Towards a parallel domain decomposition solver for immersed boundary finite element method

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joint work with
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Outline

Introduction

Parallel adaptive mesh refinement

Multilevel BDDC method

Immersed boundary FEM

Numerical results

Conclusion and outlooks

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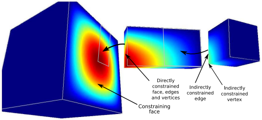
Motivations and ingredients

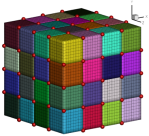
1. Adaptivity and higher order finite elements

[P. Kůs, P. Šolín, D. Andrš, *Arbitrary-level hanging nodes for adaptive hp-FEM approximations in 3D*, JCAM, 270, pp. 121–133, 2014.]

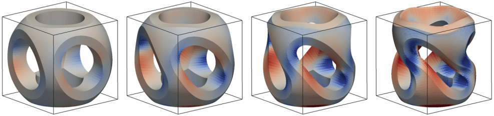


2. Nonoverlapping domain decomposition and parallel computing

[B. Sousedík, J. Šístek, and J. Mandel, *Adaptive-Multilevel BDDC and its parallel implementation*, Computing, 95 (12), pp. 1087–1119, 2013.]



3. Immersed boundary FEM



[T. Rüberg, F. Cirak, and J.M. Garcia-Aznar, *An unstructured immersed finite element method for nonlinear solid mechanics*, Advanced Modeling and Simulation in Engineering Sciences, 2016.]

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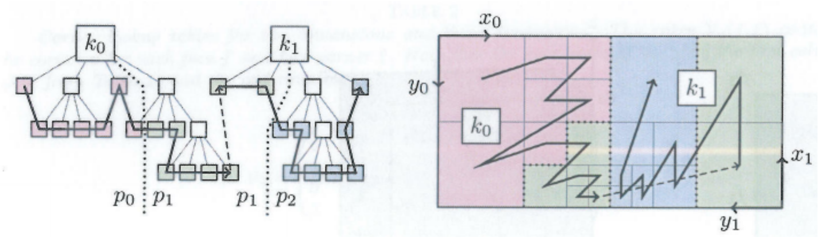
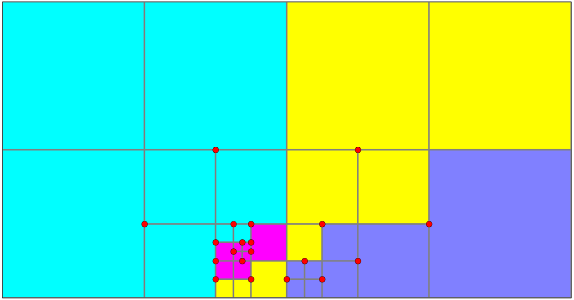
The *p4est* library



C. Burstedde, L. Wilcox, and O. Ghattas, *p4est: Scalable Algorithms for Parallel Adaptive Mesh Refinement on Forests of Octrees*, SIAM J. Sci. Comput., 3 (33), pp. 1103–1133, 2011.

Nonstandard properties of the mesh

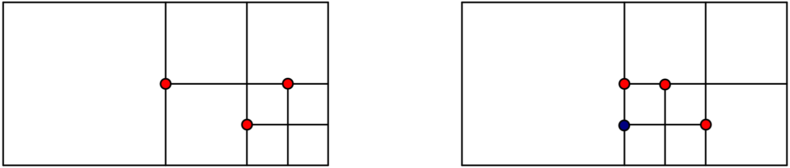


1. **Hanging nodes**
   - Hanging nodes have to be eliminated
   - They can also appear at the subdomain interface
2. **Shape of the subdomains**
   - Subdomains might be disconnected or only loosely coupled (e.g. by one node in elasticity)

Adding rules to the game

Assumptions on the mesh

- only level-1 hanging nodes allowed
- 2:1 rule
- equal order shape functions, i.e. no hp, but higher p fine



O.K. — not O.K.

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Solving the linear system

An abstract problem

$$u \in U : a(u, v) = \langle f, v \rangle \quad \forall v \in U$$

- $a(\cdot, \cdot)$ symmetric positive definite form on U
- $\langle \cdot, \cdot \rangle$ is inner product on U
- U is finite dimensional space (typically finite element functions)

Matrix form

$$u \in U : Au = f$$

- A symmetric positive definite matrix on U
- A large, sparse, condition number $\kappa(A) = \frac{\lambda_{\max}}{\lambda_{\min}} = \mathcal{O}(1/h^2)$

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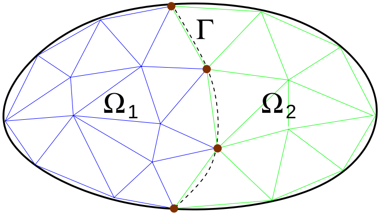
Nonoverlapping DD methods

- idea goes back to **substructuring** – a trick used in seventies to fit larger FE problems into memory



  - Ω_1, Ω_2 ... subdomains (substructures)
  - Γ ... interface
- unknowns at interface are shared by more subdomains, remaining (interior) unknowns belong to a single subdomain
- the first step is reduction of the problem to the **interface** Γ

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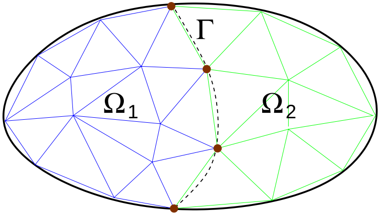

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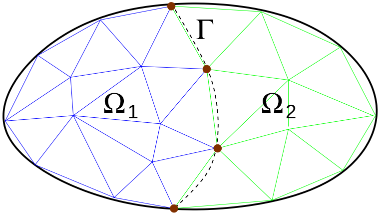

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Formation of the interface problem

- recall the matrix problem

$$Au = f$$

- reorder unknowns so that those at interior u_o^1 and u_o^2 are first, then interface u_Γ

$$\begin{bmatrix} A_{oo}^1 & & A_{o\Gamma}^1 \\ & A_{oo}^2 & A_{o\Gamma}^2 \\ A_{\Gamma o}^1 & A_{\Gamma o}^2 & A_{\Gamma\Gamma} \end{bmatrix} \begin{bmatrix} u_o^1 \\ u_o^2 \\ u_\Gamma \end{bmatrix} = \begin{bmatrix} f_o^1 \\ f_o^2 \\ f_\Gamma \end{bmatrix}$$

- eliminate interior unknowns – subdomain by subdomain = **in parallel**

$$\begin{bmatrix} A_{oo}^1 & & A_{o\Gamma}^1 \\ & A_{oo}^2 & A_{o\Gamma}^2 \\ & & S \end{bmatrix} \begin{bmatrix} u_o^1 \\ u_o^2 \\ u_\Gamma \end{bmatrix} = \begin{bmatrix} f_o^1 \\ f_o^2 \\ g \end{bmatrix}$$

$$S = \sum_{assembly} A_{\Gamma\Gamma}^i - A_{\Gamma o}^i (A_{oo}^i)^{-1} A_{o\Gamma}^i = \sum_{assembly} S^i$$

$$g = \sum_{assembly} f_\Gamma^i - A_{\Gamma o}^i (A_{oo}^i)^{-1} f_o^i = \sum_{assembly} g^i$$

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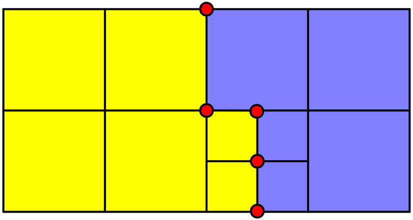

- interface Γ

Reduced (Schur complement) problem on interface Γ

$$Su_\Gamma = g$$

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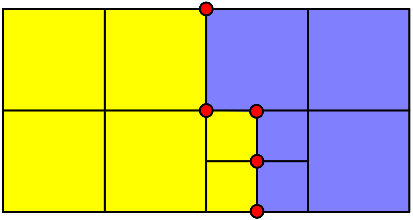
- solved by PCG



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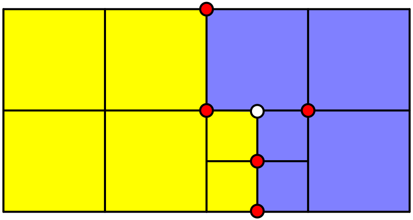
Iterative substructuring



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A practical algorithm of iterative substructuring

- In **setup**:
  1. factorize matrix A_{oo} (block diagonal = in parallel)
  2. form condensed right-hand side by solving

$$A_{oo}h = f_o,$$

and inserting $g = f_\Gamma - A_{\Gamma o}h$.

- In **each iteration**, for given p construct Sp as

$$\begin{bmatrix} A_{oo} & A_{o\Gamma} \\ A_{\Gamma o} & A_{\Gamma\Gamma} \end{bmatrix} \begin{bmatrix} w \\ p \end{bmatrix} = \begin{bmatrix} 0 \\ Sp \end{bmatrix}$$

  1. Solve (in parallel) *discrete Dirichlet problem*

$$A_{oo}w = -A_{o\Gamma}p$$

  2. Get Sp (in parallel) as

$$Sp = A_{\Gamma o}w + A_{\Gamma\Gamma}p$$

- **After iterations**, for given u_Γ, resolve (in parallel) interior unknowns by back-substitution in

$$A_{oo}u_o = f_o - A_{o\Gamma}u_\Gamma$$

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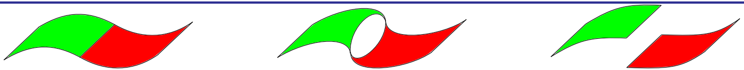
The BDDC preconditioner



U	$\subset$	$\widetilde{W}$	$\subset$	W
continuous at all nodes at interface		continuous at selected coarse dofs		no continuity at interface

- Balancing Domain Decomposition based on Constraints [Dohrmann (2003)], [Cros (2003)], [Fragakis, Papadrakakis (2003)]
- continuity at *corners*, and of averages (arithmetic or weighted) over *edges* or *faces* considered
- enough constraints to **fix floating subdomains** — $a(\cdot,\cdot)$ symmetric positive definite on $\widetilde{W}$

Variational form of $M_{BDDC} : r \longmapsto u$

$$w \in \widetilde{W} : \quad a(w,z) = \langle r, Ez \rangle \quad \forall z \in \widetilde{W}$$
$$u = Ew$$

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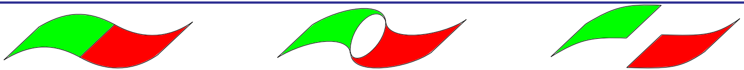

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The multilevel BDDC preconditioner

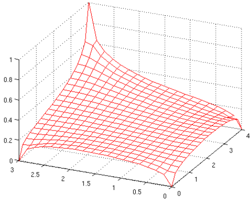
Local energy minimization problems

On each subdomain – **coarse degrees of freedom** – basis functions Ψ^i – prescribed values of coarse degrees of freedom, minimal energy elsewhere,

$$\begin{bmatrix} A^i & C^{iT} \\ C^i & 0 \end{bmatrix} \begin{bmatrix} \Psi^i \\ \Lambda^i \end{bmatrix} = \begin{bmatrix} 0 \\ I \end{bmatrix}.$$

- A^i ... local subdomain stiffness matrix
- C^i ... matrix of constraints – selects unknowns into coarse degrees of freedom

Matrix of **coarse problem** A_C assembled from local matrices $A_{Ci} = \Psi^{iT} A^i \Psi^i = -\Lambda^i$.



coarse basis fun.

Disconnected and loosely coupled subdomains

Assumption on solvability of local saddle-point systems

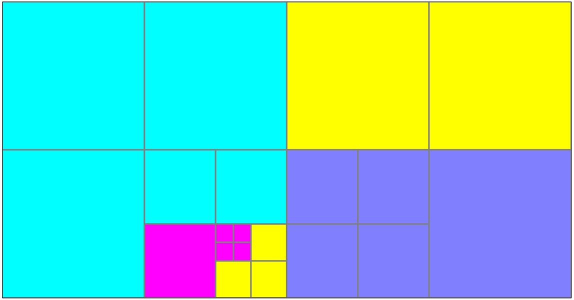
$$\mathrm{null}\, A^i \cap \mathrm{null}\, C^i = \{\mathbf{0}\}$$

- invertibility of
$$\begin{bmatrix} A^i & C^{iT} \\ C^i & 0 \end{bmatrix}$$
follows, see e.g. [Benzi, Golub, Liesen (2005)]
- satisfied if enough constraints on continuity in $\widetilde{W}$ are selected

Disconnected and loosely coupled subdomains

- more constrains needed in C^i
- more coarse basis functions Ψ^i

Disconnected and loosely coupled subdomains



- local nullspaces more complicated
- more constrains needed for each subdomain
- detect **graph components** of subdomain mesh

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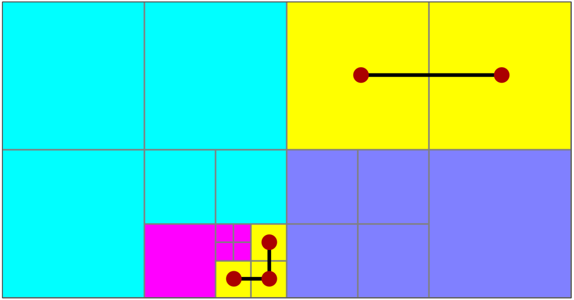

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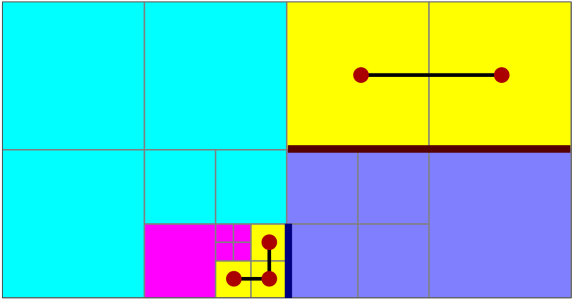

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One step of BDDC

Get residual at interface nodes $r_\Gamma^{(k)} = g - Su_\Gamma^{(k)}$ and produce **preconditioned residual** $z_\Gamma^{(k)} = M_{BDDC} r_\Gamma^{(k)}$ by

1. 1. Distribution of residual

subdomain problems | (global) coarse problem

for $i = 1, \dots, N$

$$r^i = E^{iT} r_\Gamma^{(k)}$$

$$r_C = \sum_{i=1}^{N} R_C^{iT} \Psi^{i*T} E^{iT} r_\Gamma^{(k)}$$

2. Correction of solution

$$\begin{bmatrix} A^i & C^{iT} \\ C^i & 0 \end{bmatrix} \begin{bmatrix} z^i \\ \mu^i \end{bmatrix} = \begin{bmatrix} r^i \\ 0 \end{bmatrix}$$

$$A_C u_C = r_C$$

3. Combination of subdomain and coarse corrections

$$z_\Gamma^{(k)} = \sum_{i=1}^{N} E^i \left(\Psi^i R_C^i u_C + z^i \right)$$

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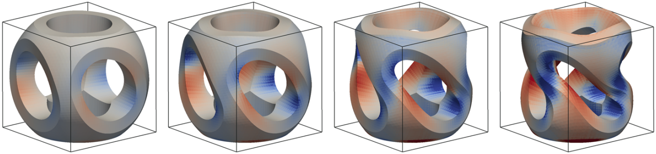
- an approach to avoiding mesh generation in FEM simulations
- robustness for geometric resolution through implicit description of the boundary

Nonstandard features compared to FEM

- weak enforcement of Dirichlet boundary conditions
- nonstandard quadrature rules
- ill-conditioning of stiffness matrices due to cut cells



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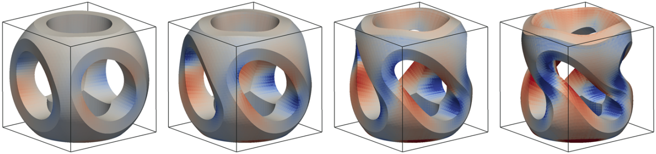

T. Rüberg, F. Cirak, and J.M. Garcia-Aznar, *An unstructured immersed finite element method for nonlinear solid mechanics*, Advanced Modeling and Simulation in Engineering Sciences, 2016.

Weak enforcement of the boundary conditions

$$u \in H^1(\Omega): \quad a(u,v) = l(v) \quad \forall v \in H^1(\Omega)$$

Penalty method

$$a(u,v) = \int_\Omega \nabla u \cdot \nabla v \, \mathrm{d}\Omega + \int_{\Gamma_D} \gamma u v \, \mathrm{d}\Gamma$$

$$l(v) = \int_\Omega f v \, \mathrm{d}\Omega + \int_{\Gamma_N} \bar{t} v \, \mathrm{d}\Gamma + \int_{\Gamma_D} \gamma \bar{u} v \, \mathrm{d}\Gamma$$

Nitsche method

$$a(u,v) = \int_\Omega \nabla u \cdot \nabla v \, \mathrm{d}\Omega - \int_{\Gamma_D} (\mathbf{n} \cdot \nabla u) v \, \mathrm{d}\Gamma - \int_{\Gamma_D} (\mathbf{n} \cdot \nabla v) u \, \mathrm{d}\Gamma + \int_{\Gamma_D} \gamma u v \, \mathrm{d}\Gamma$$

$$l(v) = \int_\Omega f v \, \mathrm{d}\Omega + \int_{\Gamma_N} \bar{t} v \, \mathrm{d}\Gamma - \int_{\Gamma_D} (\mathbf{n} \cdot \nabla v) \bar{u} \, \mathrm{d}\Gamma + \int_{\Gamma_D} \gamma \bar{u} v \, \mathrm{d}\Gamma$$

- $\gamma = \gamma_0 \alpha / h$

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- $\gamma = \gamma_0 \alpha / h$

Implementation

Parallel FEM solver with AMR and embedded domains

- experimental in-house code
- implicit geometry description
- C++ with MPI

p4est mesh manager for AMR

- rebalancing based on Z-curves
- ANSI C + MPI
- open-source (GPL)
- scalability reported for 1e5–1e6 cores

http://www.p4est.org

BDDCML equation solver

- Adaptive-Multilevel BDDC
- Fortran 95 + MPI
- open-source (LGPL)
- current version 2.5 (8/6/'15)
- tested on up to 65e3 cores and 2e9 unknowns

http://www.math.cas.cz/~sistek/software/bddcml.html

Outline

Introduction

Parallel adaptive mesh refinement

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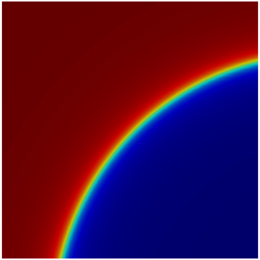
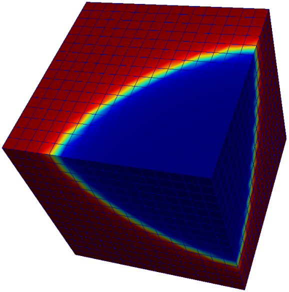
Adaptive mesh refinement

Internal layer benchmark

$$-\triangle u = f \quad \text{on} \quad (0,1)^d$$
$$u = \arctan\Big(s \cdot (r - \frac{\pi}{3})\Big)$$

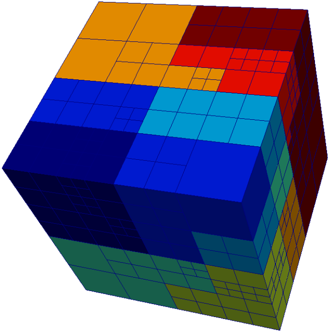


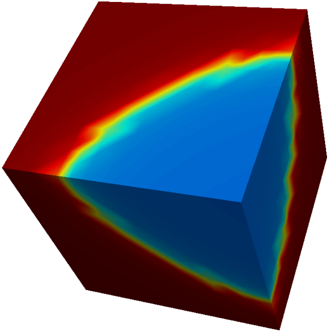


- solution exhibits sharp internal layer
- r is a distance from a given point
- s controls "steepness" of the layer

Adaptivity in 3D on 8 subdomains

- Adaptivity tested for element orders 1-4 (showed order 1)
- Guided by exact solution, using H^1 semi-norm for error calculation

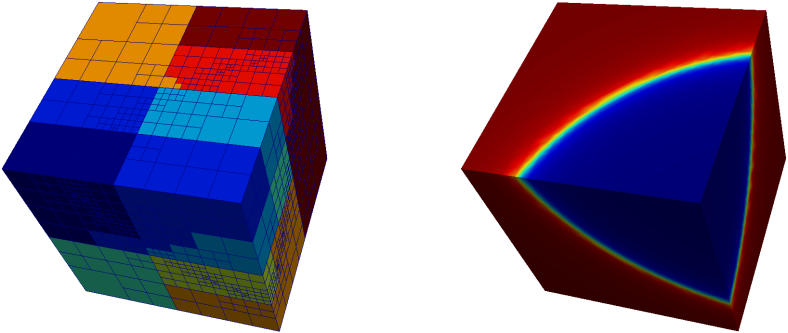




Iteration 3, mesh and solution

Adaptivity in 3D on 8 subdomains

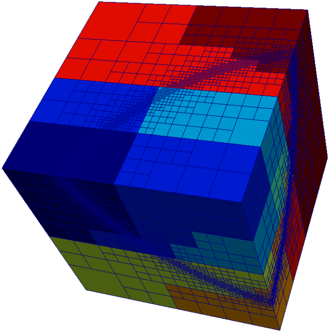
- Adaptivity tested for element orders 1-4 (showed order 1)
- Guided by exact solution, using H^1 semi-norm for error calculation

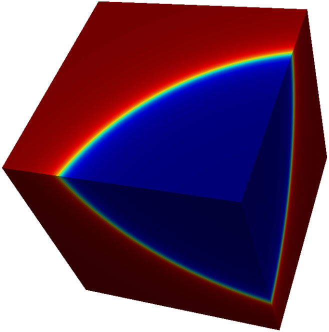


Iteration 5, mesh and solution

Adaptivity in 3D on 8 subdomains

- Adaptivity tested for element orders 1-4 (showed order 1)
- Guided by exact solution, using H^1 semi-norm for error calculation





Iteration 8, mesh and solution

Adaptivity in 3D, 3-level BDDC, linear elements

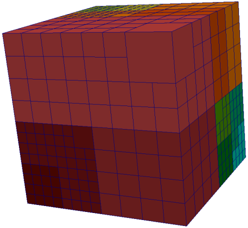
Adaptive mesh refinement

subs.	size	loc. size	PCG its.	time set-up [s]	time PCG [s]
2048/46	4913	2	**9**	2.8	1.1
2048/46	8594	4	**29**	0.55	1.6
2048/46	$2.5 \cdot 10^4$	12	**53**	0.6	3
2048/46	$1.3 \cdot 10^5$	63	**60**	0.67	3.5
2048/46	$7.0 \cdot 10^5$	342	**54**	0.89	3.5
2048/46	$3.0 \cdot 10^6$	1445	**56**	1.6	4.8
2048/46	$1.4 \cdot 10^7$	6623	**55**	2.9	10
2048/46	$6.4 \cdot 10^7$	$3.1 \cdot 10^4$	**55**	10	33
2048/46	$2.9 \cdot 10^8$	$1.4 \cdot 10^5$	**56**	61	130
2048/46	$1.3 \cdot 10^9$	$6.3 \cdot 10^5$	**51**	565	521

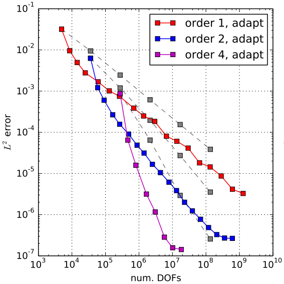
- run on *Salomon@IT4I*

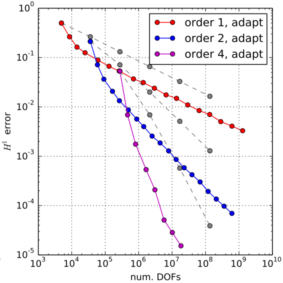
P. Kůs, J. Šístek. Coupling parallel adaptive mesh refinement with a nonoverlapping domain decomposition solver. Advances in Engineering Software, 110:34–54, 2017.

Adaptivity in 3D, 3-level BDDC, convergence order

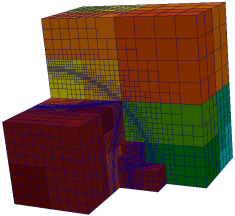


Illustrative mesh,
100K DOFs,
20 subdomains,
shown 1 – 20

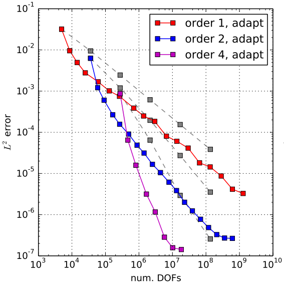


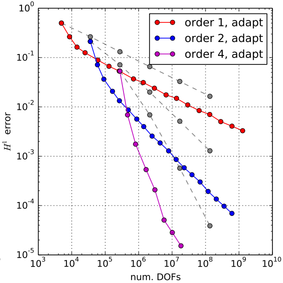


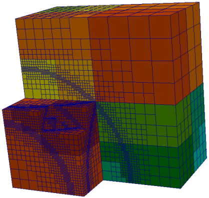
Adaptivity in 3D, 3-level BDDC, convergence order



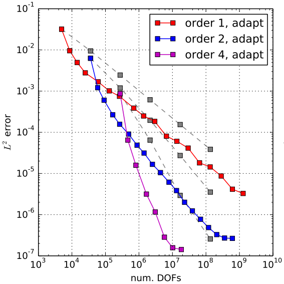
Illustrative mesh,
100K DOFs,
20 subdomains,
shown 1 – 18

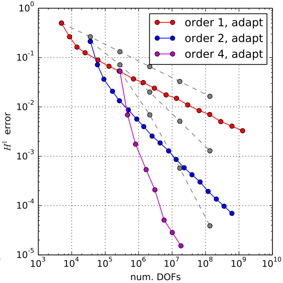


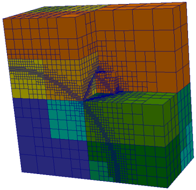




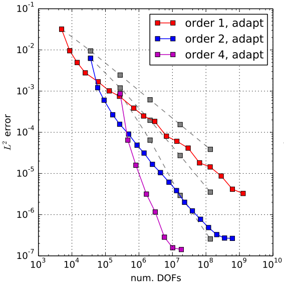
Illustrative mesh,
100K DOFs,
20 subdomains,
shown 1 – 16

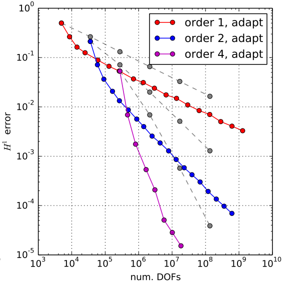




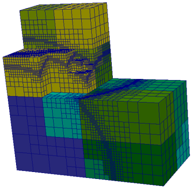


Illustrative mesh,
100K DOFs,
20 subdomains,
shown 1 – 14

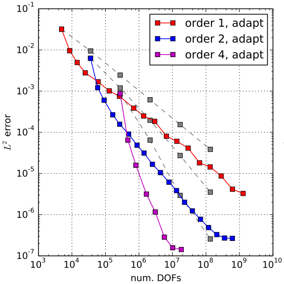


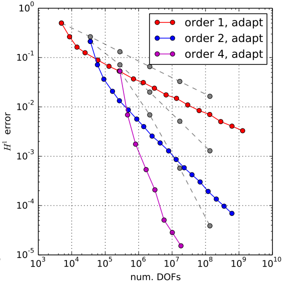


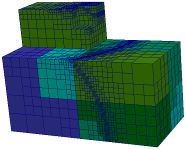
Adaptivity in 3D, 3-level BDDC, convergence order



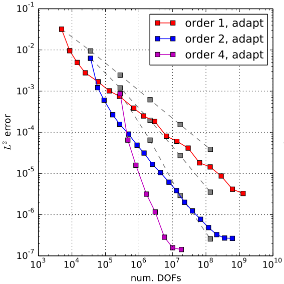
Illustrative mesh,
100K DOFs,
20 subdomains,
shown 1 – 12

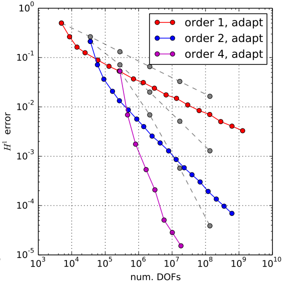


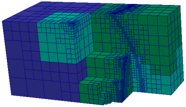




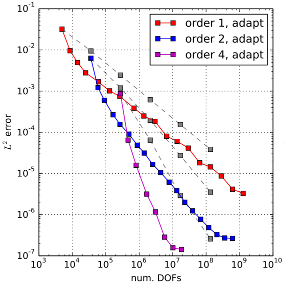
Illustrative mesh,
100K DOFs,
20 subdomains,
shown 1 – 10

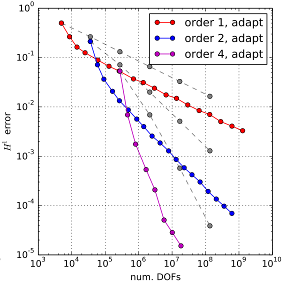






Illustrative mesh,
100K DOFs,
20 subdomains,
shown 1 – 8.





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Our use of direct solver

Two matrix factorizations

- 50% runtime (of the solver itself) spent in matrix factorizations, another 30% in back substitions (in iterations).
- We factorize two matrices on each subdomain. First A_{oo} with inner DOFs, the other with approx. 20% extra rows and columns, a saddle point problem. The first matrix is a submatrix of the second one.
- For Poisson problem and linear elasticity we use Cholesky and LDL^T decompositions, respectively. LU with pivoting used for non-symmetric problems.

$$\begin{bmatrix} A_{oo} & A_{o\Gamma} & 0 \\ A_{\Gamma o} & A_{\Gamma\Gamma} & C_\Gamma^T \\ 0 & C_\Gamma & 0 \end{bmatrix}$$

- We need to invert A_{oo} and the 3 by 3 block matrix on each subdom.
- For eliptic problems, A_{oo} is positive definite, the first 2 by 2 block matrix is positive semidefinite and the whole 3 by 3 block matrix is a saddle point problem.
- Only the part of C_i corresponding to the interface Γ is nonzero (C_Γ).

Our use of direct solver

Distibution of subdomains

- Currently we run pure MPI with one subdomain per MPI rank, trying to balance the subdomain sizes.
- This is sometimes difficult to achieve when using the parallel adaptivity of the mesh and many subdomain components.
- Having variable number of subdomains per node is appealing from various reasons, but would require a major code refactoring.

Contacts

Thank you for your attention!

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BDDCML library

http://users.math.cas.cz/~sistek/software/bddcml.html