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U.S. DEPARTMENT OF ENERGY

HPGMG BoF

High Performance Geometric Multigrid
Birds of a Feather

Introduction	*Mark Adams (LBNL)*
4th order HPGMG-FV	*Samuel Williams (LBNL)*
HPC Benchmarking	*Vladimir Marjanovic (HLRS)*
GPU Implementation of HPGMG-FV	*Simon Layton (NVIDIA)*
Questions and Discussion	*all*

4^{th} Order HPGMG-FV Implementation

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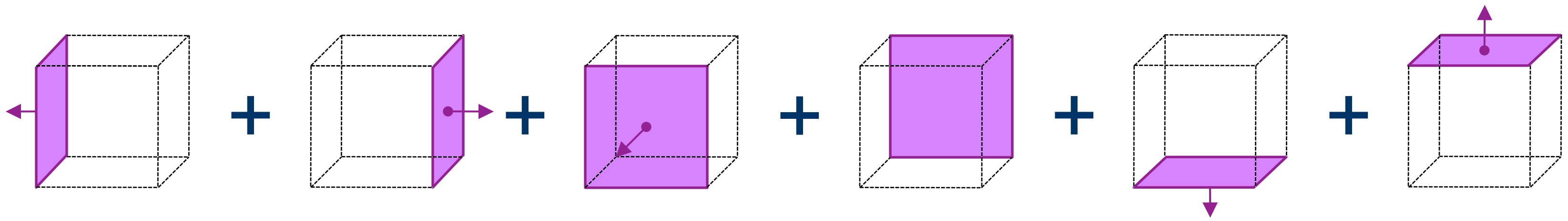
Observations of the 2nd order HPGMG-FV

- ‘Order’ describes the relationship between grid spacing and error.
- <=v0.2 implemented a 2nd order Finite Volume method.
- We found this method did not sufficiently stress HPC systems…
  - The 7pt operator and interpolation routines were heavily memory-bound on most machines (**STREAM-proxy on a single node**)
  - The Chebyshev smoother **did not stress most compilers**
  - On DDR-based architectures, the memory capacity:bandwidth balance allowed for huge problem sizes that **hid network communication**.
  - The simple 1st order boundary conditions could easily be fused with the operator and thus **sidestepped the desire to benchmark irregular parallelism and memory access**.

4^{th} order $\langle \nabla \cdot \beta \nabla u \rangle$

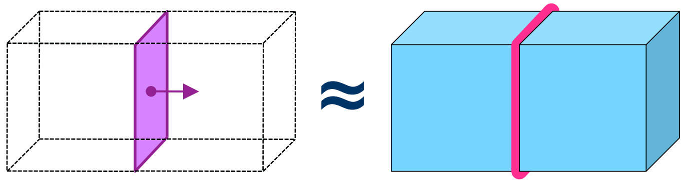
- Finite volume method expresses the average value of an operator over a cell’s volume ($\langle \nabla \cdot \beta \nabla u \rangle$) as an integral over the cell’s surface ($\langle \beta \nabla u \cdot N \rangle$).
- For 3D structured grids, each h^3 cell has 6 faces and we must calculate this term on each face….

$Lu = \langle \nabla \cdot \beta \nabla u \rangle =$



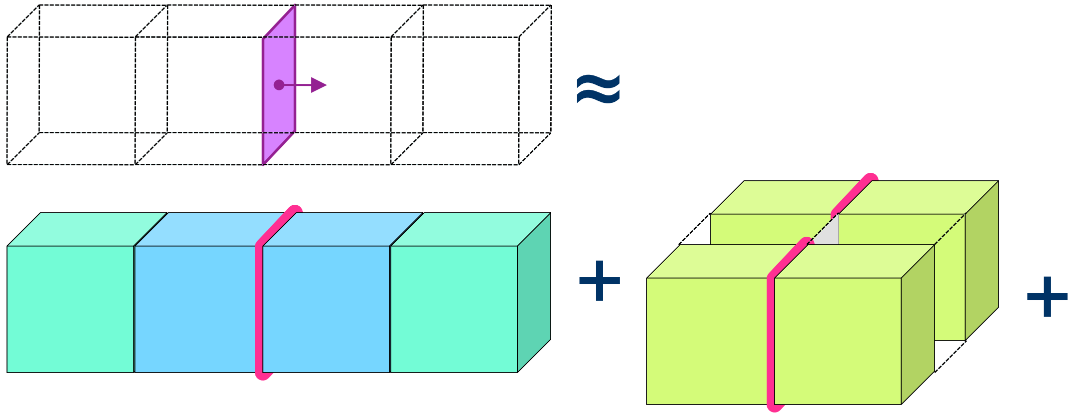
4^{th} Order Operator <∇•β∇u>

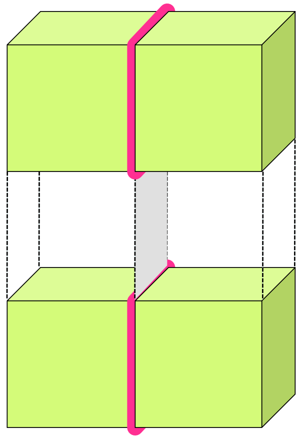
- To 2^{nd} order, we can approximate each of these flux terms as a 2-point weighted stencil…



- Hence, in 3D, 6 such terms form a 7-point variable-coefficient stencil.

- For 4^{th} order, additional terms are required…





- 25-point stencil…
  - 18 x 4-point stencils
  - 4x the floating-point operations
  - no extra DRAM data movement
  - 3x the neighbors (faces+edges)
  - 2-deep ghost zones

Choice of Smoother

- Whereas Chebyhev and Jacobi are easily SIMDized by most compilers today, we wanted a smoother to **challenge the compiler/ISA without sacrificing parallelism**.
- Out-of-place Gauss Seidel Red Black (**GSRB**) iteration…
  - Ping pong between two arrays (u and u_{new}) like Jacobi
  - Unlike Jacobi, only apply the stencil if the cell and iteration color match. Otherwise simply copy the old value to the new array.
  - Generally performs well mathematically and is insensitive to parallelism implementation choices (reproducible when threaded/vectorized)
  - Reference implementation includes stride-2, conditional, and vector variants
  - Two-pass wavefront (calculate fluxes, smooth) implementation is viable

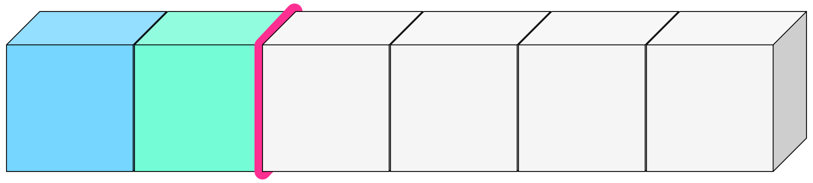
4^{th} Order Boundary Conditions

- In HPGMG-FV, as the boundary exists on cell faces, the boundary condition must be enforced prior to **every application of a stencil**.
- v0.2 and earlier used a simple, linear approximation for the zero Dirichlet boundary condition.
  - It was possible to fuse these boundary condition stencils into the operator itself
  - As such, one could **eliminate both reduced parallelism and irregular memory access** as one traverses the boundary.
  - This optimization is atypical of many real codes and undermines the benchmark's ability to evaluate the ISA/architecture/compiler/runtime response to challenging sub problems.
  - As such, it was eliminated in v0.3 and replaced with a **4^{th} order boundary condition…**

4th Order Boundary Conditions

- The 4th order boundary condition is realized by filling in ghost zone values extrapolated using interior values.
- Produces three basic families of boundary condition stencils…

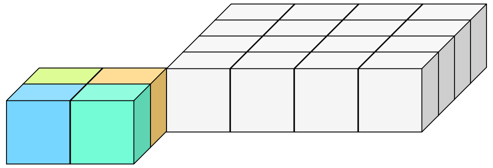
Faces



2 ghost zones x 6 symmetries

= 12 different stencil types

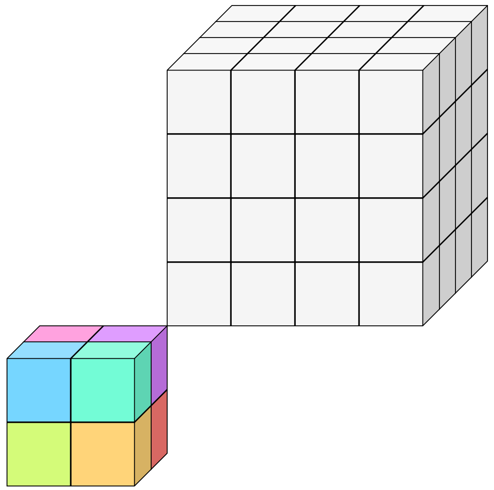
Edges



4 ghost zones x 12 symmetries

= 48 different stencil types

Corners



8 ghost zones x 8 symmetries

= 64 different stencils

4^{th} Order Boundary Conditions

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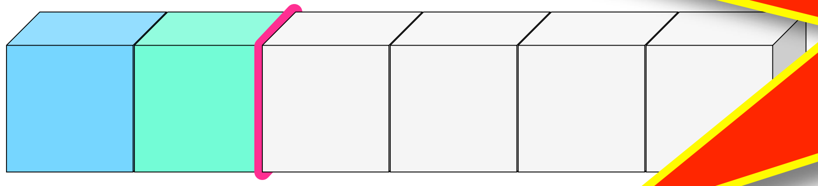
- Produces thr basic fa ondition stencils…

Each ApplyOp( ) requires over 120 stencils !

Faces



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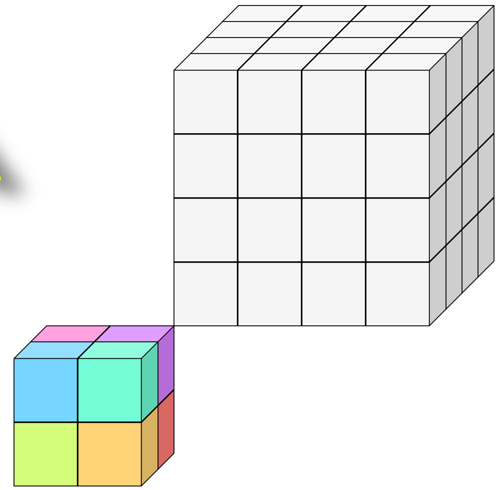


2 ghost zones x 6 symmetries
= 12 different stencil types

4 ghost zones x 12 symmetries
= 48 different stencil types

8 ghost zones x 8 symmetries
= 64 different stencils

High Order Interpolation

- For 2nd order, we used …
  - Piecewise Constant interpolation (1pt stencil) in the V-Cycles
  - Piecewise Linear interpolation (8pt stencil) for FMG's F-Cycle.
- These operations …
  - **were strongly memory-bound**
  - stressed neither core architecture nor the compiler.

- For 4th order, we now use …
  - Quadratic interpolation (**27pt stencil**) in the V-Cycles
  - Quartic interpolation (**125pt stencil**) in FMG's F-Cycle
- These operations …
  - Require communication and BCs
  - Are potentially compute-bound
  - Exercise architecture and compilers (complex symmetries can be exploited)

MPI Communication

- The operator requires communicating with face and edge neighbors
  - 3x the messages per applyOp( )
  - 2x the message size (2-deep ghost zone)
- Moreover, all interpolations now require communication with face, edge, and corner neighbors (at least 26 neighbors)

- **process0 still performs O($\log^2(P)$) ghost zone exchanges**.
- As such, at large scale, communication and coarse grid operations are relatively expensive.

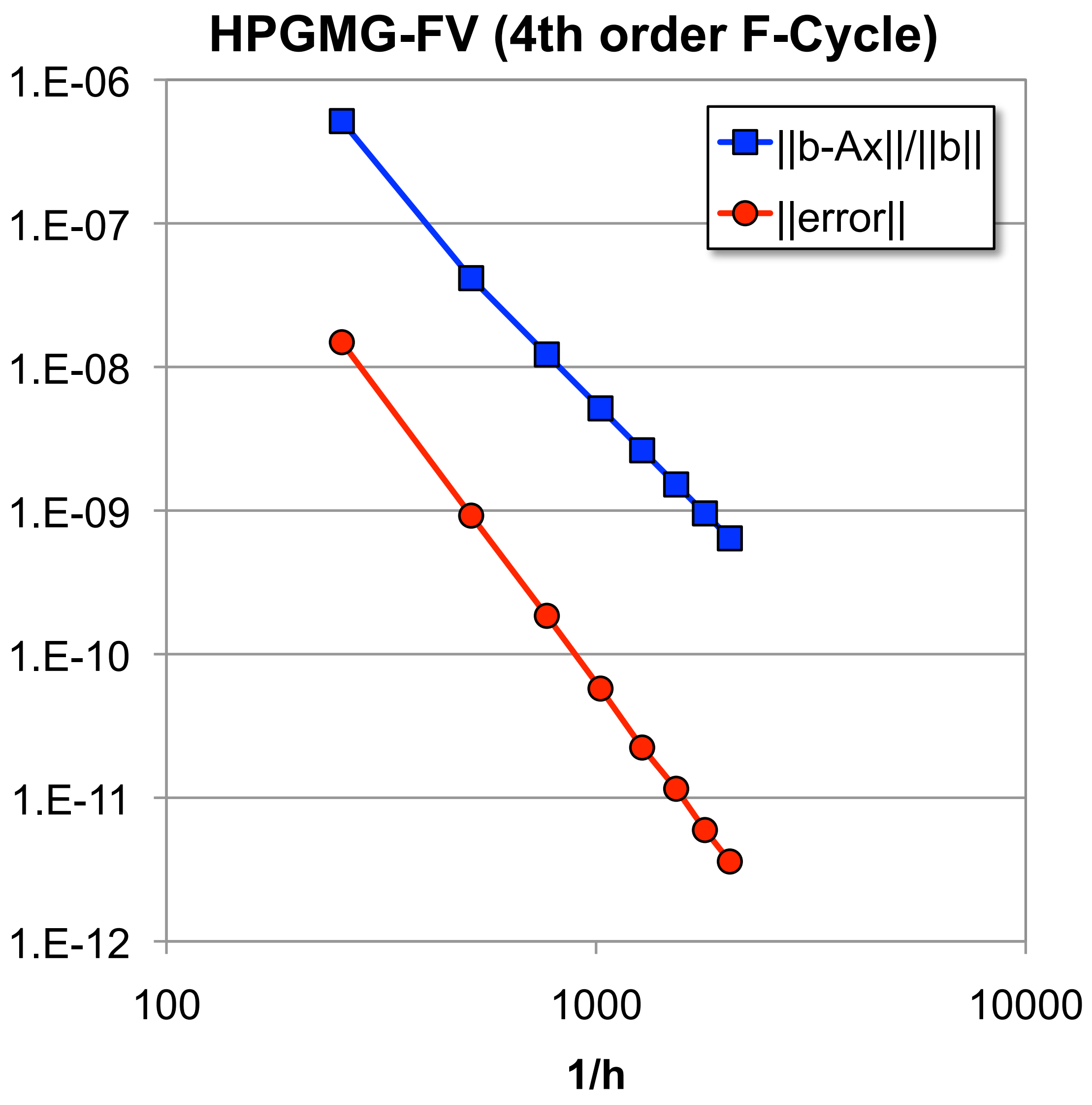
Overall Performance Implications

- The new 4th order HPGMG should …
  - perform 4x the FP operations
  - send 3x the MPI messages
  - double the MPI message size
  - move no more data from DRAM
  - attain 4th order accuracy
  - attain lower relative residual ($\sim 10^{-9}$)

- As a result, HPGMG should be more sensitive to…
  - core/cache architectural parameters
  - compiler optimizations
  - messaging overheads and network latencies
  - network injection and bisection bandwidths

Mathematical Performance

- Examine error and relative residual as a function of 1/h (e.g. problem dimension of up to $2K^3$)…
  - Error is strongly 4th order with 3 GSRB presmooths + 3 GSRB postsmooths.
  - Residual is quickly reduced ($<10^{-9}$ in one F-Cycle)
- Mathematical properties are independent of parallelism choices (processes, threads, box size, etc…)



Initial 4th Order HPGMG-FV Results

HPGMG Rank	System Name	Site	DOF/s (h)	DOF/s (2h)	DOF/s (4h)	MPI	OMP	Acc	DOF per Process	Top500 Rank
1	Mira	ALCF	5.00e+11	3.13e+11	1.07e+11	49152	64	0	36M	5
			3.95e+11	2.86e+11	1.07e+11					
2	Edison	NERSC	2.96e+11	2.46e+11	1.27e+11	10648	12	0	128M	34
3	Titan (CPU-only)	OLCF	1.61e+11	8.25e+10	2.37e+10	36864	8	0	48M	2
4	Hopper	NERSC	7.26e+10	5.45e+10	2.74e+10	21952	6	0	16M	62
5	SuperMUC	LRZ	7.25e+10	5.25e+10	2.80e+10	4096	8	0	54M	20
6	Hazel Hen	HLRS	1.82e+10	8.73e+09	2.02e+09	1024	12	0	16M	-
7	SX-ACE	HLRS	3.24e+09	1.77e+09	7.51e+08	256	1	0	32M	-
8	Babbage (MIC-only)	NERSC	7.62e+08	3.16e+08	9.93e+07	256	45	0	8M	-

Notes:
- v0.3 was made available only 3 months ago
- Mira and Babbage used optimized implementations (alignment intrinsics, loop fission to reduce prefetcher contention, OMP4 SIMD pragmas, …)
- Only 22% of SUPER MUC was available
- Babbage (KNC): 4 MPI per MIC. MPI performance was poor. Network scalability was very poor. Very Sensitive to coarse grid operations.
- Each solve performs approximately 1200 FP operations per DOF.

Initial 4th Order HPGMG-FV Results

~600 TF/s (6% of peak)

Problem sizes (N,N/8,N/64)

~355 TF/s (14% of peak)

~3.9 TF/s (24% of peak)

4K nodes is only 22% of the system

512 nodes is only 6% of the system

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FMG Weak Scaling Challenge

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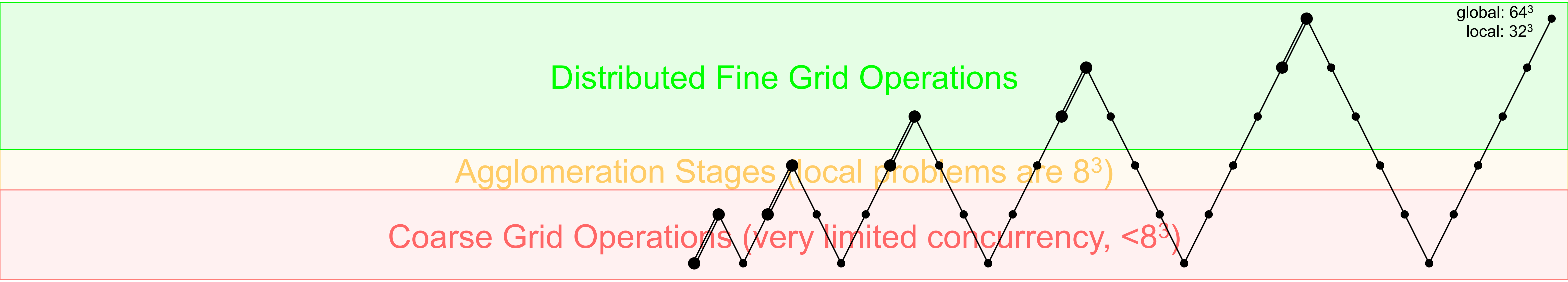

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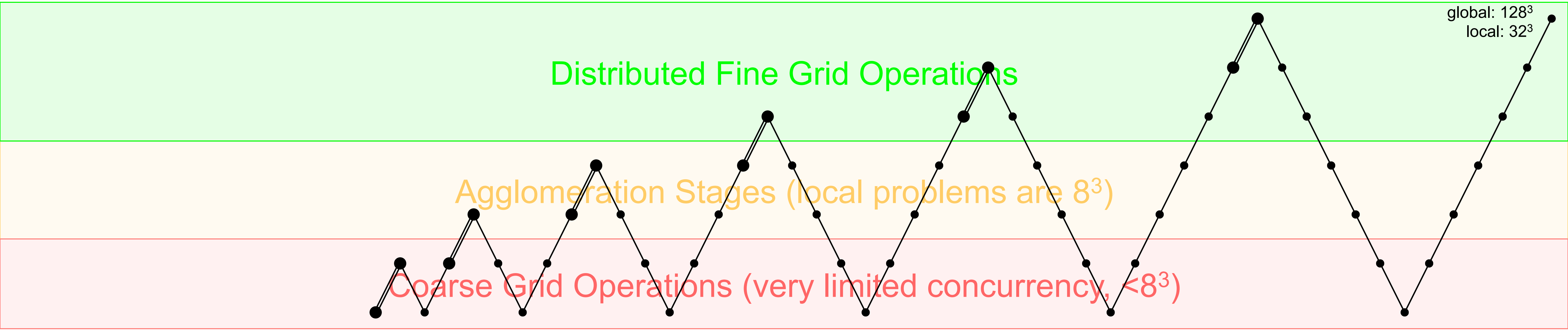
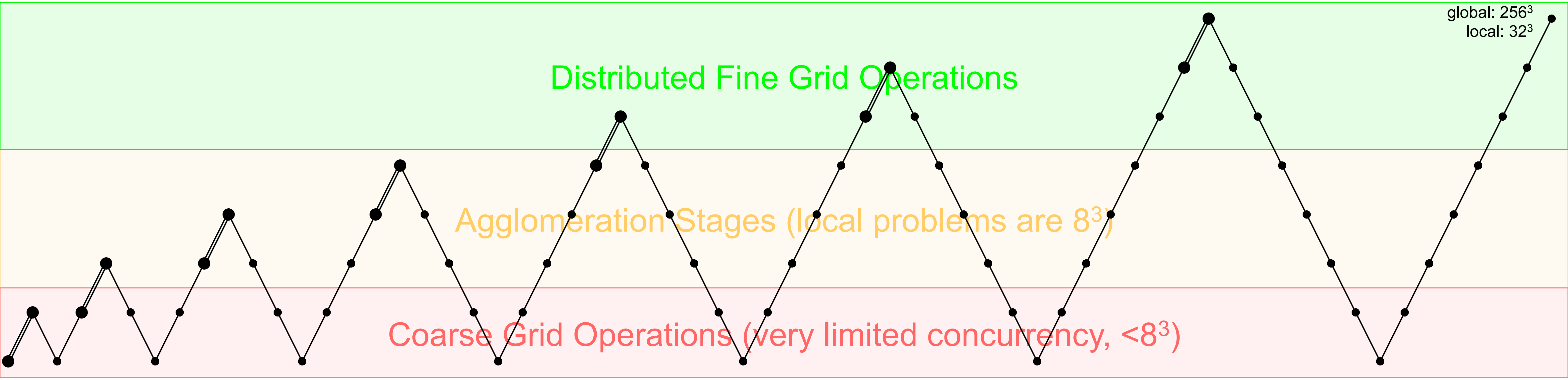


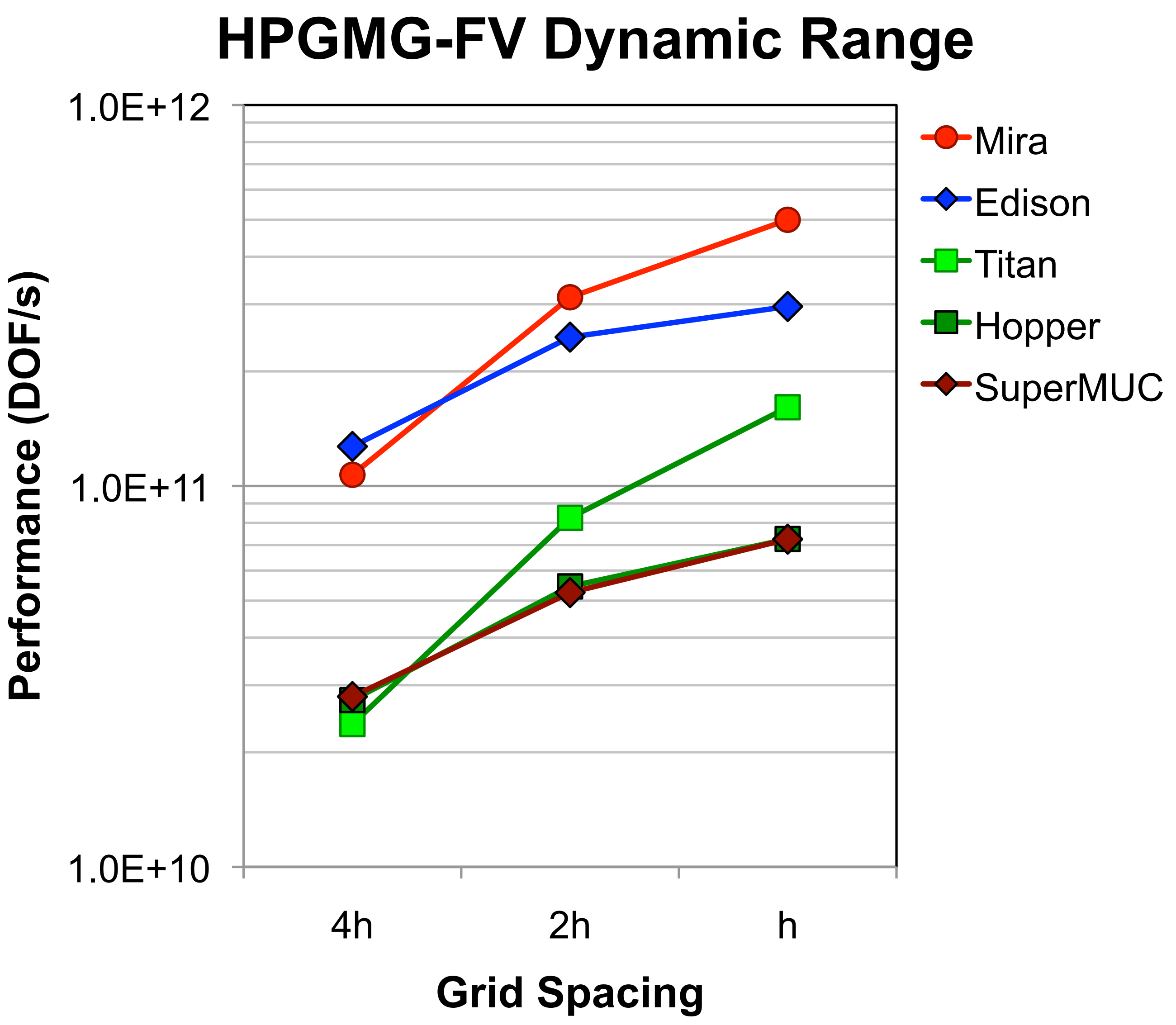
FMG Weak Scaling Challenge

- As one weak scales HPGMG-FV, coarse grid operations become an increasingly dominate fraction of the execution…
- Petascale machines can have 13+ levels !



Observations on Dynamic Range

- Dynamic Range gauges performance as a function of problem size (memory/node)
  - ‘h’ is the largest problem
  - ‘4h’ is a problem 64x (4^3) smaller
- Titan (Gemini) was found to be particularly sensitive to problem size
  - CPU-only data (apples-to-apples)
  - **7x lower performance at 4h**
- Conversely, Edison (Aries) saw only a 2.3x loss in performance at 4h
- Suggests systems are now sensitive to network architecture and memory usage
- We eagerly await HBM and GDDR-based results (lower capacity / more bandwidth)



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Questions?

HPGMG-FV is available for download:

https://bitbucket.org/hpgmg/hpgmg/

Submission Guidelines:

http://crd.lbl.gov/departments/computer-science/PAR/research/hpgmg/submission/

HPC Benchmarking

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GPU Implementation of HPGMG-FV

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Questions and Discussion