FreeFEM, PETSc, SLEPc, and HPDDM

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`https://joliv.et/FF_16th.pdf`

FreeFEM days, 16th edition

Introduction

1. Introduction
2. Using PETSc
3. How to make my code go faster?
4. Advanced functionalities
5. Domain decomposition methods
6. Conclusion

Introduction

Basic sequential functionalities

Domain specific language for FE

- mesh structure
- associated finite element spaces
- vector and matrix assemblies
- algebraic operations

Interface to other libraries

- installed by PETSc (`make petsc-slepc`)
  - MPICH (if no other MPI implementation)
  - CMake (if unavailable)
  - Bison
  - BLAS (if unavailable)
  - MUMPS (if Fortran available)
  - SuperLU_DIST (if Fortran unavailable)
  - SuperLU
  - SuiteSparse
  - *hypre*
  - [Par]METIS
  - SCOTCH
  - TetGen
  - SLEPc
  - HPDDM (if shared libraries available)
  - ARPACK (if Fortran available)
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  - Htool

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$\Longrightarrow$ sequential or parallel (with FreeFem++-mpi)

Using PETSc

Application Codes

Higher-Level Libraries and Frameworks

PETSc

TS Time Steppers
- Pseudo-Transient, Runge-Kutta, IMEX, SSP, ...
- Local and Global Error Estimators
- Adaptive Timestepping
- Event Handling
- Sensitivity via Adjoints
- ...

TAO Optimization Solvers
- PDE-Constrained
- Adjoint-Based
- Derivative-Free
- Levenberg-Marquardt
- Newton's Method
- Interior Point Methods
- ...

SNES Nonlinear Solvers
- Newton Linesearch
- Newton Trust Region
- BFGS (Quasi-Newton)
- Nonlinear Gauss-Seidel
- Successive Substitution
- Nonlinear CG
- Active Set VI
- ...

KSP Linear Solvers
- CG, GMRES, BiCGStab, FGMRES, ...
- Pipelined Krylov Methods
- Hierarchical Krylov Methods
- ...

DM Domain Management
- DMDA Regular Grids
- DMPlex Unstructured Meshes
- DMForest Forest-of-octrees AMR
- DMStag Staggered Grids
- DMNetwork Networks
- DMSwarm Particles

PC Preconditioners
- ILU/ICC
- Additive Schwarz
- Fieldsplit (Block Preconditioners)
- PCMG (Geometric Multigrid)
- GAMG (Algebraic Multigrid)
- ...

Vec Vectors

IS Index Sets

Mat Linear Operators
- AIJ (Compressed Sparse Row)
- SAIJ (Symmetric)
- BAIJ (Blocked)
- Dense
- GPU Matrices
- ...

PetscSF Parallel Communication

SLEPc Eigensolvers

Communication and Computational Kernels

MPI | BLAS/LAPACK | Kokkos | CUDA | . . .

Specific type

- `Mat` instead of `matrix`
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- `ObjectView` or `MatLoad`

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- `set(sparams = "...")` to fine-tune solvers
- `ObjectView` or `MatLoad`
- single exposed type but many implementations
  - `MatAIJ`
  - `MatSBAIJ`
  - `MatHtool`
  - `MatNest`
  - `MatShell`
  - `MatDense`
  - `MatComposite`
  - `MatIS`
  - `MatTranspose`

How to make my code go faster?

Going parallel

- no shared-memory parallelism
- distributed-memory paradigm (MPI)

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- no shared-memory parallelism
- distributed-memory paradigm (MPI)
- not fully transparent to users
- lightweight macros for workload distribution

Finite elements in parallel

Distributed-memory (MPI)

- local address space
- distribute data efficiently to minimize communication
- orthogonal to shared-memory parallelism (OpenMP)

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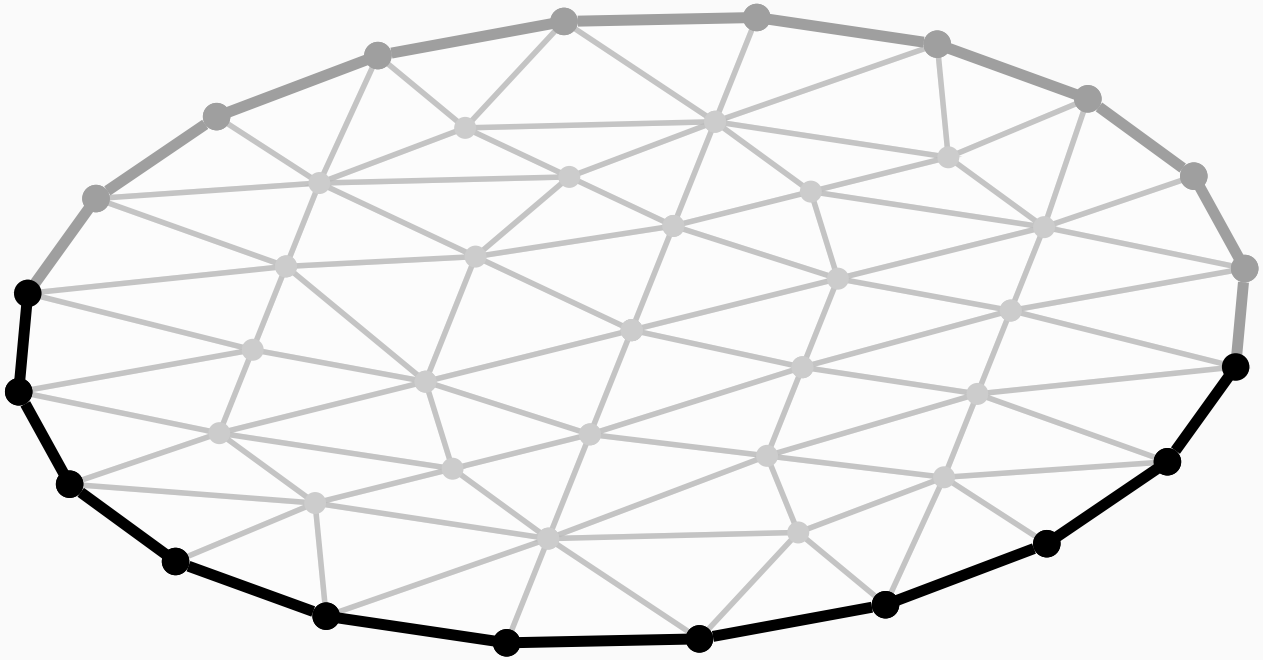

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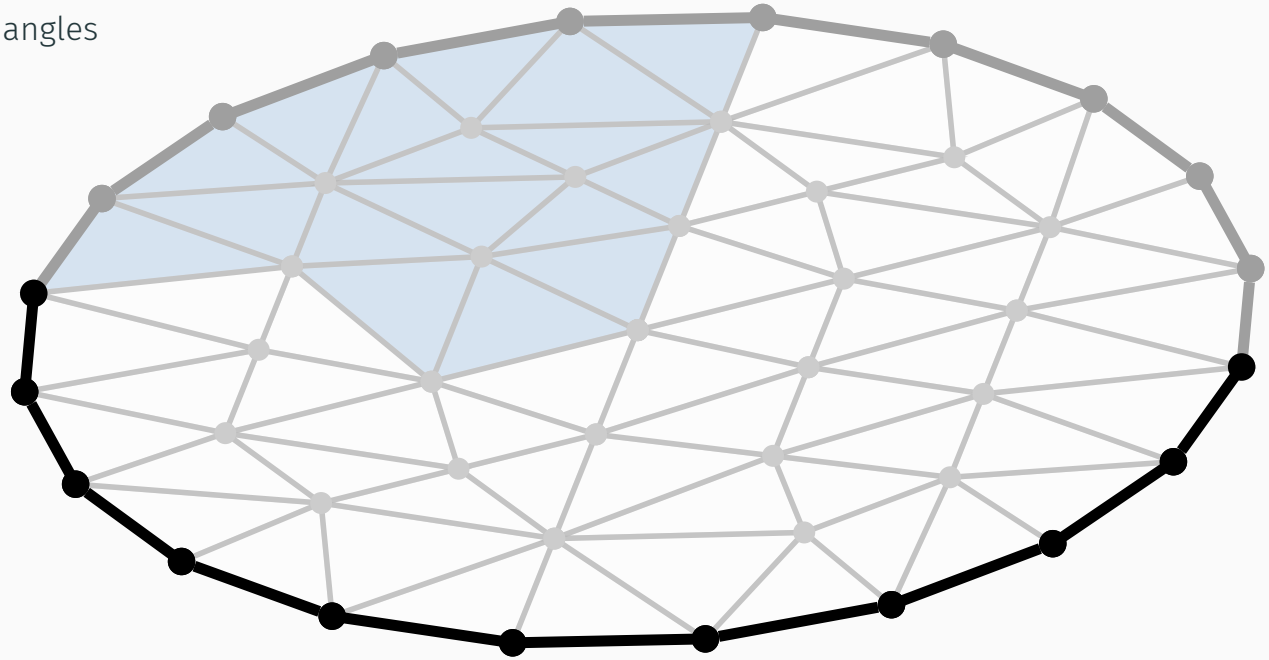
Subdomain #1: 17 triangles



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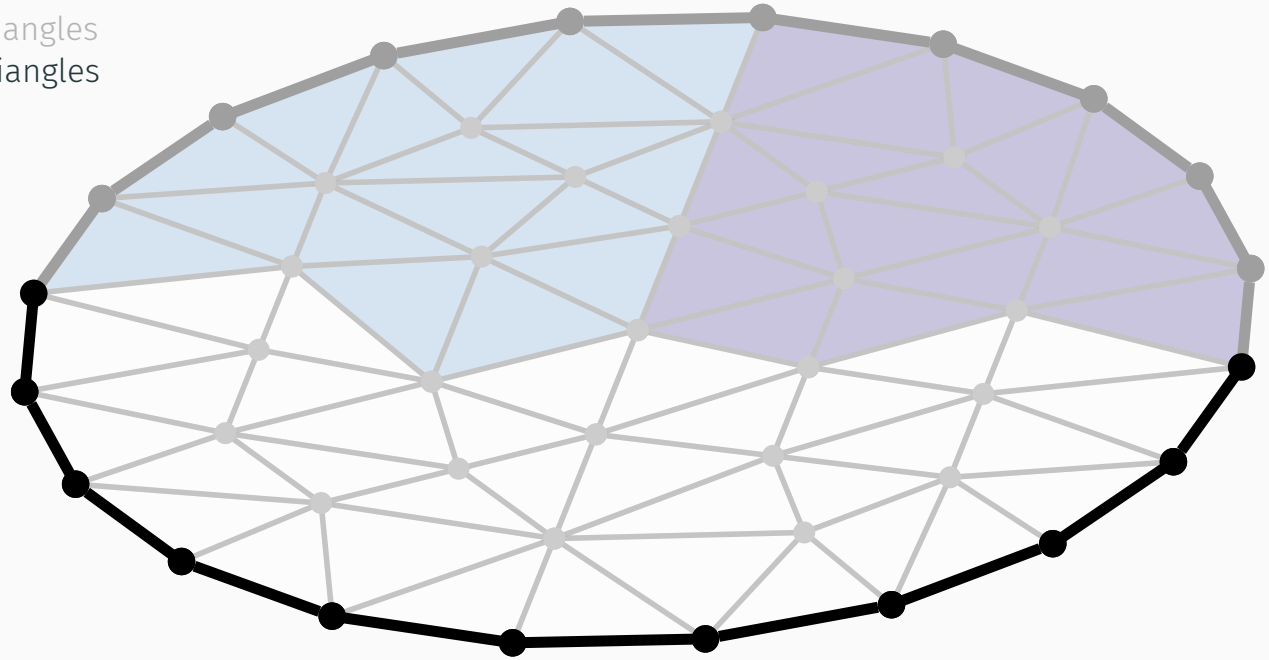

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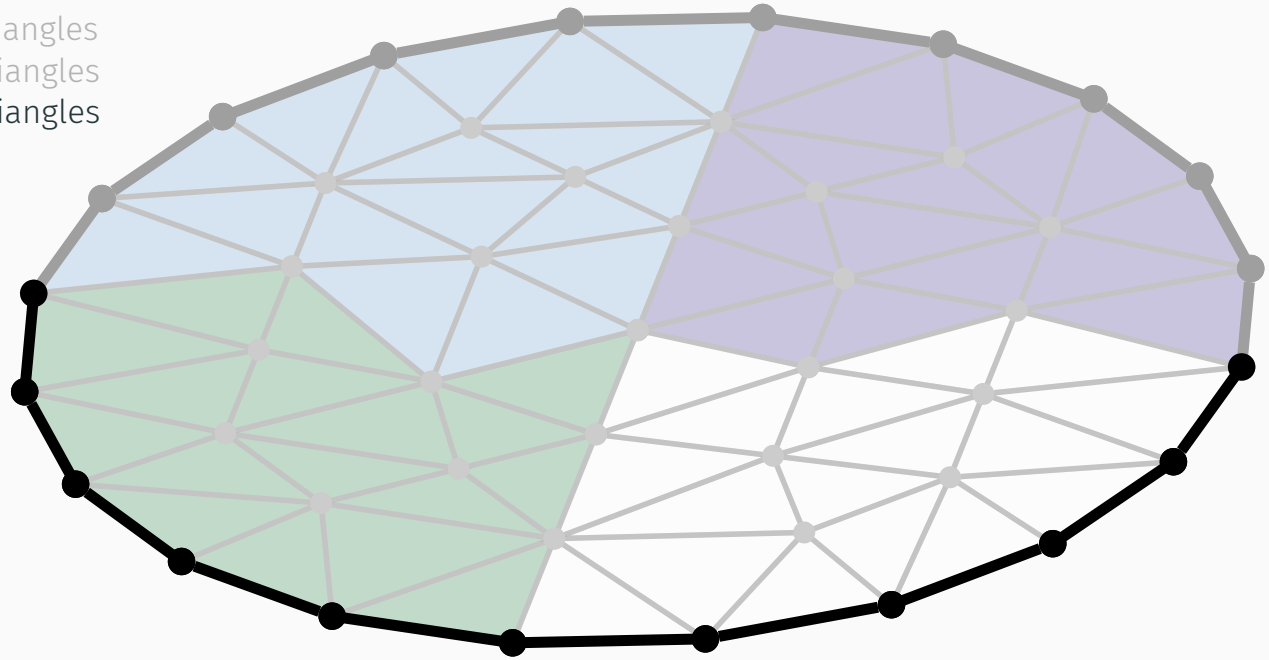

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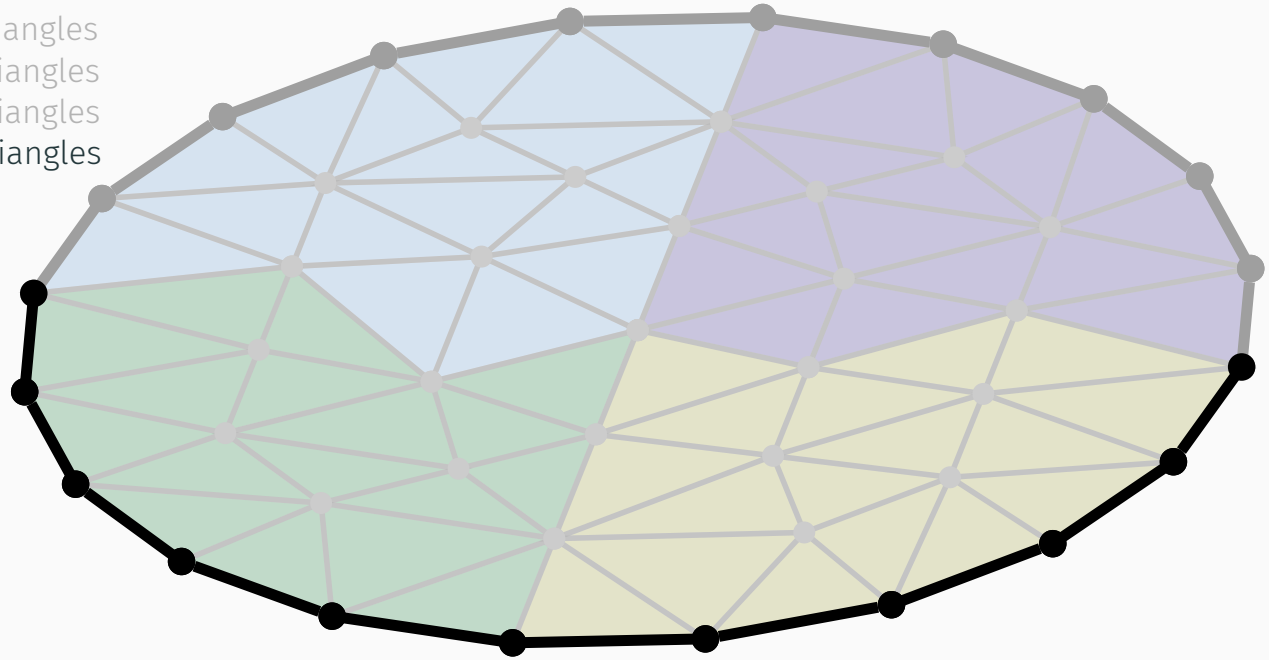

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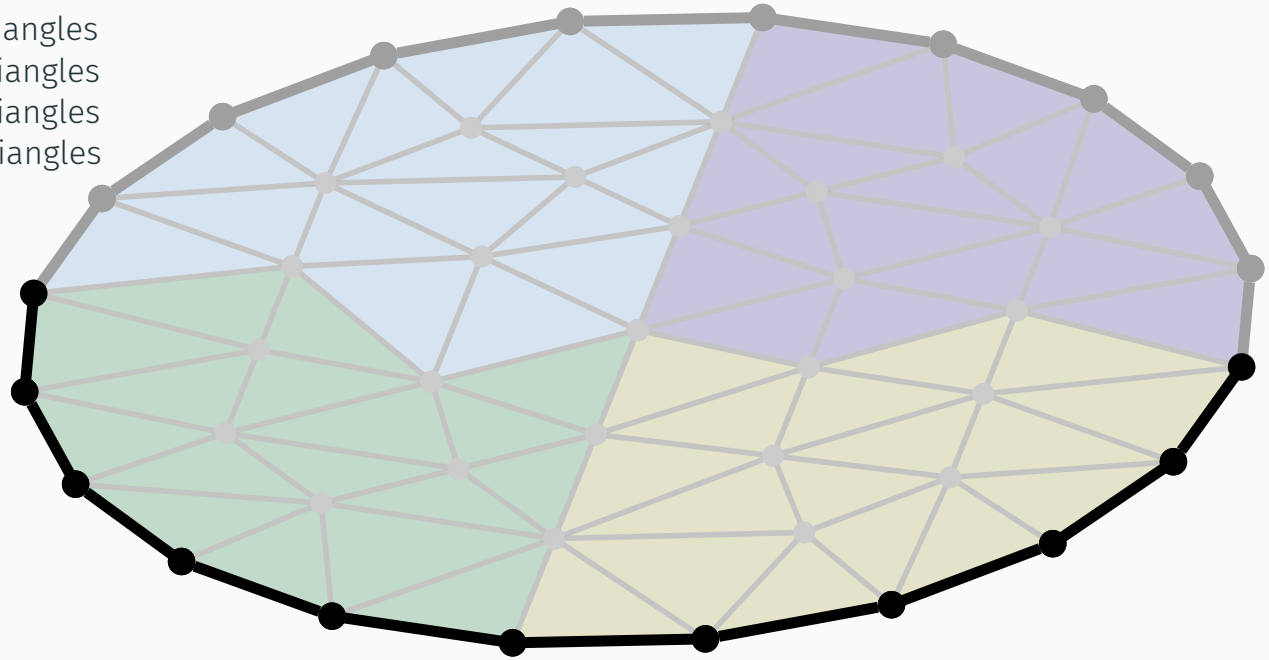


The end of the story?

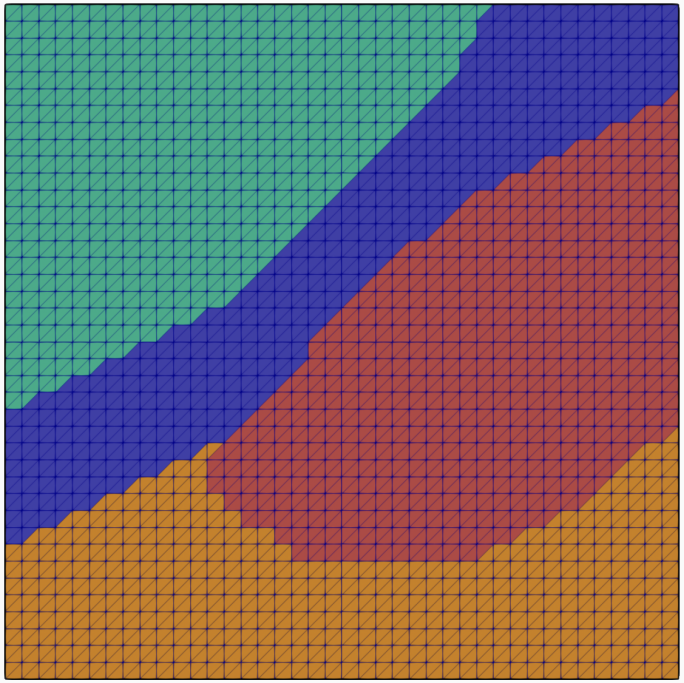
- assemblies are now easy to parallelize

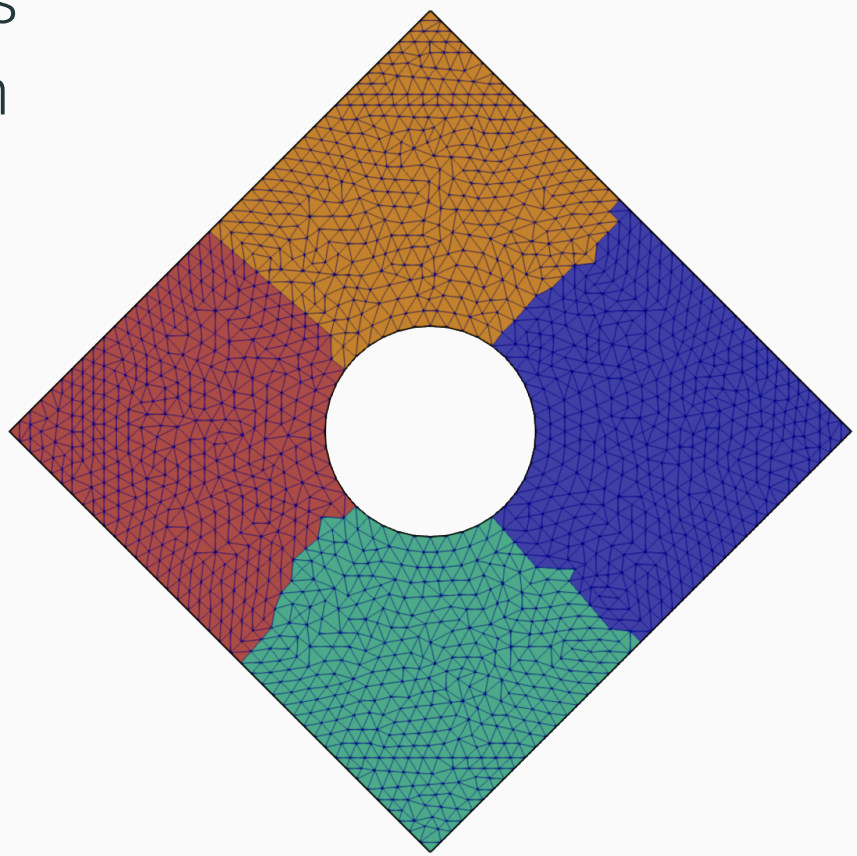
The end of the story?

- assemblies are now easy to parallelize
- many algorithms are still challenging
  - distance to a level-set
  - unstructured adaptive mesh refinement
  - nonlinear and linear solvers

Another example: interpolation

- different meshes
- different basis functions
- different decomposition





Small snippet of macro_ddm.idp

- DmeshSave
- DmeshLoad
- DmeshCreate
- MatCreate
- VecInterpolate
- MatInterpolate

Small snippet of macro_ddm.idp

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- examples, see examples/hpddm/README.md
- functionalities, see CHANGELOG.md
- https://joliv.et/FreeFem-tutorial

Advanced functionalities

Nonstandard eigensolvers

- nonlinear $T(\lambda)x = 0 \implies$ `NEPSolve`
- polynomial $\left(\sum_{i=0}^{N} \lambda^i A_i\right)x = 0, N \geqslant 2 \implies$ `PEPSolve`
- SVD $Av = \sigma u \implies$ `SVDSolve`
- more in [Roman et al., 2023]

Array of PETSc matrices

As easy as FreeFEM matrices: `Mat[int] A(N)`

Easier use of shells for preconditioners

Oseen equations: $A = \begin{bmatrix} F & B \\ B^T & C \end{bmatrix} \Longrightarrow$

```
Mat A = [[F , B],
         [B', C]]
```

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```
Mat A = [[F , B],
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```

```
Mat Object: 4 MPI processes
 type: nest
 rows=37507, cols=37507
  Matrix object:
   type=nest, rows=2, cols=2
   MatNest structure:
   (0,0) : prefix="fieldsplit_0_", type=mpiaij...
   (0,1) : type=mpiaij, rows=33282, cols=4225
   (1,0) : type=transpose, rows=4225, cols=33282
   (1,1) : prefix="fieldsplit_1_", type=mpiaij...
```

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```
Mat A = [[F , B],
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Triangular preconditioner: $\tilde{A} = \begin{bmatrix} \tilde{F} & B \\ 0 & \tilde{S} \end{bmatrix}$ with $\tilde{S}^{-1} \approx -M_p^{-1} F_p L_p^{-1}$

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```
func real[int] PCD(real[int]& in) {
    real[int] out(in.n);
    KSPSolve(Lp,in,in); MatMult(Fp,in,out);
    KSPSolve(Mp,out,out); out *= -1.0;
    return out; // = -Mp \ Fp * Lp \ in
}
set(C, parent = A, precon = PCD,
       sparams = "-fieldsplit_1_pc_type shell");
```

FEM-BEM coupling

Solve the generalized eigenvalue problem for (u, λ):

$$\begin{bmatrix} A_k & D'_k - \frac{1}{2}M^{\mathrm{tr}} \\ M^{\mathrm{tr}} & -S_k \end{bmatrix} u = \lambda \begin{bmatrix} M & 0 \\ 0 & 0 \end{bmatrix} u$$

```
Mat<complex> C;
Sk *= -1.0;
C = [[Ak , R*TDkM]
     [F2B, Sk    ]];
```

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ObjectView(C);
```

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Mat Object: 4 MPI processes
  type=nest, rows=2, cols=2
  MatNest structure:
  (0,0) : type=mpiaij, rows=10410, cols=10410
  (0,1) : type=composite, rows=10410, cols=...
  (1,0) : type=mpiaij, rows=1156, cols=10410
  (1,1) : type=htool, rows=1156, cols=1156
```

More economical MatNest

- support for dense blocks `real[int, int] d`
- pay the (memory) price twice with

```
matrix A = [[a,  d],
            [d', 0]]
```

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```
matrix A = [[a,  d],
            [d', 0]]
```

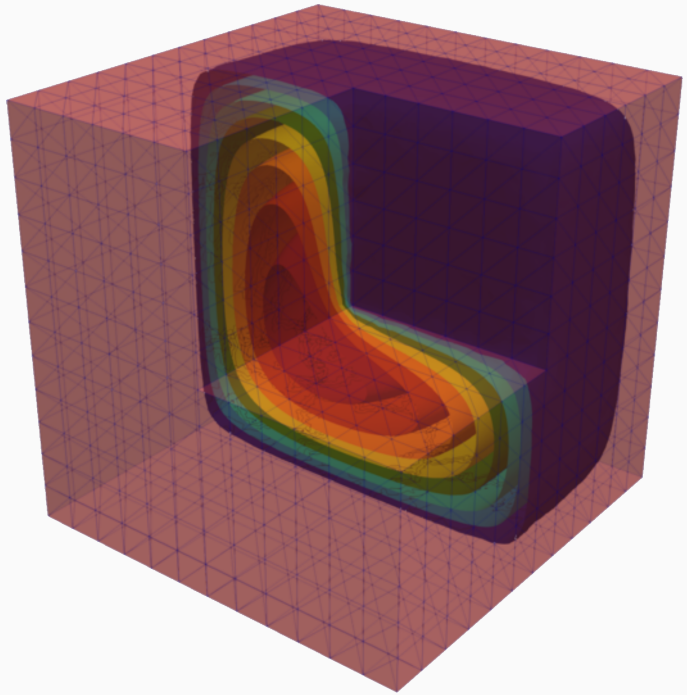
- no such overhead with

```
Mat B = [[b,  d],
         [d', 0]]
```

- the action of the transpose is computed implicitly
- `MATSOLVERMUMPS` handles `MatNest` since 3.20

Parallel mesh adaptation

- Poisson equation on the Fischera corner
- algebraic system solved with GAMG
- 128 MPI processes of Irène@TGCC



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Iteration	#2
# of tetrahedra	47k
ParMmg (sec)	2.6
transfer (sec)	2.8
GAMG (sec)	0.2

Parallel mesh adaptation

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Iteration	#2	#3
# of tetrahedra	47k	91k
ParMmg (sec)	2.6	4.9
transfer (sec)	2.8	1.9
GAMG (sec)	0.2	0.2

Parallel mesh adaptation

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Iteration	#2	#3	#4
# of tetrahedra	47k	91k	221k
ParMmg (sec)	2.6	4.9	16.2
transfer (sec)	2.8	1.9	1.4
GAMG (sec)	0.2	0.2	0.5

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Iteration	#2	#3	#4	#5
# of tetrahedra	47k	91k	221k	686k
ParMmg (sec)	2.6	4.9	16.2	22.0
transfer (sec)	2.8	1.9	1.4	1.5
GAMG (sec)	0.2	0.2	0.5	0.6

Parallel mesh adaptation

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Iteration	#2	#3	#4	#5	#6
# of tetrahedra	47k	91k	221k	686k	2.2M
ParMmg (sec)	2.6	4.9	16.2	22.0	49.9
transfer (sec)	2.8	1.9	1.4	1.5	2.7
GAMG (sec)	0.2	0.2	0.5	0.6	0.9

Parallel mesh adaptation

- Poisson equation on the Fischera corner
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Iteration	#2	#3	#4	#5	#6	#7
# of tetrahedra	47k	91k	221k	686k	2.2M	7M
ParMmg (sec)	2.6	4.9	16.2	22.0	49.9	211
transfer (sec)	2.8	1.9	1.4	1.5	2.7	11.5
GAMG (sec)	0.2	0.2	0.5	0.6	0.9	2.8

Parallel mesh adaptation

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Iteration	#2	#3	#4	#5	#6	#7	#8
# of tetrahedra	47k	91k	221k	686k	2.2M	7M	22M
ParMmg (sec)	2.6	4.9	16.2	22.0	49.9	211	180
transfer (sec)	2.8	1.9	1.4	1.5	2.7	11.5	66
GAMG (sec)	0.2	0.2	0.5	0.6	0.9	2.8	4.2

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Iteration	#2	#3	#4	#5	#6	#7	#8	#9
# of tetrahedra	47k	91k	221k	686k	2.2M	7M	22M	62M
ParMmg (sec)	2.6	4.9	16.2	22.0	49.9	211	180	299
transfer (sec)	2.8	1.9	1.4	1.5	2.7	11.5	66	87
GAMG (sec)	0.2	0.2	0.5	0.6	0.9	2.8	4.2	6.0

Parallel mesh adaptation

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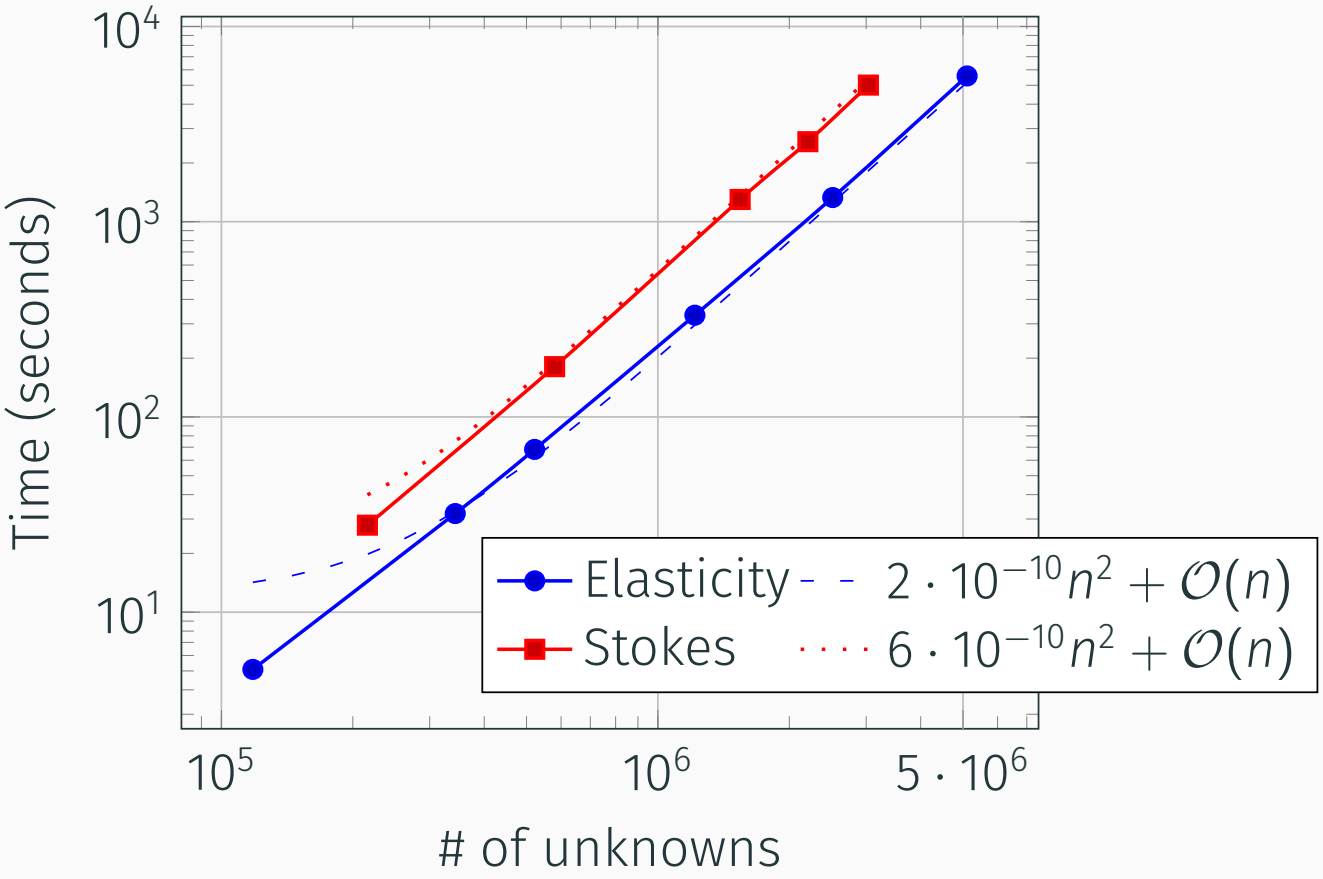
Iteration	#2	#3	#4	#5	#6	#7	#8	#9	#10
# of tetrahedra	47k	91k	221k	686k	2.2M	7M	22M	62M	170M
ParMmg (sec)	2.6	4.9	16.2	22.0	49.9	211	180	299	697
transfer (sec)	2.8	1.9	1.4	1.5	2.7	11.5	66	87	297
GAMG (sec)	0.2	0.2	0.5	0.6	0.9	2.8	4.2	6.0	—

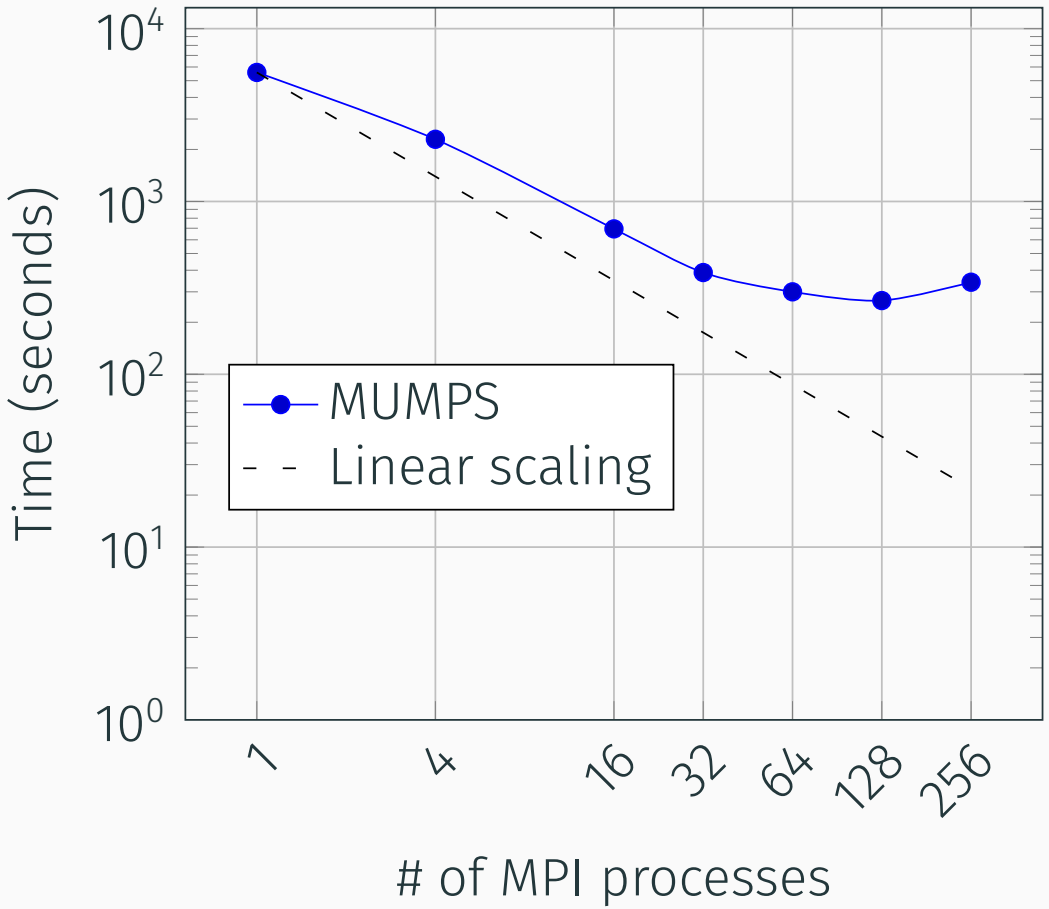
Domain decomposition methods

Complexity study of exact factorization

- 3D problems, lowest-order FE
- sequential, double-precision, exact LDL^T factorization
- `https://mumps-solver.org`



Scalability for the largest (elasticity) problem



- extremely robust solver
- difficult to reach ideal efficiency

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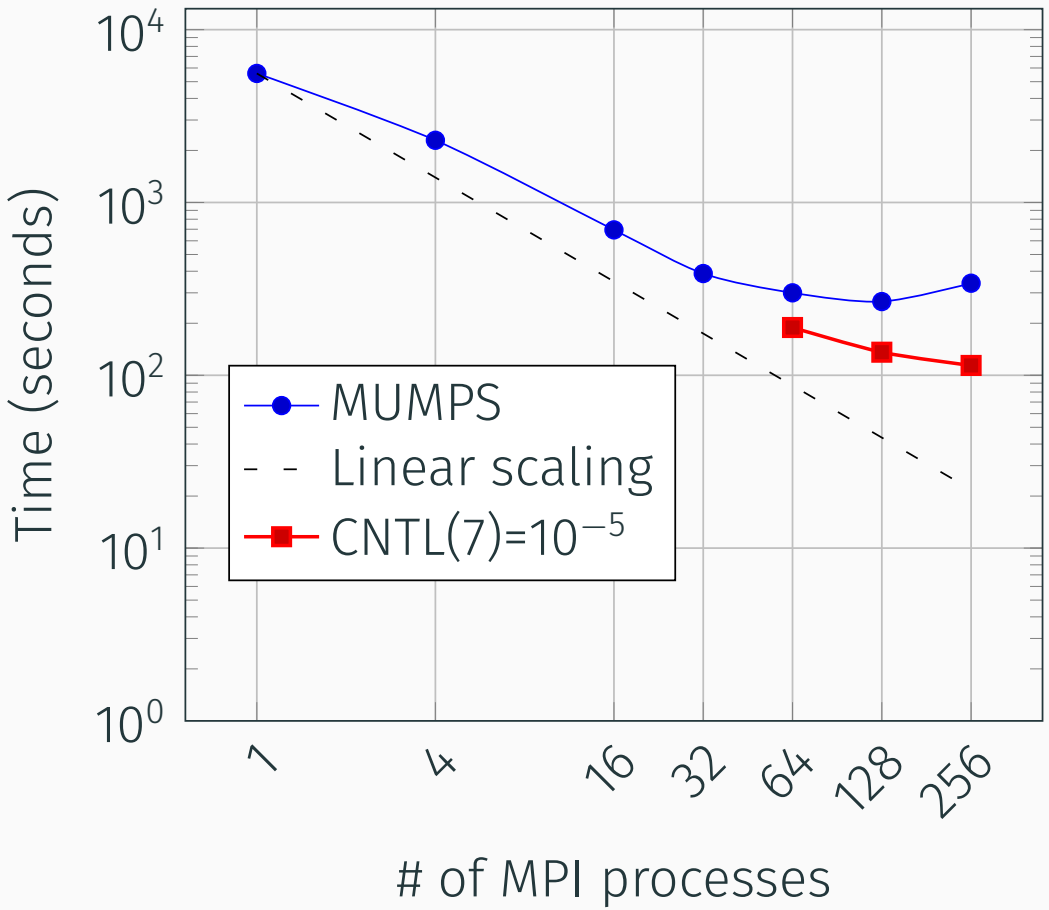
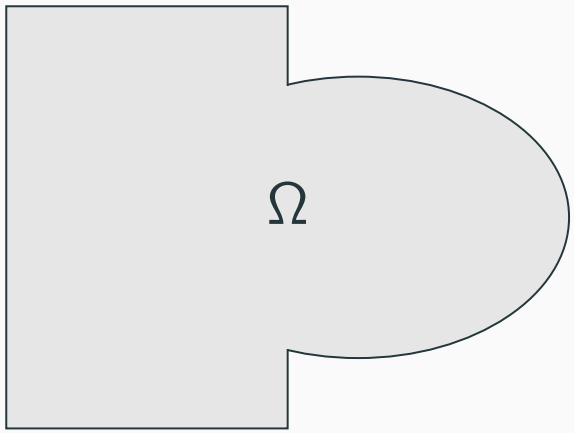


- extremely robust solver
- difficult to reach ideal efficiency
- FGMRES with a 10^{-5} tolerance, 15 iterations

Overlapping Schwarz methods

Consider the linear system: $Ax = b \in \mathbb{K}^n$



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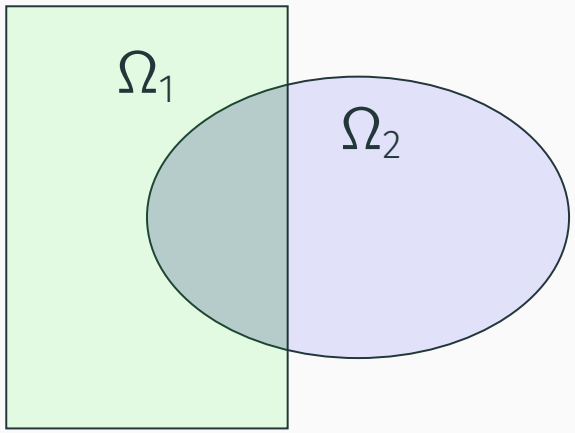
Two-way decomposition of $[\![1; n]\!]$ and restriction operators



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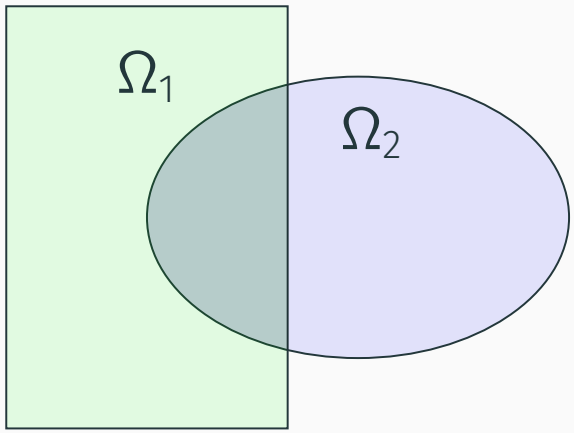
$$M_{\text{ASM}}^{-1} = \sum_{i=1}^{N=2} R_i^T (R_i A R_i^T)^{-1} R_i$$



[Schwarz, 1870]

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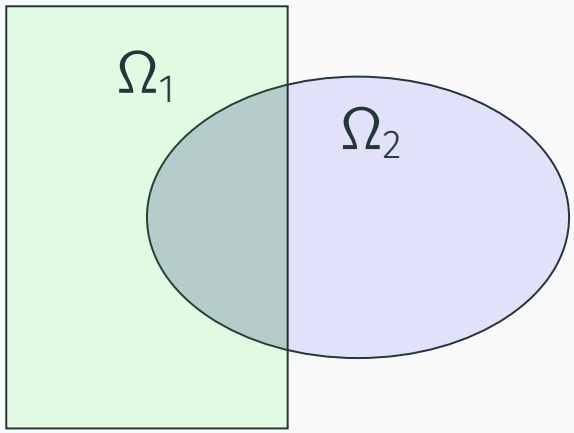
$$M_{\text{RAS}}^{-1} = \sum_{i=1}^{N=2} \tilde{R}_i^T (R_i A R_i^T)^{-1} R_i$$



[Schwarz, 1870] [Cai and Sarkis, 1999]

Overlapping Schwarz methods

Consider the linear system: $Ax = b \in \mathbb{K}^n$

Two-way decomposition of $[\![1; n]\!]$ and restriction operators

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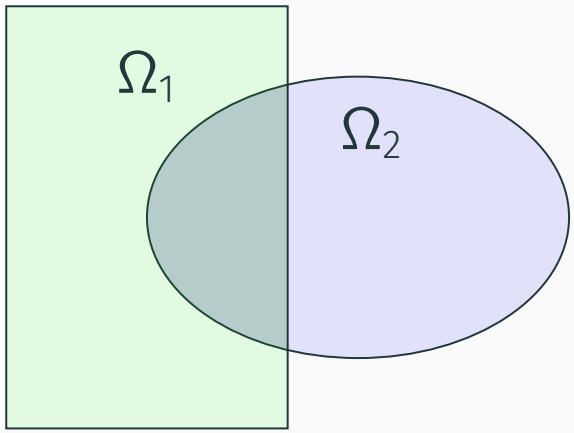

[Schwarz, 1870] [Cai and Sarkis, 1999]

$\rightarrow$ no guaranteed scalability for large N

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How to choose γ_i and $\{\Lambda_j\}_{j=1,\ldots,\gamma_i}$?

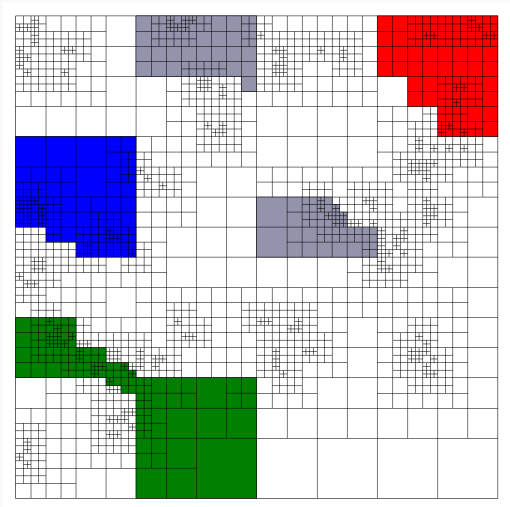
- aggressive coarsening
- capturing the “difficulties” of A
- at a moderate cost

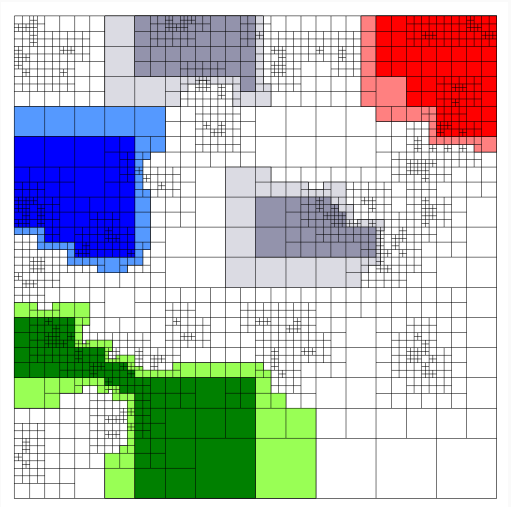
HPDDM

- specific implementation [Jolivet, Hecht, Nataf, et al., 2013]

HPDDM + PETSc

- specific implementation [Jolivet, Hecht, Nataf, et al., 2013]
- interfaced in PETSc [Jolivet, Roman, and Zampini, 2021]
  - user-provided N_i (`PCHPDDMSetAuxiliaryMat`)
  - automatically assembled on `DMPlex`





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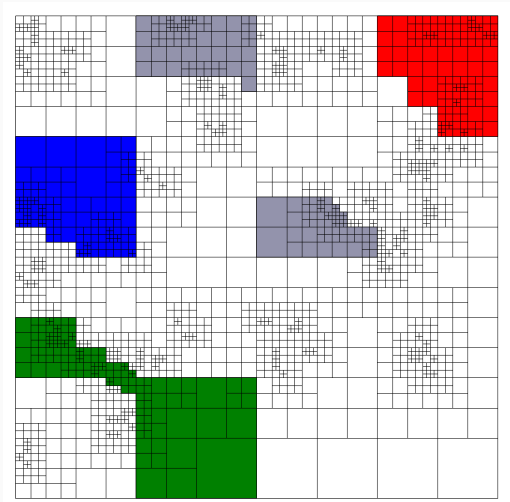
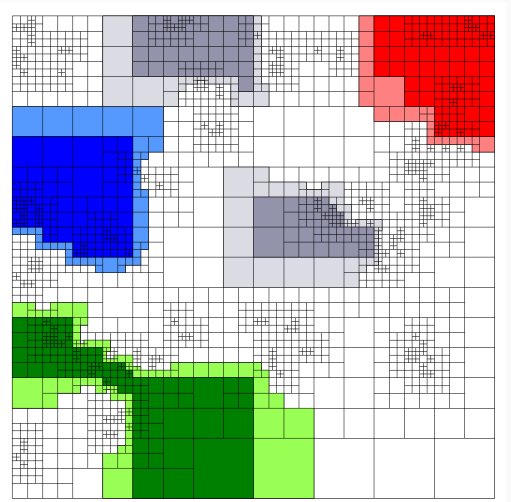
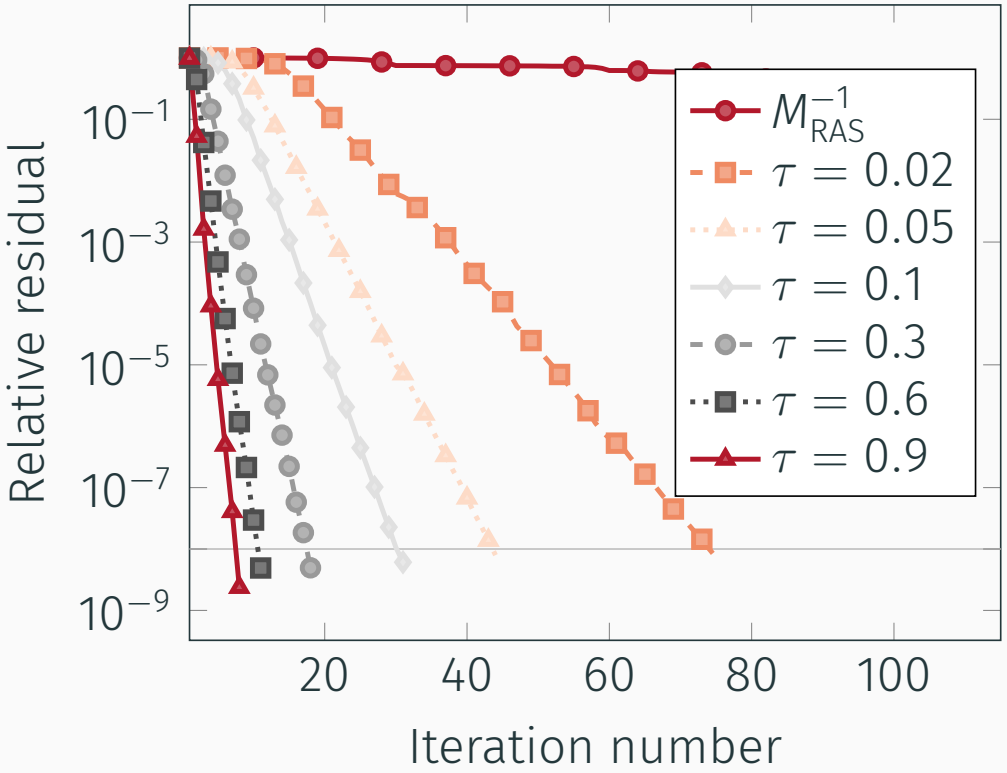




$\rightarrow$ leveraging the flexibility of PETSc for algebraic variants

Adaptive preconditioning for general systems

G3_circuit from SSMC on
256 processes [Al Daas, Jolivet, and Rees, 2023]



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0.02	739	75
0.05	1,831	44
0.1	3,608	31
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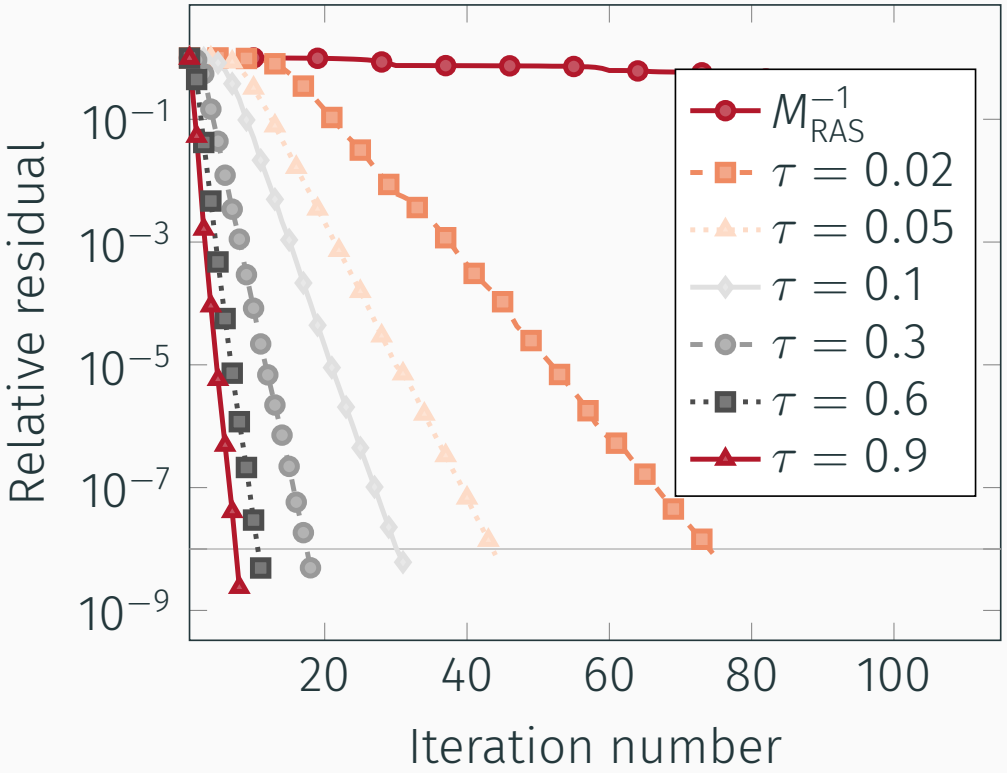

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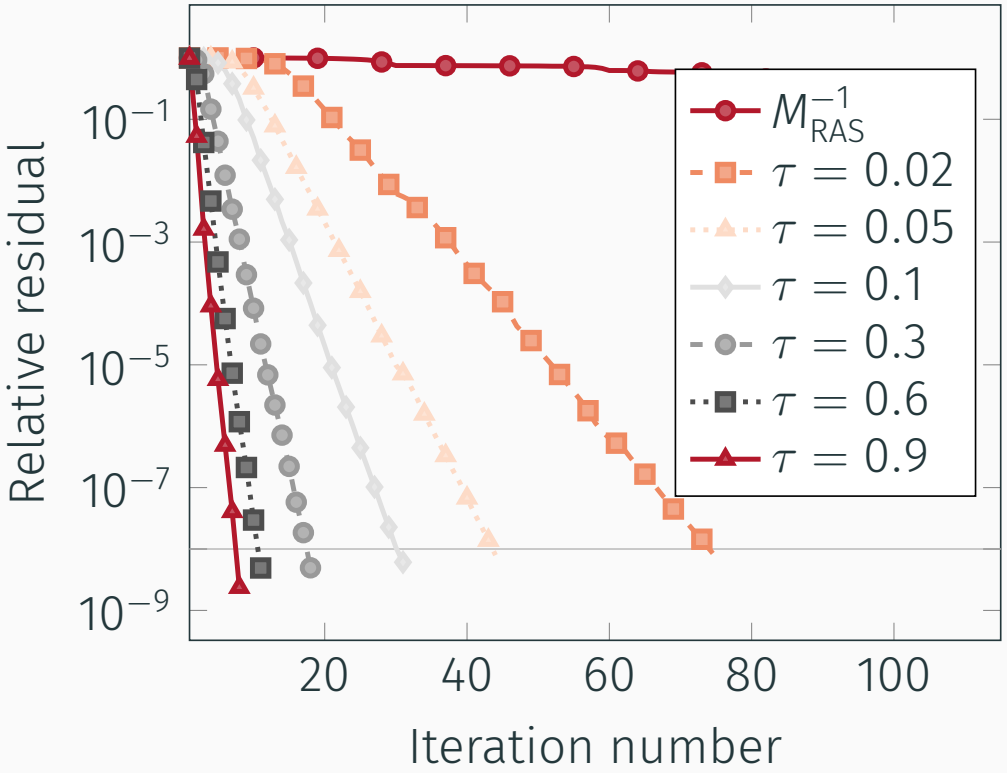

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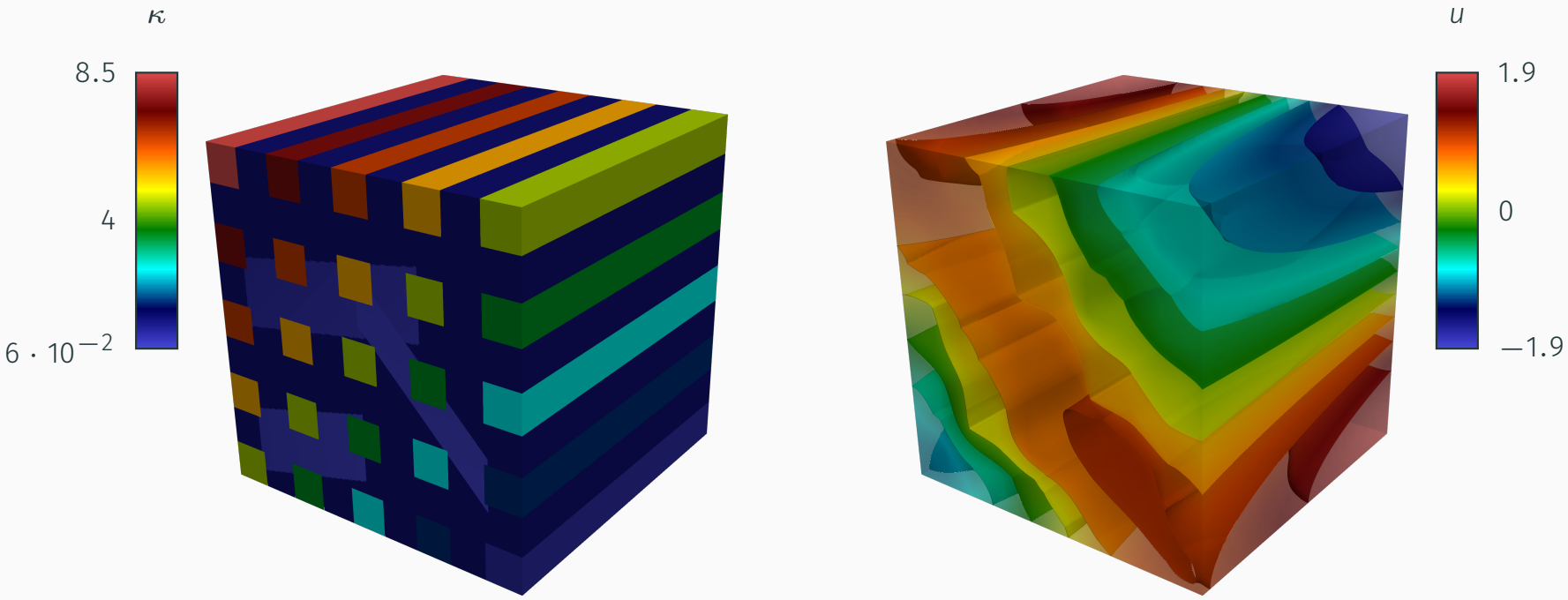
Chevron4	5	†	†
consph	93	†	†
nxp1	20	†	†

Nonlinear problem

- automatic assembly of Neumann matrices in FreeFEM
- Newton method using SNES [Brune et al., 2015]

$$-\nabla \cdot (\kappa \nabla u) - 6.2e^{u} = 0$$



(a) Coefficient distribution (b) Isosurfaces of the solution

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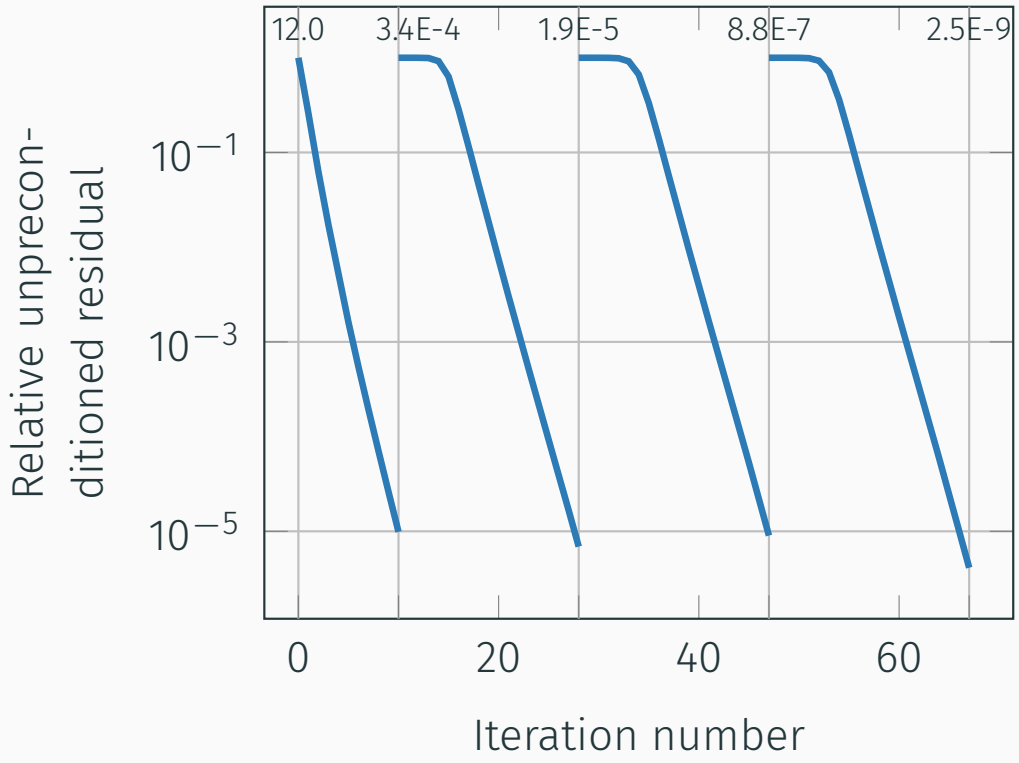

Recent extensions to saddle-point problems

$$Ax = \begin{bmatrix} A_{00} & A_{01} \\ A_{10} & A_{11} \end{bmatrix} \begin{bmatrix} x_0 \\ x_1 \end{bmatrix} = \begin{bmatrix} b_0 \\ b_1 \end{bmatrix}$$

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- apply HPDDM on the top-left block: $A_{00}^{-1} \approx M_{00,\text{deflated}}^{-1}$

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```
-prefix_push fieldsplit_1_
    -pc_type hpddm
    -pc_hpddm_schur_precondition geneo
-prefix_pop
```

- more at `stokes-block-hpddm-2d-PETSc.edp`

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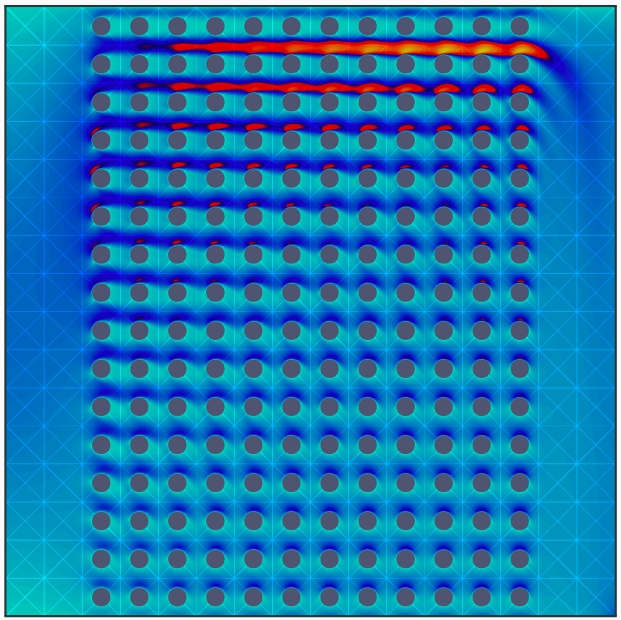
- 10^{-10} outer tolerance, 100M d.o.f., 1k MPI processes



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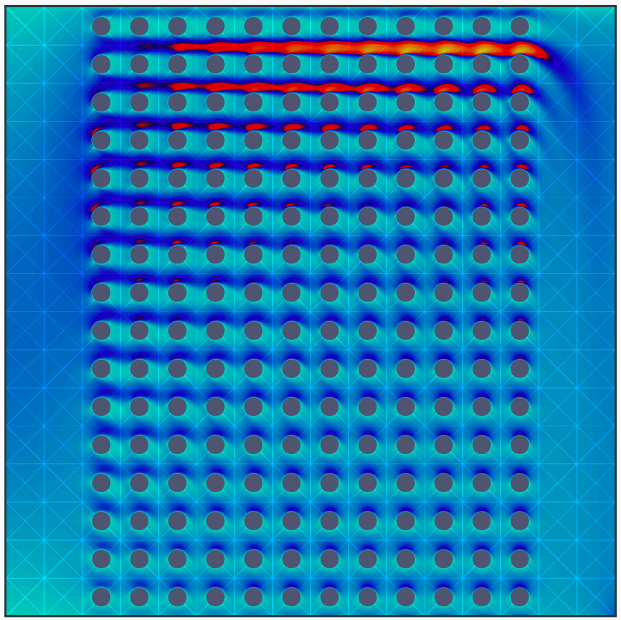

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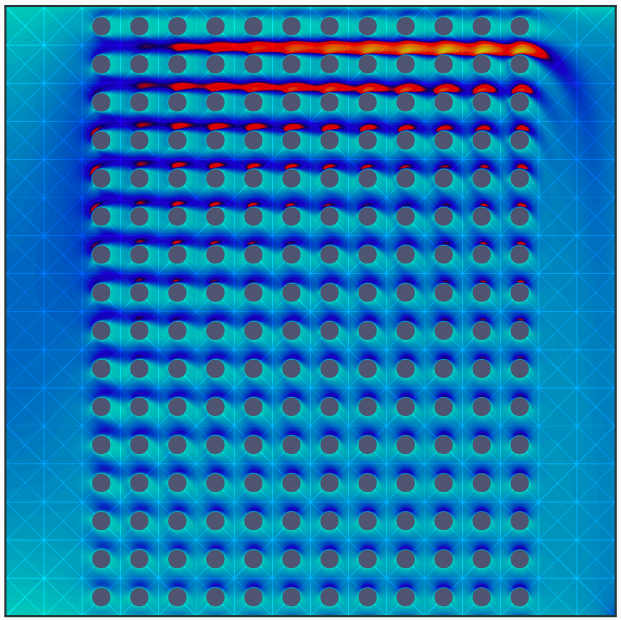

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5×10^{-4}	outer solves	A_{00} solves	S solves
GenEO	†	†	†
harmonic	6	14	6

Conclusion

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Thank you!

References 1

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