MUMPS in PETSc and HPDDM

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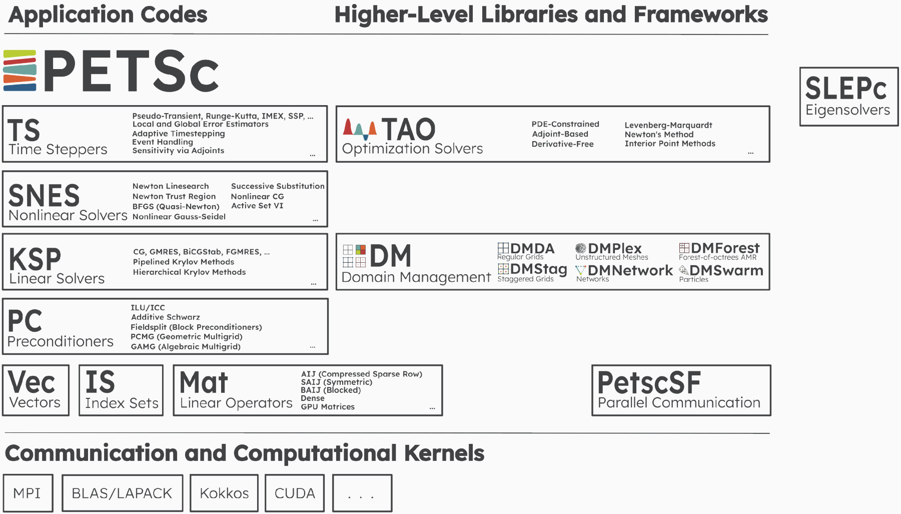
MUMPS User Days, June 23, 2023

https://joliv.et/MUD_2023.pdf



Application Codes

Higher-Level Libraries and Frameworks

PETSc

SLEPc
Eigensolvers

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

Communication and Computational Kernels

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

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  - `MatNest` (nested submatrices)

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    - `MatNest` (nested submatrices)
- runtime composability (different types and solvers)

Features since MUD 2017 in PETSc interface

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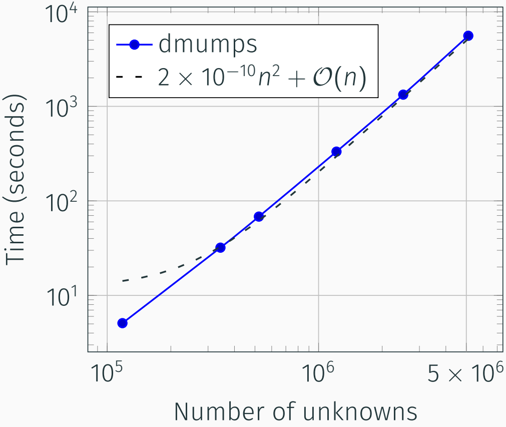
- better performance for block matrices via `ICNTL(15)`
- automatic handling of `MatSBAIJ` and `MatNest`
- different PETSc and MUMPS precision (WIP)

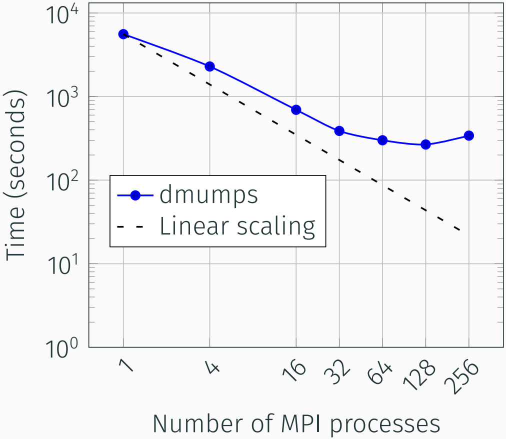
Complexity study, case #1

- 3D linear elasticity, piecewise linear FE
- sequential, double-precision, exact LDL^T factorization



→ fighting an uphill battle

Performance study for the 5M unknowns



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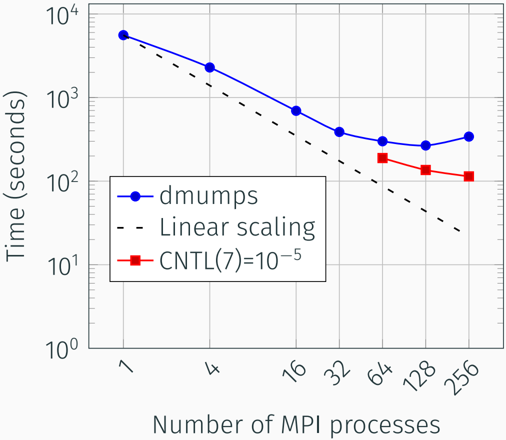

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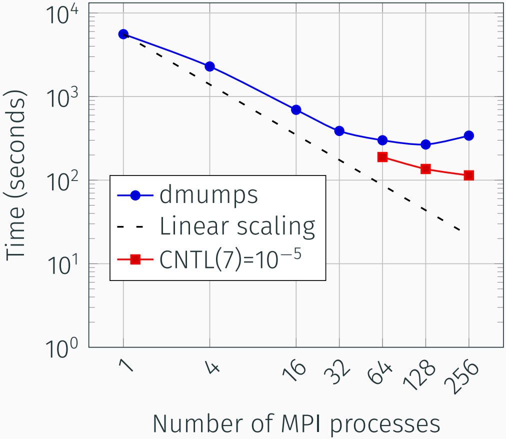

- 92% of the time (average) in numerical factorization
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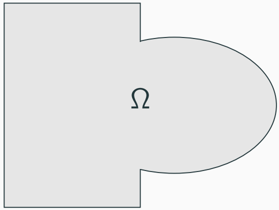
- still not quite ideal, 20% efficiency

Domain decomposition preconditioning

- global linear system $Ax = b \in \mathbb{R}^n$



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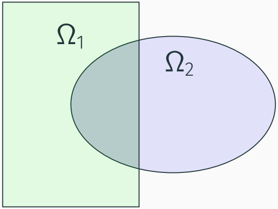
- global linear system $Ax = b \in \mathbb{R}^n$
- 2-way surjection of $[\![1; n]\!] \rightsquigarrow$ restriction operators



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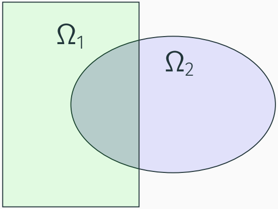
$$M_{\text{ASM}}^{-1} = \sum_{i=1}^{N=2} R_i^T (R_i A R_i^T)^{-1} R_i$$



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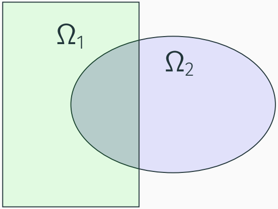

→ not so easy, M_{ASM}^{-1} doesn't scale (numerically) as $N \to +\infty$

HPDDM

- `https://github.com/hpddm/hpddm`
- spectral coarse correction $M^{-1}_{\text{additive}} = ZA_C^{-1}Z^T + M^{-1}_{\text{ASM}}$ with $A_C = Z^TAZ$

HPDDM

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- spectral coarse correction $M^{-1}_{\text{additive}} = ZA_C^{-1}Z^T + M^{-1}_{\text{ASM}}$
  with $A_C = Z^TAZ$
- three instances of MUMPS in a typical preconditioner
  - local eigensolver (computation of local "Z_i")
  - local subdomain solver $(R_iAR_i^T)^{-1}$
  - distributed coarse operator solver $(Z^TAZ)^{-1}$

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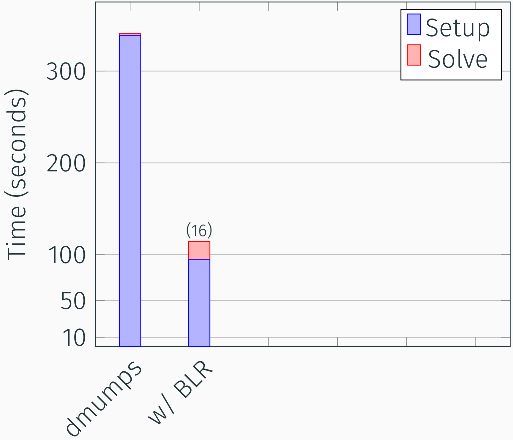
- spectral coarse correction $M^{-1}_{\text{additive}} = ZA_C^{-1}Z^T + M^{-1}_{\text{ASM}}$

  with $A_C = Z^T A Z$
- three instances of MUMPS in a typical preconditioner
  - local eigensolver
  - local subdomain solver (reuse symbolic factorization)
  - distributed coarse operator solver
- runtime flexibility
  - `-pc_hpddm_levels_1_sub_mat_mumps_…`
  - `-pc_hpddm_coarse_mat_mumps_…`

5M unknowns on 256 processes



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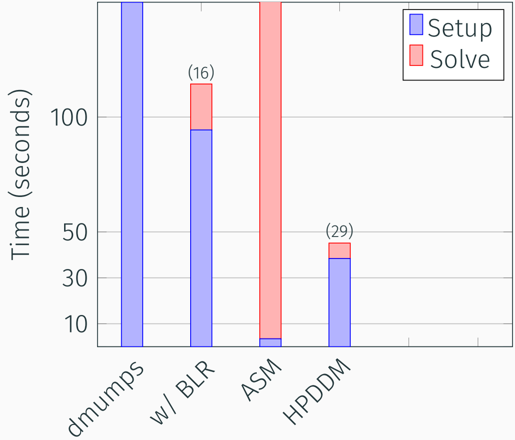

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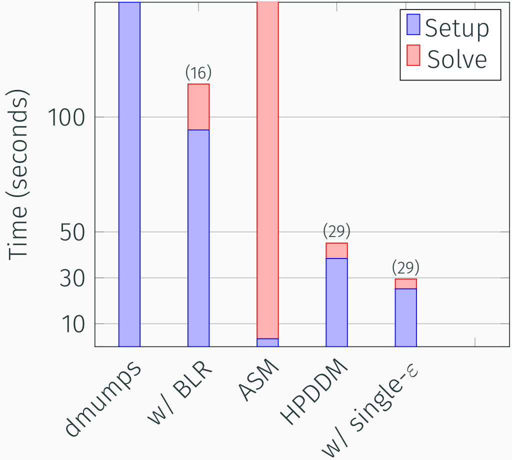

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- ○ low-precision subdomain/coarse solvers

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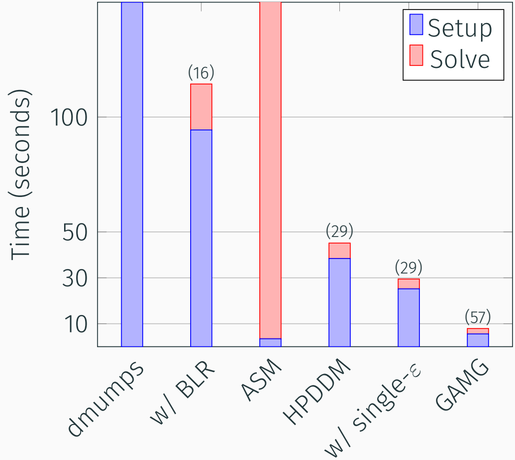
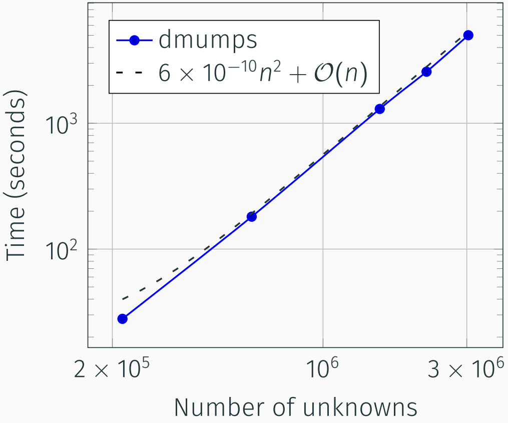


- breaking the complexity of the exact factorization
- low-precision subdomain/coarse solvers
- disclaimer: difficult to beat AMG (when it converges)

Complexity study, case #2

- 3D Stokes equation, lowest-order Taylor–Hood FE
- sequential, double-precision, exact LDL^T factorization



→ variable block size

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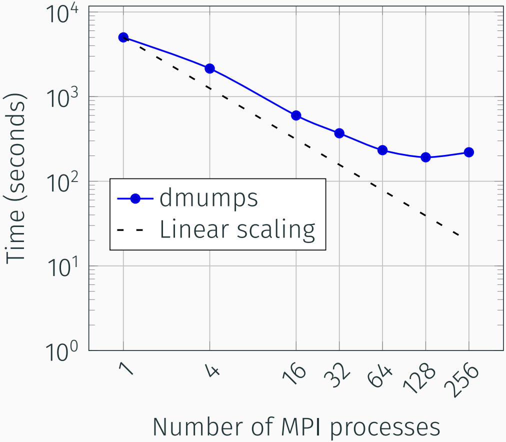

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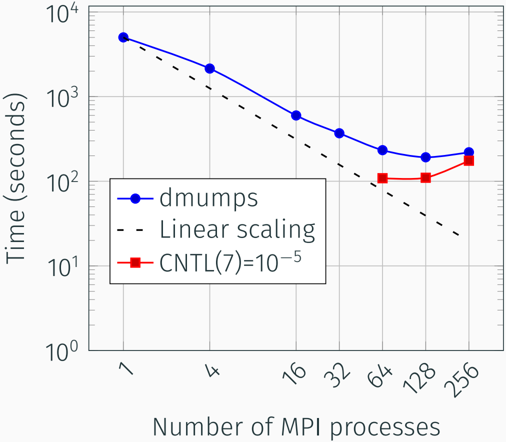

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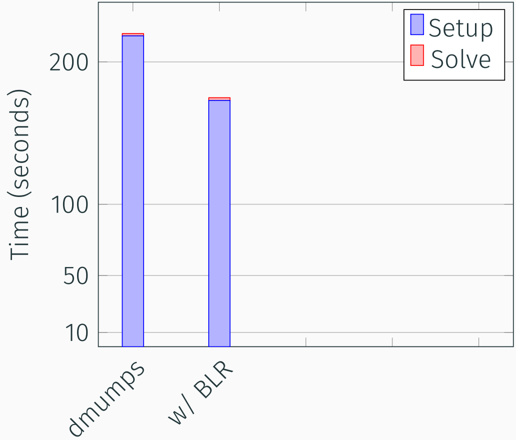

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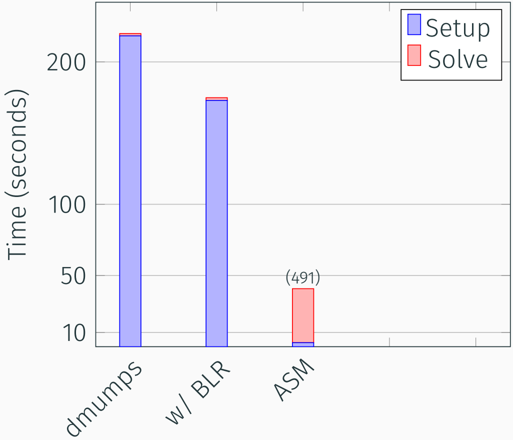

- ASM converges (albeit rather slowly)

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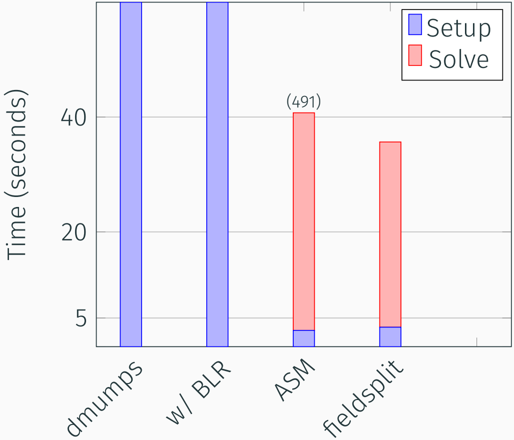

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- Schur complement: inner-outer iterations, ICNTL(15)=-3
- `-fieldsplit_0_`

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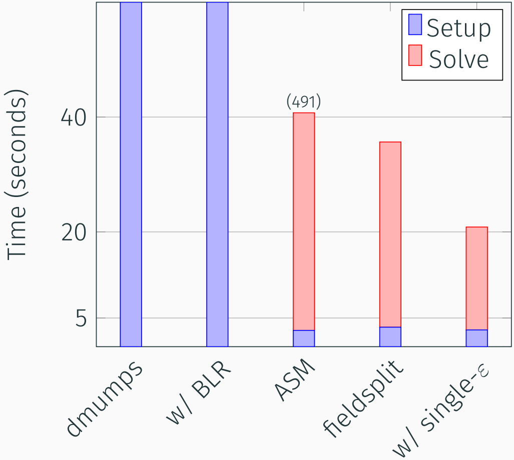

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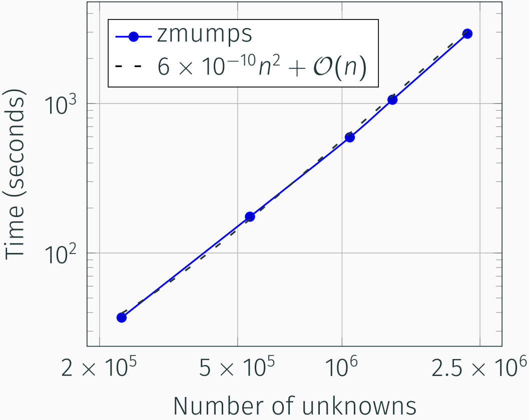
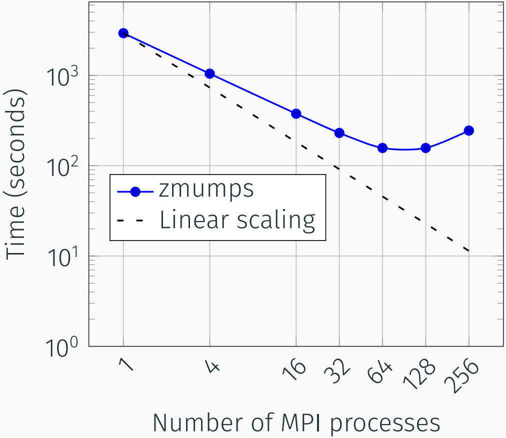


Performance study for the 2M unknowns



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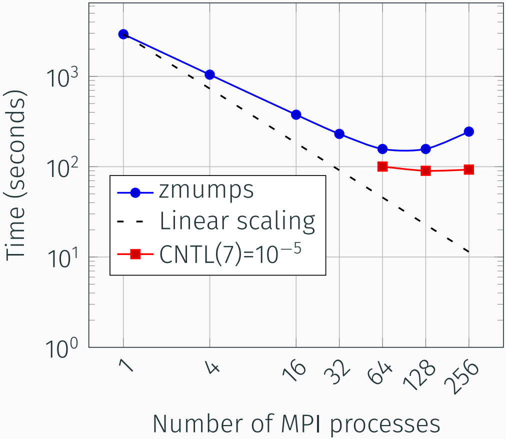

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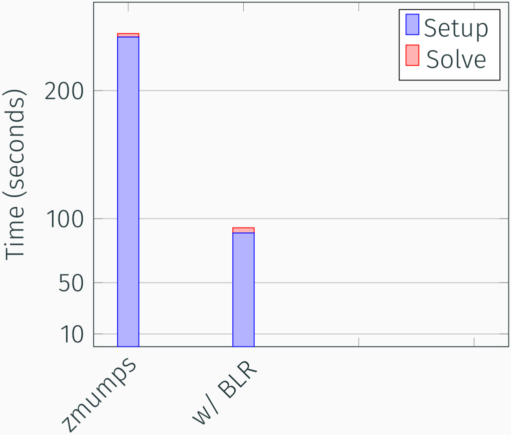

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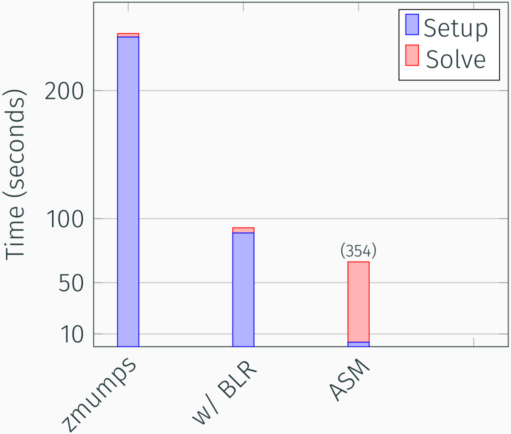

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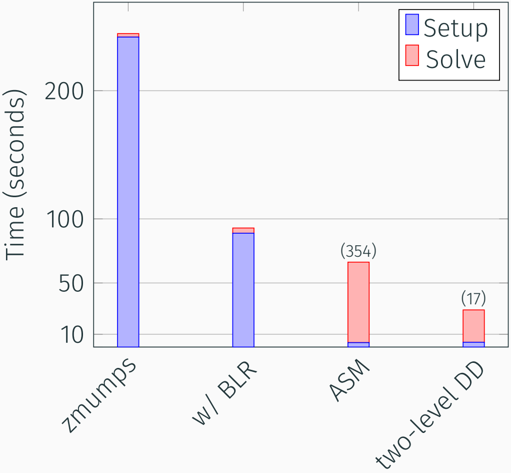

- FGMRES with a 10^{-5} tolerance
- better convergence with a coarse grid correction

Final words

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- runtime tuning
- composable solvers/preconditioners

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