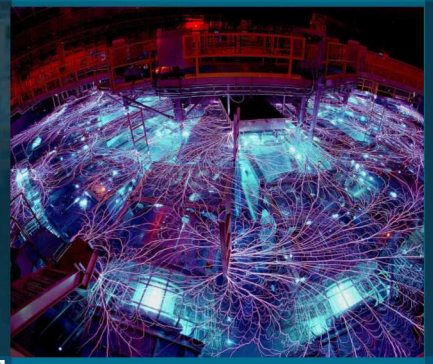
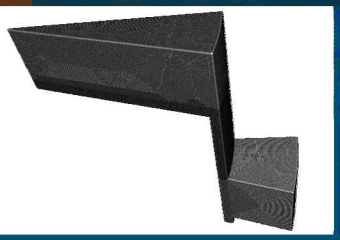
SAND2020-1793C

Linear Solvers for Plasma Simulations on Advanced Architectures





TRILINOS

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SIAM Conference on Parallel Processing, February 12-15, 2020, SAND2020-XXXX

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Outline

- Motivating application
- Governing equations
- Discretization
- Algebraic multigrid solver
- Numerical results
- Future work

Motivation

Sandia mission apps are being readied for current and emerging pre-exascale architectures, as well as future exascale architectures

- DOE ASC ATDM program
- DOE Exascale Computing Project (ECP)

EMPIRE: Sandia plasma simulation code

- Relies heavily on capabilities in Sandia's Trilinos project
  - High-performance, portable shared memory primitives
  - Sparse distributed linear algebra
  - Distributed and shared memory solvers
  - Load-balancing, time-stepping
- Requires specialized algebraic multigrid (AMG) for Maxwell's equations

EMPIRE simulations have stringent solver performance requirements (10 solves/second)

EMPIRE – Sandia plasma simulation application

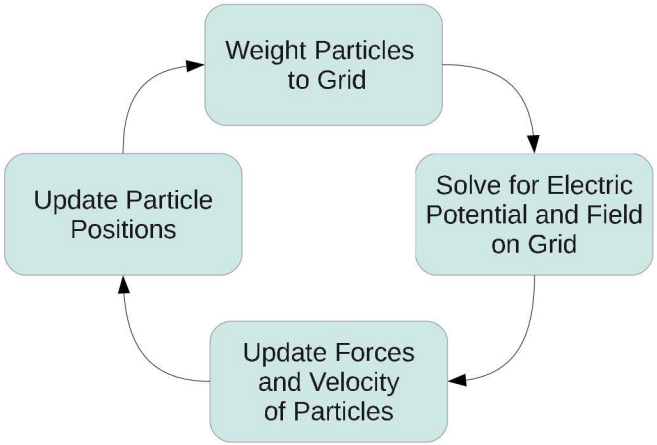
Plasma dynamics are described by Klimontovich equation

$$\frac{\partial f_i}{\partial t} + \frac{\vec{v}_i}{m} \cdot \nabla f_i + \frac{q_i}{m_i} \left(\vec{E}(x_i) + v_i \times \vec{B}(x_i) \right) \frac{\partial f_i}{\partial \vec{v}} = 0$$

for particles i with associated charge q, mass m, velocity v_i, and distribution f_i.

Particle movement coupled to electric field E and magnetic field B via Maxwell's equations.

EMPIRE uses operator-split time integration.



Bettencourt et al., *ASC ATDM Level 2 Milestone #6358: Assess Status of Next Generation Components and Physics Models in EMPIRE*, SAND2018-10100

Maxwell's Equations

$$\frac{\partial \vec{B}}{\partial t} = -\nabla \times \vec{E} \qquad \nabla \cdot (\epsilon \vec{E}) = \rho$$

$$\frac{\partial (\epsilon \vec{E})}{\partial t} = \nabla \times \mu^{-1} \vec{B} - \vec{J} \qquad \nabla \cdot \vec{B} = 0$$

$$\vec{n} \times \vec{E} = 0 \text{ on } \partial\Omega$$

electric permittivity ϵ and magnetic permeability μ.

Discretization of Maxwell's Equations

Discretized using nodal elements for $H^1(\Omega)$, Nedelec edge elements for $H(\text{curl}, \Omega)$, and Nedelec face elements for $H(\text{div}, \Omega)$.

Yields block system

$$\begin{pmatrix} \frac{1}{\Delta t}\boldsymbol{M}_B(1) & \boldsymbol{M}_B(1)\boldsymbol{C} \\ -\boldsymbol{C}^T\boldsymbol{M}_B(\mu^{-1}) & \frac{1}{\Delta t}\boldsymbol{M}_E(\varepsilon) \end{pmatrix}$$

where M_E and M_B are edge and face mass matrices, respectively

C is strong form of curl

Discretization of Maxwell's Equations (continued)

Block system can be factored

$$\begin{pmatrix} \frac{1}{\Delta t}\boldsymbol{M}_B(1) & \boldsymbol{M}_B(1)\boldsymbol{C} \\ -\boldsymbol{C}^T\boldsymbol{M}_B(\mu^{-1}) & \frac{1}{\Delta t}\boldsymbol{M}_E(\varepsilon) \end{pmatrix} = \begin{pmatrix} \frac{1}{\Delta t}\boldsymbol{M}_B(1) & \boldsymbol{0} \\ -\boldsymbol{C}^T\boldsymbol{M}_B(\mu^{-1}) & \boldsymbol{I} \end{pmatrix} \begin{pmatrix} \boldsymbol{I} & \Delta t\boldsymbol{C} \\ \boldsymbol{0} & \boldsymbol{S}_E \end{pmatrix}$$

where the Schur complement $\boldsymbol{S}_E$ is given by

$$\boldsymbol{S}_E = \frac{1}{\Delta t}\boldsymbol{M}_E(\varepsilon) + \Delta t\boldsymbol{C}^T\boldsymbol{M}_B(\mu^{-1})\boldsymbol{C} \qquad (1)$$

Challenge: $\boldsymbol{S}_E$ has large near nullspace (space of gradients)

Linear Solver Algorithm (1)

Augmenting $\boldsymbol{S_E}$ with grad-div term to reduce nullspace:

$$\overline{\boldsymbol{S}}_{\boldsymbol{E}} = \frac{1}{\Delta t}\boldsymbol{M}_{\boldsymbol{E}}(\varepsilon) + \Delta t\left\{\boldsymbol{C}^{\boldsymbol{T}}\boldsymbol{M}_{\boldsymbol{B}}(\mu^{-1})\boldsymbol{C} + \boldsymbol{M}_{\boldsymbol{E}}(1)\boldsymbol{G}\boldsymbol{M}_{\rho}(\mu)^{-1}\boldsymbol{G}^{\boldsymbol{T}}\boldsymbol{M}_{\boldsymbol{E}}(1)\right\}$$

Solving (1) is equivalent to solving:

$$\begin{pmatrix} \overline{\boldsymbol{S}}_{\boldsymbol{E}} & \frac{1}{\Delta t}\boldsymbol{M}_{\boldsymbol{E}}(\varepsilon)\boldsymbol{G} \\ \frac{1}{\Delta t}\boldsymbol{G}^{\boldsymbol{T}}\boldsymbol{M}_{\boldsymbol{E}}(\varepsilon) & \frac{1}{\Delta t}\boldsymbol{G}^{\boldsymbol{T}}\boldsymbol{M}_{\boldsymbol{E}}(\varepsilon)\boldsymbol{G} \end{pmatrix} \begin{pmatrix} \tilde{\vec{c}}_{\boldsymbol{E}} \\ \tilde{\vec{c}}_{\rho} \end{pmatrix} = \begin{pmatrix} \vec{F} \\ \boldsymbol{G}^{\boldsymbol{T}}\vec{F} \end{pmatrix} \qquad (2)$$

where

$$\boldsymbol{S}_{\boldsymbol{E}}\vec{\boldsymbol{c}}_{\boldsymbol{E}} = \vec{F}$$

$$\vec{E} = \tilde{\vec{c}}_{\boldsymbol{E}} + \boldsymbol{G}\tilde{\vec{c}}_{\rho}$$

$$\tilde{\vec{c}}_{\boldsymbol{E}} = \boldsymbol{M}_{\boldsymbol{E}}(1)^{-1}\boldsymbol{C}\boldsymbol{M}_{\boldsymbol{B}}(\mu^{-1})\tilde{\vec{c}}_{\boldsymbol{B}}$$

Bochev et al., *An algebraic multigrid approach based on a compatible gauge reformulation of Maxwell's equations*, 2008.

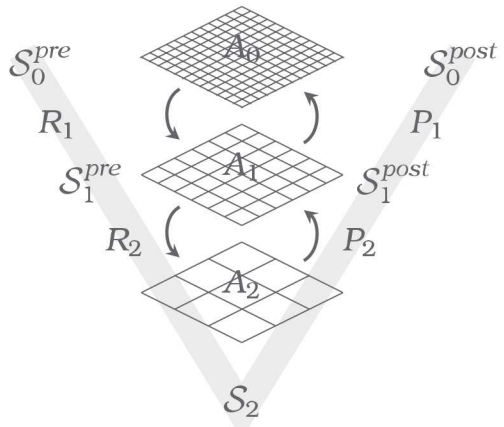
Linear Solver Algorithm (2)

Equation (2) can be solved with CG and Maxwell-specific algebraic multigrid preconditioner

- Block diagonal preconditioner
  - Off-diagonal coupling is ignored
- (1,1) block is edge-based vector Laplacian, requires special prolongator
- (2,2) block is node-based Laplacian

Multigrid: scalable solution method for linear systems arising from elliptic PDEs

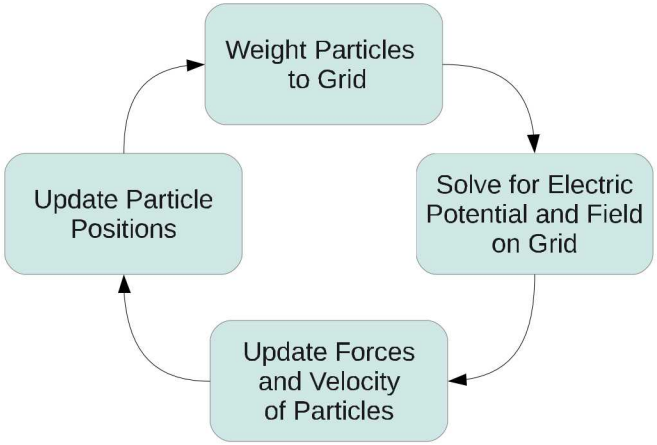
- Idea: capture error at multiple resolutions:
  - **Smoothing** reduces oscillatory error (high energy)
  - **Coarse grid correction** reduces smooth error (low energy)
- Algebraic multigrid (AMG)
- Preconditioner generates A_i's, R_i's, P_i's



Bochev et al., *An algebraic multigrid approach based on a compatible gauge reformulation of Maxwell's equations*, 2008.

Overall EMPIRE Solve

Recall that the Maxwell solve is part of overall EMPIRE solution process;

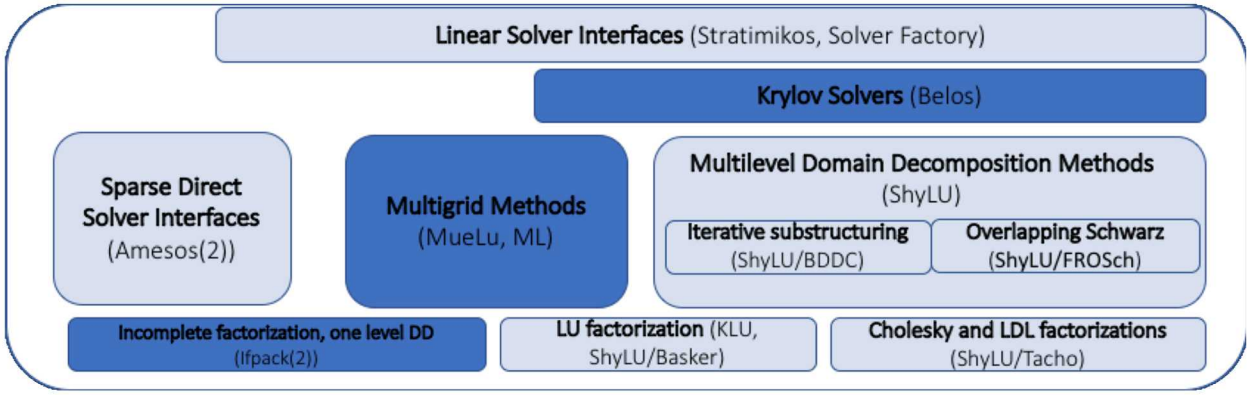


AMG preconditioner is set up only once, and then applied at each time step.

Efficiency of linear preconditioner apply is paramount.

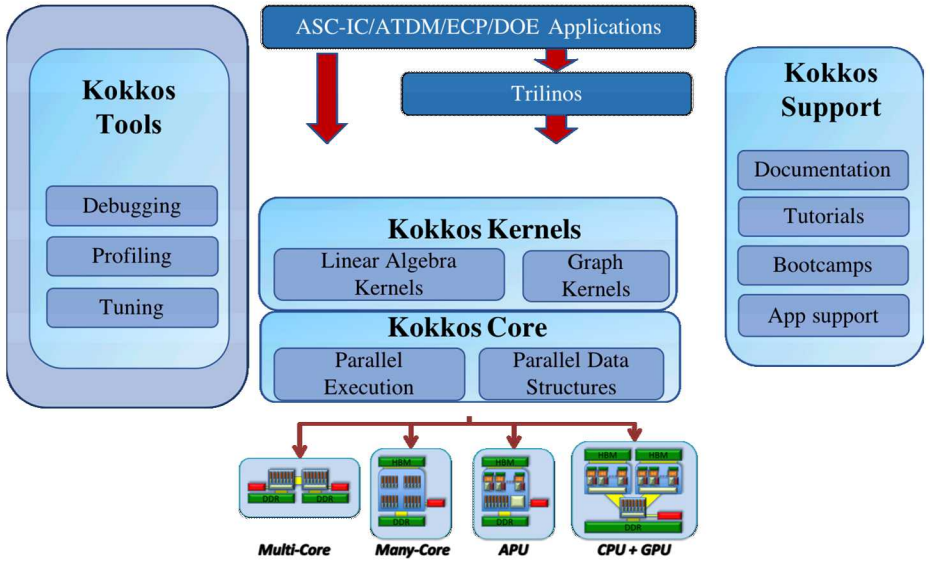
Software

Trilinos Project

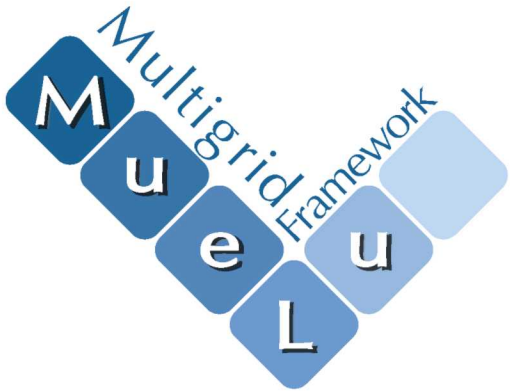


github.com/trilinos/Trilinos

github.com/kokkos



MueLu Multigrid Library



Unstructured algorithms

- classic smoothed aggregation (SA)
- non-symmetric AMG
- AMG for Maxwell's equations

Structured Algorithms

- semi-coarsening AMG
- geometric MG
- structured-grid aggregation-based MG

Leverages many other Trilinos scientific libraries

- Shared memory parallelism from Kokkos → architecture portability
- Sparse distributed linear algebra: Tpetra
- Distributed smoothers: Ifpack2
- Shared memory smoothers, SpGEMM, distance-2 coloring: Kokkos-Kernels
- Load balancing: Zoltan2
- Direct Solvers: Amesos2

Numerical Results

EMPIRE Particle-in-Cell Numerical Experiments

SNL Vortex cluster

- 54 compute nodes
  - Dual socket IBM Power 9, four Nvidia Tesla V100 GPUs
- Interconnect: fat tree Infiniband
- gcc 7.3.1, Spectrum MPI 10.3.0, CUDA 10.1.243
- Application readiness testbed for Sierra supercomputer @ LLNL

Source: SAND-2019-10835R

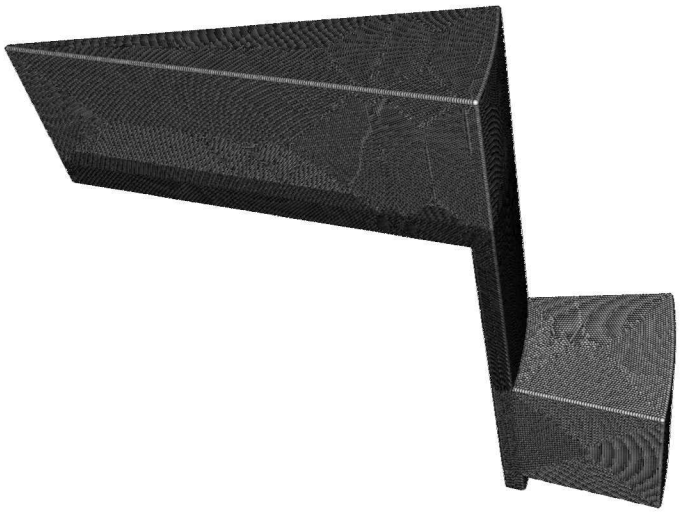
"BDot" mesh

- Small: 10.9m elements, 1.87m nodes
  - Dynamic CFL range: 0.86 to 16.9
- Refined: 85m elements, 14.8m nodes
  - Dynamic CFL range: 0.64 to 16.9

"Cavity" mesh

- 39.1m elements, 6.8m nodes
- Dynamic CFL range: 0.25 to 13.5

1 MPI rank/GPU



Linear Solver Details

Recall the system that we are solving:

$$\begin{pmatrix} \frac{1}{\Delta t}\boldsymbol{M}_B(1) & \boldsymbol{M}_B(1)\boldsymbol{C} \\ -\boldsymbol{C}^T\boldsymbol{M}_B(\mu^{-1}) & \frac{1}{\Delta t}\boldsymbol{M}_E(\epsilon) \end{pmatrix} = \begin{pmatrix} \frac{1}{\Delta t}\boldsymbol{M}_B(1) & \boldsymbol{0} \\ -\boldsymbol{C}^T\boldsymbol{M}_B(\mu^{-1}) & \boldsymbol{I} \end{pmatrix} \begin{pmatrix} \boldsymbol{I} & \Delta t\boldsymbol{C} \\ \boldsymbol{0} & \boldsymbol{S}_E \end{pmatrix}$$

$\boldsymbol{S}_E$ solved with Conjugate Gradient + Maxwell AMG

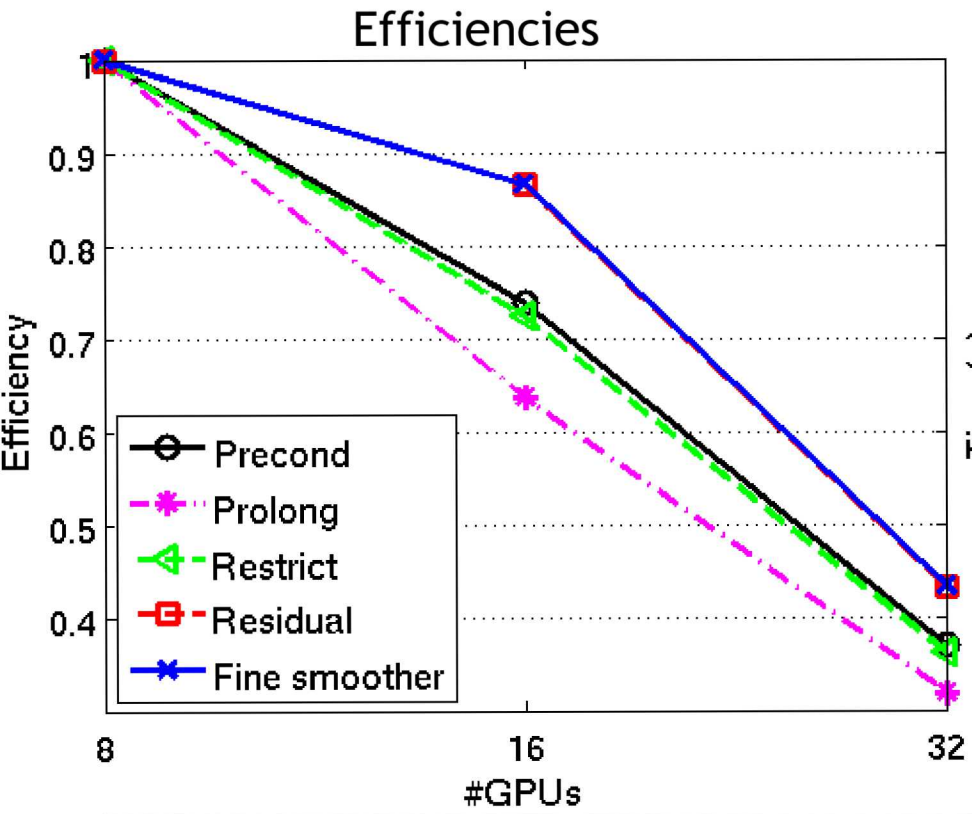
Maxwell AMG preconditioner is set up only once, applied over many timesteps

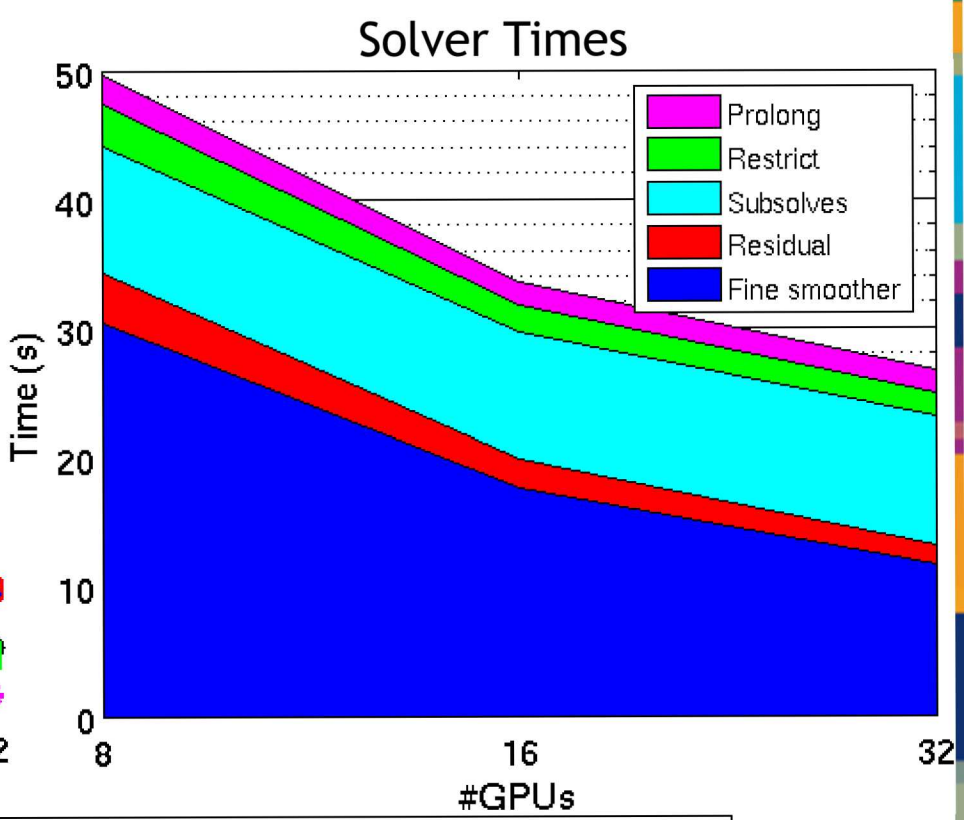
Fine grid smoother: degree 4 Chebyshev polynomial

We will use 2x2 block diagonal (additive) variant

- (1,1) block: single level, degree 6 Chebyshev
- (2,2) block: single level, degree 6 Chebyshev

Bdot: AMG Strong Scaling on "Small" Mesh

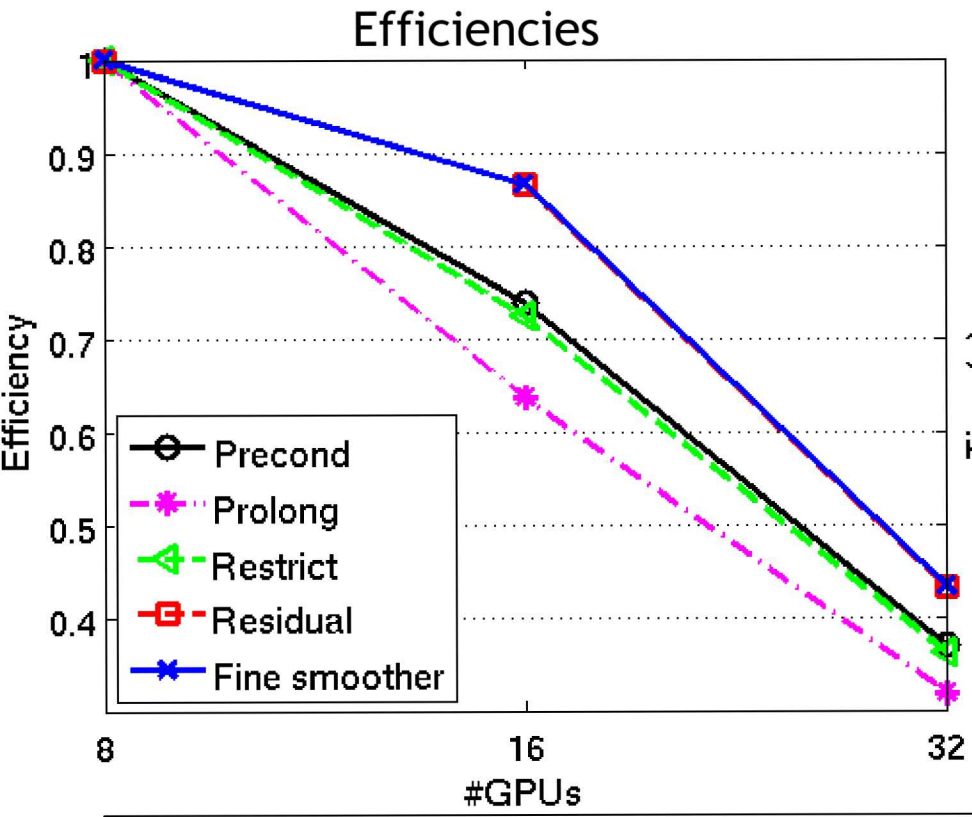


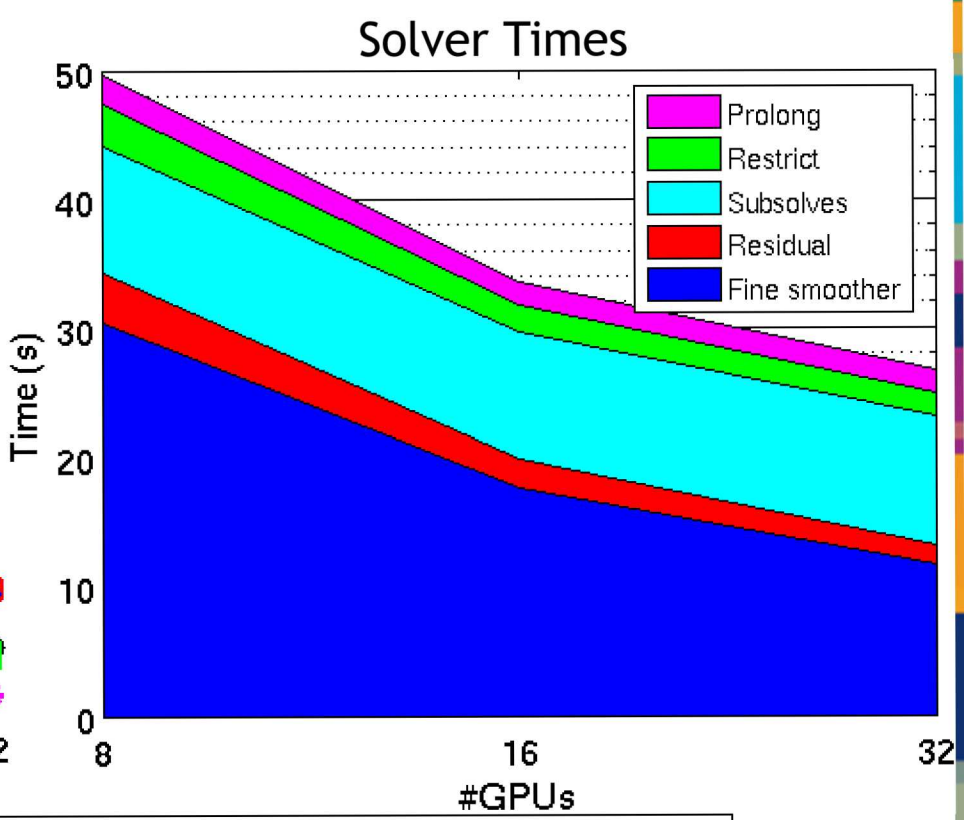


200 timesteps

#GPUs	8	16	32
#Edges/device	1.62M	809k	405k
#Nodes/device	235k	117k	59k

Bdot: AMG Strong Scaling on "Small" Mesh





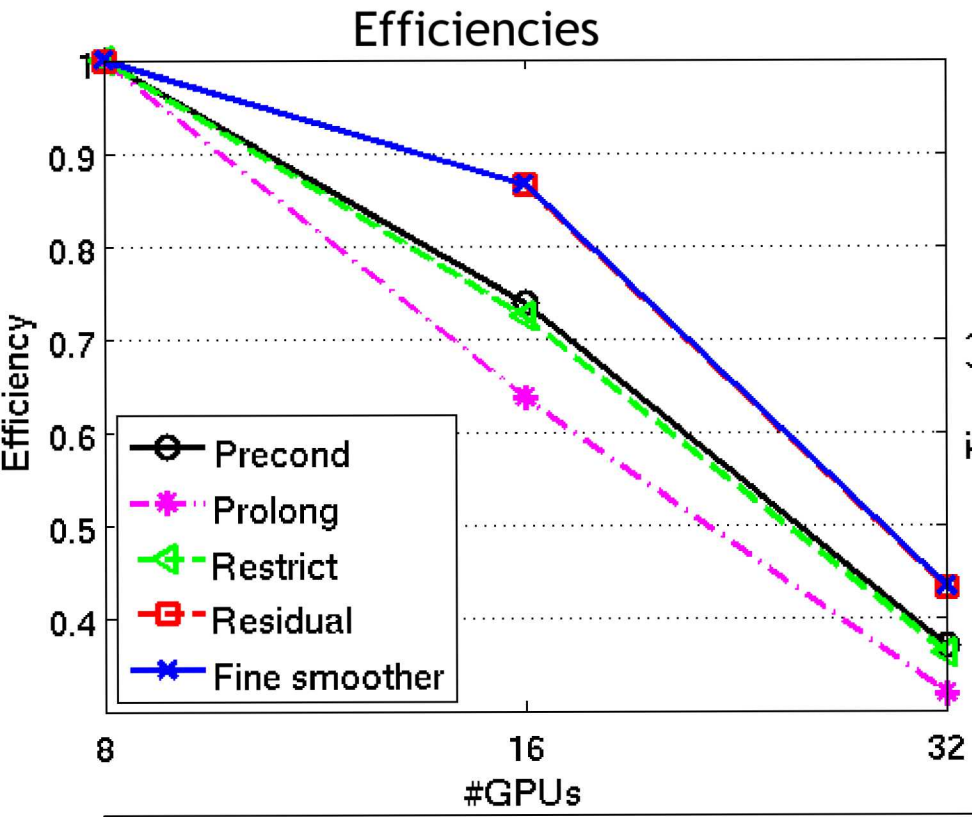
200 timesteps

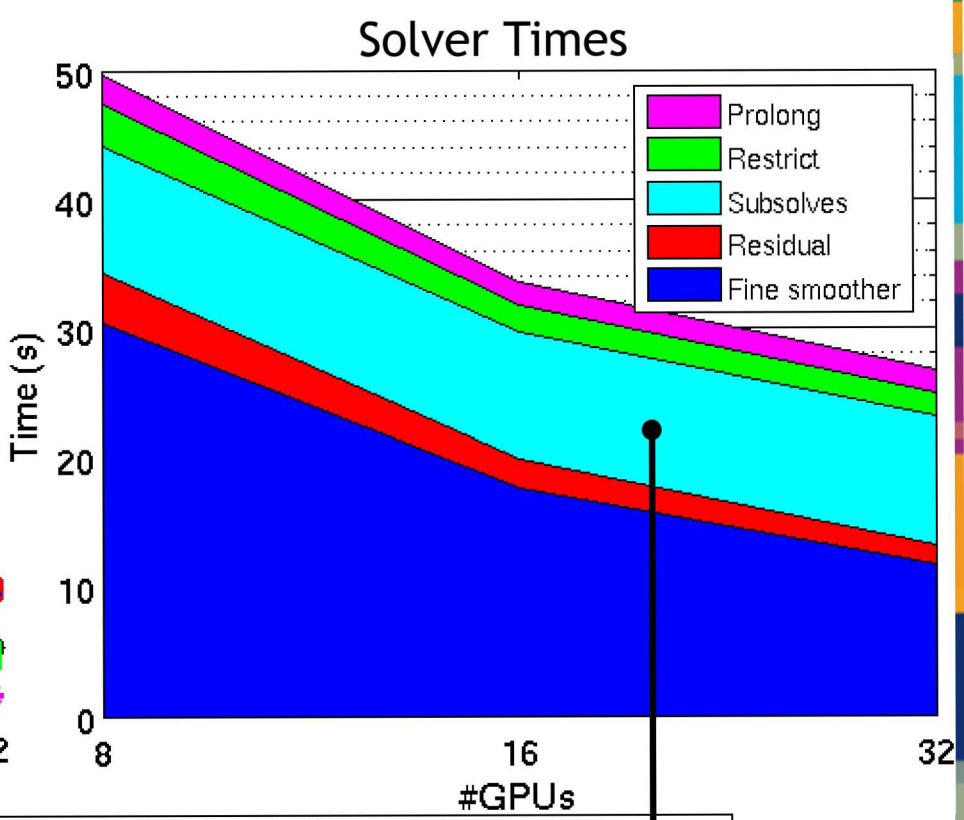
AMG is 70-80% of total linear solve time

6 solves/sec @ 32 GPUs

Chebyshev smoother (matvec kernel) efficiency drops off at @ 32 GPUs

Bdot: AMG Strong Scaling on "Small" Mesh





200 timesteps

AMG is 70-80% of total linear solve time

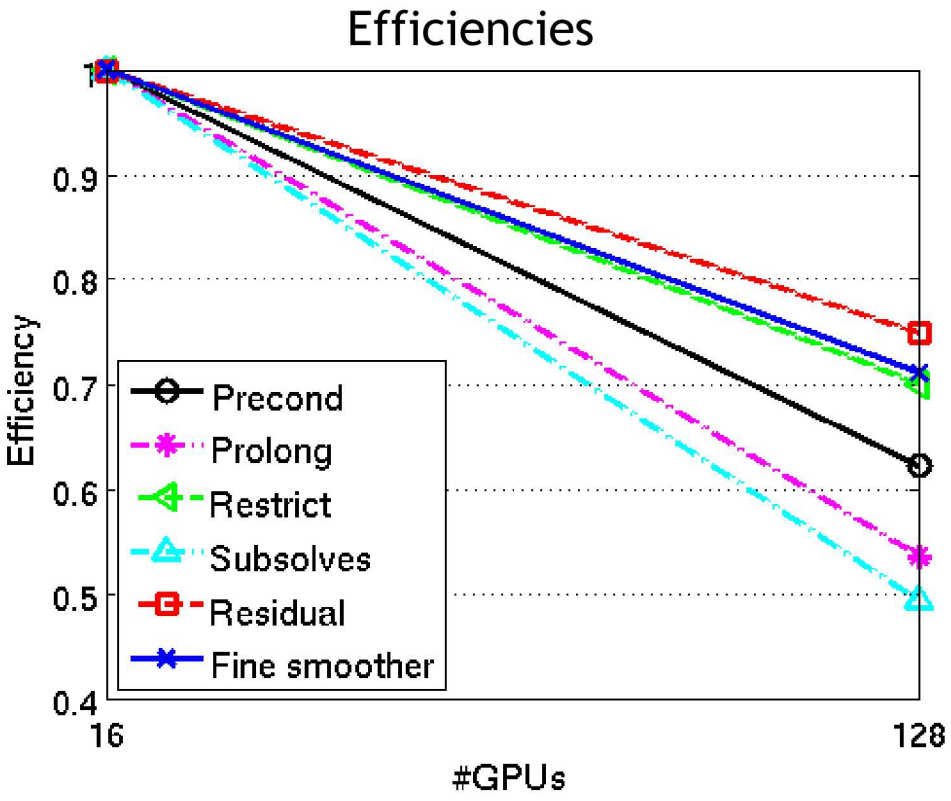
6 solves/sec @ 32 GPUs

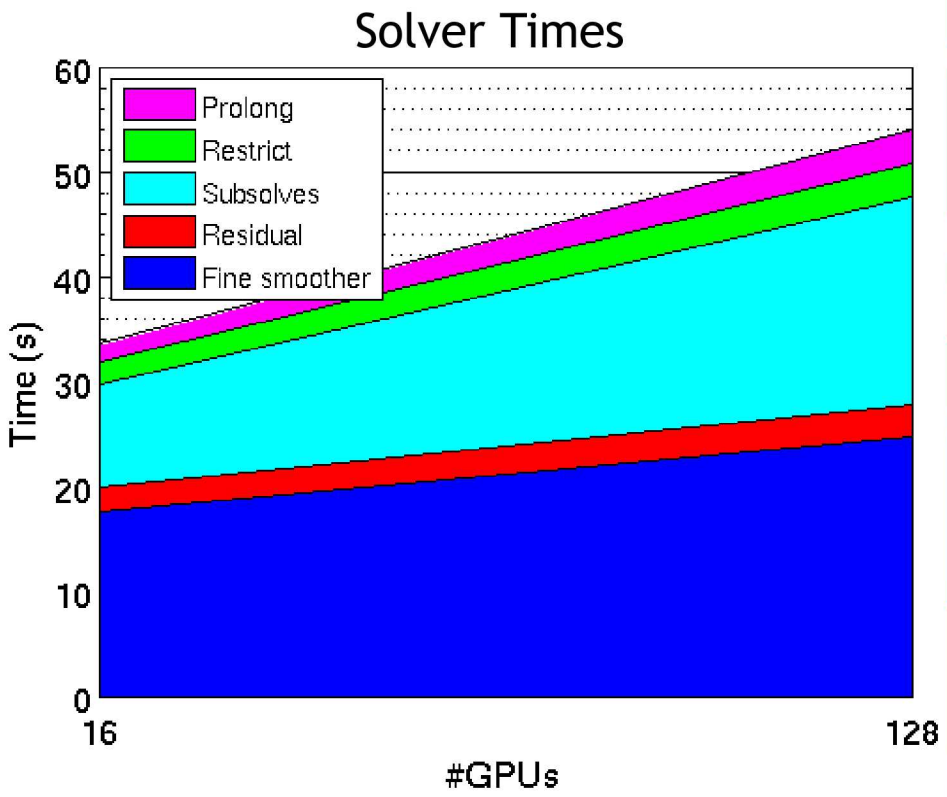
Chebyshev smoother (matvec kernel) efficiency drops off at @ 32 GPUs

Subsolves migrated to small number of devices

- Effect of rebalancing, so no speedup expected

Bdot: AMG Weak Scaling





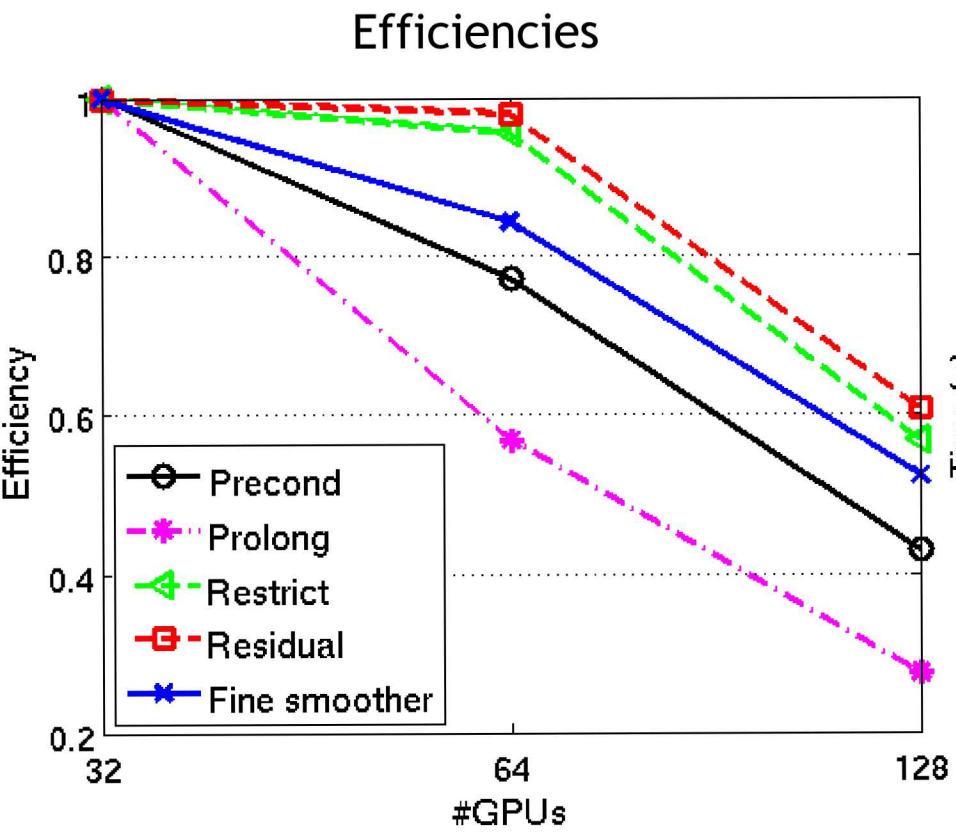
200 timesteps

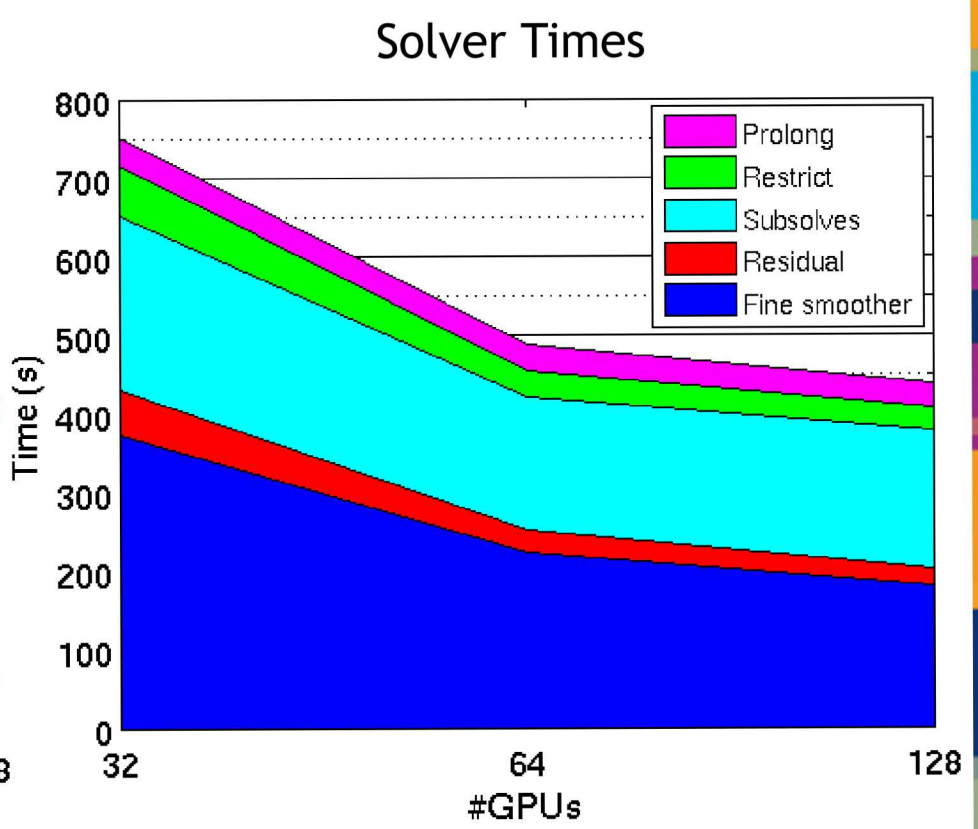
AMG is 75-80% of total linear solve time

4.5 solves/sec @ 16 GPUs

3 solves/sec @ 128 GPUs

Cavity: AMG Strong Scaling

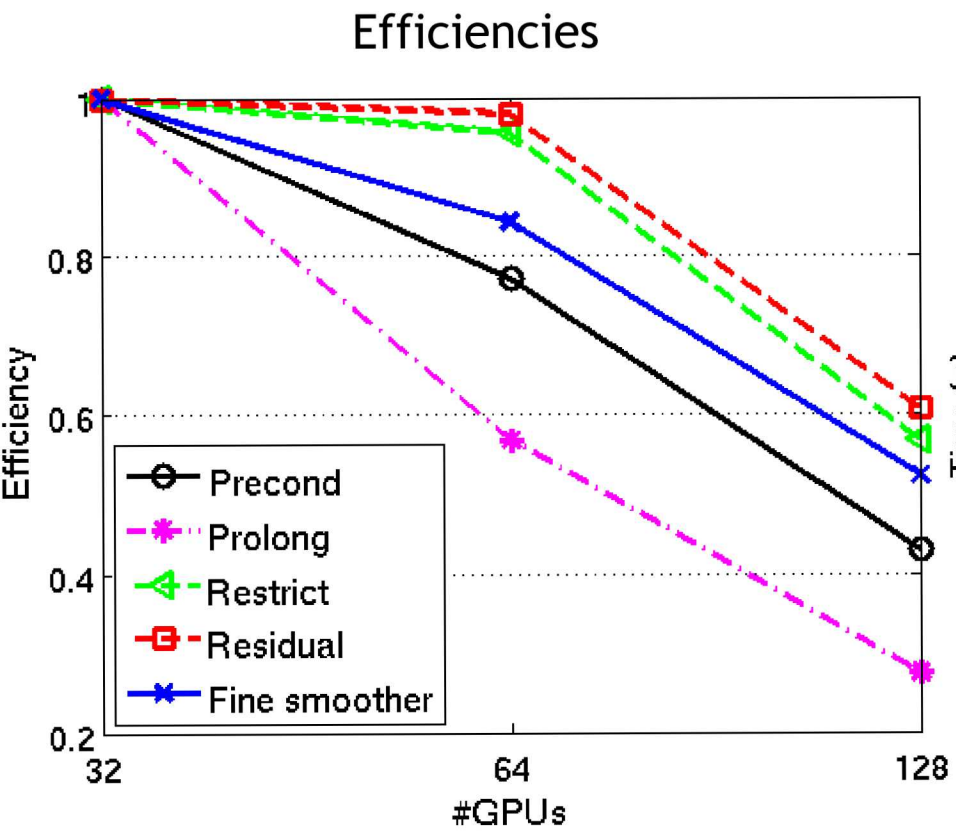


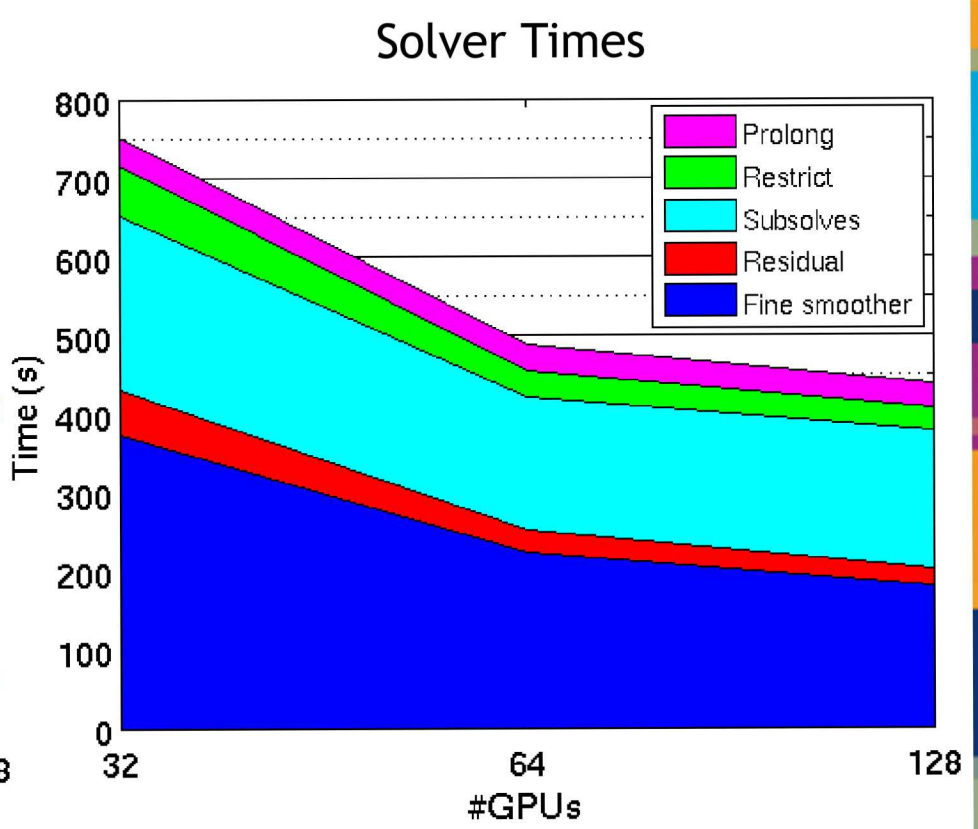


2000 timesteps

#GPUs	32	64	128
#Edges/device	1.46M	728k	364k
#Nodes/device	213k	106k	53k

Cavity: AMG Strong Scaling





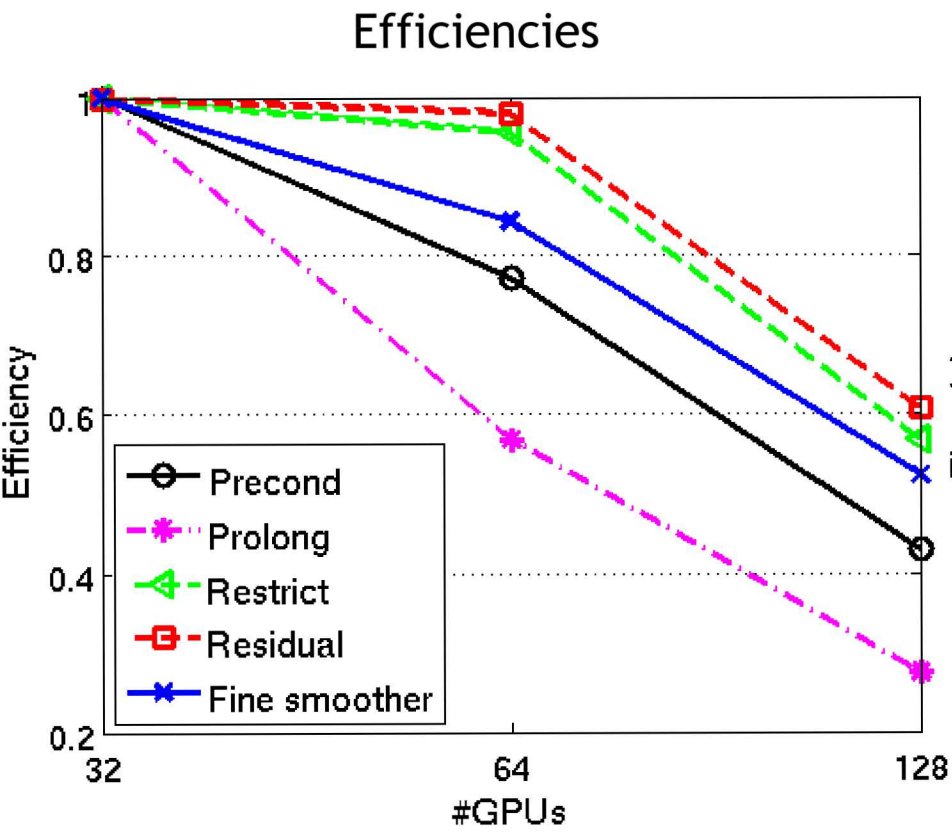
2000 timesteps

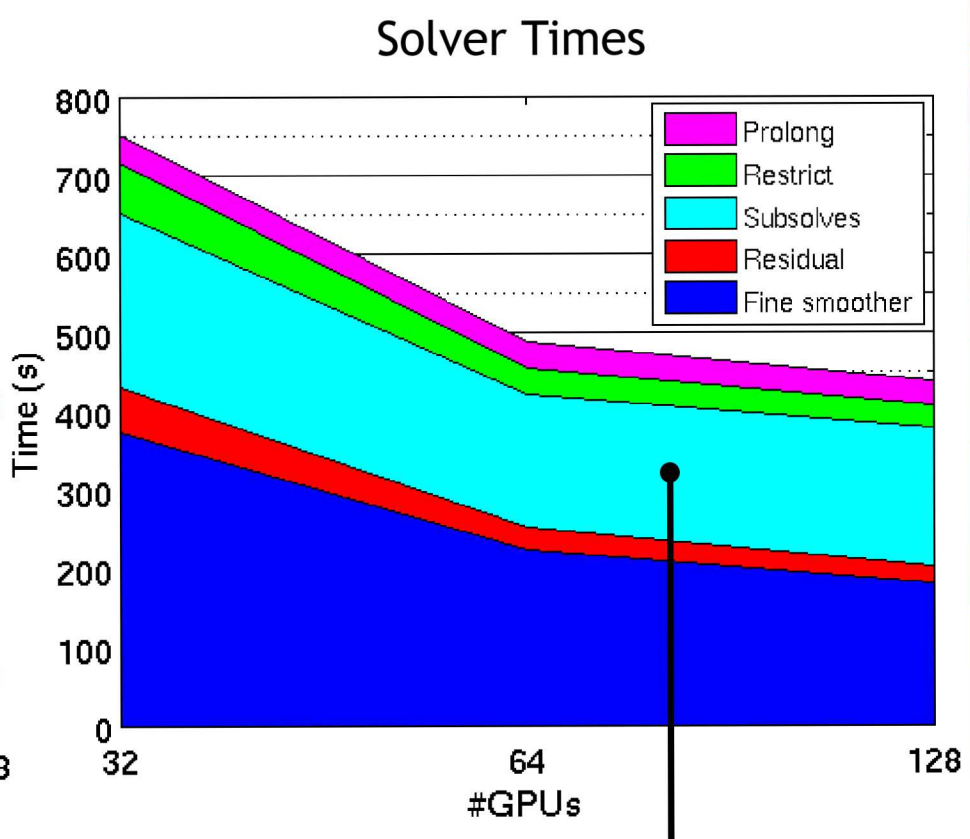
AMG is ~80% of total linear solve time

3.8 solves/sec @ 128 GPUs

At 128 GPUs, subsolve and fine grid smoother are roughly same cost

Cavity: AMG Strong Scaling





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3.8 solves/sec @ 128 GPUs

At 128 GPUs, subsolve and fine grid smoother are roughly same cost

Subsolves always occur on same number of devices

- Effect of rebalancing, so efficiency drop expected

Future Work / Concluding Remarks

Assess solver performance on larger cavity meshes on Sierra platform

s-step Chebyshev smoother

- Single halo exchange but with larger message
- Followed by *s* local matrix-vector products

Related talks

- M. Bettencourt, "Towards Exascale Plasma Simulations using PIC Algorithms", Wedn. pm, MS5
- L. Berger-Vergiat, "MueLu's Algorithmic Performance on GPUs", Thursday p.m. MS34
- C. Siefert, "State of the Tpetra Linear Solver Stack", Friday a.m., MS41