Scalable Linear Solvers for the Next Generation: Applications in Oxy-Coal Clean Energy Boiler Design

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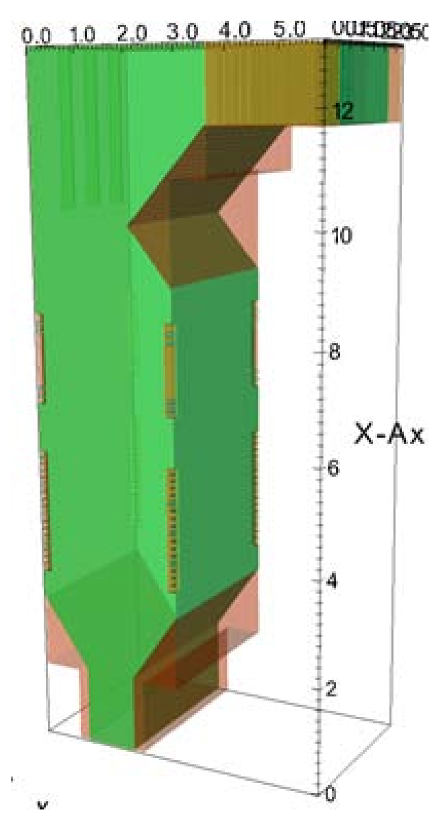
Introduction and Motivation

- Coal is our most abundant energy source
- Conventional coal power plants are significant sources of green house gases and other pollutants entering our atmosphere.
- Retrofit existing power plants for **Oxy-Combustion**

Oxy-Combustion Benefits

- High CO_2 capture rates
- Retrofit existing facilities
- Environmentally friendly
- Use existing coal resources



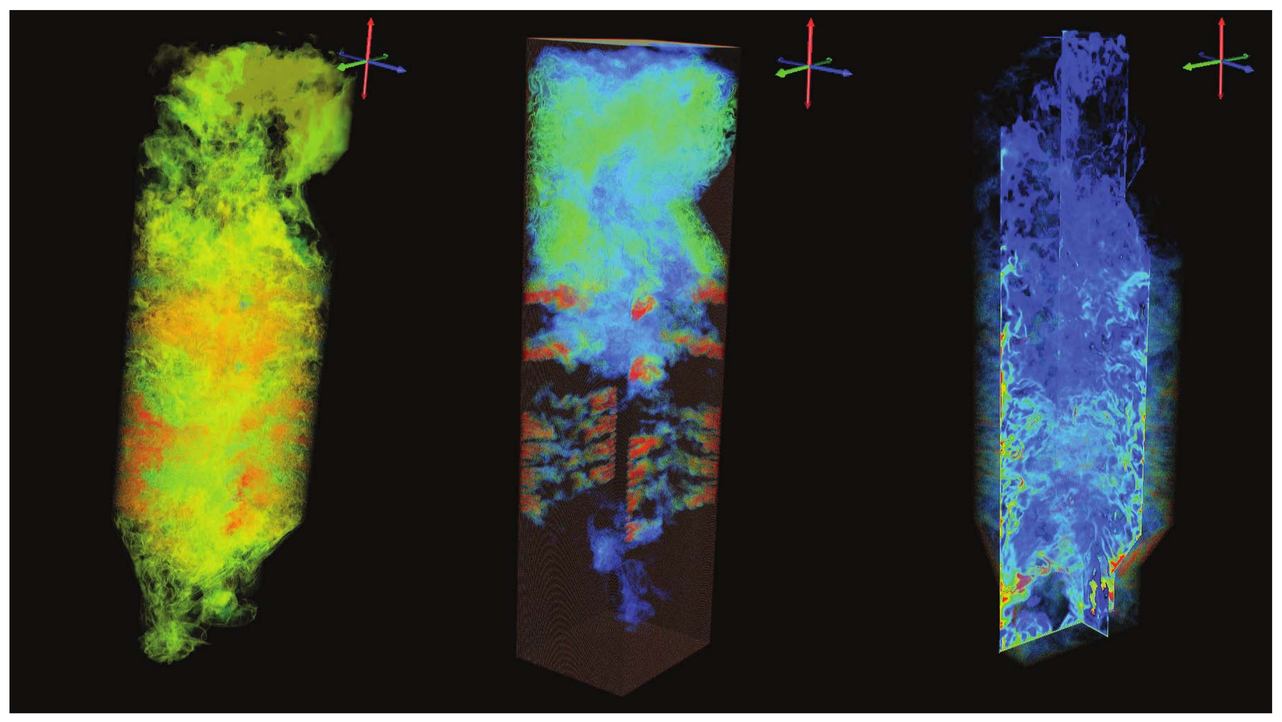
Oxy-Combustion Challenges

- Require new oxy-fuel firing systems
- Performance, efficiency and cost effectiveness are still being evaluated
- Evaluate performance in test systems and ***SIMULATION***
- Validation/Verification & Uncertainty Quantification (VV/UQ)

Exascale Energy Problem Design

Alstom Clean Oxy-Coal Boiler

- Need LES resolution for 350 MW problem
- 9×10^{12} simulation cells
- Estimates 50-100 million cores to simulate problem in 48 hours of wall clock time



Gas Temperature O_2 Concentration Particle Concentration

Simulation Challenges

For a portion of the Alstom Boiler Simulation, it is necessary to solve the fully incompressible Navier-Stokes equations within the ARCHES combustion component

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \mathbf{u} = 0 \quad (1)$$

$$\frac{\partial \rho \mathbf{u}}{\partial t} = \mathbf{F} - \nabla p; \mathbf{F} \equiv -\nabla \cdot \rho \mathbf{u}\mathbf{u} + \mu \nabla^2 \mathbf{u} + \rho g \quad (2)$$

$$\nabla^2 p = \nabla \cdot \mathbf{F} + \frac{\partial^2 \rho}{\partial t^2} \equiv R \quad (3)$$

- Pressure Poisson equation (3) is large and sparse
- Time required to solve (3) is the dominant factor in time per timestep.
- 10^{10} unknowns on 10^6 processors
- Solver **MUST** be scalable (weak) – Use Multi-Grid Solvers, i.e. Hypre (LLNL)

Use Hypre Efficiently

- **ELIMINATE** startup costs for solver communication at each timestep
- Share key data structures between Hypre and Uintah's Datawarehouse
- Chose the right pre-conditioner (PFMG) and relaxer (Red Black Gauss-Seidel)
- Skip levels during the coarsening/refining stage when the solution is smooth

Hypre Setup Costs

Titan Cores Startup	2K	4K	8K	16K	32K	64K	128K
	0.02	0.13	0.25	0.25	0.50	0.75	3.89
Jaguar Cores Startup	3K	6K	12K	24K	48K	96K	192K
	1.54	1.10	1.22	2.04	2.4	2.9	22.11

Weak Scalability Model for Solver Time

- Solver time as a function of the number of Cores
- Power law relationship $(time = a * Cores^m)$

$$\log(time) = \log(a) + m \log(Cores) \quad (4)$$

- Use empirical data to determine the slope (m) of the curve fit to predict scalability at Core counts on future/larger machines
- Evaluate individual multi-grid steps to determine scaling bottlenecks

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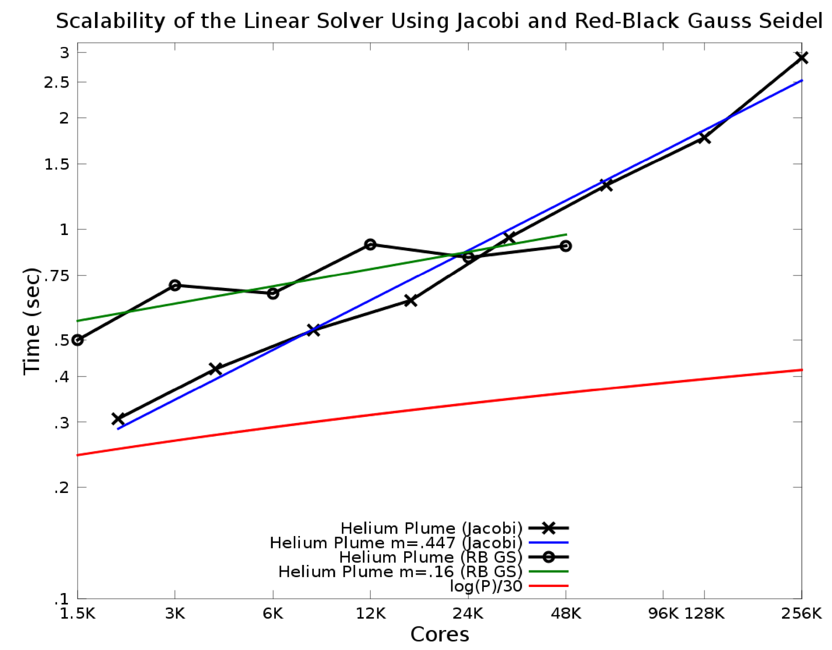
- Continuing work will use DOE ALCC allocation CMB026 for time on Titan when it becomes available in late 2012

Results

Two test problems were chosen to study solver scalability, a Taylor-Green problem and a Helium Plume problem.

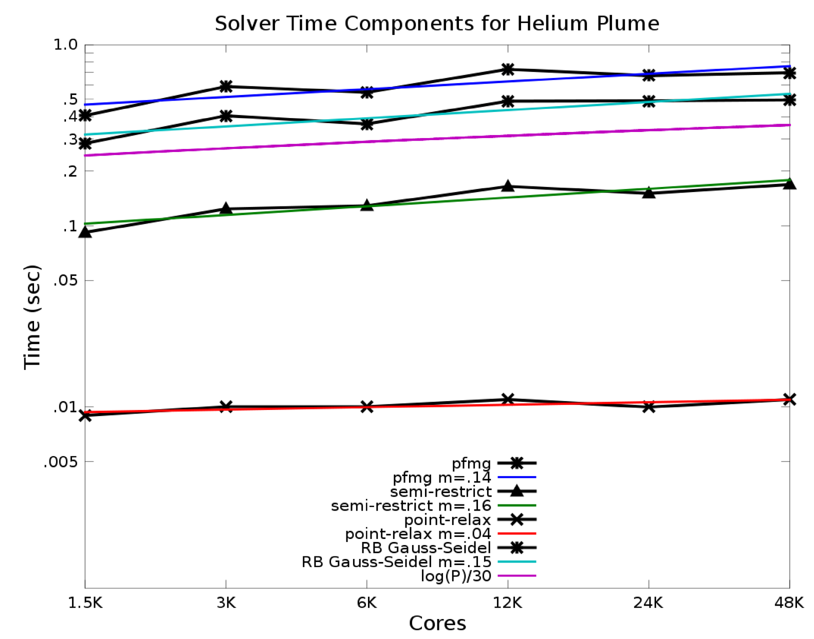


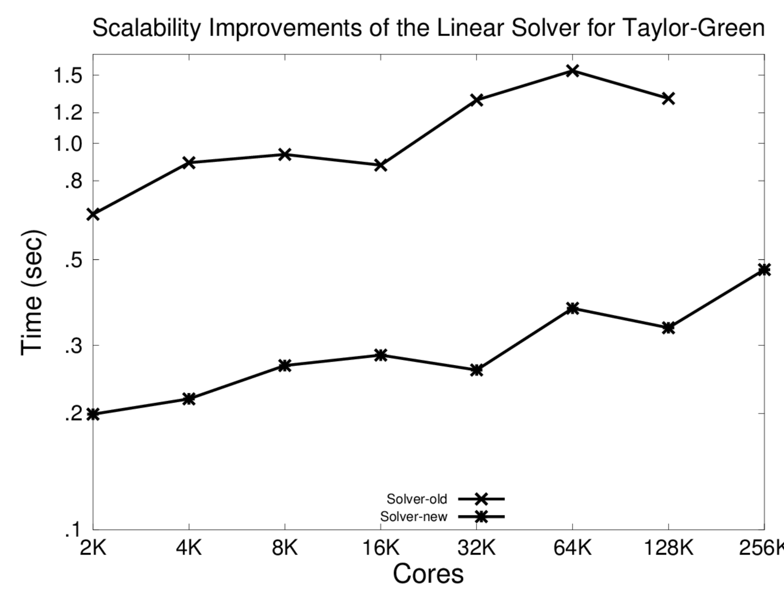
Relaxation Scheme Comparison

- Choice of correct relaxer has a significant effect on the scalability
- Red Black Gauss Seidel relaxation scheme has significantly better scaling characteristics over the simpler Jacobi point-wise smoother.

Multi-Grid Step Breakdown

- Use (4) to model the timing of individual steps of the multi-grid solve.
- Pre-conditioner (PFMG) and Relaxation Phase (RB GS) determine the overall slope of the scalability curve.





Scalability Improvements

- Scales remarkably well up to 256K cores
- Weakly scalable solver with a log(P) dependency for global communication
- Correct pre-conditioner (PFMG)
- Best relaxation scheme (RB GS)
- Skip levels during coarsening & refining
- Eliminate set-up costs

Future Work & References

Tune the solve phase for the complex Alstom Boiler Runs. Anticipated that during the course of any simulation, the ever evolving complex dynamics will require different solver parameters and schemes, i.e. pre-conditioners and relaxers to perform efficiently.

1. *Schmidt, J.; Berzins, M.; Thornock, J.; Saad, T.; Sutherland, J., "Large Scale Parallel Solution of Incompressible Flow Problems using Uintah and hypre", Technical Report, No. UUSCI-2012-002, SCI Institute, Univeristy of Utah, 2012.*

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