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
4th Order HPGMG-FV Implementation

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Observations of the 2\textsuperscript{nd} order HPGMG-FV

- ‘Order’ describes the relationship between grid spacing and error.
- $\leq v0.2$ implemented a 2\textsuperscript{nd} 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 1\textsuperscript{st} order boundary conditions could easily be fused with the operator and thus sidestepped the desire to benchmark irregular parallelism and memory access.
**4th order \(<\nabla \cdot \beta \nabla u>\)**

- Finite volume method expresses the average value of an operator over a cell’s volume (\(<\nabla \cdot \beta \nabla u>\)) as an integral over the cell’s surface (\(<\beta \nabla u \cdot N>\)).

- For 3D structured grids, each \(h^3\) cell has 6 faces and we must calculate this term on each face:

\[
Lu = <\nabla \cdot \beta \nabla u> = \quad + \quad + \quad + \quad + \quad +
\]
4\textsuperscript{th} Order Operator $\langle \nabla \cdot \beta \nabla u \rangle$

- To 2\textsuperscript{nd} order, we can approximate \textit{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\textsuperscript{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

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Hence, in 3D, 6 such terms form a 7-point variable-coefficient stencil.
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 \( u_{\text{new}} \)) 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
4th 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 4th order boundary condition…
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
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- 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

Each ApplyOp() requires over 120 stencils!
High Order Interpolation

For 2\textsuperscript{nd} 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 4\textsuperscript{th} 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)
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 4\textsuperscript{th} 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 4\textsuperscript{th} 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 $4^{th}$ 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

<table>
<thead>
<tr>
<th>HPGMG Rank</th>
<th>System Name</th>
<th>Site</th>
<th>DOF/s (h)</th>
<th>DOF/s (2h)</th>
<th>DOF/s (4h)</th>
<th>MPI</th>
<th>OMP</th>
<th>Acc</th>
<th>DOF per Process</th>
<th>Top500 Rank</th>
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<tr>
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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 problem sizes (N,N/8,N/64) (6% of peak)

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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!

Distributed Fine Grid Operations
Agglomeration Stages (local problems are $8^3$)
Coarse Grid Operations (very limited concurrency, <$8^3$)
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)
Acknowledgements

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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

Vladimir Marjanovic
High Performance Computing Center Stuttgart (HLRS)
Questions and Discussion