

A Roofline Performance Analysis of an Algebraic Multigrid Solver

Alex Druinsky, Brian Austin, Sherry Li, Osni Marques, Eric Roman and Samuel Williams

Lawrence Berkeley National Laboratory

Goal: Develop a performance model of an optimal-order resilient solver for PDEs, using high-order discretization elements and AMG, combined with low-rank sparse factorizations.

Two-grid Adaptive Smoothed Aggregation Spectral AMG Method^{1,2}

- Pre-smoothing: $y = x_i + M^{-1}(b - Ax_i)$
- Coarse grid correction
 - restrict the residual: $r_c = P^T(b - Ay)$
 - coarse grid equation: $A_c x_c = r_c$
 - update fine grid iterate: $z = y + Px_c$
- Post-smoothing: $x_{i+1} = z + M^{-T}(b - Az)$

- ❖ Agglomerates of elements, aggregates of vertices
- ❖ P (interpolation operator): Chebyshev-based polynomial; sparse; requires eigenvectors of agglomerates and SVD
- ❖ M (smoother): Chebyshev-based polynomial; sparse
- ❖ Coarse grid solver:
 - ❖ PCG (Gauss-Seidel or Jacobi)
 - ❖ HSS (FGMRES)

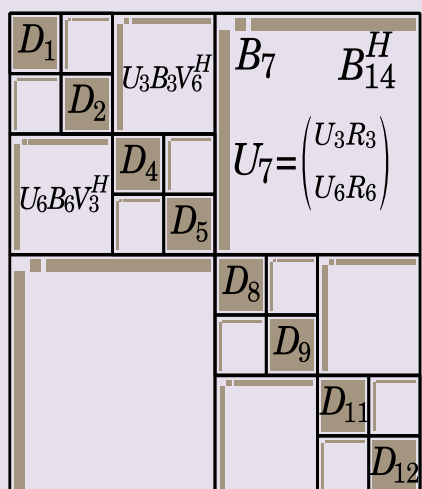
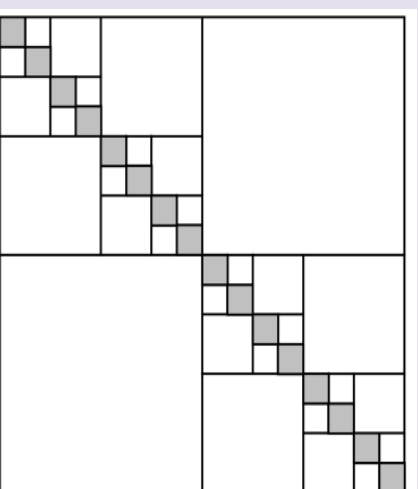
$$P = S \begin{bmatrix} \bar{P}_1 & & \\ & \bar{P}_2 & \\ & & \ddots \\ & & & \bar{P}_{na} \end{bmatrix}$$

$S = \text{smoother}$
 $\bar{P}_i = \text{set of eigenvectors (depends on tolerance } \theta)$
 $na = \text{number of agglomerates}$

Hierarchically Semi-Separable (HSS) Low-rank Sparse Solver and Preconditioner^{3,4}

- ❖ HSS structure for dense, but data-sparse structured matrices (examples: BEM, integral equations, PDEs with smooth kernels)
- ❖ Matrix off-diagonal blocks are rank deficient
- ❖ Recursion leads to hierarchical partitioning, nested bases lead to nearly linear complexity

hierarchical partition SVD with nested bases matrix block representation

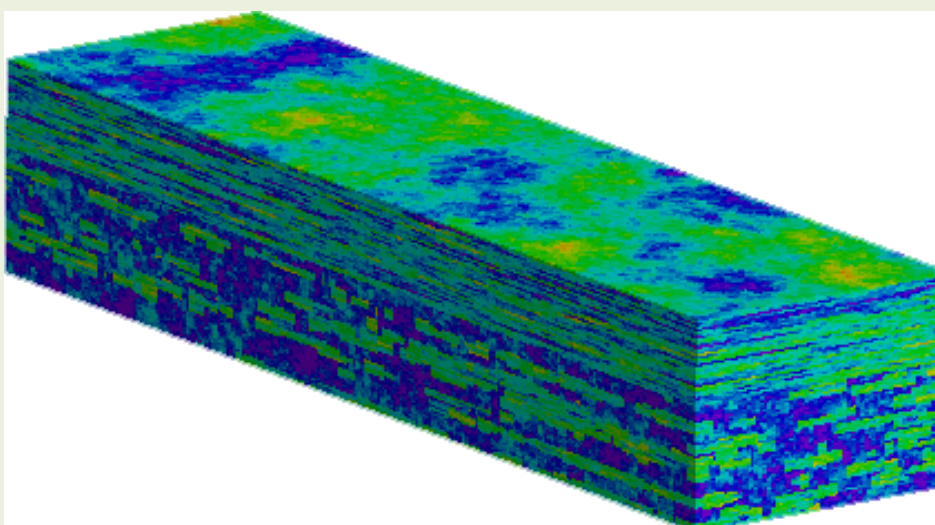


$$A = \begin{bmatrix} D_1 & U_1 B_1 V_2^T & U_3 B_3 V_6^T \\ U_2 B_2 V_1^T & D_2 & \\ U_6 B_6 V_4^T & & D_5 \end{bmatrix}$$

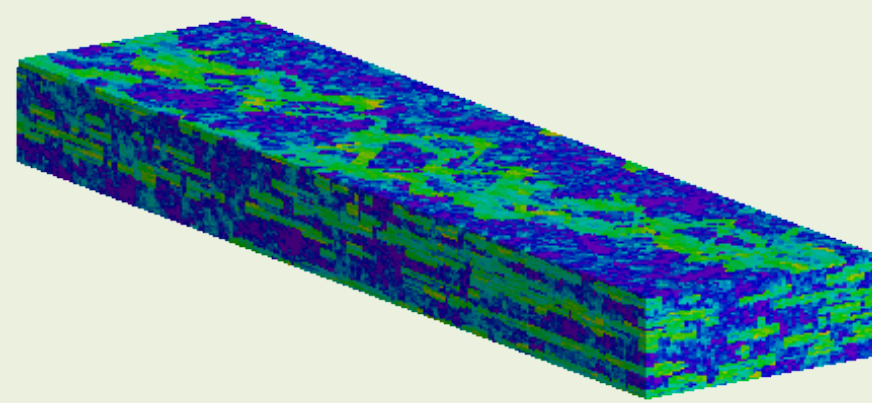
Case Study: SPE10 Benchmark (model 2)⁵

- Model of a formation in the Brent oil field; 1200'x2200'x170' (fine scale cell size is 20'x10'x2'). The top 70 ft (35 layers) represents the Tarbert formation; the bottom 100 ft (50 layers) represents Upper Ness (fluvial).
- Modelled described by Brinkman equations⁶

$$\begin{cases} -\nu \Delta u + k(x)u + \nabla p = f(x) & \forall x \in \Omega \\ \text{div } u = 0 & \forall x \in \Omega \\ Bu = g & \text{on } \partial\Omega \end{cases}$$

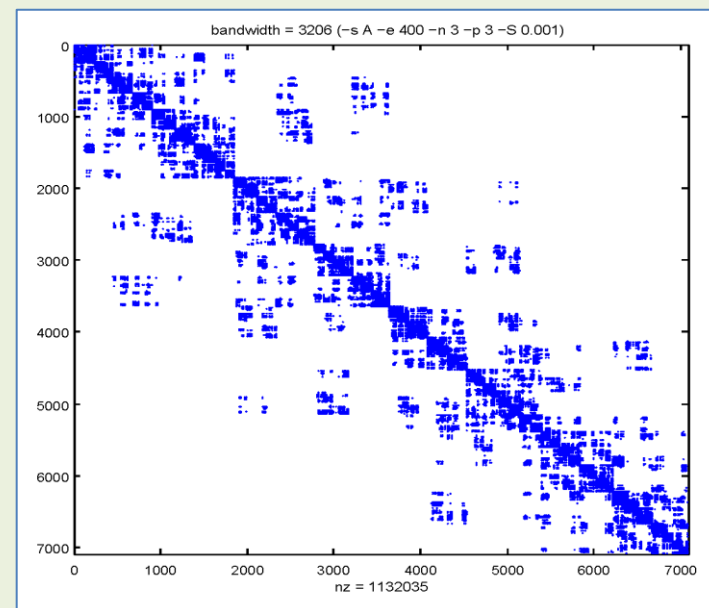
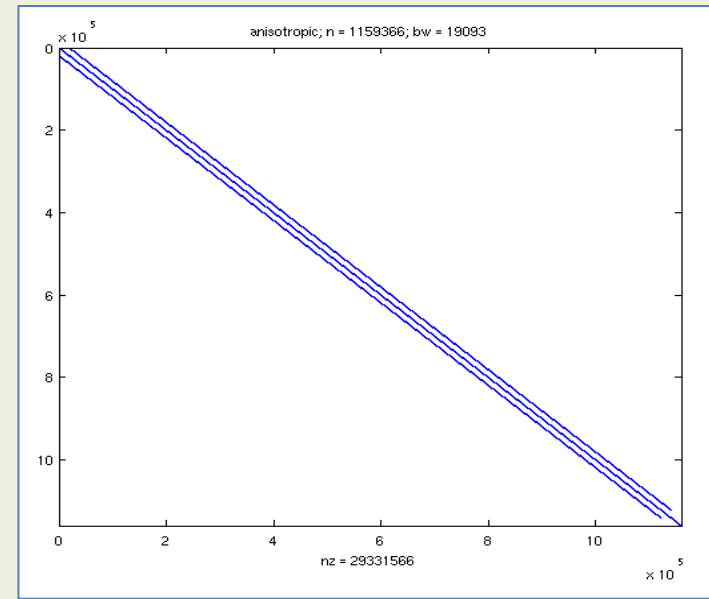


porosity of the whole model



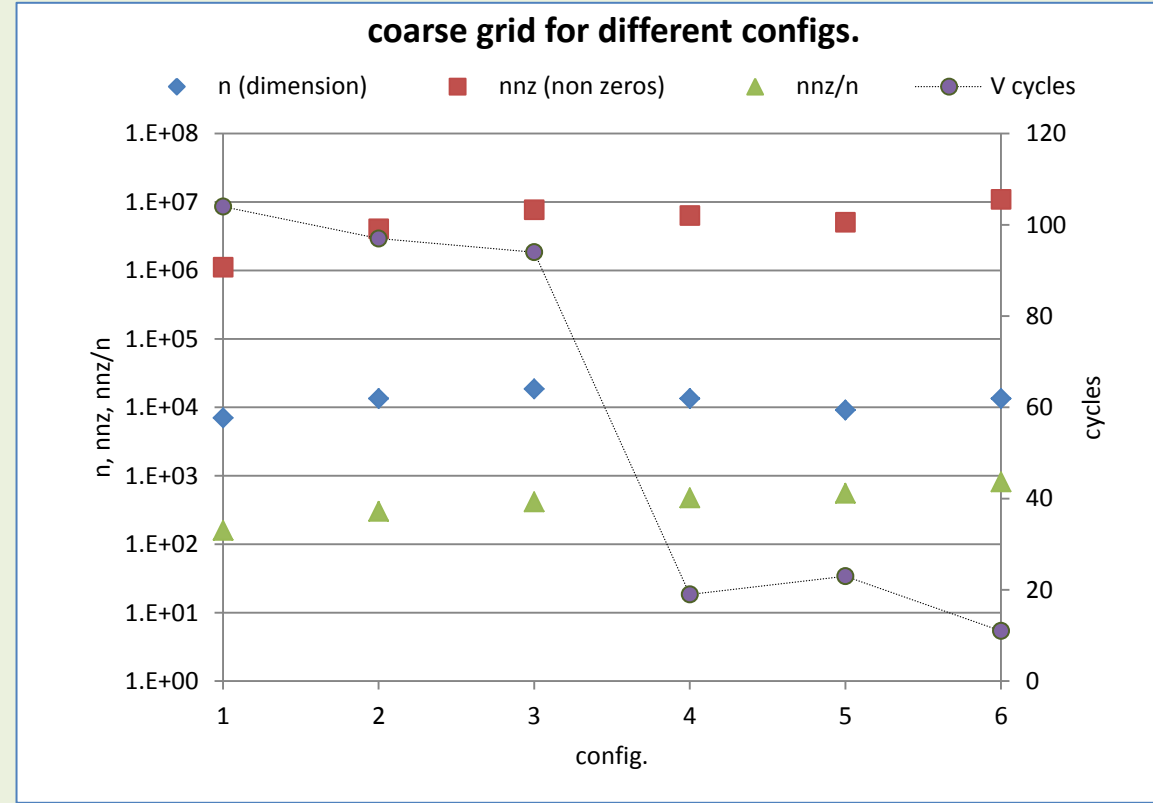
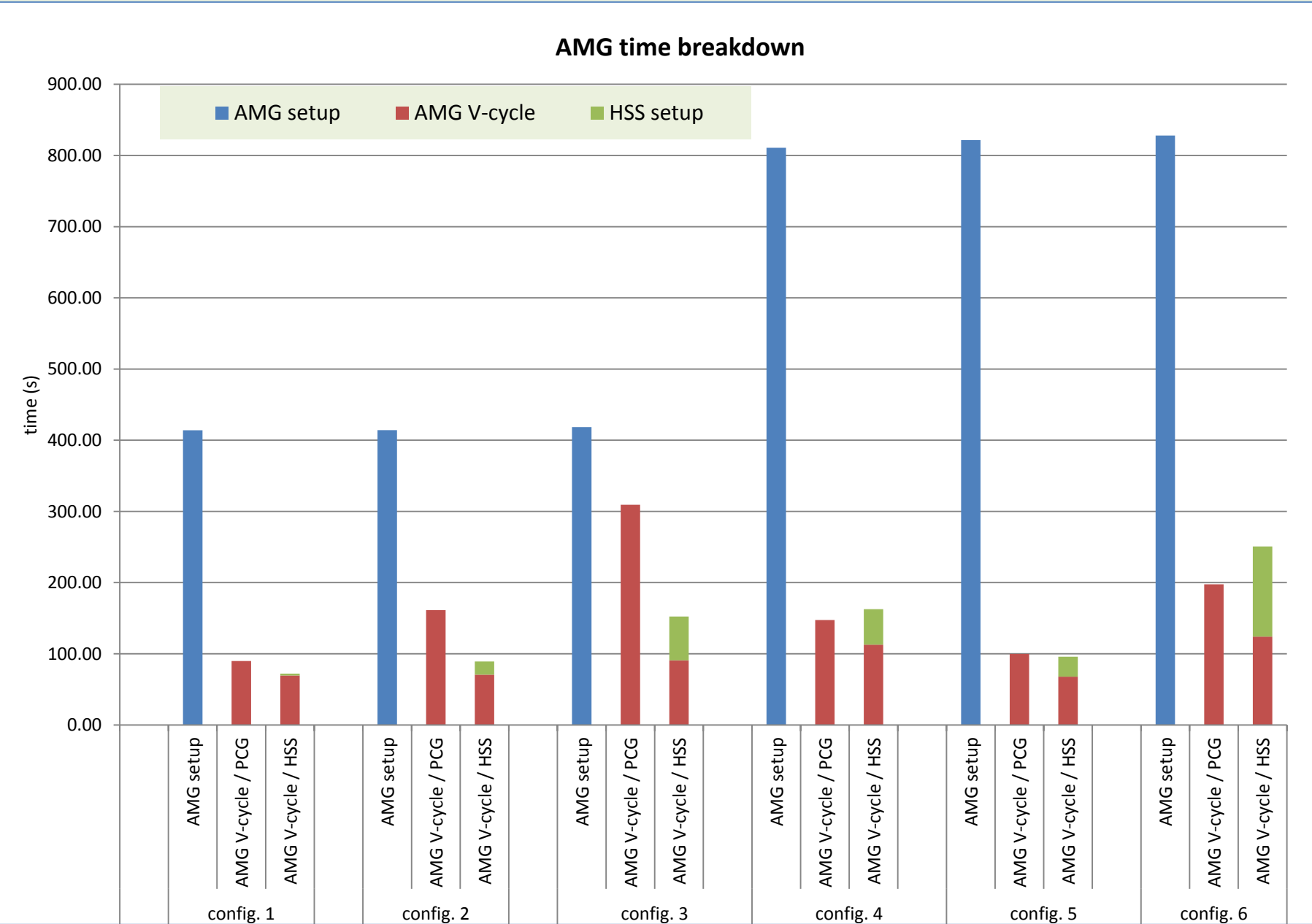
part of the Upper Ness sequence

fine grid
 $n \approx 1.16 M$
 $nnz \approx 30.63 M$
 $nnz/n \approx 26$



coarse grid
(sample)

- ❖ Parameters for AMG code: elements per agglomerate (e), degrees of polynomials for M and P (v), spectral tolerance (θ).
- ❖ Target platform: Cray XC30 (Edison @ NERSC), 12-core Intel Ivy Bridge at 2.4 GHz; L1 and L2 caches with 64 KB and 256 KB, respectively; 30-MB L3 cache shared by the 12 cores (only one core used in the experiments below, OpenMP work in progress).
- ❖ Increasing the number of elements per agglomerate leads to a smaller but denser coarse grid, reduces the number of AMG cycles, but with a much costlier AMG hierarchy construction.
- ❖ For our purposes the important parameter is the spectral tolerance, as P becomes sparser for small tolerances (HSS derives much more benefits from sparse P).



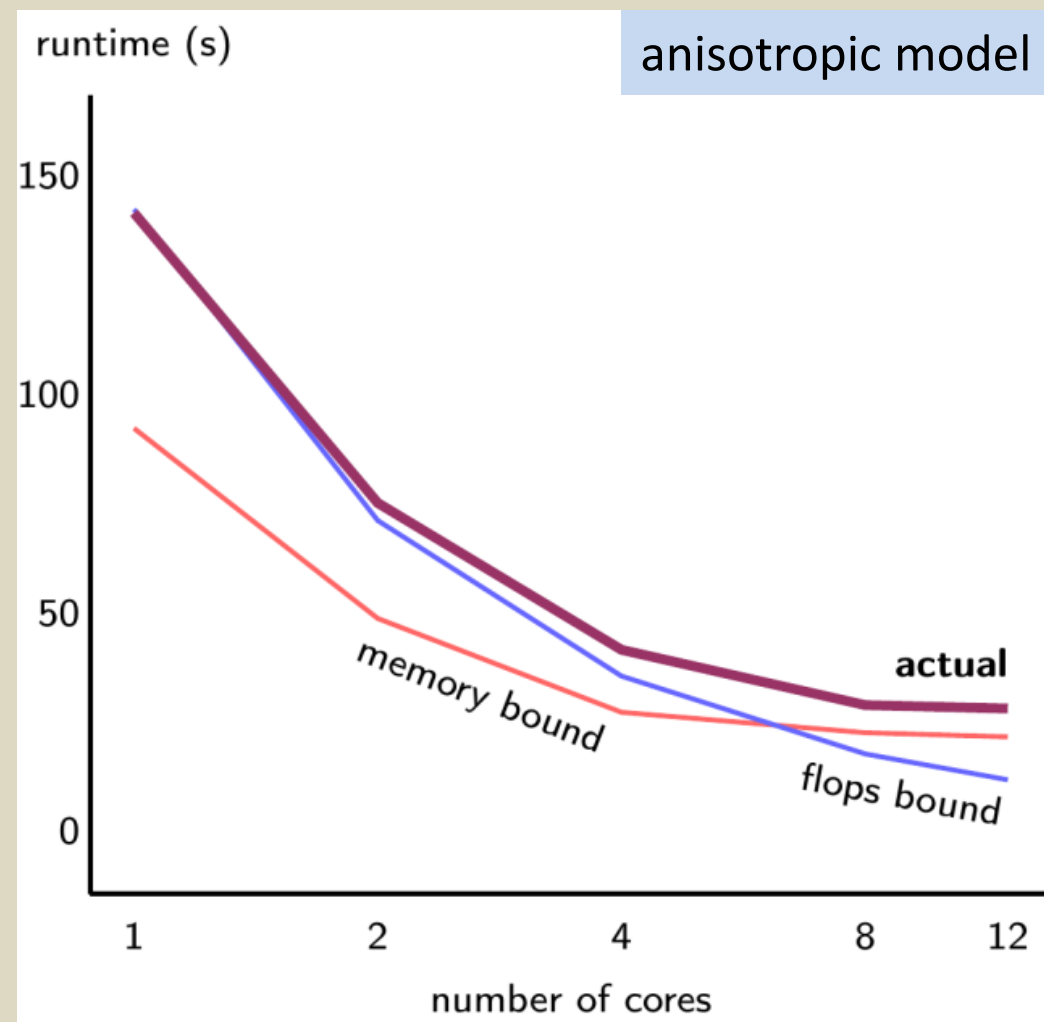
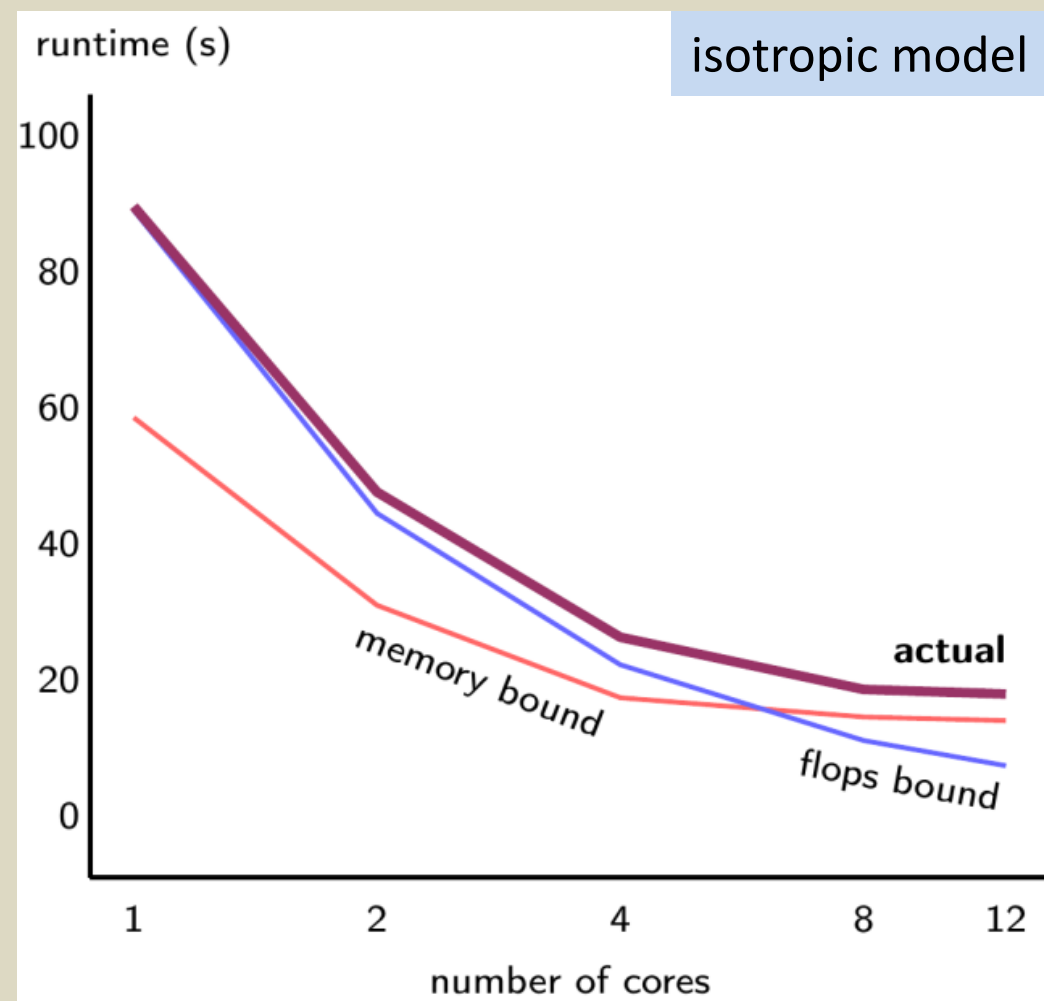
config.	e	v	θ
1	400	3	0.001
2	400	3	0.003
3	400	3	0.005
4	1000	3	0.003
5	1000	5	0.003
6	1000	5	0.005

Performance Analysis

- A roofline performance model⁷ identifies performance bounds and bottlenecks.
- We are looking at the AMG cycle part of the algorithm (ignoring the hierarchy).
- Memory traffic and flops are expressed as simple functions of parameters (number of zeros, matrix dimensions, etc.)
- Byte and flop counts translate into lower bounds on runtimes.

stage	bytes	flops
pre- and post-smooth	$(3v + 1)(12nza + 3 \cdot 8n)$	$2(3v + 1)(nza + 2n)$
restrict	$12nza + 12nzp + 3 \cdot 8n$	$2(nza + nzp)$
coarse solve (PCG/J)		
multiply by A_c	$12nzc$	$2nzc$
preconditioner	$2 \cdot 8n_c$	n_c
vector operations	$5 \cdot 8n_c$	$2 \cdot 5n_c$
interpolate	$12nzp + 8n$	$2nzp$
termination criterion	$12nza + 4 \cdot 8n$	$2(nza + n)$

Runtime bounds and actual runtime for config. 1 ($e=400, v=3, \theta=0.001$) on one socket of the Cray XC30. Effective Gflops ranges from 1.6 for 1 core through 19.2 for 12 cores, obtained by dividing the machine peak rate by 12, based on the assumption that the compiler does not generate optimized code. STREAM benchmark bandwidths: DRAM bandwidths range from 13.2 through 48.5; L3 ranges from 21 through 210.1 GB/s. The estimates are based on traffic between DRAM and L3 for the fine grid matrix and between L3 and L2 for the coarse grid matrix.



Conclusions

- For SPE10, convergence is not impaired by a small spectral tolerance and performance is improved.
- Roofline bound analysis is quite accurate (within 20%) for the PCG/GS solver, but remains an open problem for HSS (FGMRES)

References

- D. Kalchev, C. Ketelsen and P. Vassilevski, Two-Level Adaptive Algebraic Multigrid for a Sequence of Problems with Slowly Varying Random Coefficients, SIAM J. Sci. Comp., 35:1215-1234, 2013.
- M. Brezina and P. Vassilevski, Smoothed Aggregation Spectral Element Agglomeration AMG: SA-pAMGe, LLNL-PROC-490083, June 29, 2011.
- J. Xia, S. Chandrasekaran, M. Gu and X. S. Li, Fast Algorithms for Hierarchically Semiseparable Matrices Numer. Linear Algebra Appl., 17:953-976, 2010.
- S. Wang, X.S. Li, J. Xia and M. de Hoop, Efficient Scalable Algorithms for Solving Dense Linear Systems with Hierarchically Semiseparable Structures, SIAM J. Sci. Comp., 35:519-544, 2013.
- Society of Petroleum Engineers. <http://www.spe.org/web/csp/datasets/set02.htm>
- U. Villa, Scalable Efficient Methods for Incompressible Fluid-dynamics in Engineering Problems, PhD Thesis, Emory University, 2012.
- S. Williams, A. Waterman, and D. Patterson, Roofline: An Insightful Visual Performance Model for Multicore Architectures, Commun. ACM, 52:65-76, 2009.

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