Relaxing the Role of Corners in BDDC with Perturbed Formulation

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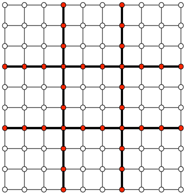
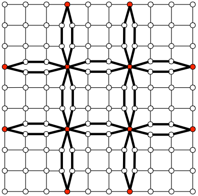
What is BDDC?

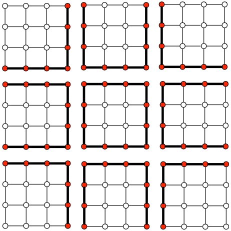
BDDC = Balancing Domain Decomposition by Constraints [Dohrmann '03]

- is an iterative substructuring method (non-overlapping DD)
- belongs to the family of BDD methods [Mandel '93] which are essentially Neumann-Neumman methods [De Roeck, Le Tallec, Vidrascu '92; Glowinski, Wheeler '88] with a coarse space.
- has "the same" spectrum with FETI-DP [Farhat et al., '01] (see [Mandel, Dohrmann, Tezaur '05; Brenner, Sung '07])
- can be analyzed using the Additive Schwarz framework proposed by [Dryja, Widlund '95]
- uses additive coarse grid correction (coarse duty and fine duties can be overlapped [Badia's talk on Tuesday] [Badia, Martin, Principe '14])

BDDC Space, Coarse Functions and Constraints







$V_h(\Omega)$ $\subset$ $\widetilde{V}$ $\subset$ $\hat{V} = \prod_{i=}^{N} V_h(\Omega)|_{\Omega_i}$

globally continuous — discontinuous across Γ

fully coupled — partially coupled — fully decoupled

- BDDC space: $\widetilde{V} = \widehat{V}$+constraints
- coarse functions ":=" values at constrains + minimizing energy ($\dim$(coarse space) = #constraints)
- constraints are chosen s.t. local problems and coarse problem are well-posed (invertible)

Choices of Constraints for BDDC

Typical types of constraint are:

1. value at a subdomain corner (for invertibility & convergence)
2. average value on a subdomain edge/face (for convergence)

Work on corner detection algorithms includes:

- [Dorhmann '03, Lesoinne '03]: "corner-based" selection
- [Klawonn and Widlund '04]: "edge-based" on selection of corners
- [Šístek et al. '12]: face-based selection of corners

Motivation

- Corner detection mechanism can be complicated
- For domains with complex geometry, connected subdomains are not guaranteed by mesh partitioners (ParMETIS, PT-Scotch)
- Do not want to use change of basis
- For some situation, we want to have a minimal coarse space (eliminate corners and possibly either edges or faces)

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Can we formulate a BDDC method that

- is scalable (Accuracy)
- works with all types of constrains, partitions (Robustness)
- works without corner detection, change of basis (Simplicity)

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Can we formulate a BDDC method that

- is scalable (Accuracy)
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- works without corner detection, change of basis (Simplicity)

YES! USE PERTURBED FORMULATION!

Model problem

Find $u \in V_h(\Omega) \subset H_0^1(\Omega)$ such that

$$a(u, v) = F(v), \text{ for all } v \in V_h(\Omega),$$

where $a(u, v) = \int_\Omega \nabla u \cdot \nabla v dx,\ F(v) = \int_\Omega f v dx,\ f \in L_2(\Omega).$

(Results can be extended for linear elasticity!!!)

- non-overlapping decomposition: $\Omega = \cup_{j=1}^N \Omega_j, \quad \Omega_j \cap \Omega_k = \emptyset$
- restriction: $u_j = u|_{\Omega_j}, v_j = v|_{\Omega_j}$ and $a_j(u_j, v_j) = \int_\Omega u_j v_j dx$
- interface: $\Gamma = \cup_{j=1}^N (\partial\Omega_j \backslash \Omega)$

Interface Problem

$$V_h(\Omega) = V(\Omega\backslash\Gamma) \oplus V(\Gamma), \quad V(\Omega\backslash\Gamma) \perp_{a(\cdot,\cdot)} V(\Gamma)$$
$$V(\Omega\backslash\Gamma) = \{v \in V_h(\Omega) : v(x) = 0 \quad \forall\, x \in \Gamma\}$$

For any $u \in V_h$, there exists an unique decomposition

$$u = u^\circ + \bar{u}, \quad u^\circ \in V_h(\Omega\backslash\Gamma),\ \bar{u} \in V(\Gamma)$$

- $u^\circ = \sum_{i=1}^{N} u_i^\circ$ can be founded by solving decoupled Dirichlet problems on subdomains
- $\bar{u}$ is the solution of the interface problem:

$$S_h\bar{u} = f_h, \text{ where } S_h : V_h(\Gamma) \to V(\Gamma)',\ f_h \in V(\Gamma)'$$

S_h: *global Schur complement operator*, $\langle S_h v_1, v_2\rangle := a(v_1, v_2)$
f_h : $\langle f_h, v\rangle := F(v)$

BDDC formulates a preconditioner for S_h

Ingredients of BDDC

1. Constraint set $\mathcal{C}$
2. Spaces:
   - BDDC interface space:
     $\mathcal{H}_\mathcal{C} = \{v \in L^2(\Omega) : v_j = v|_{\Omega_j} \in \mathcal{H}_j = V(\Gamma)|_{\Omega_j},\ v \text{ satisfies } \mathcal{C}\}$
   - fine spaces:
     $\mathcal{H}^f = \{v \in \mathcal{H}_\mathcal{C} : v \text{ satisfies zero-constraints } \mathcal{C}\}, \quad \mathcal{H}^f_j = \mathcal{H}^f|_{\Omega_j}$
   - coarse space: $\mathcal{H}_\mathcal{C} = \mathcal{H}^c \oplus \mathcal{H}^f, \quad \mathcal{H}^c \perp_{a(\cdot,\cdot)} \mathcal{H}^f$
3. (Coarse/fine) Schur operators: $S_0 : \mathcal{H}^c \to (\mathcal{H}^c)', \quad S_j : \mathcal{H}^f_j \to (\mathcal{H}^f_j)'$

$$\langle S_0 v, w \rangle = a(v, w), \quad \langle S v_j, w_j \rangle = a_j(v_j, w_j)$$

4. Injection/extension maps: $E_0 : \mathcal{H}^c \to \mathcal{H}_\mathcal{C},\ E_j : \mathcal{H}^f_j \to \mathcal{H}_\mathcal{C}$
5. Averaging projection: $P_\Gamma : \mathcal{H}_\mathcal{C} \to V(\Gamma)$

$$P_\Gamma v = \frac{1}{|\mathcal{N}(p)|} \sum_{j \in \mathcal{N}} v_j(p), \quad \mathcal{N}(p) = \{1 \le j \le N : p \in \Gamma_j\}$$

BDDC Formulation

1. Constraint set $\mathcal{C}$
2. Spaces: $\mathcal{H}_{\mathcal{C}} = \mathcal{H}^c \oplus \mathcal{H}^f, \quad \mathcal{H}^c \perp_{a(\cdot,\cdot)} \mathcal{H}^f$
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5. Averaging projection: $P_\Gamma : \mathcal{H}_{\mathcal{C}} \to V(\Gamma)$

$$\boxed{B_{\text{BDDC}} = (P_\Gamma E_0) S_0^{-1} (P_\Gamma E_0)^t + \sum_{j=1}^{N} (P_\Gamma E_j) S_j^{-1} (P_\Gamma E_j)^t}$$

Currently: $\mathcal{C}$ is chosen s.t S_0 and S_j are positive (invertible)!!!

BDDC Formulation

1. Constraint set $\mathcal{C}$
2. Spaces: $\mathcal{H}_{\mathcal{C}} = \mathcal{H}^c \oplus \mathcal{H}^f, \quad \mathcal{H}^c \perp_{a(\cdot,\cdot)} \mathcal{H}^f$
3. (Coarse/fine) Schur operators: $S_0 : \mathcal{H}^c \to (\mathcal{H}^c)', \quad S_j : \mathcal{H}_j^f \to (\mathcal{H}_j^f)'$

$$\langle S_0 v, w \rangle = a(v,w), \quad \langle S v_j, w_j \rangle = a_j(v_j, w_j)$$

4. Injection/extension maps: $E_0 : \mathcal{H}^c \to \mathcal{H}_{\mathcal{C}},\ E_j : \mathcal{H}_j^f \to \mathcal{H}_{\mathcal{C}}$
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Currently: $\mathcal{C}$ is chosen s.t S_0 and S_j are positive (invertible)!!!

Can we use different bilinear forms instead?

Perturbed Bilinear Forms

Our inspiration: [Dryja, Widlund '95] on "Schwarz methods of Neumann-Neumann type"

Consider a bilinear form $\widetilde{a}(\cdot,\cdot)$ satisfying the following properties:

1. sufficiently close:

$$C_{\mathrm{l}}\,\widetilde{a}(v,v) \le a(v,v) \le C_{\mathrm{u}}\,\widetilde{a}(v,v) \quad \forall v \in H_0^1(\Omega)$$

$C_{\mathrm{l}},\ C_{\mathrm{u}}$ are independent of H, h and N

2. positive substructure components:

$$\widetilde{a}(v,w) = \sum_{j=1}^{J} \widetilde{a}_j(v_j, w_j), \quad \forall v, w \in H_0^1(\Omega)$$

where $\widetilde{a}_j(\cdot,\cdot)$ are positive definite in $H_0^1(\Omega)|_{\Omega_j}$

Ingredients of Perturbed BDDC

1. Constraint set $\mathcal{C}$: any combination of C, E, F and no change of basis)

2. Spaces: $V_h(\Omega) = V(\Omega\backslash\Gamma) \oplus \widetilde{V}(\Gamma), \quad V(\Omega\backslash\Gamma) \perp_{\widetilde{a}(\cdot,\cdot)} \widetilde{V}(\Gamma)$
$\widetilde{\mathcal{H}}_{\mathcal{C}} = \{v \in L^2(\Omega) : v_j = v|_{\Omega_j} \in \widetilde{\mathcal{H}}_j = \widetilde{V}(\Gamma)|_{\Omega_j}, \ v \text{ satisfies } \mathcal{C}\}$
   - fine spaces:
     $\widetilde{\mathcal{H}}^f = \{v \in \widetilde{\mathcal{H}}_{\mathcal{C}} : v \text{ satisfies zero-constraints } \mathcal{C}\}, \quad \widetilde{\mathcal{H}}^f_j = \widetilde{\mathcal{H}}^f|_{\Omega_j}$
   - coarse space: $\widetilde{\mathcal{H}}_{\mathcal{C}} = \widetilde{\mathcal{H}}^c \oplus \widetilde{\mathcal{H}}^f, \quad \widetilde{\mathcal{H}}^c \perp_{\widetilde{a}(\cdot,\cdot)} \widetilde{\mathcal{H}}^f$

3. (Coarse/fine) Schur operators: $\widetilde{S}_0 : \widetilde{\mathcal{H}}^c \to (\widetilde{\mathcal{H}}^c)', \quad \widetilde{S}_j : \widetilde{\mathcal{H}}^f_j \to (\widetilde{\mathcal{H}}^f_j)'$

$$\langle \widetilde{S}_0 v, w\rangle = \widetilde{a}(v,w), \quad \langle \widetilde{S} v_j, w_j\rangle = \widetilde{a}_j(v_j, w_j)$$

4. Injection/extension maps: $\widetilde{E}_0 : \widetilde{\mathcal{H}}^c \to \widetilde{\mathcal{H}}_{\mathcal{C}}, \ \widetilde{E}_j : \widetilde{\mathcal{H}}^f_j \to \widetilde{\mathcal{H}}_{\mathcal{C}}$

5. Averaging projection: $P_\Gamma : \widetilde{\mathcal{H}}_{\mathcal{C}} \to \widetilde{V}(\Gamma)$

6. Connection projection: $Q_\Gamma : \widetilde{V}(\Gamma) \to V(\Gamma)$

$$(Q_\Gamma \widetilde{v})(p) = \widetilde{v}(p), \quad \forall\, \widetilde{v} \in \widetilde{V}_h(\Gamma), \ p \in \Gamma_h$$

Perturbed BDDC Formulation

1. Constraint set $\mathcal{C}$: any combination of C (Corner), E (Edge), F (Face))
2. Spaces: $\widetilde{\mathcal{H}}_{\mathcal{C}} = \widetilde{\mathcal{H}}^c \oplus \widetilde{\mathcal{H}}^f, \quad \widetilde{\mathcal{H}}^c \perp_{\widetilde{a}(\cdot,\cdot)} \widetilde{\mathcal{H}}^f$
3. (Coarse/fine) Schur operators: $\widetilde{S}_0 : \widetilde{\mathcal{H}}^c \to (\widetilde{\mathcal{H}}^c)', \quad \widetilde{S}_j : \widetilde{\mathcal{H}}_j^f \to (\widetilde{\mathcal{H}}_j^f)'$
4. Injection/extension maps: $\widetilde{E}_0 : \widetilde{\mathcal{H}}^c \to \widetilde{\mathcal{H}}_{\mathcal{C}}, \ \widetilde{E}_j : \widetilde{\mathcal{H}}_j^f \to \widetilde{\mathcal{H}}_{\mathcal{C}}$
5. Averaging projection: $P_\Gamma : \widetilde{\mathcal{H}}_{\mathcal{C}} \to \widetilde{V}(\Gamma)$
6. Connection projection: $Q_\Gamma : \widetilde{V}(\Gamma) \to V(\Gamma)$

$$\widetilde{B}_{\mathsf{BDDC}} = (Q_\Gamma \widetilde{P}_\Gamma E_0)\widetilde{S}_0^{-1}(Q_\Gamma \widetilde{P}_\Gamma E_0)^t + \sum_{j=1}^{N} (Q_\Gamma \widetilde{P}_\Gamma E_j)\widetilde{S}_j^{-1}(Q_\Gamma \widetilde{P}_\Gamma E_j)^t$$

No need to implement Q_Γ!!!

Choices of Perturbation

1. Perturbation with full mass

$$\widetilde{a}(u,v) = a(u,v) + \frac{1}{L^2}\int_\Omega uv\,dx = \int_\Omega \nabla u \cdot \nabla v\,dx + \frac{1}{L^2}\int_\Omega uv\,dx,$$

where $L = \mathrm{diameter}(\Omega)$.
Note that: in [Dryja, Widlund '95]

$$\widetilde{a}_j(u,v) = a_j(u,v) + \frac{1}{{H_j}^2}\int_{\Omega_j} uv\,dx$$

2. Perturbation with mass on interface (Robin perturbation)

$$\widetilde{a}(u,v) = a(u,v) + \frac{H^{n-1}}{L^n}\int_\Gamma uv\,ds = \int_\Omega \nabla u \cdot \nabla v\,dx + \frac{H^{n-1}}{L^n}\int_\Gamma uv\,ds$$

Convergence Result

Lemma 1

For any $v \in V_h(\Gamma)$, *we have*

$$\langle S_h v, v\rangle \geq \min_{\substack{v=\sum_{j=0}^{N} Q_j \widetilde{v}_j \\ \widetilde{v}_0 \in \widetilde{\mathcal{H}}^c,\, \widetilde{v}_j \in \widetilde{H}_j^f,\, (1\leq j \leq N)}} \sum_{j=0}^{N} \langle \widetilde{S}_j \widetilde{v}_j, \widetilde{v}_j \rangle, \quad Q_j = Q_\Gamma \widetilde{P}_\Gamma \widetilde{E}_j$$

(*i.e.* $\lambda_{\min}(\widetilde{B}_{\mathsf{BDDC}} S_h) \geq 1/C_{\mathrm{u}}$)

$$\langle S_h v, v\rangle \lesssim [1 + \ln(H/h)]^2 \min_{\substack{v=\sum_{j=0}^{N} Q_j \widetilde{v}_j \\ \widetilde{v}_0 \in \widetilde{\mathcal{H}}^c,\, \widetilde{v}_j \in \widetilde{H}_j^f,\, (1\leq j \leq N)}} \sum_{j=0}^{N} \langle \widetilde{S}_j \widetilde{v}_j, \widetilde{v}_j \rangle$$

(*i.e.* $\lambda_{\max}(\widetilde{B}_{\mathsf{BDDC}} S_h) \lesssim [1 + \ln(H/h)]^2$)

Lemma 1: Ingredients for Proof

Follow [Klawonn, Widlund, Dryja '02, Brenner, Sung '07] with modifications:

- The decomposition:

$$v = Q_\Gamma \widetilde{v} = Q_\Gamma \widetilde{P}_\Gamma \widetilde{I}_0 \widetilde{v}_0 + \sum_{j=1}^{J} Q_\Gamma \widetilde{P}_\Gamma \widetilde{E}_j \widetilde{v}_j = \sum_{j=0}^{J} Q_j \widetilde{v}_j .$$

- Switching the bilinear forms: $\widetilde{a}(\widetilde{v},\widetilde{v}) \le \widetilde{a}(v,v) \le C_{\mathrm{u}} a(v,v)$
- Acceptable paths exists even when only E (Edges) or F (faces) are selected:

$$\widetilde{w} = \widetilde{v}_j - Q_j \widetilde{v}_j = \sum_{j=1}^{N} \left(\sum_{c \in C_j} \widetilde{w}_c + \sum_{e \in E_j} \widetilde{w}_e + \sum_{f \in F_j} \widetilde{w}_f \right)$$

  - Acceptable edge path [Klawonn, Widlund, Dryja '02]
  - Acceptable face path [Klawonn, Widlund, Dryja 'DD13]

Theorem 2

There exist a positive constant C, independent of h, H and N, such that

$$\kappa(\widetilde{B}_{\mathsf{BDDC}} S_h) = \frac{\lambda_{\max}(\widetilde{B}_{\mathsf{BDDC}} S_h)}{\lambda_{\min}(\widetilde{B}_{\mathsf{BDDC}} S_h)} \leq C \left(1 + \ln \frac{H}{h}\right)^2 .$$

Software and Machines

FEMPAR (in-house developed HPC software):

Finite Element Multiphysics PARallel software

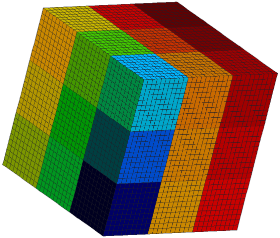
- Massively parallel for FE simulation of multiphysics PDEs
- Interfaces to external multi-threaded sparse direct solvers (PARDISO, HSL_MA87, etc.) and serial AMG preconditioners (HSL_MI20)

1. **MareNostrum** at Barcelona Super Computer Center: Intel SandyBridge processors, Infiniband interconnection (shared) 1.1 Petaflops, 100.8 TB memory, 3056 compute nodes, 48896 cores
2. **HLRN-III** in Hanover, Germany: Cray XC30 0.9 Petaflops, 105 TB memory, 936 compute nodes, 22464 cores

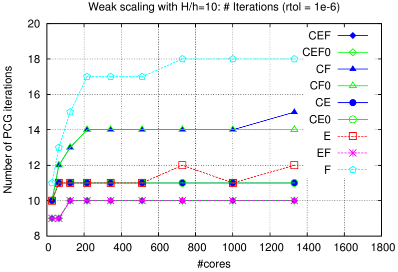
Poisson's Equation on the Unit Cube

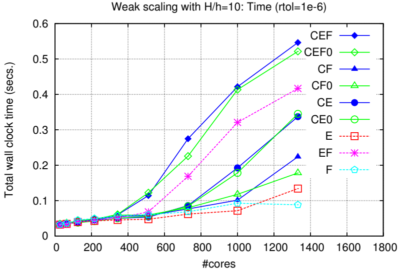
Problem Data:

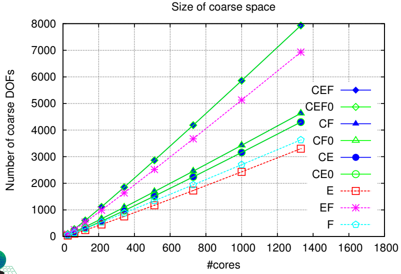
- Domain: $[0\ 1] \times [0\ 1] \times [0\ 1]$
- Zero Dirichlet condition on the whole boundary
- RHS f is chosen to have a predefined solution
- Structured hexahedral mesh
- Regular partition with $m \times m \times m,\ m = 2, \ldots, 11$ subdomains
- $H/h = 10, 30$



Poisson's Equation: Perturbation w. Full Mass & $H/h = 10$

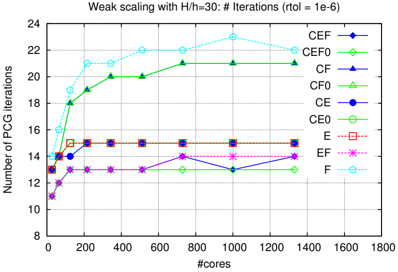


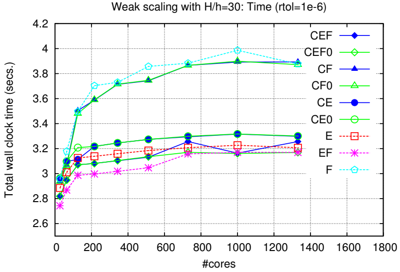


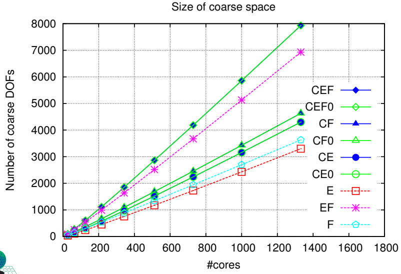


- *0: without perturbation
- CEF_CD: CEF with corner detection
- the rest: with perturbation

Poisson's Equation: Perturbation w. Full Mass & $H/h = 30$





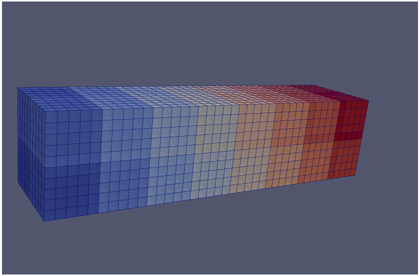


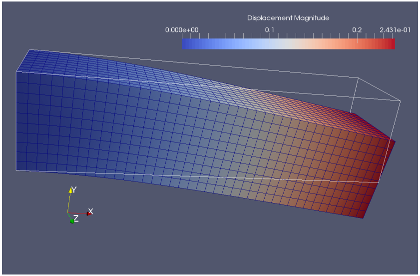
- *0: without perturbation
- CEF_CD: CEF with corner detection
- the rest: with perturbation

Elasticity: Long Beam Problem

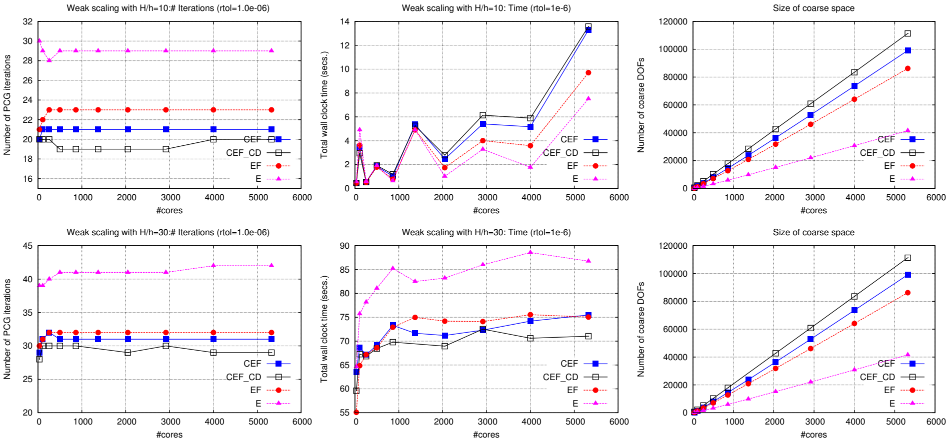
Problem Data:

- Domain: $[0\ \ 2] \times [0\ \ 0.5] \times [0\ \ 0.5]$
- BCs: fixing face $\{x = 0\}$
- External force: $F = [0.0\ \ -0.005\ \ 0.0]^T$
- Structured hexahedral mesh
- Regular partition with $4m \times m \times m,\ m = 2, \ldots, 11$ subdomains
- $H/h = 10, 30$



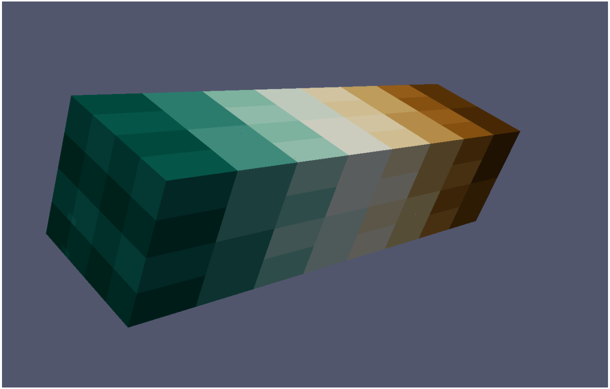


Elasticity: Long Beam - Robin Perturbation



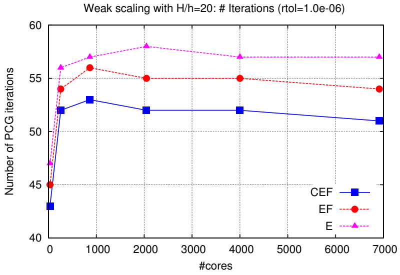
Works with perturbation or corner detection [Šístek et al.] only

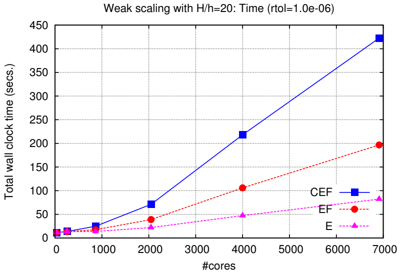
Linear Elasticity: Long Beam - Disconnected Subdomains

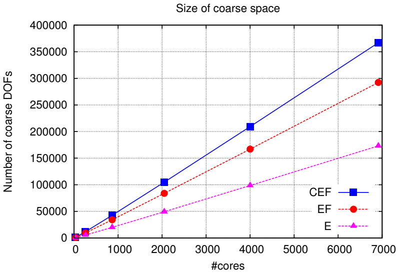


- $4m^3, m = 2, 4, \ldots, 12$ subdomains, half of them are disconnected with 4 disconnected parts each
- corner detection failed

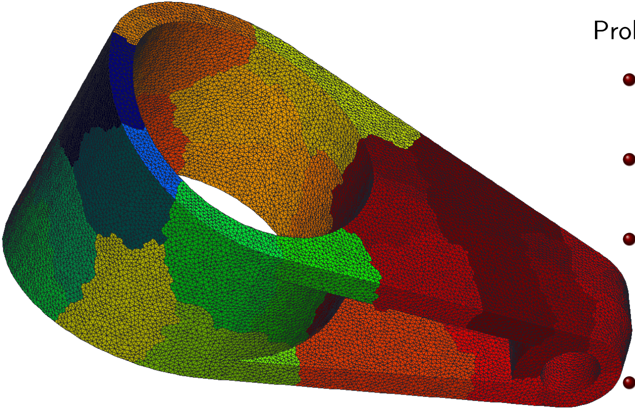
Linear Elasticity: Long Beam - Disconnected Subdomains







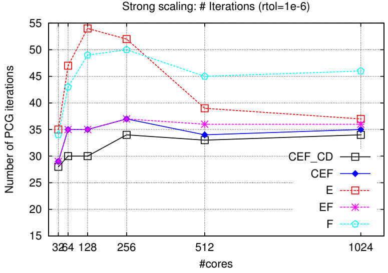
Elasticity: Cross Link Problem

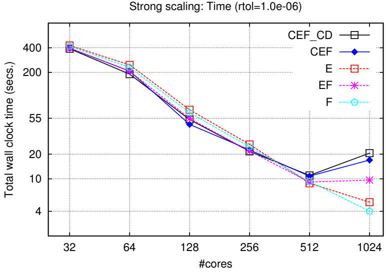


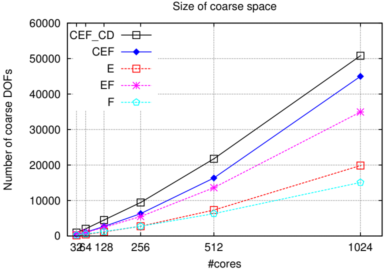
Problem Data:

- BCs: fixing inner interfaces of the two holes
- External force: $F = [1.0 \;\; 1.0 \;\; 1.0]^T$
- Unstructured tetrahedral mesh with 4.5M DoFs, 25M elements (not the one shown)
- Partitioned by METIS

Linear Elasticity: CrossLink - Robin







Conclusions and Future Work

Conclusions:

- we have formulated a new BDDC preconditioner with perturbed formulation
- the new method
  - is scabable
  - works with all types of constraints, partitions
  - work without corner detection, change of basis
- we demonstrated that in building coarse space, having small precondition number might not be the ultimate goal but having small size coarse space

Future Work

- inexact/approximate BDDC with perturbation (already got good numerical results for Poisson's problem)
- algebraic perturbation

Thank you!

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