Parallel Multigrid Tutorial

19th Copper Mountain Conference on Multigrid Methods

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References and Acknowledgements

- "Introduction to Parallel Computing", Blaise Barney
  – https://computing.llnl.gov/tutorials/parallel_comp/

- "A Parallel Multigrid Tutorial", Jim Jones
  – Copper Mountain tutorial in 1999, 2005, & 2007

- "A Parallel Computing Tutorial", Ulrike Meier Yang
  – IMA Tutorial at Workshop on Fast Solution Techniques, Nov 2010

Outline

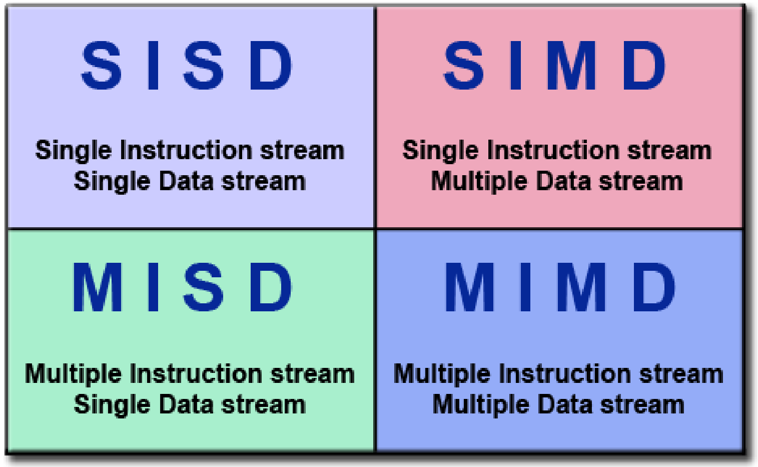
- Parallel Computing
  - Classical computer taxonomy
  - Programming models
  - Parallel performance metrics
  - Parallelizing PDE-based problems

- Parallel Multigrid
  - Parallel Algebraic Multigrid
  - Parallel Multigrid Software Design
  - Some Current Research Topics

Parallel Computing

Classical Taxonomy of Computers due to Michael Flynn in 1972

- Classifies by instruction stream and data stream



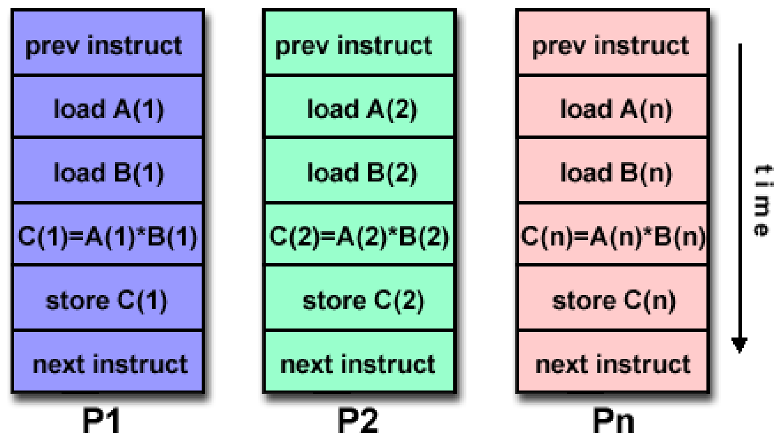
SISD Single Instruction stream Single Data stream	**SIMD** Single Instruction stream Multiple Data stream
MISD Multiple Instruction stream Single Data stream	**MIMD** Multiple Instruction stream Multiple Data stream

- Two main types of parallel systems today
  - SIMD: GPUs, Intel Knights Landing (KNL)
  - MIMD: Most supercomputers, clusters, multi-core PCs

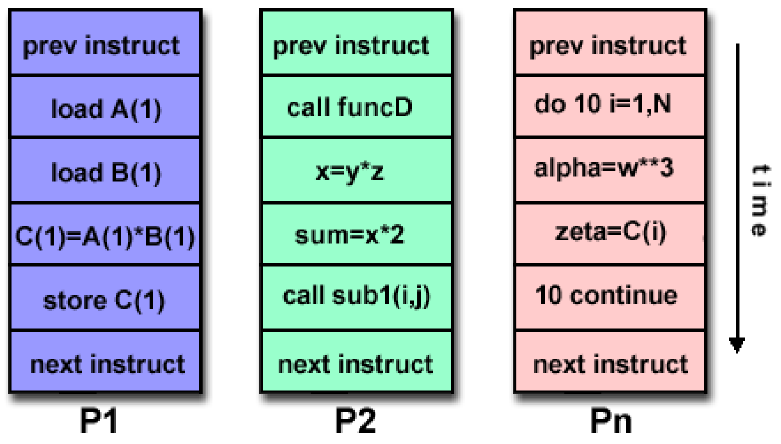
- Recent supercomputers are MIMD with SIMD subcomponents

SIMD vs MIMD in Pictures

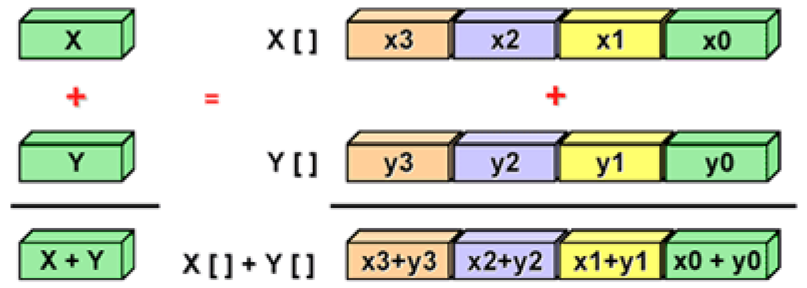
SIMD: instruction stream is the same



MIMD: instruction stream is different

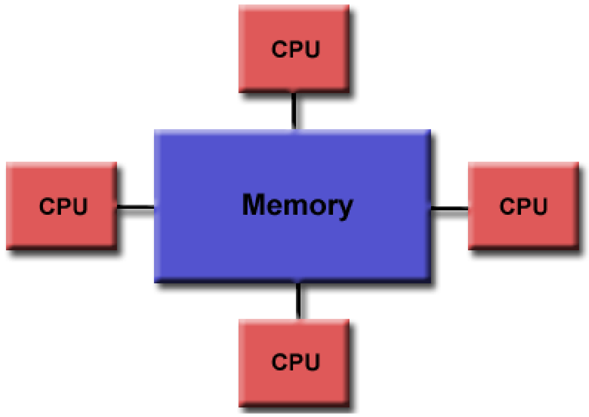


Example SIMD computation: vector addition

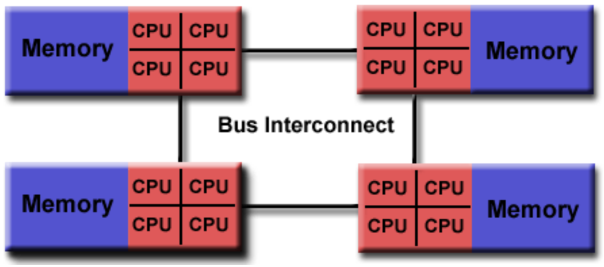


Parallel Computer Memory Architectures – Shared Memory

- All processors can access the same memory
- Uniform memory access (UMA):
  - Same access time to memory
- Non-uniform memory access (NUMA)
  - Different access times to different memories
- Advantages:
  - User-friendly programming perspective to memory (global address space)
  - Data sharing is fast
- Disadvantages:
  - Lack of scalability between memory and CPUs
  - Programmer responsible to ensure "correct" access of global memory



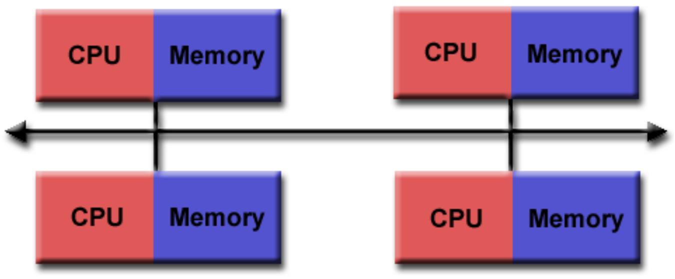
Shared Memory (UMA)



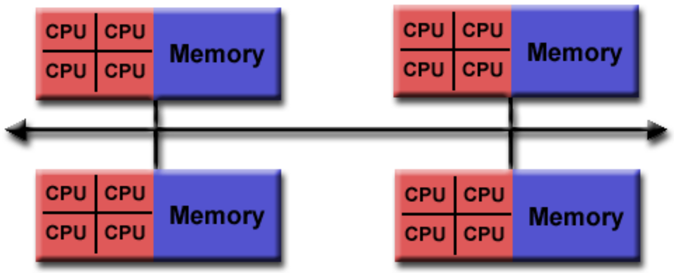
Shared Memory (NUMA)

Parallel Computer Memory Architectures – Distributed Memory

- Require a communication network to connect inter-processor memory
- Advantages:
  - — Memory is scalable with number of processors
  - — No memory interference or overhead for trying to keep cache coherency
- Disadvantages:
  - — Programmer responsible for data communication between processors
  - — Difficult to map data structures to memory
- Hybrid Distributed-Shared Memory
  - — Generally used for today's largest and fastest computers



Distributed Memory



Hybrid Architecture

Parallel Programming Models

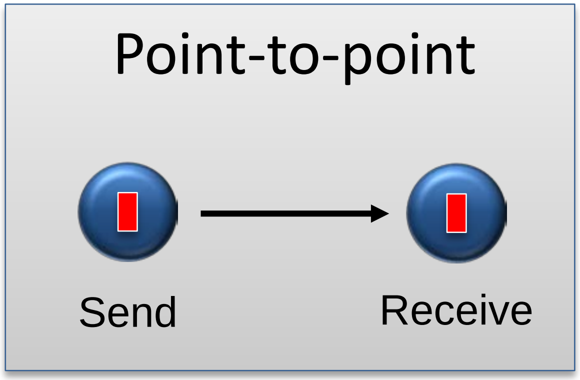
- Shared memory (without threads)
  - API in many operating systems, SHMEM
- Shared memory with threads
  - POSIX Threads (Pthreads), OpenMP (1997)
- Message Passing
  - MPI (Message Passing Interface, 1994)
- Data Parallel
  - Also referred to as Partitioned Global Address Space (PGAS) model
  - Coarray Fortran, Unified Parallel C (UPC), Global Arrays, X10, Chapel
- Hybrid
  - MPI+OpenMP, MPI+CUDA, etc.

- All of these can be implemented on any architecture
  - Most common approach – Single Program Multiple Data (SPMD)

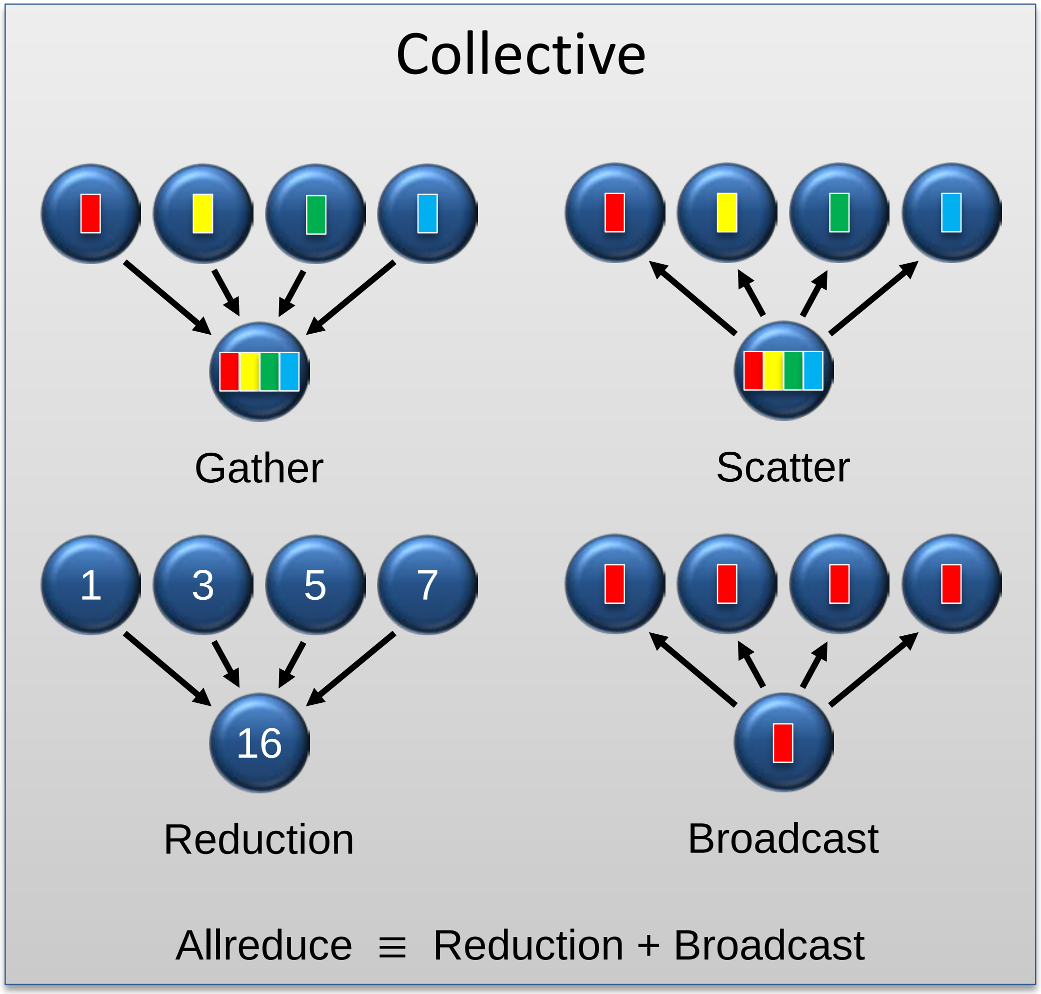
This tutorial will discuss parallel multigrid from a distributed-memory message-passing viewpoint

- Will mostly use conceptual diagrams and descriptions
- Will not focus on implementation details and specific code
- MPI and OpenMP will be the primary languages mentioned

Communication – Two basic types

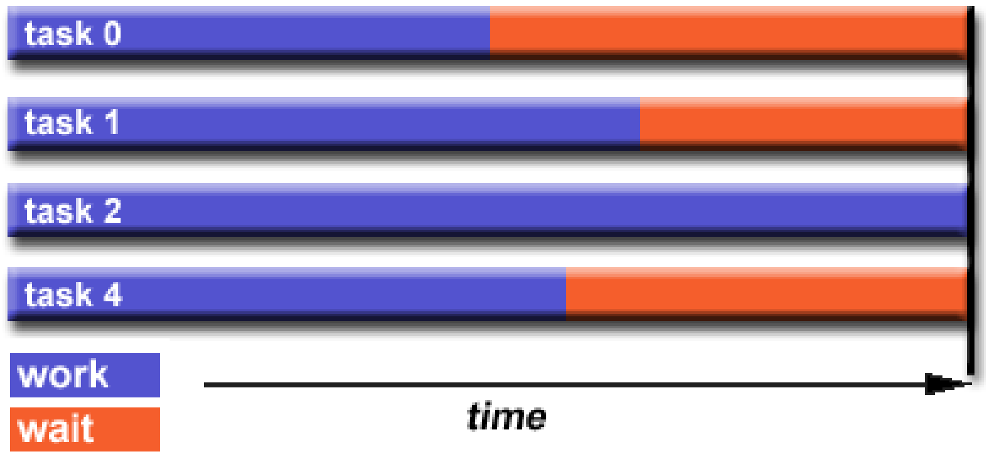


- MG codes mainly use
  - Send, Receive
  - Allreduce (MPI routine)
- Gather and Scatter are not scalable



Load balancing

- Keep all tasks busy all of the time
  - Minimize idle time
- The slowest task will determine the overall performance



Parallel Computing Performance Metrics

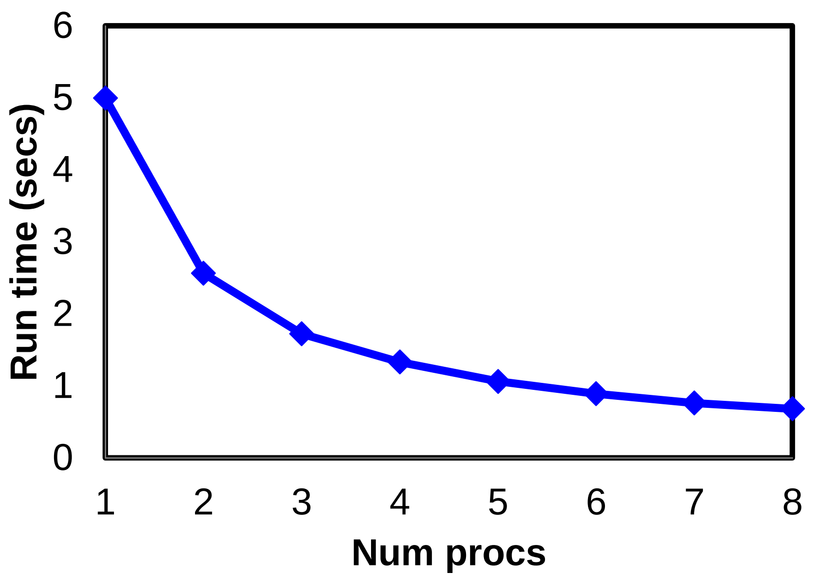
- Let $T(N,P)$ be the time to solve a problem of size N using P processors

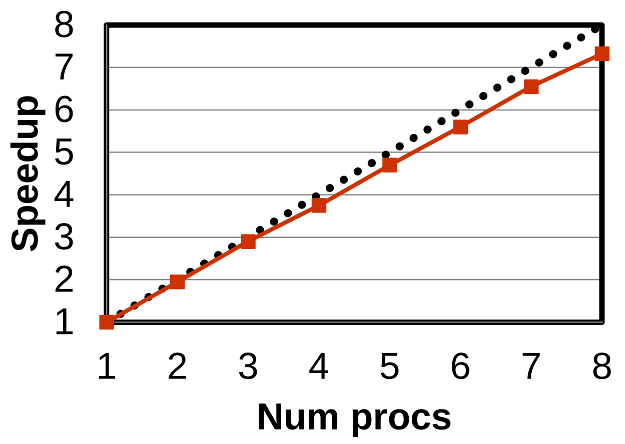
- Strong scaling – problem size is fixed
  - Speedup: $S(N,P) = T(N,1) \,/\, T(N,P)$
  - Efficiency: $E(N,P) = S(N,P) \,/\, P$

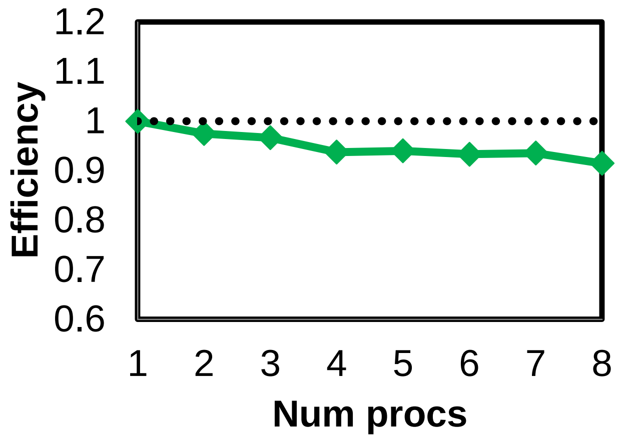
- Weak scaling – problem size is proportional to P
  - Scaled Efficiency: $SE(N,P) = T(N,1) \,/\, T(PN,P)$

- An algorithm is scalable if $T(PN,P) \leq C$ for all P
  - Ideally C is a constant, but this is not always possible
  - For multigrid, C grows as $\log P$ (this is optimal for some problems)

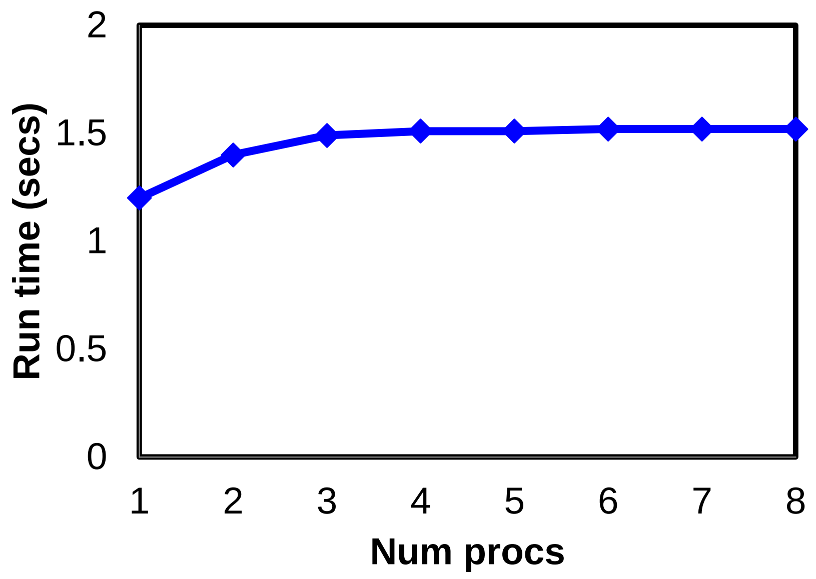
Strong Scaling – fix the problem size and increase the number of processors

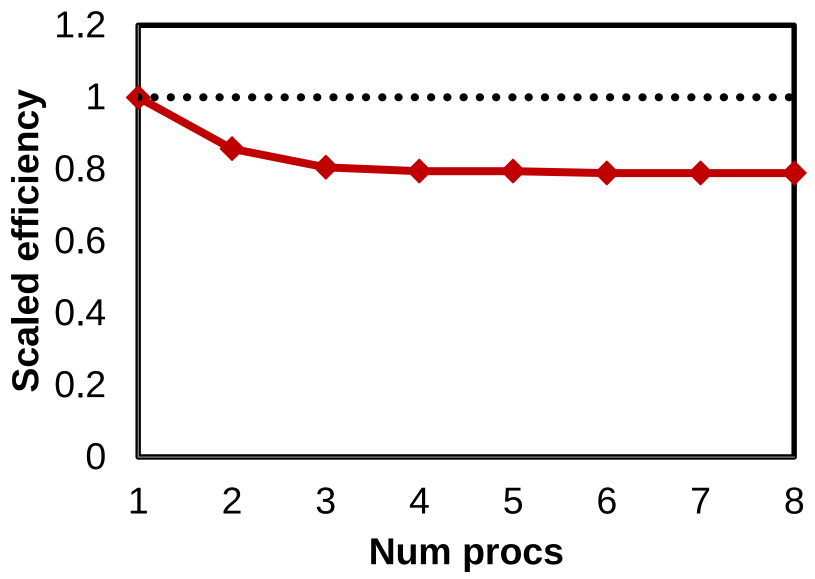






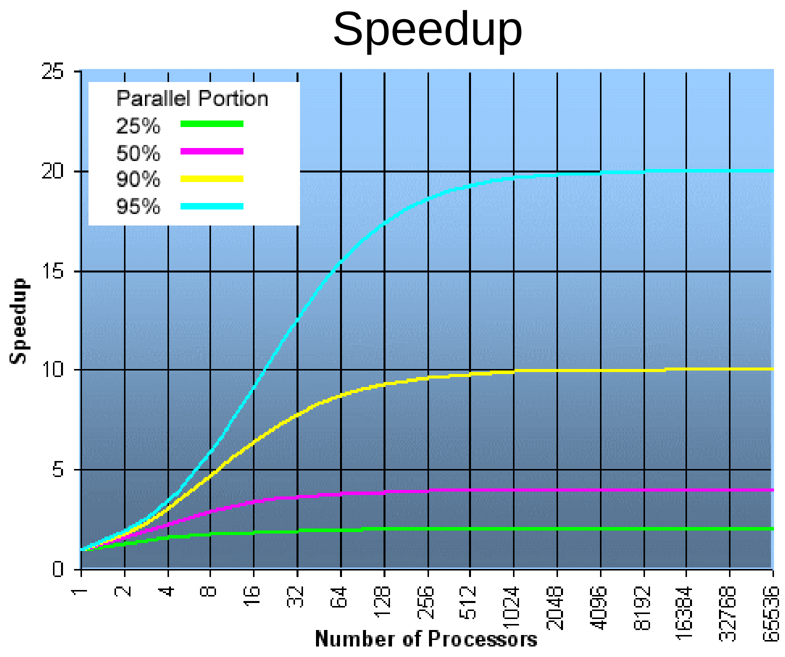
Weak Scaling – increase the problem size and the number of processors proportionately

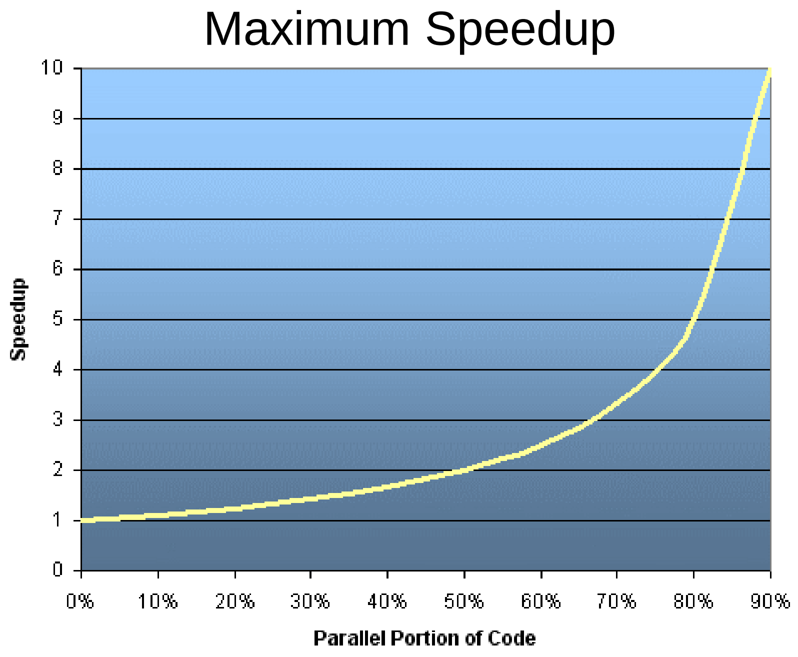




Amdahl's Law models speedup as a function of the serial (non-parallelizable) component of a code

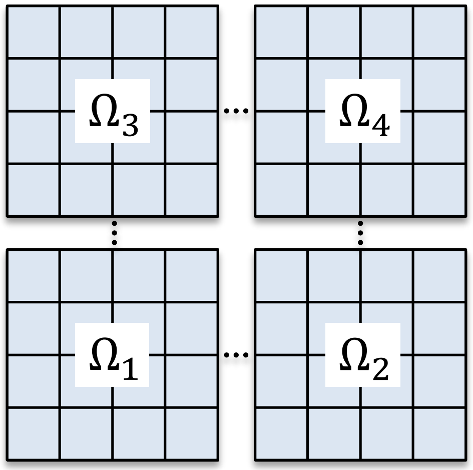
$$\text{Speedup} = \frac{1}{\underbrace{F}_{\text{Parallelizable fraction}}/\underbrace{P}_{\text{Num processors}} + \underbrace{(1-F)}_{\text{Serial fraction}}} < \boxed{\frac{1}{(1-F)}} \leftarrow \text{Maximum Speedup}$$





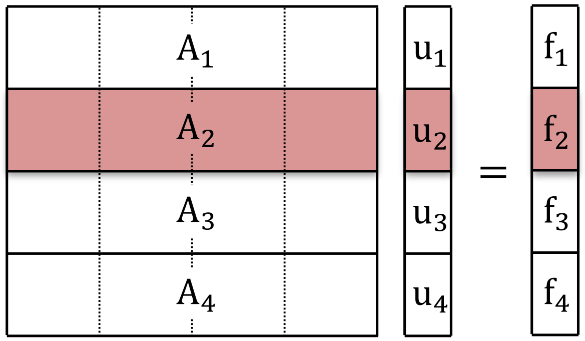
Domain partitioning is the primary approach for parallelizing PDE-based problems

- Example grid Ω partitioned into 4 subdomains Ω_p



- Processor p owns data associated with Ω_p

- Example sparse linear system resulting from a discretized PDE (e.g., 5-pt cell-centered discretization of $\Delta u = f$)

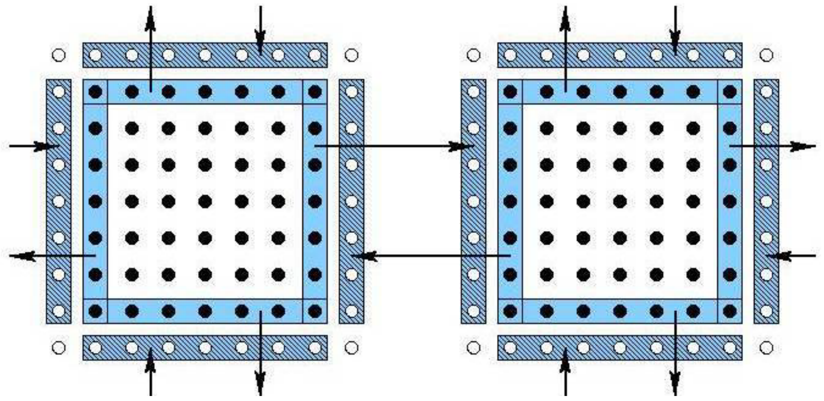


- Each 5-pt stencil corresponds to a row of A

- Processor p owns A_p, u_p, f_p

Basic linear algebra operations are at the core of parallel multigrid algorithms

- Matrix-vector multiply: Ax
- On each processor p:
  - Exchange subdomain boundary data with “nearest neighbors” (MPI Send/Recv)
  - Compute local product $A_p x_p$



- Vector addition: $z = x + y$

z_0	=	x_0	+	y_0	← Proc 0
z_1	=	x_1	+	y_1	← Proc 1
z_2	=	x_2	+	y_2	← Proc 2

- Vector product: $s = x^T y$
  - Compute local product then $s_0 + s_1 + s_2$ (MPI Allreduce)

s_0	=	x_0	*	y_0	← Proc 0
s_1	=	x_1	*	y_1	← Proc 1
s_2	=	x_2	*	y_2	← Proc 2

Parallel programming models provide useful incite into expected performance

- Most common communication/computation model
  - Simple, but effective for providing qualitative understanding
  - Better models account for message contention, network topology, etc.

$$T_{comm} = \alpha + m\beta \quad \text{(communicate m doubles)}$$

$$T_{comp} = m\gamma \quad \text{(compute m flops)}$$

- Values for α, β, γ vary across machines, but communication generally dominates, especially network latency

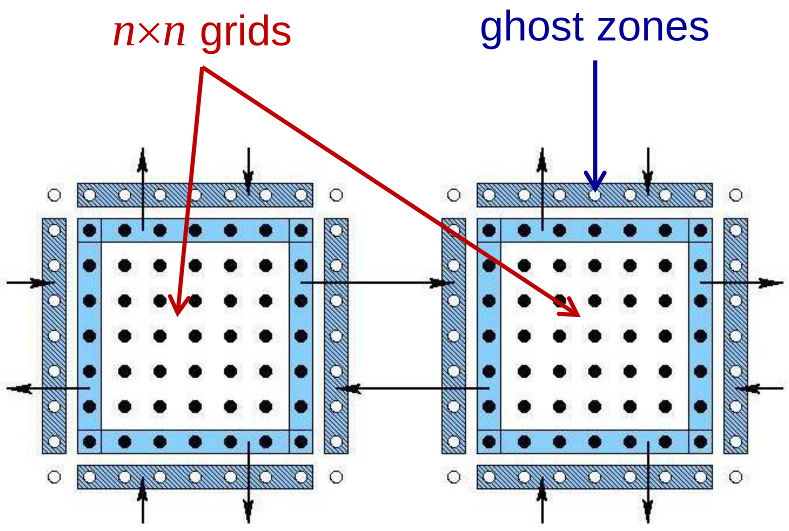
Typical relationship: $\alpha = 10^4\gamma; \quad \beta = 10^1\gamma$

- For sparse linear algebra (especially multigrid), developing approaches to minimize communication is key

Parallel model for matrix-vector multiply – 5-pt discretization of 2D Laplace equation

- On each processor p:
  - Exchange subdomain boundary data with "nearest neighbors"
  - Compute local product $A_p x_p$
- Total time determined by slowest processor
- Time to do a matvec
  - 4 communications of size n data (assuming bi-directional)
  - $5n^2$ computations (multiply-adds)

$$T \approx 4\alpha + 4n\beta + 5n^2\gamma$$

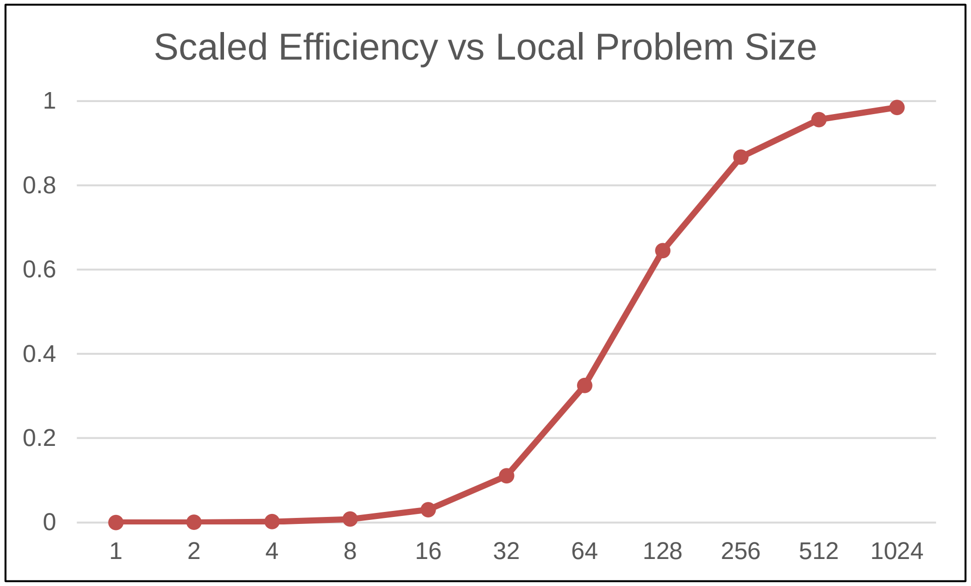


5-pt stencil

$$\begin{bmatrix} & -1 & \\ -1 & 4 & -1 \\ & -1 & \end{bmatrix}$$

Increase local problem size for efficiency

- Large local problem size → computations dominate

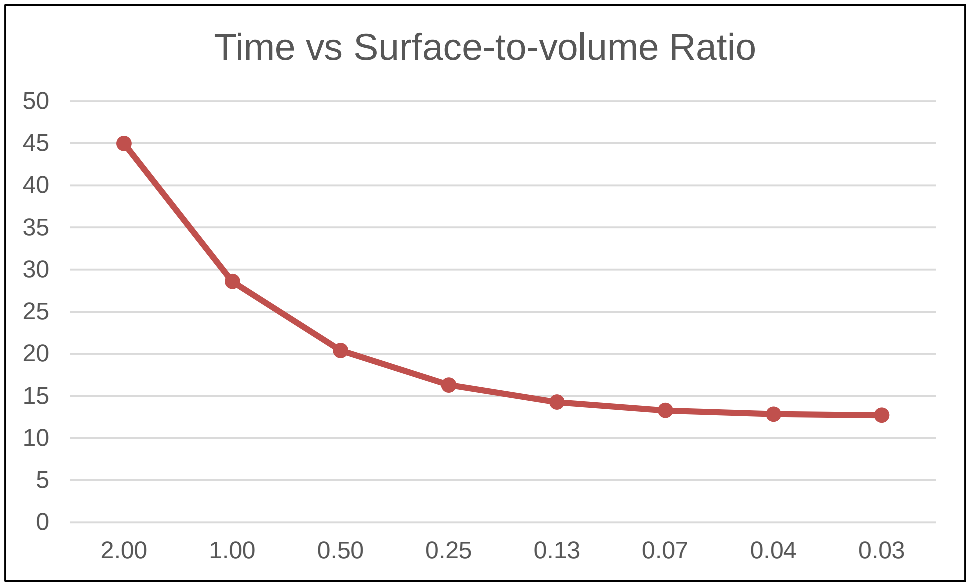


- It's not always possible to increase problem size
  — Competition for memory with the rest of the application

- Easy to make an algorithm look good by choosing large problem
  — Better to show both large and small cases

Minimize surface-to-volume ratio for speed

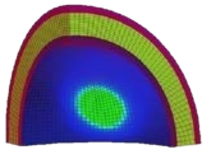
- Consider a local volume of size 16,384 (=128^2), but for rectangles of varying dimensions
  - — Large surface-to-volume ratio = long thin rectangle (1 x 16,384)
  - — Smallest ratio = a cube (128 x 128)



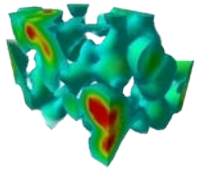
Parallel Multigrid

Multigrid will play an important role for addressing exascale challenges

- For many applications, the fastest and most scalable solvers are multigrid methods

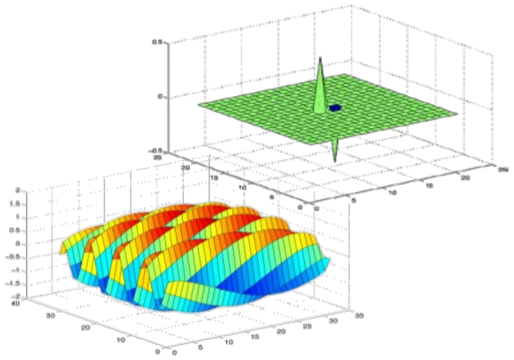

Elasticity / Plasticity

- Exascale solver algorithms will need to:
  - Exhibit extreme levels of parallelism (exascale → 1B cores)
  - Minimize data movement & exploit machine heterogeneity
  - Demonstrate resilience to faults

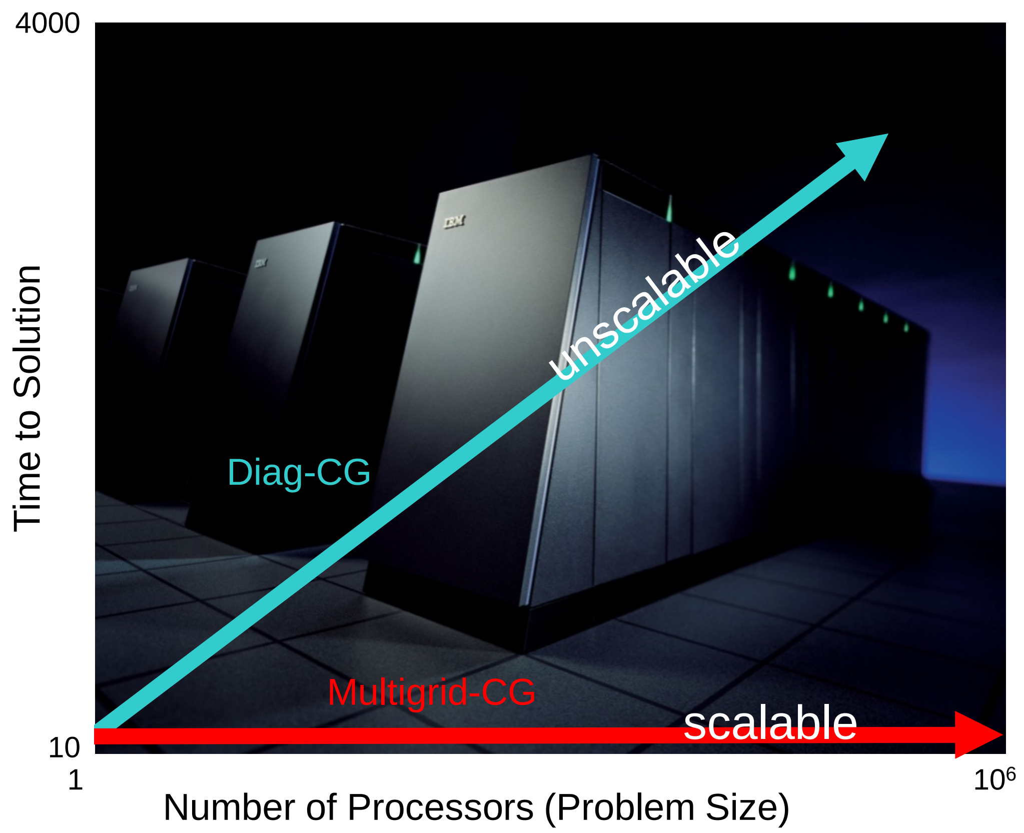

Quantum Chromodynamics

- Multilevel methods are ideal
  - Key feature: Optimal O(N)

- Research challenge:
  - No optimal solvers yet for some applications, even in serial!
  - Parallel computing increases difficulty

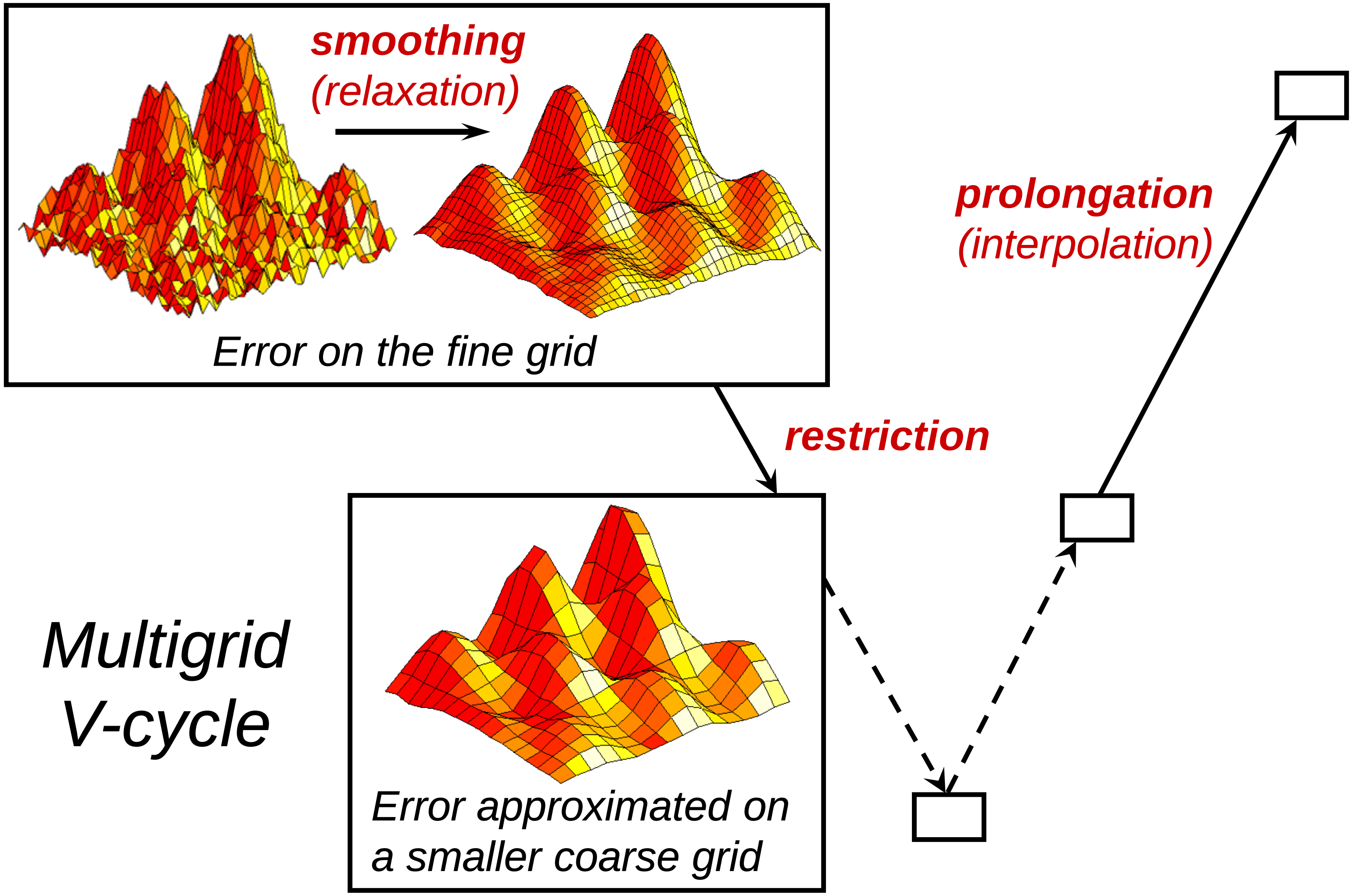

Helmholtz Modes

Multigrid solvers have $O(N)$ complexity, and hence have good scaling potential



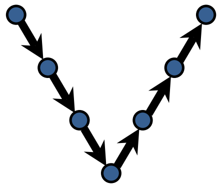
- Weak scaling – want constant solution time as problem size grows in proportion to the number of processors

Multigrid (MG) uses a sequence of coarse grids to accelerate the fine grid solution

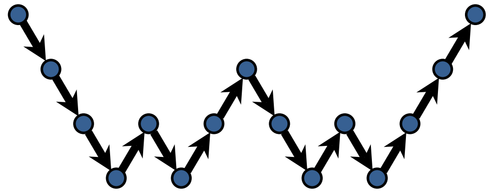


Comments on multigrid cycles

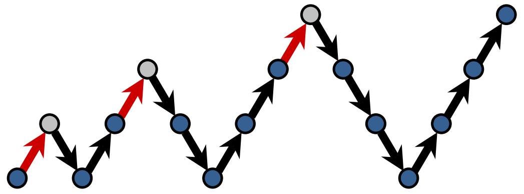
- V-cycle:
  - Most commonly used cycle
  - $O(N)$ work satisfies $||e|| \leq \varepsilon$ for fixed tolerance ε



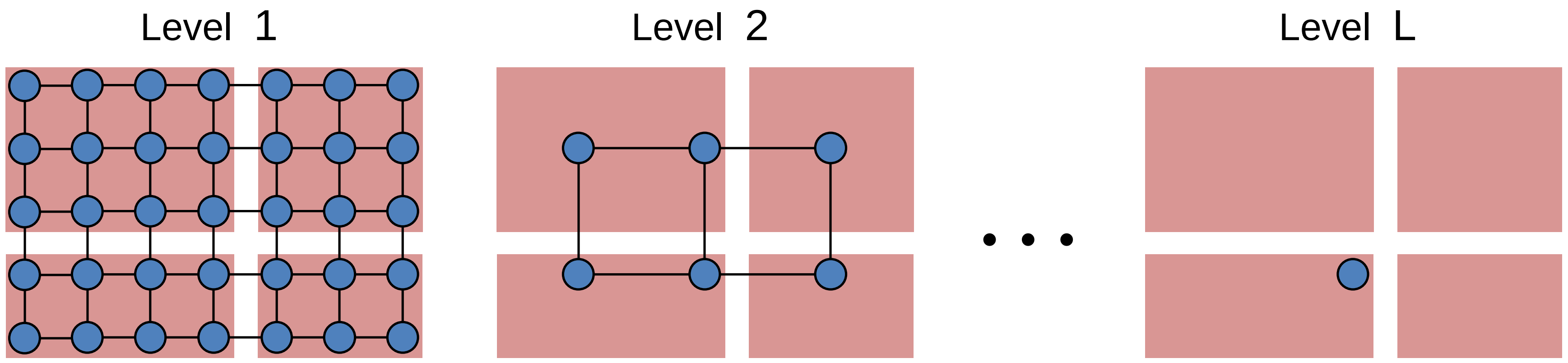
- W-cycle:
  - More robust than V-cycles
  - $O(N)$ work satisfies $||e|| \leq \varepsilon$
  - Not scalable in parallel (discussed later)



- FMG V-cycle:
  - $O(N)$ work satisfies $||e|| \leq kh^p$ where h^p is discretization accuracy



Straightforward MG parallelization yields optimal-order performance for V-cycles



- ~ 1.5 million idle cores on Sequoia!
- Multigrid has a high degree of concurrency
  - Size of the sequential component is only O(log N)!
  - This is often the minimum size achievable
- Parallel performance model has the expected log term

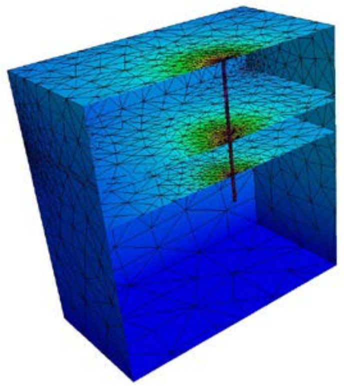
$$T_V = O(\log N)(\text{comm latency}) + O(\Gamma_p)(\text{comm rate}) + O(\Omega_p)(\text{flop rate})$$

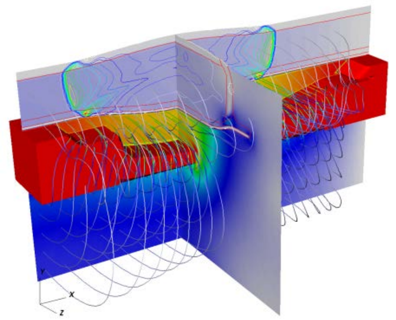
Parallel computing imposes restrictions on multigrid algorithm development

- Avoid sequential techniques
  - Classical AMG coarsening
  - Gauss-Seidel smoother
  - Cycles with large sequential component
    - F-cycle: O($\log^2$ N)
    - W-cycle: O($2^{\log N}$) = O(N)

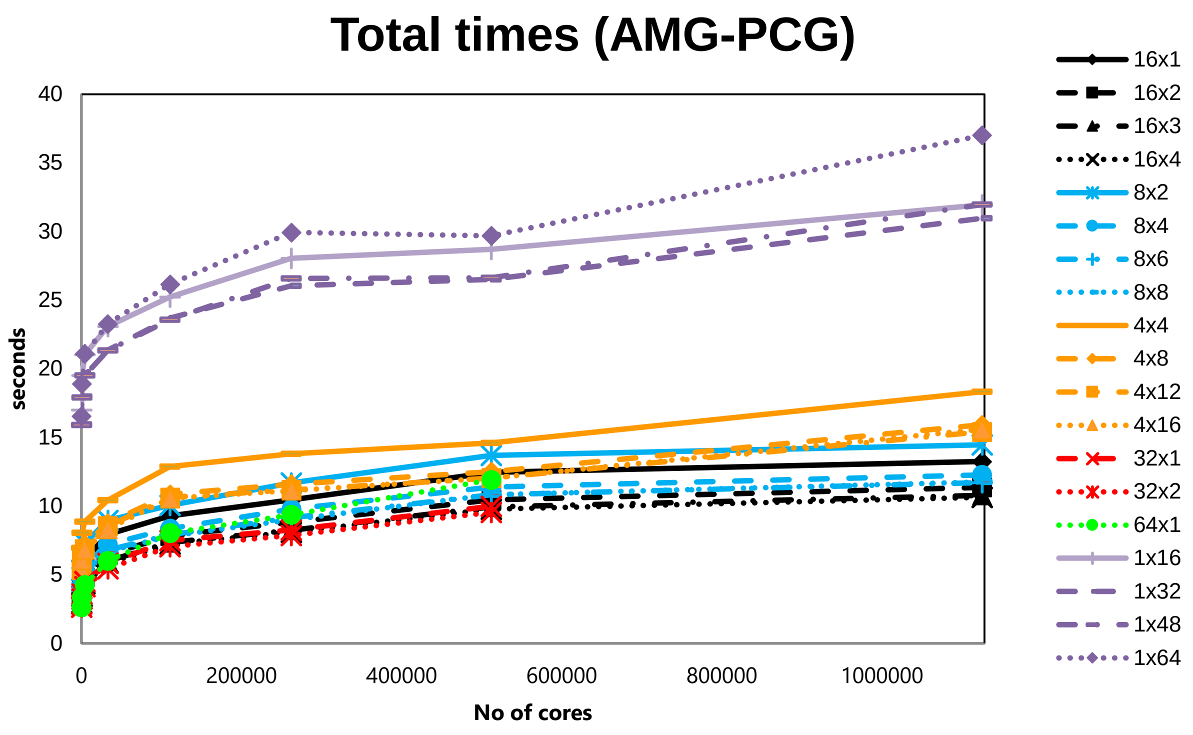
- Control communication
  - Galerkin coarse-grid operators (P^TAP) can lead to high communication costs in AMG

- Need both CS and Math advances!
  - New methods have new convergence and robustness characteristics
  - Successful addressing issues so far


10x speedup for subsurface problems with new coarsening and interpolation approach

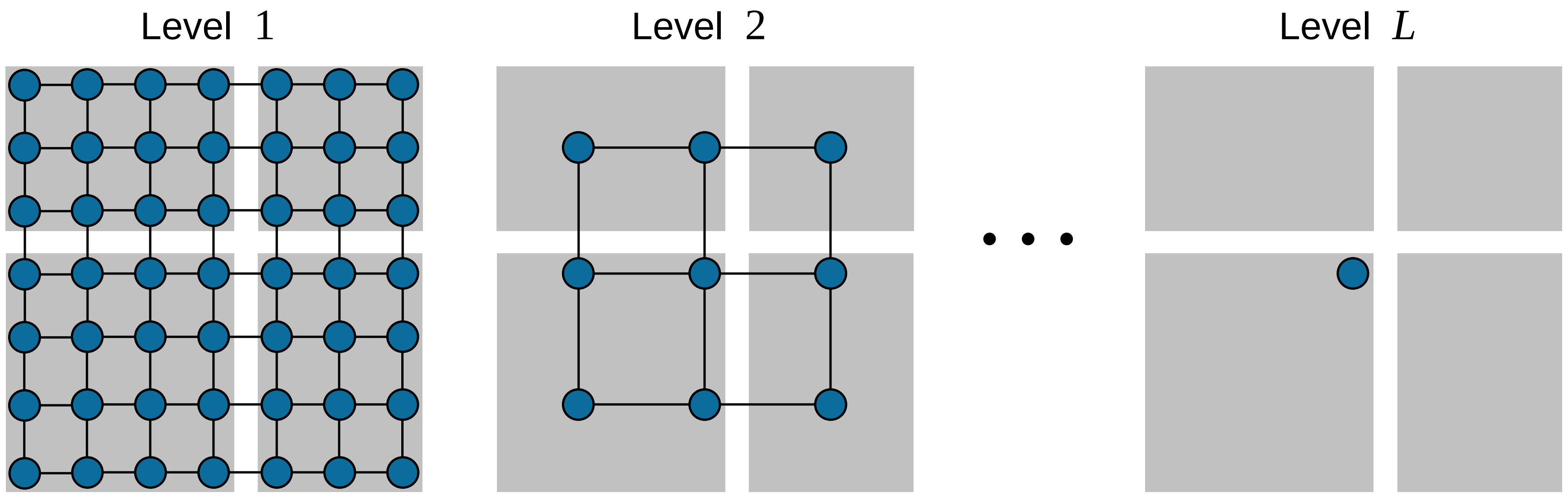

Magnetic flux compression generator simulation enabled by MG smoother research

Parallel AMG in *hypre* now scales to 1.1M cores on Sequoia (IBM BG/Q)



- *m* x *n* denotes *m* MPI tasks and *n* OpenMP threads per node
- Largest problem above: 72B unknowns on 1.1M cores

Approach for parallelizing multigrid is straightforward data decomposition



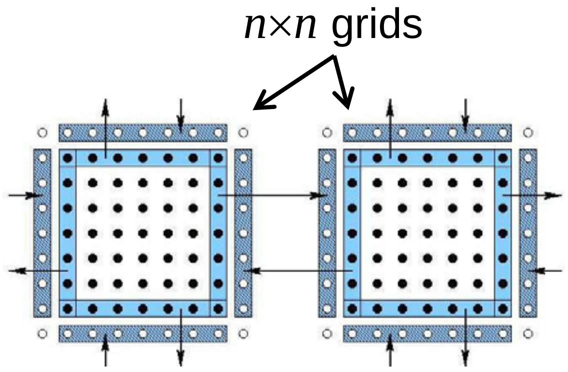
- Basic communication pattern is "nearest neighbor"
  - Relaxation, interpolation, & Galerkin not hard to implement
- Different neighbor processors on coarse grids
- Many idle processors on coarse grids (100K+ on BG/L)
  - Algorithms to take advantage have had limited success

Straightforward parallelization approach is optimal for V-cycles on structured grids (5-pt Laplacian example)

- Standard communication / computation models

$$T_{comm} = \alpha + m\beta \quad \textit{(communicate m doubles)}$$

$$T_{comp} = m\gamma \quad \textit{(compute m flops)}$$



- Time to do relaxation

$$T \approx 4\alpha + 4n\beta + 5n^2\gamma$$

- Time to do relaxation in a V(1,0) multigrid cycle

$$\begin{aligned} T_V &\approx (1+1+\cdots)4\alpha + (1+1/2+\ldots)4n\beta + (1+1/4+\ldots)5n^2\gamma \\ &\approx (\log N)4\alpha + (2)4n\beta + (4/3)5n^2\gamma \end{aligned}$$

- For achieving optimality in general, the *log* term is unavoidable!

- More precise:

$$T_{V,better} \approx T_V + (\log P)(4\beta + 5\gamma)$$

A closer look at the idle processor problem

- The idle processor problem seems severe, but standard parallel V-cycle multigrid performance has optimal order

$$T_V \approx (\log N)4\alpha + (2)4n\beta + (4/3)5n^2\gamma$$

- What are the limits of what we can achieve by trying to use idle processors to accelerate convergence?

- Consider an ideal setting:
  - Fine grid of size N distributed across P procs with n rows per proc (hence $N=nP$)
  - Constant coarsening factor f and grid complexity bound $F=1/(1-1/f)$ (example: 3D cube with full coarsening → $f=8$, $F=8/7$)

- Assume multigrid takes CN work to converge and we don't know how to do less work than this

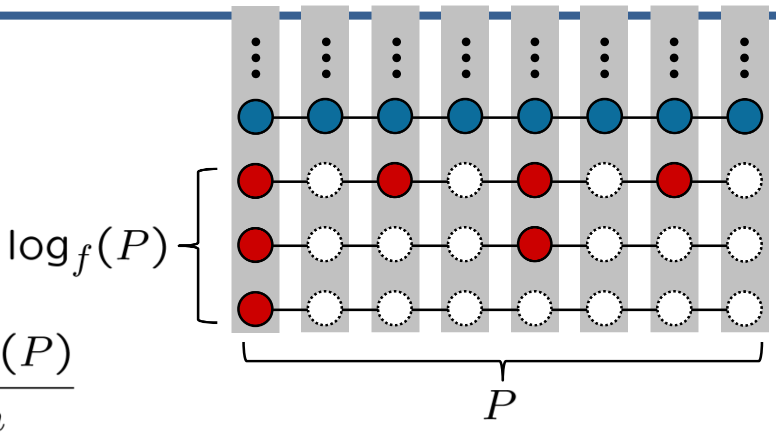
A closer look at the idle processor problem (2)

- Work potential

$$\log_f(P)P - (FP - P)$$

- Best speedup per V-cycle

$$\frac{FN + \log_f(P)P - FP + P}{FN} \leq 1 + \frac{\log_f(P)}{n}$$



- Overall speedup assuming at least one V-cycle is required

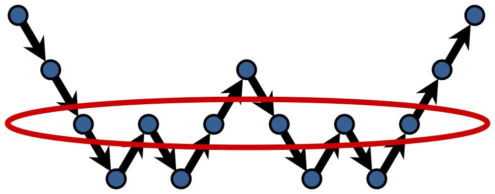
$$\max\left\{1 + \frac{\log_f(P)}{n}, \frac{C}{F}\right\}$$

- Only makes sense if n is very small
  - Example: 3D Laplace on 1M procs: $\log_8(P) < 7$
- And this analysis is extremely optimistic!
  - Assumes computations in cycle 2 can be done before cycle 1

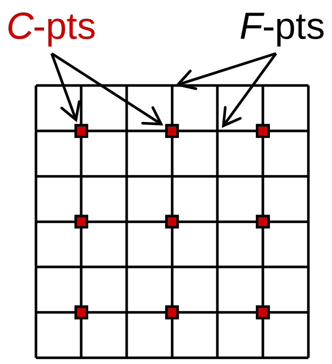
Additional comments on parallel multigrid

- W-cycles scale poorly:

$$T_W \approx (2^{\log N})4\alpha + (\log N)4n\beta + (2)5n^2\gamma$$



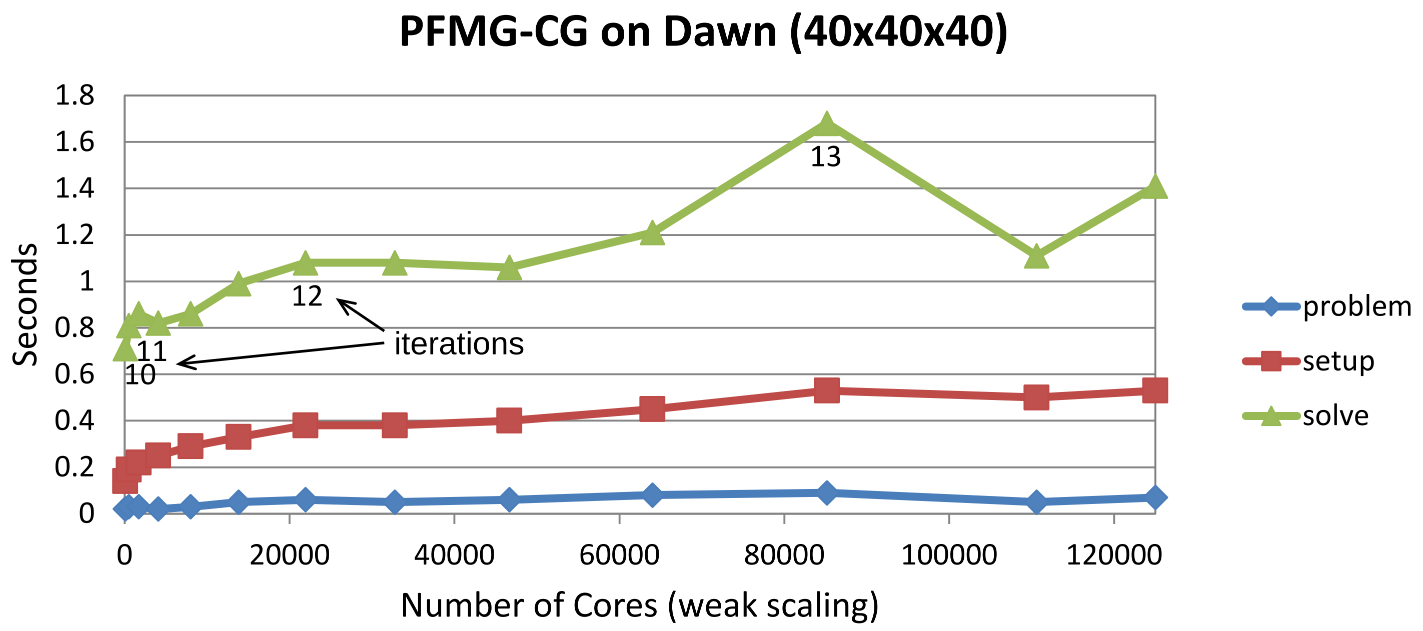
- Lexicographical Gauss-Seidel is too sequential
  - Use red/black or multi-color GS
  - Use weighted Jacobi, hybrid Jacobi/GS, L1
  - Use *C*-*F* relaxation (Jacobi on *C*-pts then *F*-pts)
  - Use Polynomial smoothers



- Parallel smoothers are often less effective

- Survey on parallel multigrid, paper on parallel smoothers:
  - "A Survey of Parallelization Techniques for Multigrid Solvers," Chow, Falgout, Hu, Tuminaro, and Yang, *Parallel Processing For Scientific Computing*, Heroux, Raghavan, and Simon, editors, SIAM, series on Software, Environments, and Tools (2006)
  - "Multigrid Smoothers for Ultra-Parallel Computing," Baker, Falgout, Kolev, and Yang, *SIAM J. Sci. Comput.*, 33 (2011), pp. 2864-2887.

Example weak scaling results on Dawn (an IBM BG/P system at LLNL) in 2011



- Laplacian on a cube; 40^3 = 64K grid per processor; largest had 8 billion unknowns
- PFMG is a semicoarsening multigrid solver in *hypre*
- Constant-coefficient version - 1 trillion unknowns on 131K cores in 83 seconds
- Can improve setup (these results already use the assumed partition algorithm described later)

Parallel Algebraic Multigrid (AMG)

Preliminaries… the Galerkin coarse-grid operator

- As before, consider solving the $N \times N$ linear system

$$Au = f$$

- Let P be prolongation (interpolation) and P^T restriction

- The coarse-grid operator is defined by the Galerkin procedure, $A_c = P^T A P$

- This gives the "best" coarse-grid correction in the sense that the solution e_c of the coarse system

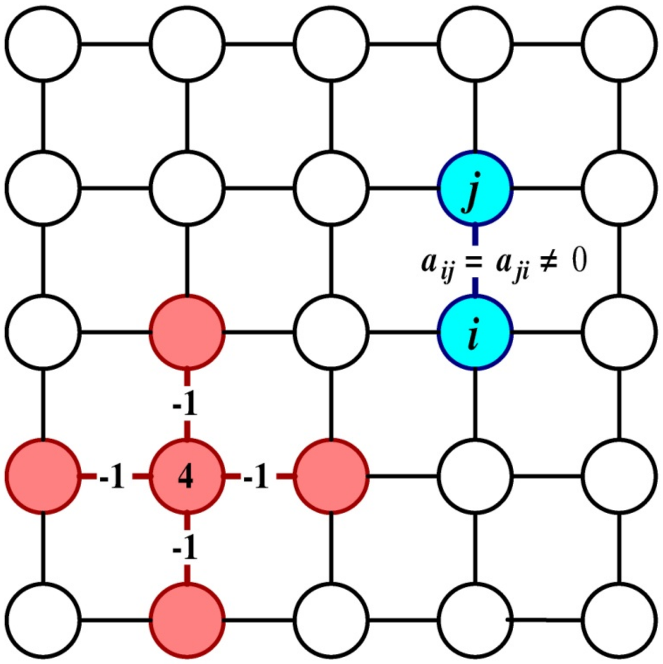
$$A_c e_c = P^T r$$

satisfies

$$e_c = \text{arg min} \; \|e - P e_c\|_A$$

Preliminaries… AMG "grids"

- Matrix adjacency graphs play an important role in AMG:
  - grid = set of graph vertices
  - grid point i = vertex i
- As a visual aid, it is highly instructive to relate the matrix equations to an underlying PDE and discretization
- We will often draw the grid points in their geometric locations
- Remember that AMG doesn't actually use this geometric information!



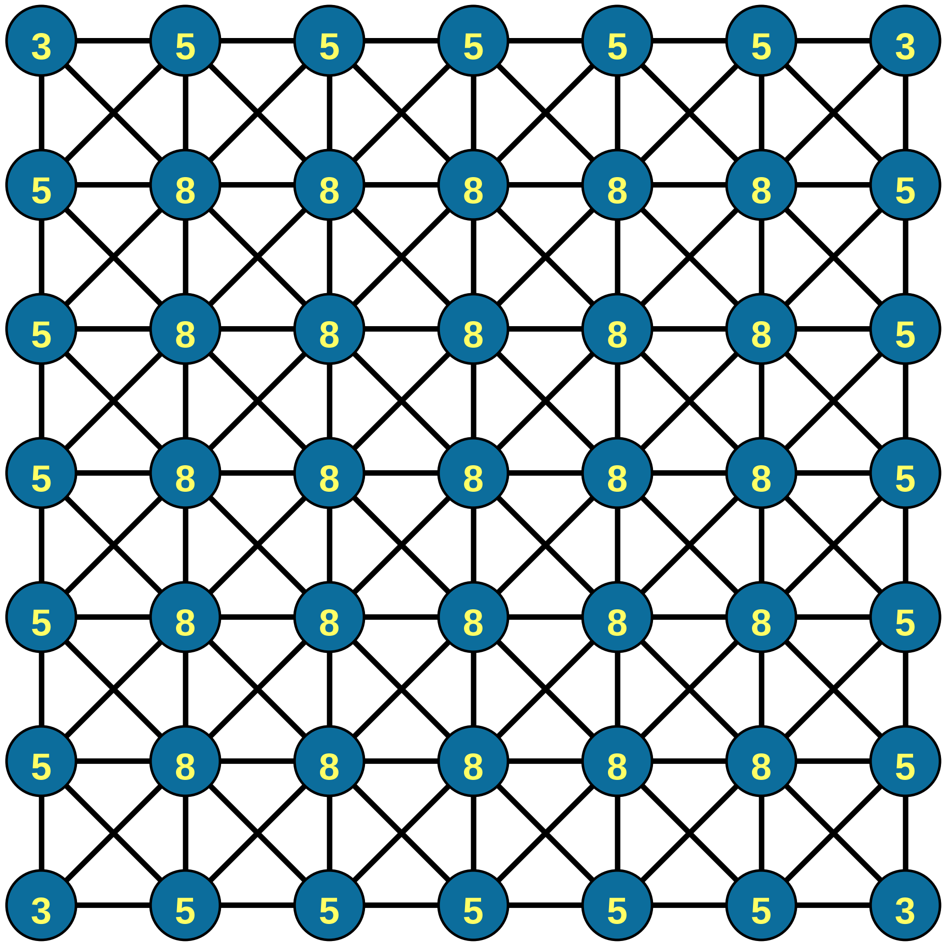
Choosing the coarse grid

- Classical AMG (C-AMG) – coarse grid is a subset of the fine grid

- The basic coarsening procedure is as follows:
  - Define a strength matrix A_s by deleting weak connections in A
  - First pass: Choose an independent set of fine-grid points based on the graph of A_s
  - Second pass: Choose additional points if needed to satisfy interpolation requirements

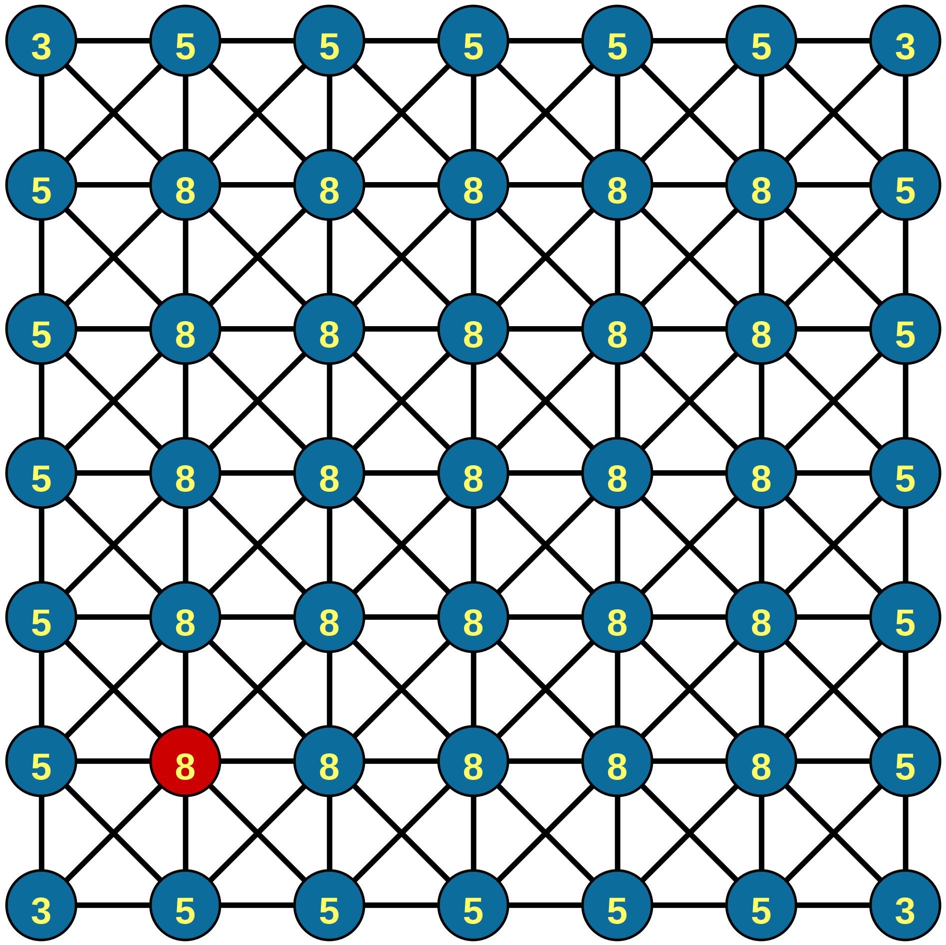
- Coarsening partitions the grid into *C*- and *F*-points

C-AMG coarsening



- **select C-pt with maximal measure**
- **select neighbors as F-pts**
- **update measures of F-pt neighbors**

C-AMG coarsening



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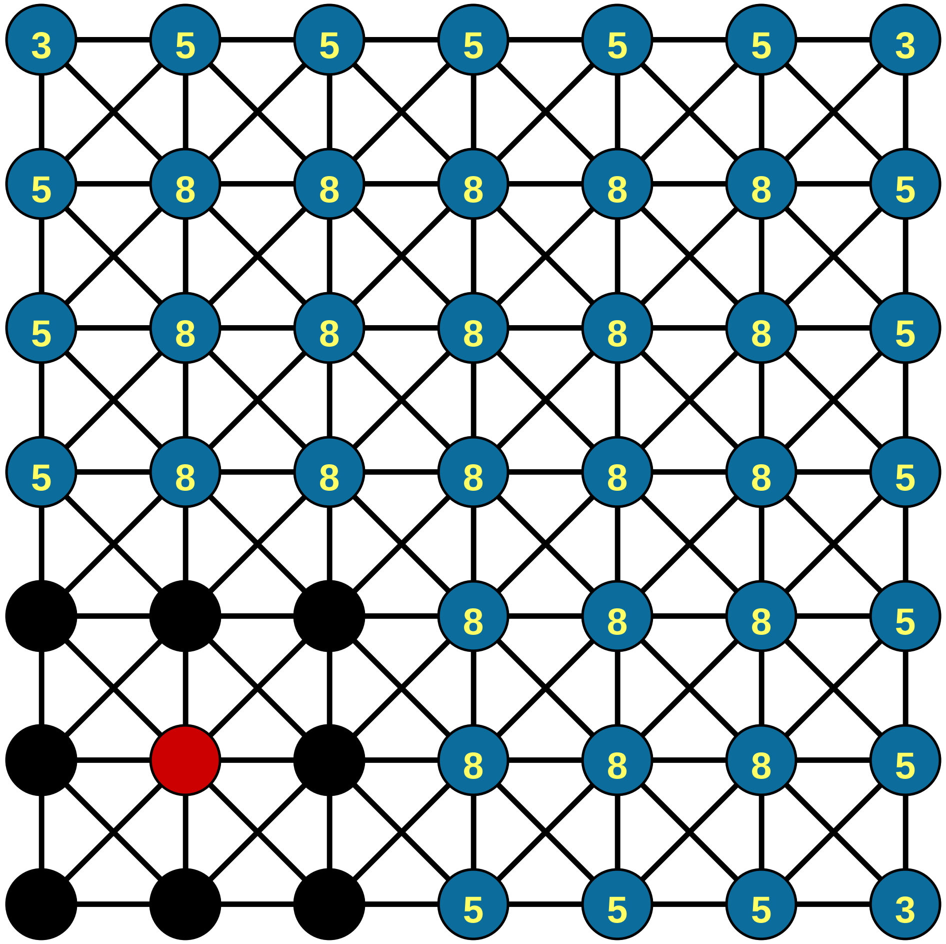
C-AMG coarsening



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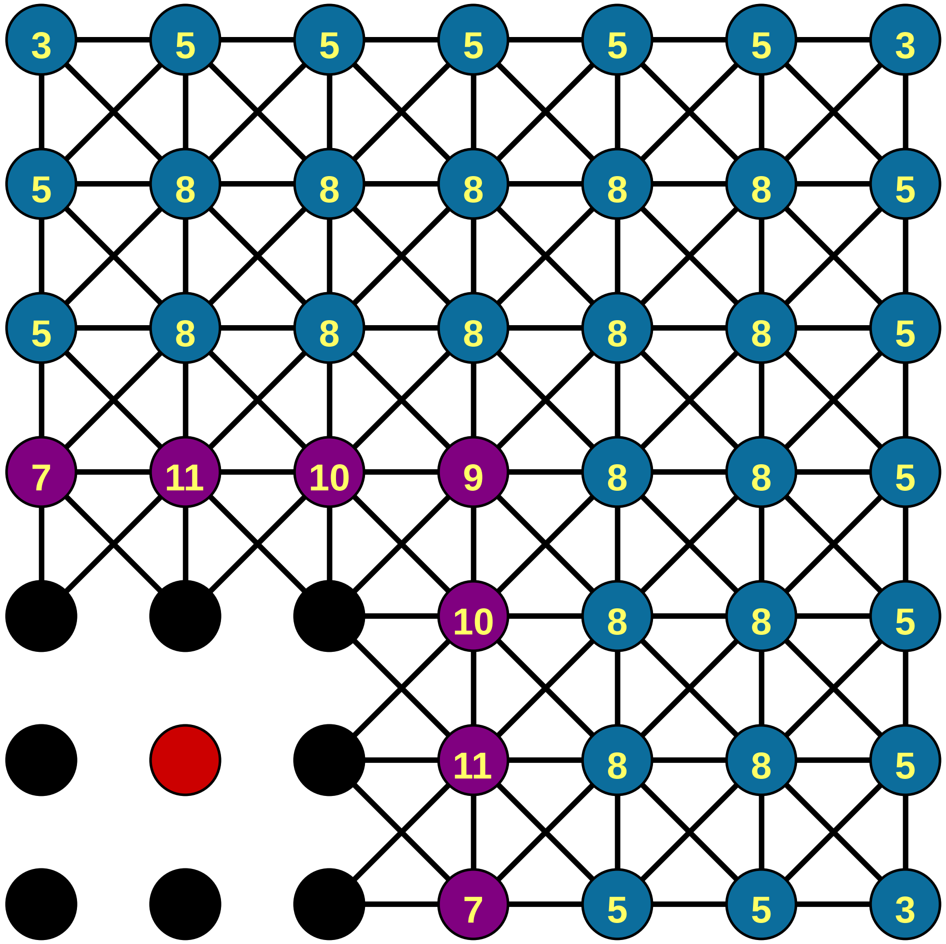
C-AMG coarsening



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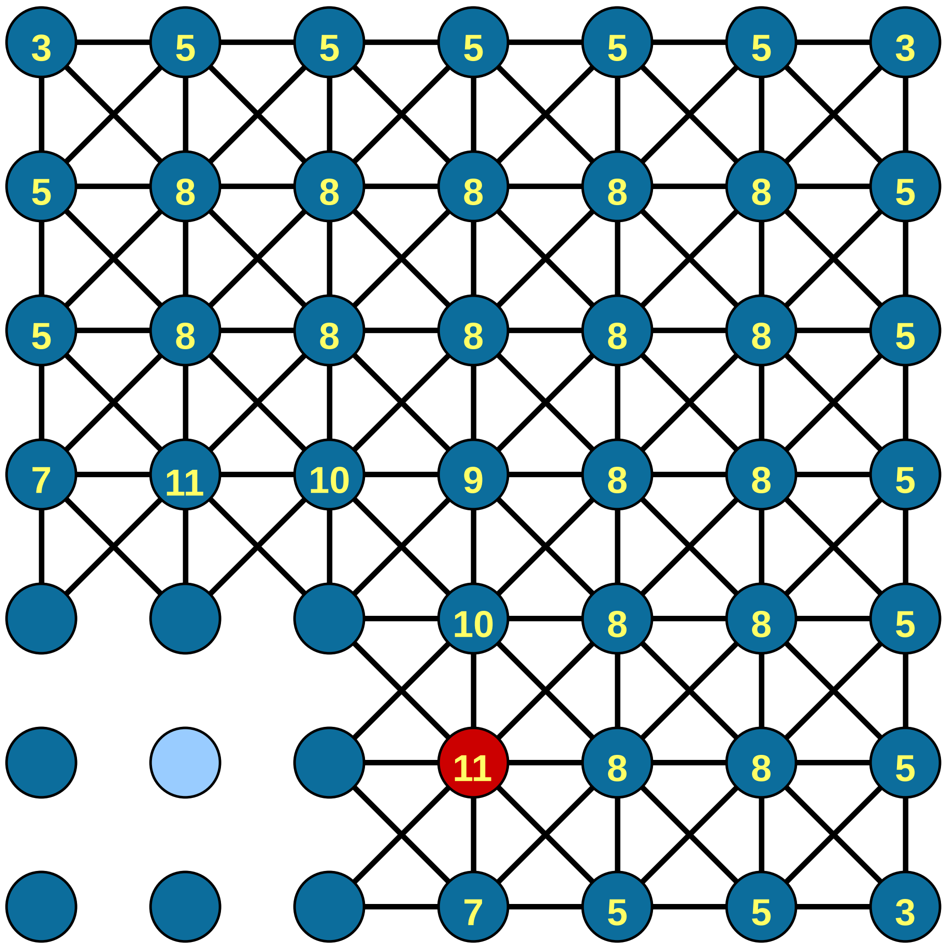
C-AMG coarsening



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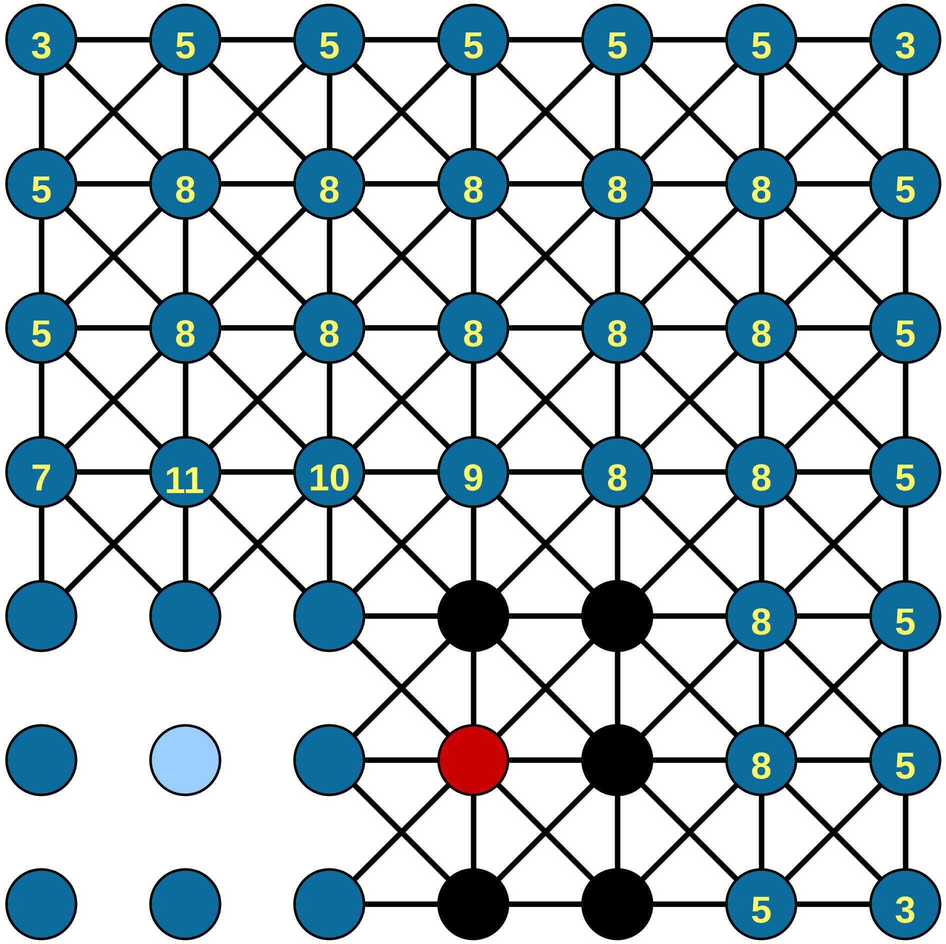
C-AMG coarsening



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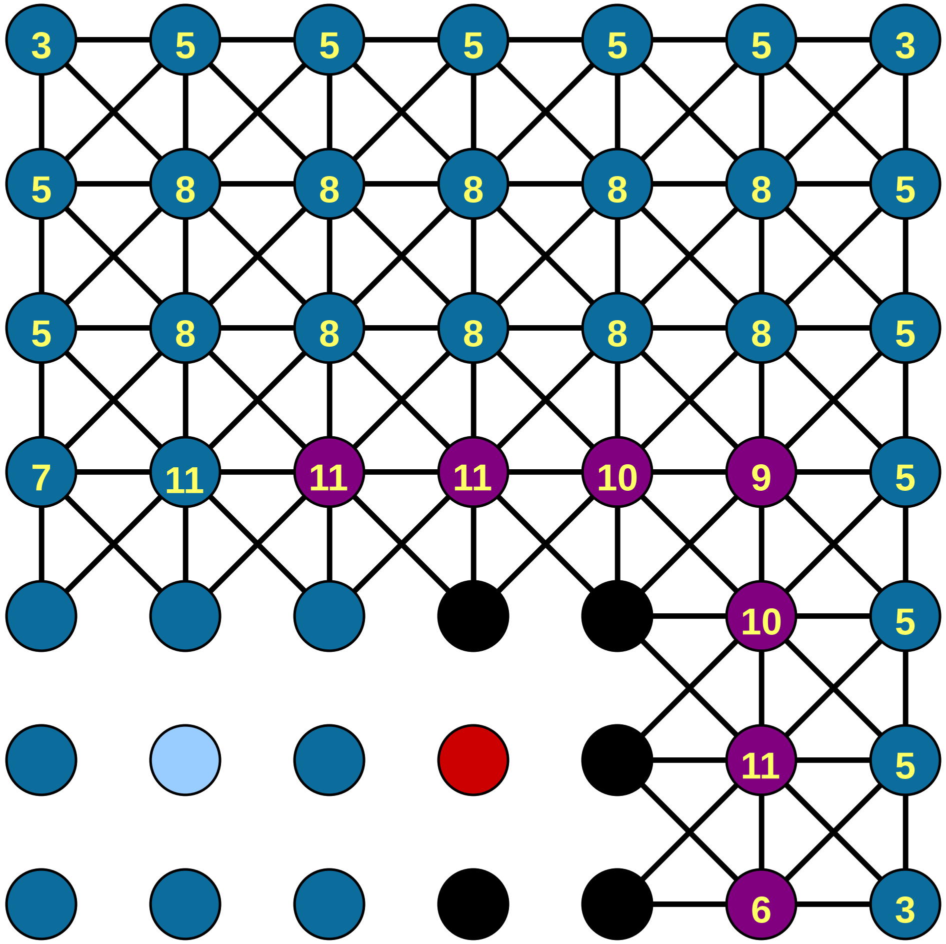
C-AMG coarsening



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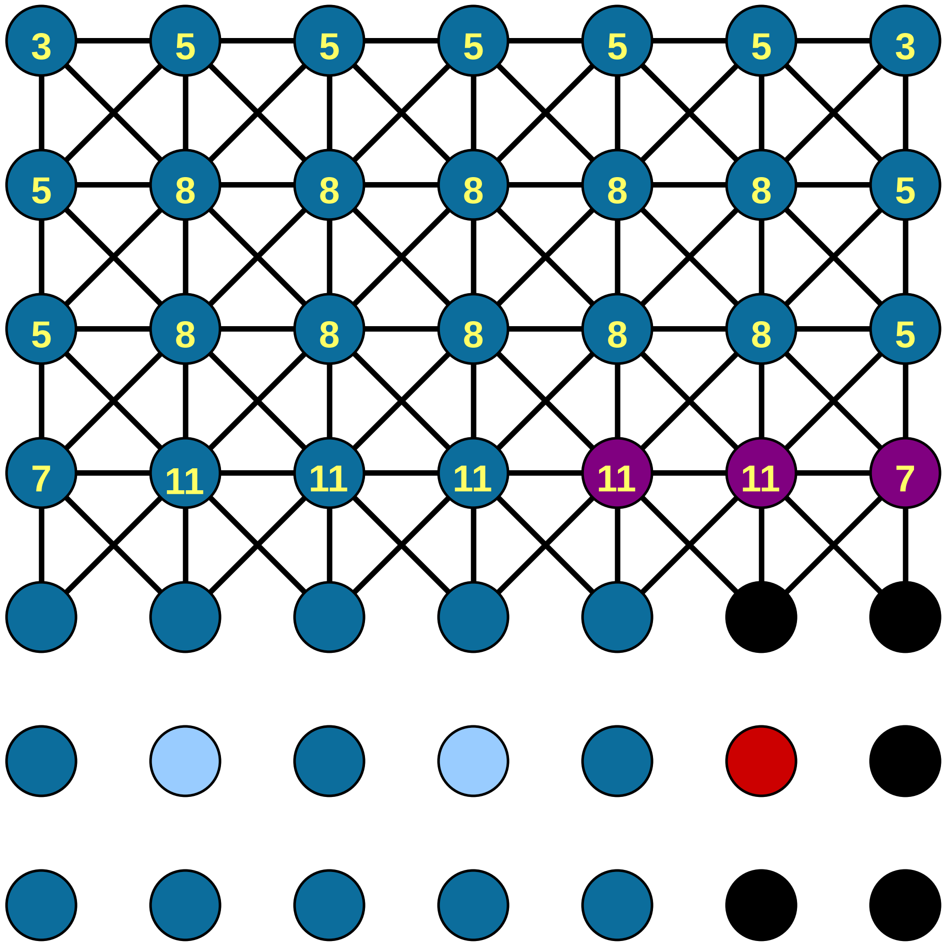
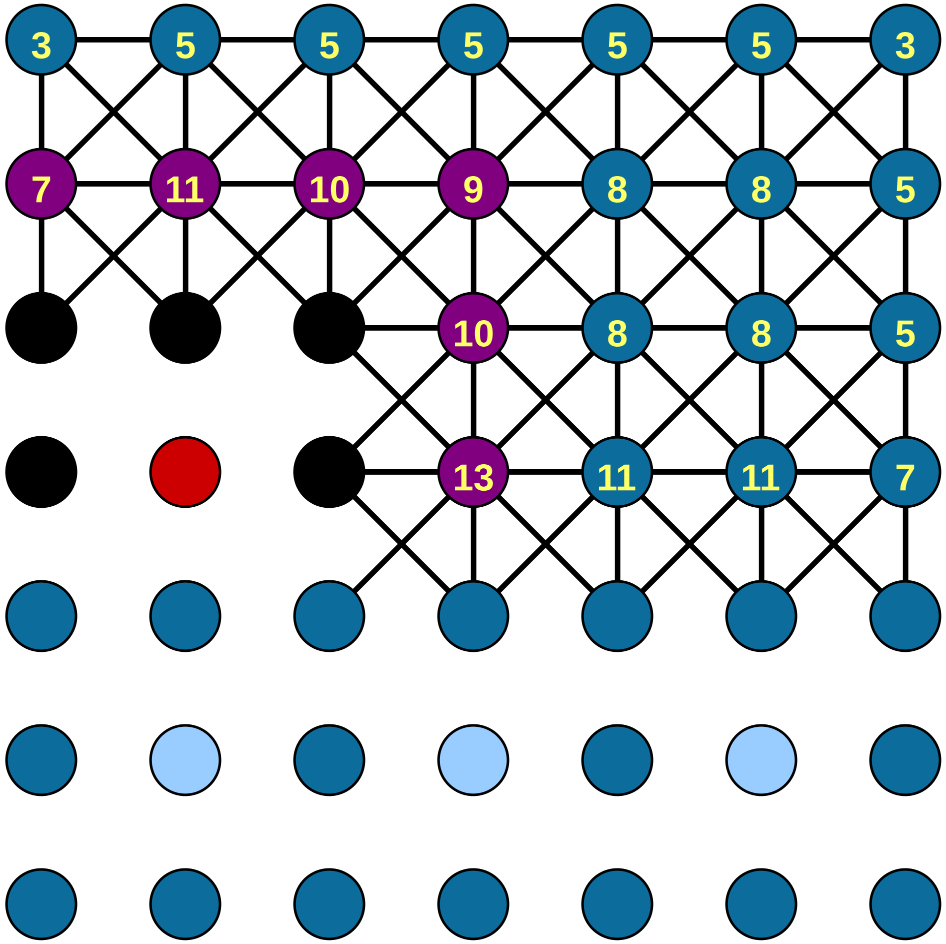
C-AMG coarsening



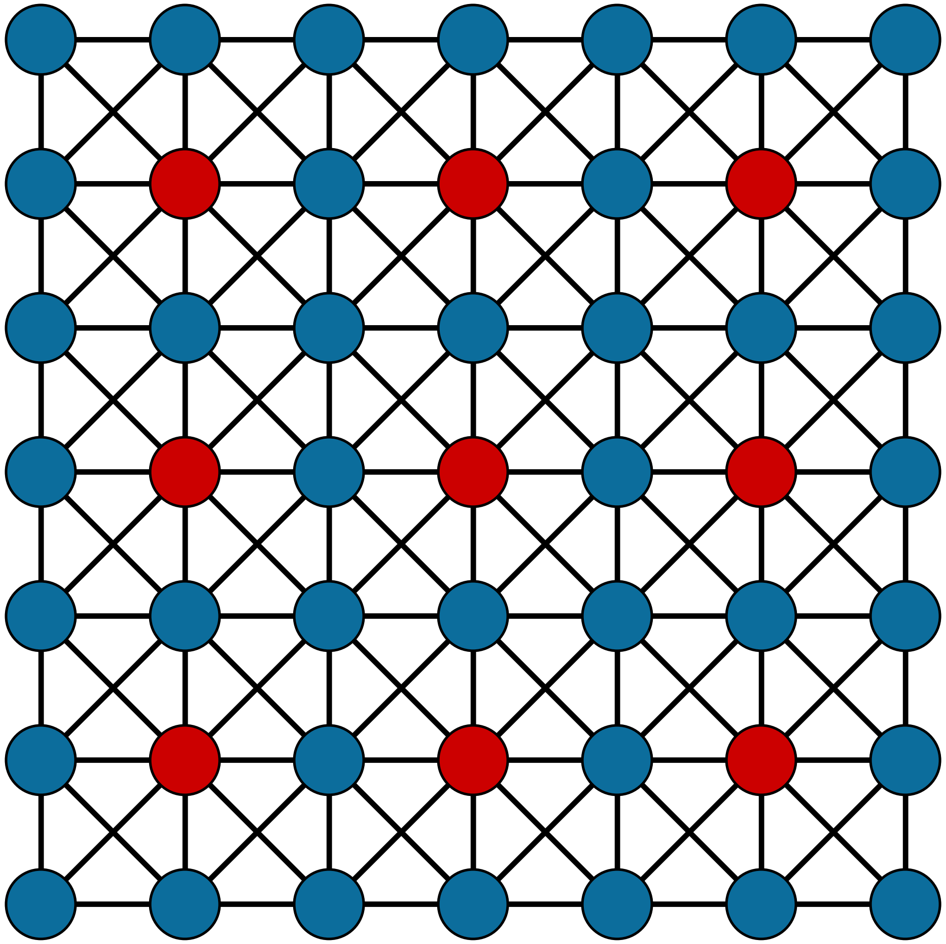
- select C-pt with maximal measure
- select neighbors as F-pts
- update measures of F-pt neighbors

C-AMG coarsening



- select C-pt with maximal measure
- select neighbors as F-pts
- update measures of F-pt neighbors

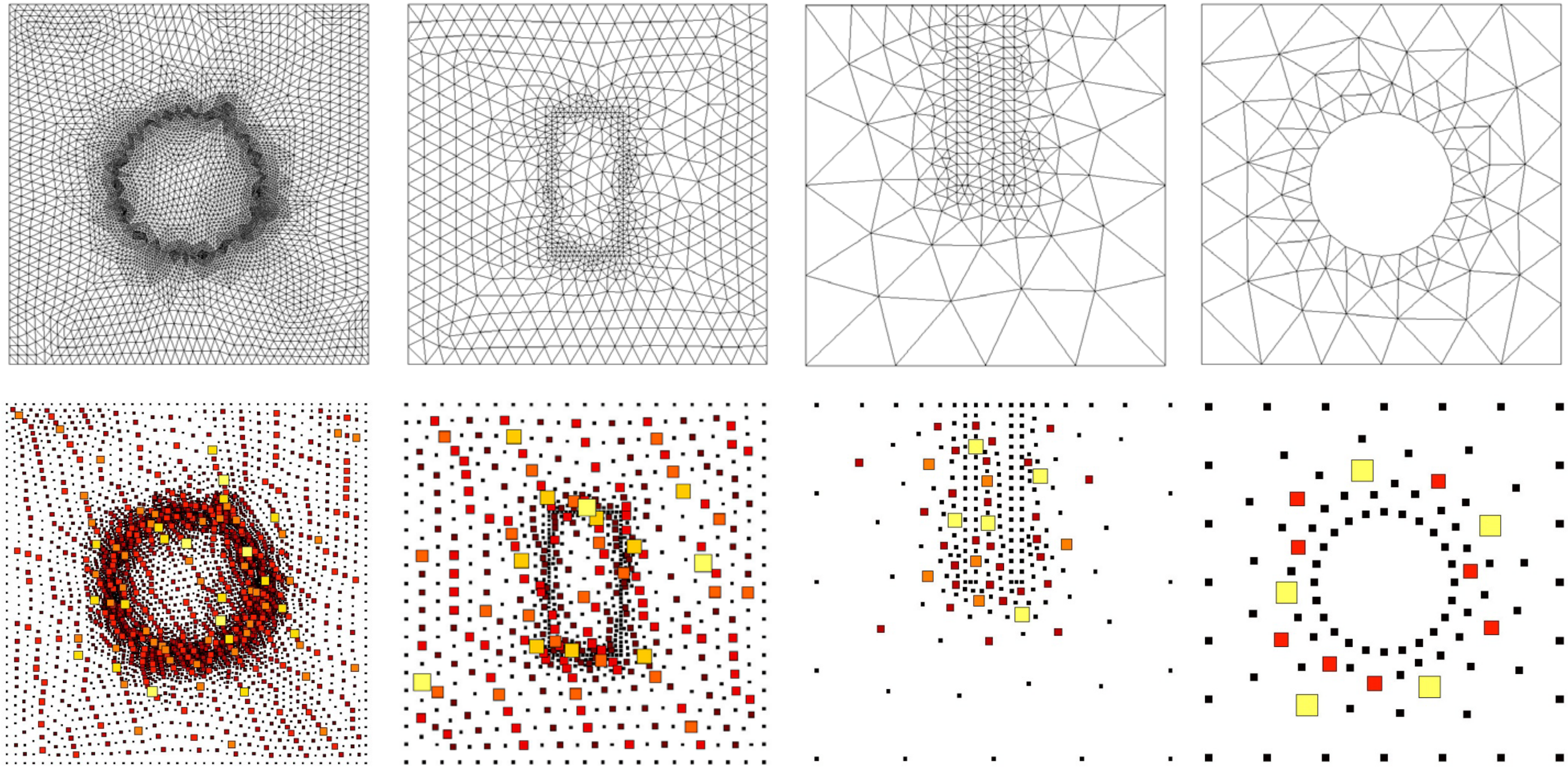
C-AMG coarsening is inherently sequential



- select C-pt with maximal measure
- select neighbors as F-pts
- update measures of F-pt neighbors

AMG grid hierarchies for several 2D problems

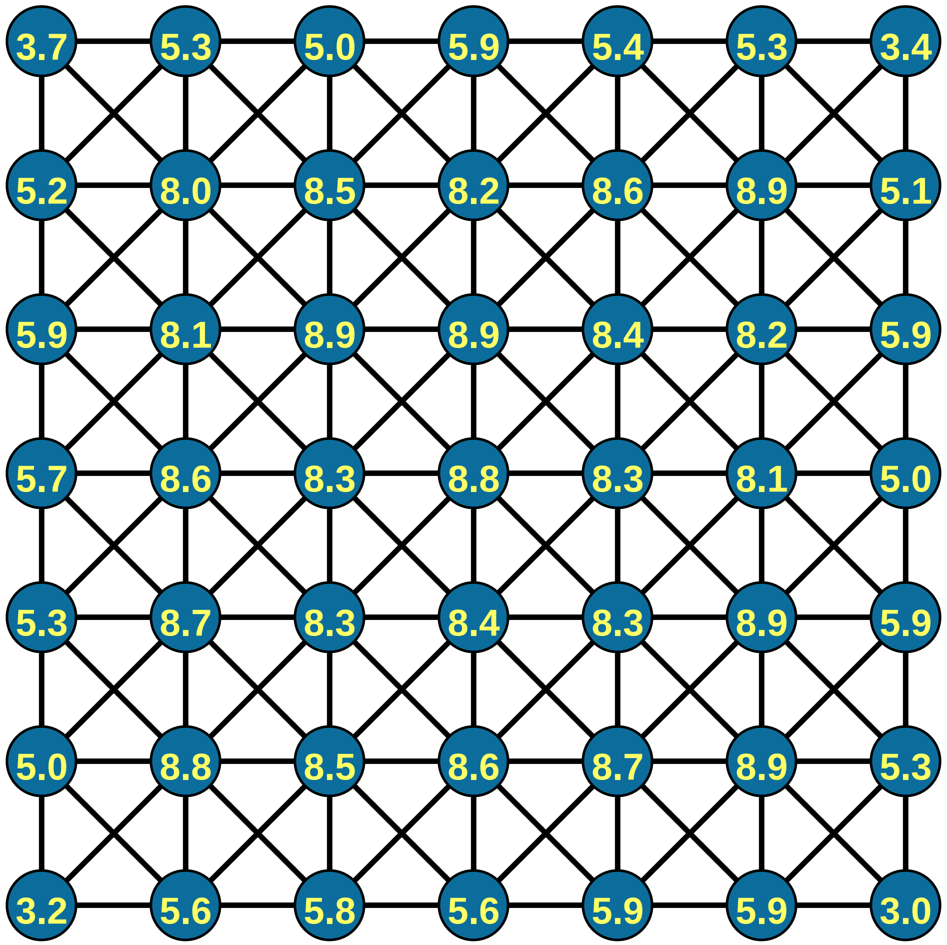
domain1 - 30^o	domain2 - 30^o	pile	square-hole



Parallel Coarsening Algorithms

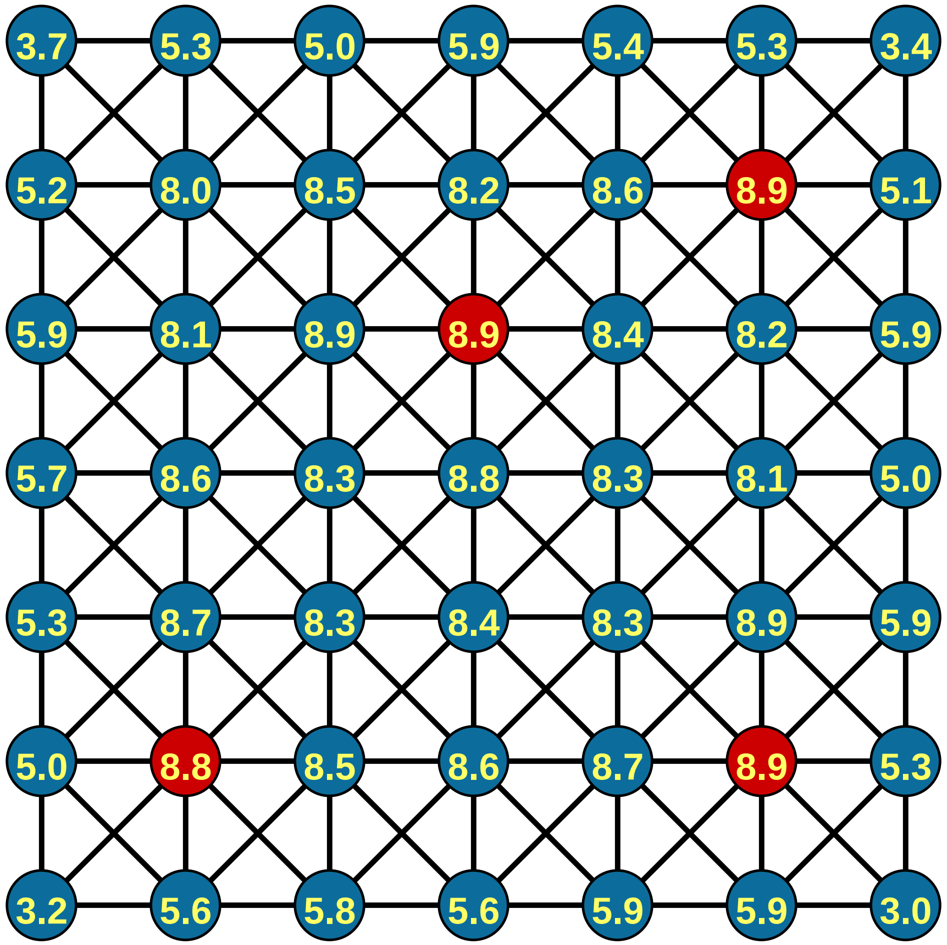
- C-AMG coarsening algorithm is inherently sequential
- Several parallel algorithms (in *hypre*):
  - CLJP (Cleary-Luby-Jones-Plassmann) – one-pass approach with random numbers to get concurrency (illustrated next)
  - Falgout – C-AMG on processor interior, then CLJP to finish
  - PMIS – CLJP without the 'C'; parallel version of C-AMG first pass
  - HMIS – C-AMG on processor interior, then PMIS to finish
  - CGC (Griebel, Metsch, Schweitzer) – compute several coarse grids on each processor, then solve a global graph problem to select the grids with the best "fit"
  - …
- Other parallel AMG codes use similar approaches

CLJP coarsening is fully parallel



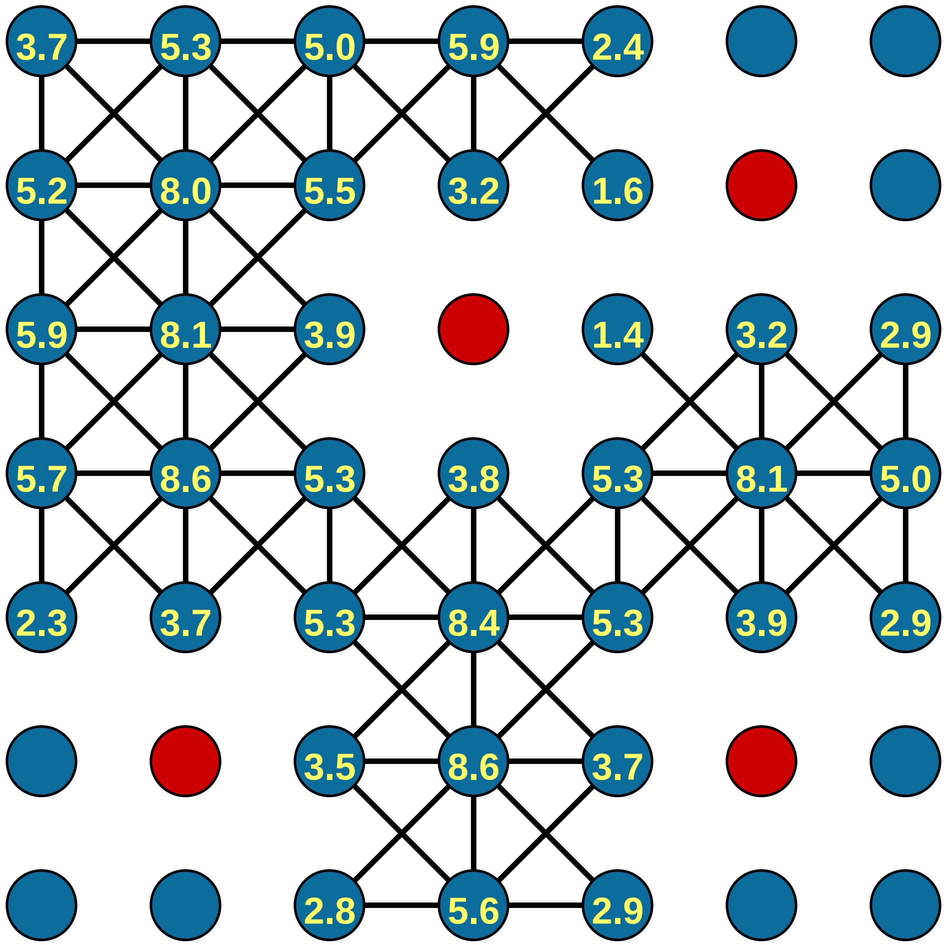
- **select C-pts with maximal measure locally**
- **remove neighbor edges**
- **update neighbor measures**

CLJP coarsening is fully parallel



- **select C-pts with maximal measure locally**
- **remove neighbor edges**
- **update neighbor measures**

CLJP coarsening is fully parallel



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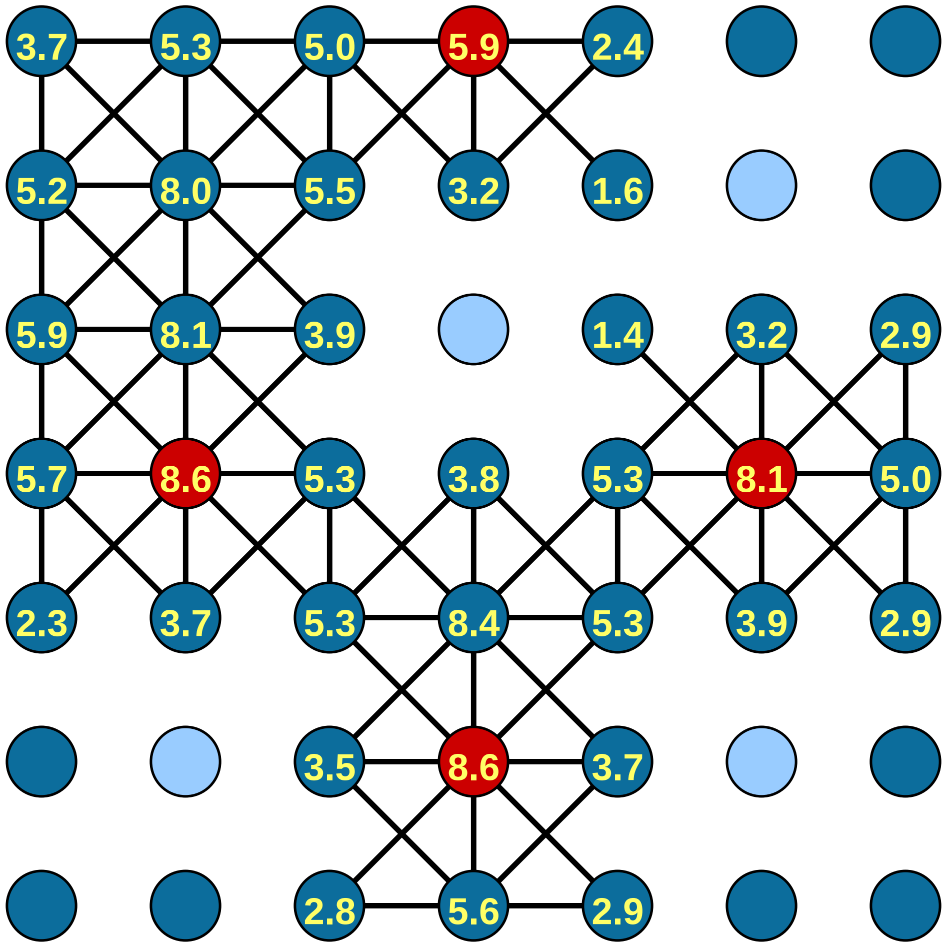
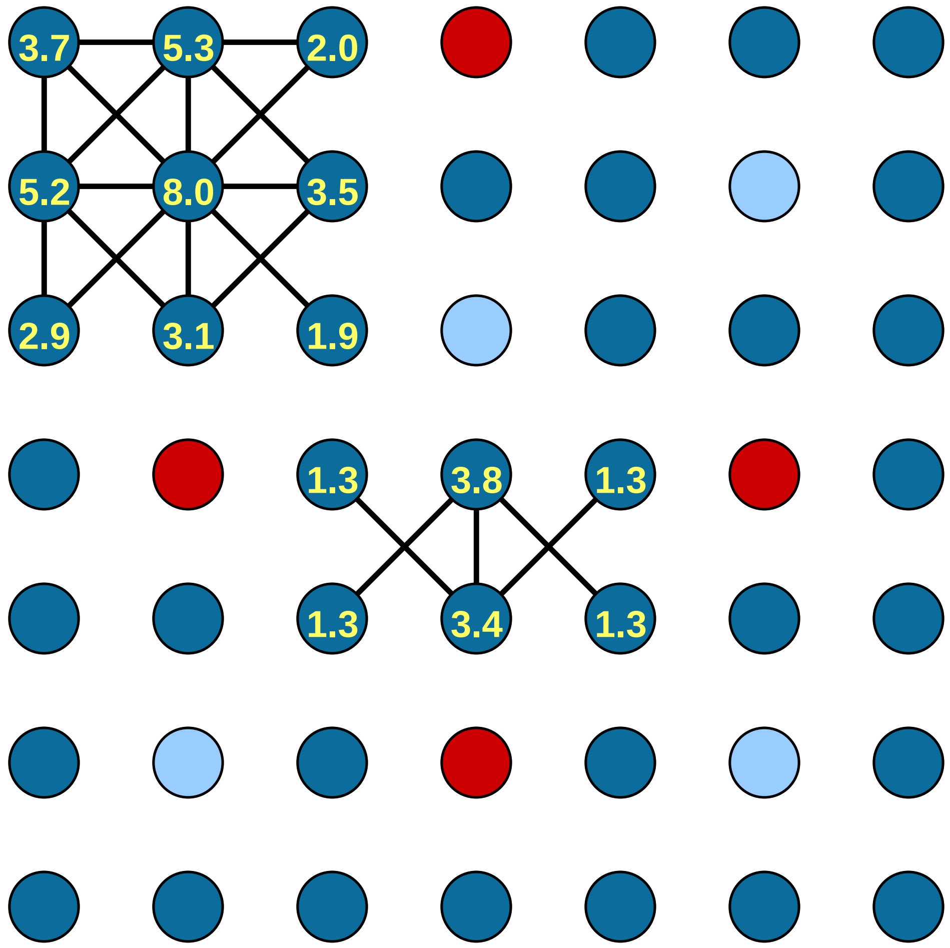
- update neighbor measures

CLJP coarsening is fully parallel



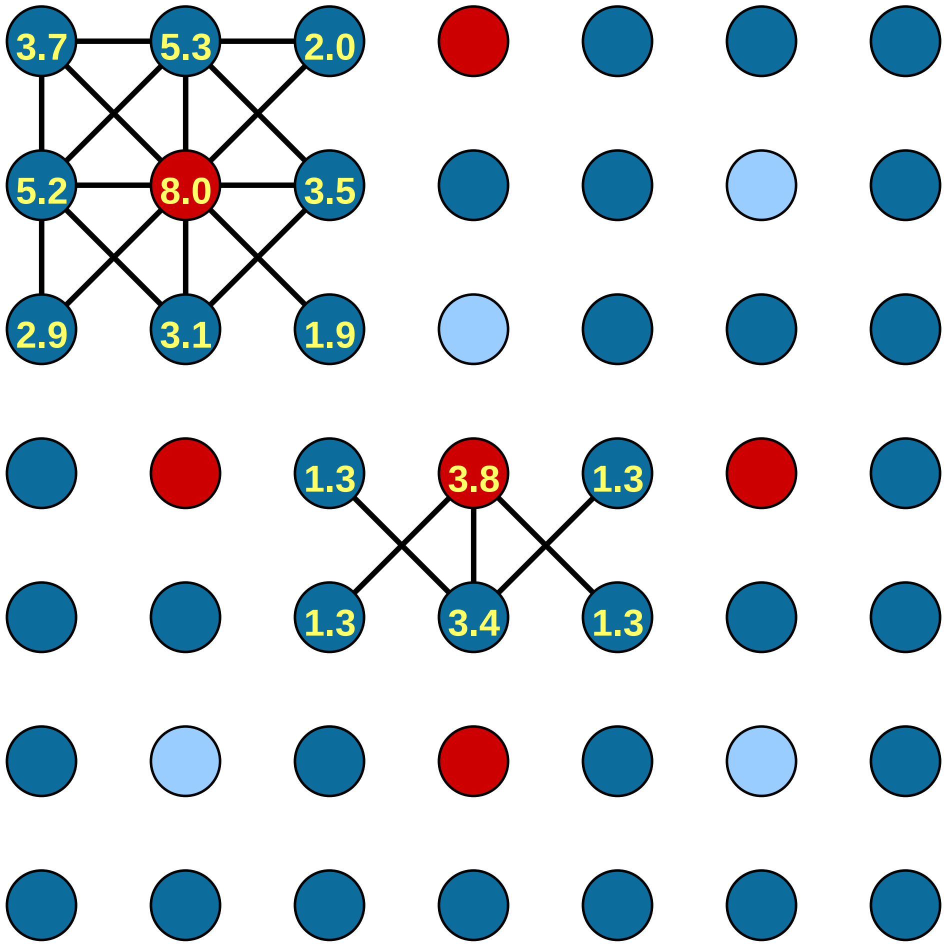
- select C-pts with maximal measure locally
- remove neighbor edges
- update neighbor measures

CLJP coarsening is fully parallel



- select C-pts with maximal measure locally
- remove neighbor edges
- update neighbor measures

CLJP coarsening is fully parallel



- select C-pts with maximal measure locally
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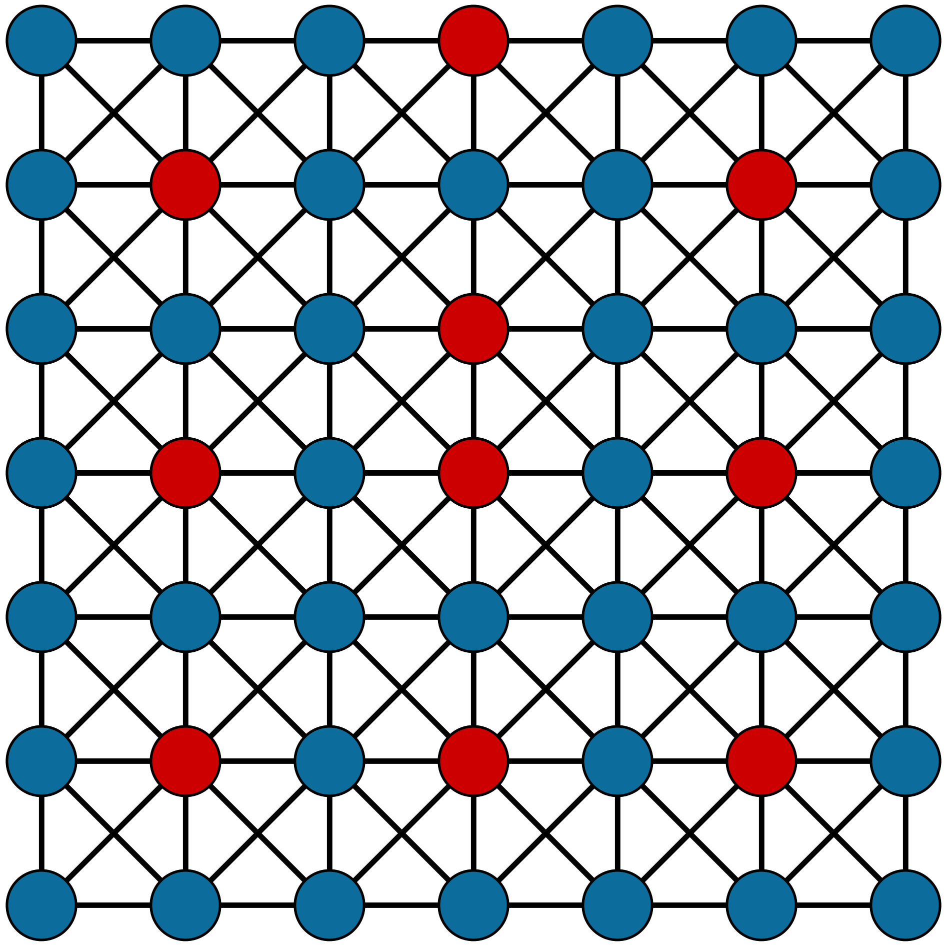
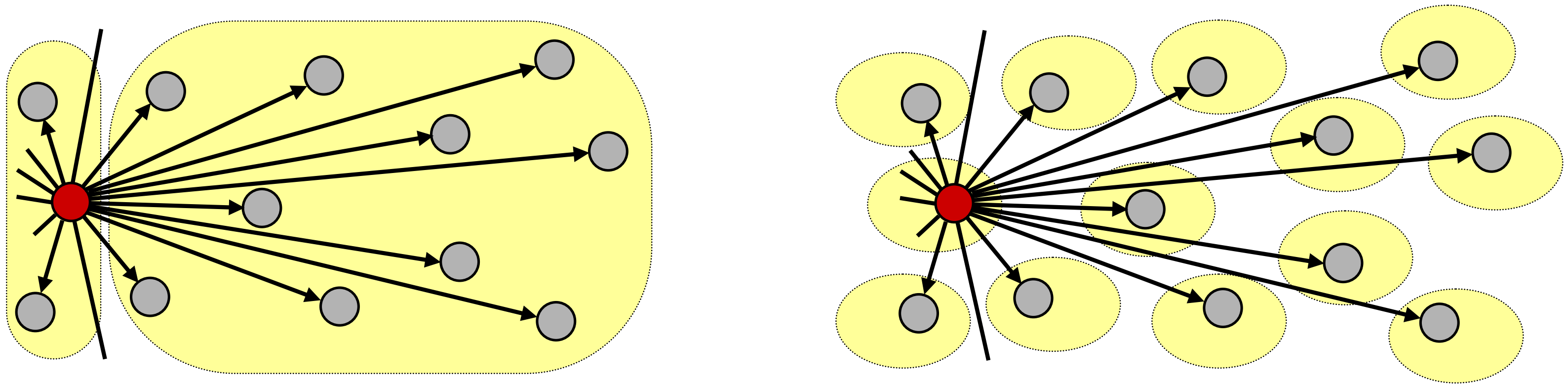
CLJP coarsening is fully parallel



- **10 C-points selected**
- **Standard AMG selects 9 C-points**

Parallel coarse-grid selection in AMG can produce unwanted side effects

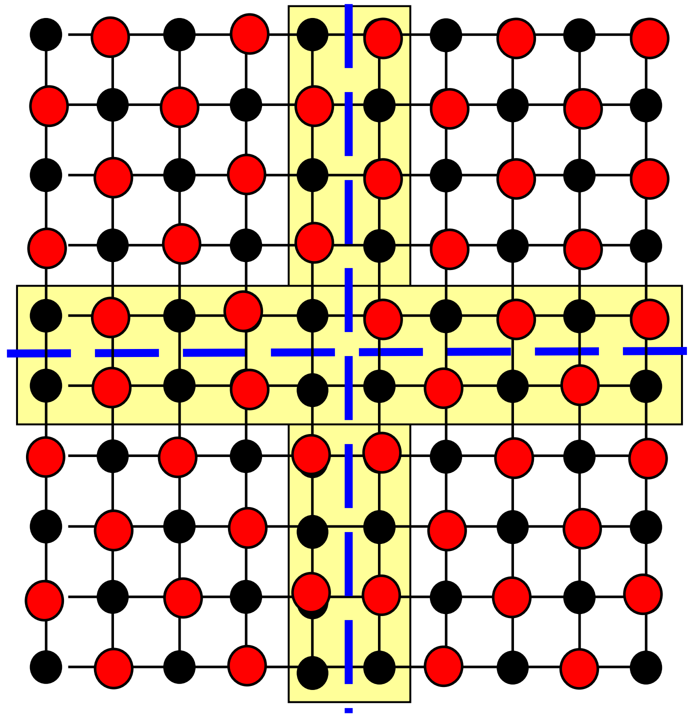
- Non-uniform grids can lead to increased operator complexity and poor convergence
- Operator "stencil growth" reduces parallel efficiency



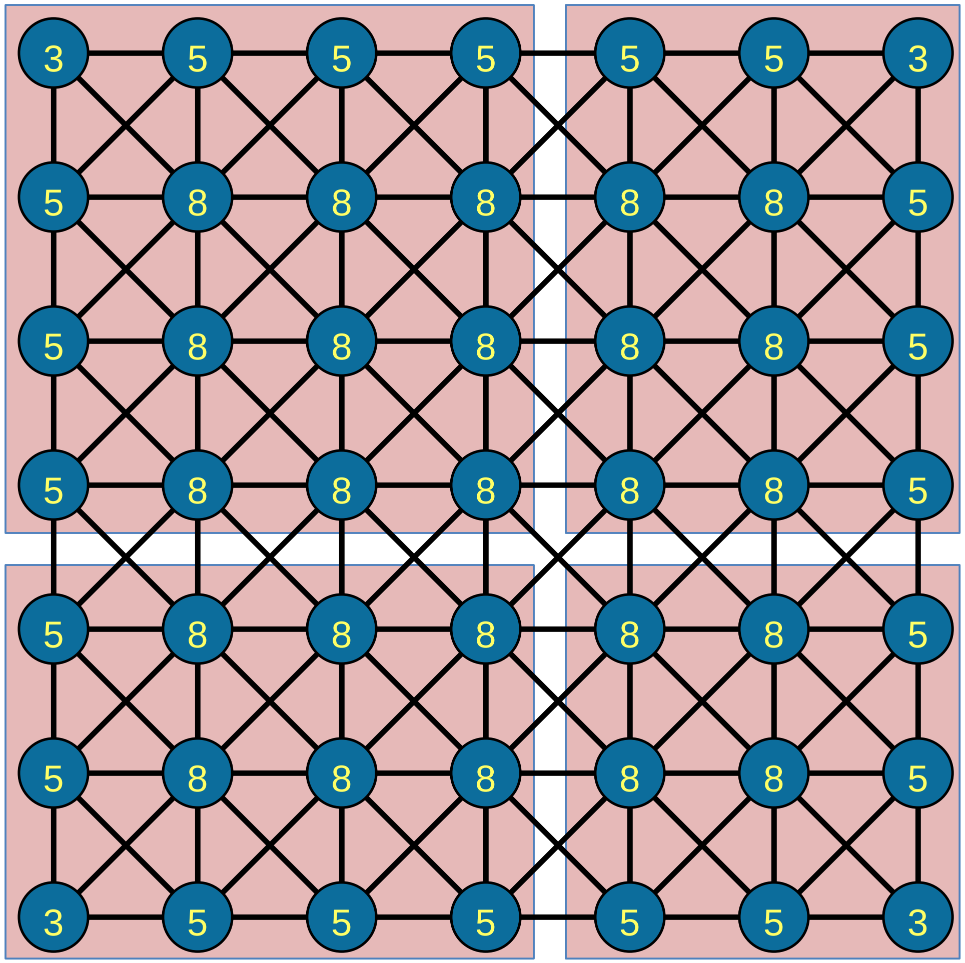
- Currently no guaranteed ways to control complexity
- Can ameliorate with more aggressive coarsening
- Requires long-range interpolation approaches

More aggressive coarsening in parallel – PMIS eliminates the second pass

- Parallel coarsening algorithms – perform sequential algorithm on each processor, then deal with processor boundaries

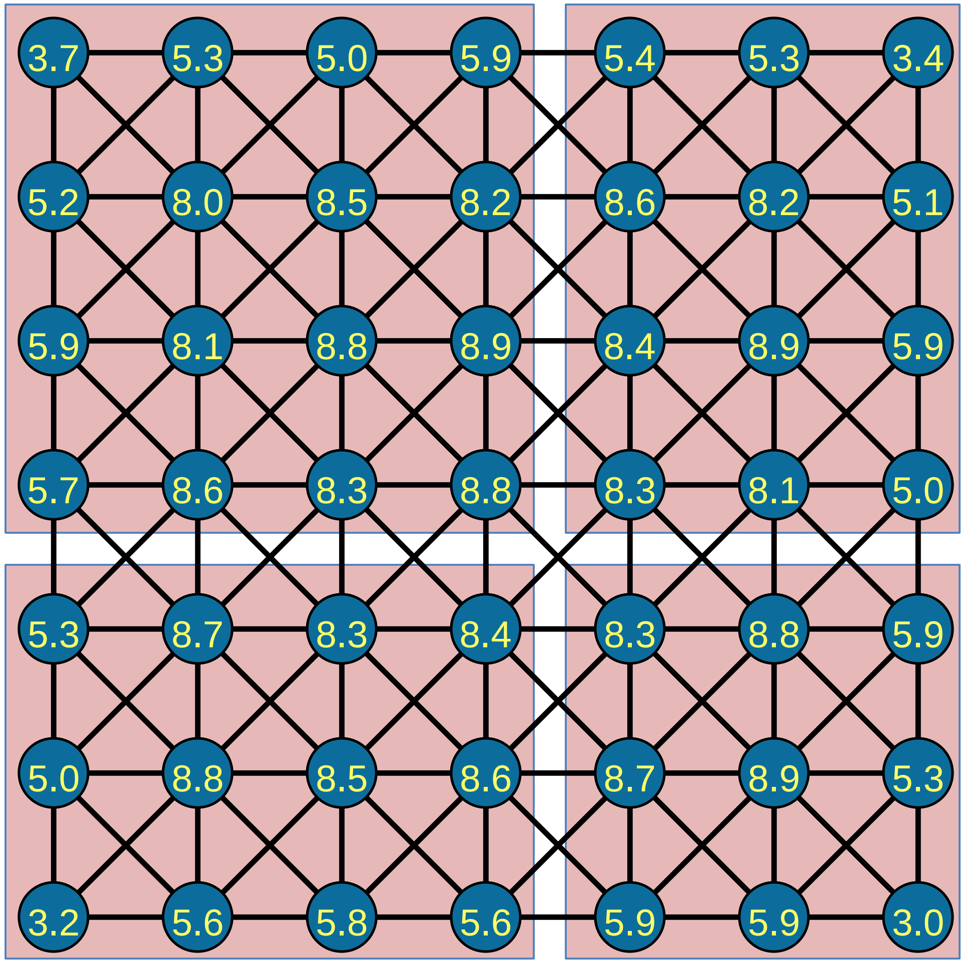


PMIS: start



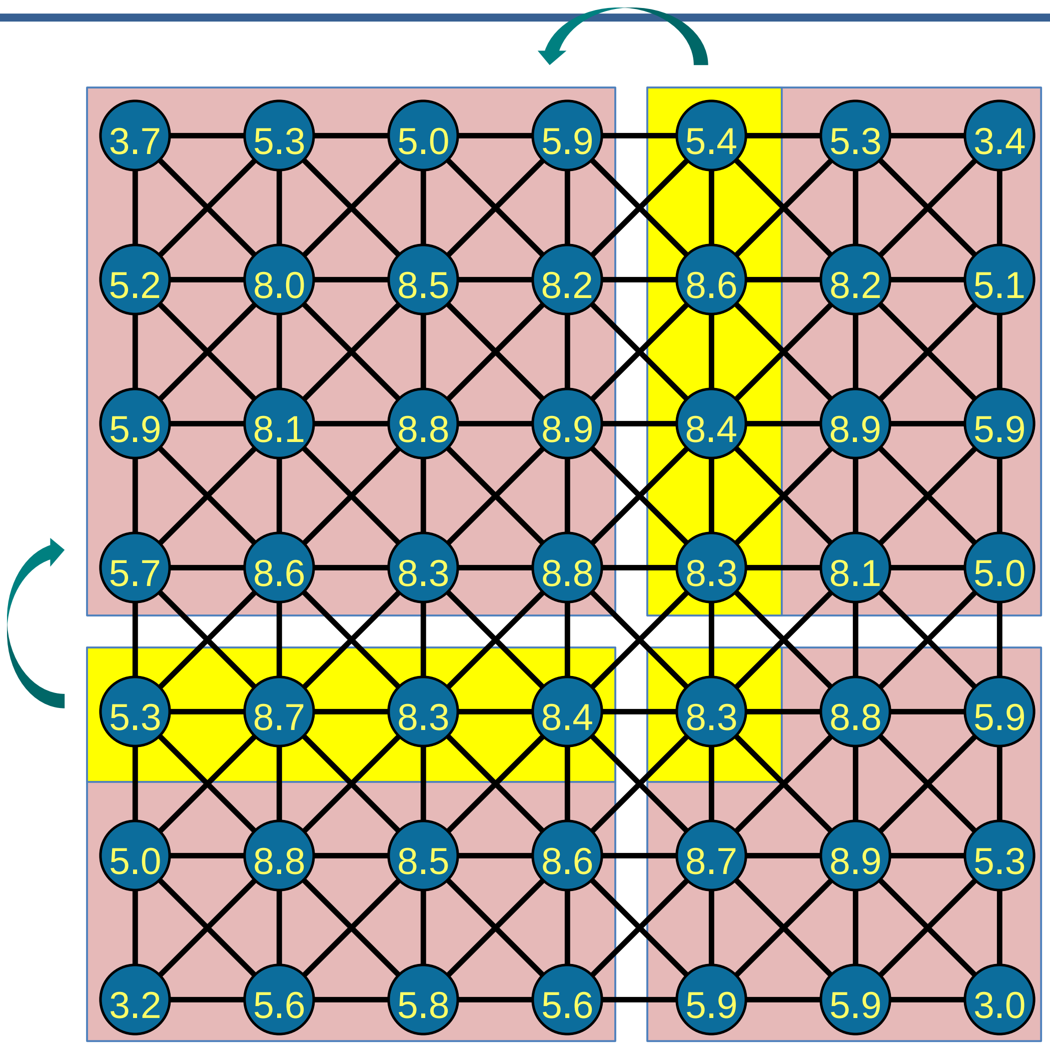
- select C-pt with maximal measure
- select neighbors as F-pts

PMIS: add random numbers



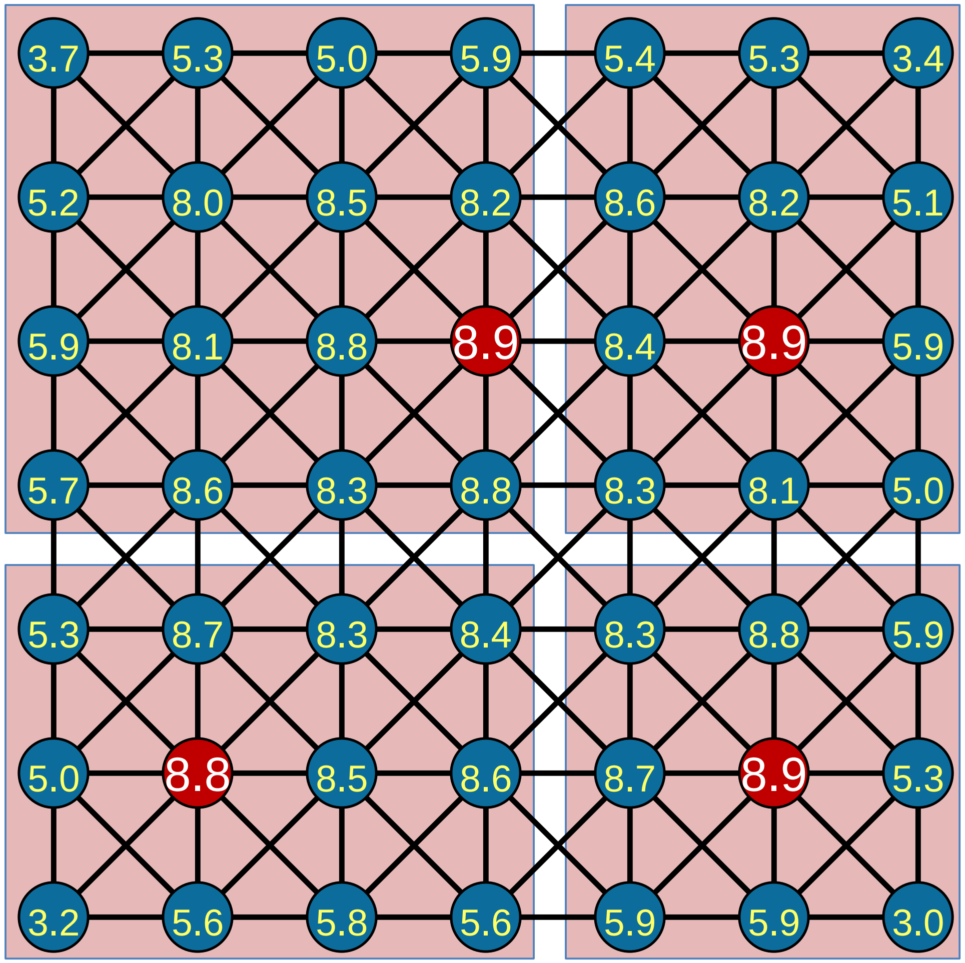
- select C-pt with maximal measure
- select neighbors as F-pts

PMIS: exchange neighbor information



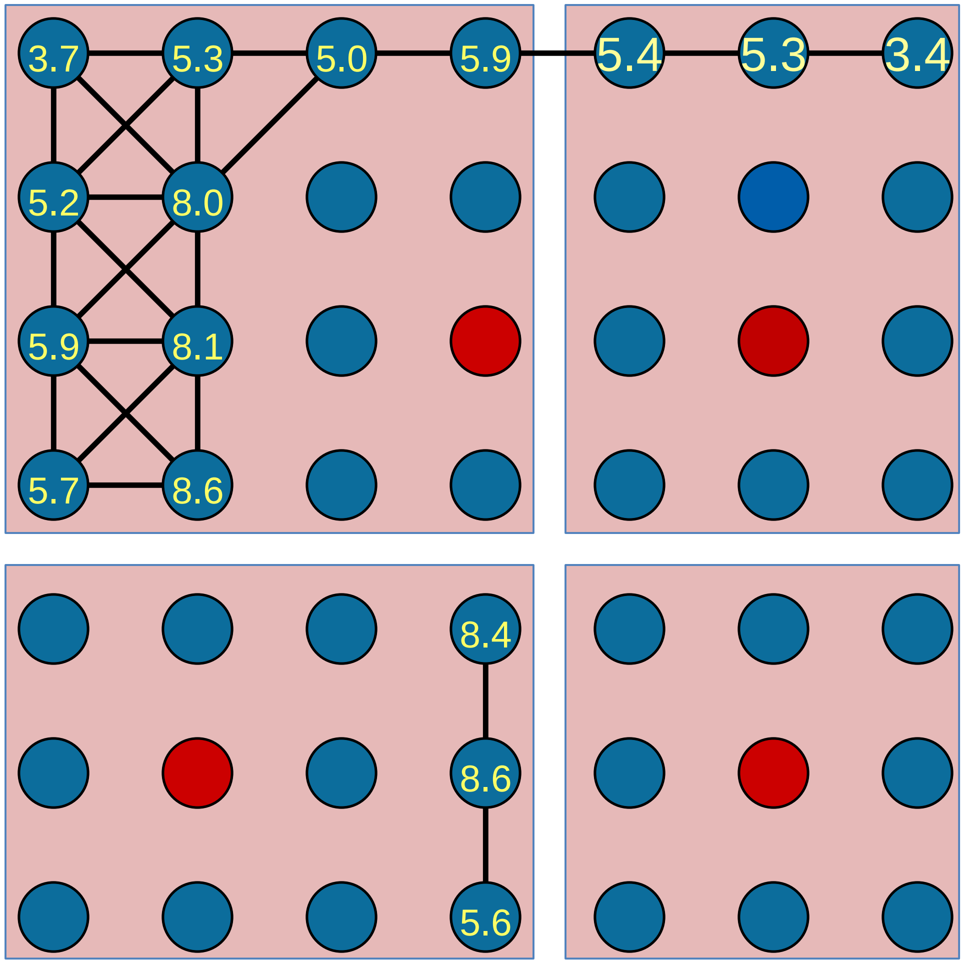
- select C-pt with maximal measure
- select neighbors as F-pts

PMIS: select



- select C-pts with maximal measure locally
- make neighbors F-pts

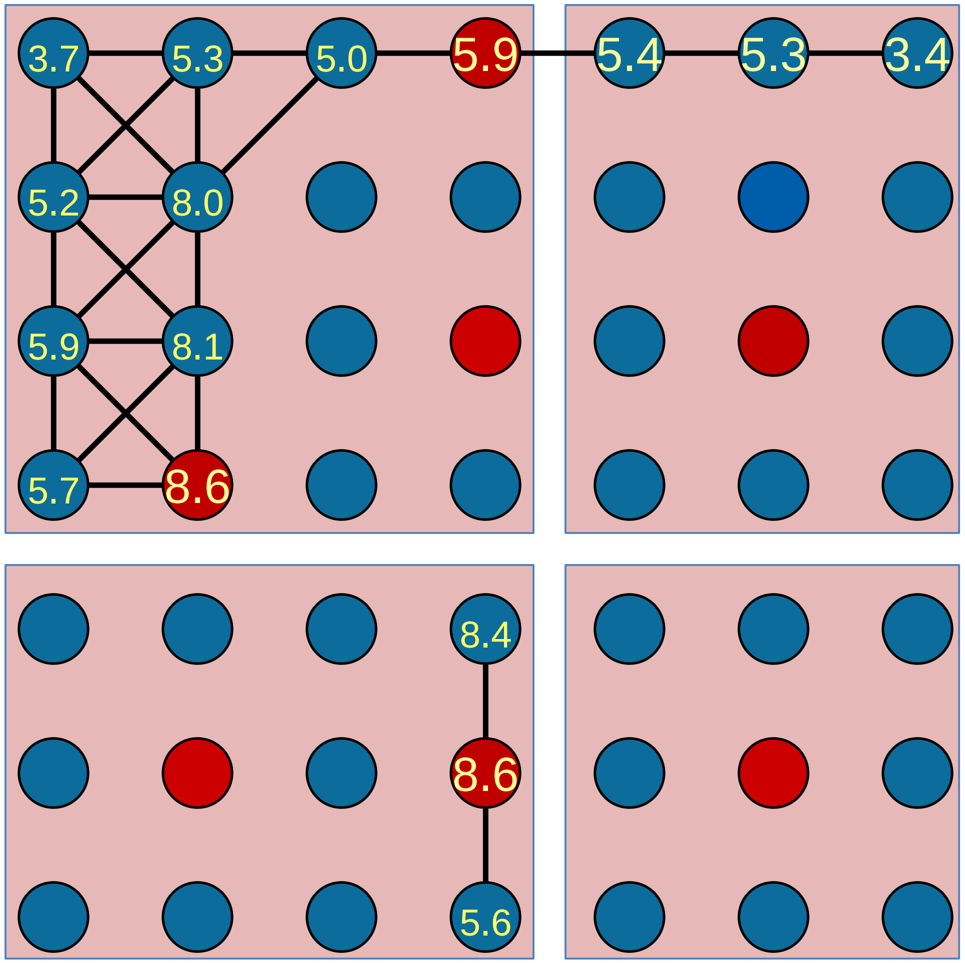
PMIS: update 1



- select C-pts with maximal measure locally

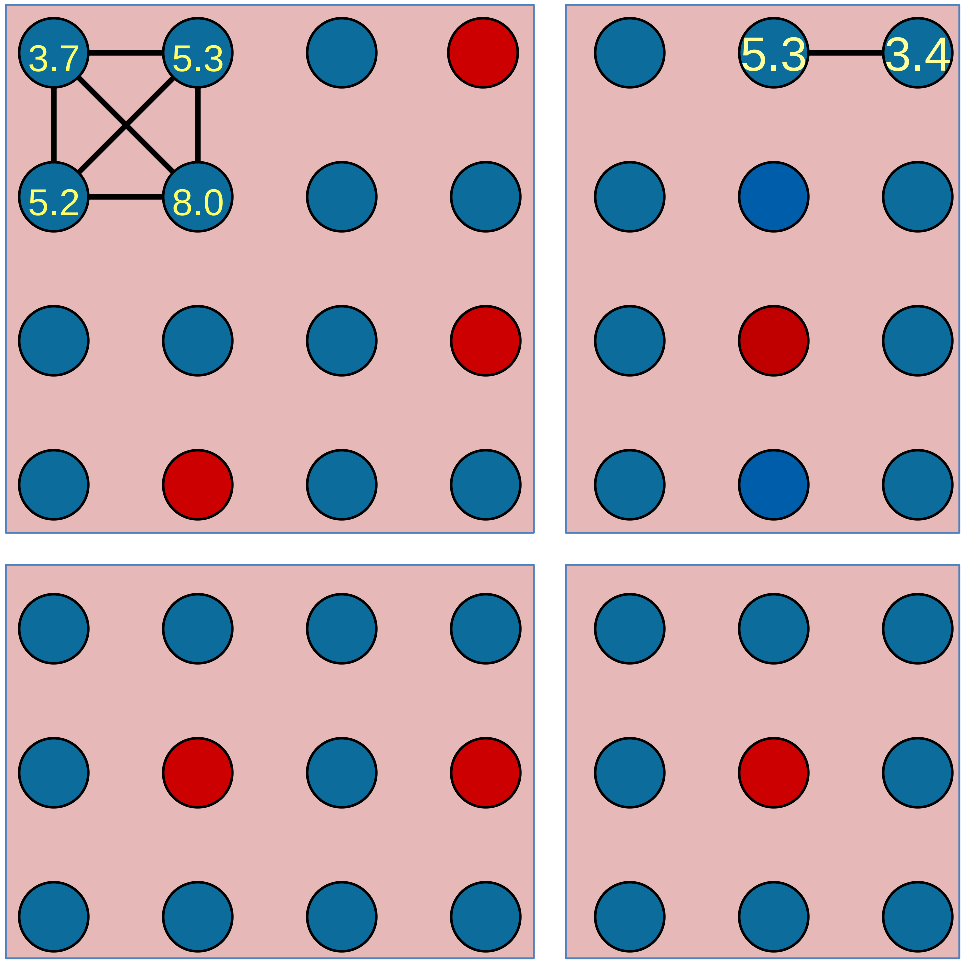
- make neighbors F-pts
(requires neighbor
 info)

PMIS: select



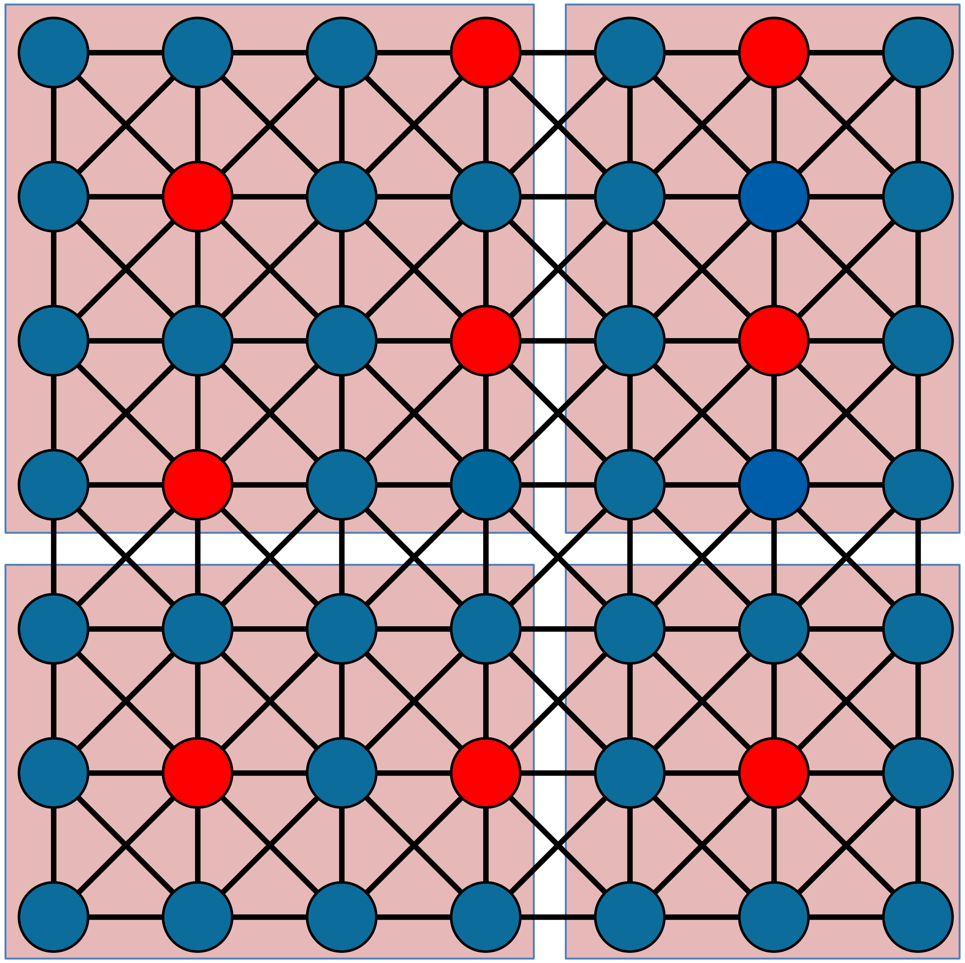
- select C-pts with maximal measure locally
- make neighbors F-pts

PMIS: update 2



- select C-pts with maximal measure locally
- make neighbors F-pts

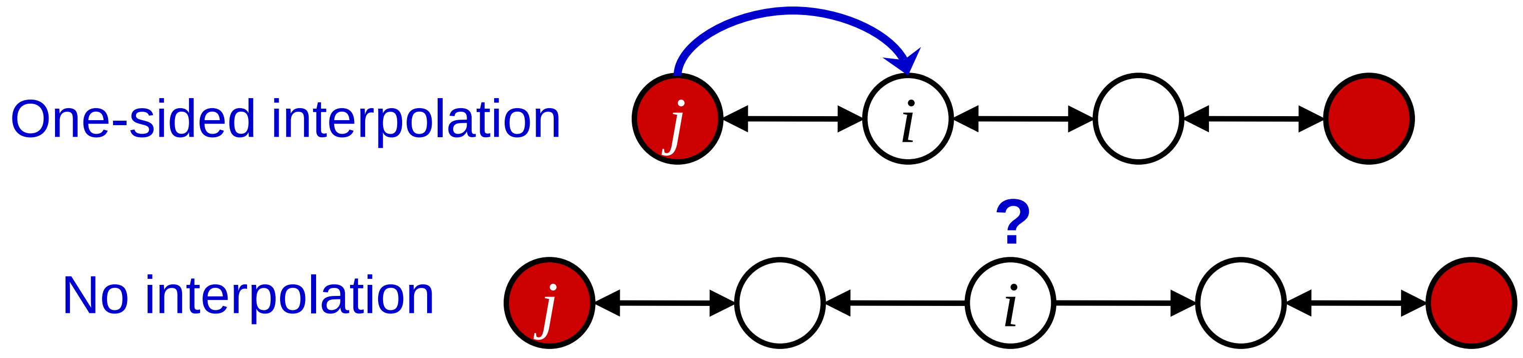
PMIS: final grid



- select C-pts with maximal measure locally
- make neighbor F-pts
- remove neighbor edges

C-AMG interpolation is not suitable for more aggressive coarsening

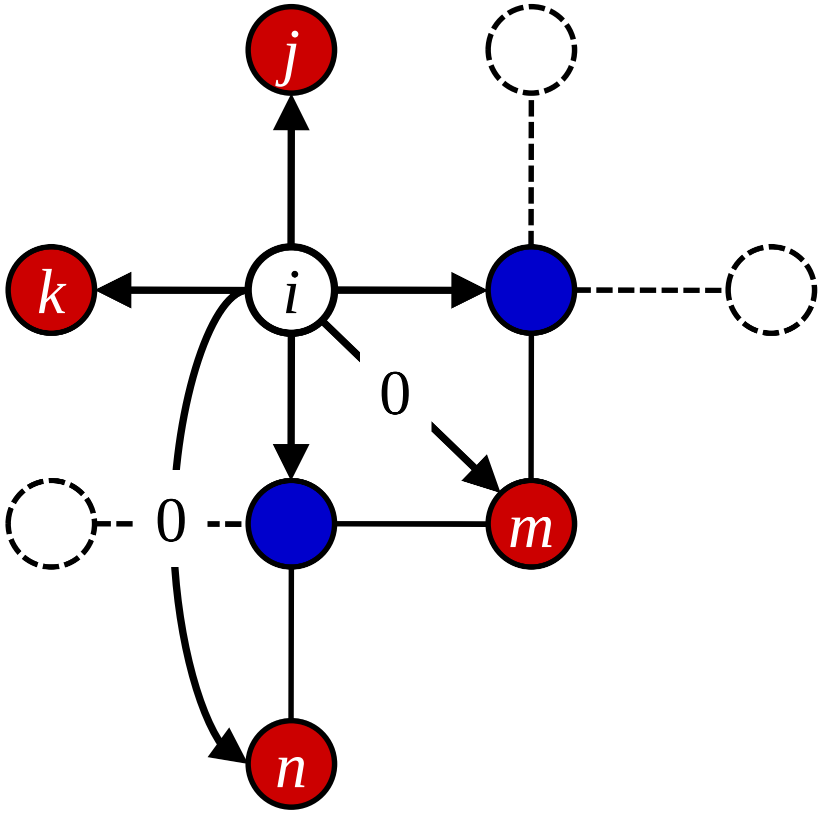
- PMIS is parallel and eliminates the second pass, which can lead to the following scenarios:



- Want above *i*-points to interpolate from both *C*-points
- Long-range (distance two) interpolation!

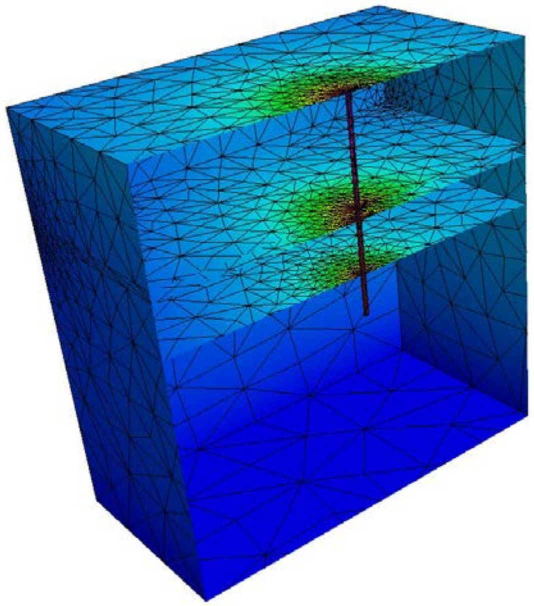
One possibility for long-range interpolation is extended interpolation

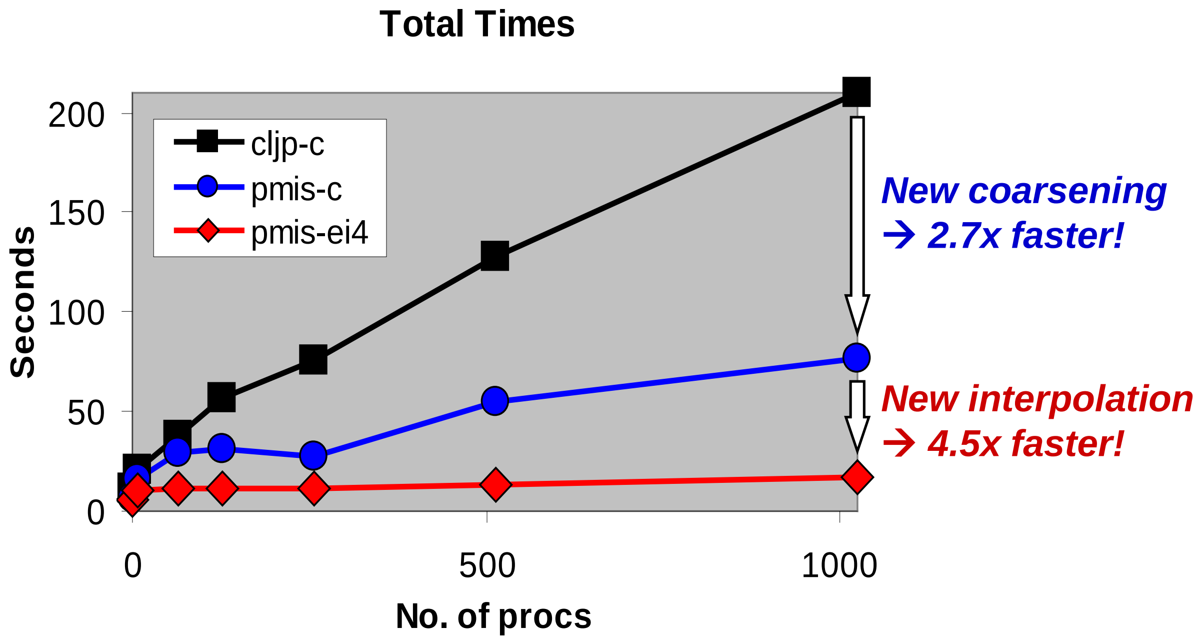
- C-AMG: $C_i = \{j,k\}$
- Long-range: $C_i = \{j,k,m,n\}$
- Extended interpolation – apply C-AMG interpolation to an extended stencil
- Extended+i interpolation is the same as extended, but also collapses to point *i*
- Improves overall quality



New parallel coarsening and long-range interpolation methods improve scalability

- Unstructured 3D problem with material discontinuities
- About 90K unknowns per processor on MCR (Linux cluster)
- AMG - GMRES(10)





Agglomeration of coarsest grid

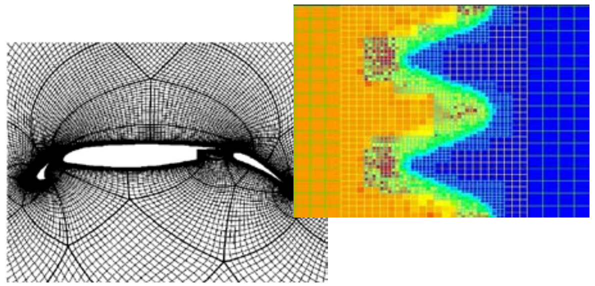
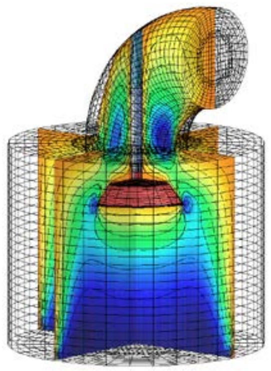
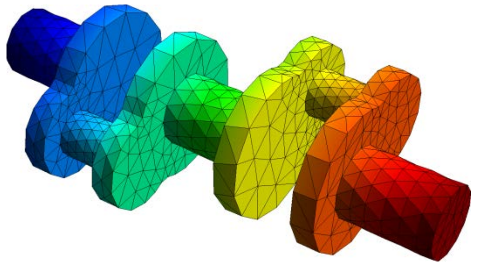
- One technique that can be useful is to gather (agglomerate) the system matrix at some coarse level to a single processor
- This costs O(log P) communications, but so does simply continuing the V-cycle
- This helps when the matrix rows have grown in complexity
  - Avoids cost of communicating with many neighbors

Multigrid Software Design

hypre
high performance preconditioners

Simulation codes present a wide array of challenges for scalable linear solver libraries

- Different applications
  - Diffusion, elasticity, magnetohydrodynamics (MHD)
- Different discretizations and meshes
  - Structured, block-structured, structured AMR, overset, unstructured

- Different languages – C, C++, Fortran
- Different programming models – MPI, OpenMP
- Scalability beyond 100,000 processors!

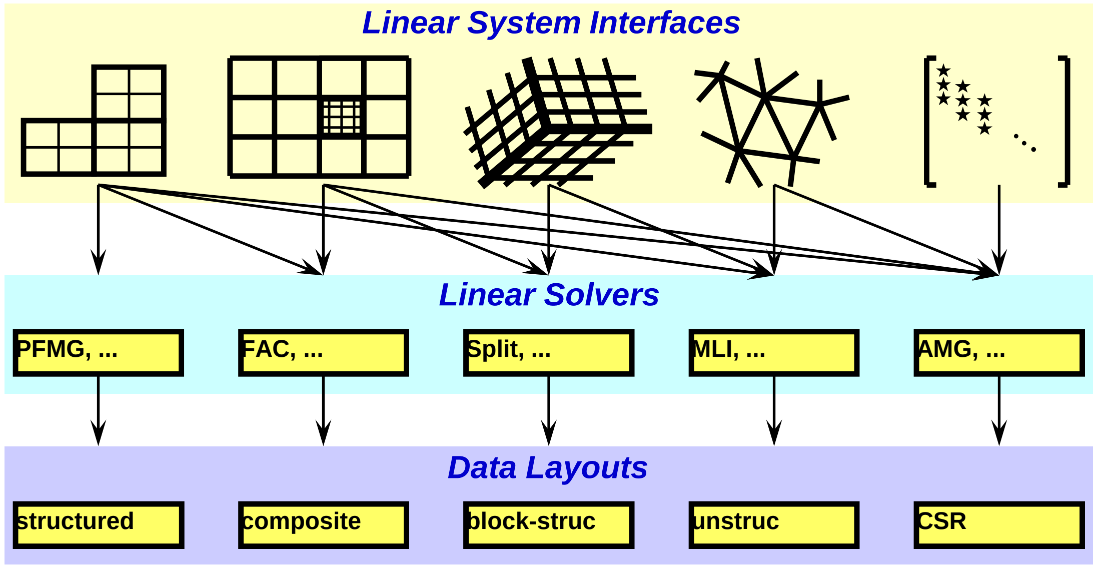
Challenge: Software design

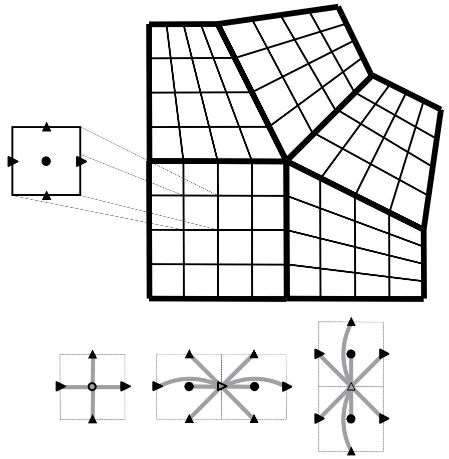
- The “best” solver for a given application usually takes advantage of the setting
  - structured grids, constant coefficients, FE discretization, etc.

- Traditional linear solver libraries take in only generic matrix-vector information

- How do we supply these “best solvers” in library form?

Unique software interfaces in *hypre* provide efficient solvers not available elsewhere





Block-structured grid with 3 variable types and 3 discretization stencils

- Example: *hypre*'s interface for semi-structured grids
  — Based on "grids" and either "stencils" or "finite elements" (new)
  — Allows for specialized solvers for structured AMR
  — Also provides for more general solvers like *AMG*

Challenge: Parallel implementation

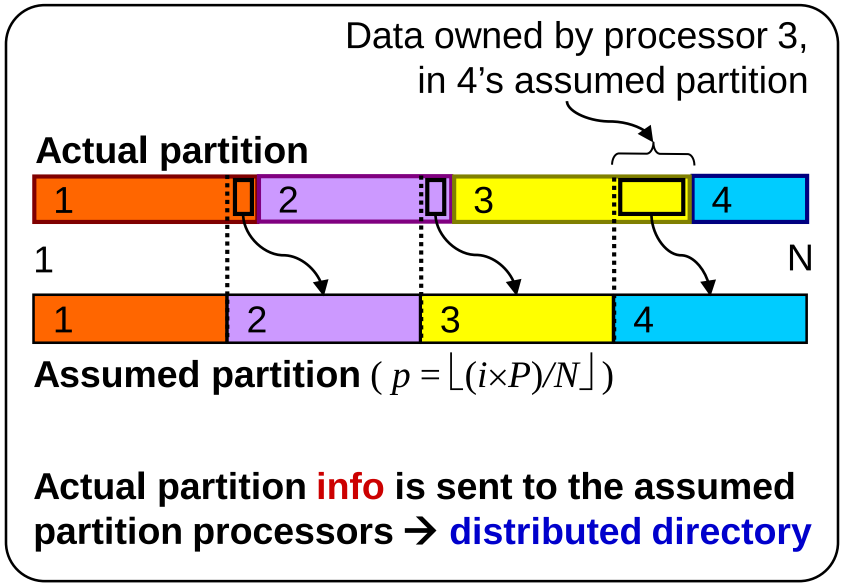
- Simple algorithms can be used for modest numbers of processors (< 100)
  - e.g., store O(P) data and do $O(P^2)$ computations to determine send/receive patterns

- On large numbers of processors (1K – 10K), algorithms get more complex
  - e.g., store O(P) data and do O(P) computations to determine send/receive patterns

- What about 100K – 1B processors?

Assumed partition (AP) algorithm enables scaling to 100K+ processors

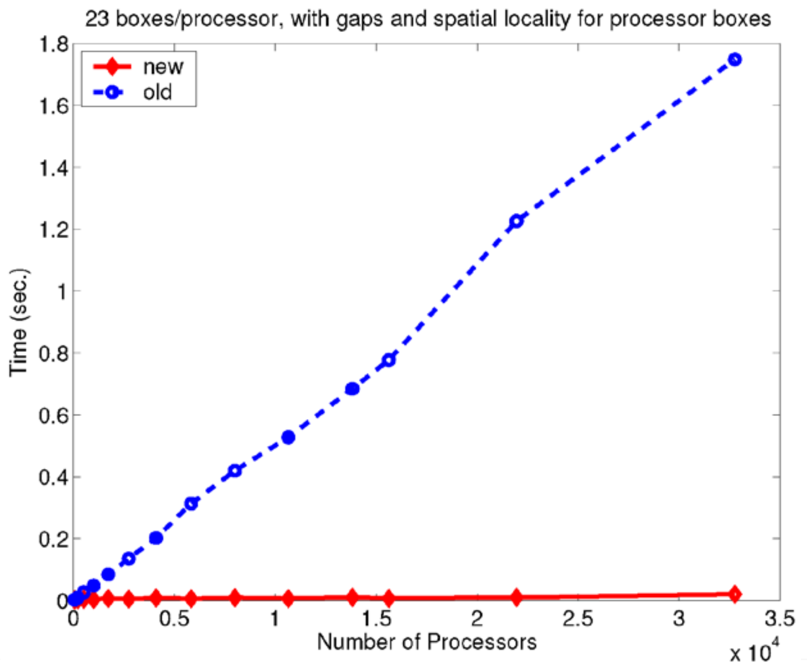
- Answering global distribution questions previously required $O(P)$ storage & computations
- On BG/L, $O(P)$ storage may not be possible
- AP algorithm requires
  - $O(1)$ storage
  - $O(\log P)$ computations
- Default approach in *hypre*
- AP has general applicability beyond *hypre*

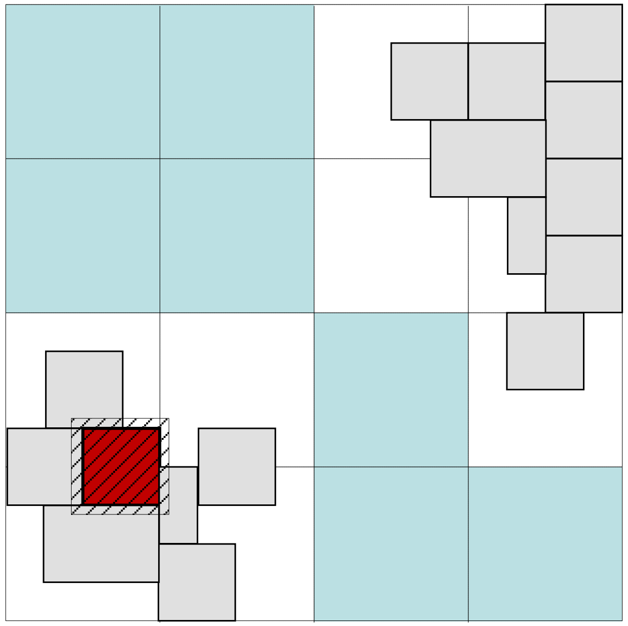

Data owned by processor 3, in 4's assumed partition
Actual partition
1
2
3
4
1
N
1
2
3
4
Assumed partition ($p = \lfloor (i \times P)/N \rfloor$)

Actual partition info is sent to the assumed partition processors → distributed directory

Assumed partition (AP) algorithm is more challenging for structured AMR grids

- AMR can produce grids with “gaps”
- Our AP function accounts for these gaps for scalability
- Demonstrated on 32K procs of BG/L



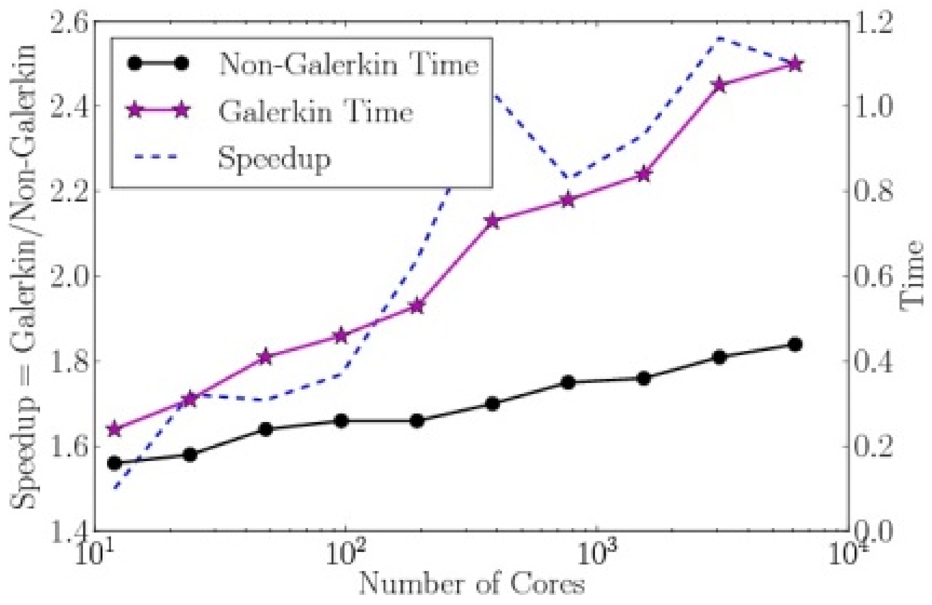


Simple, naïve AP function leaves processors with empty partitions

Some Recent Research Topics

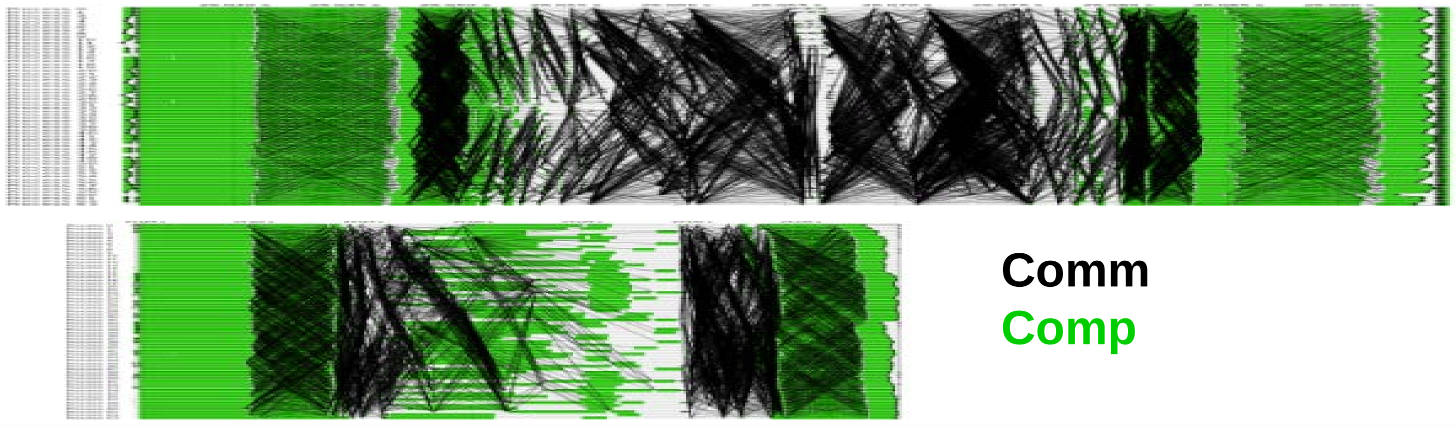
Recent spatial-MG research focuses on reducing parallel communication costs (1)

- Non-Galerkin AMG replaces the usual coarse-grid operators with sparser ones
  - Speedups from 1.2x - 2.4x over existing AMG
  - In *hypre* 2.10.0b



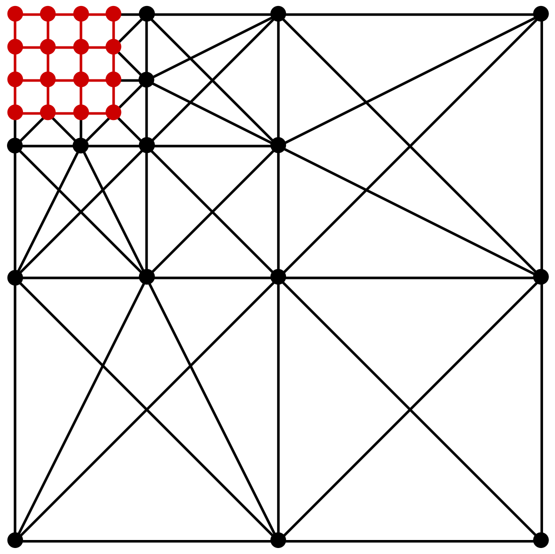
Recent spatial-MG research focuses on reducing parallel communication costs (2)

- Mult-additive AMG exploits a theoretical identity to inherit the parallelization benefits of additive methods and the convergence properties of multiplicative
  - Additive MG is good at overlapping communication and computation, but converges slower than multiplicative MG
  - Speedups of 2x over existing AMG
  - In *hypre* 2.10.0b



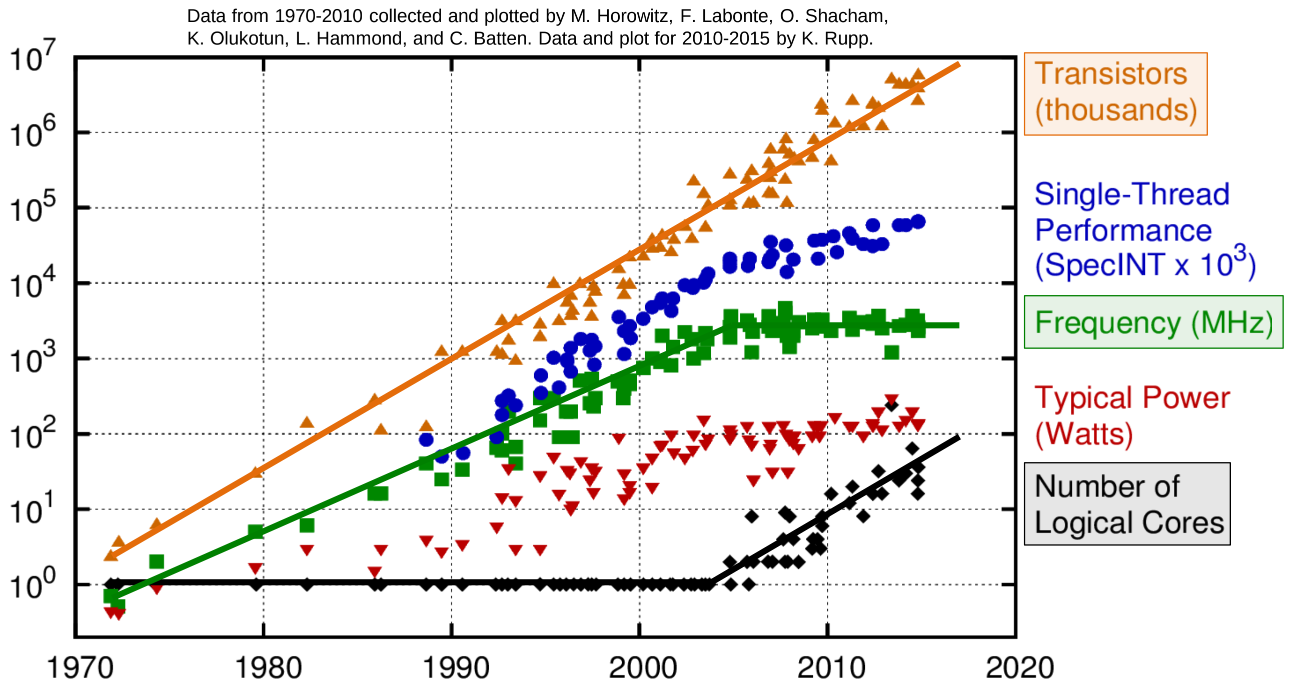
Recent spatial-MG research focuses on reducing parallel communication costs (3)

- AMG domain decomposition (AMG-DD) employs cheap global problems to speed up convergence
  - Constructs problems algebraically from an existing method
  - Potential for FMG convergence with only log N latency (vs $\log^2$ N)!
  - Implementing parallel code



Parallel Time Integration (Parallel Multigrid in Time)

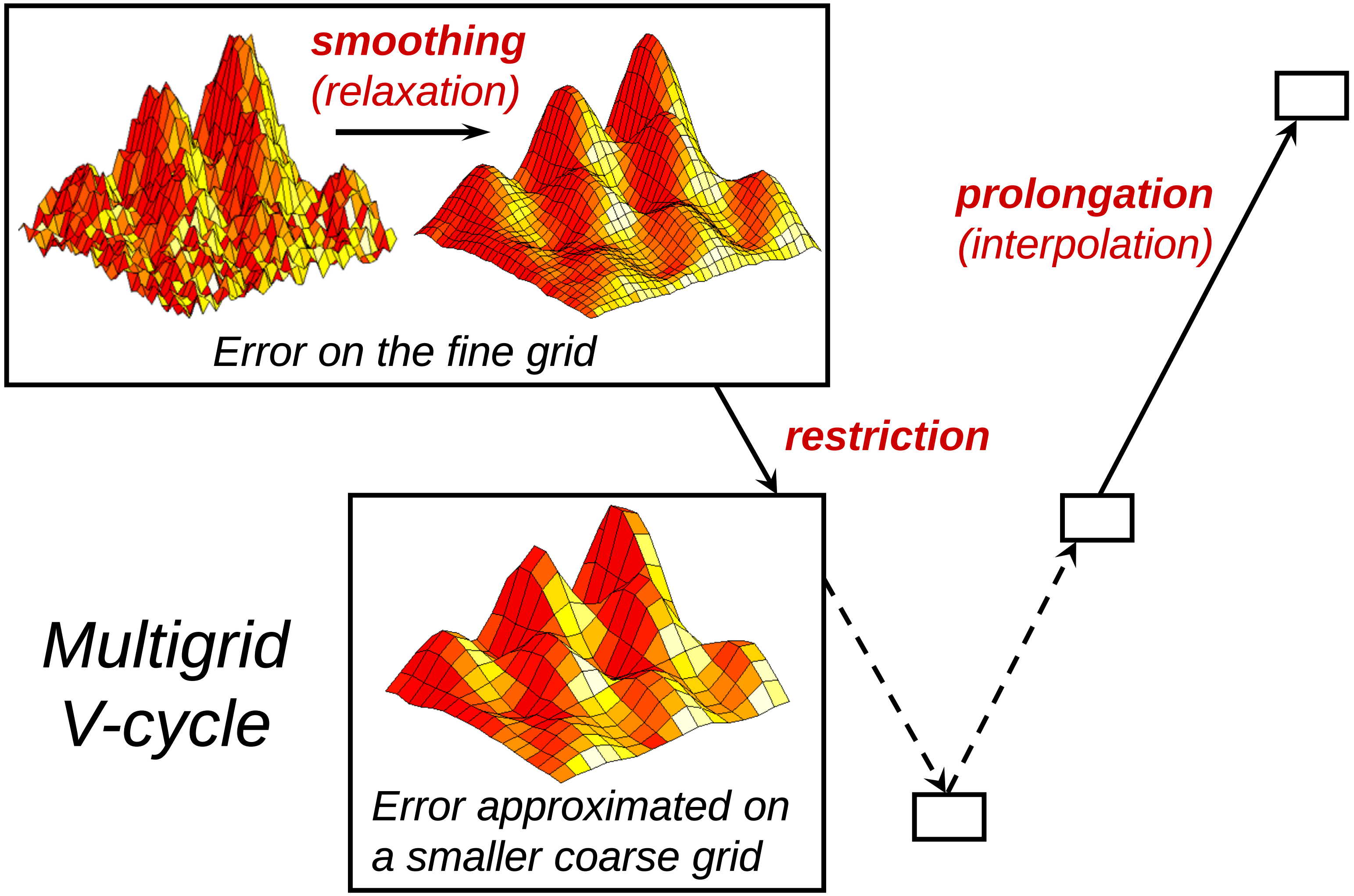
Parallel time integration is a major paradigm shift driven by hardware design realities



- Architecture trend: flat clock rates, more concurrency
  - Traditional time stepping is becoming a sequential bottleneck

- Continued advancement in scientific simulation will require algorithms that are parallel in time

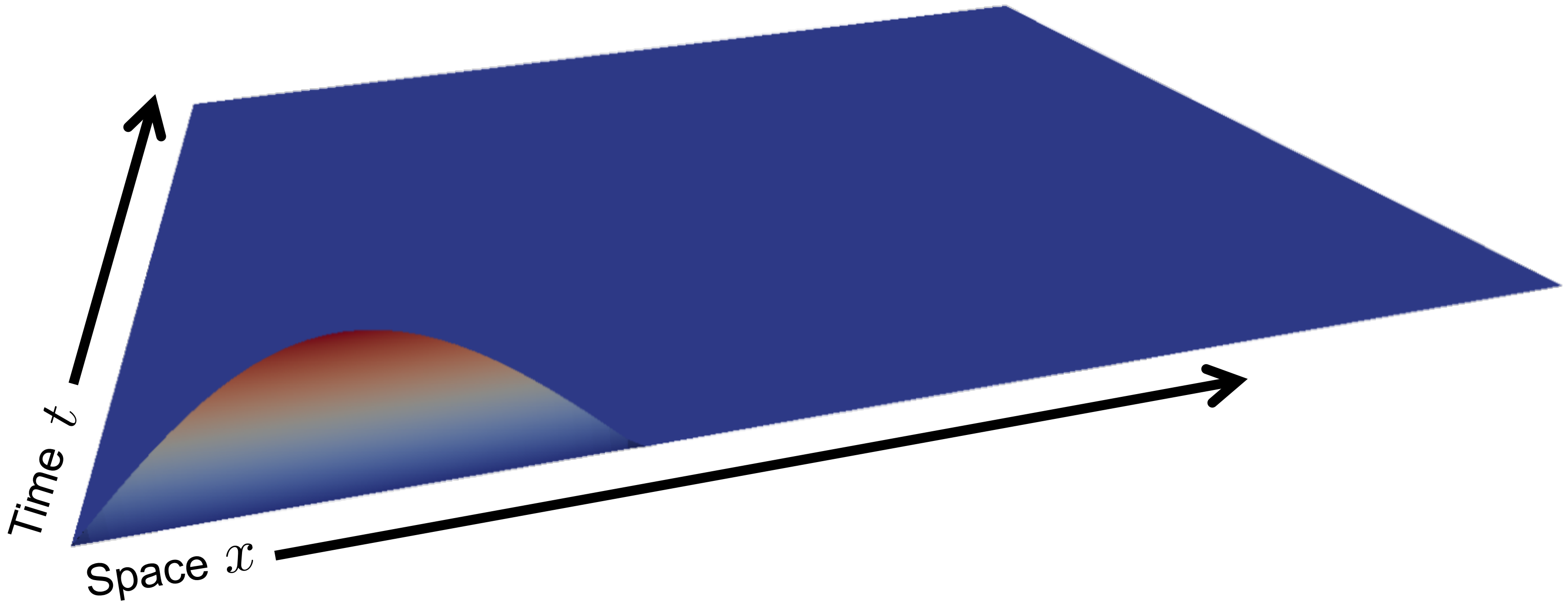
One approach for parallel-in-time: apply multigrid ideas to the (space-)time dimension



Multigrid V-cycle

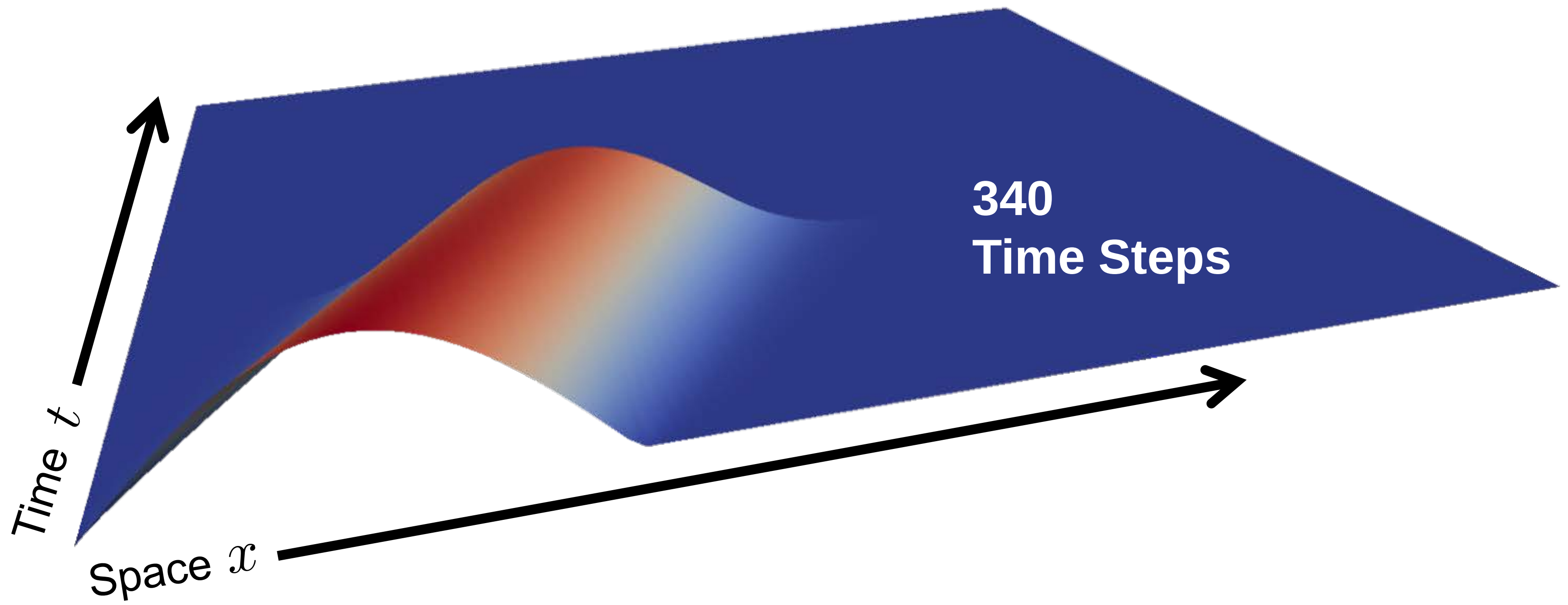
Time stepping is sequential

- Simple advection equation, $u_t = -cu_x$
- Initial condition is a wave



Time stepping is sequential

- Simple advection equation, $u_t = -cu_x$
- Wave propagates serially through space



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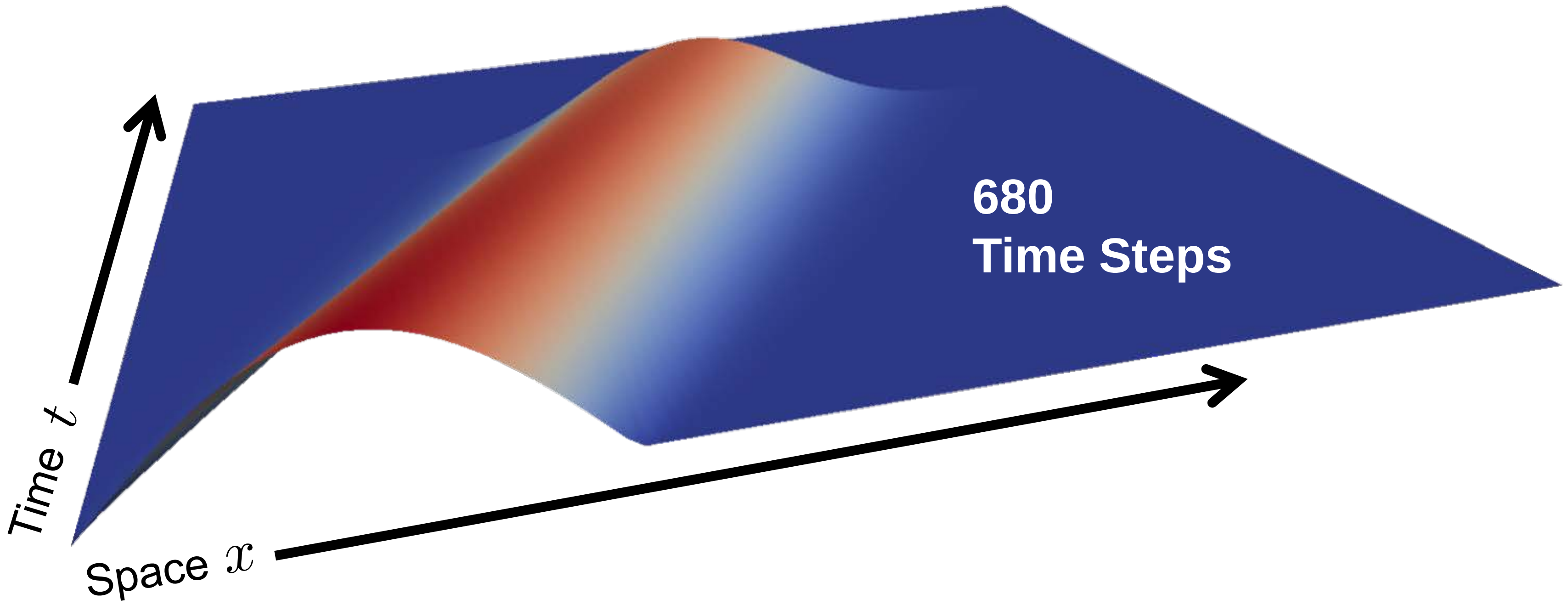

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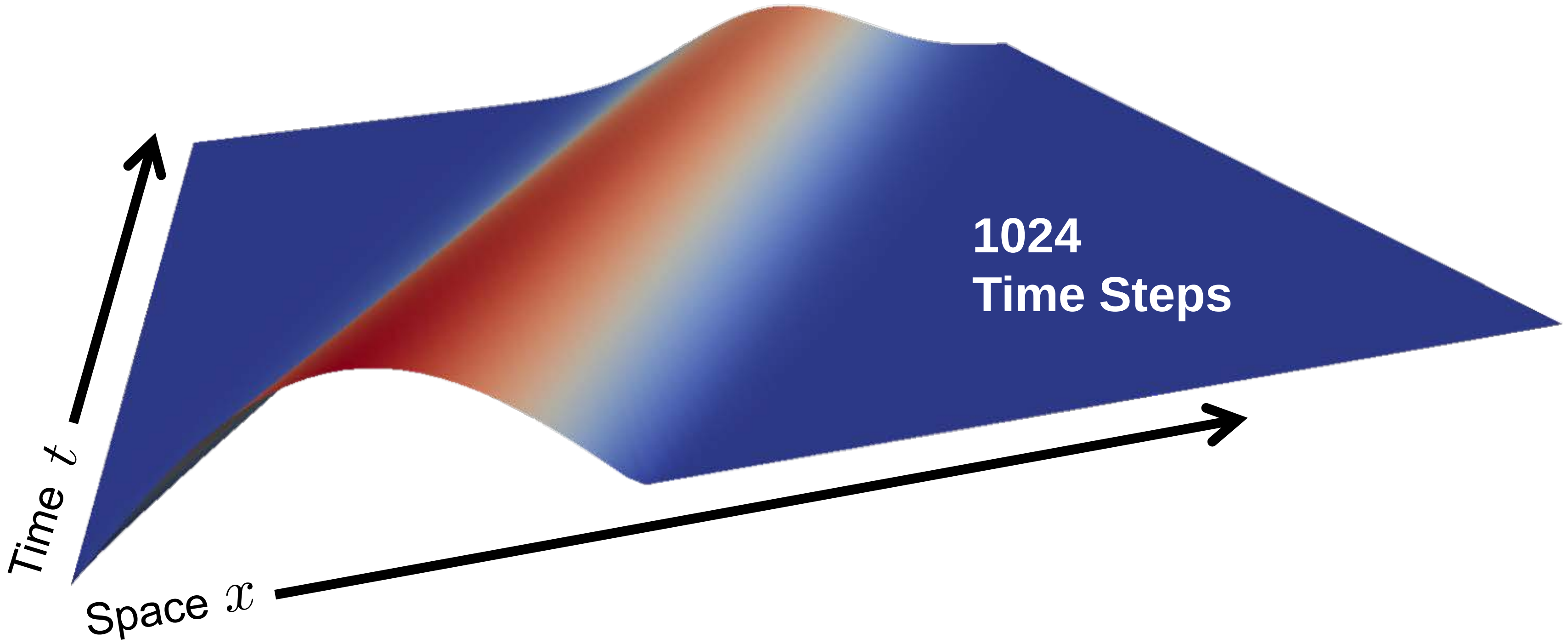
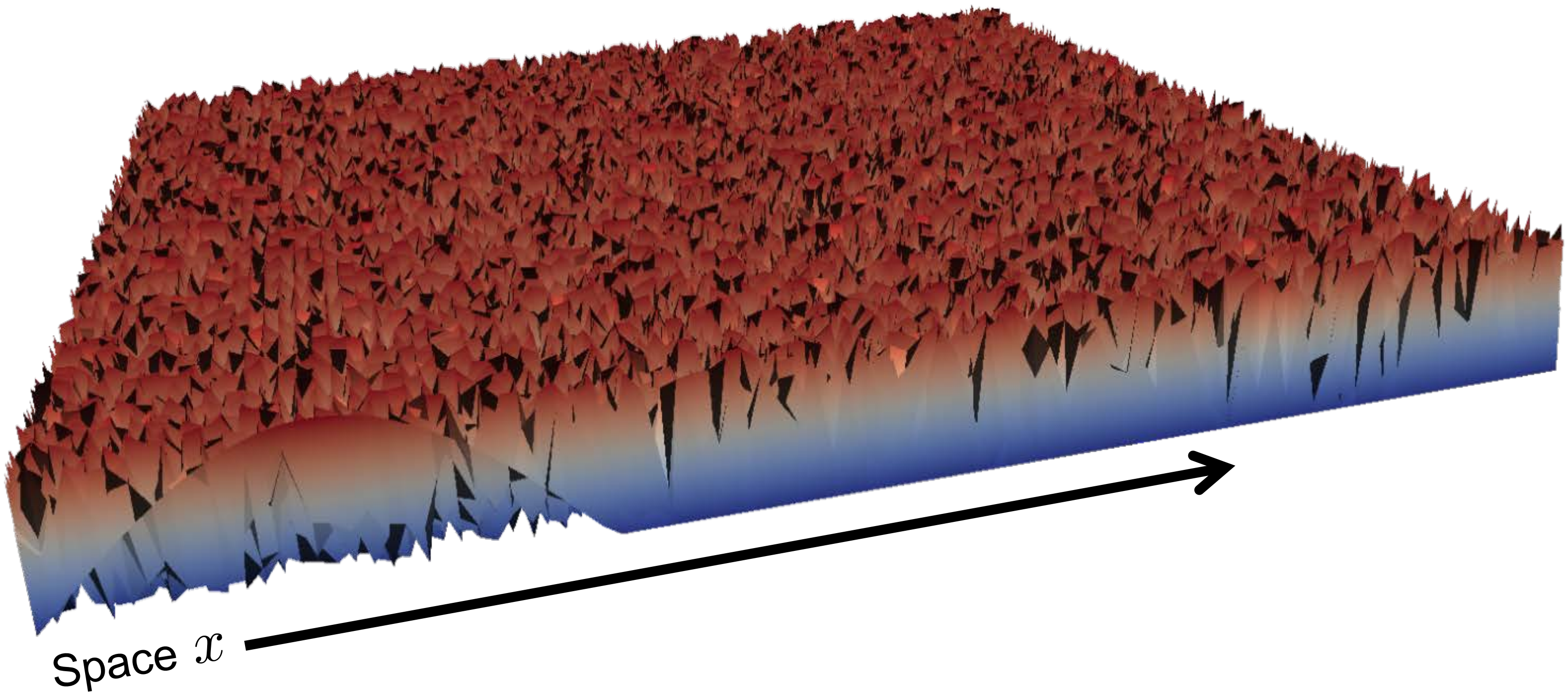


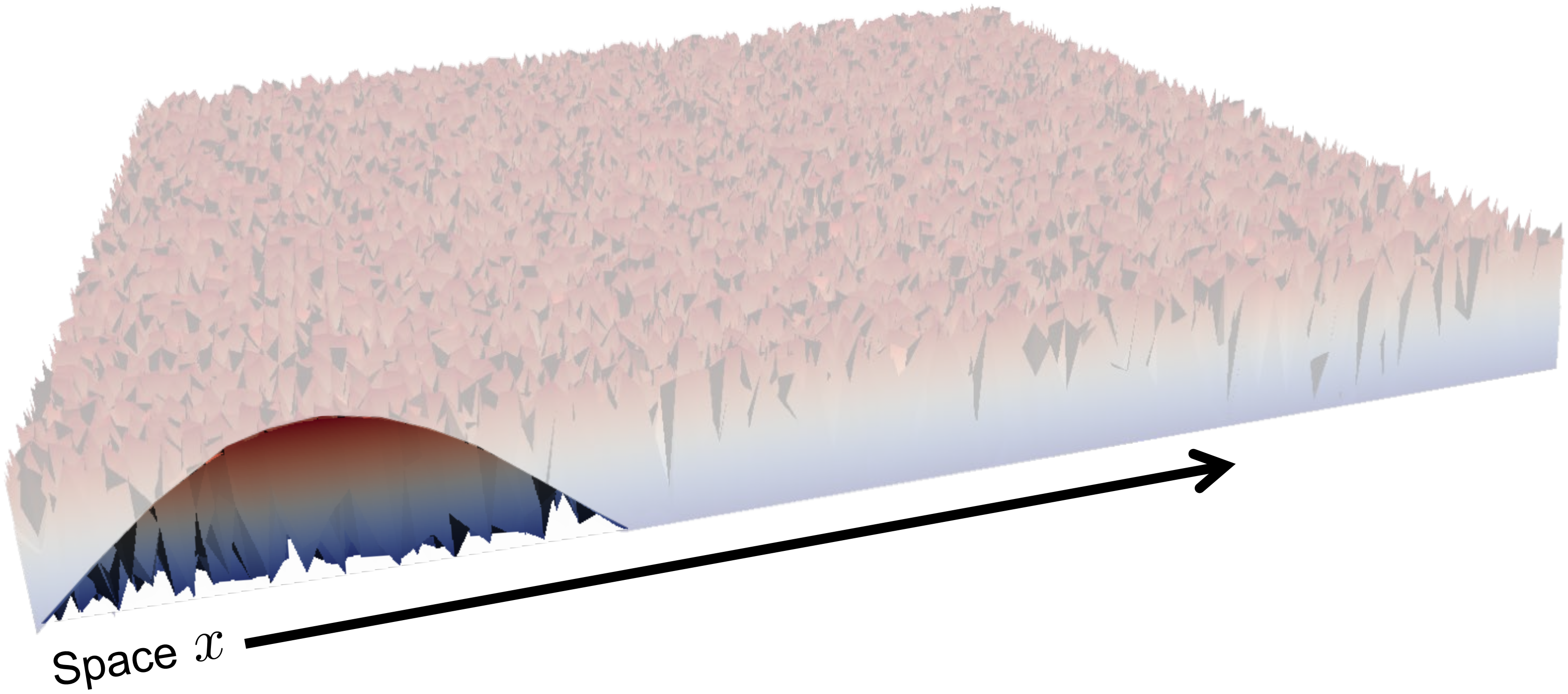
Multigrid-in-time converges to the serial space-time solution in parallel

- Simple advection equation, $u_t = -cu_x$
- Random initial space-time guess (only for illustration)



Multigrid-in-time converges to the serial space-time solution in parallel

- Simple advection equation, $u_t = -cu_x$
- Initial condition is a wave



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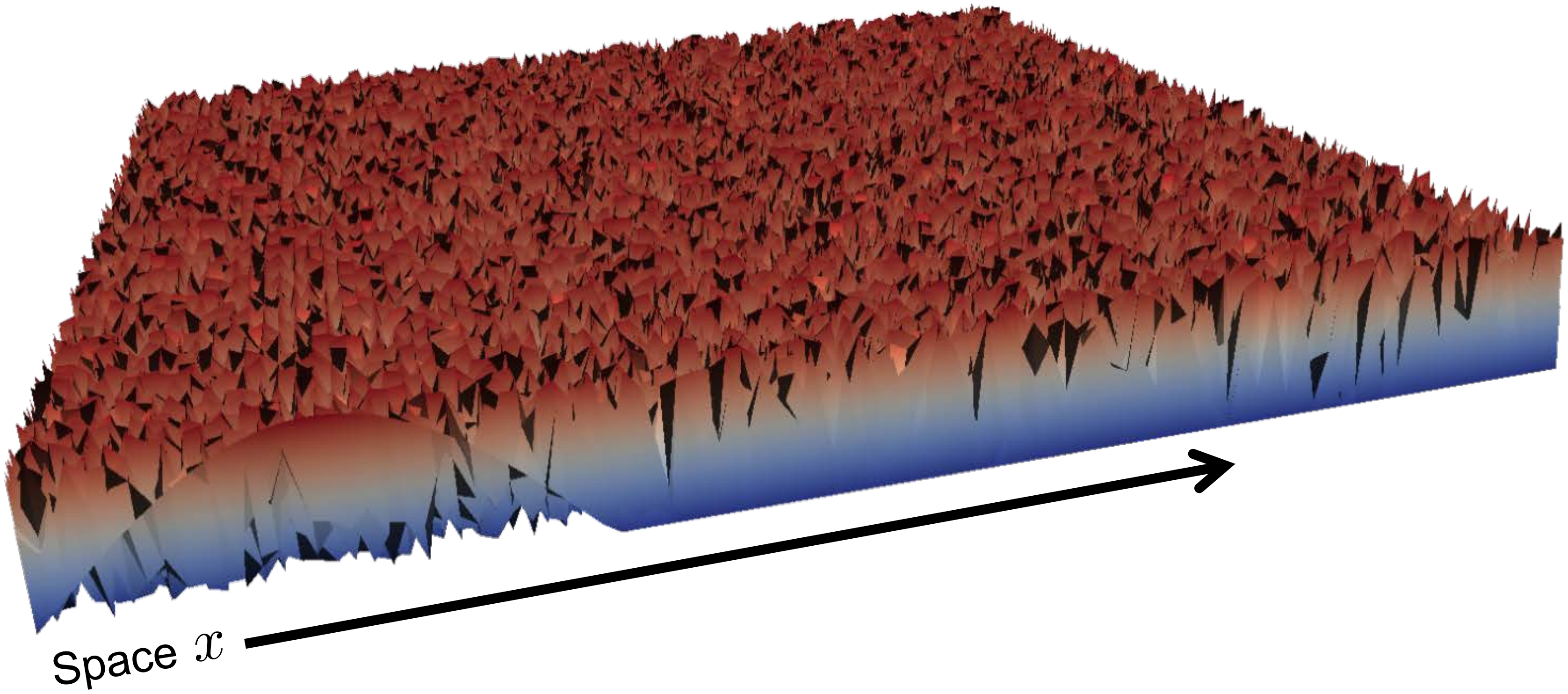
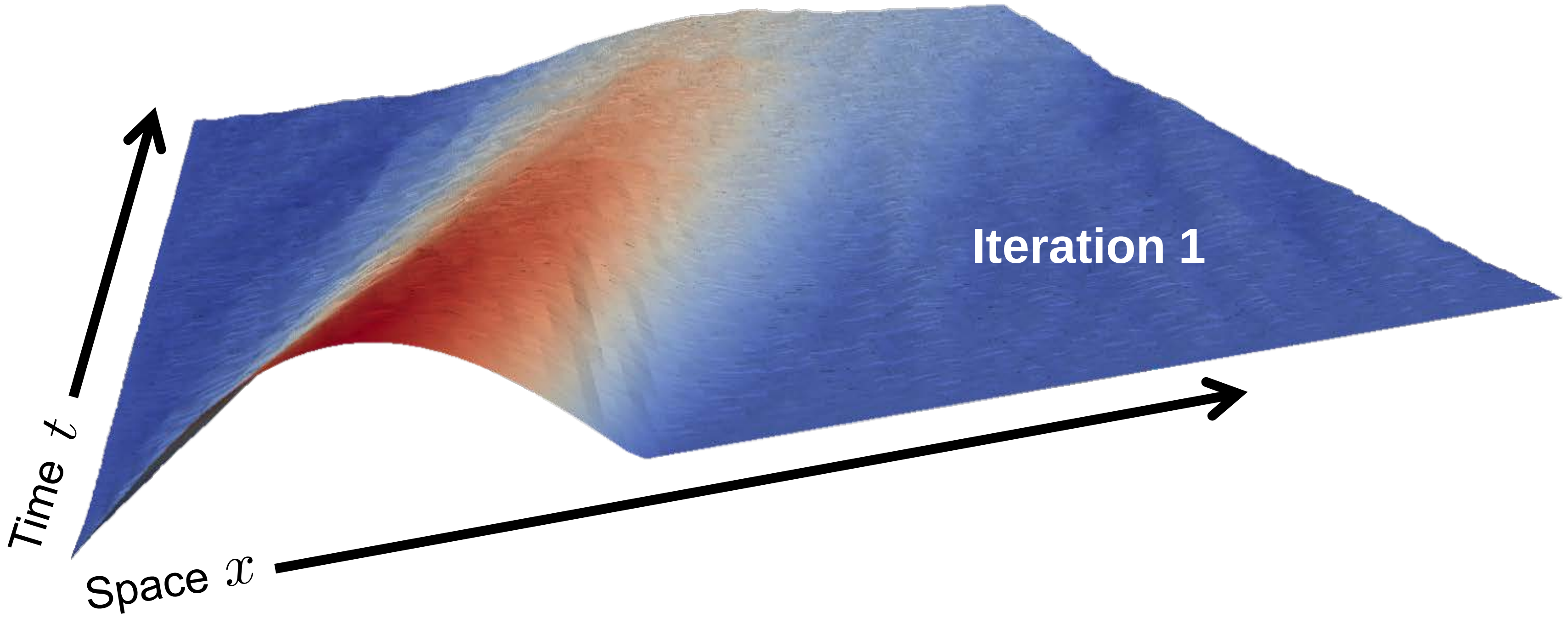


Multigrid-in-time converges to the serial space-time solution in parallel

- Simple advection equation, $u_t = -cu_x$
- Multilevel structure allows for fast data propagation



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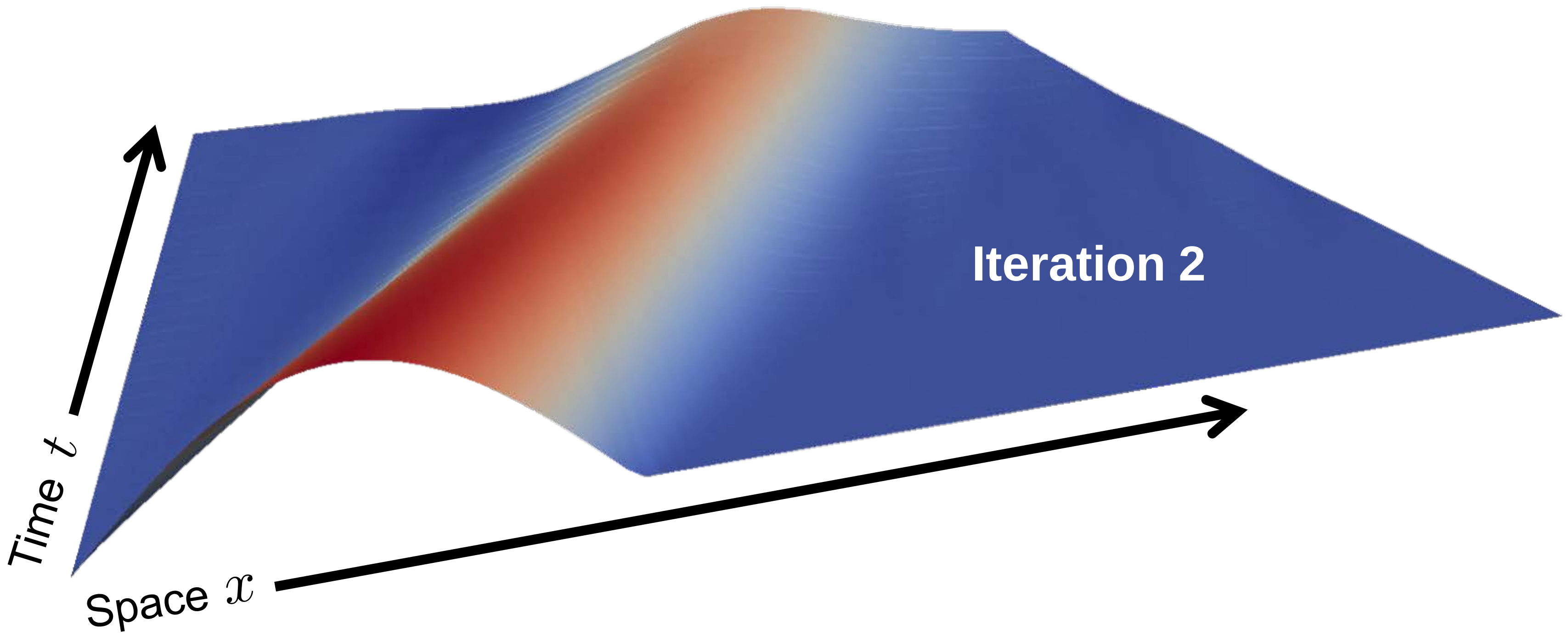

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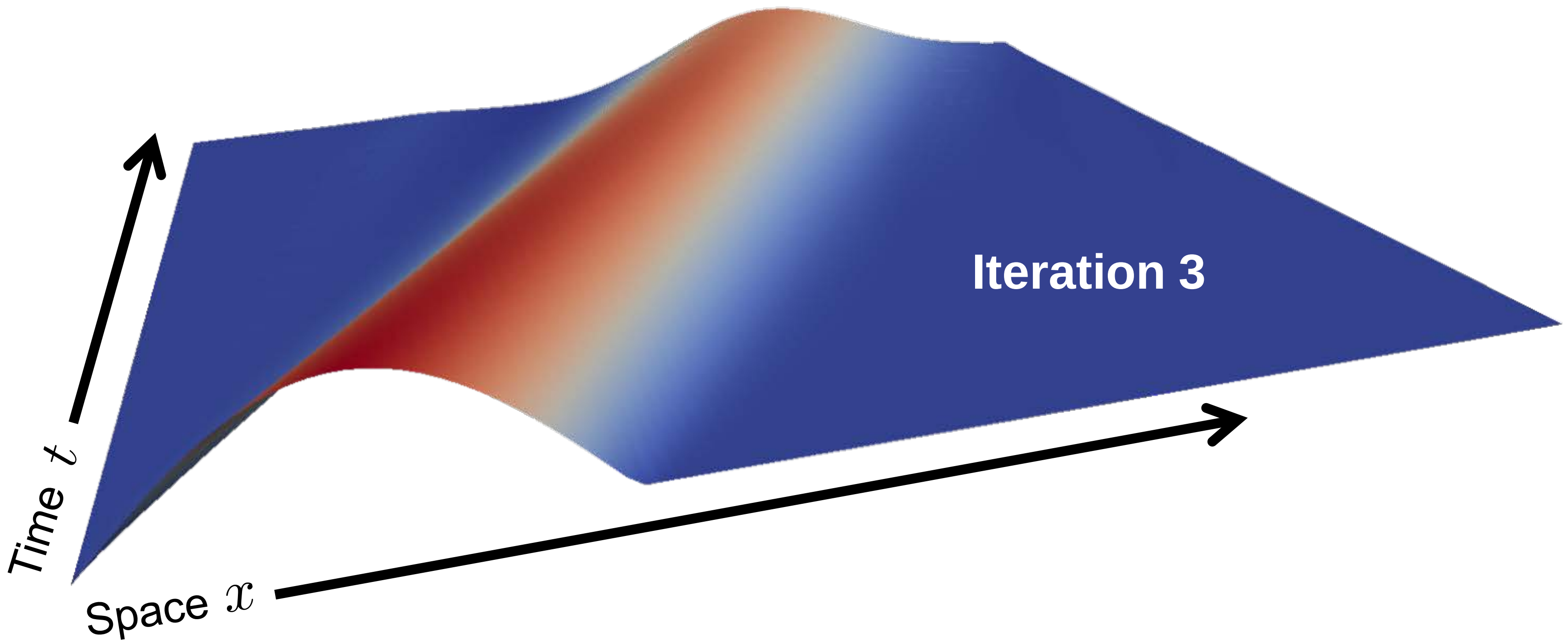
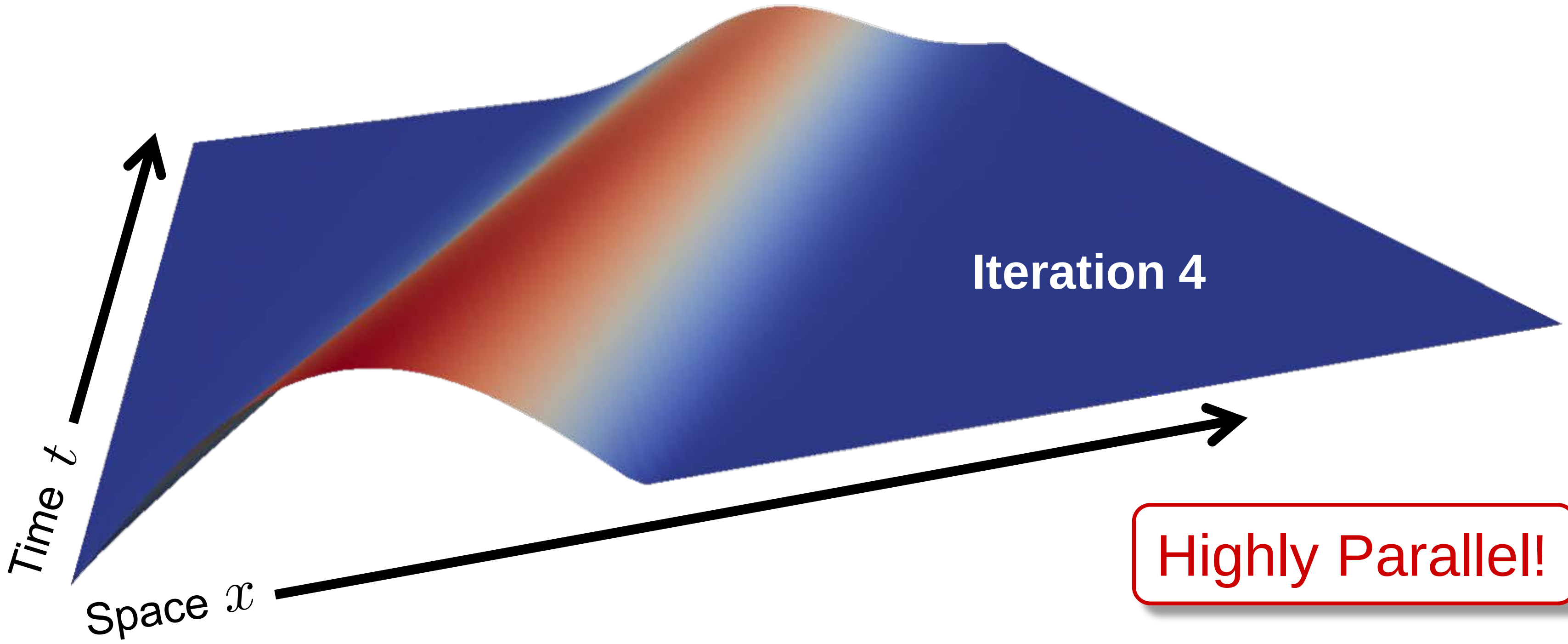


Multigrid-in-time converges to the serial space-time solution in parallel

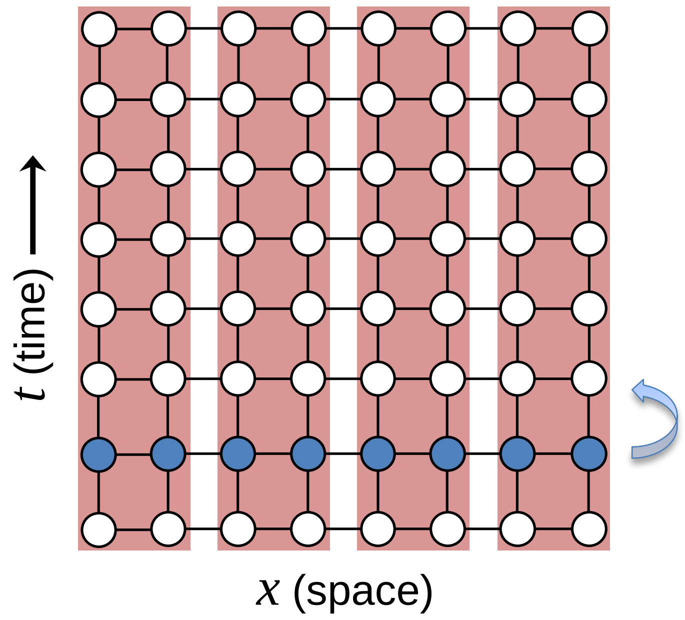
- Simple advection equation, $u_t = -cu_x$
- Already very close to the solution



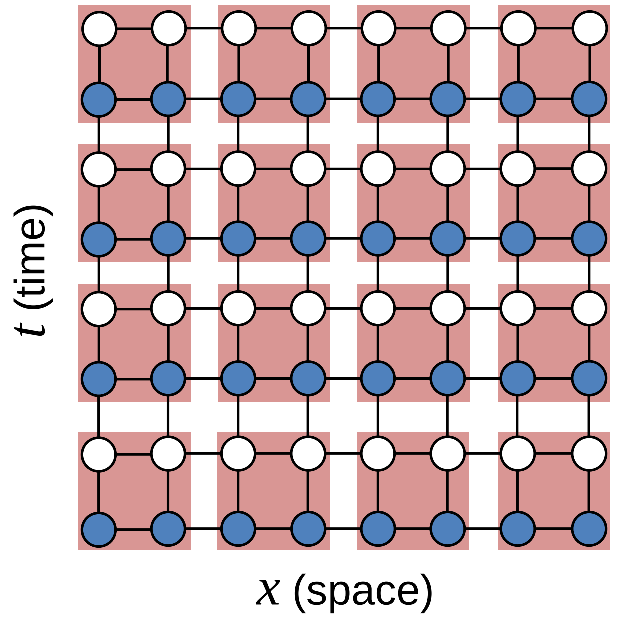
Highly Parallel!

Significantly more parallel resources can be exploited with multigrid in time

Serial time stepping



Multigrid in time



- ⊖ Parallelize in space only
- ⊕ Store only one time step

- ⊕ Parallelize in space and time
- ⊖ Store several time steps

It's useful to view the time integration problem as a large block matrix system

- General one-step method

$$\boldsymbol{u}_i = \Phi_i(\boldsymbol{u}_{i-1}) + \boldsymbol{g}_i, \quad i = 1, 2, \ldots, N$$

- Linear setting: time marching = block forward solve
  - $O(N)$ direct method, but sequential

$$A\mathbf{u} \equiv \begin{pmatrix} I & & & \\ -\Phi & I & & \\ & \ddots & \ddots & \\ & & -\Phi & I \end{pmatrix} \begin{pmatrix} \boldsymbol{u}_0 \\ \boldsymbol{u}_1 \\ \vdots \\ \boldsymbol{u}_N \end{pmatrix} = \begin{pmatrix} \boldsymbol{g}_0 \\ \boldsymbol{g}_1 \\ \vdots \\ \boldsymbol{g}_N \end{pmatrix} \equiv \mathbf{g}$$

- The MGRIT approach is based on multigrid reduction (MGR) methods (approximate cyclic reduction)
  - $O(N)$ iterative method, but highly parallel
  - Non-intrusive – user only provides time integrator Φ

The MGRIT approach builds as much as possible on existing codes and technologies

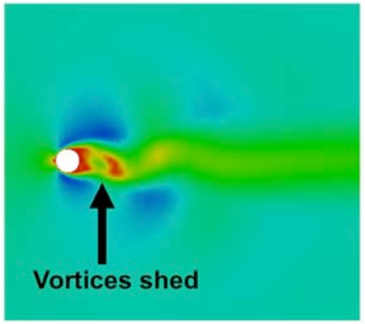
- Combines algorithm development, theory, and software proof-of-principle

- Goal: Create concurrency in the time dimension
- Non-intrusive, with unchanged time discretization
  - Implicit, explicit, multistep, multistage, …
- Converges to same solution as sequential time stepping
- Extends to nonlinear problems with FAS formulation

$$\begin{pmatrix} I & & & \\ -\Phi & I & & \\ & \ddots & \ddots & \\ & & -\Phi & I \end{pmatrix}$$

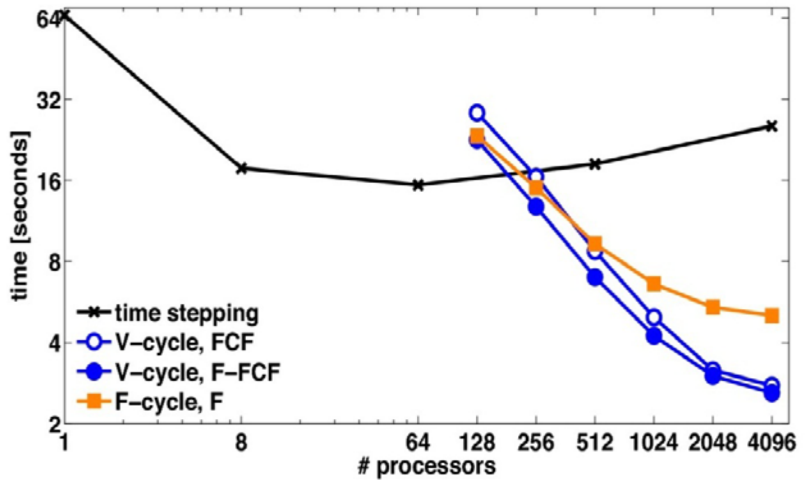
- XBraid is our open source implementation of MGRIT
  - User defines two objects and writes several wrapper routines (Step)
  - Only stores *C*-points to minimize storage

- Many active research topics, applications, and codes
  - Adaptivity in space and time, moving meshes, BDF methods, …
  - Linear/nonlinear diffusion, advection, fluids, power grid, elasticity, …
  - MFEM, hypre, Strand2D, Cart3D, LifeV, CHeart, GridDyn



Parallel speedups can be significant, but in an unconventional way

- Parallel time integration is driven entirely by hardware
  - Time stepping is already *O*(*N*)
- Useful only beyond some scale
  - There is a crossover point
  - Sometimes need significantly more parallelism just to break even
  - Achievable efficiency is determined by the space-time discretization and degree of intrusiveness



3D Heat Equation: 33^3 x 4097, 8 procs in space, 6x speedup

- The more time steps, the more speedup potential
  - Applications that require lots of time steps benefit first
  - Speedups (so far) up to 49x on 100K cores

Nearly 50 years of research exists but has only scratched the surface

- Earliest work goes back to 1964 by Nievergelt
  - Led to multiple shooting methods, Keller (1968)
- Space-time multigrid methods for parabolic problems
  - Hackbusch (1984); Horton (1992); Horton and Vandewalle (1995)
  - The latter is one of the first optimal & fully parallelizable methods to date
- Parareal was introduced by Lions, Maday, and Turinici in 2001
  - Probably the most widely studied method
  - Gander and Vandewalle (2007) show that parareal is a two-level FAS multigrid method
- Discretization specific work includes
  - Minion, Williams (2008, 2010) – PFASST, spectral deferred correction, FAS
  - DeSterck, Manteuffel, McCormick, Olson (2004, 2006) – FOSLS
- Research on these methods continues to ramp up!
  - Ruprecht, Krause, Speck, Emmett, Langer, … this is not an exhaustive list
- Recent review: Gander (2015), "50 years of time parallel time integration"

CASC

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Thank You!

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