A User-Friendly Highly Scalable AMG Solver

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1. Motivation (1)

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Many application software need an efficient solver for linear systems from (or related to) the discretization of PDEs like

$$-\text{div}(D\,\textbf{grad}(u)) + \mathbf{v}\,\textbf{grad}(u) + c\,u \;=\; f \qquad (+BC)$$

- De facto standard for a long time: direct solvers
  To substitute them one needs
  - a black box solver
    (we provide the matrix & rhs, it returns the solution)
  - that is robust
    (stable performance with respect to changes in the BC, PDE coeff., geometry & discretization grid)
- Efficient solver means:
  solve the system in near linear time: $\frac{\text{elapsed}}{n\times\#\text{cores}} \approx$ (small) cst

1. Motivation (2)

Multigrid methods:

often robust, always efficient $\rightarrow$ good candidates

AMG variants: designed to work black box

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- In principle, yes: AMG stands for Algebraic Multigrid, where "algebraic" means that all algorithmic components are derived from the matrix itself

  $\rightarrow$ the user passes the matrix to the soft and that's it

- In practice, many people use an AMG software without knowing much about it

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  but many others experienced struggling with variant selection and parameters tuning before getting satisfactory results

2. Aggregation-based AMG (1)

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Principle: Keep many features common to AMG methods

- Basic two-grid scheme which alternates smoothing iterations and coarse grid corrections
  - Gauss–Seidel for smoothing
  - Coarse grid correction based on a prolongation matrix P built from the system matrix A

    P is $n \times n_c$ (n_c : number of coarse variables)

    The coarse grid matrix is $A_c = P^T A P$

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- Proceed recursively

  Set up phase: to define coarser and coarser levels

  Solve phase: approximate solution of coarse systems based on the two grid scheme at coarse level

2. Aggregation-based AMG (2)

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This is achieved with prolongation P based on plain aggregation

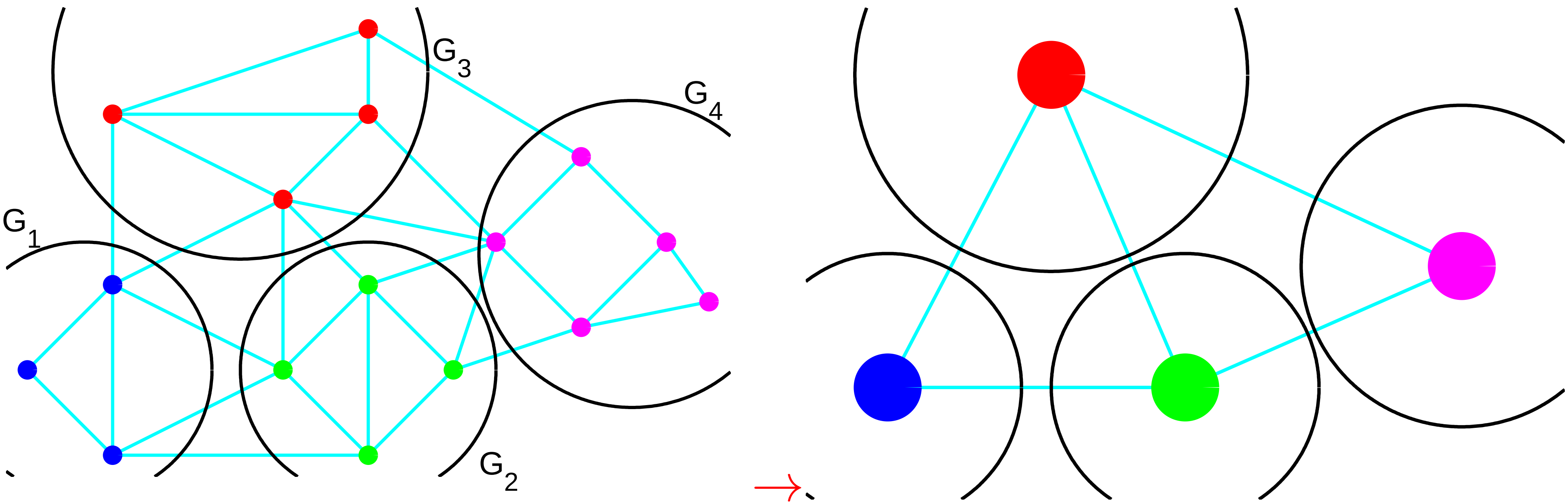
Coarsening by plain aggregation

Coarse unknowns: 1 per aggregate and vice-versa

Prolongation P : piecewise constant

Coarse grid matrix: obtained by a simple summation

$$P_{iJ} = \begin{cases} 1 & \text{if } i \in G_J \\ 0 & \text{otherwise} \end{cases} \quad , \qquad (A_c)_{ij} = \sum_{k \in G_i} \sum_{\ell \in G_j} a_{k\ell}$$



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Convergence analysis

Under some assumptions, it can be shown that the two-grid spectral radius (or condition number) is bounded as a function of

$$K = \max_{i=1,\dots,n_c} K_{G_i}$$

where K_{G_i} is a quantity associated to aggregate G_i that is easy (and relatively cheap) to assess

K_{G_i} characterize thus the quality of the aggregate G_i

The theory is rigorous for M-matrices (possibly nonsymmetric), with heuristic extensions to matrices with nonnegative row-sum (in practice, works as long as the negative offdiagonal connections “dominate” the positive ones)

2. Aggregation-based AMG (5)

Quality aware aggregation algorithm

Basic principle: build aggregates in a greedy fashion, trying to optimize the quality indicator K_{G_i} while keeping it in any case within prescribed bounds

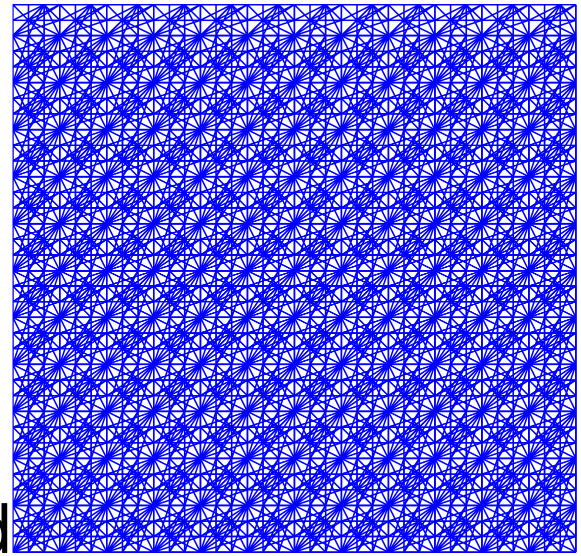
In that way, some minimal convergence properties are guaranteed, making the method particularly robust

(The two-grid convergence rate is under control)

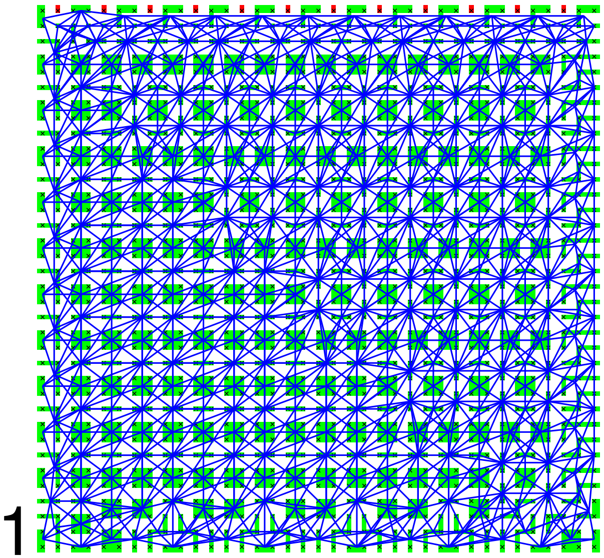
2. Aggregation-based AMG (6)

Illustration of how it may work

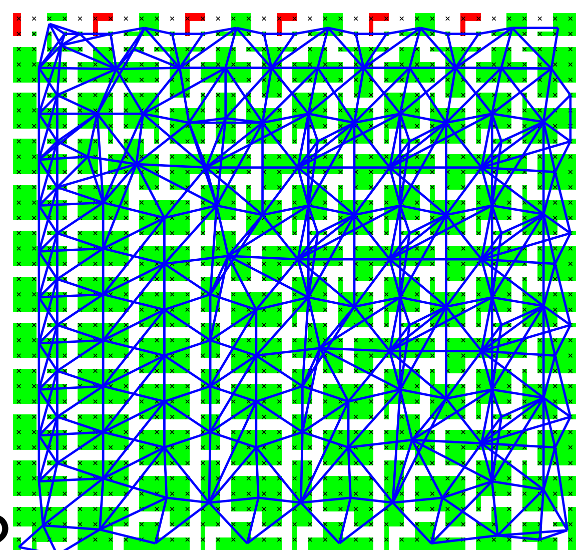
Regular grid, 3rd order finite elements (p3) for Poisson
($nnz(A) \approx 16\,n$)



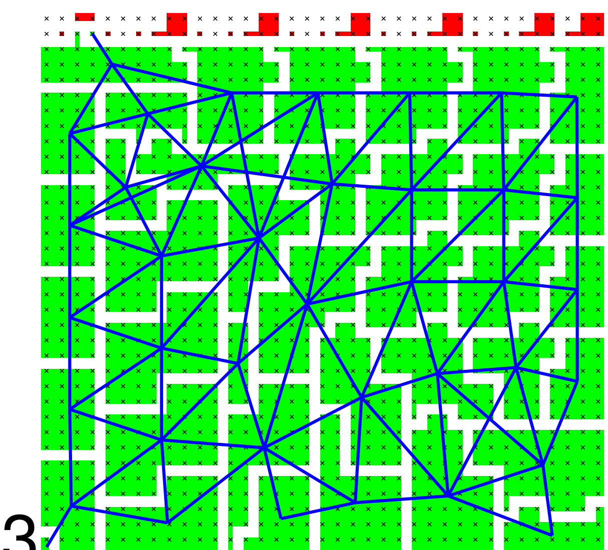
Fine grid



Level 1



Level 2



Level 3

2. Aggregation-based AMG (7)

No free lunch theorem:

We gained something, where are the downsides?

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No free lunch theorem:

We gained something, where are the downsides?

(1) The two-grid convergence rate is not as good as can be with more classical AMG methods

However, using the method as a preconditioner for CG or GMRES/GCR, the impact on the number of iterations is limited and can be offset by

- a cheaper setup
- a lower cost per iteration, thanks to
  - cheap smoothing
    (only 1 GS sweep for pre- and post-smoothing)
  - lighter coarse grid matrices
    (with less rows and less nonzero entries per row)

2. Aggregation-based AMG (8)

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In a multigrid algorithm, the coarse systems $A_c\mathbf{u}_c = \mathbf{r}_c$
are approximately solved with a few iterations of the
two-grid method at the considered (coarse) level
(recursivity: this way one moves to a further coarser level)

- 1 stationary iteration: V-cycle
- 2 stationary iterations: W-cycle

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- 1 stationary iteration: V-cycle
- 2 stationary iterations: W-cycle
- 2 iter. with Krylov (CG/GMRES) acceleration: K-cycle

  Same workflow and about the same cost as with the W-cycle,
  but major robustness enhancement

Iterative solution with AGgregation-based algebraic MultiGrid

Linear system solver software package

- Black box
- FORTRAN 90 (easy interface with C & C++)
- Matlab interface

```
>>  x=agmg(A,y);
>>  x=agmg(A,y,1);   % SPD case
```

- Free academic license
  Professional version available (with extra features)

3. AGMG (robustness study) (2)

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Robustness

Assessed on a large test suite of discrete second order elliptic PDEs, comprising

- problems on 2D/3D regular grids and on 2D/3D unstructured grids, some with strong local refinement
- problems with (big) jumps and/or (large) anisotropy in the PDE coefficients
- symmetric (SPD) and nonsymmetric problems (2D/3D convection-diffusion with dominating convection)
- finite difference and finite element (up to $p4$) discretizations

Size: Minimal: 5×10^5 – Maximal: $3. \times 10^7$

nnz per row: Minimal: $5.$ – Maximal: $74.$

3. AGMG (robustness study) (3)

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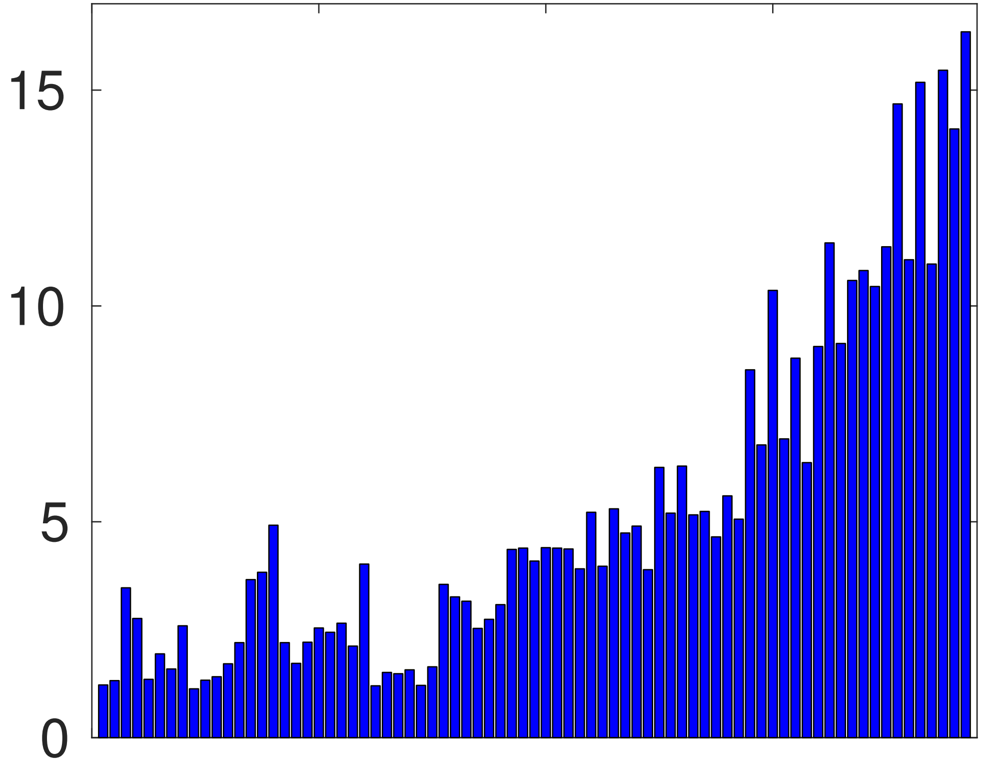
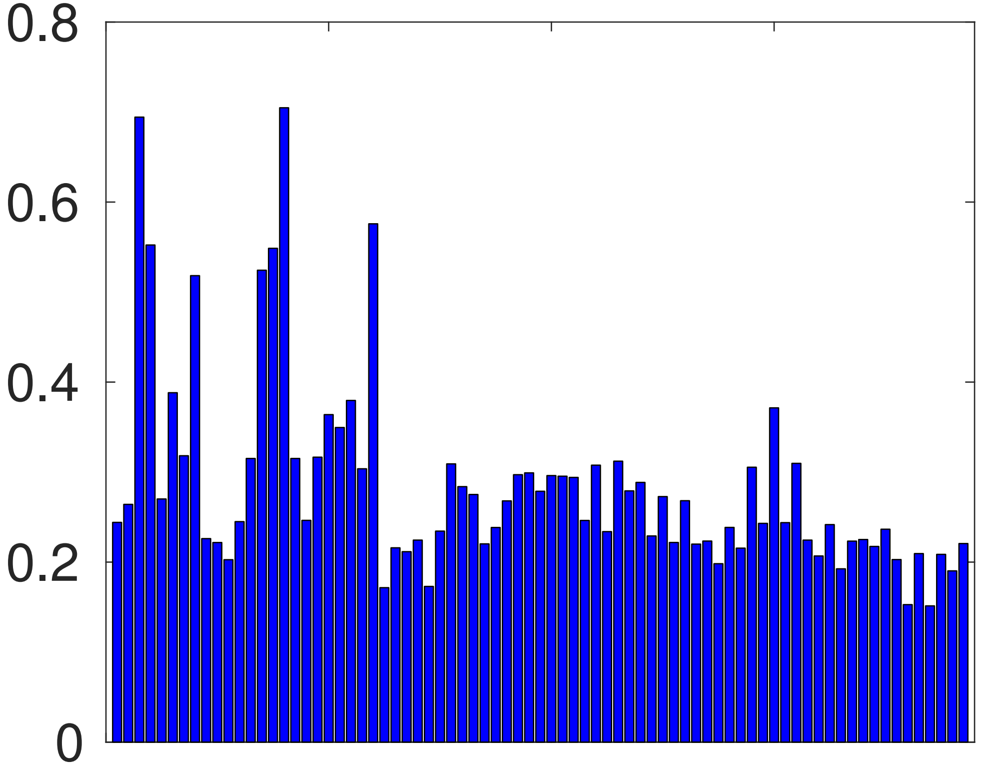
Time per unknown



Time per nnz



Total wall clock time in microseconds per unknown or nnz

– vs – problem index

(problems ordered by increasing number of nnz per row)

(Desktop workstation – Intel XEON E5-2620 at 2.10GHz – 2017)

3. AGMG (comparative study) (4)

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Comparison with some other methods

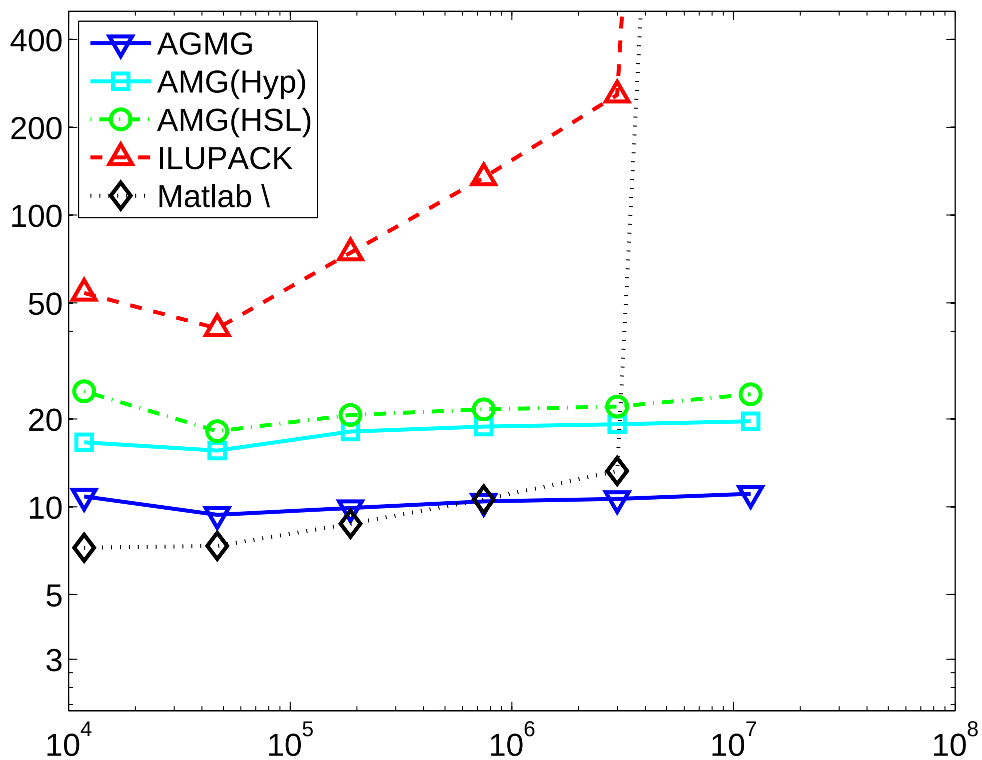
- AMG(Hyp): a classical AMG method (Hypre library)
- AMG(HSL): a classical AMG method (HSL library)
- ILUPACK: efficient threshold-based ILU preconditioner
- Matlab \: Matlab sparse direct solver (UMFPACK)

All methods but the last with Krylov subspace acceleration

Iterations stopped when $\frac{\|\mathbf{r}_k\|}{\|\mathbf{r}_0\|} < 10^{-6}$

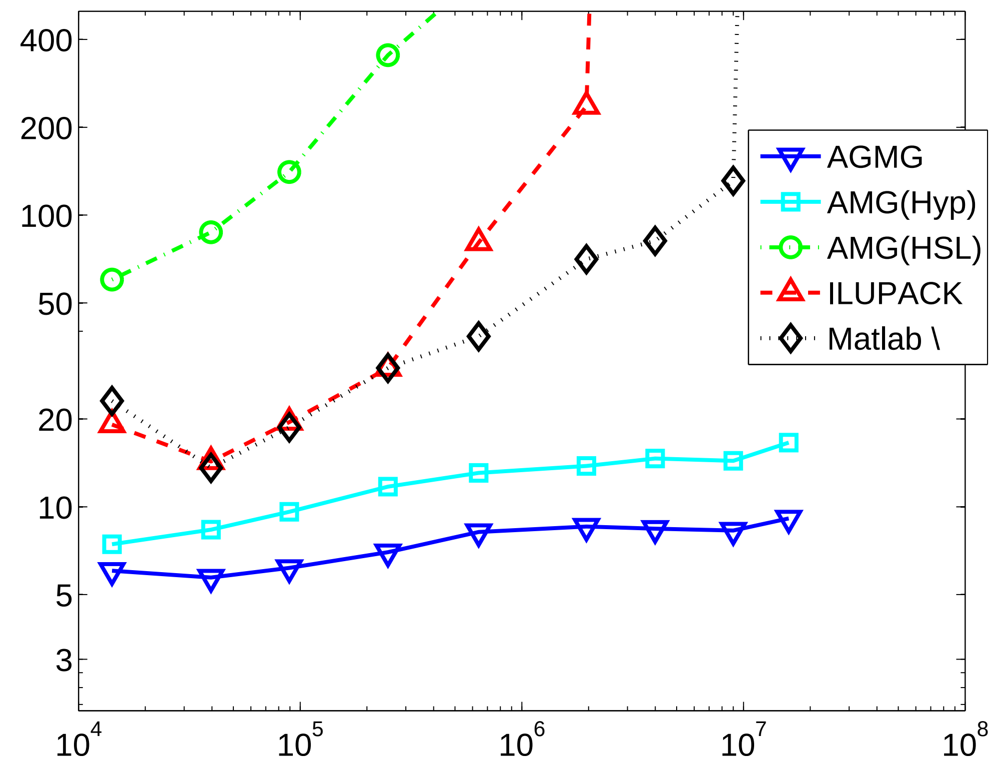
3. AGMG (comparative study) (5)

Poisson 2D, FE(P3)



(33% of nonzero offdiag > 0)

Convection-Diffusion 2D, FD



(circulating flow, $\nu = 10^{-6}$)

Wall clock time in microseconds per unknown – vs – # unknowns

(Computing node – Intel XEON L5420 processors at 2.50GHz – 2012)

3. AGMG (comparative study) (6)

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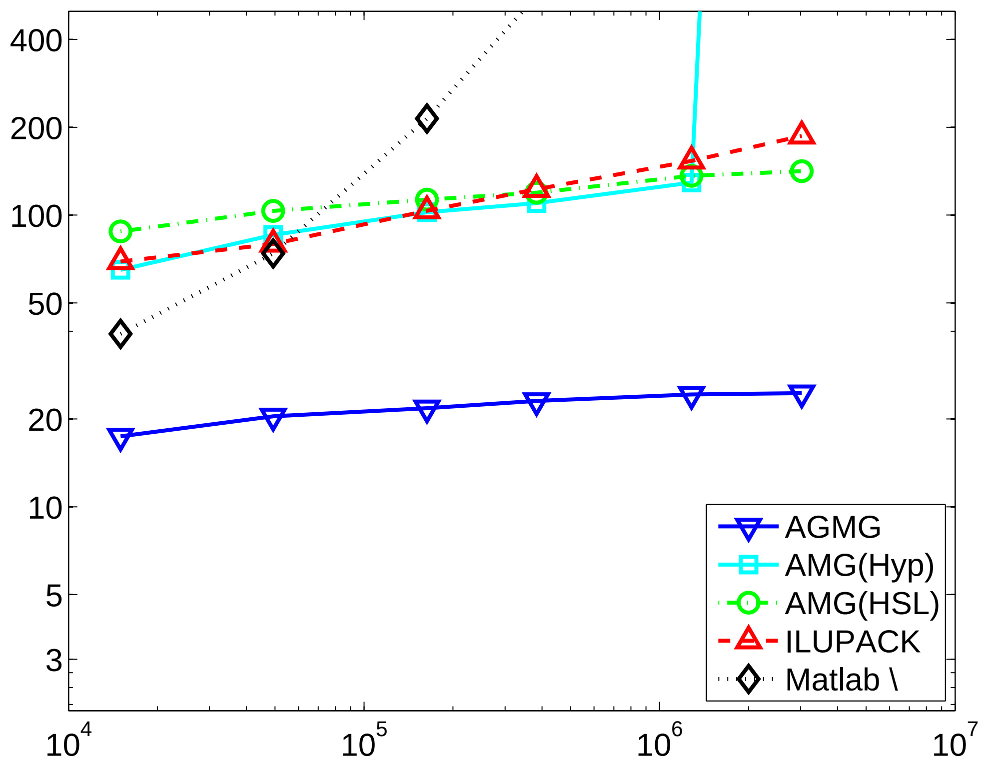
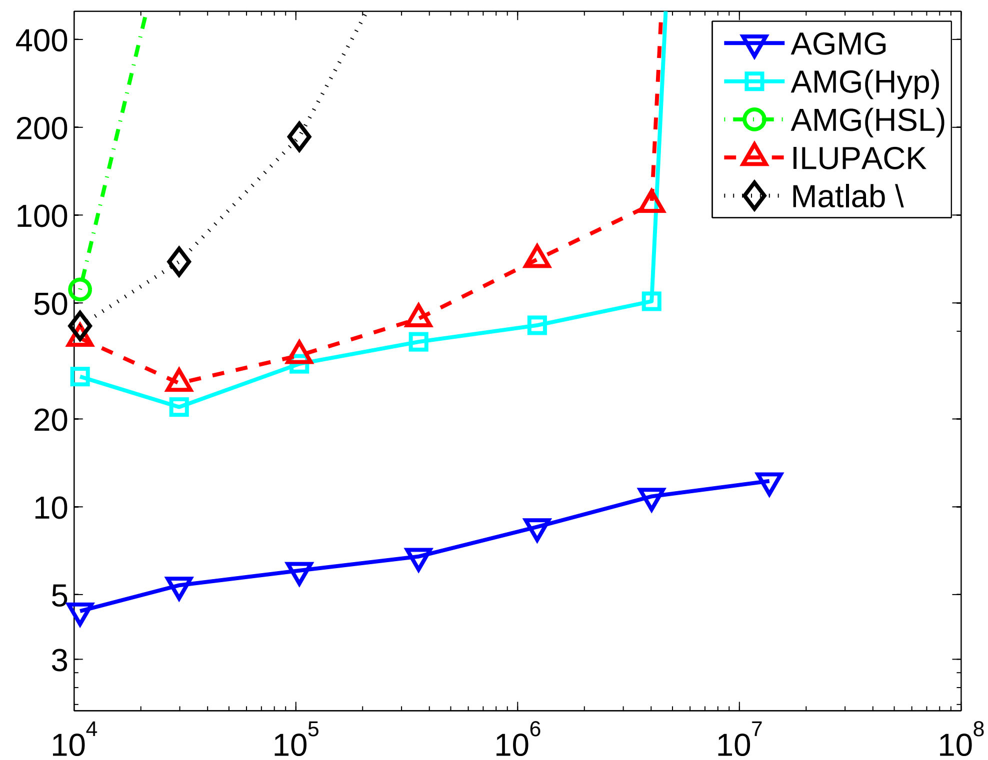
POISSON 3D, FE(P3)



(51% of nonzero offdiag > 0)

CONVECTION-DIFFUSION 3D, FD



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General strategy

Partitioning of the unknowns $\rightarrow$ distribution of matrix rows

- Setup phase
  Aggregation algorithm: unchanged but aggregates are only formed with unknowns in a same partition

  $\rightarrow$ inherently parallel

  Only few communications needed to form the next coarse grid matrix

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- **Solve phase**
  - Smoothing: Truncated Gauss-Seidel, ignoring connections between different partitions $\rightarrow$ inherently parallel
  - Grid transfer operations: inherently parallel

4. Parallelization (2)

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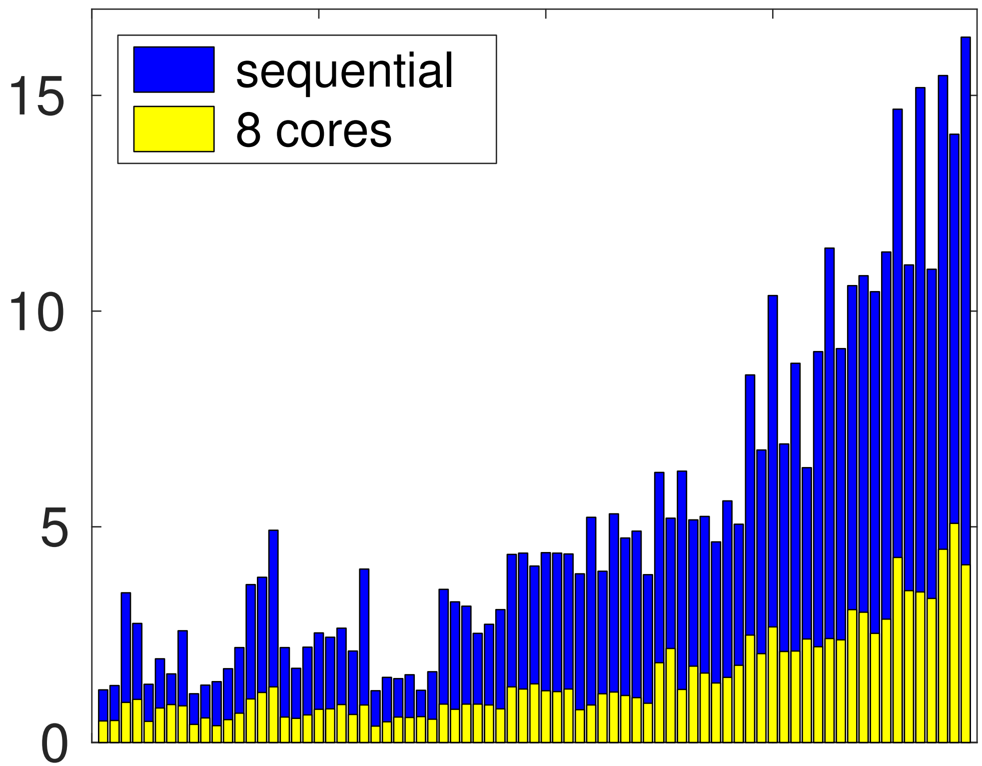
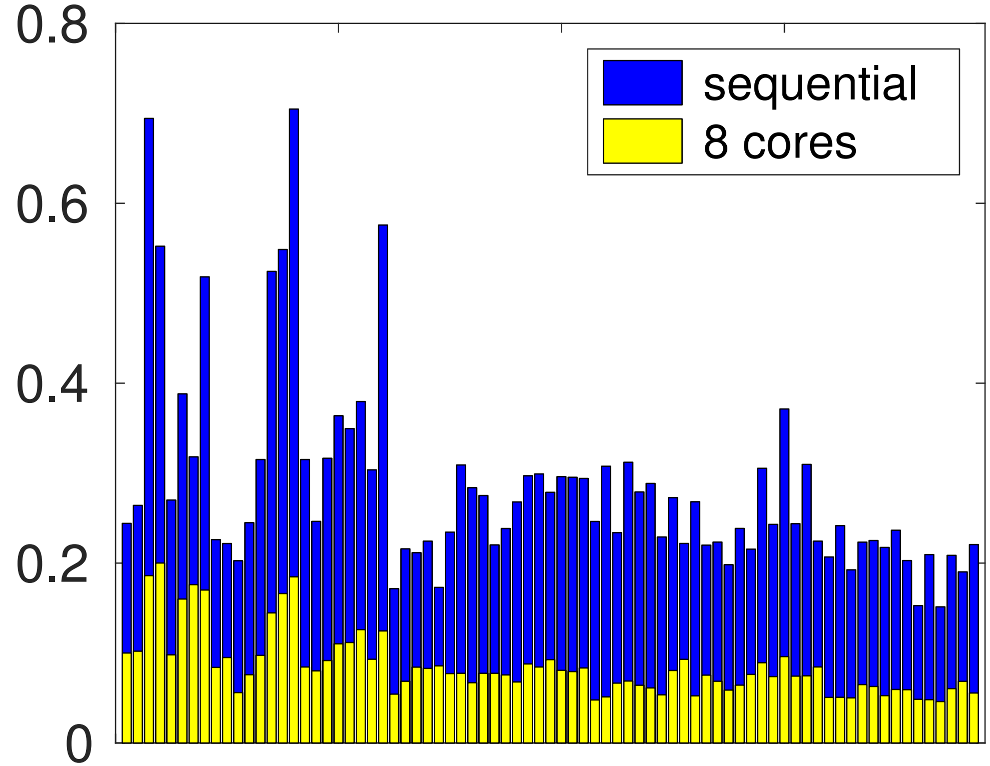
Nothing more needed for efficient multithreading (OpenMP)

Global results for the test suite:

Time per unknown



Time per nnz



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MPI: the Bottom level solver can be a bottleneck

- More frequently called than with the V-cycle
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- Sequential AGMG uses a sparse direct solver, but parallel versions of these do not scale well enough
- Thus: dedicated Iterative bottom level solver
  Rationale:
  - only a small % of total flops
    $\rightarrow$ some suboptimality is harmless
  - few unknowns involved
    $\rightarrow$ needs a method that scales well despite this

  Our choice:
  a simplified two-level domain decomposition method

4. Parallelization (4)

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Iterative bottom level solver

- Aggregation-based two-grid method
  (one further level: very coarse grid)
- All unknowns on a same process form 1 aggregate
  (very coarse grid: size = number of processes (cores))
- Better smoother:
  Block Jacobi
  (sparse direct solver for the local part of the matrix)
- Solution of very coarse grid systems:
  Sparse direct solver

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Iterative bottom level solver for massive parallelism

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- Better smoother:
  ~~Block Jacobi~~
  ~~(sparse direct solver for the local part of the matrix)~~
  Apply sequential AGMG to the local part of the matrix
  Allows us to use only 4 levels whatever the matrix size
- Solution of very coarse grid systems:
  ~~Sparse direct solver~~
  AGMG again, sequential or parallel within subgroups of processes (depending on the size of the systems)

4. Parallelization (5)

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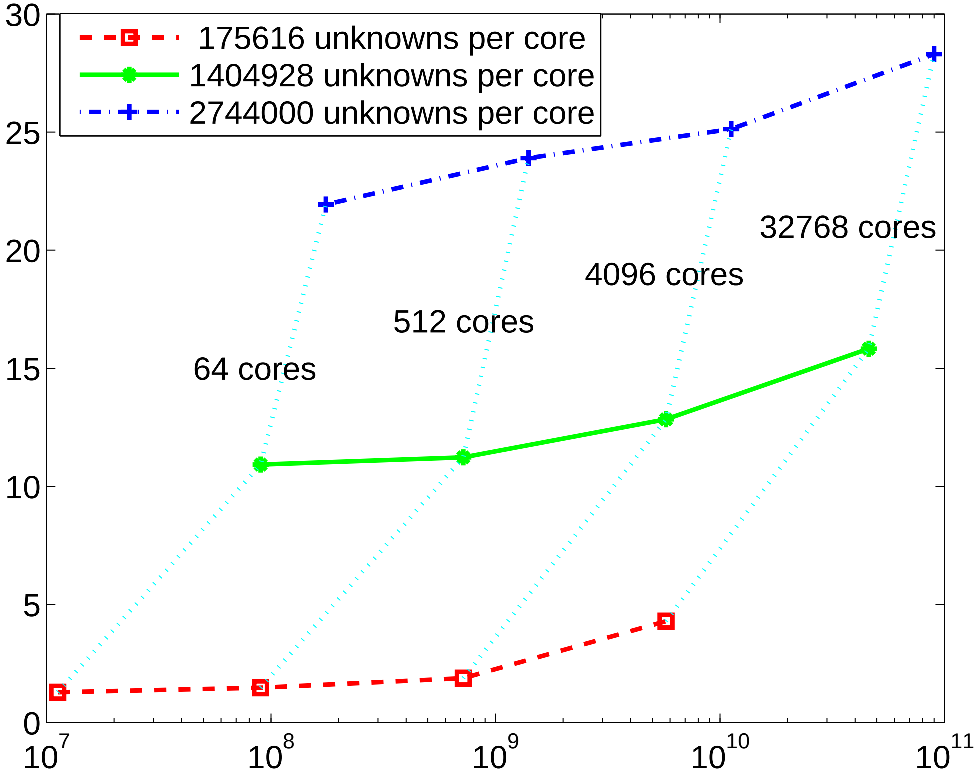
Performance of AGMG on supercomputers

3D Poisson (FD) on HERMIT (HPC – Cray XE6 – 2014)

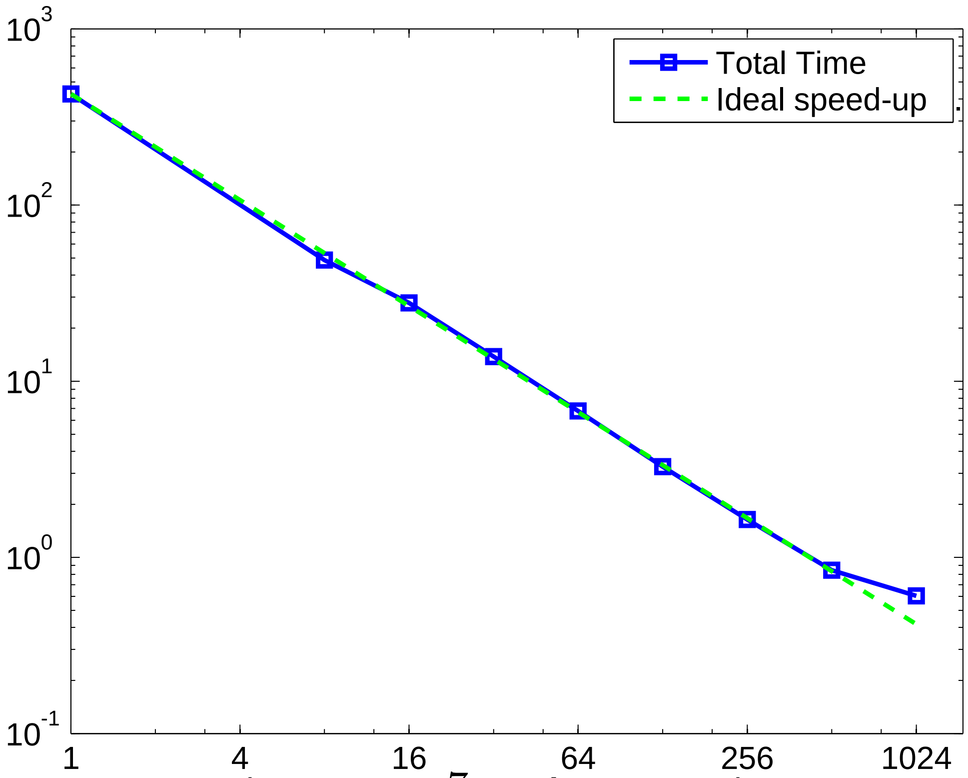
Weak scalability

Time – vs – # unknowns



Strong scalability

Time – vs – number of cores



Times reported are total wall clock times in seconds

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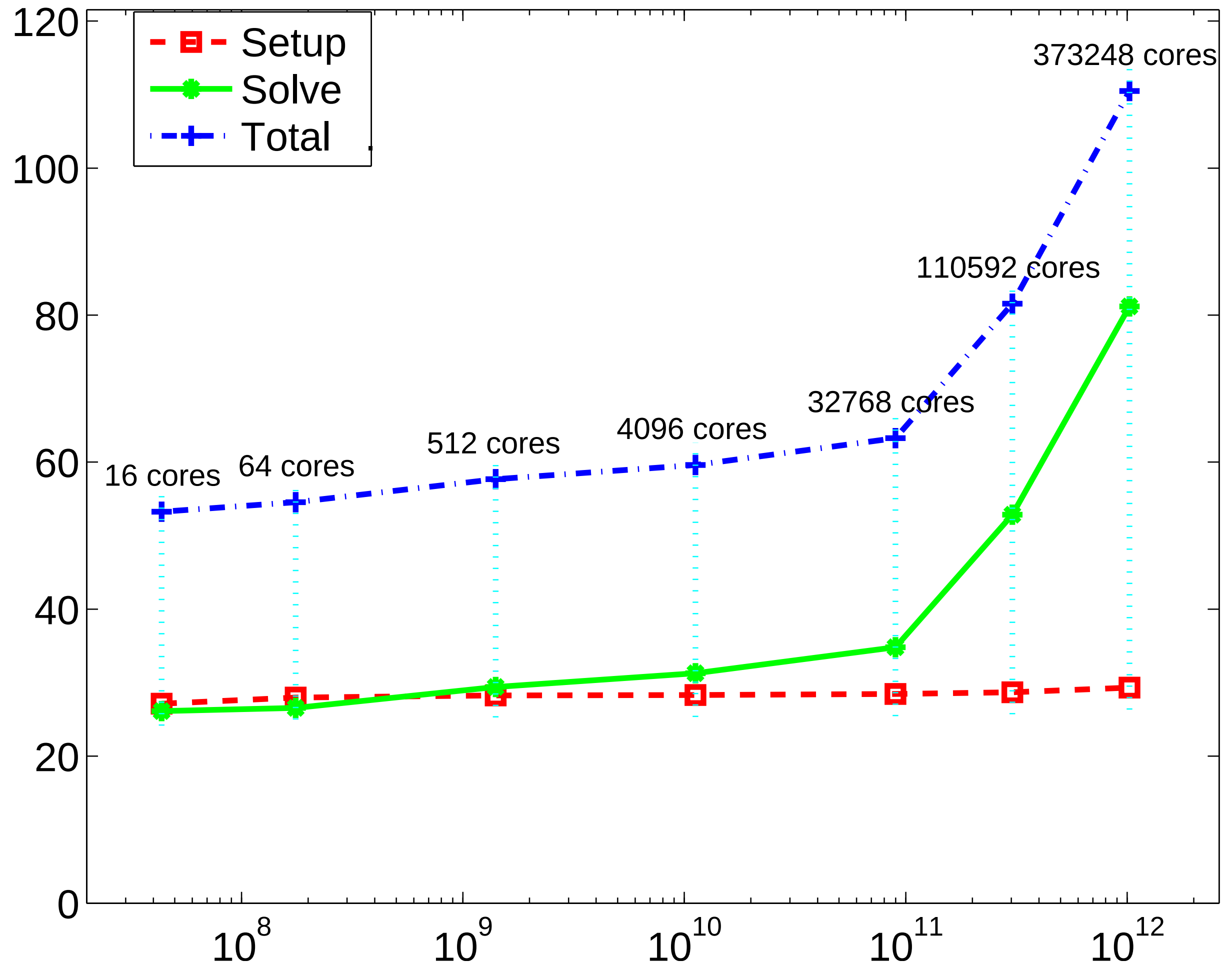

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5. Extensions

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Stokes problems

- Simple algebraic transformation to reinforce the weight of the diagonal blocks (literally: pre-conditioning)
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  $\rightarrow$ monolithic AMG, faster than block preconditioning

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Graph Laplacians

- Standard aggregation based on multiple pairwise matching is inefficient for some exotic sparsity patterns
- Robustness recovered with Degree aware Rooted Aggregation (DRA)

  . . . can be also combined with quality control
- The resulting method is significantly faster than LAMG

6. Conclusions

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- Can be faster than other state-of-the-art solvers
- Fairly small setup time: especially well suited when only a modest accuracy is needed

Selected references

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The K-cycle

- Recursive Krylov-based multigrid cycles (with P. S. Vassilevski), NLAA, 2008

Two-grid analysis of aggregation-based methods

- Algebraic analysis of aggregation-based multigrid (with A. Napov), NLAA, 2011

AGMG and quality aware aggregation

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