phi_i(x) \cdot n(x)\, ds$$

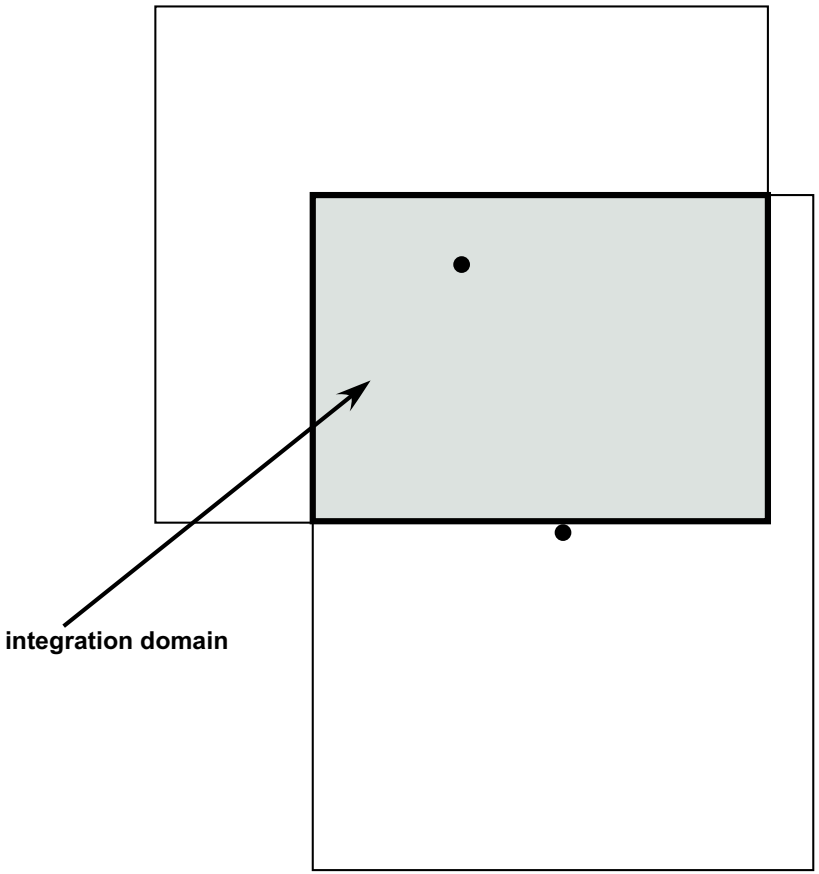
- Number of publications on the subject.
- Patch test type and some mathematical analysis.

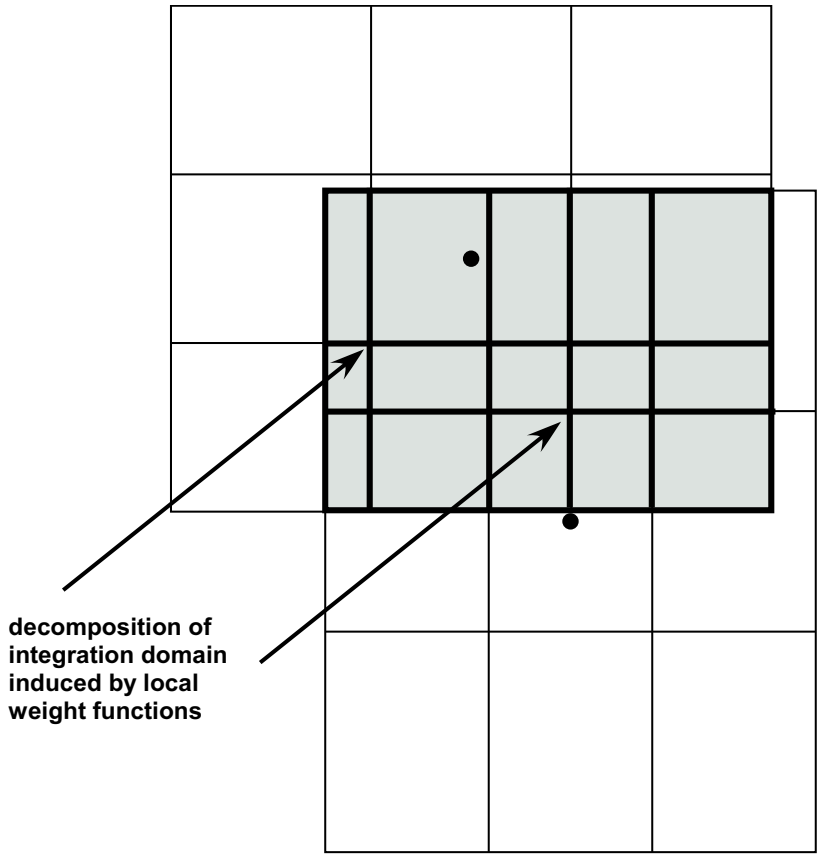
Dynamics

Extension to implicit / explicit dynamics?

schweitzer@scai.fraunhofer.de

Meshfree Methods: “Correct” Numerical Integration

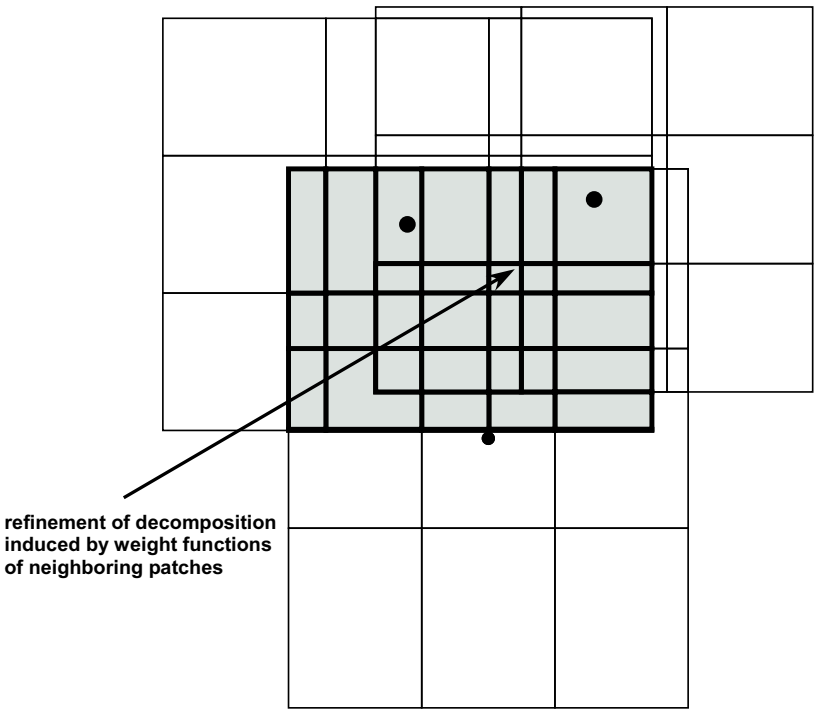


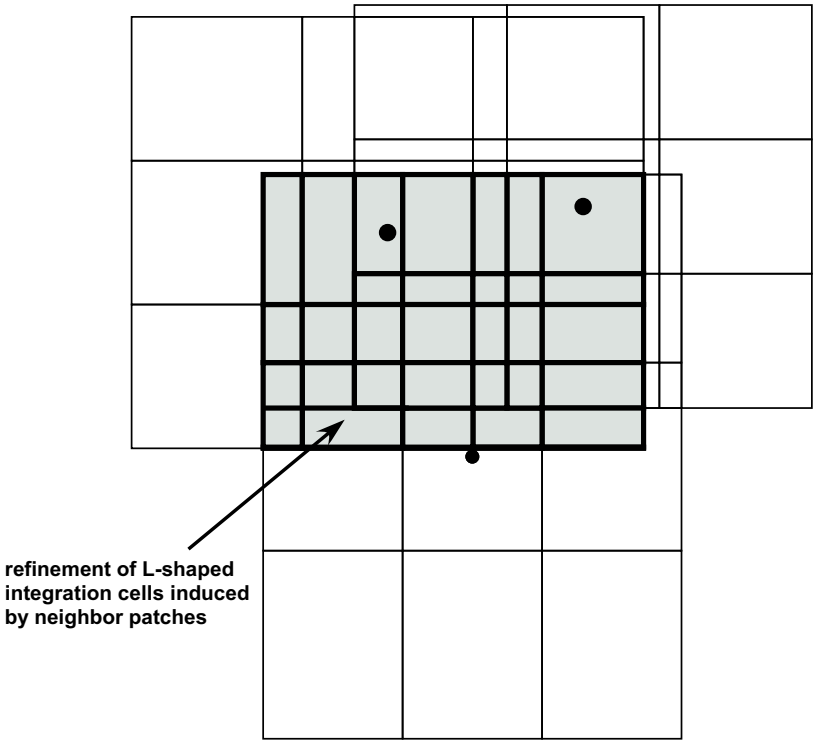


- Minimal integration domains, i.e. respect supports of basis functions.
- Respect internal structure of weight/kernel.

schweitzer@scai.fraunhofer.de

Meshfree Methods: “Correct” Numerical Integration





- Respect all neighbors.
- Resolve non-convex integration domains.

May yield much larger number of integration domains/points!

Optimal Approximation Spaces

Historic goals

- Simpler domain approximation than mesh generation.
- Less constraints in adaptive refinement.
- Easy construction of approximations with arbitrary smoothness.
- Allows for large deformations.

Modern (mathematical) goals

- Convergence order independent of regularity of problem/solution.

MLS & RKPM

- Allows for arbitrary smoothness via weight/kernel.
- Allows for *h*-adaptivity ✓, *p*-adaptivity × (multiscale RKPM ✓).
- Allows for discontinuities via weight/kernel/visibility criterion.
- More general basis functions?
- Linear solvers, stability and explicit dynamics?

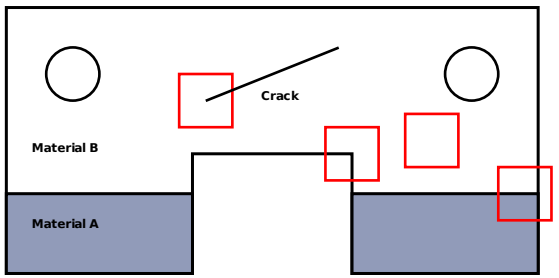
schweitzer@scai.fraunhofer.de

Decomposition of $u \in H^s(\Omega)$

$$u = u_{\text{smooth}} + u_{\text{jump}} + u_{\text{singular}}$$

Efficient approximation of u

- Higher order polynomials for u_{smooth}.
- Discontinuous basis functions for u_{jump}.
- Singular basis functions for u_{singular}.



Localization by partition of unity

- Consider a partition of unity (PU) $\{\varphi_i\}$ with $\omega_i := \text{supp}(\varphi_i)$

$$u = \sum_{i=1}^{N} \varphi_i u = \sum_{i=1}^{N} \left(\varphi_i u_{\text{smooth}} + \varphi_i u_{\text{jump}} + \varphi_i u_{\text{singular}} \right).$$

- Localization of approximation: $u|_{\omega_i} \approx u_i \in V_i(\omega_i) = \text{span}\langle \vartheta_i^k \rangle$.
- Smooth splicing of local spaces

$$V^{\text{PU}} := \sum_{i=1}^{N} \varphi_i V_i(\omega_i) = \sum_{i=1}^{N} \varphi_i (\mathcal{P}^{p_i} + \mathcal{E}_i).$$

- *No* compatability restrictions as in FEM (local/parallel).
- Approximation by $V_i(\omega_i)$, functions φ_i just "glue".

schweitzer@scai.fraunhofer.de

Meshfree Methods: Partition of Unity Methods

Definition (Partition of Unity)

Let $\{\varphi_i : i = 1, \ldots, N\}$ be a collection of N Lipschitz functions with

$$\sum_{i=1}^{N} \varphi_i \equiv 1 \text{ on } \overline{\Omega}, \quad \|\varphi_i\|_{L^\infty(\mathbb{R}^D)} \leq C_\infty, \quad \|\nabla\varphi_i\|_{L^\infty(\mathbb{R}^D)} \leq \frac{C_\nabla}{\operatorname{diam}(\omega_i)}.$$

Local approximation spaces

$$V_i(\operatorname{supp}(\varphi_i)) = V_i(\omega_i) = \mathcal{P}^{p_i} + \mathcal{E}_i = \operatorname{span}\langle\vartheta_i^n\rangle = \operatorname{span}\langle\psi_i^s\rangle + \operatorname{span}\langle\eta_i^t\rangle$$

Global PUM space

$$V^{\mathrm{PU}} = \sum_{i=1}^{N} \varphi_i V_i = \operatorname{span}\langle\varphi_i\vartheta_i^n\rangle$$

schweitzer@scai.fraunhofer.de

Partition of Unity Methods: Notation

Arbitrary function $u \in V^{\mathrm{PU}}$

$$u(x) = \sum_{i=1}^{N} \sum_{m=1}^{d_{V_i}} u_i^m \varphi_i(x) \vartheta_i^m(x)$$

Local contributions from $V_i(\omega_i)$

$$u_i(x) = \sum_{m=1}^{d_{V_i}} u_i^m \vartheta_i^m(x)$$

Coefficient-vectors and moment-vectors

$$\tilde{u} = (u_{(i,m)}), \quad \hat{f} = (\langle f, \varphi_i \vartheta_i^m \rangle)$$

schweitzer@scai.fraunhofer.de

Partition of Unity Methods: Approximation Properties

PUM error bound (Babuška, Melenk)

Let φ_i be an admissible PU. Assume that on each patch $\Omega \cap \omega_i$, the function f can be approximated by a function $v_i \in V_i$ such that

$$\|f - v_i\|_{L^2(\Omega\cap\omega_i)} \leq \hat{\epsilon}_i, \quad \text{and} \quad \|\nabla(f - v_i)\|_{L^2(\Omega\cap\omega_i)} \leq \tilde{\epsilon}_i$$

hold for all $i = 1, \ldots, N$. Then the function

$$v := \sum_{i=1}^{N} \varphi_i v_i \in V^{\mathrm{PU}} \subset H^1(\Omega)$$

satisfies the global estimates

$$\begin{aligned} \|f - v\|_{L^2(\Omega)} &\leq \sqrt{\Lambda} C_\infty \Big(\sum_{i=1}^{N} \hat{\epsilon}_i^2 \Big)^{1/2}, \\ \|\nabla(f - v)\|_{L^2(\Omega)} &\leq \sqrt{2\Lambda} \Big(\sum_{i=1}^{N} \big(\frac{C_\nabla}{\mathrm{diam}(\omega_i)} \big)^2 \hat{\epsilon}_i^2 + C_\infty^2 \tilde{\epsilon}_i^2 \Big)^{1/2}. \end{aligned}$$

Partition of Unity Methods: Selection of Local Enrichments

Enrichments

- Exact enrichments
  - Known singularitites (e.g. $\eta(x) = \|x - x_0\|^\alpha$),
  - Known discontinuities (e.g. $\eta(x) = \cos(\frac{\theta_c}{2})$)
- Approximate enrichments:
  - Singularities $\eta(x) = \|x - x_0\|^\beta$
  - Discontinuities $\eta(x) = H_\pm(x - c)$
  - Boundary layers $\eta(x) = \exp(1 - \mathrm{dist}(x, c))$
  - Radial component of solution
- Numerical enrichments:
  - Cell problems (with/without global-local-approach)
  - Reconstruction of experimental data (or reduced order basis)
  - Eigenfunctions of local problems

Goals

- Optimal fine level approximation: Error minimization.
- Acceptable coarse level approximation: Fast & robust solution.
- Load-balancing in local and global operations.

schweitzer@scai.fraunhofer.de

Partition of Unity Methods: Evaluation of Approximation Quality

Notation

$$u = u_s + u_r, \quad u_r \in H^2(\Omega), \quad u^{\mathrm{PU}} = \sum_{i=1}^{N} \varphi_i \underbrace{(\psi_i + \eta_i)}_{\in \mathcal{P}^{p_i} + \mathcal{E}_i}$$

Optimal Convergence

$$\|u - w_i\| = \|u_r + u_s - \psi - \eta\| \leq \|u_r - \psi_i\| + \|u_s - \eta_i\|$$

Since $u_s|_{\omega_i} \in \mathcal{E}_i$, choice of $\eta_i = u_s$ yields

$$\|u - w_i\|_{L^2(\omega_i \cap \Omega)} \leq \|u_r - \psi_i\|_{L^2(\omega_i \cap \Omega)} \leq c\, h_i^t \|u_r\|_{H^t(\omega_i \cap \Omega)},$$

and

$$\|\nabla(u - w_i)\|_{L^2(\omega_i \cap \Omega)} \leq \|\nabla(u_r - \psi_i)\|_{L^2(\omega_i \cap \Omega)} \leq c\, h_i^{t-1} \|u_r\|_{H^t(\omega_i \cap \Omega)}.$$

schweitzer@scai.fraunhofer.de

Partition of Unity Methods: Super-Convergence in Enrichment Zone

Considering a different splitting

$$u = \underbrace{\operatorname{Proj} u}_{\in \mathcal{P}^{p_i}} + \underbrace{(u - \operatorname{Proj} u)}_{\in H^1(\Omega) \setminus \mathcal{P}^{p_i}}$$

Local spaces $V_i = \mathcal{P}^{p_i} \oplus \mathcal{E}_i \setminus \mathcal{P}^{p_i}$. Estimates now take the form

$$\|u - w_i\| \leq \|\operatorname{Proj} u - \psi\| + \|(u - \operatorname{Proj} u) - \eta\| = \|(u - \operatorname{Proj} u) - \eta\|.$$

There exists η_s such that

$$\|u - w_i\| \leq \|(u - \operatorname{Proj} u) - \eta\| \leq \|\underbrace{(u - \operatorname{Proj} u) - \eta_s}_{\in H^m(\omega_i \cap \Omega)} - \eta_r\|.$$

Error Bound?

$$\|(u - \operatorname{Proj} u) - \eta_s - \eta_r\| \leq C(\omega_i) \, \|(u - \operatorname{Proj} u) - \eta_s\|$$

Numerical measurement of

$$C_V(\omega_i) := \frac{\|u - w_i\|}{\|u - \operatorname{Proj} u\|}, \, C_{\mathcal{E}}(\omega_i) := \frac{\|(u - \operatorname{Proj} u) - \eta\|}{\|u - \operatorname{Proj} u\|}.$$

schweitzer@scai.fraunhofer.de

Exact enrichments: Linear fracture mechanics

Goal

Error minimization of finest level (accuracy of SIF)

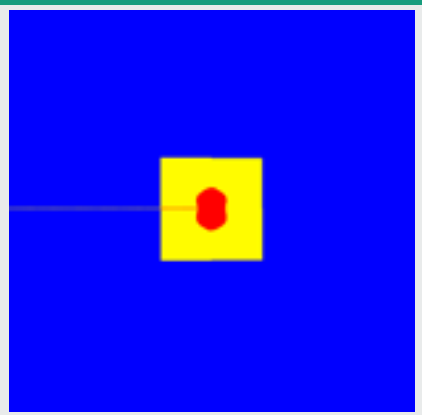
- Displacement discontinuous across crack

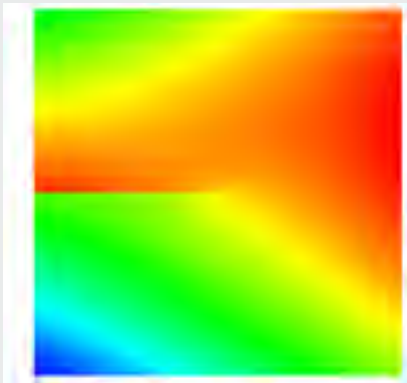
$$\mathcal{E}_i = \mathcal{P}^{p_i} \cdot H^C$$

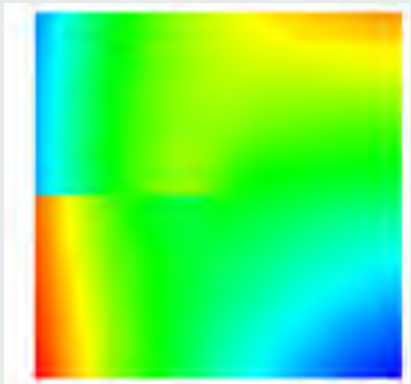
- Stress is singular at crack tip (i.e. gradient of displacement)

$$\mathcal{E} = \{\sqrt{r}\cos\frac{\theta}{2}, \sqrt{r}\sin\frac{\theta}{2}, \sqrt{r}\sin\theta\sin\frac{\theta}{2}, \sqrt{r}\sin\theta\cos\frac{\theta}{2}\}.$$

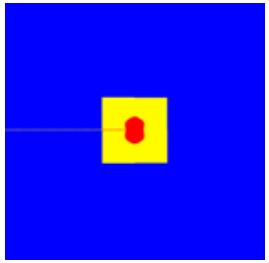
Enrichment zone & exact solution

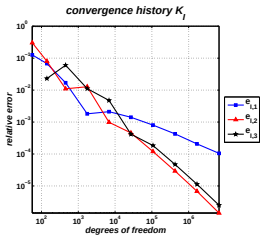


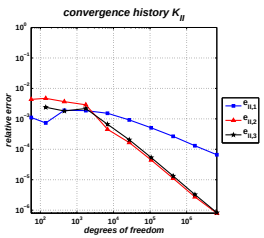


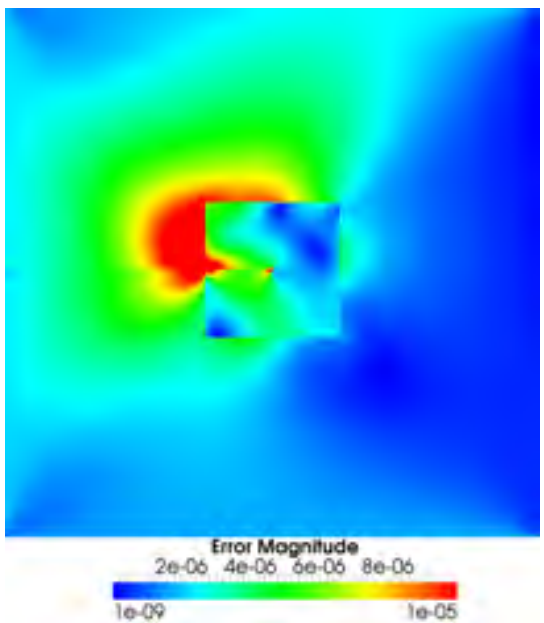


Exact enrichments: Linear fracture mechanics









J	dof	N	$e_{L\infty}$	$\rho_{L\infty}$	e_{L2}	ρ_{L2}	e_{H1}	ρ_{H1}
with respect to Ω								
4	1748	256	7.044_3	0.90	3.425_3	1.00	3.677_2	0.56
5	6836	1024	2.349_3	0.81	9.265_4	0.96	1.795_2	0.53
6	26996	4096	7.999_4	0.78	2.410_4	0.98	8.893_3	0.51
7	107252	16384	2.751_4	0.77	6.121_5	0.99	4.508_3	0.49
8	427508	65536	9.501_5	0.77	1.535_5	1.00	2.215_3	0.51
9	1686716	262144	3.273_5	0.78	3.820_6	1.01	9.948_4	0.58
with respect to E_1								
4	236	16	5.745_2	0.53	3.112_2	0.66	1.050_1	0.56
5	528	36	1.915_2	1.36	7.083_3	1.84	4.028_2	1.19
6	1448	100	6.521_3	1.07	1.594_3	1.48	1.434_2	1.02
7	4632	324	2.243_3	0.92	3.639_4	1.27	5.082_3	0.89
8	16376	1156	7.747_4	0.84	8.482_5	1.15	1.802_3	0.82
9	61368	4356	2.670_4	0.81	2.020_5	1.09	6.441_4	0.78
with respect to E_2								
4	56	4	6.977_2	—	5.785_2	—	9.873_2	—
5	236	16	2.327_2	0.76	1.435_2	0.97	5.154_2	0.45
6	528	36	7.923_3	1.34	3.201_3	1.86	1.984_2	1.19
7	1448	100	2.725_3	1.06	6.776_4	1.54	7.085_3	1.02
8	4632	324	9.410_4	0.91	1.449_4	1.33	2.518_3	0.89
9	16376	1156	3.242_4	0.84	3.227_5	1.19	8.986_4	0.82
with respect to E_3								
5	56	4	3.072_2	—	2.693_2	—	4.728_2	—
6	236	16	1.046_2	0.75	6.846_3	0.95	2.523_2	0.44
7	528	36	3.597_3	1.33	1.476_3	1.91	9.733_3	1.18
8	1448	100	1.242_3	1.05	2.967_4	1.59	3.481_3	1.02
9	4632	324	4.279_4	0.92	6.060_5	1.37	1.244_3	0.88

$$e := \| u - u_I^{PU} \|, \qquad \rho := \log\left(\frac{e_I}{e_{I-1}}\right) / \log\left(\frac{\text{dof}_I}{\text{dof}_{I-1}}\right)$$

Optimal: $\rho_{L2} = \frac{2}{2}$, $\rho_{H1} = \frac{1}{2}$ classical (h^γ) via $d \cdot \rho = \gamma$

schweitzer@scai.fraunhofer.de

Partition of Unity Methods: Enrichment Strategies

Extremly Greedy

Use “perfect” enrichment, i.e. the true solution. Thus, there is no error and therefore no convergence rate.

Traditional

Use a local space which contains the singular component of the solution.

- Multi-dimensional enrichment space.
- Just one dof fixed by solution!
- Remaining dofs should provide some additional approximation.

schweitzer@scai.fraunhofer.de

Numerical Setup & Measurements

Pure Approximation Problem

$$u = \begin{pmatrix} x^2 + y^2 - 1 \\ 1 + x^3 + y^3 \end{pmatrix}, \quad \Omega = (-1, 1)^2$$

Enrichment

Geometric crack tip enrichment in $(-0.25, 0.25)^2$

Measurements

- Local errors $C_{\mathcal{E}}(\omega_i) := \frac{\|(u - \mathbf{Proj}\, u) - \eta\|}{\|u - \mathbf{Proj}\, u\|}$.
- Local errors $C_V(\omega_i) := \frac{\|u - w_i\|}{\|u - \mathbf{Proj}\, u\|}$.
- Local quotients $Q = \frac{C_{\mathcal{E}}(\omega_i)}{C_V(\omega_i)}$
- Local convergence rates $\gamma_{\mathcal{D},L^2}$ and $\gamma_{\mathcal{D},H^1}$.

schweitzer@scai.fraunhofer.de

Local Convergence Behavior in L^2

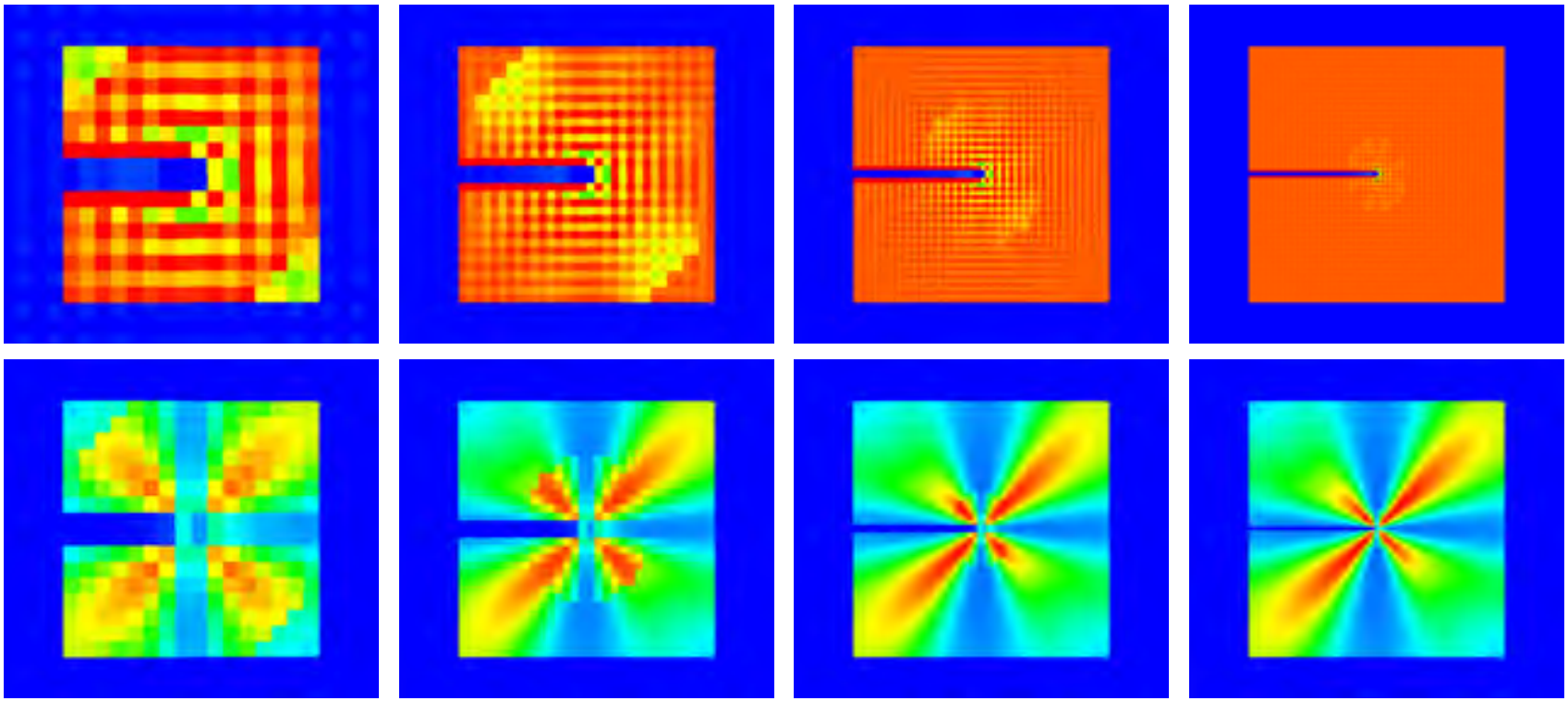


Figure 1: Contour plot of the convergence rate $\gamma_{\mathcal{D},L^2}$ (top row; blue$=2$, red$=3$), the quotient Q_{L^2} (bottom row; blue$=1$, red$=1.75$), on levels $J = 7, 8, 9, 10$ (left to right).

schweitzer@scai.fraunhofer.de

Local Convergence Behavior in H^1

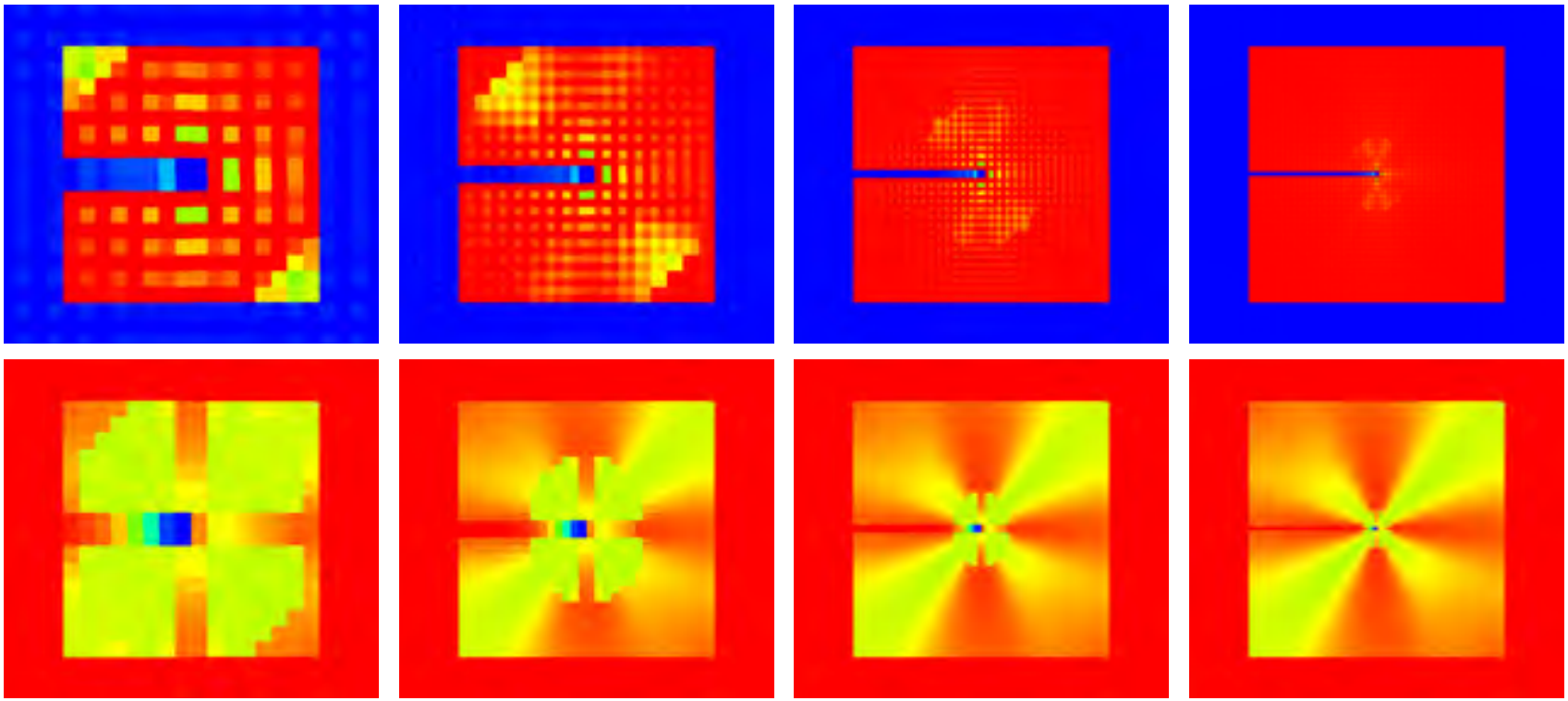


Figure 2: Contour plot of the convergence rate $\gamma_{\mathcal{D},H^1}$ (top row; blue$=1$, red$=2$), and the quotient Q_{H^1} (bottom row; blue$=0.75$, red$=1$), on levels $J = 7, 8, 9, 10$ (left to right).

schweitzer@scai.fraunhofer.de

Global Convergence Behavior

J	dof	N	$e_{L\infty}$	$\rho_{L\infty}$	$\gamma_{L\infty}$	e_{L2}	ρ_{L2}	γ_{L2}	e_{H1}	ρ_{H1}	γ_{H1}
with respect to Ω											
4	1748	256	5.148_{3}	0.98	1.91	2.882_{3}	1.00	1.96	7.820_{2}	0.52	1.01
5	6836	1024	1.323_{3}	1.00	1.96	7.309_{4}	1.01	1.98	3.940_{2}	0.50	0.99
6	26876	4096	3.329_{4}	1.01	1.99	1.839_{4}	1.01	1.99	2.026_{2}	0.49	0.96
7	105636	16384	8.240_{5}	1.02	2.01	4.614_{5}	1.01	1.99	9.965_{3}	0.52	1.02
8	419748	65536	2.025_{5}	1.02	2.02	1.155_{5}	1.00	2.00	4.332_{3}	0.60	1.20
9	1674660	262144	5.080_{6}	1.00	1.99	2.889_{6}	1.00	2.00	2.481_{3}	0.40	0.80
with respect to E_1											
4	368	36	2.924_{3}	2.28	3.18	4.993_{4}	2.14	2.98	5.718_{2}	1.45	2.03
5	1160	100	6.964_{4}	1.25	2.07	7.903_{5}	1.61	2.66	1.808_{2}	1.00	1.66
6	3968	324	1.746_{4}	1.13	2.00	1.303_{5}	1.47	2.60	5.930_{3}	0.91	1.61
7	13704	1156	4.327_{5}	1.13	2.01	2.215_{6}	1.43	2.56	2.006_{3}	0.87	1.56
8	51528	4356	1.077_{5}	1.05	2.01	3.822_{7}	1.33	2.53	6.930_{4}	0.80	1.53
9	200904	16900	2.689_{6}	1.02	2.00	6.666_{8}	1.28	2.52	2.419_{4}	0.77	1.52
with respect to E_2											
4	236	16	2.368_{3}	1.69	3.51	4.042_{4}	1.66	3.44	5.220_{2}	1.30	2.69
5	528	36	6.835_{4}	1.54	1.79	5.771_{5}	2.42	2.81	1.438_{2}	1.60	1.86
6	1448	100	1.713_{4}	1.37	2.00	8.291_{6}	1.92	2.80	4.085_{3}	1.25	1.82
7	4408	324	4.245_{5}	1.25	2.01	1.233_{6}	1.71	2.75	1.197_{3}	1.10	1.77
8	14496	1156	1.048_{5}	1.17	2.02	1.931_{7}	1.56	2.67	3.579_{4}	1.01	1.74
9	53088	4356	2.569_{6}	1.08	2.03	3.109_{8}	1.41	2.63	1.136_{4}	0.88	1.66
with respect to E_3											
4	56	4	2.368_{3}	—	—	4.827_{4}	—	—	6.930_{2}	—	—
5	236	16	6.835_{4}	0.86	1.79	9.568_{5}	1.13	2.33	2.448_{2}	0.72	1.50
6	528	36	1.713_{4}	1.72	2.00	1.424_{5}	2.37	2.75	7.188_{3}	1.52	1.77
7	1448	100	4.245_{5}	1.38	2.01	2.050_{6}	1.92	2.80	2.038_{3}	1.25	1.82
8	4408	324	1.048_{5}	1.26	2.02	3.038_{7}	1.72	2.75	5.880_{4}	1.12	1.79
9	14496	1156	2.569_{6}	1.18	2.03	4.751_{8}	1.56	2.68	1.789_{4}	1.00	1.72

The enrichment has nothing to do with the solution - yet higher order convergence!

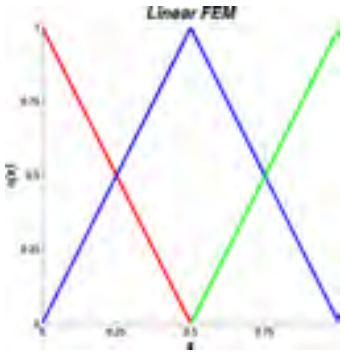
schweitzer@scai.fraunhofer.de

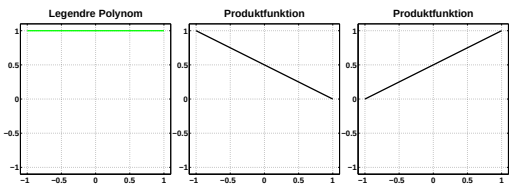
Partition of Unity Methods: Selection of the PU (XFEM/GFEM)

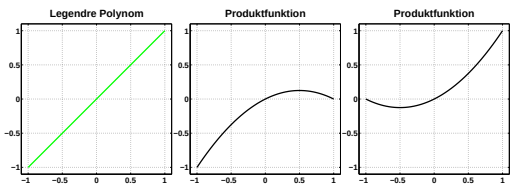
$$V^{\mathrm{PU}} = \sum_{i=1}^{N} \varphi_i \; V_i = \sum_{i=1}^{N} \varphi_i \; \mathcal{P}^{p_i} + \sum_{i=1}^{N} \varphi_i \; \mathcal{E}_i$$

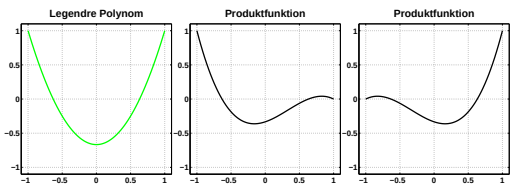
Linear FEM as PU

- Consider interval $[0, 1]$ mit $\varphi_{\mathbf{0}}^{\mathrm{FEM}}$, $\varphi_{\mathbf{1}}^{\mathrm{FEM}}$, $V_i = \{1, x\}$.
- Products of functions $\varphi_i^{\mathrm{FEM}} \psi_i^n$ quadratic polynomials.
- Number of functions $\#\{\varphi_i^{\mathrm{FEM}} \psi_i^n\} = 4$.









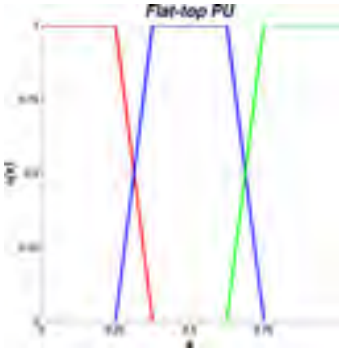
- Approximation benefits from higher reproducing properties of PU.
- Selection of local spaces *not* completely local (blending elements).
- Global stability *not* implied by local stability.
- Recently introduced: Stable GFEM (Babuška & Banerjee)

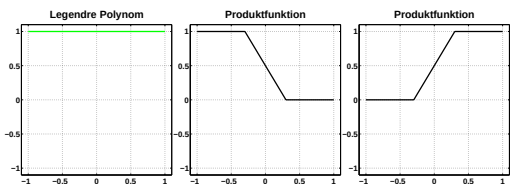
schweitzer@scai.fraunhofer.de

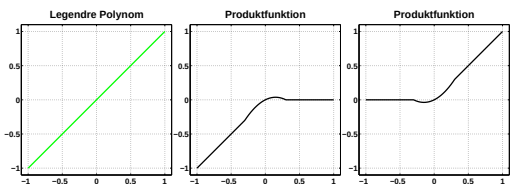
Partition of Unity Methods: Selection of the PU (PPUM/HPC)

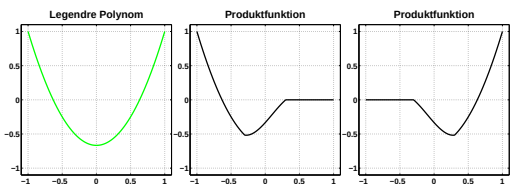
Flat-top PU

- Ensure $\varphi_i \equiv 1$ on $\omega_{i,\mathrm{FT}} \subset \omega_i = \mathrm{supp}(\varphi_i)$, $|\omega_{i,\mathrm{FT}}| \approx |\omega_i|$.
- Global independence implied by local independence on $\omega_{i,\mathrm{FT}}$.
- Supports are *smaller* than in FEM.









- Order of global approximation inherited from local orders.
- Complete independence of local spaces, no compatibility.
- Global stability implied by local stability.

schweitzer@scai.fraunhofer.de

Partition of Unity Methods: Stability

Lemma (Stability)

Let the local spaces V_i for $i = 1, \dots, N$ and their respective basis functions ϑ_i^m for $m = 1, \dots, d_i$ satisfy

$$\kappa_{1,i}^{-1}\ \mu(\omega_{\mathrm{FT},i} \cap \Omega) \sum_{m=1}^{d_i} (u_i^m)^2 \quad \leq \quad \|u_i\|^2_{L^2(\omega_{\mathrm{FT},i} \cap \Omega)}, \tag{3}$$

$$\|u_i\|^2_{L^2(\omega_i \cap \Omega)} \quad \leq \quad \kappa_{2,i}\ \mu(\omega_i) \sum_{m=1}^{d_i} (u_i^m)^2 \tag{4}$$

for any $u_i = \sum_{m=1}^{d_i} u_i^m \vartheta_i^m \in V_i$. Moreover, let $\mu(\omega_i) \asymp h^d$ and assume that the PU has the flat-top property. Then the product functions $\varphi_i \vartheta_i^m$ are a basis for the global PUM space V^{PU} and there holds

$$K_1^{-1} \Big(\sum_{i=1}^{N} \sum_{m=1}^{d_i} (u_i^m)^2 \Big)^{\frac{1}{2}} \leq h^{-\frac{d}{2}} \|u^{\mathrm{PU}}\|_{L^2(\Omega)} \leq K_2 \Big(\sum_{i=1}^{N} \sum_{m=1}^{d_i} (u_i^m)^2 \Big)^{\frac{1}{2}} \tag{5}$$

where $u^{\mathrm{PU}} = \sum_{i=1}^{N} \varphi_i u_i \in V^{\mathrm{PU}}$ with

$$K_1 = \min_{i=1,\dots,N} \kappa_{1,i} \text{ and } K_2 = \sqrt{\Lambda} \max_{i=1,\dots,N} \kappa_{2,i}.$$

schweitzer@scai.fraunhofer.de

Proof of Lemma

With the help of properties of an admissible PU we easily obtain the upper bound

$$\|u^{\mathrm{PU}}\|^2_{L^2(\Omega)} = \int_\Omega \Big(\sum_{i=1}^N \varphi_i(x) u_i(x) \Big)^2 \, dx \leq \Lambda C_\infty^2 \sum_{i=1}^N \|u_i\|^2_{L^2(\omega_i \cap \Omega)}.$$

For the respective lower bound we utilize the flat-top property (**??**). Obviously, there holds

$$\|u^{\mathrm{PU}}\|^2_{L^2(\Omega)} \geq \sum_{j=1}^N \int_{\omega_{\mathrm{FT},j} \cap \Omega} \Big(\sum_{i=1}^N \varphi_i(x) u_i(x) \Big)^2 \, dx.$$

Observe that a flat-top PU has a particular Kronecker property

$$\varphi_i|_{\omega_{\mathrm{FT},j}} = \delta_{ij}$$

which yields the estimate

$$\|u^{\mathrm{PU}}\|^2_{L^2} \geq \sum_{j=1}^N \int_{\omega_{\mathrm{FT},j}} u_j^2(x) \, dx = \sum_{j=1}^N \|u_j\|^2_{L^2(\omega_{\mathrm{FT},i} \cap \Omega)}.$$

The assertion then follows from (**??**) and (**??**).

Partition of Unity Methods: Construction of Stable Basis

$$V_i(\omega_i) = \mathcal{P}_i^{p_i}(\omega_i) + \mathcal{E}_i(\omega_i) = \mathcal{P}_i^{p_i}(\omega_i) + \mathcal{E}|_{\omega_i}$$

- Different scaling of $\mathcal{P}_i^{p_i}(\omega_i)$ and $\mathcal{E}|_{\omega_i}$.
- Local linear dependence / ill-conditioning of restrictions $\mathcal{E}|_{\omega_i}$.
- Overlap of $\mathcal{P}_i^{p_i}(\omega_i)$ and $\mathcal{E}|_{\omega_i}$.

All can be eliminated easily and automatically!

schweitzer@scai.fraunhofer.de

Partition of Unity Methods: Construction of Stable Basis

Enforce $\kappa_{1,i} = 1$, check $\kappa_{2,i}$ during computation.

- Orthogonalize $\langle \psi_i^t \rangle$ and $\langle \eta_i^s \rangle$ separately.

$$M = ODO^T, OO^T = \mathbb{I}, D = \text{diag}(\lambda)$$

  Remove small eigenfunctions with small eigenvalues $\tilde{O}$, $\tilde{D}$.
- Compute $\mathcal{E} \setminus \mathcal{P}^{p_i}$ by Schurcomplement.
- Compute Orthogonal Basis.

Local transformation/projection (parallel)!

$$V_i = \mathcal{P}^{p_i} + \mathcal{E} \approx \mathcal{P}^{p_i} \oplus D = \mathcal{P}^{p_i} \oplus \mathcal{E} \setminus \mathcal{P}^{p_i}$$

schweitzer@scai.fraunhofer.de

Partition of Unity Methods: Construction of Stable Basis

Consider local mass matrix on ω_i (on $\omega_{i,\mathsf{FT}}$)

$$(M^i)_{n,m} := \int_{\omega_{i,\mathsf{FT}} \cap \Omega} \vartheta_i^n \vartheta_i^m \, dx \quad \text{für alle } m, n$$

$$M_i = \begin{pmatrix} M^i_{\mathcal{P},\mathcal{P}} & M^i_{\mathcal{P},\mathcal{E}} \\ M^i_{\mathcal{E},\mathcal{P}} & M^i_{\mathcal{E},\mathcal{E}} \end{pmatrix} \qquad \begin{aligned} O_{\mathcal{P}}^T M^i_{\mathcal{P},\mathcal{P}} O_{\mathcal{P}} &= D_{\mathcal{P}} \\ O_{\mathcal{E}}^T M^i_{\mathcal{E},\mathcal{E}} O_{\mathcal{E}} &= D_{\mathcal{E}} \end{aligned}$$

Stable basis for $V_i = \mathcal{P}^{p_i} + \mathcal{E}_i \approx \mathcal{P}^{p_i} \oplus \mathcal{D}_i$ mit $\mathcal{D}_i \approx \mathcal{E} \setminus \mathcal{P}^{p_i}$ via

$$S_i^{\mathcal{E}\setminus\mathcal{P}} := \begin{pmatrix} D_{\mathcal{P}}^{-1/2} O_{\mathcal{P}}^T & 0 \\ -\tilde{D}_{\mathcal{D}}^{-1/2} \tilde{O}_{\mathcal{D}}^T M^*_{\mathcal{E},\mathcal{P}} D_{\mathcal{P}}^{-1/2} O_{\mathcal{P}}^T & \tilde{D}_{\mathcal{D}}^{-1/2} \tilde{O}_{\mathcal{D}}^T \tilde{D}_{\mathcal{E}}^{-1/2} \tilde{O}_{\mathcal{E}}^T \end{pmatrix}$$

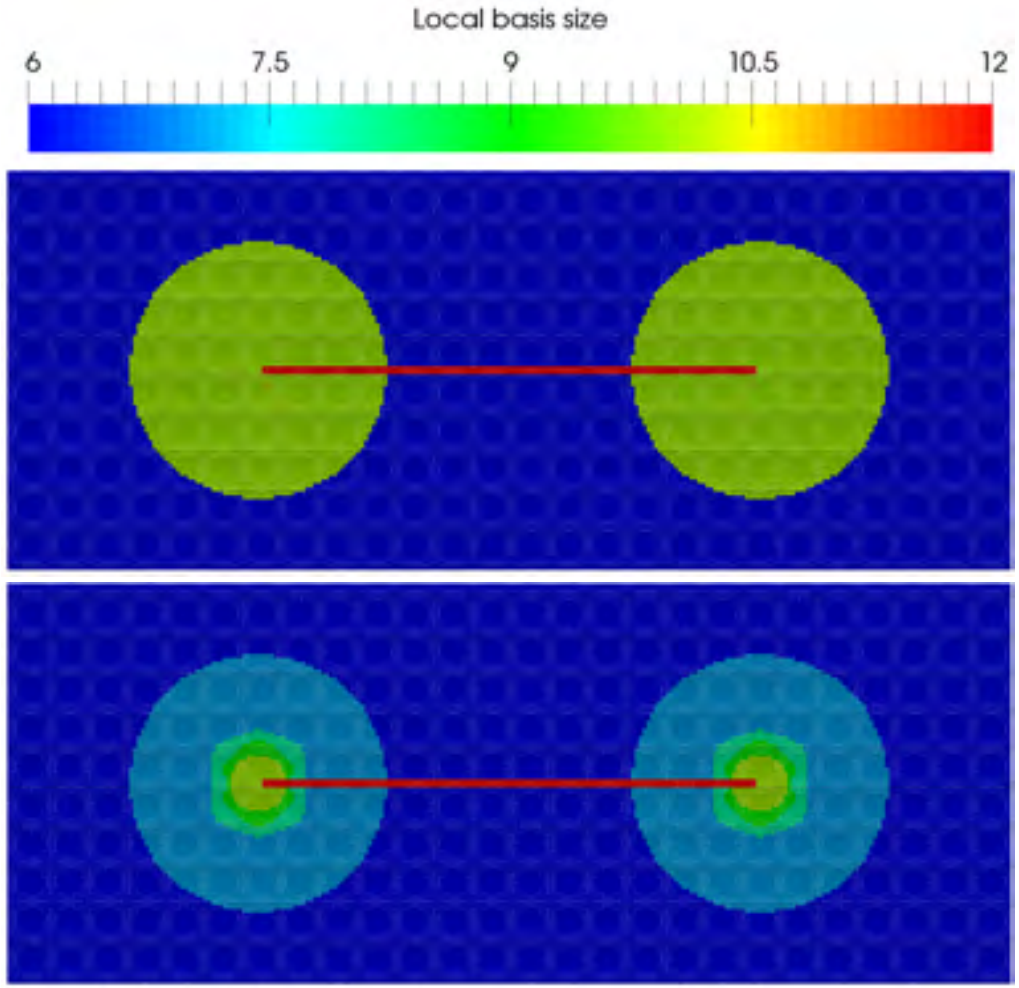
Post-Processing

Block-diagonal operator P can easily applied (in parallel)

$$A_{\text{stable}} = PAP^T$$

schweitzer@scai.fraunhofer.de

Partition of Unity Methods: Construction of Stable Basis



schweitzer@scai.fraunhofer.de

Partition of Unity Methods: Essential Boundary Conditions

Nitsche's Methods

Just as described above but with $\beta = h_i^{-1/2}\gamma$, i.e. localized.

- Need to compute weak formulation.
- Need to compute regularization parameter.
- Requires second order PDE — not applicable to explicit dynamics.

Conforming Approach

- Limit case of regularization $\rightarrow \infty$.
- Kernel of trace operator yields "interior" basis functions.
- Complement yields "boundary" basis functions.
- Due to flat-top we can localize the trace!

Conforming Treatment: Limit case $\beta \to \infty$

Short-hand notation

$$
\begin{aligned}
V_\Omega &:= \{v \in V^{\mathrm{PU}} \mid \mathbf{supp}(v) \cap \Gamma_D = \emptyset\},\\
V_{D,n,K} &:= \{v \in V^{\mathrm{PU}} \mid \mathbf{supp}(v) \cap \Gamma_D \neq \emptyset \text{ and } \mathcal{B}_{D,n}(v) = (v \cdot n)|_{\Gamma_D} = 0\},\\
V_{D,n,I} &:= \{v \in V^{\mathrm{PU}} \mid \mathbf{supp}(v) \cap \Gamma_D \neq \emptyset \text{ and } \mathcal{B}_{D,n}(v) = (v \cdot n)|_{\Gamma_D} \neq 0\}.
\end{aligned}
$$

Limit problem

$$
a_\infty(u,v) = \begin{cases}
\displaystyle\int_\Omega \boldsymbol{\sigma}(u) : \boldsymbol{\epsilon}(v)\, dx & v \in V_\Omega,\\
\displaystyle\int_\Omega \boldsymbol{\sigma}(u) : \boldsymbol{\epsilon}(v)\, dx - \int_{\Gamma_D} (n \cdot \boldsymbol{\sigma}(v)n)n \cdot u\, ds & v \in V_{D,n,K},\\
\displaystyle\int_{\Gamma_D} (u \cdot n)(v \cdot n)\, ds & v \in V_{D,n,I},
\end{cases} \tag{6}
$$

$$
\langle l_\infty, v\rangle = \begin{cases}
\displaystyle\int_\Omega fv\, dx + \int_{\Gamma_N} g_N v\, ds & v \in V_\Omega,\\
\displaystyle\int_\Omega fv\, dx + \int_{\Gamma_N} g_N v\, ds - \int_{\Gamma_D} g_{D,n}(n \cdot \boldsymbol{\sigma}(v)n)\, ds & v \in V_{D,n,K},\\
\displaystyle\int_{\Gamma_D} g_{D,n}(v \cdot n)\, ds & v \in V_{D,n,I}.
\end{cases} \tag{7}
$$

schweitzer@scai.fraunhofer.de

Conforming Treatment: Limit case $\beta \to \infty$

Since $\mathcal{B}_{D,n}(u) = g_{D,n}$ for $v \in V_{D,n,K}$ simplifies to

$$\int_\Omega \boldsymbol{\sigma}(u) : \boldsymbol{\epsilon}(v)\, dx = \int_\Omega fv\, dx + \int_{\Gamma_N} g_N v\, ds \tag{8}$$

for all $v \in V_\Omega + V_{D,n,K}$. For $v \in V_{D,n,I}$ we have

$$\int_{\Gamma_D} (u \cdot n)(v \cdot n)\, ds = \int_{\Gamma_D} g_{D,n}(v \cdot n)\, ds \tag{9}$$

In matrix-form

$$A = \begin{pmatrix} A_{K,K} & A_{K,I} \\ 0 & B_{I,I} \end{pmatrix}, \qquad \hat{f} = \begin{pmatrix} \hat{f}_K \\ \hat{g}_I \end{pmatrix}. \tag{10}$$

Thus

$$\tilde{u}_I = B_{I,I}^{-\mathbf{1}} \hat{g}_I, \quad \tilde{u}_K = A_{K,K}^{-\mathbf{1}} (\hat{f}_K - A_{K,I} \tilde{u}_I). \tag{11}$$

- Standard in FEM.
- Kernel of trace $\mathcal{B}_{D,n}$ on PUM space not known a priori.
- Global operation - prohibitively expensive.

Conforming Treatment: Limit case $\beta \to \infty$

Obviously for an arbitrary PPUM function u^{PU}

$$\mathcal{B}_{D,n}(u^{\mathrm{PU}}) = 0 \quad \Longleftarrow \quad \mathcal{B}_{D,n}(\vartheta_i^m) = 0 \quad \text{for all } (i, m) \tag{12}$$

If PU satisfies a flat-top condition on Dirichlet boundary even

$$\mathcal{B}_{D,n}(u^{\mathrm{PU}}) = 0 \quad \Longleftrightarrow \quad \mathcal{B}_{D,n}(\vartheta_i^m) = 0 \quad \text{for all } (i, m) \tag{13}$$

- Equivalence only needed for global inverse of $B_{I,I}$.
- Implication is sufficient for local approximation.
- Analogous approach to preconditioner to attain splitting/basis.

From

$$(M_i^{D,n})_{k,l} = \int_{\Gamma_{D,n}} (\vartheta_i^k \cdot n)(\vartheta_i^l \cdot n)\, ds. \tag{14}$$

construct

$$V_i = V_{i,K} \oplus V_{i,I}$$

Leading to

$$\sum_{i=1}^{N} \varphi_i V_i = V^{\mathrm{PU}} = V_K^{\mathrm{PU}} \oplus V_I^{\mathrm{PU}} := \sum_{i=1}^{N} \varphi_i V_{i,K} \oplus \sum_{i=1}^{N} \varphi_i V_{i,I} \tag{15}$$

schweitzer@scai.fraunhofer.de

Partition of Unity Methods: Solvers

Multilevel Iteration $\mathcal{M}_{\gamma}^{\nu_1,\nu_2}(k, x_k, b_k)$

1. if $k > 0$:
   - 1.1 For $l = 1, \ldots, \nu_1$: Set $x_k = \mathrm{S}_k^1(x_k, b_k)$.
   - 1.2 Set $d_{k-1} := I_k^{k-1}(b_k - A_k x_k)$.
   - 1.3 Set $e_{k-1} := 0$.
   - 1.4 For $i = 1, \ldots, \gamma$: $e_{k-1} = \mathcal{M}_{\gamma}^{\nu_1,\nu_2}(k-1, e_{k-1}, d_{k-1})$.
   - 1.5 Set $x_k = C_k(x_k, e_{k-1}) := x_k + I_{k-1}^k e_{k-1}$.
   - 1.6 For $l = 1, \ldots, \nu_2$: Set $x_k = \mathrm{S}_k^2(x_k, b_k)$.
2. else:
   - 2.1 Set $x_k = A_k^{-1} b_k$.

Fast Convergence

1. Approximation property of I_{k-1}^k.
2. Smoothing property of S_k^p.
3. $\mathrm{Im}(\mathrm{S}_k^p) \sim \mathrm{Im}(I_{k-1}^k) \sim \mathrm{Ker}(C_k)$

schweitzer@scai.fraunhofer.de

Partition of Unity Methods: Interlevel Transfer Operators

- Shape functions are *non-interpolatory*.
- Function spaces V_{PU}^{k-1} and V_{PU}^{k} are *nonnested*

$$\varphi_{i,k-1}\psi_{i,k-1}^{n} \neq \sum \beta_{j,k}^{m}\varphi_{j,k}\psi_{j,k}^{m}.$$

- Variational assumption, Galerkin identity

$$A_{k-1} = I_{k}^{k-1} A_k I_{k-1}^{k}$$

  is *not* valid.

Choices for prolongation I_{k-1}^{k}

- Global-to-global L^2-projection $I_{k-1}^{k} = \Pi_{k-1}^{k}$.
- Global-to-local L^2-projection $I_{k-1}^{k} = \widehat{\Pi}_{k-1}^{k}$.
- Local-to-local L^2-projection $I_{k-1}^{k} = \widetilde{\Pi}_{k-1}^{k}$.

schweitzer@scai.fraunhofer.de

PUM L^2-Projections: Localization

From the basic PUM error estimate [Babuška, Melenk]

$$\|v - v^{\mathrm{PU}}\|^2_{L^2(\Omega)} \leq C \sum_i \|v - v_i\|^2_{L^2(\omega_i \cap \Omega)},$$

where

$$v_i := \sum_n u_i^n \psi_i^n, \quad \text{and} \quad v^{\mathrm{PU}} := \sum_i \varphi_i v_i = \sum_i \varphi_i \sum_n u_i^n \psi_i^n$$

we know that it is sufficient to control the local errors

$$\|v - v_i\|_{L^2(\omega_i \cap \Omega)}$$

on each cover patch ω_i.

Global-to-local L^2-projection

With $v = u_{k-1}^{\mathrm{PU}}$ and $v^{\mathrm{PU}} = I_{k-1}^k u_{k-1}^{\mathrm{PU}}$

$$\| u_{k-1}^{\mathrm{PU}} - I_{k-1}^k u_{k-1}^{\mathrm{PU}} \|_{L^2(\Omega)}^2 \leq C \sum_i \| u_{k-1}^{\mathrm{PU}} - u_{i,k} \|_{L^2(\omega_{i,k} \cap \Omega)}^2$$

Localize trial space:

- Project *global* coarse functions u_{k-1}^{PU} onto *local* fine functions $u_{i,k}$.
- Need to consider all *geometric* interlevel neighbors

$$\omega_{i,k} \cap \omega_{j,k-1} \neq \emptyset.$$

- *Global-to-local* projection $\widehat{\Pi}_{k-1}^k = (\widetilde{M}_k^k)^{-1} (\widehat{M}_{k-1}^k)$

$$\begin{aligned} (\widetilde{M}_k^k)_{(i,n),(i,m)} &:= \langle \psi_{i,k}^m, \psi_{i,k}^n \rangle_{L^2(\omega_{i,k} \cap \Omega)} \\ (\widehat{M}_{k-1}^k)_{(i,n),(j,m)} &:= \langle \varphi_{j,k-1} \psi_{j,k-1}^m, \psi_{i,k}^n \rangle_{L^2(\omega_{i,k} \cap \Omega)}. \end{aligned}$$

Local-to-local L^2-projection

Localize test space:

- Due to *hierarchy* of cover patches exactly one coarse patch $\omega_{\tilde{i},k-1}$ for each fine patch $\omega_{i,k}$, such that $\omega_{i,k} \subseteq \omega_{\tilde{i},k-1}$.
- With triangle inequality

$$\begin{aligned} \|u_{k-1}^{\mathrm{PU}} - u_{i,k}\|_{L^2(\omega_{i,k}\cap\Omega)} \quad \leq \quad & \|u_{k-1}^{\mathrm{PU}} - u_{\tilde{i},k-1}\|_{L^2(\omega_{i,k}\cap\Omega)} + \\ & \|u_{\tilde{i},k-1} - u_{i,k}\|_{L^2(\omega_{i,k}\cap\Omega)}. \end{aligned}$$

- First term small by definition, i.e. $u_{k-1}^{\mathrm{PU}} = u_{\tilde{i},k-1}$ on subset of $\omega_{\tilde{i},k-1} \supset \omega_{i,k}$.
- Second term allows to project *local* coarse functions $u_{k-1,\tilde{i}}$ onto *local* fine functions $u_{i,k}$.

schweitzer@scai.fraunhofer.de

Partition of Unity Methods: Selection of Smoothers

Successive Subspace Correction Method

For all $l = 1, \ldots, N$:

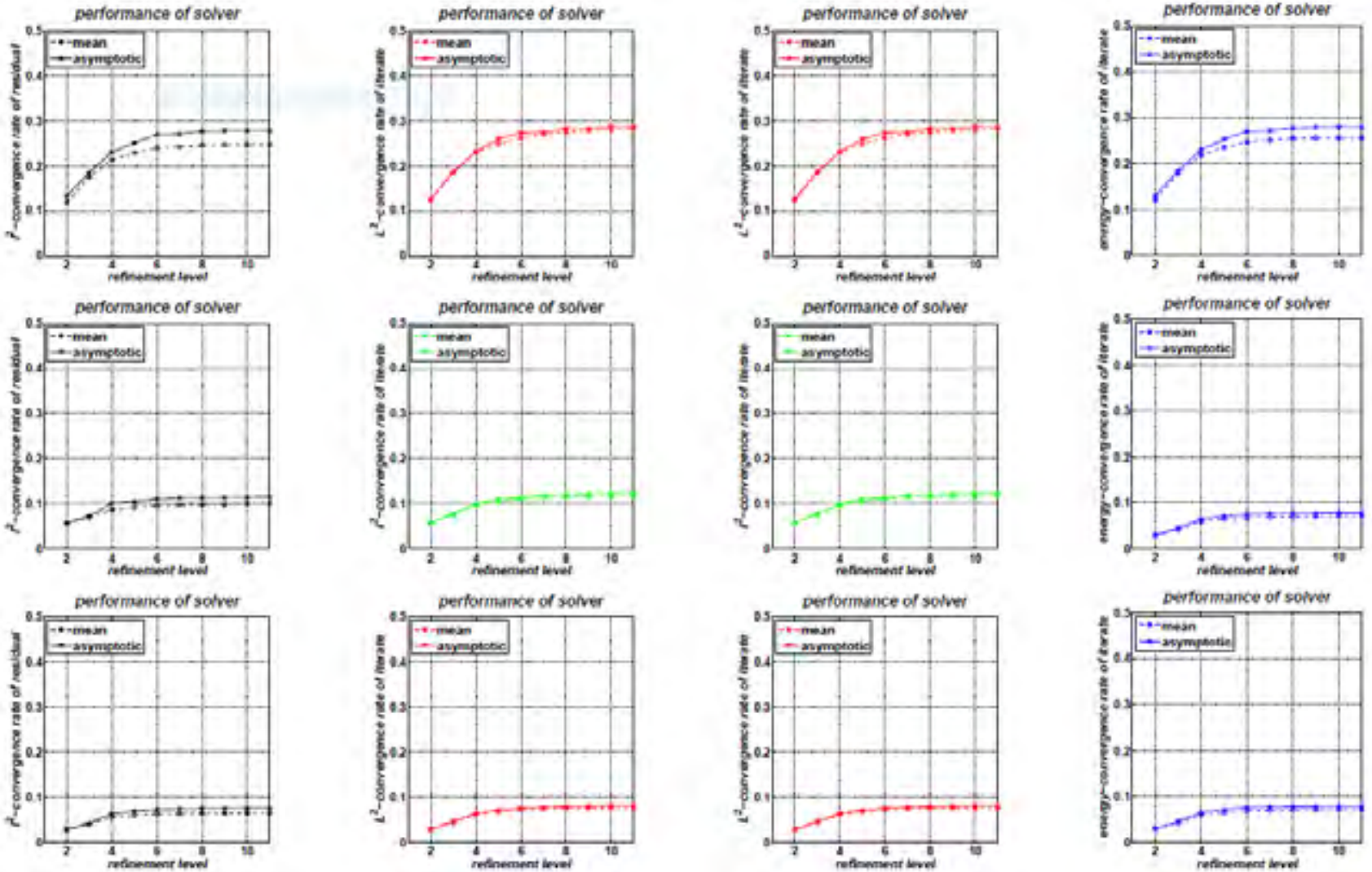
- Compute local residual $\hat{f}_l := P_l^T(\hat{f} - A\tilde{u})$.
- Solve subspace problem $(P_l^T A\, P_l)\tilde{u}_l A_{l,l}\tilde{u}_l = \hat{f}_l$.
- Update global iterate $\tilde{u} = \tilde{u} + P_l\tilde{u}_l$.

Subspace Definitions:

- Scalar smoother:
$$\mathcal{V}_{i,n} := \{v \in V^{\mathrm{PU}} \mid v = \varphi_i v_i^n \psi_i^n\}$$
- Block smoother:
$$\mathcal{V}_i := \varphi_i V_i^p = \{v \in V^{\mathrm{PU}} \mid v = \sum_n \varphi_i v_i^n \psi_i^n\}$$
- Multiplicative overlapping Schwarz:
$$\widetilde{\mathcal{V}}_l := \sum_{\omega_i \cap \omega_l \neq \emptyset} \mathcal{V}_i = \{v \in V^{\mathrm{PU}} \mid v = \sum_{i \in C_l} \varphi_i \sum_n v_i^n \psi_i^n\}$$

schweitzer@scai.fraunhofer.de

Partition of Unity Methods: Evaluation of Multilevel Solver



Convergence rates for the multilevel $V(s, s)$-cycles with $s = \mathbf{1}, \mathbf{3}, \mathbf{5}$ (top to bottom row) and block-Gauss–Seidel smoothing.

Solver efficiency: $\mathbf{Cost}(A^{-\mathbf{1}} \cdot b) \approx \mathbf{15}\,\mathbf{Cost}(A \cdot x)$

schweitzer@scai.fraunhofer.de

Partition of Unity Methods: Expicit Dynamics

Model problem

$$u_{tt}(x,t) = \Delta u(x,t) \quad (x,t) \in \Omega \times (0,T)$$

Central differences in time

$$u(\cdot, t_{n+1}) = (\delta t)^2 \Delta u(\cdot, t_n) + 2u(\cdot, t_n) - u(\cdot, t_{n-1}) =: f(\cdot) \quad \text{in } \Omega.$$

Galerkin in space

Given $f \in L^2(\Omega)$ find $u^h \in V^h \subset L^2(\Omega)$ such that for all $v^h \in V^h$

$$\langle f - u^h, v^h \rangle_{L^2(\Omega)} = 0$$

Mass matrix problem

Let $\hat{f} = (f_i)$, $M = (M_{i,j})$ where $f_i = \langle f, \phi_i \rangle_{L^2(\Omega)}$, $M_{i,j} = \langle \phi_j, \phi_i \rangle_{L^2(\Omega)}$

$$M\tilde{u} = \hat{f}$$

schweitzer@scai.fraunhofer.de

L^2-Approximation Problem

Global L^2-projection

$$\Pi_{L^2(\Omega)} : L^2(\Omega) \to V^h, \quad f \mapsto u^h, \quad M\tilde{u} = \hat{f}$$

Properties of consistent mass matrix

- Symmetric positive definit
- Well-conditioned and sparse
- Explicit inverse expensive

Approximation of the mass matrix: Lumping in FEM

Approximate sparse M by diagonal $\bar{M}$ via classical approaches

- Direct mass lumping:
  Kronecker property
- Variational mass lumping:
  Numerical integration, polynomial basis
- Template mass lumping

schweitzer@scai.fraunhofer.de

Partition of Unity Method

Improved PUM error bound

Let φ_i be an admissible and non-negative PU. Then, there hold the global estimates

$$\|f - v\|_{L^2(\Omega)} \leq \sqrt{C_\infty}\Big(\sum_{i=1}^{N} \hat{\epsilon}_i^2\Big)^{1/2},$$

$$\|\nabla(f - v)\|_{L^2(\Omega)} \leq \sqrt{2}\Big(\sum_{i=1}^{N} \Lambda\big(\frac{C_\nabla}{\operatorname{diam}(\omega_i)}\big)^2 \hat{\epsilon}_i^2 + C_\infty \tilde{\epsilon}_i^2\Big)^{1/2}.$$

Proof.

$$\Big(\sum_{i=1}^{N} \varphi_i(x)(f(x) - v_i(x))\Big)^2 = \Big(\sum_{i=1}^{N} \big(\sqrt{\varphi_i(x)}\big)\big(\sqrt{\varphi_i(x)}(f(x) - v_i(x))\big)\Big)^2$$

Cauchy-Schwarz

$$\Big(\sum_{i=1}^{N} \varphi_i(x)(f(x) - v_i(x))\Big)^2 \leq \sum_{j=1}^{N} \varphi_j(x) \sum_{i=1}^{N} \varphi_i(x)(f(x) - v_i(x))^2 \leq \sum_{i=1}^{N} \varphi_i(x)(f(x) - v_i(x))^2$$

schweitzer@scai.fraunhofer.de

L^2-projection onto V^{PU}

Global L^2-projection onto V^{PU}

$$\Pi_{L^2(\Omega)} : L^2(\Omega) \to V^{\mathrm{PU}}, \quad f \mapsto u^h, \quad M\tilde{u} = \hat{f}$$

Consistent mass matrix

$$M = (M_{(i,n),(j,m)}), \quad M_{(i,n),(j,m)} = \langle \varphi_j \vartheta_j^m, \varphi_i \vartheta_i^n \rangle_{L^2(\Omega)},$$

Moment-vector

$$\hat{f} = (f_{(i,n)}), \quad f_{(i,n)} = \langle f, \varphi_i \vartheta_i^n \rangle_{L^2(\Omega)}.$$

Re-interpretation of moments

$$\begin{aligned} f_{(i,n)} &= \langle f, \varphi_i \vartheta_i^n \rangle_{L^2(\Omega)} = \int_\Omega f \varphi_i \vartheta_i^n \, dx = \int_{\Omega \cap \omega_i} f \varphi_i \vartheta_i^n \, dx \\ &= \langle f | \varphi_i | \vartheta_i^n \rangle_{L^2(\Omega \cap \omega_i)} = \langle f, \vartheta_i^n \rangle_{L^2(\Omega \cap \omega_i, \varphi_i)} \end{aligned}$$

$$L^2(\Omega \cap \omega_i, \varphi_i) := \{ u \in L^2(\Omega) : \|u\|^2_{L^2(\Omega \cap \omega_i, \varphi_i)} := \int_{\Omega \cap \omega_i} \varphi_i |u|^2 \, dx < \infty \}$$

L^2-projection onto V^{PU}: The Local Perspective

$$L^2(\Omega \cap \omega_i, \varphi_i) := \{u \in L^2(\Omega) : \|u\|^2_{L^2(\Omega\cap\omega_i,\varphi_i)} := \int_{\Omega\cap\omega_i} \varphi_i |u|^2 \, dx < \infty\}$$

Local L^2-projection onto V^{PU}

$$\bar{\Pi}_{L^2(\Omega)} : L^2(\Omega) \to V^{\mathrm{PU}}, \quad f \mapsto \bar{u}, \quad \bar{M}\tilde{\bar{u}} = \hat{f}$$

Localized mass matrix

$$\bar{M} = (\bar{M}_{(i,n),(j,m)}), \quad \bar{M}_{(i,n),(j,m)} = \begin{cases} 0 & i \neq j \\ \langle \vartheta_i^m | \varphi_i | \vartheta_i^n \rangle_{L^2(\Omega\cap\omega_i)} & i = j \end{cases}$$

- Construction is independent of local spaces (enrichments, order)
- Consistent right-hand side $\hat{f}$
- Block-diagonal matrix $\bar{M}$
- Symmetric positive definite $\bar{M}$

schweitzer@scai.fraunhofer.de

Consistent vs. Lumped Mass Matrix

Lemma

The approximation $\bar{u} \in V^{\mathrm{PU}}$ obtained by local projection $\bar{\Pi}_{L^2(\Omega)}$ satisfies

$$\|f - \bar{u}\|_{L^2(\Omega)} \leq \sqrt{C_\infty} \Big(\sum_{i=1}^{N} \hat{\epsilon}_i^2 \Big)^{1/2}.$$

Moreover, the operator $\bar{M} - M$ is symmetric positive semi-definite.

Conservation $u = \Pi f = \bar{\Pi} f = \bar{u}$

For all $\tilde{w} \in \ker(\bar{M} - M)$ holds

$$\|w\|^2_{L^2(\Omega)} = \tilde{w}^T M \tilde{w} = \tilde{w}^T \bar{M} \tilde{w}.$$

If $w \in L^2(\Omega)$ such that $w|_{\Omega \cap \omega_i} \in V_i$ then $\tilde{w} \in \ker(\bar{M} - M)$.

schweitzer@scai.fraunhofer.de

Further Properties

Interpretation: Classical FEM

Linear FEM space $V^{\mathrm{FE}} = V^{\mathrm{PU}} = \operatorname{span}\langle \phi_i \rangle$ if $V_i = \operatorname{span}\langle 1 \rangle$. Thus,

$$\bar{M}_{i,i} = \int_\Omega \phi_i \, dx = \int_\Omega \sum_{j=1}^{N} \phi_j \phi_i \, dx = \sum_{j=1}^{N} \int_\Omega \phi_j \phi_i \, dx = \sum_{j=1}^{N} M_{i,j}.$$

Application to GFEM/XFEM

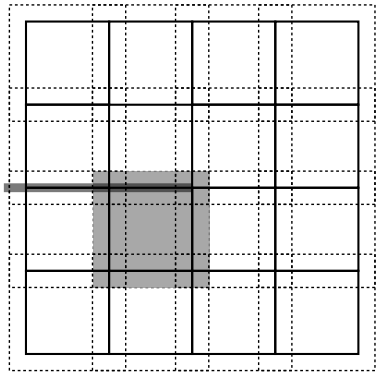
$\bar{M}$ always invertible if local basis stable with respect to $L^2(\Omega \cap \omega_i, \varphi_i)$.

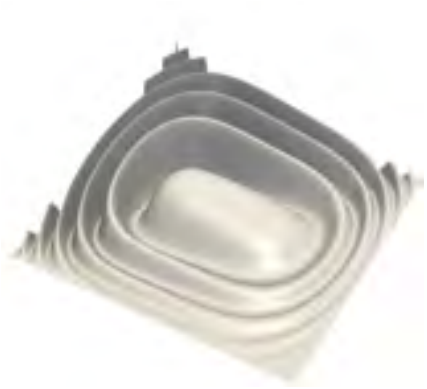
Convergence: Discontinuous Galerkin

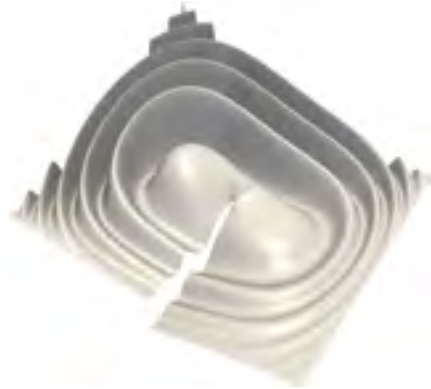
As $\varphi_i \to \chi_{\omega_i}$ we find $\bar{M}$ and M become the consistent mass matrix of the resulting discontinuous space $V = \sum_{i=1}^{N} \chi_{\omega_i} V_i$

schweitzer@scai.fraunhofer.de

Approximation Results







Experimental setup: Projections $u := \Pi f$ and $\bar{u} := \bar{\Pi} f$

- Overlapping patches $\omega = \alpha \cdot \mathcal{C}$ from uniform grid cells $\mathcal{C}$ ($\alpha = 1.1, 1.5, 1.9$).
- Polynomial degree $p = 1, 3, 5$ for smooth solution.
- Additional crack tip and discontinuous enrichment in fixed zone for singular solution.
- Relative errors:

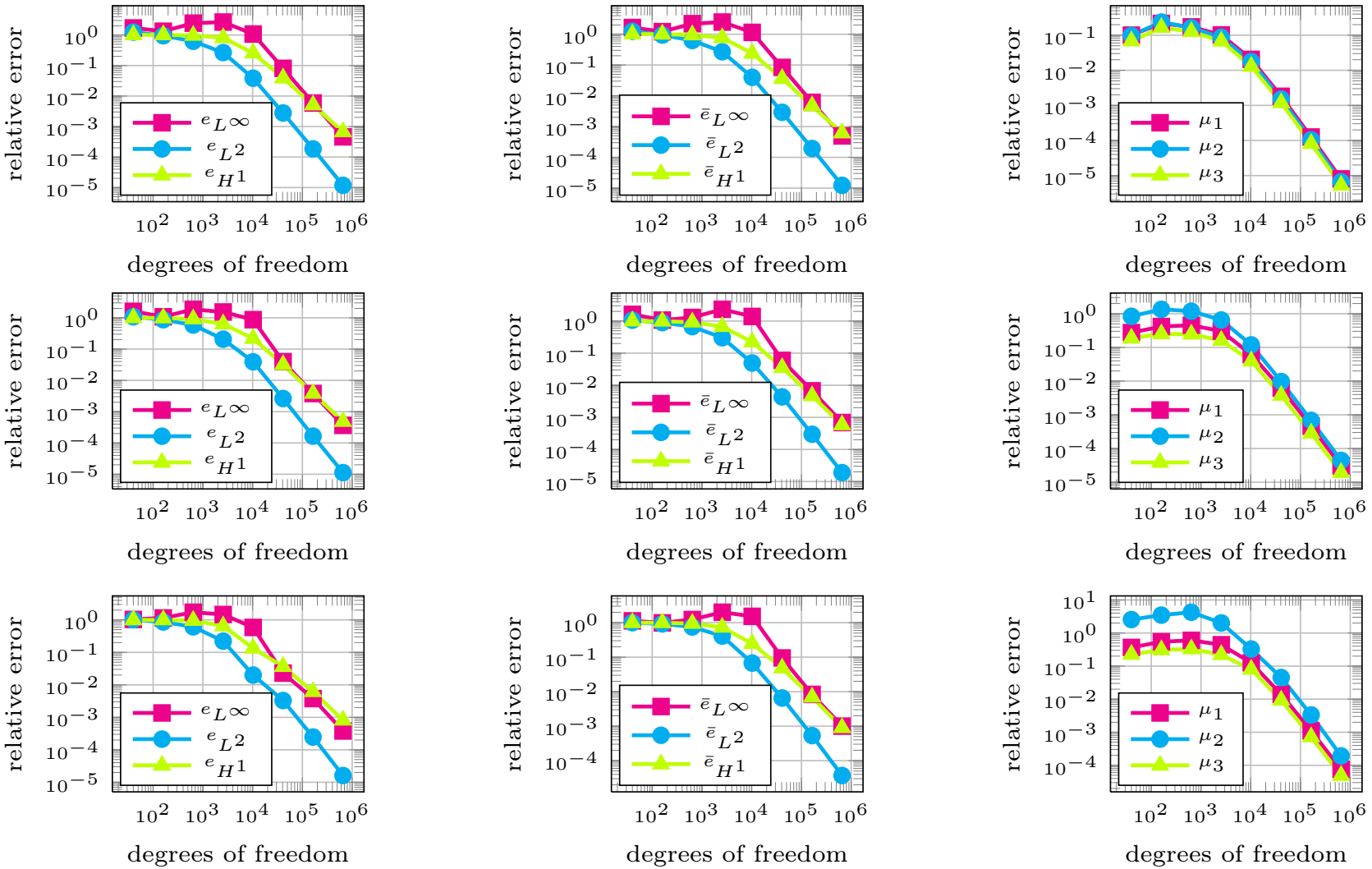
$$e_{L^\infty} := \frac{\|f-u\|_{L^\infty}}{\|f\|_{L^\infty}}, \quad e_{L^2} := \frac{\|f-u\|_{L^2}}{\|f\|_{L^2}}, \quad e_{H^1} := \frac{\|f-u\|_{H^1}}{\|f\|_{H^1}},$$

- Relative defects in mass and kinetic energy:

$$\mu_1 := \sqrt{\frac{\tilde{\bar{u}}^T \bar{M} \tilde{\bar{u}} - \tilde{u}^T M \tilde{u}}{\tilde{u}^T M \tilde{u}}}, \quad \mu_2 := \sqrt{\frac{\tilde{u}^T (\bar{M} - M) \tilde{u}}{\tilde{u}^T M \tilde{u}}}, \quad \mu_3 := \sqrt{\frac{\tilde{\bar{u}}^T (\bar{M} - M) \tilde{\bar{u}}}{\tilde{u}^T M \tilde{u}}}$$

schweitzer@scai.fraunhofer.de

Approximation Results

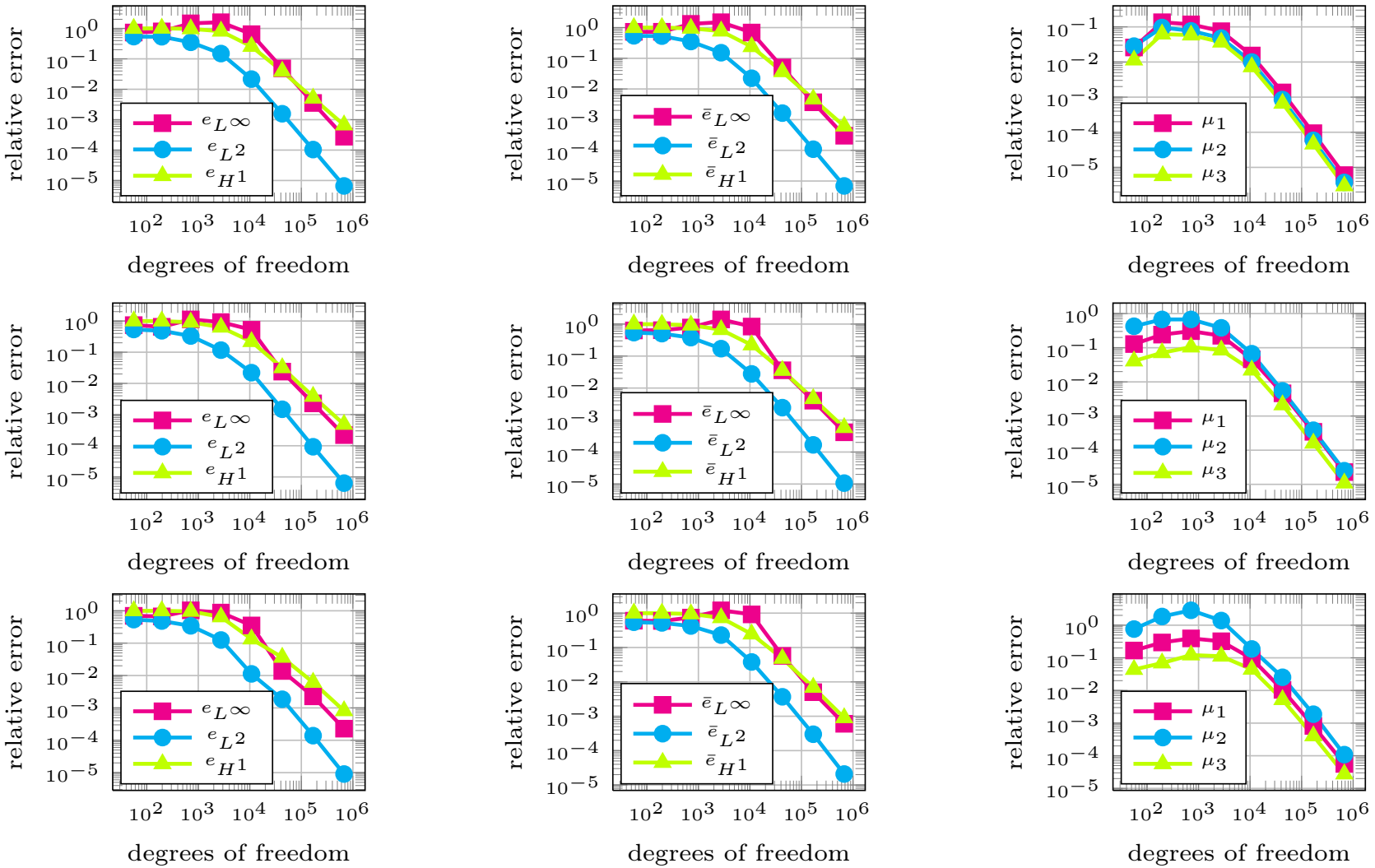


Smooth solution: $p = 3$ and $\alpha = 1.1, 1.5, 1.9$ (top to bottom)

schweitzer@scai.fraunhofer.de

Fraunhofer SCAI

Approximation Results



Singular solution: Enrichment, $p = 3$ and $\alpha = 1.1, 1.5, 1.9$ (top to bottom)

schweitzer@scai.fraunhofer.de

Time-Stepping Results: Properties

Conservation

$$(\bar{M} - M)x = \lambda x, \quad \ker(\bar{M} - M) \supseteq \mathcal{P}^p$$

Critical time-step

$$Kx = \lambda Mx, \quad Kx = \lambda \bar{M}x,$$

Stability limit on time-step:

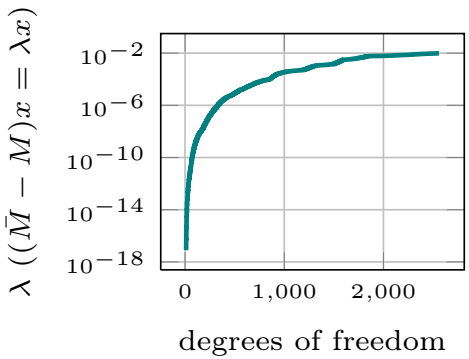
$$\delta t_{\text{critical}} \leq \frac{2}{\sqrt{\lambda_{\max}}},$$

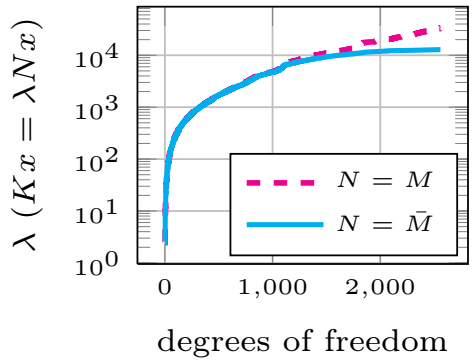
Preconditioner

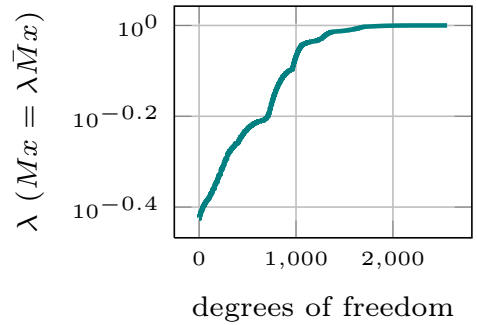
$$Mx = \lambda \bar{M}x, \quad \dim\{x : \lambda = 1\}$$

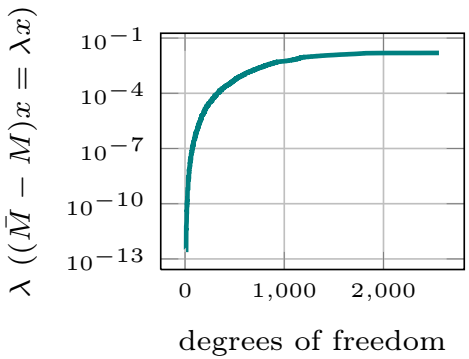
schweitzer@scai.fraunhofer.de

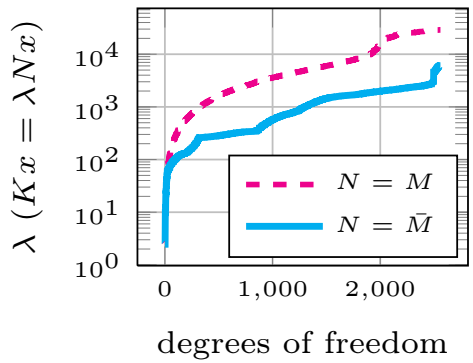
Time-Stepping Results: Properties

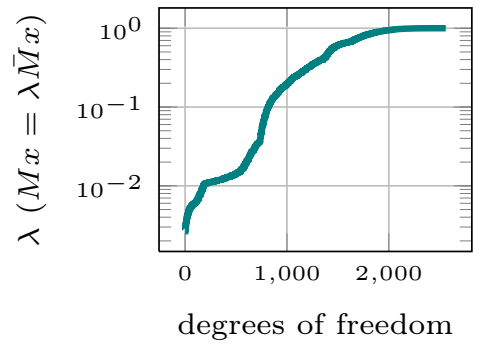


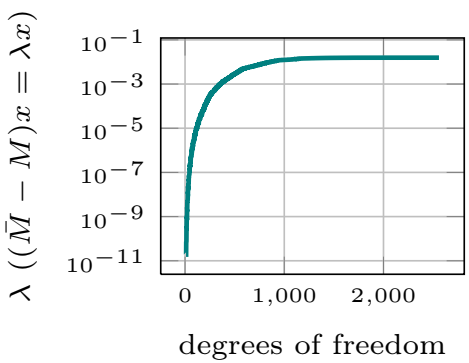


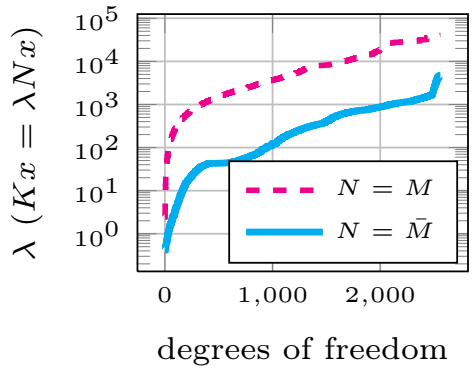


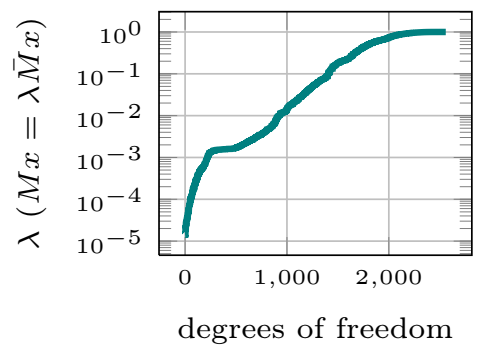








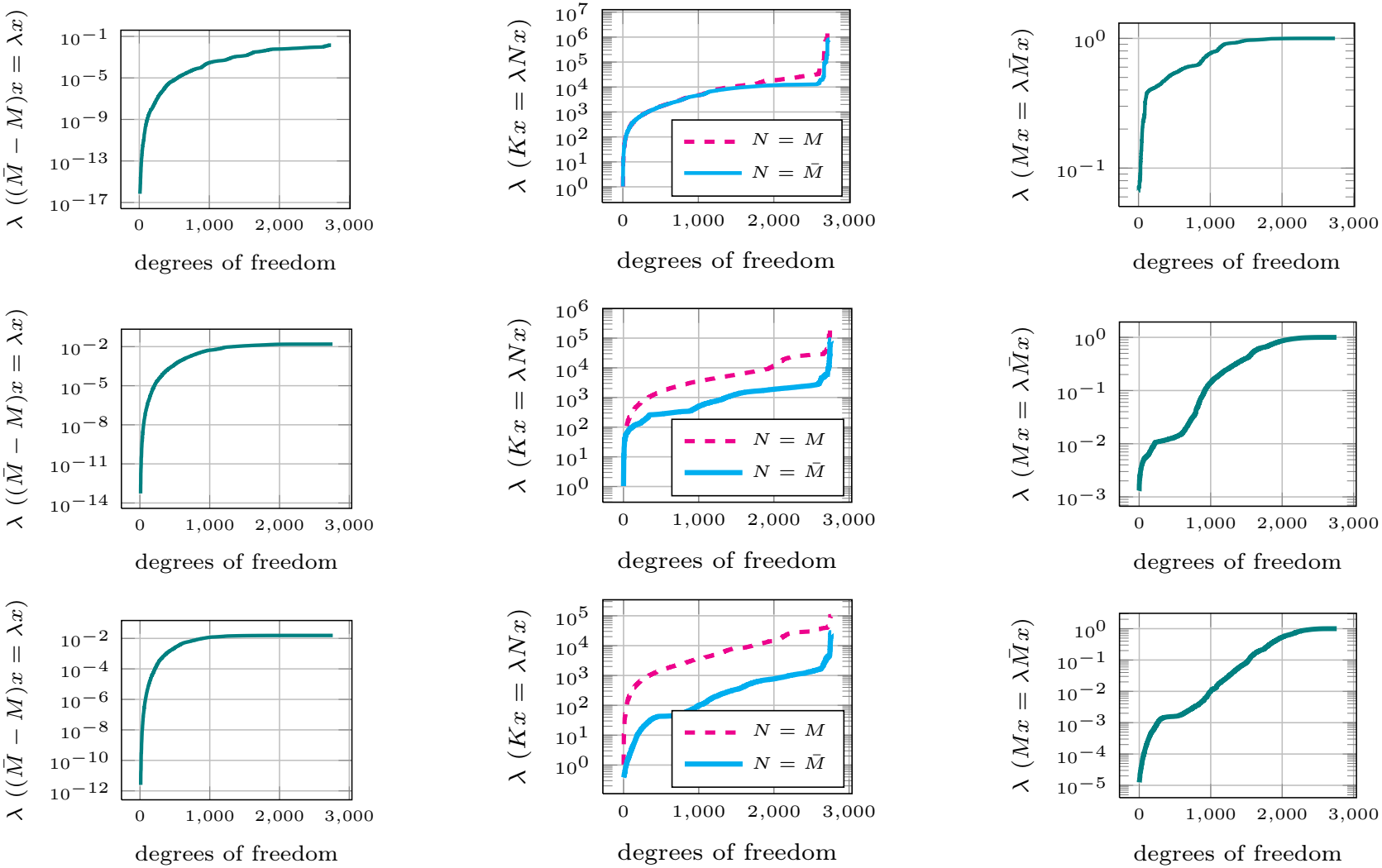




Smooth solution: $p = 3$ and $\alpha = 1.1, 1.5, 1.9$ (top to bottom)

schweitzer@scai.fraunhofer.de

Time-Stepping Results: Properties



Singular solution: Enrichment, $p = 3$ and $\alpha = 1.1, 1.5, 1.9$ (top to bottom)

Time-Stepping Results: Slit membrane

Model problem

$$\begin{aligned} u_{tt} &= \Delta u \quad \text{in } \Omega \times (0,T), & u_t(\cdot,0) &= 0 \quad \text{in } \Omega, \\ u(\cdot,0) &= \gamma \quad \text{in } \Omega, & u(x,t) &= 0 \quad \text{for } x \in \partial\Omega,\, t > 0, \end{aligned}$$

Central difference time-stepping

Displacement u, velocity v and acceleration a:

$$N\tilde{a}_n = K\tilde{u}_n, \quad \tilde{v}_{n+1/2} = \delta t_{n+1/2}\tilde{a}_n + \tilde{v}_{n-1/2}$$

where $N \in \{M, \bar{M}\}$ and

$$\tilde{u}_{n+1} = \delta t_n \tilde{v}_{n+1/2} + \tilde{u}_n$$

Experimental setup

Overlap of $\alpha = 1.3$ on 32×32 grid, $p = 3$ and enrichment.

schweitzer@scai.fraunhofer.de

Time-Stepping Results: $|(u - \bar{u})(\cdot, t_n)| \in [0, 2 \cdot 10^{-3}]$

Snapshots $t_n = 500 n \delta t$ with $n \in \{1, 2, \ldots, 20\}$ (up to 10^4 time-steps).

schweitzer@scai.fraunhofer.de

Movie

Time-Stepping Results: Explicit Nonlinear Elasticity

schweitzer@scai.fraunhofer.de

Movie