CERFACS

CENTRE EUROPÉEN DE RECHERCHE ET DE FORMATION AVANCÉE EN CALCUL SCIENTIFIQUE

Highly robust iterative, domain decomposition solvers and load balancing aspects in the setup phase

[joint work with A. Klawonn (U Cologne) and O. Rheinbach (TU Freiberg)]

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EoCoE

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Find $u \in H_0^1(\Omega, \partial\Omega_D)^3$, such that

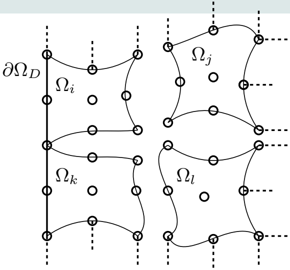
$$\begin{aligned} a(u,v) &= \int_\Omega 2\mu\varepsilon(u) : \varepsilon(v)\mathrm{d}x + \int_\Omega \lambda \mathrm{div}(u)\mathrm{div}(v)\mathrm{d}x \\ &= f(v) = \int_\Omega f \cdot v\mathrm{d}x + \int_{\partial\Omega_N} g \cdot v\mathrm{d}s \quad \forall v \in H_0^1(\Omega, \partial\Omega_D)^3 \end{aligned} \tag{1}$$

- $\Omega \subset \mathbb{R}^3$ bounded polyhedral domain,
- $\partial\Omega_D \subset \partial\Omega$ a closed subset of nonvanishing measure and $\partial\Omega_N := \partial\Omega \setminus \partial\Omega_D$.
- $H_0^1(\Omega, \partial\Omega_D)^k := \{v \in H^1(\Omega)^k : v = 0 \text{ on } \partial\Omega_D\}$,
- λ and μ the Lamé constants depending on Young's modulus $\mathsf{E}(x) > 0$, and Poisson's ratio $0 < \nu(x) < \frac{1}{2}$ for all $x \in \Omega$.
- $f : \Omega \to \mathbb{R}^3$ volume force
- $g : \partial\Omega_N \to \mathbb{R}^3$ surface force

Initial domain decomposition steps:

- Divide Ω into N nonoverlapping subdomains Ω_i, $i = 1, \ldots, N$,
- assemble local stiffness matrices $K^{(i)}$ and load vectors $f^{(i)}$, $i = 1, \ldots, N$.

$\rightarrow$ the decoupled problems lead to 'floating subdomains'.



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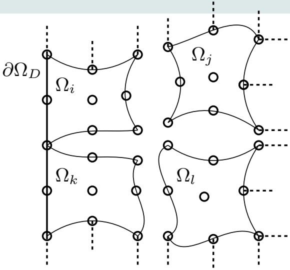
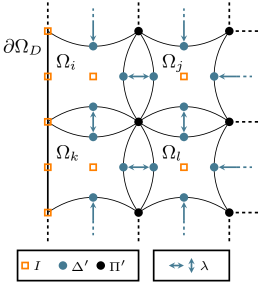


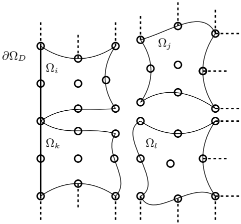
FETI-DP **FETI-DP**

- Subdivide the set of variables into inner (I), a priori dual (Δ') and primal (Π') variables (nodes/dofs).
- Enforce continuity (in each iteration step) at primal variables (nodes/dofs) by subassembly.
- Enforce continuity (at convergence) at dual variables (nodes/dofs) by Lagrange multipliers λ.



Initial system after domain decomposition:

$$\underbrace{\begin{bmatrix} K^{(1)} & & \\ & \ddots & \\ & & K^{(N)} \end{bmatrix}}_{=:K} \underbrace{\begin{bmatrix} u^{(1)} \\ \vdots \\ u^{(N)} \end{bmatrix}}_{=:u} = \underbrace{\begin{bmatrix} f^{(1)} \\ \vdots \\ f^{(N)} \end{bmatrix}}_{=:f}$$



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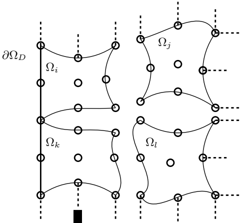
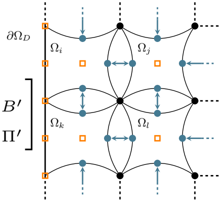


FETI-DP **FETI-DP**

$$\begin{bmatrix} K_{II}^{(1)} & K_{I\Delta'}^{(1)} & & & & \widetilde{K}_{\Pi' I}^{(1)T} \\ K_{\Delta' I}^{(1)} & K_{\Delta'\Delta'}^{(1)} & & & & \widetilde{K}_{\Pi'\Delta'}^{(1)T} \\ & & \ddots & & & \vdots \\ & & & K_{II}^{(N)} & K_{I\Delta'}^{(N)} & \widetilde{K}_{\Pi' I}^{(N)T} \\ & & & K_{\Delta' I}^{(N)} & K_{\Delta'\Delta'}^{(N)} & \widetilde{K}_{\Pi'\Delta'}^{(N)T} \\ \widetilde{K}_{\Pi' I}^{(1)} & \widetilde{K}_{\Pi'\Delta'}^{(1)} & \cdots & \widetilde{K}_{\Pi' I}^{(N)} & \widetilde{K}_{\Pi'\Delta'}^{(N)} & \widetilde{K}_{\Pi'\Pi'} \end{bmatrix} =: \begin{bmatrix} K_{B'B'} & \widetilde{K}_{\Pi' B'}^{T} \\ \widetilde{K}_{\Pi' B'} & \widetilde{K}_{\Pi'\Pi'} \end{bmatrix}$$



and the introduction of LM λ yields the system: $\begin{bmatrix} K_{B'B'} & \widetilde{K}_{\Pi' B'}^{T} & B^T \\ \widetilde{K}_{\Pi' B'} & \widetilde{K}_{\Pi'\Pi'} & O \\ B & O & O \end{bmatrix} \begin{bmatrix} u_B' \\ \tilde{u}_\Pi' \\ \lambda \end{bmatrix} = \begin{bmatrix} f_B' \\ \tilde{f}_{\Pi'} \\ 0 \end{bmatrix}$

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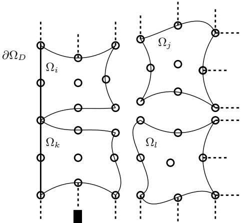
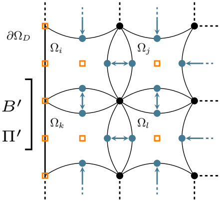


FETI-DP **FETI-DP**

$$\begin{bmatrix} K^{(1)}_{II} & K^{(1)}_{I\Delta'} & & & & \widetilde{K}^{(1)T}_{\Pi' I} \\ K^{(1)}_{\Delta' I} & K^{(1)}_{\Delta'\Delta'} & & & & \widetilde{K}^{(1)T}_{\Pi'\Delta'} \\ & & \ddots & & & \vdots \\ & & & K^{(N)}_{II} & K^{(N)}_{I\Delta'} & \widetilde{K}^{(N)T}_{\Pi' I} \\ & & & K^{(N)}_{\Delta' I} & K^{(N)}_{\Delta'\Delta'} & \widetilde{K}^{(N)T}_{\Pi'\Delta'} \\ \widetilde{K}^{(1)}_{\Pi' I} & \widetilde{K}^{(1)}_{\Pi'\Delta'} & \cdots & \widetilde{K}^{(N)}_{\Pi' I} & \widetilde{K}^{(N)}_{\Pi'\Delta'} & \widetilde{K}_{\Pi'\Pi'} \end{bmatrix} =: \begin{bmatrix} K_{B'B'} & \widetilde{K}^T_{\Pi' B'} \\ \widetilde{K}_{\Pi' B'} & \widetilde{K}_{\Pi'\Pi'} \end{bmatrix}$$



and the introduction of LM λ yields the system: $\begin{bmatrix} \widetilde{K} & B^T \\ B & O \end{bmatrix} \begin{bmatrix} \widetilde{u} \\ \lambda \end{bmatrix} = \begin{bmatrix} \widetilde{f} \\ 0 \end{bmatrix}$

Unpreconditoned system: after reducing to the Lagrange multipliers:

$$\boxed{F := B\widetilde{K}^{-1}B^T\lambda = B\widetilde{K}^{-1}\widetilde{f} =: d}$$

$$F = \underbrace{B_{B'}K_{B'B'}^{-1}B_{B'}^T}_{\text{local solvers}} + \underbrace{B_{B'}K_{B'B'}^{-1}\widetilde{K}_{B'\Pi'}\widetilde{S}_{\Pi'\Pi'}^{-1}\widetilde{K}_{\Pi'B'}K_{B'B'}^{-1}B_{B'}^T}_{\text{coarse problem; coupled!}}.$$

Dirichlet-Preconditioner: $M_D^{-1} := B_D S B_D^T$ (Sum of local operators!)

1. S: Schur complement of K after elimination of the interior variables
2. B_D: appropriately scaled jump operator on Δ'; scaling depends on coefficients

Standard FETI-DP is PCG solving

$$M_D^{-1}F\lambda = M_D^{-1}d$$

For more details, see, e.g., Farhat et al. (2001), Farhat et al. (2000), Mandel/Tezaur (2001), Klawonn et al. (2002), Klawonn/Widlund (2006), Klawonn/Rheinbach (2007) and the references therein.

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- almost incompressible materials

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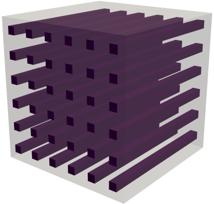

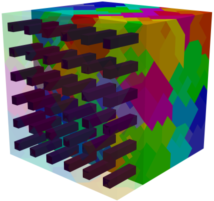

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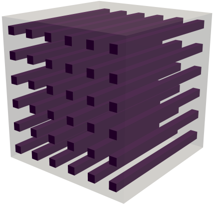
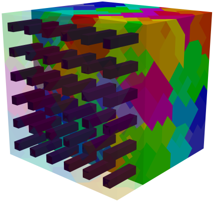


Standard FETI-DP^{*1}

N	$\lvert\Pi'\rvert$	cond	iter	time	$\lVert r^{(i)}\rVert$
216	9,828	2.09e+6	>5000	480s	5.61e-05^{*2}

Table: Compressible linear elasticity of a matrix material with E_1=1 surrounding beams with E_2=1e+6. 1.02e+6 degrees of freedom. $\mathcal{P}_2$ elements.



- $*1$: FETI-DP w/ Dirichlet precond., vertex + edge average coarse space.
- $*2$: relative reduction by a factor of 1e-4 after 5000 iterations.
- N: number of subdomains and cores
- $\lvert\Pi'\rvert$: size of the corresponding nonadaptive (a priori) coarse space.
- cond: condition number of the preconditioned FETI-DP operator.
- iter: number of iterations of the PCG algorithm.
- $\lVert r^{(i)}\rVert$: true residual norm
- time: total runtime (in seconds)

- Solve (local) eigenvalue problems for a priori tolerances (nonexhaustive)

  Our approach Klawonn/Kühn/Rheinbach (2016,2017,2018,2019)

  based on Mandel/Sousedík (2007), Sousedík (2008), Klawonn/Radtke/Rheinbach (2016).

  Related works: Bjørstad/Koster/Krzyzanowski (2001), Bjørstad/Krzyzanowski (2002), Sousedík (2010), Galvis/Efendiev (2010), Nataf/Xiang/Dolean (2010), Nataf/Xiang/Dolean/Spillane (2011), Dolean/Nataf/Scheichl/Spillane (2012), Šístek/Mandel/Sousedík (2012), Sousedík/Šístek/Mandel (2013), Spillane/Rixen (2013), Dohrmann/Pechstein (2013,2017), Jolivet/Hecht/Nataf/Prud'homme (2014), Spillane (2014,2016), Klawonn/Radtke/Rheinbach (2014,2015), Kim/Chung (2015), Gosselet/Rixen/Roux/Spillane (2015), Radtke (2015), Zampini (2016), Gander/Loneland/Rahman (TR2015), Beirão da Veiga/Pavarino/Scacchi/Widlund/Zampini (2017), Calvo/Widlund (2016), Oh/Widlund/Zampini/Dohrmann (2017), Haferssas/Jolivet/Nataf (2017), Kim/Chung/Wang (2017), Heinlein/Klawonn/Knepper/Rheinbach (2018), Bovet/Parret-Fréaud/Spillane/Gosselet (2017), Eikeland/Marcinkowski/Rahman (TR2016), Barrenechea/Bosy/Dolean (2018), Marcinkowski/Rahman (2018), Agullo/Giraud/Poirel (2019), Al Daas/Grigori (2019), ...

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- Enforce constraints based on computed eigenvectors:
  - Implementation I: Optional Lagrange Multipliers or Saddle Point Problems

    (Farhat/Lesoinne/Pierson (2000), Mandel/Dohrmann/Tezaur (2004), Mandel/Sousedík (2007), ...)
  - Implementation II: Deflation and Balancing (FETI-DP only)

    (Nicolaides (1987), Dostál (1988), Nabben/Vuik (2006), Domorádová(Jarošová)/Dostál (2007), Jarošová/Klawonn/Rheinbach (2012), Klawonn/Rheinbach (2012), ...)
  - Implementation III: (Generalized) Transformation-of-Basis approach

    (Klawonn/Widlund (2001,2006), Klawonn/Widlund/Dryja (2002), Li/Widlund (2005), Klawonn/Rheinbach (2006, 2007), ..., Klawonn/Kühn/Rheinbach (TR2017, ETNA 2018))

Define $P_D := B_D^T B$ and $\widetilde{S}$: Schur complement on the interface, coupled in some primal variables.

- Condition number bound for standard FETI-DP with coarse space Π':

$$\boxed{|P_D w|_{\widetilde{S}} \leq C|w|_{\widetilde{S}} \quad \forall w : w \text{ cont. in } \Pi' \quad \Rightarrow \kappa(M_D^{-1}F) \leq C.}$$

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$$\boxed{|P_D w|_{\widetilde{S}} \geq \text{TOL} |w|_{\widetilde{S}}}$$

  to set up second coarse space Π.

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- Attention: P_D and $\widetilde{S}$ are global operators!

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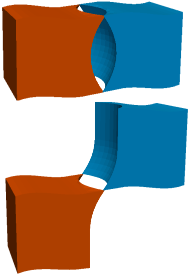


$P_D := B_D^T B$ and $\widetilde{S}$: Schur complement on the interface, coupled in some primal variables.

- Adaptive FETI-DP approach based on the P_D estimate:
  $\mathcal{Z}$ (face or edge of $\{\Omega_i, \Omega_s\}$): $P_{D,\mathcal{Z}}$ and $\widetilde{S}_{is}$: localized P_D and $\widetilde{S}$;
  TOL: a priori tolerance. Use w_{is}^l, $l = 1, 2, \ldots$ with

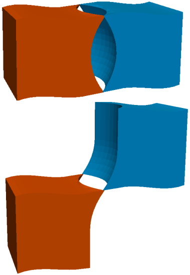
$$\boxed{|P_{D,\mathcal{Z}} w_{is}^l|_{\widetilde{S}_{is}} \geq \text{TOL} |w_{is}^l|_{\widetilde{S}_{is}}}$$

to set up a second coarse space Π

$\rightarrow$ use of a transformation:

continuity in Π means

orthogonality to span$\{w_{is}^l : l = 1, 2, \ldots\}$!



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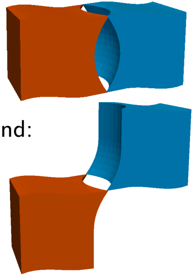


- From local $P_{D,\mathcal{Z}}$ to global P_D to condition number bound:
  For adaptive FETI-DP with coarse space $\Pi' \cup \Pi$:

  $$\boxed{\begin{gathered} |P_D w|_{\widetilde{S}} \leq \text{TOL}\cdot\text{G} |w|_{\widetilde{S}} \quad \forall w \,:\, w \text{ cont. in } \Pi' \cup \Pi \\ \Rightarrow \kappa(M_D^{-1} F) \leq \text{TOL}\cdot\text{G}. \end{gathered}}$$

- local eigenvector constraints $\rightsquigarrow$ global condition number bound
- depending on user-defined TOL, in practice (and geometrical constants, in theory)

Theorem

All vertices primal.

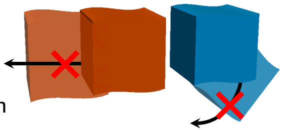
- $N_{\mathcal{F}}$: *maximum number of faces of a subdomain*
- $N_{\mathcal{E}}$: *maximum number of edges of a subdomain*
- $M_{\mathcal{E}}$: *maximum multiplicity of an edge*
- TOL: *user-defined tolerance for solving the local eigenproblems*

FETI-DP with local adaptive constraints enforced by generalized transformation-of-basis approach, satisfies

$$\kappa(\widehat{M}_T^{-1}\widehat{F}) \leq 4\max\{N_{\mathcal{F}}, N_{\mathcal{E}} M_{\mathcal{E}}\}^2 \text{TOL}.$$

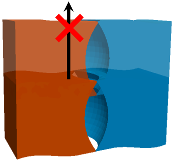
Klawonn/Kühn/Rheinbach (SISC 2016, TR2017, ETNA 2018)

Π_{is}:



- e.g., Ω_i and Ω_s share a face $\mathcal{Z}$
- two projections Π_{is} and $\overline{\Pi}_{is}$ (matrix-free) to remove rigid body modes
- For $\mu_{is}^l \geq$TOL, we solve the generalized eigenvalue problem

$\overline{\Pi}_{is}$:

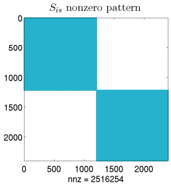


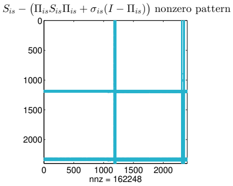
$$\overline{\Pi}_{is}\Pi_{is}P_{D,\mathcal{Z}}^T \begin{bmatrix} S_i & 0 \\ 0 & S_s \end{bmatrix} P_{D,\mathcal{Z}}\Pi_{is}\overline{\Pi}_{is}w_{is}^l$$

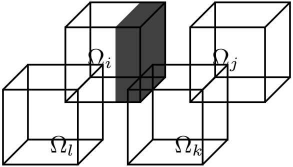
$$= \mu_{is}^l(\overline{\Pi}_{is}(\Pi_{is}\begin{bmatrix} S_i & 0 \\ 0 & S_s \end{bmatrix}\Pi_{is} + \sigma(I - \Pi_{is}))\overline{\Pi}_{is} + \sigma(I - \overline{\Pi}_{is}))w_{is}^l.$$

either on rank i or rank s.

$\rightsquigarrow$ computational overhead and load balance?

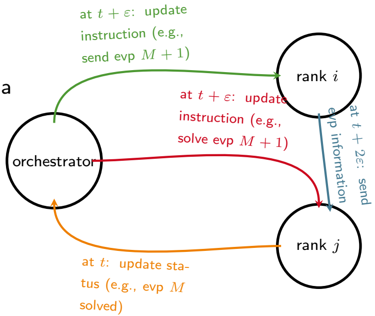


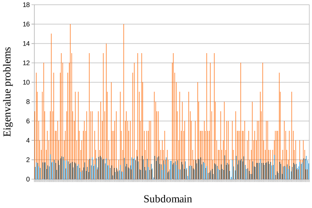


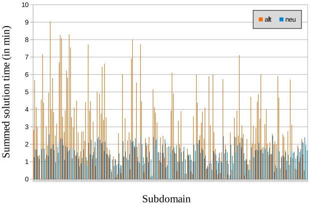


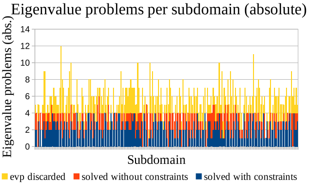
- C/C++, PETSc 3.8.0, and SLEPc 3.8.0
- rough solution of the eigenvalue problems
- only a subset of eigenvalue problems is solved
- for eigenvalue problem setup: **nonblocking** and **point-to-point**, plain MPI (`MPI_IRecv` and `MPI_Isend`) communication
- one **orchestrating rank**
  - **collecting** and **distributing** the eigenvalue problems (i.e., index information) **a priori** (via `MPI_Scatterv` and `MPI_Bcast`)
  - **supervising** the solution process and **redistributing (in runtime!)** the eigenvalue problems (i.e., index information) via **nonblocking** and **point-to-point** communication

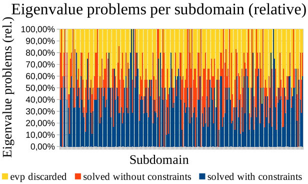
$\rightarrow$ **enhanced load balancing**!

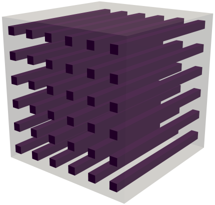


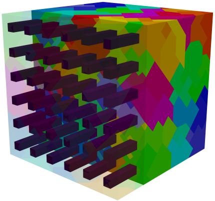

Eigenvalue problems
Subdomain
18
16
14
12
10
8
6
4
2
0


Summed solution time (in min)
Subdomain
alt
neu
10
9
8
7
6
5
4
3
2
1
0


Eigenvalue problems per subdomain (absolute)
Eigenvalue problems (abs.)
Subdomain
14
12
10
8
6
4
2
0
evp discarded
solved without constraints
solved with constraints


Eigenvalue problems per subdomain (relative)
Eigenvalue problems (rel.)
Subdomain
100,00%
90,00%
80,00%
70,00%
60,00%
50,00%
40,00%
30,00%
20,00%
10,00%
0,00%
evp discarded
solved without constraints
solved with constraints





Standard FETI-DP^{*1}

$\lvert\Pi'\rvert$	$\lvert\Pi\rvert$	cond	iter	time	$\lVert r^{(i)}\rVert$
9,828	-	2.09e+6	>5000	480s	5.61e-05^{*2}

Adaptive FETI-DP^{*3}

$\lvert\Pi'\rvert$	$\lvert\Pi\rvert$	cond	iter	time	$\lVert r^{(i)}\rVert$
9,483	4,129	54.85	61	143s	5.35e-09^{*4}

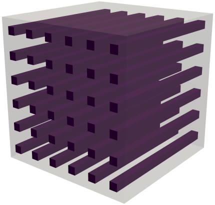
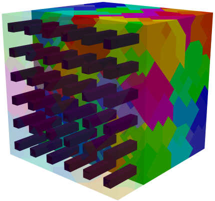


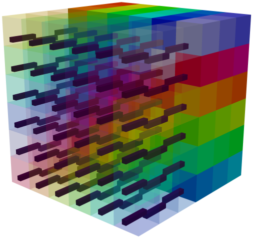
Table: Compressible linear elasticity of a matrix material with E_1=1 surrounding beams with E_2=1e+6. $\mathcal{P}_2$ elements. 216 subdomains and cores, 1.02e+6 degrees of freedom



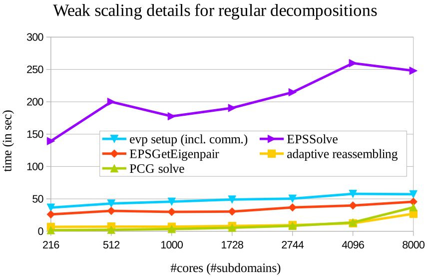
- $*1$: FETI-DP w/ Dirichlet precond., vertex + edge average coarse space.
- $*2$: relative reduction by a factor of 1e-4 after 5000 iterations.
- $*3$: Adaptive FETI-DP (Klawonn/Kühn/Rheinbach (2016-2019)) with single vector KrylovSchur eigensolver
- $*4$: relative reduction by a factor of 1e-8 after 61 iterations.
- $\lvert\Pi'\rvert$: size of the corresponding nonadaptive (a priori) coarse space.
- cond: condition number of the preconditioned FETI-DP operator.
- iter: number of iterations of the PCG algorithm.
- $\lVert r^{(i)}\rVert$: true residual norm
- time: total runtime (in seconds)

Composite material:

- regular decomposition of the unit cube: N subdomains
- zero Dirichlet boundary conditions on the entire boundary
- homogeneous $\nu = 0.3$
- inhomogeneous E $\in \{1, 1e+6\}$ in form of $N^{2/3}$ chopped beams (as illustrated)



Example: $N = 216$
subdomains in different colors
high coefficients $1e + 6$ in dark purple

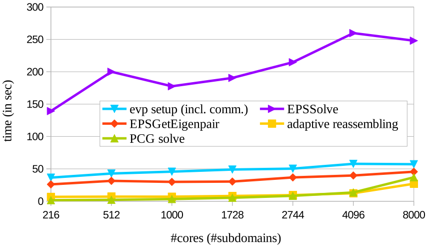

Weak scaling details for regular decompositions
time (in sec)
300
250
200
150
100
50
0
216
512
1000
1728
2744
4096
8000
#cores (#subdomains)
evp setup (incl. comm.)
EPSSolve
EPSGetEigenpair
adaptive reassembling
PCG solve

N (#cores-1)	cond.	iter	$\lvert\Pi'\rvert$	$\lvert\Pi\rvert$	nnz (coarse)	d.o.f.	time	eff.
216	14.02	35	375	1677	2.04e+5	1.17e+6	209s	**100%**
512	20.12	39	1029	4175	5.43e+5	2.74e+6	274s	76%
1000	24.60	43	2187	8551	1.18e+6	5.31e+6	266s	78%
1728	27.91	47	3993	15512	2.25e+6	9.15e+6	283s	74%
2744	30.22	50	6591	25545	3.82e+6	1.45e+7	320s	65%
4096	32.90	52	10125	39173	5.98e+6	2.16e+7	381s	55%
8000	39.39	59	20577	79097	1.24e+7	4.20e+7	409s	51%

Table: Compressible linear elasticity of a matrix material with $E_1=1$ surrounding chopped beams and E_2=1e+6. $\mathcal{P}_2$ elements. Block size 10 for KrylovSchur eigensolver.

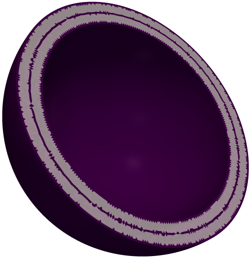
- N (#cores-1): number of subdomains and cores-1
- cond: condition number of the preconditioned FETI-DPo perator.
- iter: number of iterations of the PCG algorithm.
- nnz (coarse): nonzeros in the coarse matrix
- $\lvert\Pi'\rvert$: size of the corresponding nonadaptive (a priori) coarse space
- $\lvert\Pi\rvert$: size of the corresponding adaptive (a posteriori) coarse space
- d.o.f.: total number of degrees of freedom
- time: total runtime (in seconds)
- eff: efficiency of the algorithm

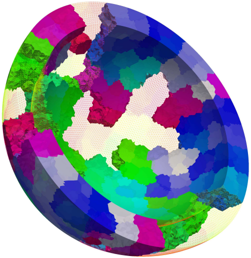
Weak scaling details for regular decompositions



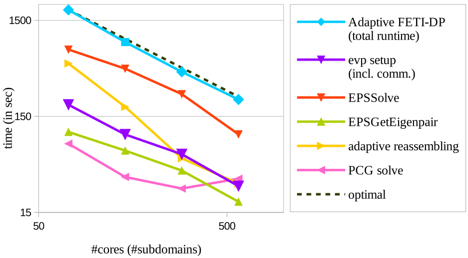
Composite material:

- hemisphere
- unstructured mesh
- zero Dirichlet boundary conditions on the upper part
- zero Neumann boundary conditions elsewhere
- homogeneous $\nu = 0.3$
- inhomogeneous E $\in\{1,1e+6\}$ in form of layers (as illustrated)
- 2.6 million degrees of freedom





Strong scaling behavior of adaptive FETI-DP and essential code parts

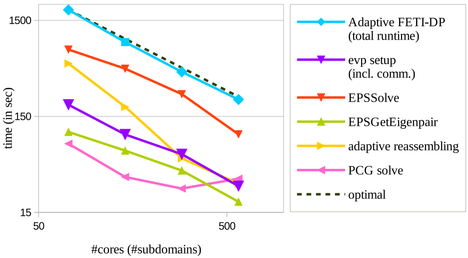


N (#cores-1)	cond.	iter	$\|\Pi'\|$	$\|\Pi\|$	nnz (coarse)	time	eff.
72	109.21	89	1248	4733	2.97e+6	1925s	**100%**
144	80.62	80	3003	9392	6.46e+6	890s	108%
288	77.20	81	9843	13704	1.33e+7	436s	110%
576	72.02	74	24033	16251	2.17e+7	224s	107%

Table: Compressible linear elasticity on a hemisphere; a soft material with E_1=1 in layers with a stiff material with E_2=1e+6. $\mathcal{P}_2$ elements. 2.6 million degrees of freedom. Single vector KrylovSchur eigensolver.

- N (#cores-1): number of subdomains and cores-1
- cond: condition number of the preconditioned FETI-DP operator.
- iter: number of iterations of the PCG algorithm.
- nnz (coarse): nonzeros in the coarse matrix
- $|\Pi'|$: size of the corresponding nonadaptive (a priori) coarse space
- $|\Pi|$: size of the corresponding adaptive (a posteriori) coarse space
- time: total runtime (in seconds)
- eff: efficiency of the algorithm

Strong scaling behavior of adaptive FETI-DP and essential code parts



ν	cond.	iter	$\lvert\Pi' \cup \Pi\rvert$
0.45	**6.52**	27	4085
0.499	**7.34**	30	4736
0.49999	**6.81**	28	4909
0.4999999	**6.81**	28	4913
0.499999999	**6.81**	28	4913

Table: Almost incompressible linear elasticity of a homogeneous cubic material with E=1 and ν as given, decomposed into 64 subdomains. $\mathcal{Q}_2\mathcal{P}_0$ elements.

- ν: Poisson ratio
- cond: condition number of the preconditioned FETI-DP operator.
- iter: number of iterations of the PCG algorithm.
- $\lvert\Pi' \cup \Pi\rvert$: size of the corresponding coarse space

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Thank you for your kind attention!

- Parallel results:
  A. Klawonn, M. J. Kühn, O. Rheinbach
  "Parallel adaptive FETI-DP using
  lightweight asynchronous dynamic load balancing"
  Technical Report: CDS-TR-2019-7

- Theoretical details:
  A. Klawonn, M. Kühn, O. Rheinbach
  "Adaptive Coarse Spaces for FETI-DP in Three Dimensions"
  SIAM J. Sci. Comput., Vol. 38(5), pp. A2880–A2911.