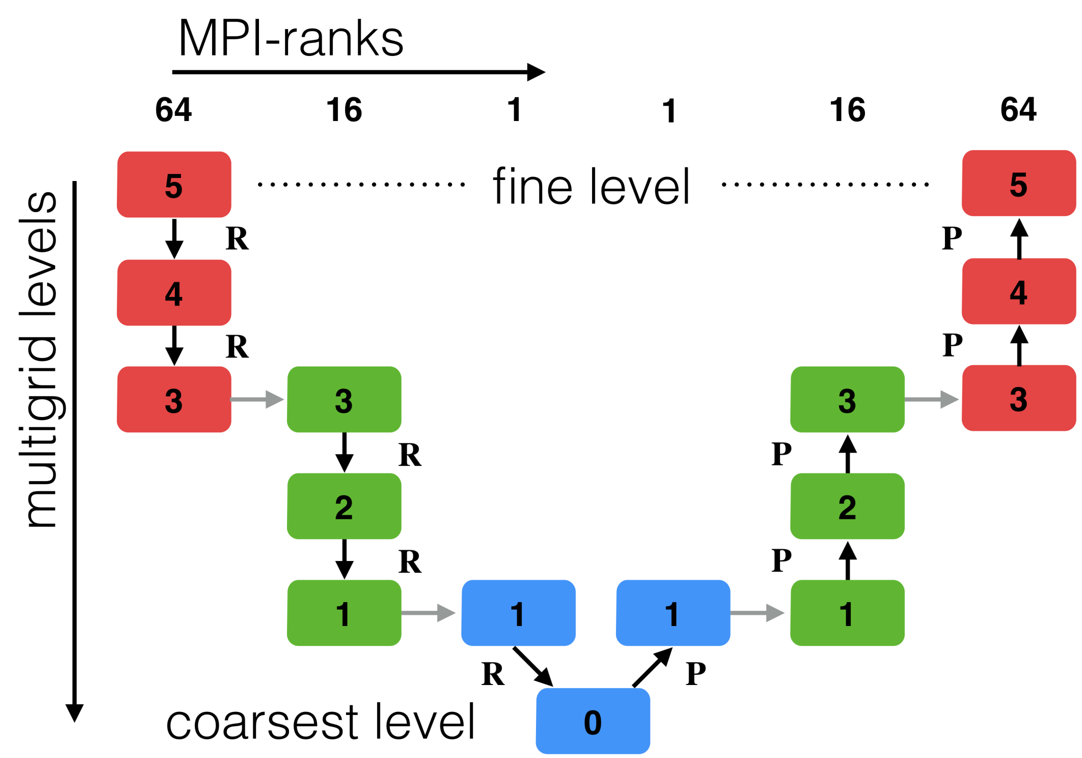
Extreme-scale Multigrid Components within PETSc



Dave A. May (ETH Zürich), **Patrick Sanan** (USI Lugano, ETH Zürich), **Karl Rupp**, **Matthew G. Knepley** (Rice University), **Barry F. Smith** (Argonne National Lab)

Outline

1. **Motivation** : The need for (easy-to-use) agglomeration within extreme-scale geometric multigrid

2. **Implementation** :
    1. The `PCTelescope` implementation
    2. Use cases

3. **Numerical Experiments**

4. **Future Development** : Extensions for unstructured grids

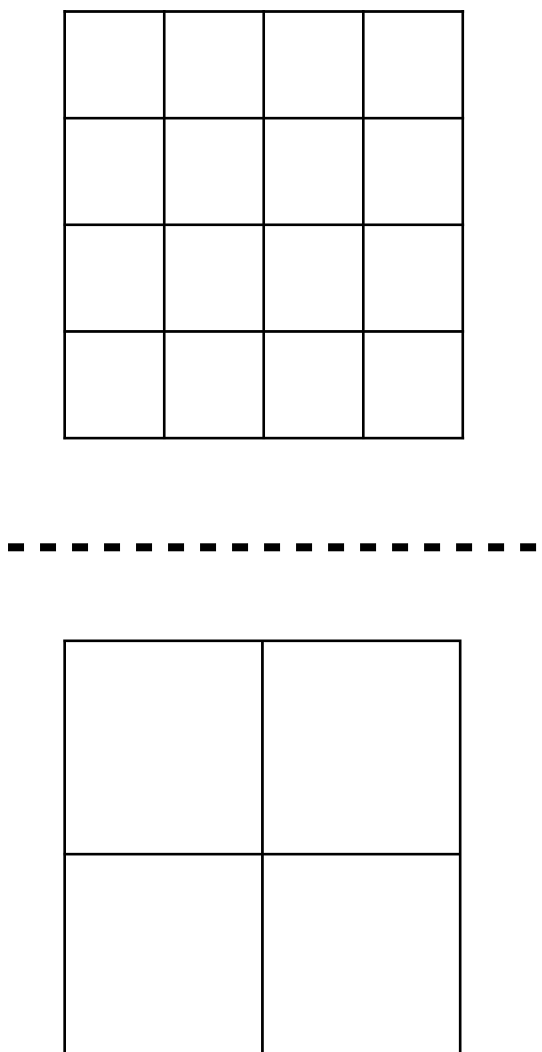
The Need for Agglomeration in Parallel Multigrid

Re-discretised Geometric Multigrid (RMG)

Given $Ax = b$ let v denote our guess for x

Two-level RMG algorithm (Simplest Form)

FINE Ω^h



COARSE Ω^{2h}

"Smooth" N times

$$v = v + \omega(b - Av)$$

Compute residual

$$r^h = b - Av$$

Restrict $r^h \to \Omega^{2h}$, yielding r^{2h}

Compute error

Solve $A^{2h}e^{2h} = r^{2h}$

Interpolate $e^{2h} \to \Omega^h$, yielding e^h

Compute residual correction

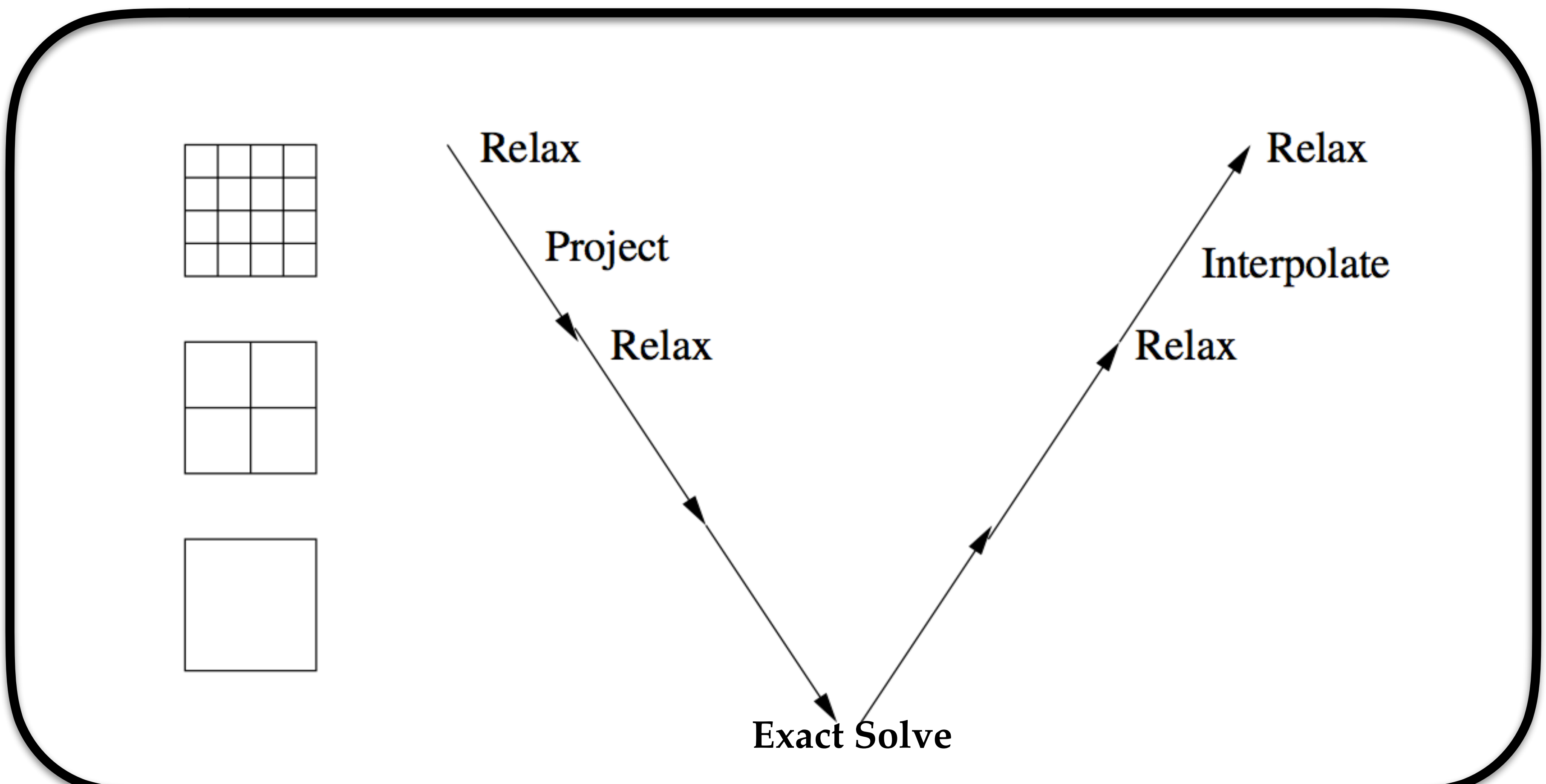
$$v = v + e^h$$

"Smooth" N times

$$v = v + \omega(b - Av)$$

Re-discretised Geometric Multigrid (RMG)

- Ingredients
  - A mesh hierarchy (fine → coarse) on which will discretise our PDE
  - A restriction operator (maps field from fine → coarse)
  - An interpolation operator (maps field from coarse → fine)
  - A smoother on each level
  - A coarse grid solver



Why Multigrid (MG)?

- Theoretically optimal solve time *O(n)* ⟶ **scalable**

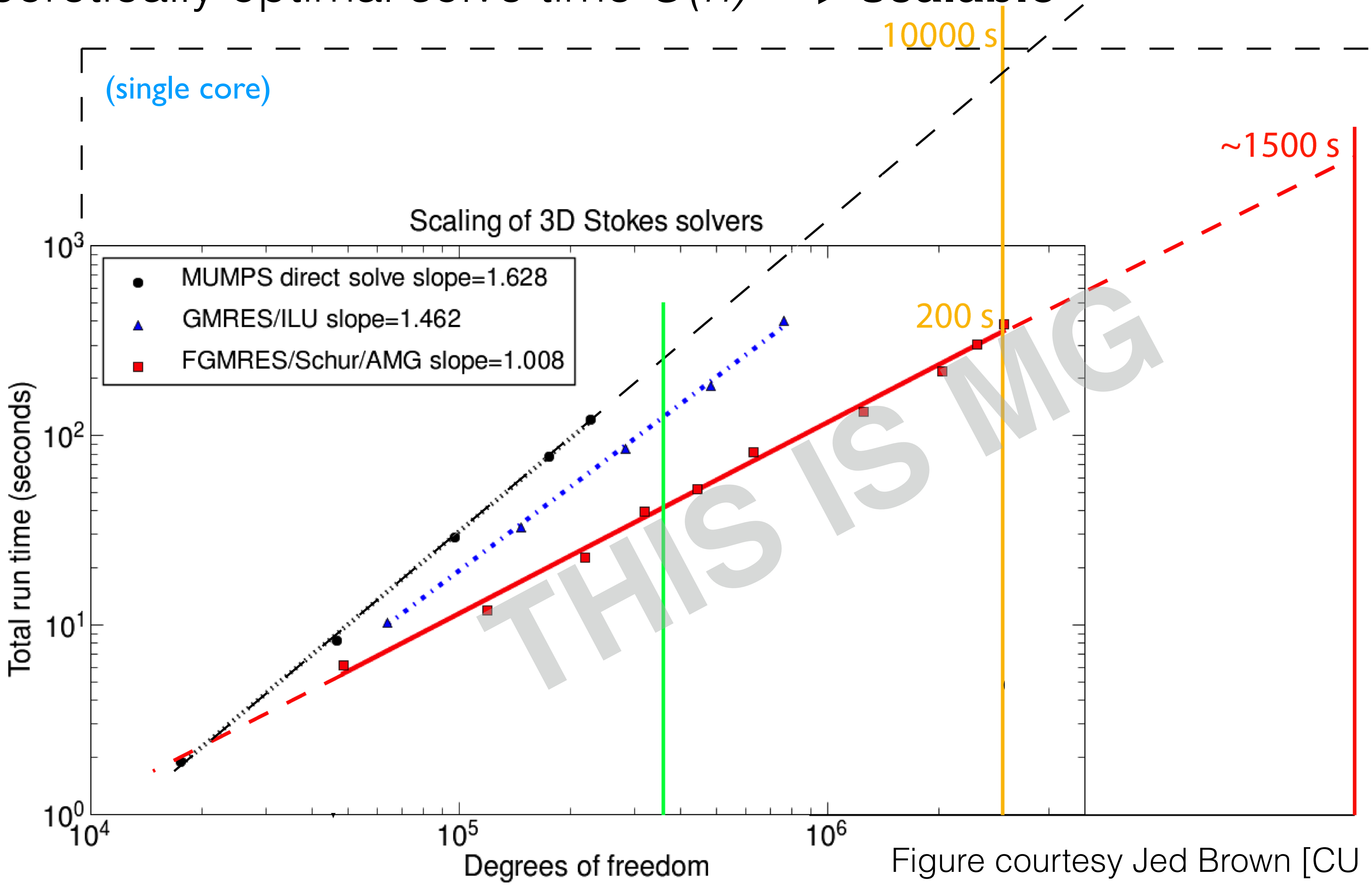


Figure courtesy Jed Brown [CU Boulder]

3000 km x 2000 km x 200 km - 3 velocity components

with mesh resolution of 11 km --> 110 million unknowns

with mesh resolution of 20 km --> 1.8 million unknowns

with mesh resolution of 34 km --> 0.34 million unknowns

Why Are More Levels Better?

- Fewer levels implies the coarse grid will contain a large number of unknowns. Recall that the coarse grid correction requires an accurate solve (usually expensive, non-scalable).
- *Optimality of MG comes from having a tiny coarse grid problem.*

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Two-level method

Mesh	Time	Factor
17^3	1.22E-02	-
33^3	1.25E-01	10x
65^3	3.87E+00	31x
129^3	1.42E+02	63x

Mesh	Levels	Time	Factor
17^3	2	1.22E-02	-
33^3	3	7.14E-02	6x
65^3	4	6.51E-01	9x
129^3	5	5.48E+00	8x
257^3	6	4.37E+01	8x

`$PETSC_DIR/src/ksp/ksp/examples/tutorials/ex45.c`

- *When RMG breaks down and the effective coarsest grid is not "coarse enough" ➔ change to another scalable method*

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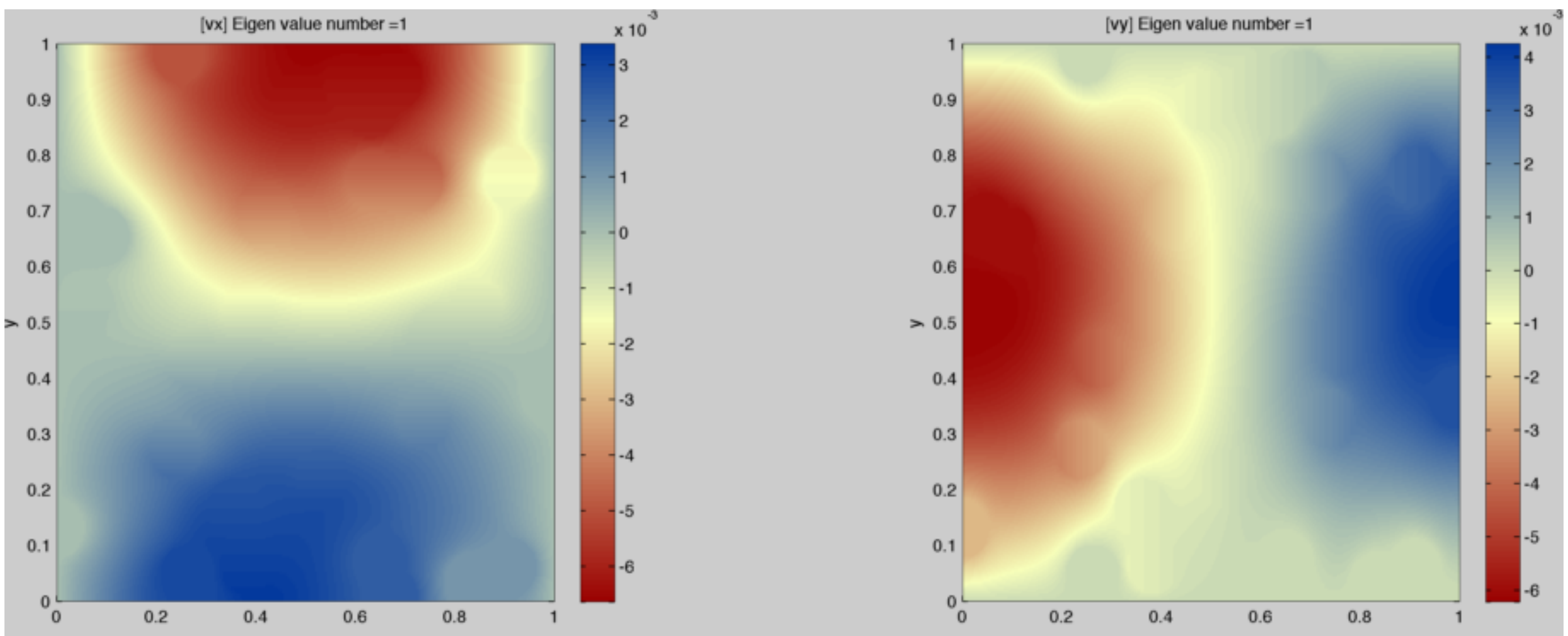
- *When RMG breaks down and the effective coarsest grid is not "coarse enough" → change to another scalable method*

Multigrid in Parallel

- Multigrid levels are sometimes limited in practice
  - Practical restrictions often apply; e.g. a minimum of 1 finite element per rank
  - "Empty" ranks may still impose collective communication costs
  - Coarse grids may be limited in their ability to resolve features



- A multigrid V-cycle (with an exact coarse grid solve) is all-to-all communication, with a **fundamental *log(P)* communication cost**

Multigrid in Parallel - Where to Communicate?

- Should the cost be incurred within a solve on a coarse grid?
  - AMG or another multilevel method (e.g. `PCGAMG`)
    - Setup stage doesn't scale for AMG
    - Shifts the question but doesn't fundamentally answer it
  - Hierarchical Krylov methods [May et. al CMAME 2015]
    - Doesn't scale forever - network latency eventually dominates
  - Redundant solve on all cores (PETSc's `PCREDUNDANT`)
    - Slow and expensive
- Or at intermediate points in the hierarchy? ⟶ **Agglomeration**
  - **As we coarsen, use smaller sets of processors (MPI ranks)**
  - Allows balance of communication and computation
  - Well-known, but requires implementation effort

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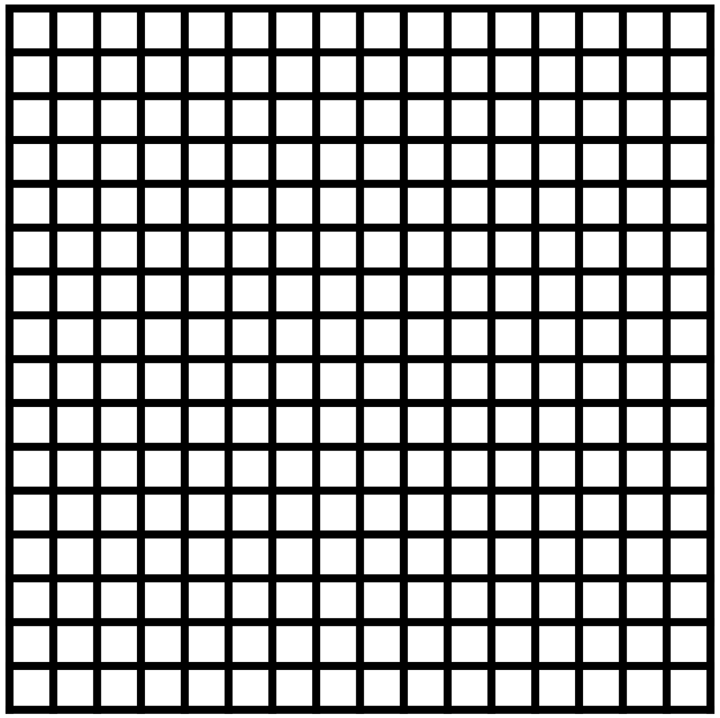
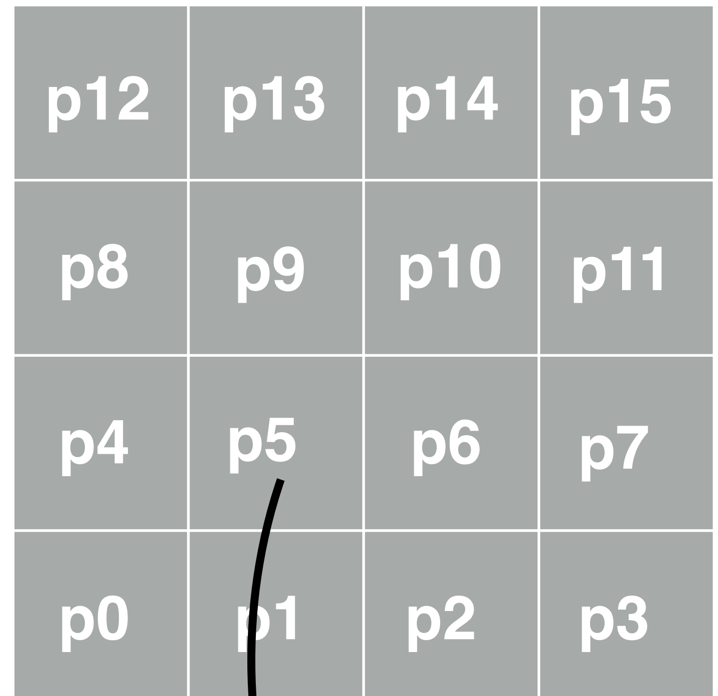
`PCBDDC`
`PCGAMG`

Repartitioning Coarse Grids

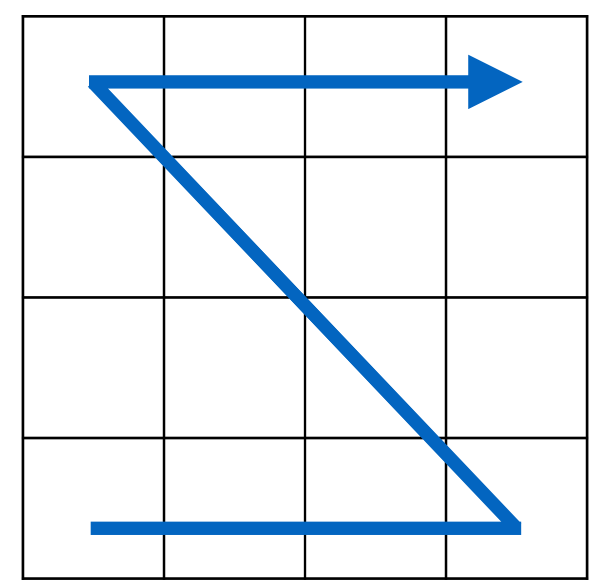
Mesh: 16 x 16 elements



Partition: 4 x 4 processors



Local element ordering (p5)



We wish to solve

$$A^{16}x^{16} = b^{16}$$

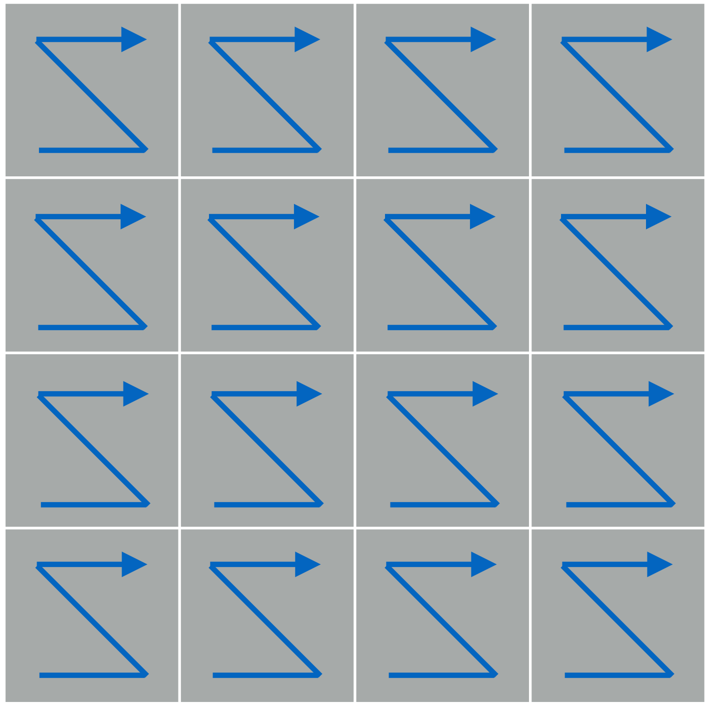
on a smaller number of processors

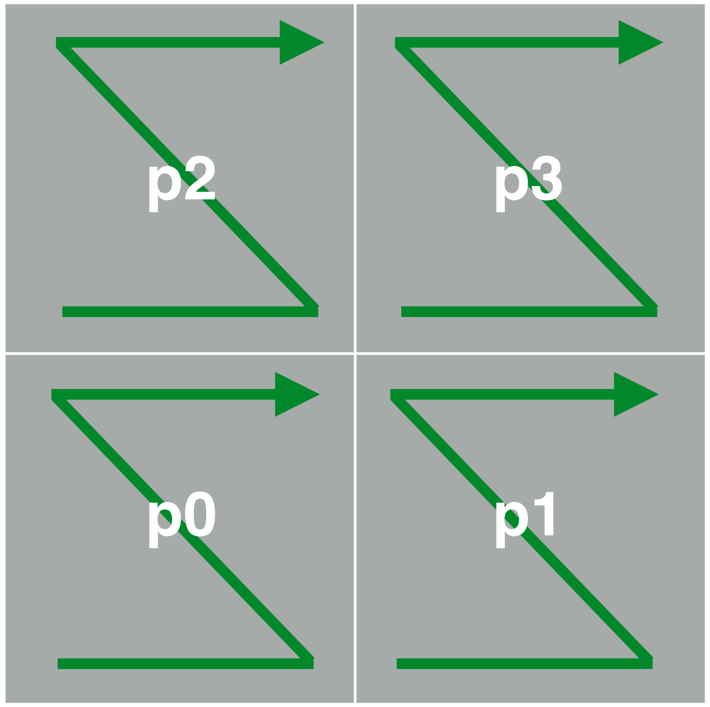
Repartitioning Coarse Grids

Repartition: 2 x 2 processors

A^{16}

b^{16}





A^4

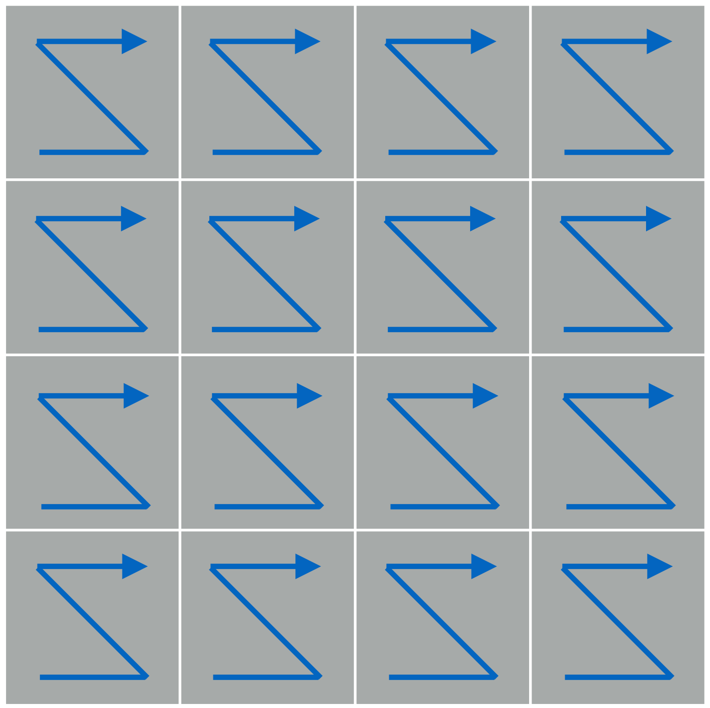
b^4

x^4

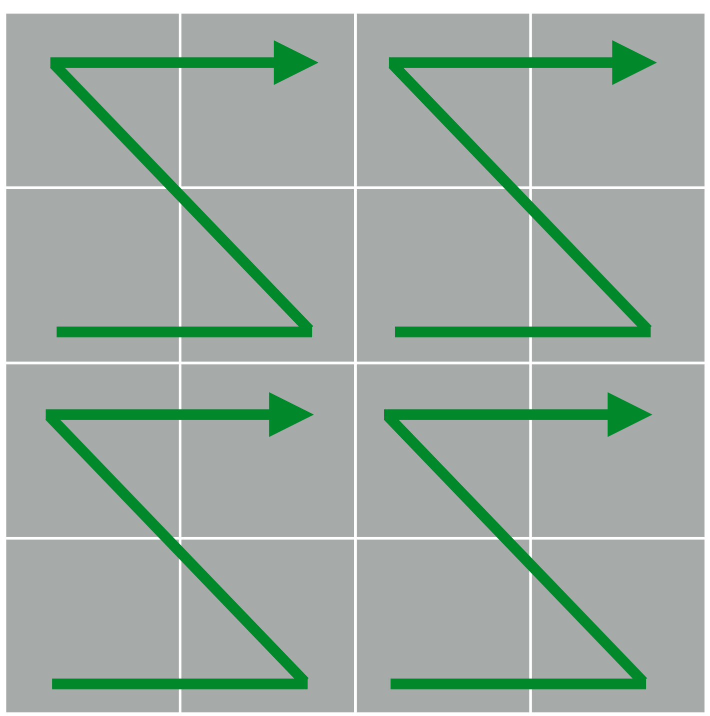
Repartitioning Coarse Grids

A^{16}

b^{16}



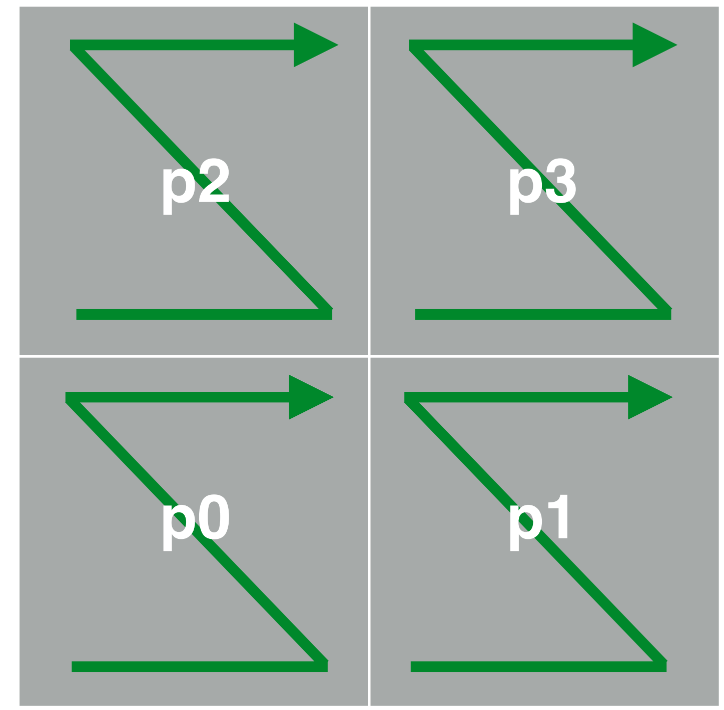
P^T



$A^{16\to 4}$

$b^{16\to 4}$

Repartition: 2 x 2 processors



A^4

b^4

x^4

$$\boldsymbol{A}^{16\to 4} = \boldsymbol{P}^T \boldsymbol{A}^{16} \boldsymbol{P}$$

$$\boldsymbol{A}^4 = \mathrm{GATHER}[\boldsymbol{A}^{16\to 4}]$$

$$\boldsymbol{b}^{16\to 4} = \boldsymbol{P}^T \boldsymbol{b}^{16}$$

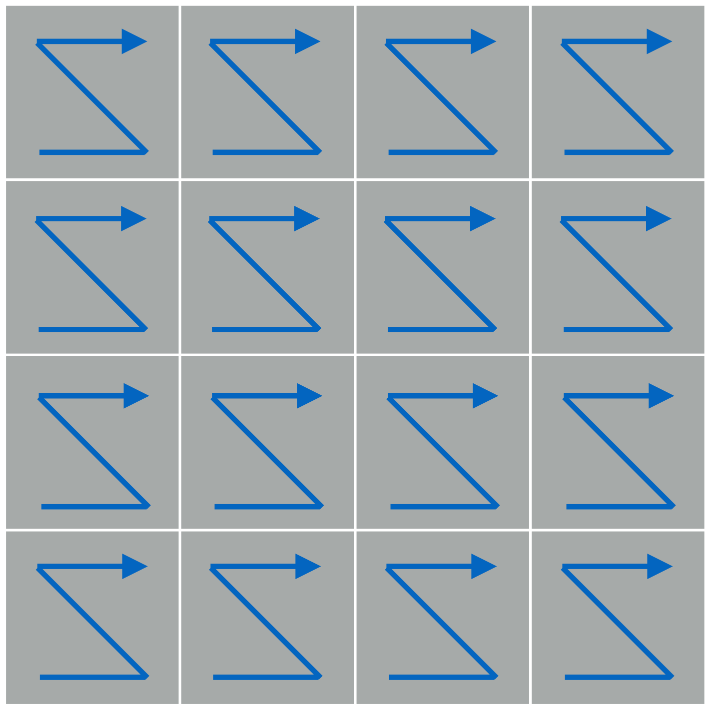
$$\boldsymbol{b}^4 = \mathrm{GATHER}[\boldsymbol{b}^{16\to 4}]$$

Perform solve $\quad \boldsymbol{A}^4 \boldsymbol{x}^4 = \boldsymbol{b}^4$

$$\boldsymbol{x}^{4\to 16} = \mathrm{SCATTER}[\boldsymbol{x}^4]$$

$$\boldsymbol{x}^{16} = \boldsymbol{P}\boldsymbol{x}^{4\to 16}$$

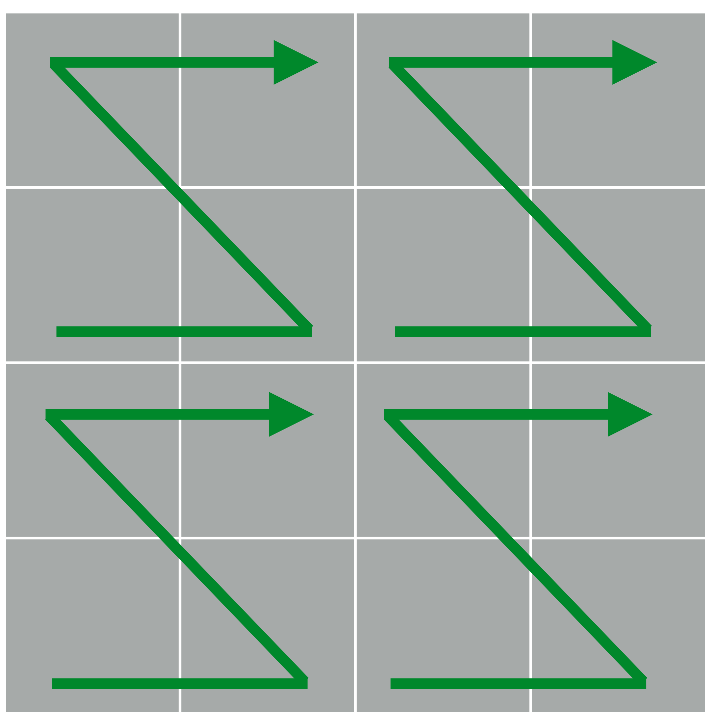
Repartitioning Coarse Grids



A^{16}

b^{16}

P^T



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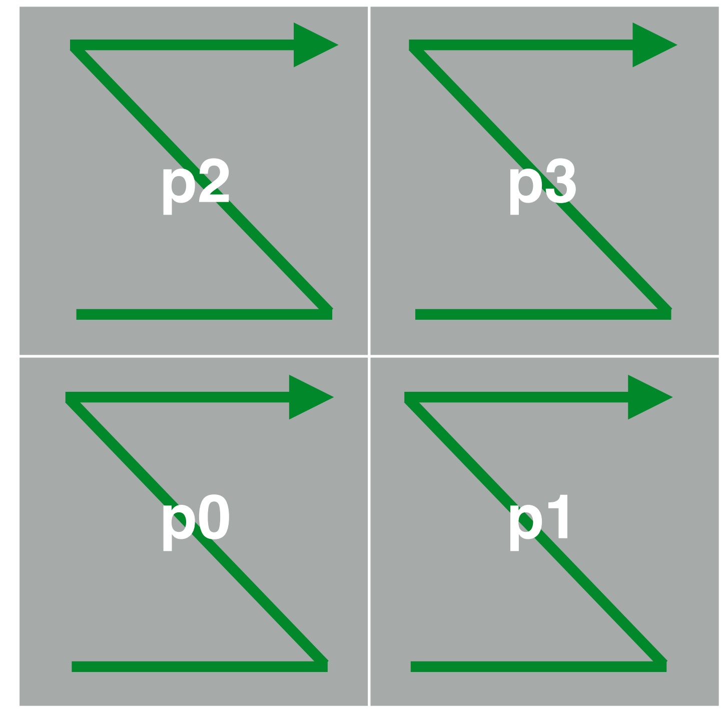

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Repartitioning Coarse Grids

Repartition: 2 x 2 processors

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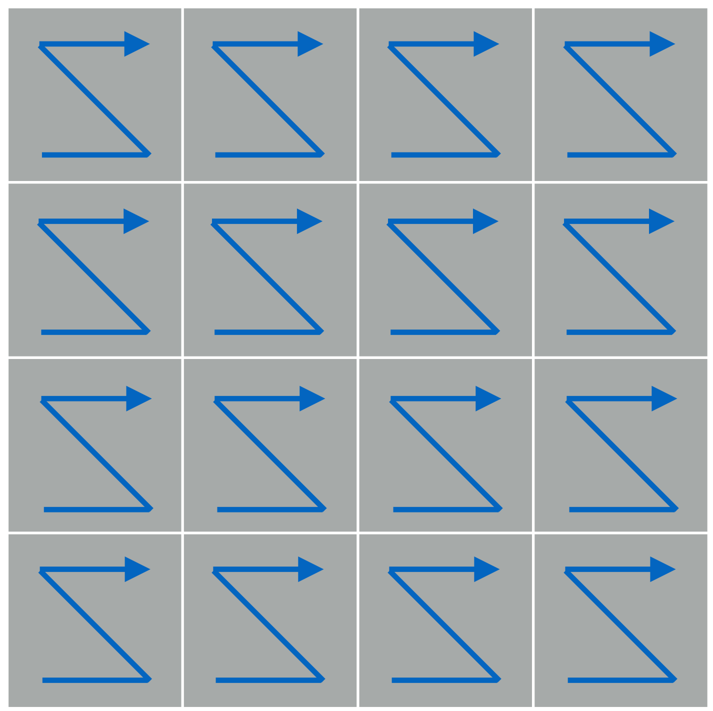
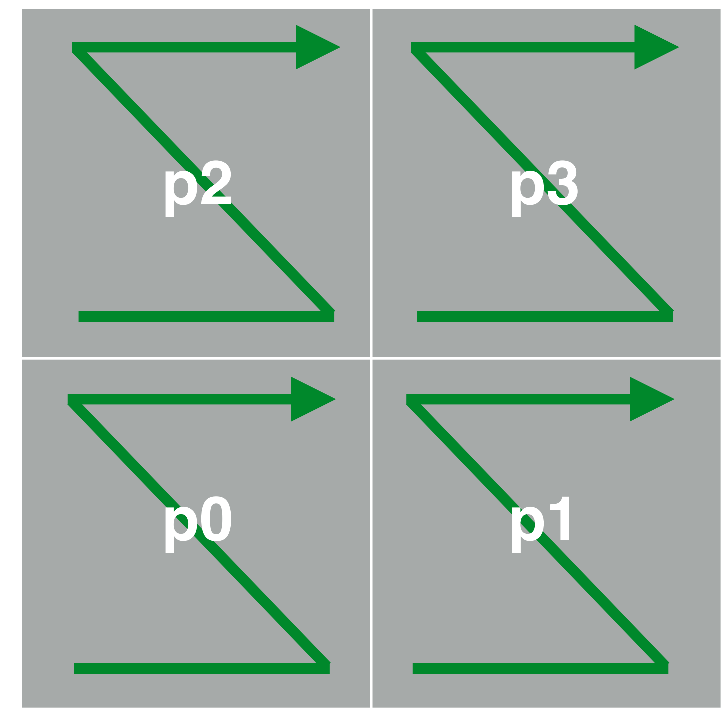
b^{16}



$\xleftarrow{P}$

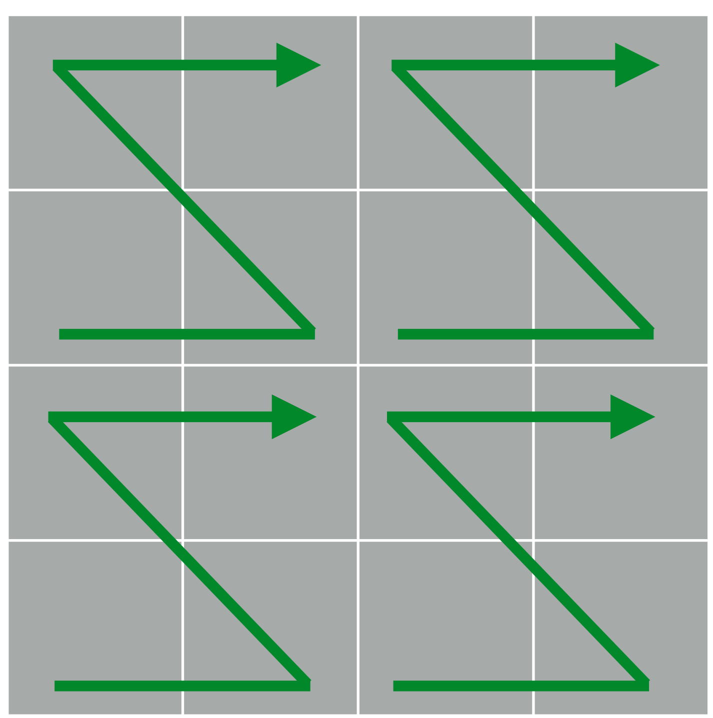


A^4

b^4

x^4

$P^T \downarrow$



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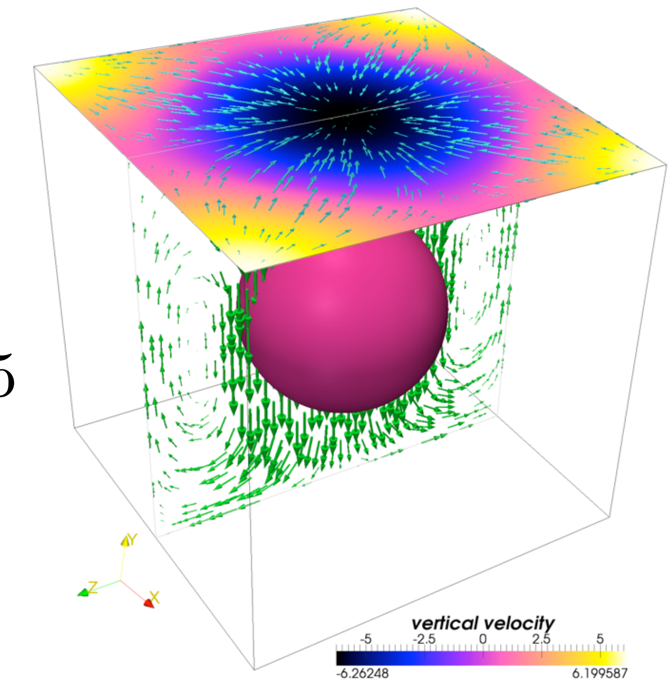
Linear Stokes Solver: Strong Scaling



- 96^3 Q2-P1 elements
- 3-level method
- Chebyshev(10)/Jacobi
- Coarse grid solvers:
  - Hierarchical Krylov
  - `PCGAMG`
  - Repartitioned (custom precursor to `PCTelescope`) by a factor of 16

$$R = 0.25$$
$$\Delta\eta = 10^4$$

Wall clock times (sec)

MPI-ranks		64	512	4096
Strategy	Task			
H-Krylov	Coarse solve	1.8872e+02	3.3849e+01	9.1787e+00
	Smoother	4.8848e+02	5.1566e+01	7.2146e+00
	Solve	9.9545e+02	1.1651e+02	1.9926e+01
GAMG	Coarse solve	3.3929e+01	4.8522e+00	3.6687e+00
	Smoother	3.4835e+02	4.3411e+01	6.9875e+00
	Solve	5.9950e+02	7.4663e+01	2.1039e+01
Repartitioned	Coarse solve	1.4028e+02	1.7607e+01	2.9893e+00
	Nested coarse solve	1.5587e+01	1.9563e+00	3.3214e−01
	Smoother	3.0379e+02	3.8059e+01	5.6223e+00
	Solve	6.4287e+02	8.0635e+01	1.1826e+01

Linear Stokes Solver: Strong Scaling

- 96^3 Q2-P1 elements
- 3-level method
- Chebyshev(10)/Jacobi
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  - Hierarchi[illegible]
  - **PCGAMG**
  - Repartiti[illegible]

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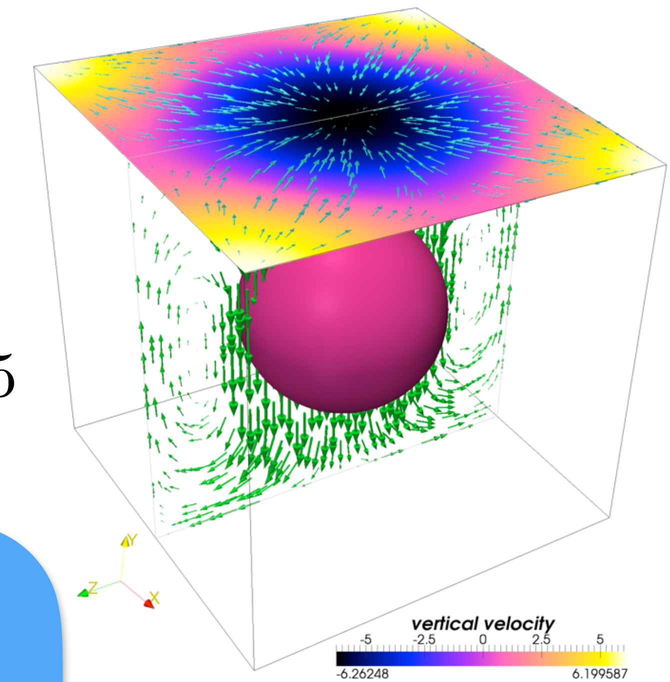


```
-mg_coarse_ksp_type fgmres
-mg_coarse_pc_type ksp
-mg_coarse_ksp_ksp_type chebyshev
-mg_coarse_ksp_ksp_max_it <maxit>
-mg_coarse_ksp_ksp_norm_type none
-mg_coarse_ksp_ksp_convergence_test skip
-mg_coarse_ksp_pc_type <pctype>
```

64 → 4096 ranks

Wall clock times (sec)

MPI-rank[illegible]		[illegible]	[illegible]	12[illegible]
Strategy				
H-Krylov	[illegible]	[illegible]	[illegible]	[illegible]
	Smoother	4.8848e+02	[illegible]	[illegible]
	Solve	9.9545e+02	1.1651e+02	1.9926e+01
GAMG	[illegible]	[illegible]3929e+01	[illegible]	[illegible]
	Smoother	[illegible]4835e+02	[illegible]	[illegible]
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Repartitio[illegible]	[illegible]	[illegible]e+02	1.7607e+01	2.9893e+00
	[illegible]	[illegible]	[illegible]	[illegible]
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	Solve	6.4287e+02	8.0635e+01	1.1826e+01

78% Strong scaling efficiency

```
-mg_coarse_pc_type gamg
```

45% Strong scaling efficiency

```
-mg_coarse_pc_type ????
```

85% Strong scaling efficiency

Linear Stokes Solver: Strong Scaling

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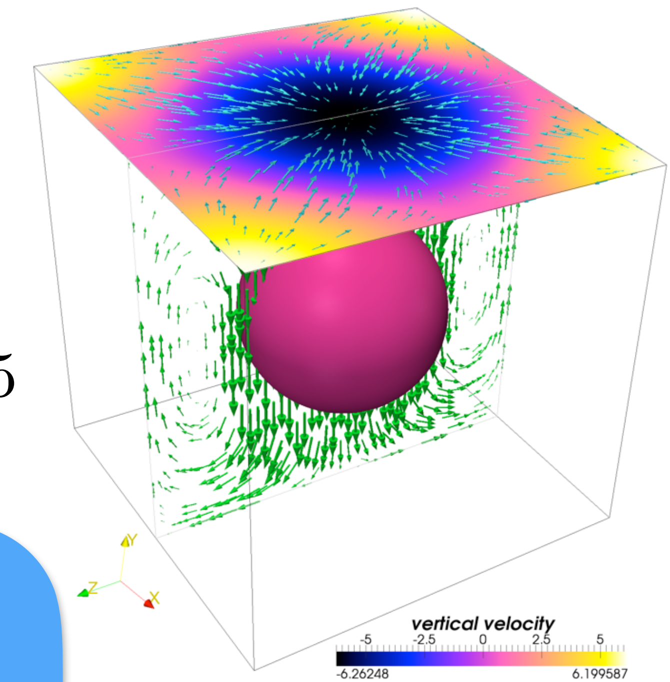


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	[illegible]	[illegible]	[illegible]	[illegible]
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```
-mg_coarse_pc_type telescope
```

85% Strong scaling efficiency

PCTelescope: *Agglomeration in PETSc*

Flavours of Multigrid for Variable Coefficients

[Chan & Wan, JCP, 2000]

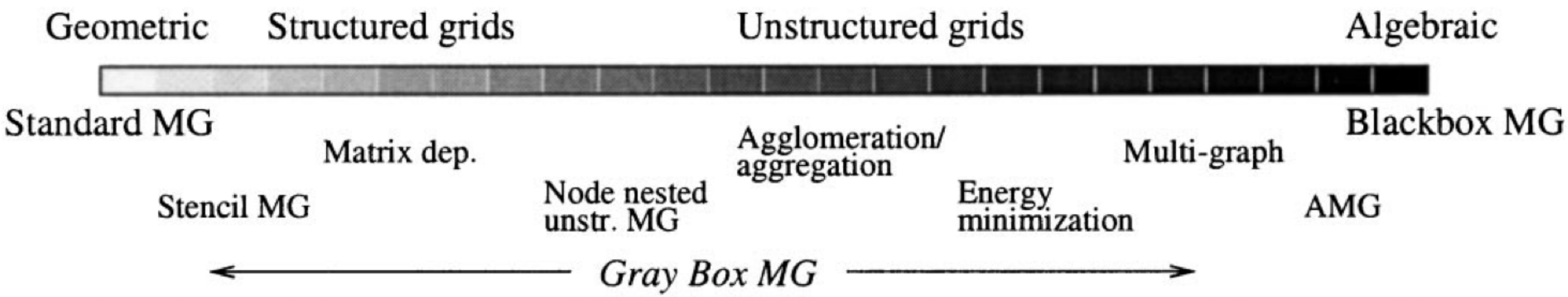

Fig. 1. A spectrum of multigrid methods.

Cheap (“Weak”)

Expensive (“Robust”)

Flavours of Multigrid for Variable Coefficients

[Chan & Wan, JCP, 2000]

Make **modular** and **simple**

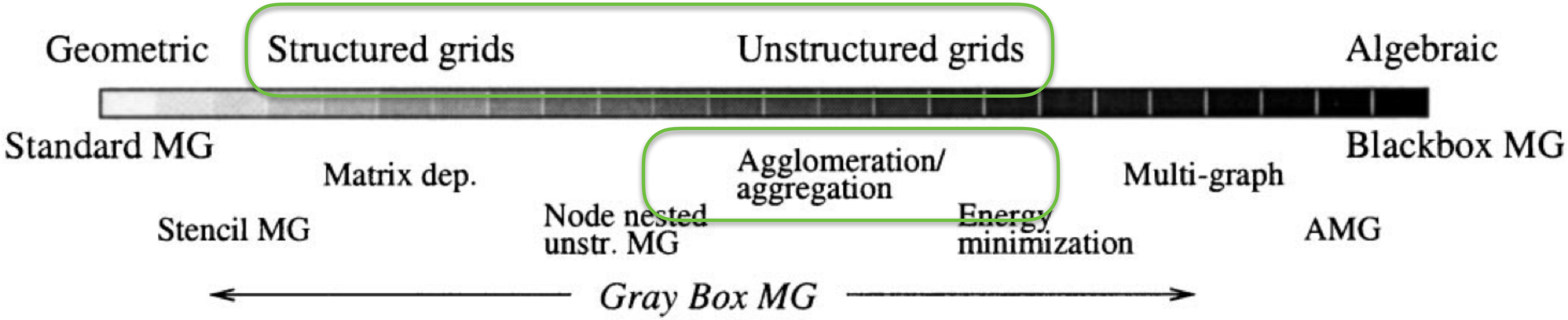

Fig. 1. A spectrum of multigrid methods.

Cheap (“Weak”)

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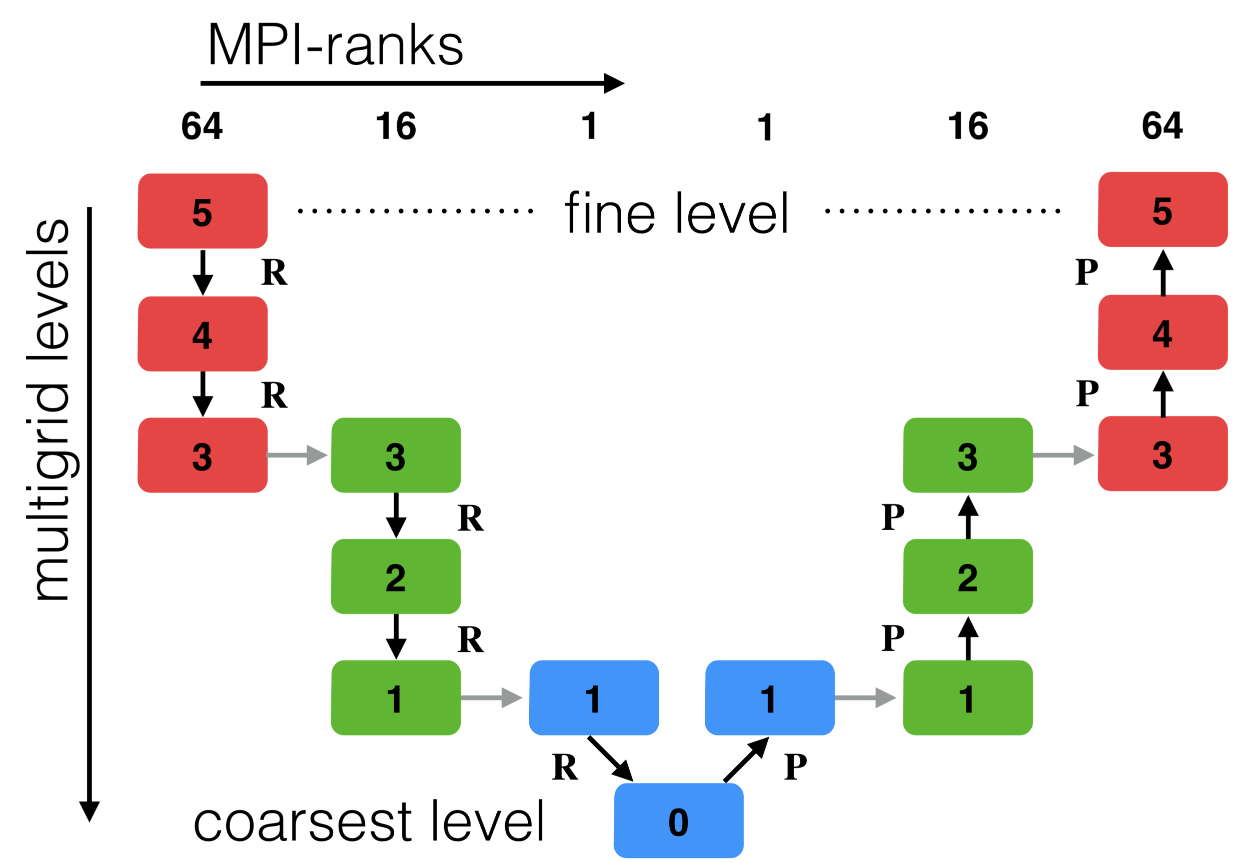
Implementing Agglomeration for Multigrid

- Not new, not impossible to implement*, but as an extreme-scale component, **rarely implemented at first, and often not at all** if code is insufficiently modular
- Predictive performance models are lacking, so **runtime configurability is useful**
- Agglomeration has uses outside of MG



*See our paper for many references

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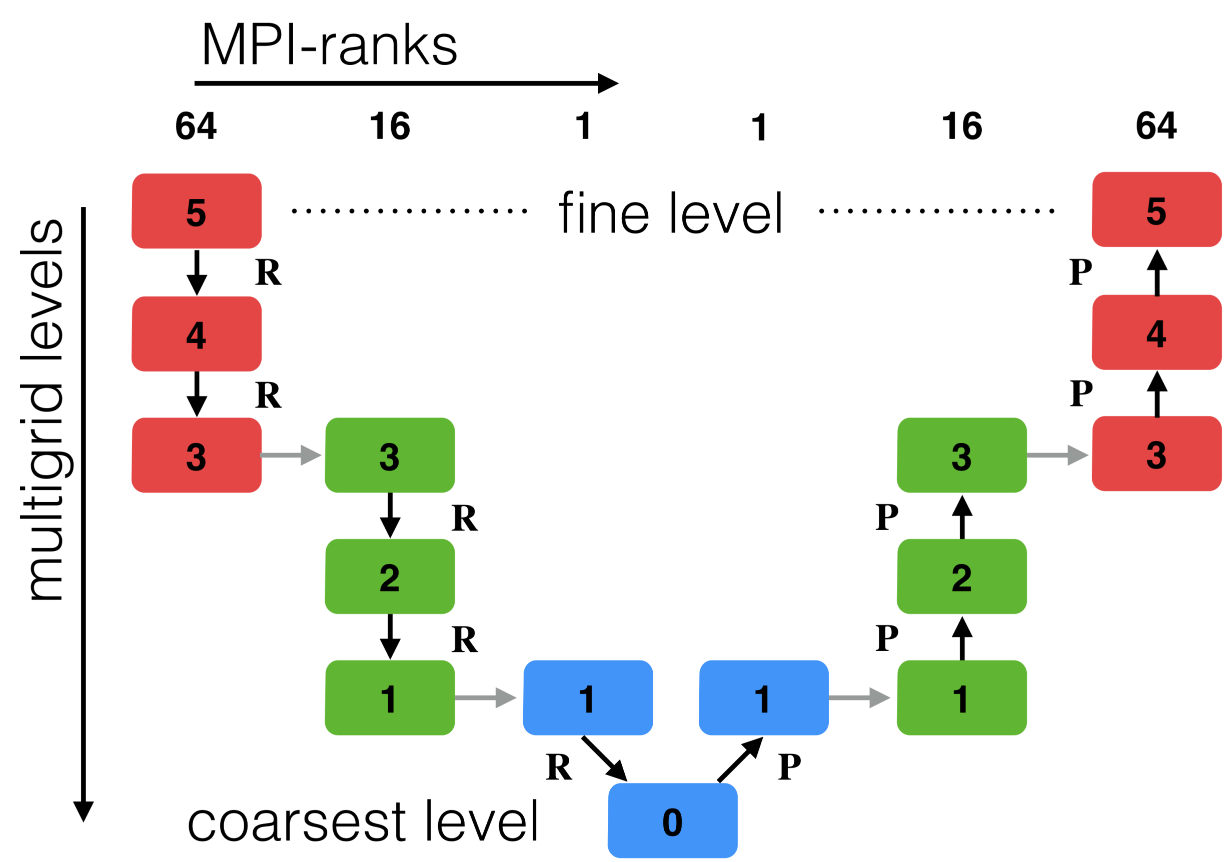


- We implement agglomeration as a **preconditioner** within PETSc, to provide a reusable building block
  - Simple, composable design
  - Not optimal for all usage, particularly in memory footprint.
- We focus on agglomeration which is **aware of domain connectivity** via PETSc's `DM` class

*See our paper for many references

Design Philosophy

- **P**ortable, **E**xtensible **T**oolkit for **S**cientific **c**omputation
- **P**ortable, **E**xtensible **T**oolkit for **S**olver **c**omposability ?
- Composable building blocks
  - `KSP` : iterative linear solver
  - `PC` : preconditioner within `KSP`
    - Also used for direct solvers
    - Nested `KSP` objects as subsolvers or smoothers
  - `SNES` : nonlinear solver
  - `DM` : domain management
- **Runtime configurability** is a central design decision.
  - experimentation usually required to choose solver parameters
  - Solvers and subsolvers addressed with **options prefixes**

```
-stokes_fieldsplit_u_mg_levels_2_ksp_type sor
```

Anatomy of a Prefix

Name of a **PC** type (**PCSOR**)

Custom prefix for a linear solver (**KSP**)

Option for **PC**

`-stokes_fieldsplit_u_mg_levels_2_pc_type sor`

Prefix for smoother within **PCMG**

Prefix for a block sub-solver within **PCFIELDSPLIT**

DM

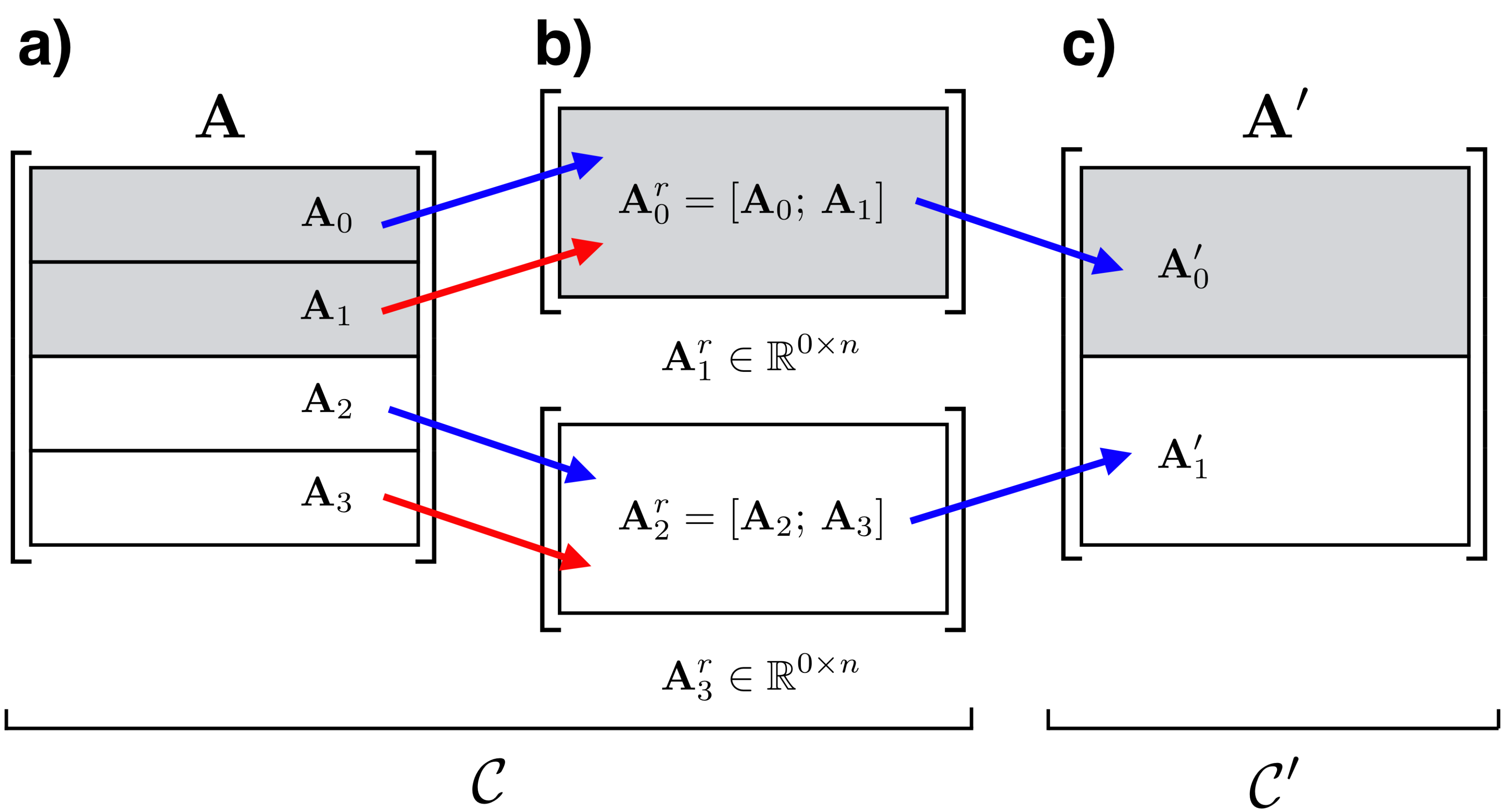
- A class to provide the required interface between solvers and distributed domains
- Geometric primitives, topological relationships between them, and field information

PCMG

- It's not entirely obvious that a solver library should include domain information
- However, geometric multigrid is facilitated with this information, so `PCMG` couples strongly to `DM`
- `PCTelescope` is also "`DM` aware"
- Following the design pattern of providing composable, nestable solvers, the smoothers on each level of the multigrid hierarchy, as well as the coarse grid solver, are `KSP` objects

PCTelescope Design - Assembled Matrices

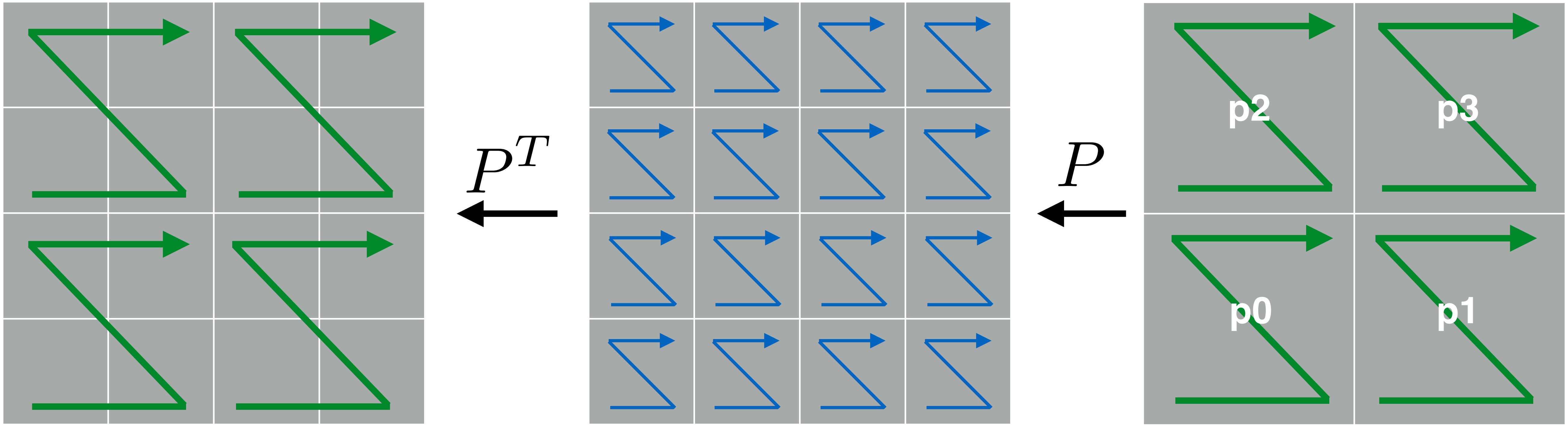
1. Given an MPI communicator $\mathcal{C}$, create a new communicator $\mathcal{C}'$.
2. Repartition the input matrix $\mathbf{A}$ and vector $\mathbf{x}$ onto $\mathcal{C}'$, yielding $\mathbf{A}'$ and $\mathbf{x}'$.
3. Apply a Krylov method to solve $\mathbf{A}'\mathbf{y}' = \mathbf{x}'$ on $\mathcal{C}'$.
4. Scatter the solution $\mathbf{y}'$ to $\mathcal{C}$ to obtain $\mathbf{y}$.



Nullspaces attached to $\mathbf{A}$ are automatically propagated!

DM Repartitioning

- PETSc allows `DM`'s to be associated with `KSP` objects, which in turn makes them available to `PC`'s like `PCTelescope`
- `PCTelescope` can automatically repartition regular 2D and 3D grids represented with `DMDA` objects
- This involves constructing a permutation to account for the new ordering



Use Cases

Multigrid with Truncation

Use an LU routine as a coarse grid solver:

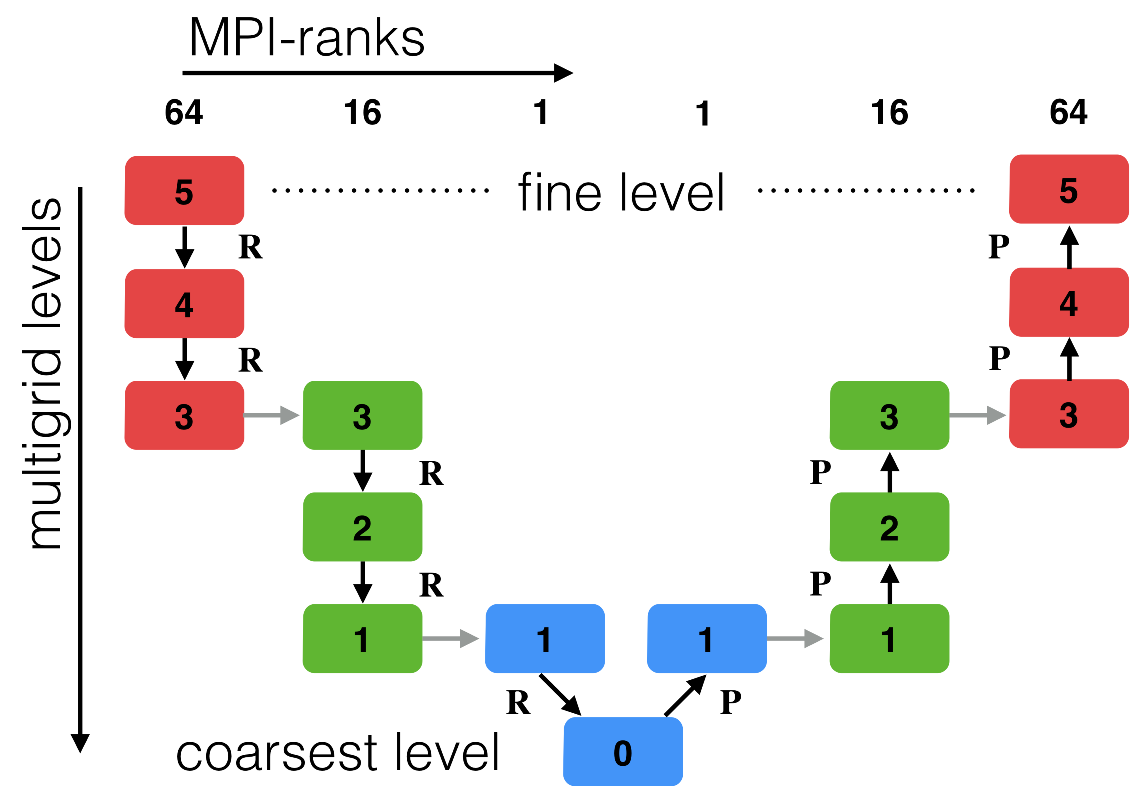
```
-pc_type mg
-pc_mg_levels <N>
-mg_coarse_pc_type telescope
-mg_coarse_pc_telescope_reduction_factor <r>
-mg_coarse_telescope_pc_type lu
-mg_coarse_pc_telescope_subcomm_type
[contiguous,interlaced]
```

Interface to your sequential or parallel direct solver of choice

(recent addition in PETSc `master`)

First **np/r** ranks, or every **r**th rank?

Repartitioned Coarse Grids




```
-pc_type mg
-pc_mg_levels 2
-pc_mg_galerkin
-mg_coarse_pc_type telescope
-mg_coarse_pc_telescope_reduction_factor 4

-mg_coarse_telescope_pc_type mg
-mg_coarse_telescope_pc_mg_levels 2
-mg_coarse_telescope_pc_mg_galerkin
-mg_coarse_telescope_mg_coarse_pc_type telescope
-mg_coarse_telescope_mg_coarse_pc_telescope_reduction_factor 16

-mg_coarse_telescope_mg_coarse_telescope_pc_type mg
-mg_coarse_telescope_mg_coarse_telescope_pc_mg_levels 2
-mg_coarse_telescope_mg_coarse_telescope_pc_mg_galerkin
```

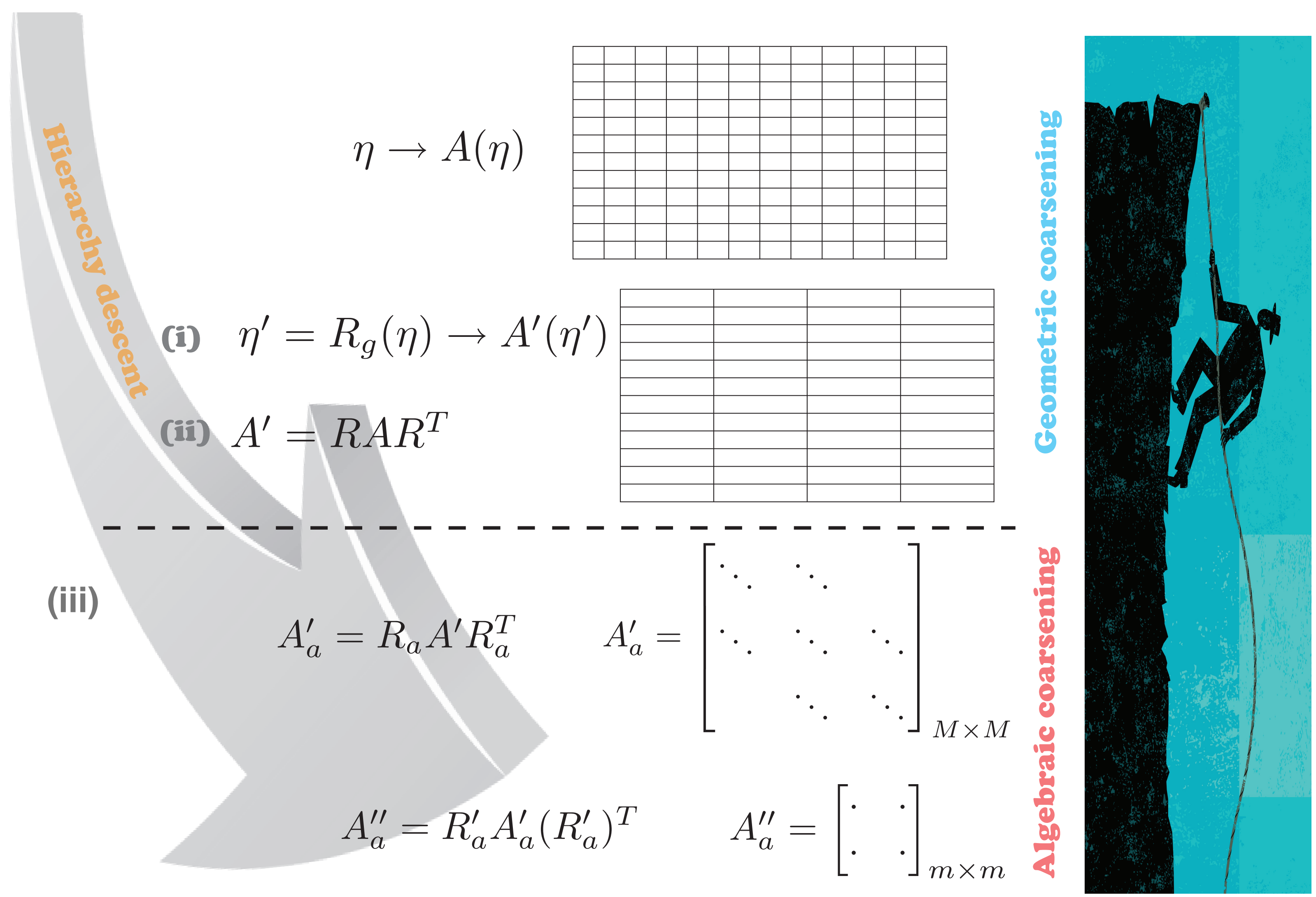
Hybrid Coarse Operator Construction

```
-pc_type mg
-pc_mg_levels <N1>
-mg_coarse_pc_type telescope
-mg_coarse_pc_telescope_reduction_factor <r>
-mg_coarse_telescope_pc_type mg
-mg_coarse_telescope_pc_mg_levels <N2>
-mg_coarse_telescope_pc_mg_galerkin
-mg_coarse_telescope_mg_coarse_pc_type gamg
```

Re-disc. geom. MG

Galerkin MG

Algebraic MG



Subdomain Smoothers with Constant Size

```
-pc_type mg
-pc_mg_levels <N>
-mg_levels_pc_type telescope
-mg_levels_pc_telescope_reduction_factor <rn>
-mg_levels_telescope_pc_type bjacobi
-mg_levels_telescope_sub_pc_type <xxx>
```

Smoothers with Different Spatial Decomposition

```
-pc_type mg
-pc_mg_levels <N>
-mg_levels_pc_type telescope
-mg_levels_pc_telescope_reduction_factor <r>
-mg_levels_telescope_repart_da_processors_z 1
```

Edison

2.57 PFlop/s peak

Numerical Experiments

Piz Daint

7.787 PFlop/s peak

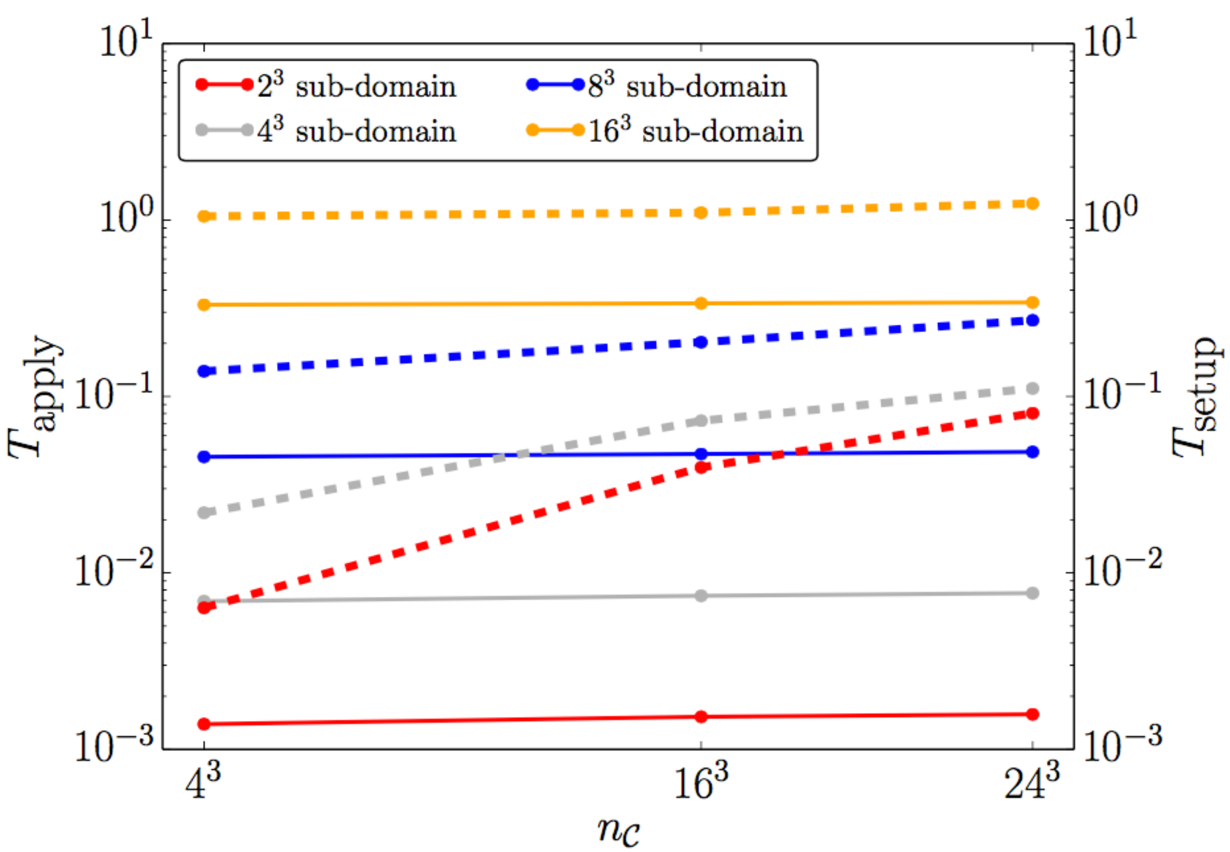
2,968m peak courtesy Sascha M. Schnepp

Agglomeration Profiling

- Profile Setup and Application times for `PCTelescope` on Piz Daint
- 3D FD Laplacian (N^3 DOF)
  - `$PETSC_DIR/src/ksp/ksp/examples/tutorials/ex45.c`

n_C	N	r	T_{setup} (s)	T_{apply} (s)
64	8	8	1.64E−03	8.11E−05
64	8	16	1.77E−03	1.00E−04
64	8	32	1.88E−03	1.51E−04
64	8	64	2.05E−03	2.80E−04
4096	32	8	3.02E−02	5.63E−04
4096	32	16	3.82E−02	3.84E−04
4096	32	32	3.19E−02	3.74E−04
4096	32	64	3.12E−02	6.21E−04
13824	48	8	4.37E−02	4.30E−04
13824	48	16	4.55E−02	3.53E−04
13824	48	32	5.76E−02	5.58E−04
13824	48	64	5.50E−02	5.62E−04

- 3D Q1-Q1 stabilized Stokes problem (M^3 elements)
  - `$PETSC_DIR/src/ksp/ksp/examples/tutorials/ex42.c`



n_C	M	r	T_{setup} (s)	T_{apply} (s)
64	8	8	6.34E−03	1.39E−03
64	8	16	1.02E−02	2.06E−03
64	8	32	1.23E−02	3.26E−03
64	8	64	1.72E−02	4.44E−03
4096	32	8	3.96E−02	1.53E−03
4096	32	16	4.93E−02	2.58E−03
4096	32	32	5.76E−02	4.20E−03
4096	32	64	7.39E−02	7.33E−03
13824	48	8	8.04E−02	1.58E−03
13824	48	16	8.91E−02	2.60E−03
13824	48	32	1.02E−01	4.20E−03
13824	48	64	1.30E−01	7.37E−03

Repartitioning at Scale

- 3D linear elasticity example, run on Edison
- Q2 finite elements implemented on top of `DMDA`
- FGMRES preconditioned with a single V-cycle of geometric multigrid
- Strong-scaling test to stress communication
- “Easy” with constant coefficents: variable coefficients cause further problems for the truncated approach

M	levels	N_L	ranks	$T_{\mathrm{setup}}^{tele}$ (s)	T_{solve} (s)
32	2	2	16^3	–	8.34E−01
32	2, 3	4	16^3, 4^3	8.56E−02	5.23E−01
32	2, 3, 3	6	16^3, 4^3, 1	9.54E−02	1.27E−01
64	2	2	32^3	–	1.48E+01
64	2, 3	4	32^3, 8^3	2.30E−01	1.40E−01
64	2, 3, 3	6	32^3, 8^3, 2^3	3.71E−01	1.82E−01
64	2, 2, 3	5	32^3, 16^3, 4^3	3.43E−01	1.39E−01
64	2, 2, 3, 3	7	32^3, 16^3, 4^3, 1	3.71E−01	1.51E−01

Hybrid CPU-GPU Subdomain Smoothers

- On a hybrid system, one may wish to use agglomerated communicators with a single rank per available accelerator
- We can do so on Piz Daint, assigning a single rank per GPU in the agglomerated communicator
- This allows comparison of SpMV performanceFrom the command line
  - With no need for threads (flat MPI + subcommunicators)

	CPU (8 MPI-ranks)			GPU		
M	Time (s)	GF/s	E/s	Time (s)	GF/s	E/s
4	8.89E−03	11.99	720k	2.43E−02	4.40	264k
8	1.27E−01	6.96	402k	5.90E−02	14.99	865k
12	4.15E−01	7.3	417k	1.91E−01	15.91	908k
24	3.15E+00	7.79	439k	1.44E+00	17.09	963k

Hybrid CPU-GPU Subdomain Smoothers

- We can also compare time to solution of a full solve using GPU subdomain smoothers

M	levels	overlap	T_{setup} (s)	Its.	T_{solve} (s)
8	2	–	1.12E−02	12	4.27E−02
12	3	–	4.41E−02	16	2.06E−01
24	3	–	1.88E−01	13	1.55E+00
48	4	–	1.29E+00	11	9.92E+00
8	2	0	5.49E−01	12	2.2813e-01
12	2	0	2.52E+00	16	2.3985e-01
24	3	0	4.94E+00	13	**1.28E+00**
48	4	0	3.58E+01	11	**6.66E+00**
8	2	1	5.95E−01	12	2.40E−01
12	2	1	1.10E+00	16	4.30E−01
24	3	1	5.55E+00	13	**1.52E+00**
48	4	1	2.30E+01	11	**7.34E+00**

Future Development: Agglomeration for Multigrid on Unstructured Meshes

Extending to Support Unstructured Grids

- PETSc supports unstructured grids via the `DMPlex` class
- Ordering is more complicated
  - “Reduction factor” is less clear
  - Permutation and Scatter objects more complex to generate
- More attached structure must be considered and repartitioned
- Regardless, all required operations are algebraic and can be defined - the key is to lower the burden on a typical user
- Proposed Solution
  - When working with `DMPlex` (or more exotic `DM` implementations), return the responsibility of defining the reduced communicator and required mappings to the `DM`, requiring a call to `DMPlexGetReducedComm()`

Concluding Remarks

- Subdomain agglomeration in extreme-scale geometric multigrid allows for scalability
- This pattern can be encapsulated as a component with preconditioner semantics
- A single simple design, aware of operator nullspaces and underlying domain descriptions, can be effectively used in several ways
  - Coarse grid agglomeration in multigrid
  - Efficient construction of agglomerated subdomains to use with factorization-based sub-solvers
  - Efficient construction of agglomerated subdomains for use with coprocessors associated with multiple CPU cores in a flat MPI environment

Concluding Remarks

`PCTelescope` available in PETSc 3.7

- Composable tool for MPI rank agglomeration, implemented as a PETSc `PC`
- Aware of operator nullspaces and structured grids (`DMDA`)
- Useful for multigrid hierarchies as well as other tasks requiring agglomeration
- Controllable at runtime from the command line
- Main use case: (hybrid) MG hierarchies
- Auxiliary use cases: easy plumbing to define nested operators
- Also supports matrix-free / unassembled operators
  - Override `DMCreateMatrix()` and use `KSPSetComputeOperators()`

Thank You for Your Attention, and Try It Out!

- `PCTelescope` in current PETSc release 3.7.x
  - `mcs.anl.gov/petsc`
- Ongoing improvements in PETSc **`master`**
  - `https://bitbucket.org/petsc/petsc`
- Get in touch if you are interested in the development of `PCTelescope` for unstructured meshes used `DMPlex`
  - `dave.may@erdw.eth.ch`
  - `patrick.sanan@{usi.ch,erdw.ethz.ch}`
- Paper:
  - Dave A. May, Patrick Sanan, Karl Rupp, Matthew G. Knepley, and Barry F. Smith. 2016. **Extreme-Scale Multigrid Components within PETSc**. In Proceedings of the Platform for Advanced Scientific Computing Conference (PASC '16)

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