报告来源：2019年IDAJ中国CAE/MBD技术大会

CONVERGE 3.0 Results and Looking Ahead to 3.1

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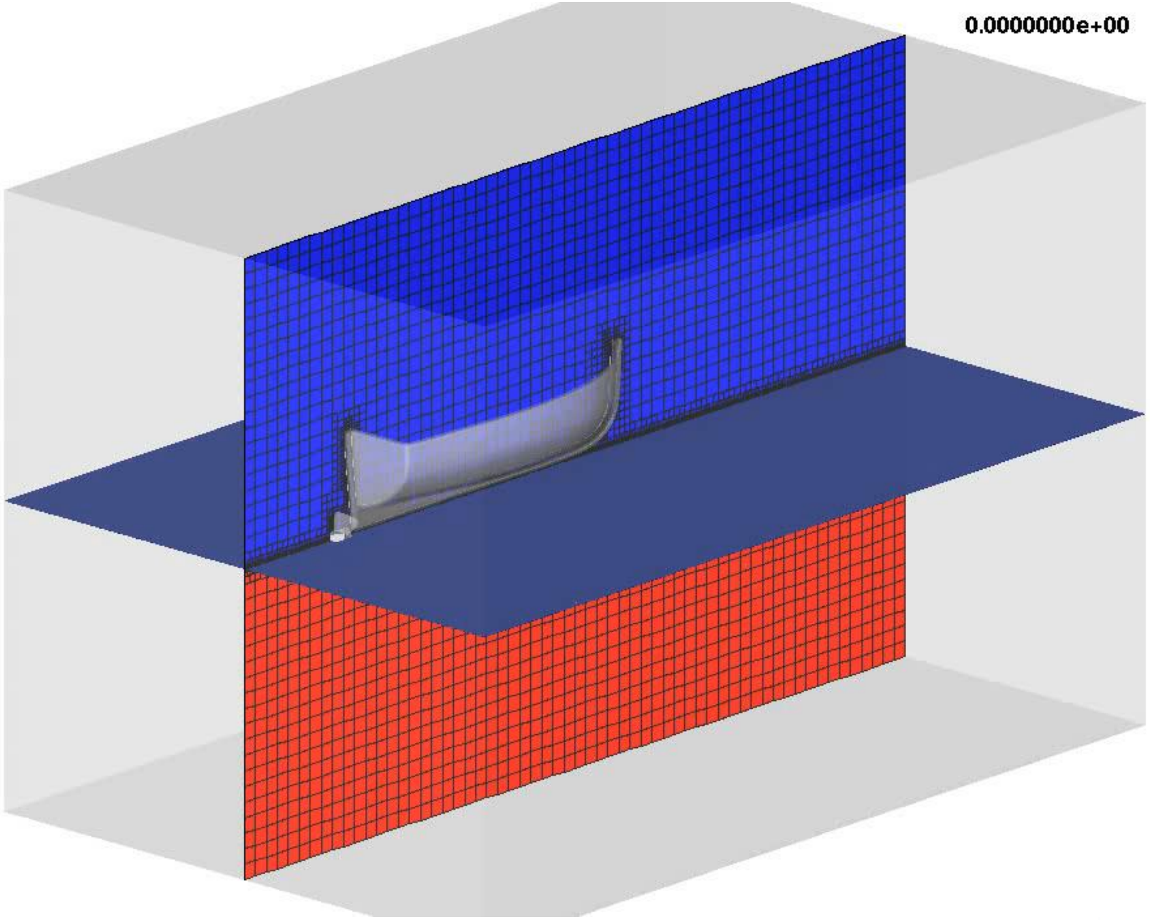
CONVERGE CFD SOFTWARE

Overview

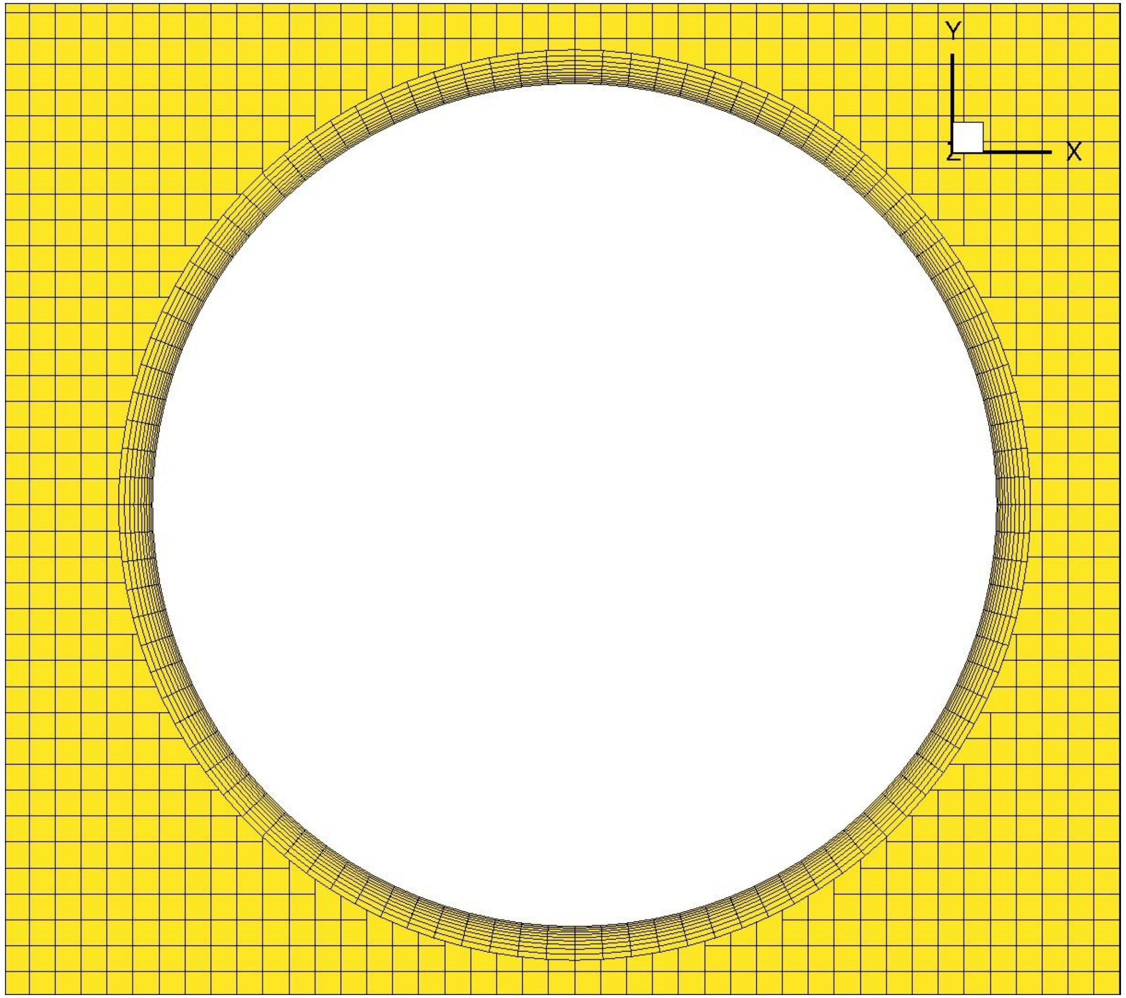
- 3.0 Updates
  - Inlaid grid examples
  - Solver
  - Combustion
- Scaling Results
  - FlameD
  - SI8
- 2.4 vs. 3.0 Results Comparison
- 3.1 Features



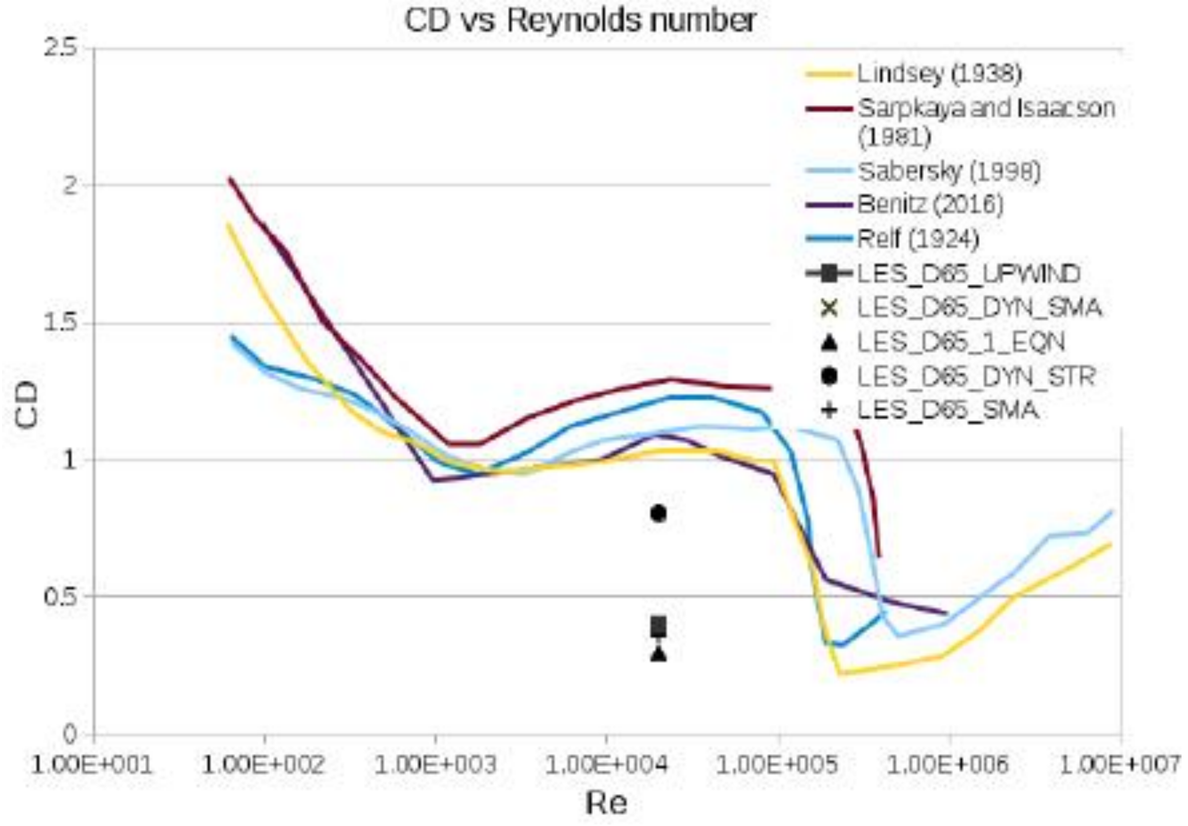
Inlaid Mesh

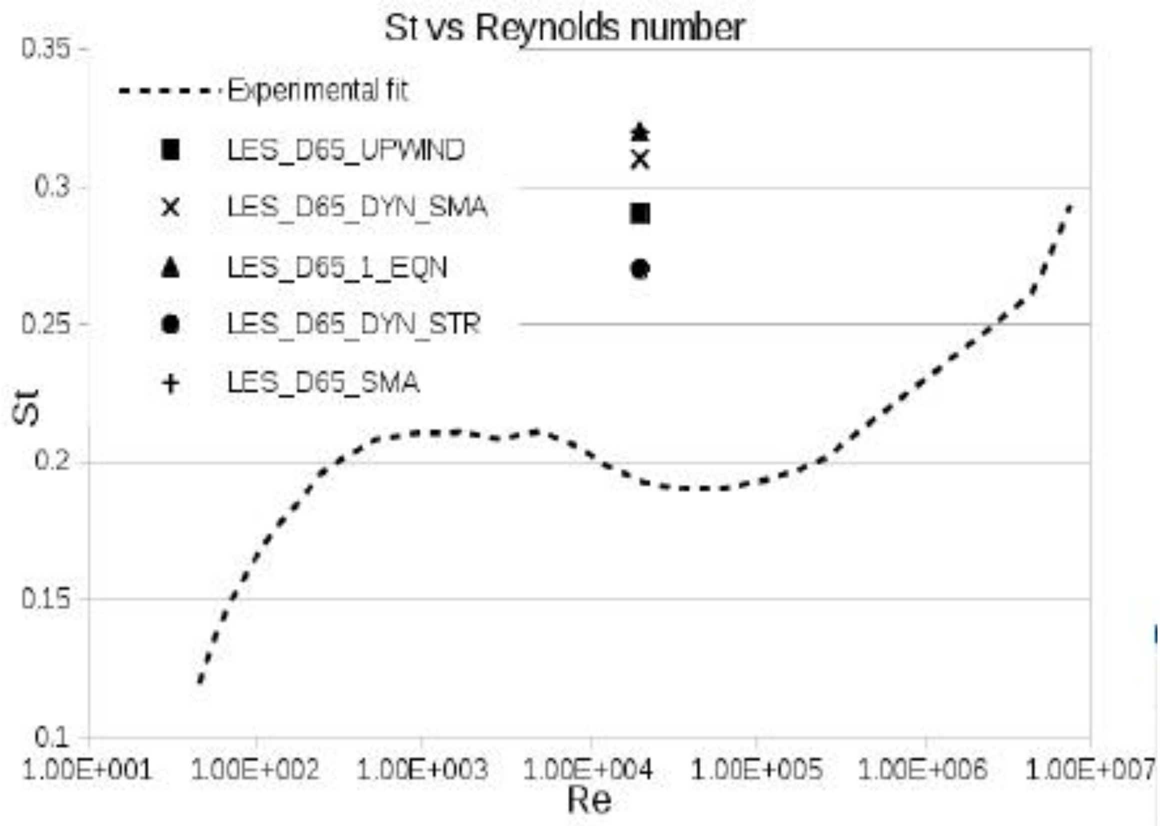
Inlaid Mesh Application—Flow Over a Cylinder

- Incompressible flow
- Re = 20,000
- Cartesian and inlaid mesh cases run at various resolutions
- Compared to experimental drag and vortex shedding frequency

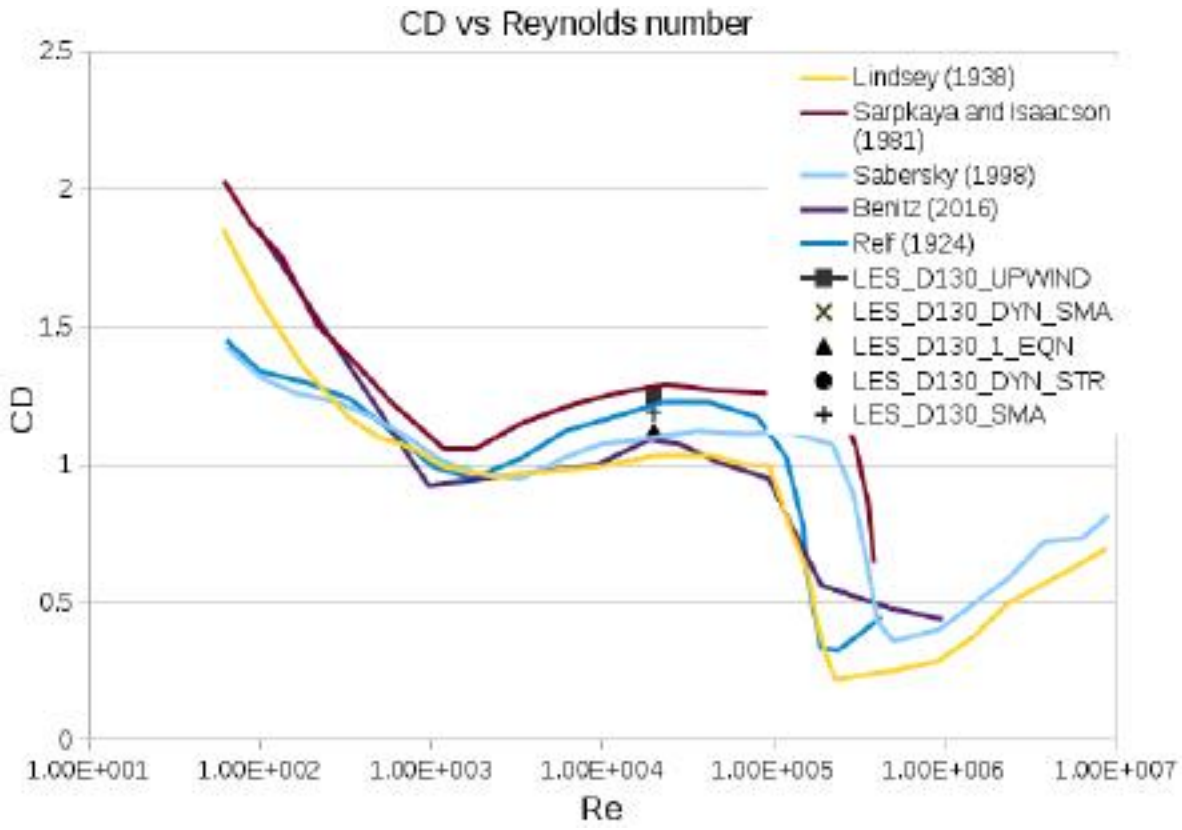


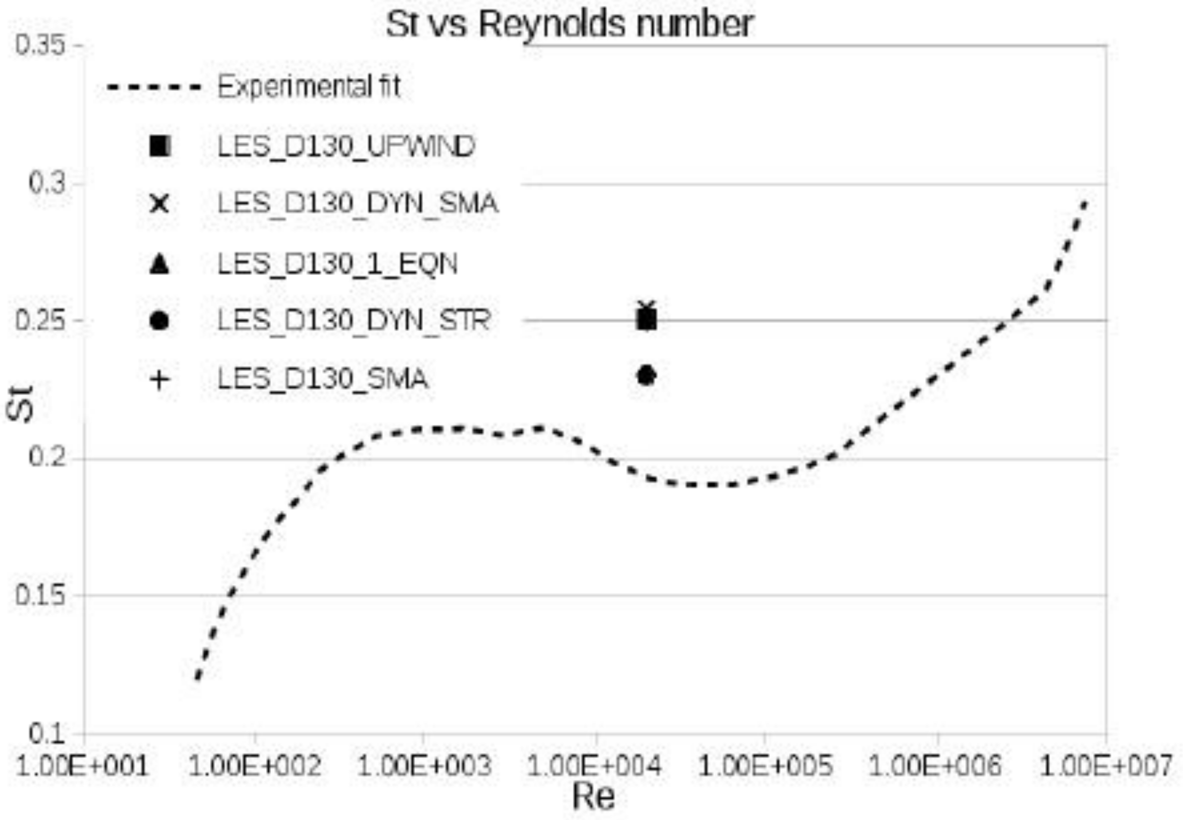
Cartesian: Coarse Grid (~100,000 cells)



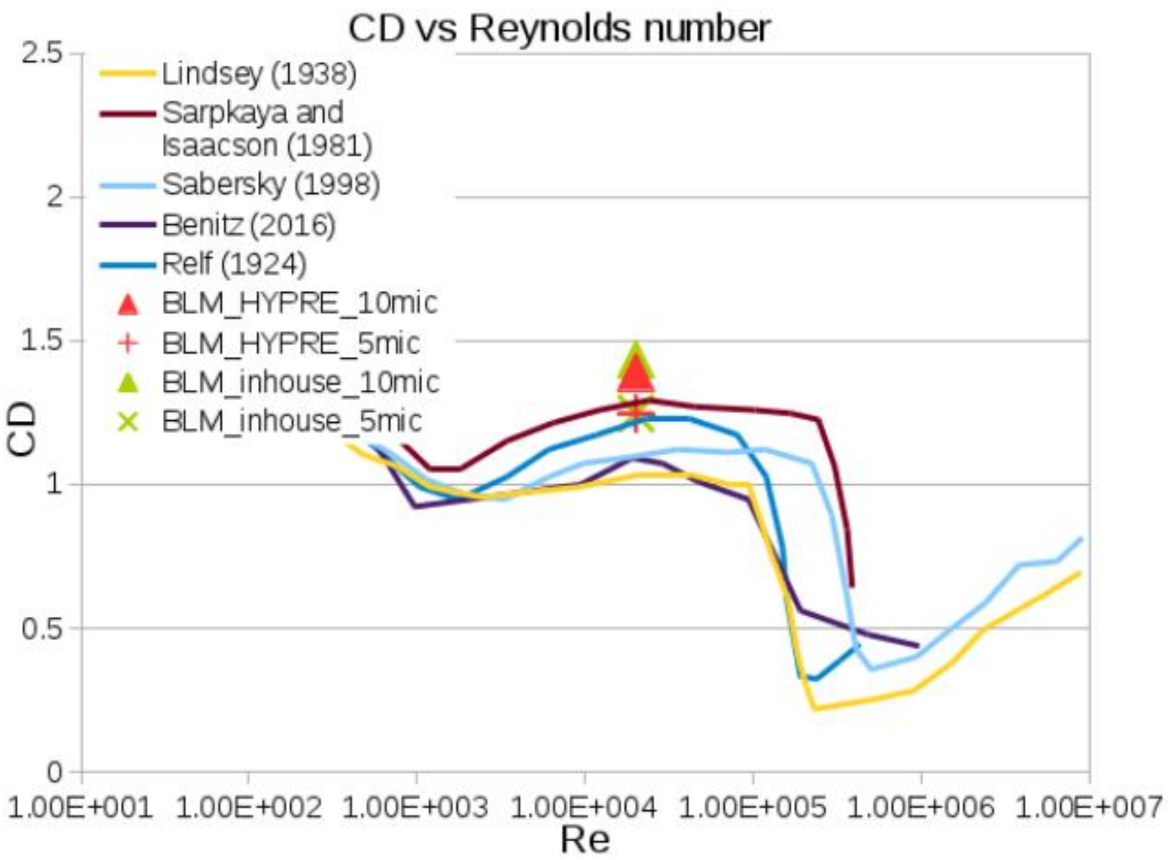


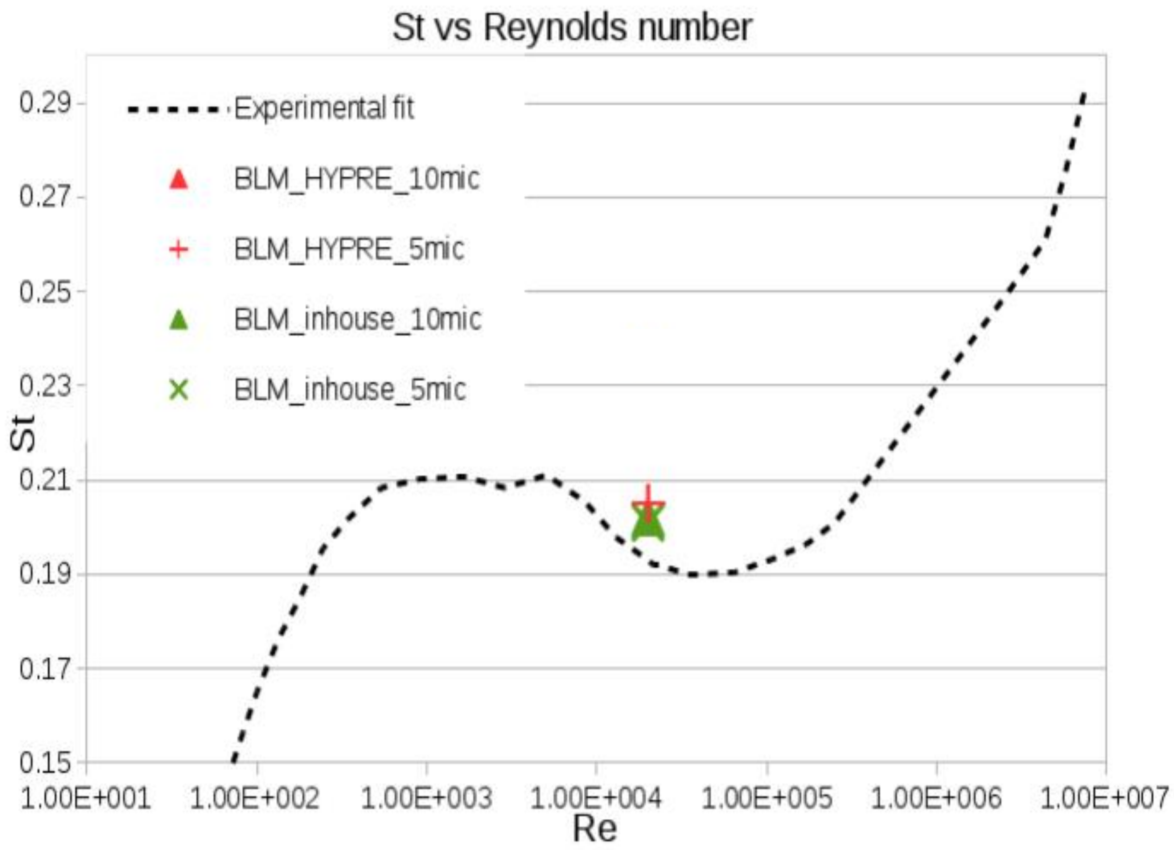
Cartesian: Fine Grid (~300,000 cells)





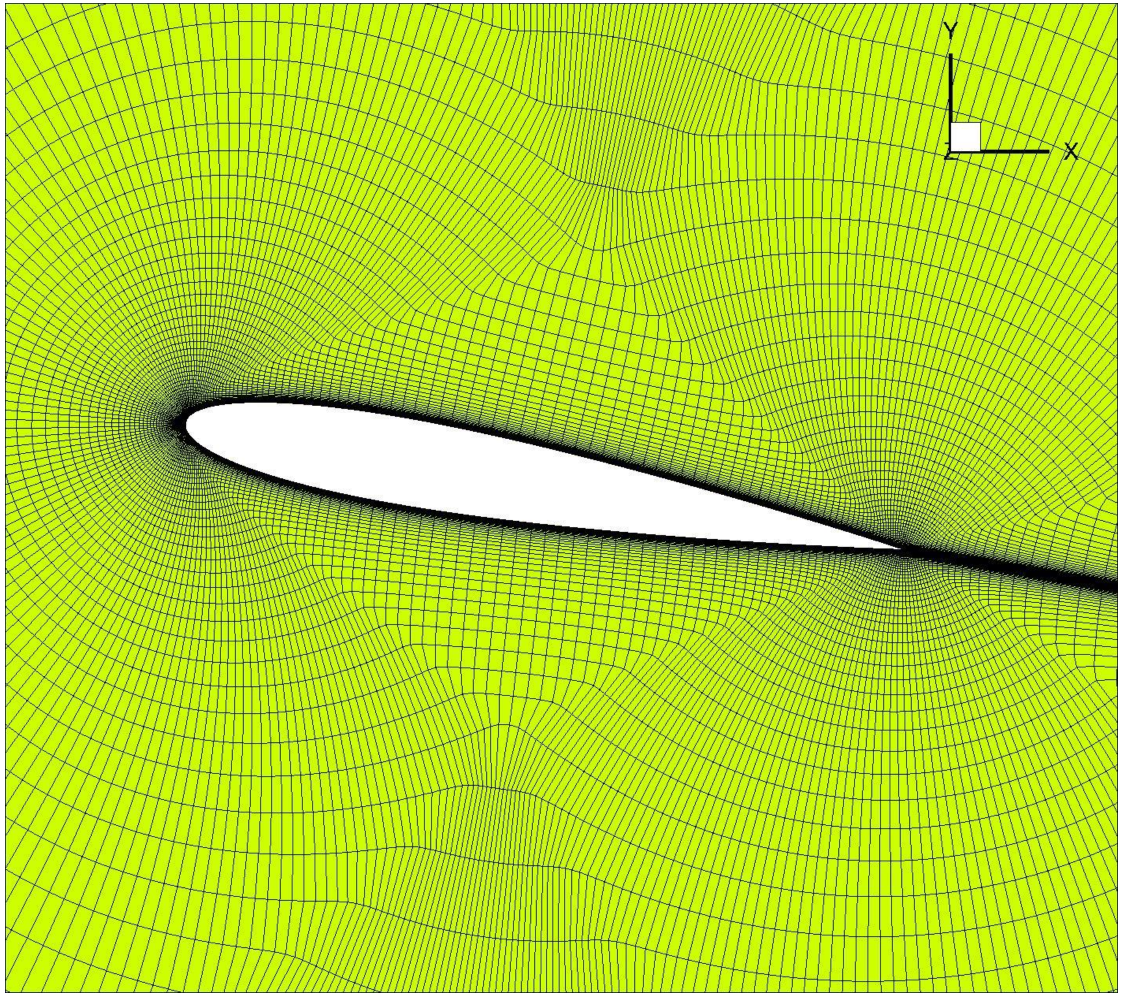
Inlaid Grid (~80,000 cells)



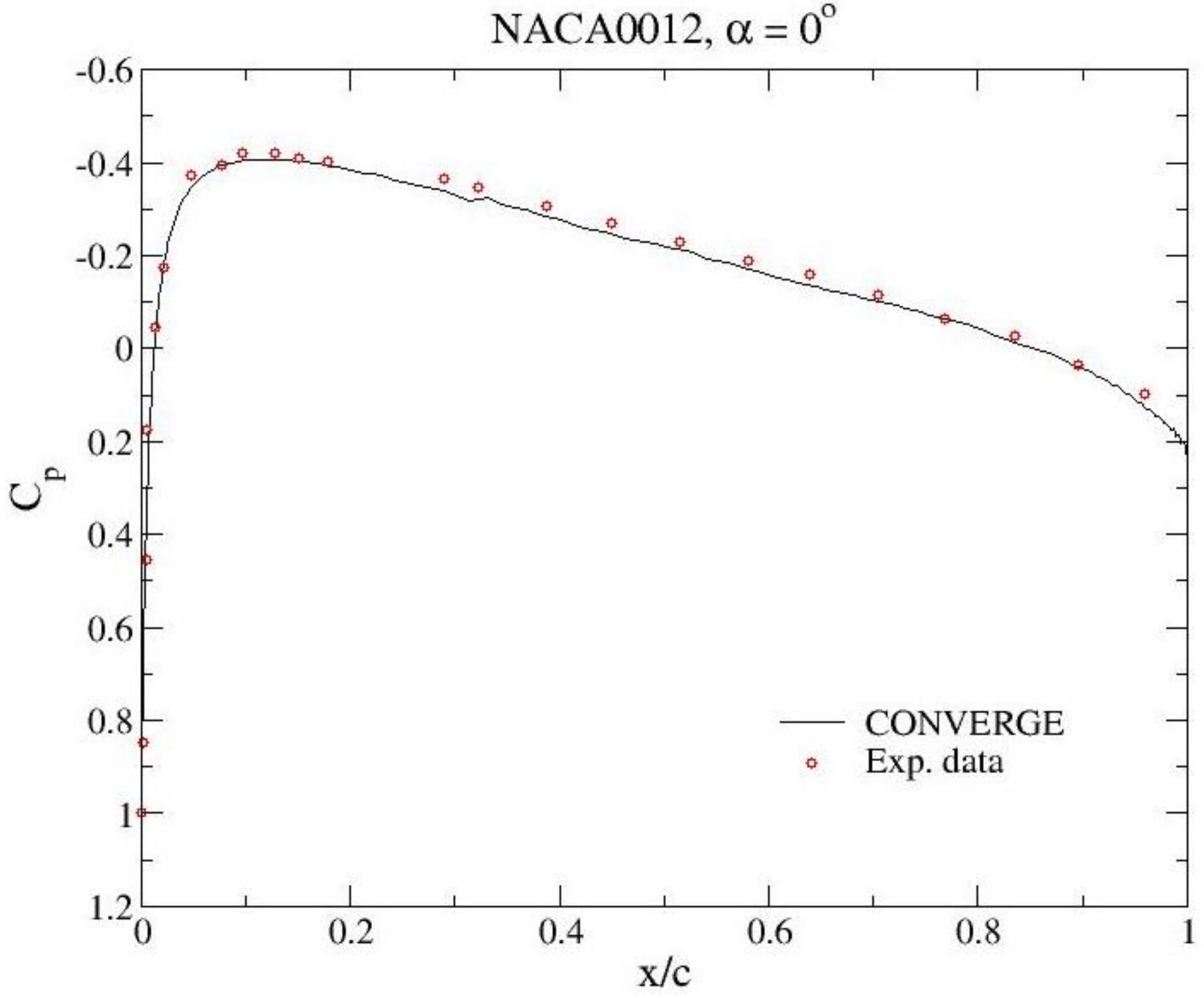


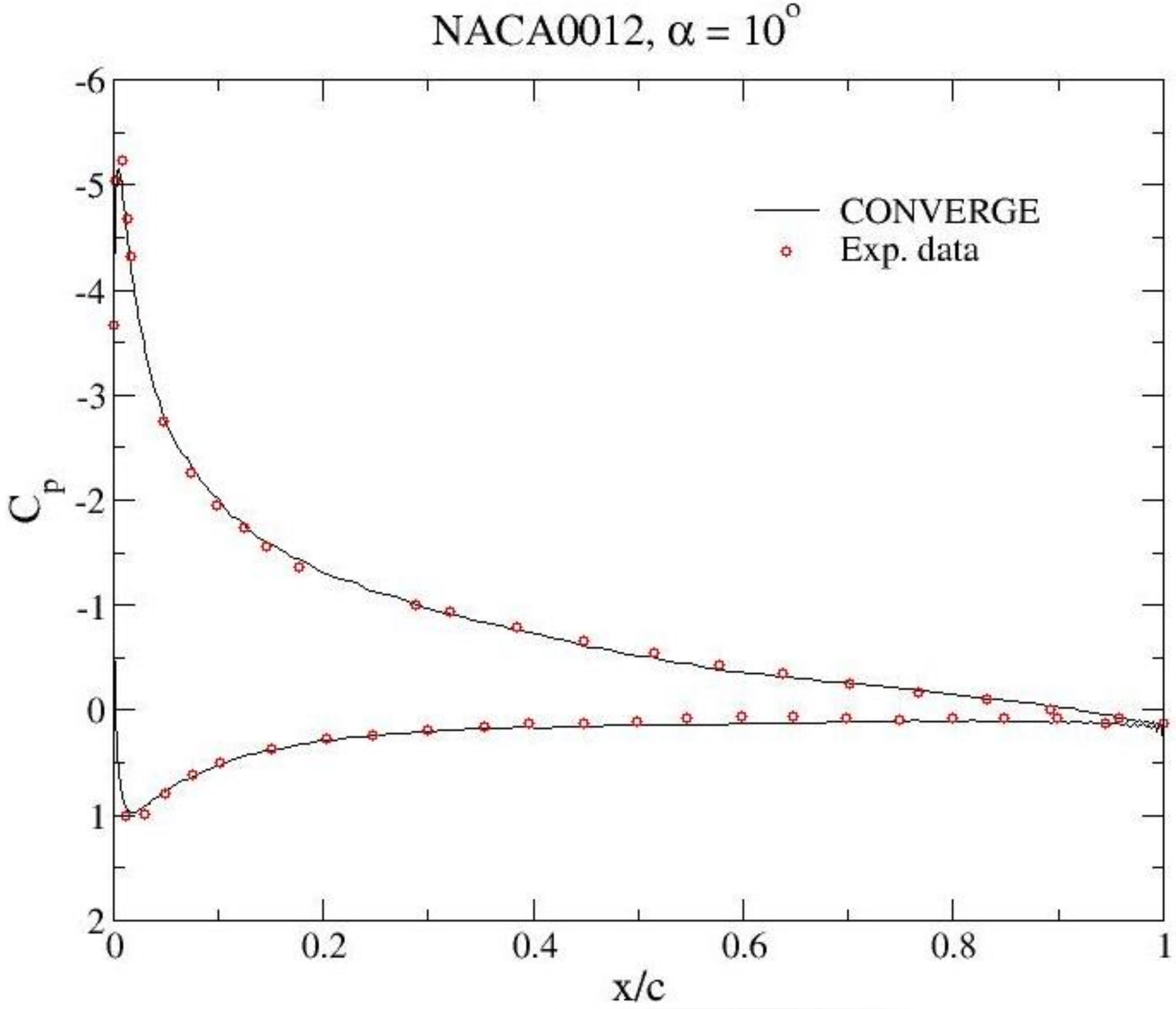
Inlaid Mesh Application—Airfoil

- NACA 0012 symmetric airfoil
- Grid is supplied as a industry-standard benchmark
  - Entire grid imported and treated as an inlaid mesh
- Three configurations were simulated
  - $\alpha = 0^o, 10^o, 15^o$



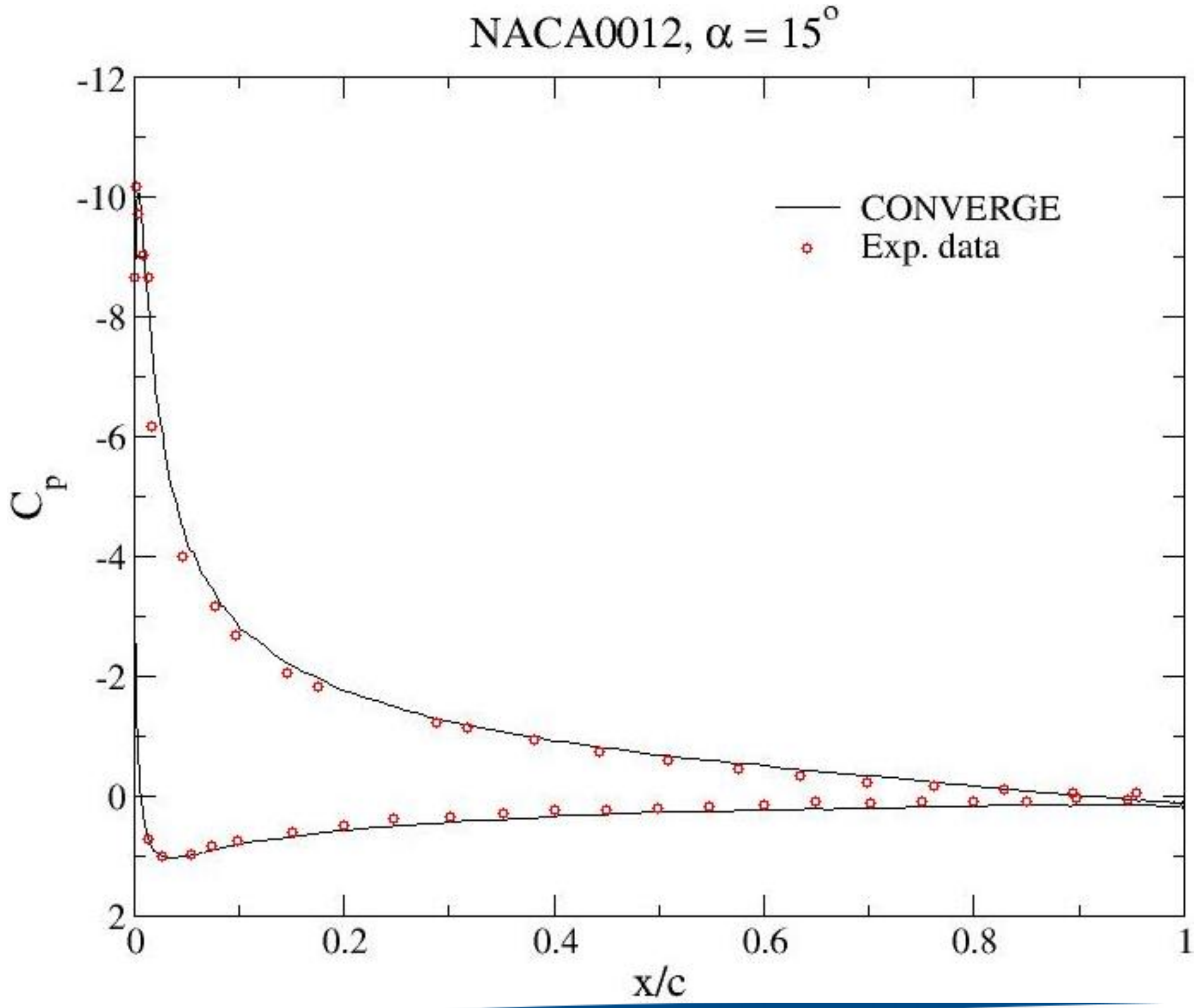
Inlaid Mesh Application—Airfoil





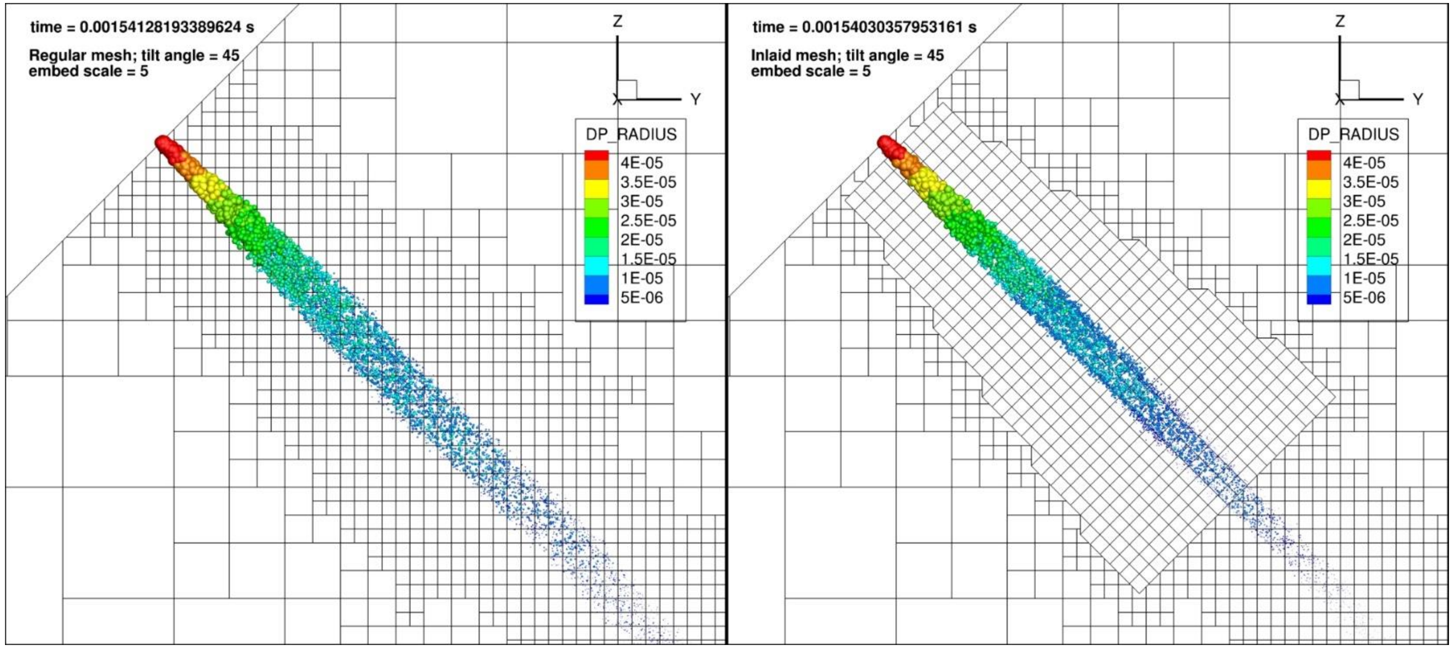
Inlaid Mesh Application—Airfoil

- Overall good match with exp. data, especially as near-wall cell spacing reduced
- Trying to use only cartesian grid for airfoil case fails



Inlaid Mesh Application—Spray

- Jet penetration can be sensitive to grid alignment on coarse meshes
- Example case: ECN Spray A, single nozzle, tilted to 45 *deg*
  - Compare results to a non-tilted Spray A case setup
  - Inlaid mesh along the spray axis minimizes the numerical differences between the 0 *deg* and 45 *deg* configurations
- Spray aligned inlaid mesh may be harmful when there is crossflow present



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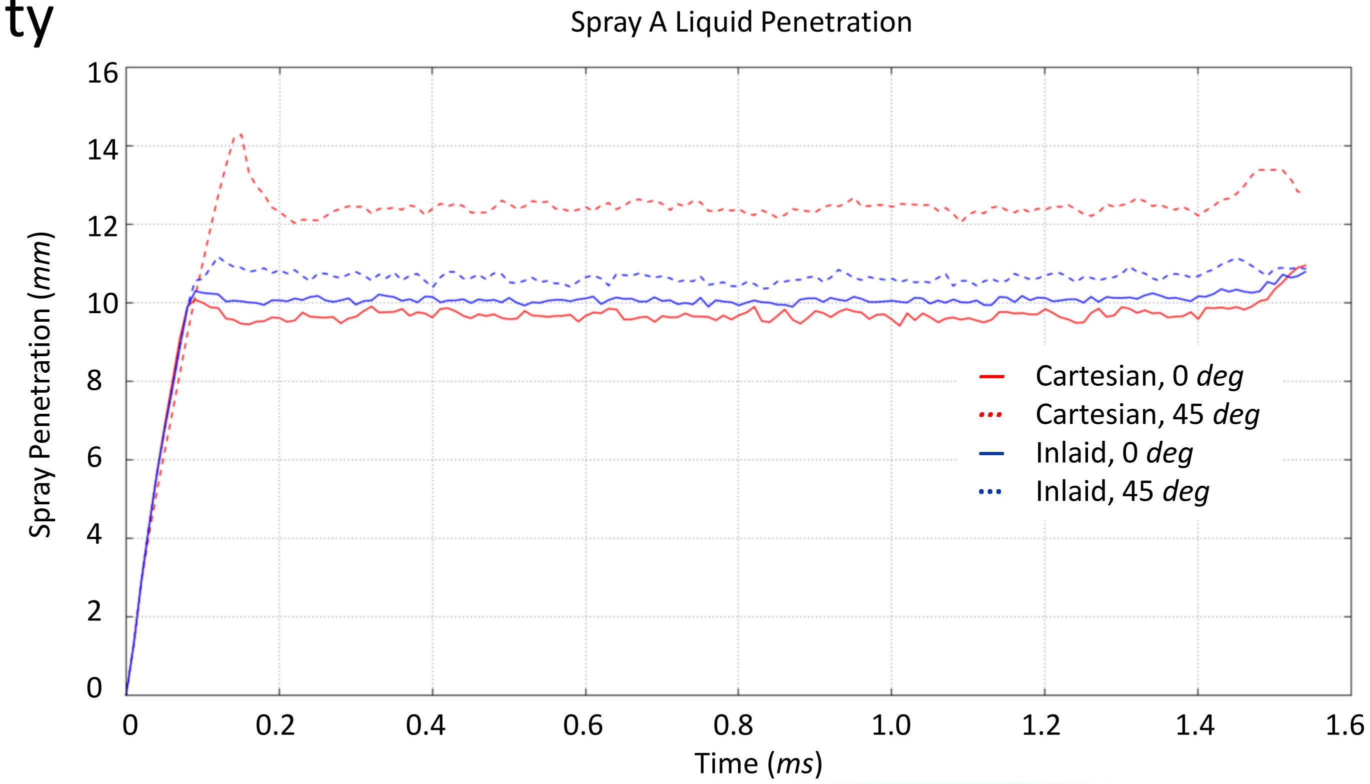
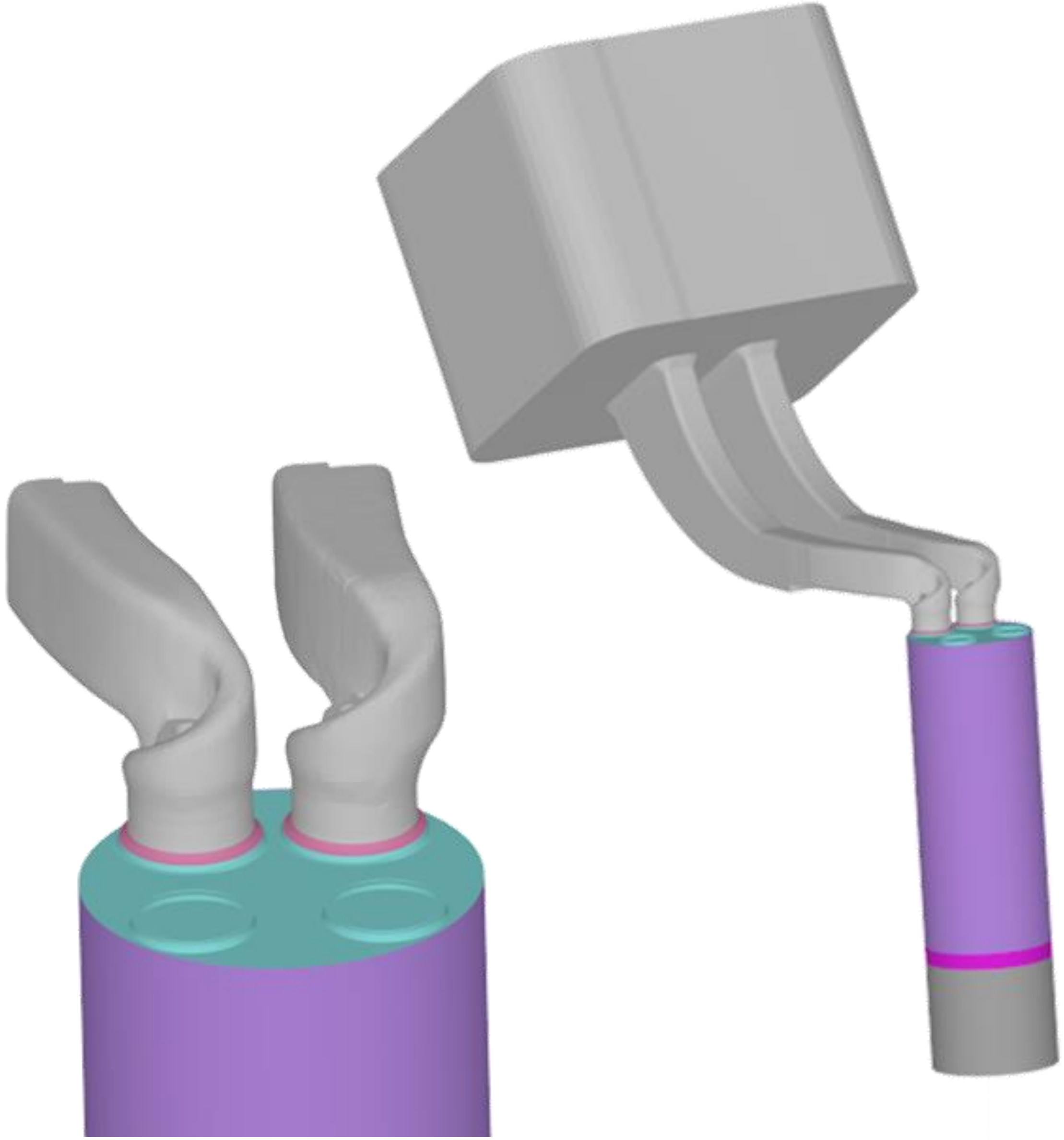
Inlaid Mesh Application—Spray

- For approximately the same cell count (about 5% fewer cells), the inlaid mesh case shows much less grid sensitivity
  - Embed scale 5
  - *dx_min* = 0.25 *mm*
  - Approximately 150,000 cells
- The Cartesian setup could reduce or eliminate this grid sensitivity, but it would require more cells



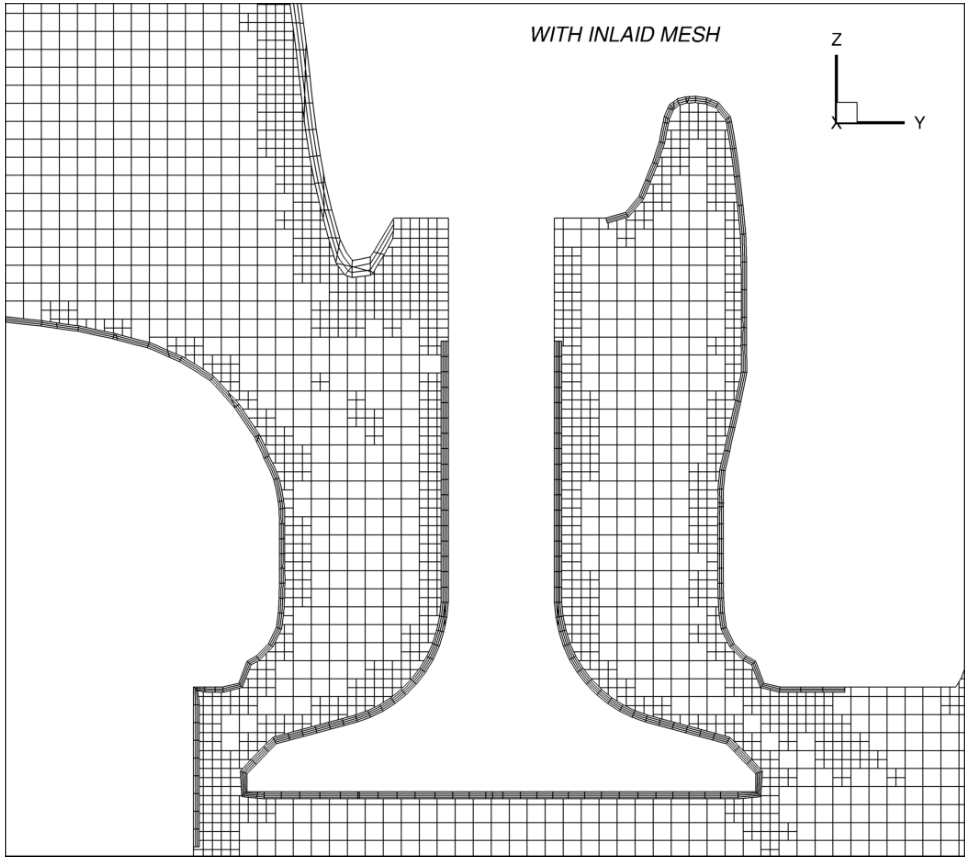
Flowbench Simulation

- Intake port flow
- 6 mm lift
- Cartesian grid:
  - 4 mm base
  - 0.5 mm AMR
  - 0.25 mm boundary embedding
  - 1M cells
- Inlaid grid
  - 5 layers of cells on valve and seat walls
  - 0.5 mm AMR
  - 0.9 M cells
- Inlaid case initialized from Cartesian case results
  - This process is not automated yet

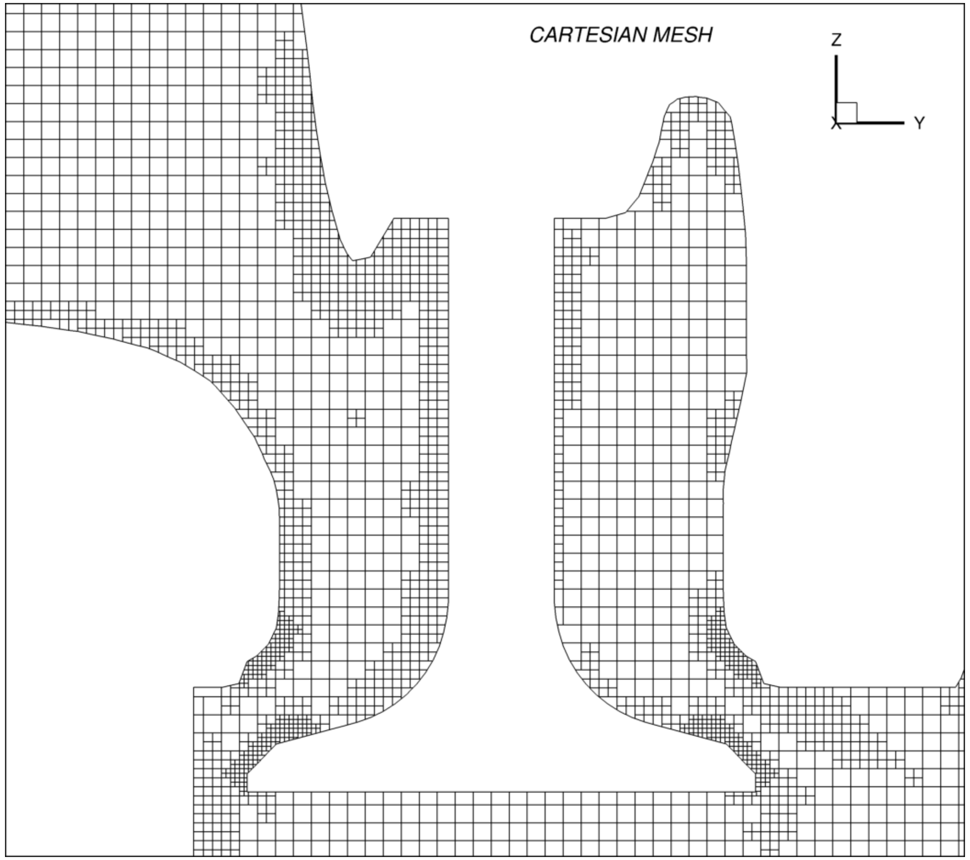


Mesh for Flowbench Simulation

Inlaid Mesh

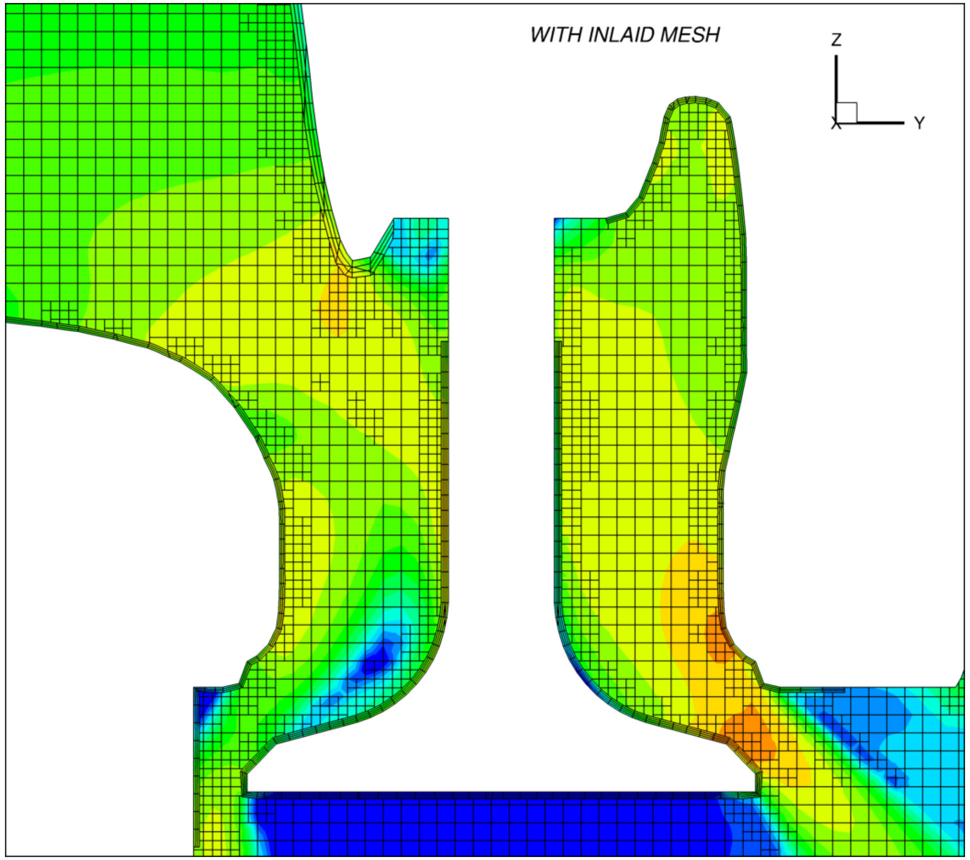


Cartesian Mesh

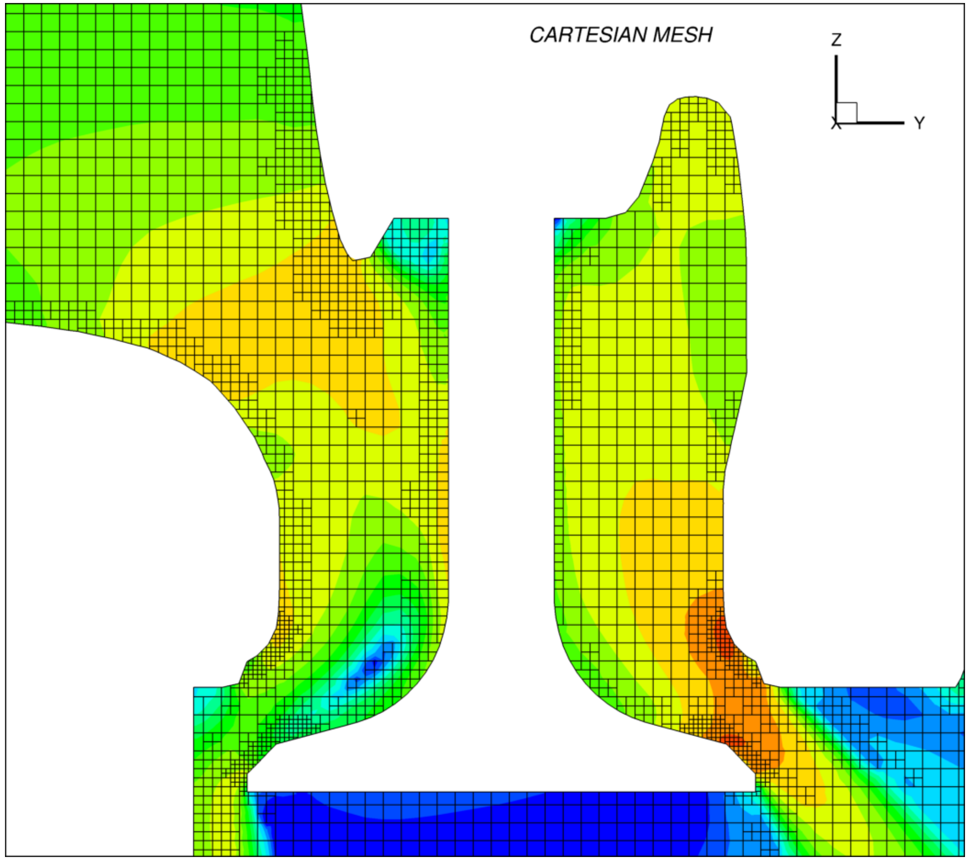


Flowbench Velocity

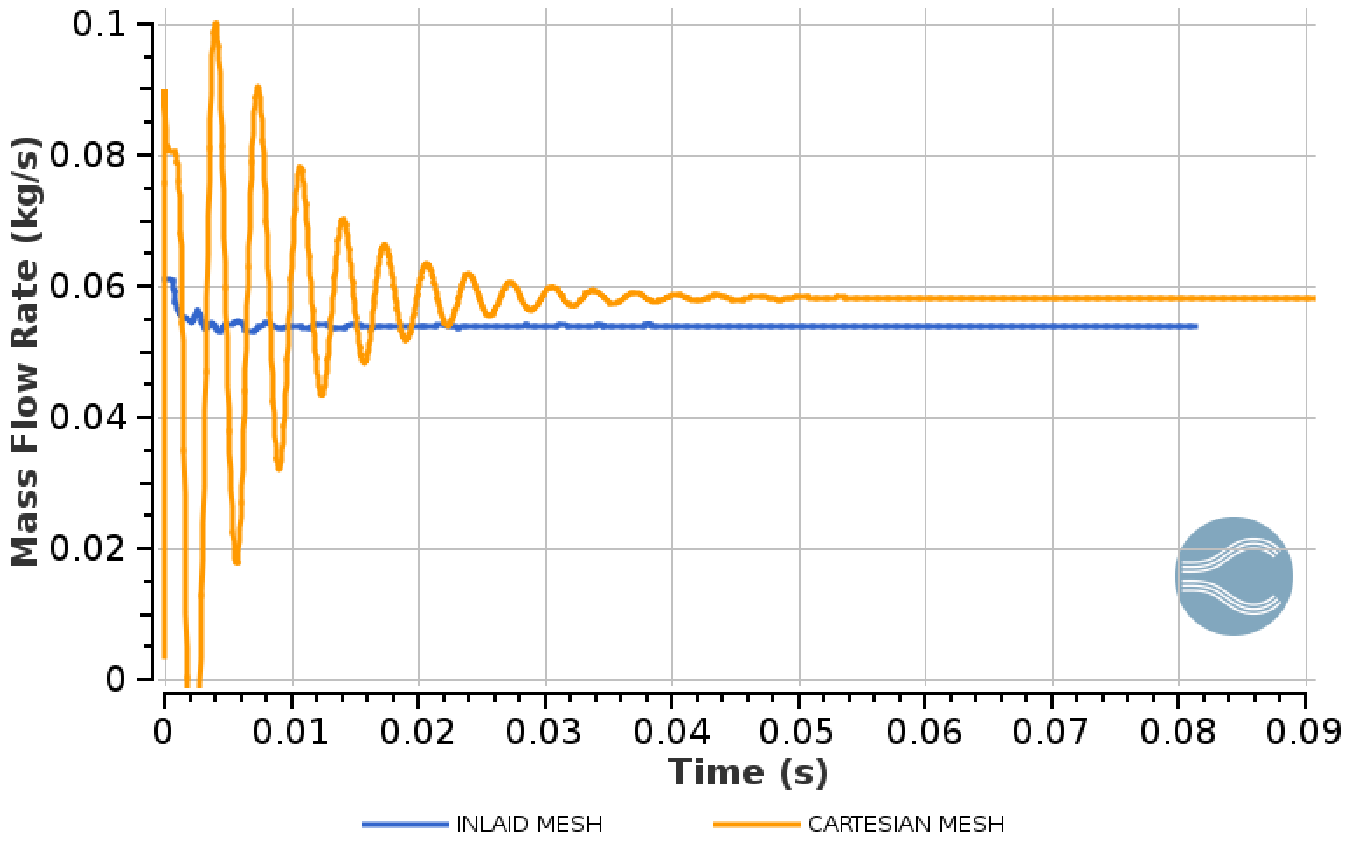
Inlaid Mesh



Cartesian Mesh



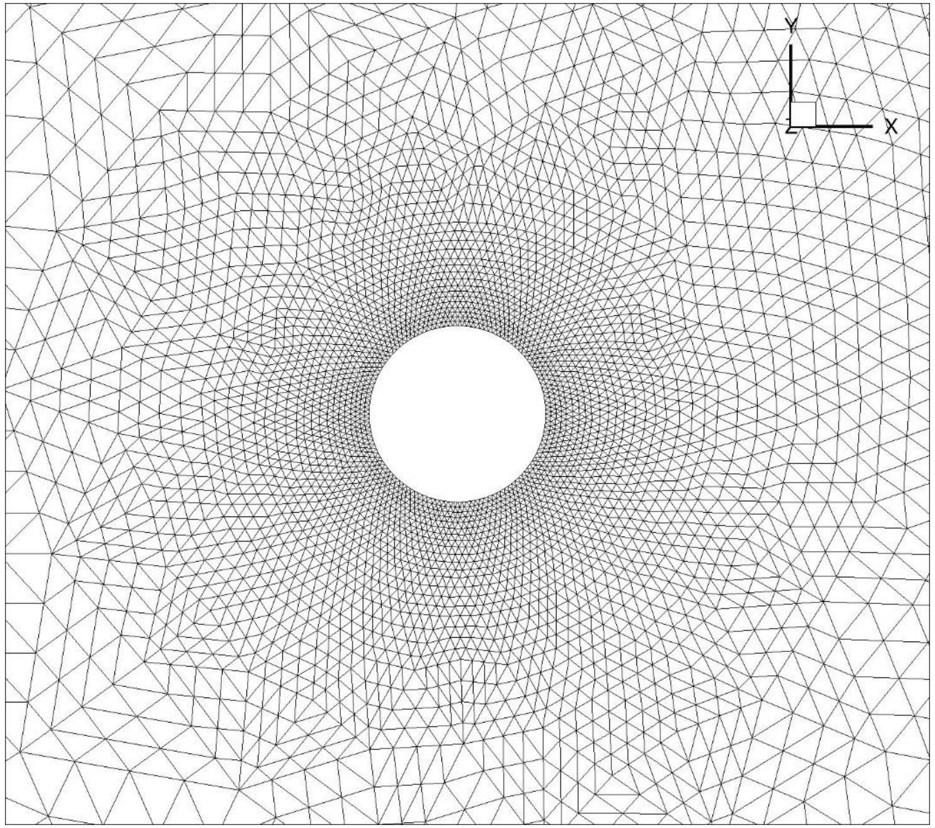
Flowbench Predicted Flowrate

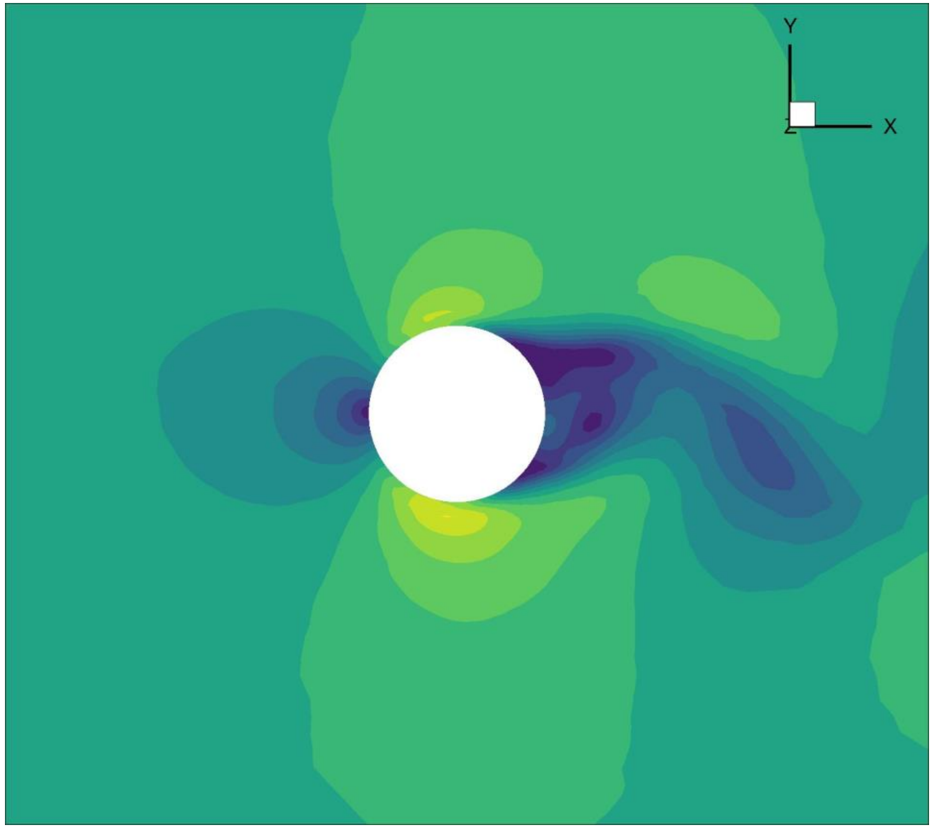


Insufficient resolution at the boundaries typically overpredicts flowrate.
As desired, the inlaid grid case reduces the predicted flowrate.

Importing A Grid as an Inlaid Grid

- CONVERGE can import and run a grid created in another software
- All grid types are supported





SIMPLE Solver

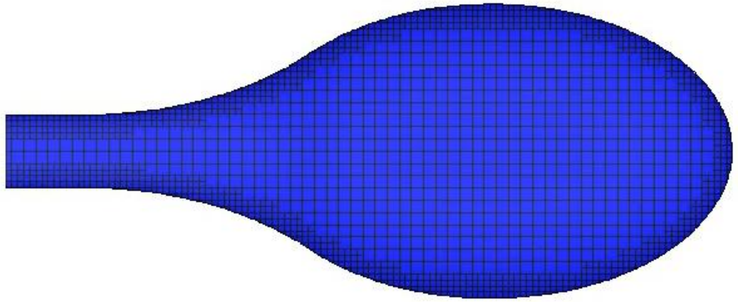
SIMPLE (modified) algorithm

- The current PISO algorithm in CONVERGE assumes that the changes in the diffusion term of momentum equation are negligible after velocity corrections in each PISO loop
- SIMPLE accounts for the above effects by re-solving momentum equation in each SIMPLE loop.
- SIMPLE is required when the local viscous effect is large, e.g. high viscosity flows, well resolved boundary layers, etc.
- SIMPLE may be more accurate when time-step is large
- The steady-state solver uses large pseudo-timesteps, so SIMPLE can be useful for speeding up steady-state simulations

Pressure-Based Solver

Pressure-Based Solver in CONVERGE

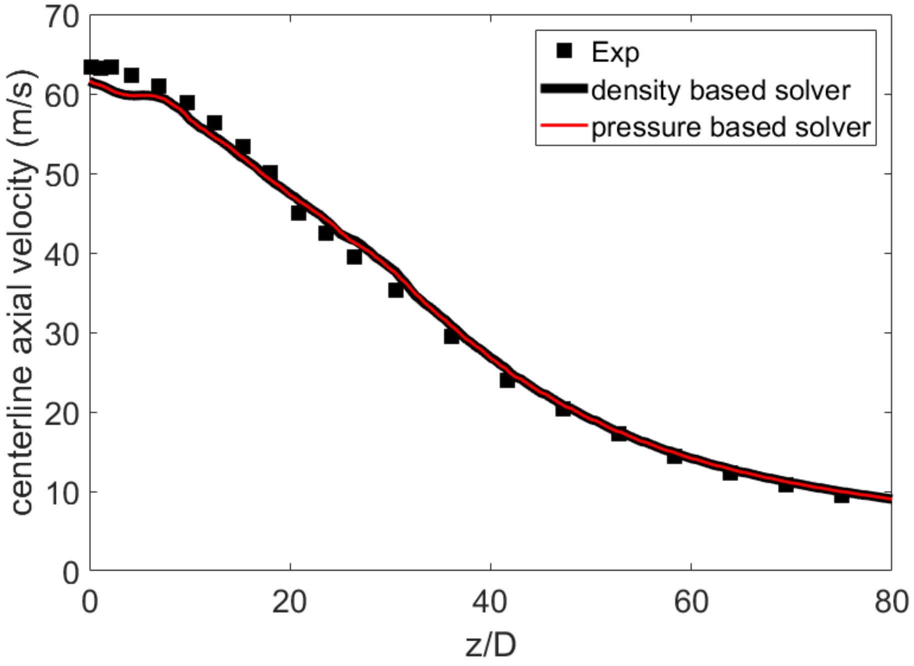
- Even though the conventional solver in CONVERGE solves a Lapacian equation for pressure, it is a density based solver
  - Pressure and density are not strictly coupled each timestep
  - Coupling is handled through a correction term in the pressure equation which keeps density and pressure loosely linked
  - By being density-based, conventional solver conserves density and species
- A modification to transport solver in CONVERGE allows for a new pressure-based solver
  - Density is derived from pressure through the equation of state
  - Can result in faster runtimes for low Mach number cases where perfect conservation is not necessary

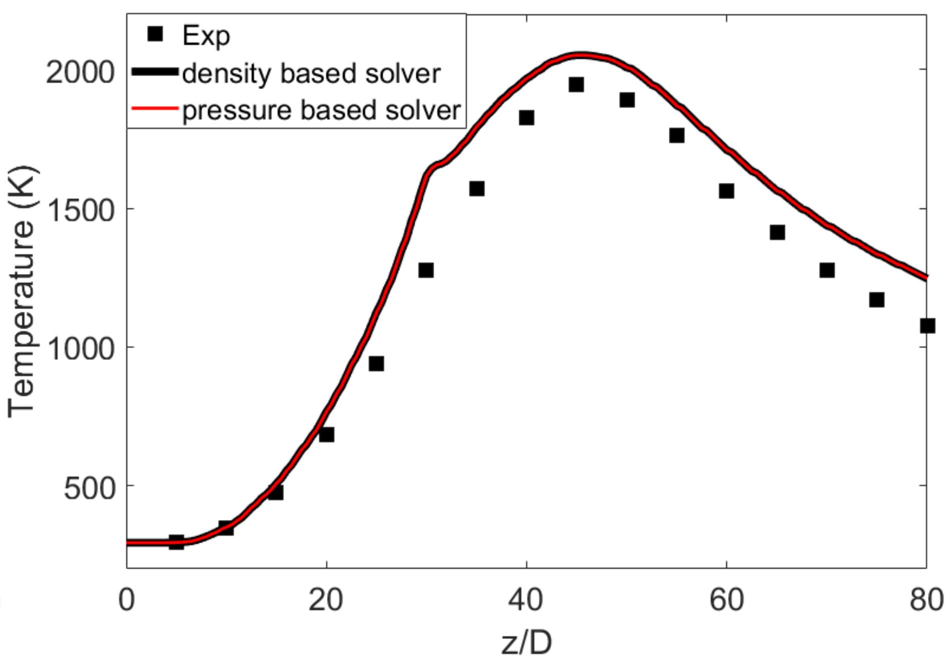


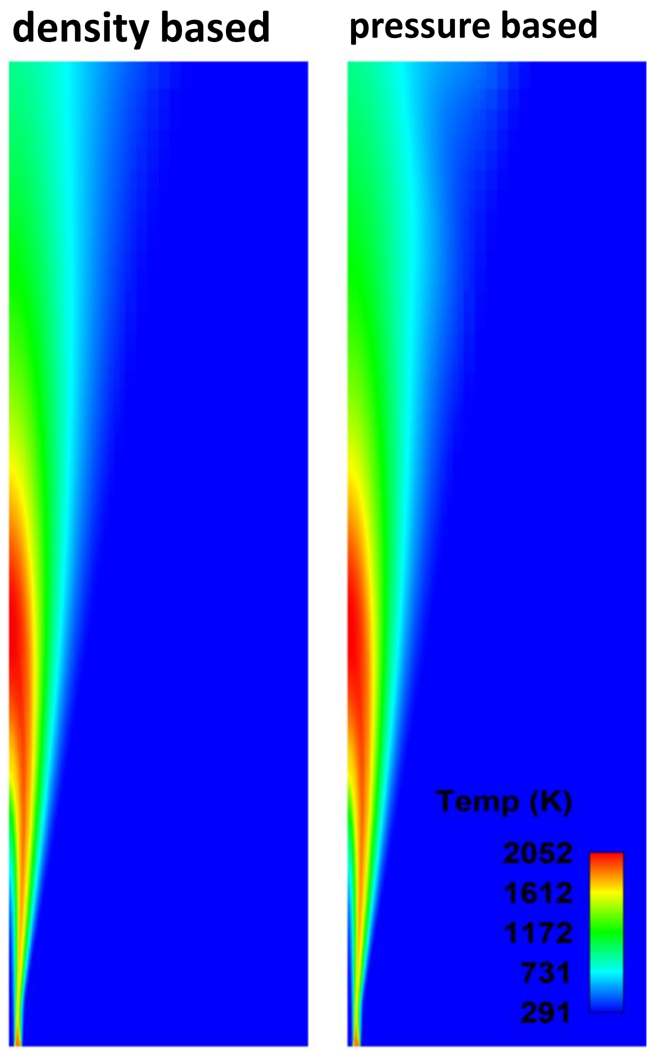
Flame D Steady State Solver Comparison

RANS Sandia Flame D case (CFL=36) running on 24 core:

steady state solver	density based	pressure based
wall clock time (sec)	5422	3052



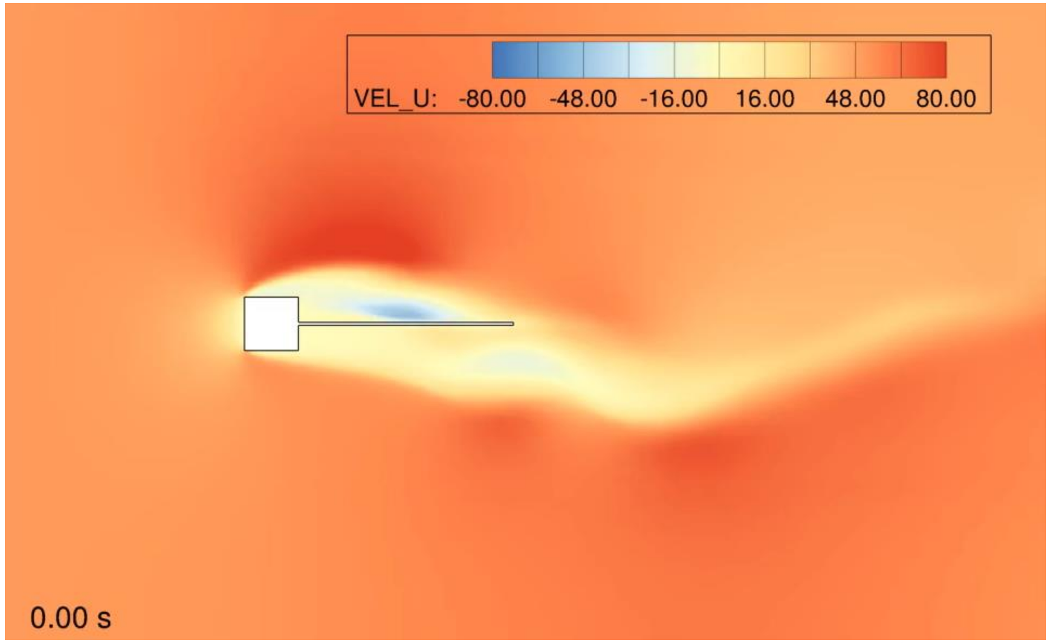




UDFs

User-Defined Functions

- CONVERGE 3.0 features an application programming interface (API) to serve as a layer between CONVERGE and your UDFs
  - UDFs are not copied snippets of CONVERGE source code
  - UDFs access to the main solver is more flexible, but more explicit
    - UDFs do not have access to a set of global variables
    - You instruct the UDF and CONVERGE what information will be passed from one to the other
  - UDFs do not need to be recompiled for each minor release



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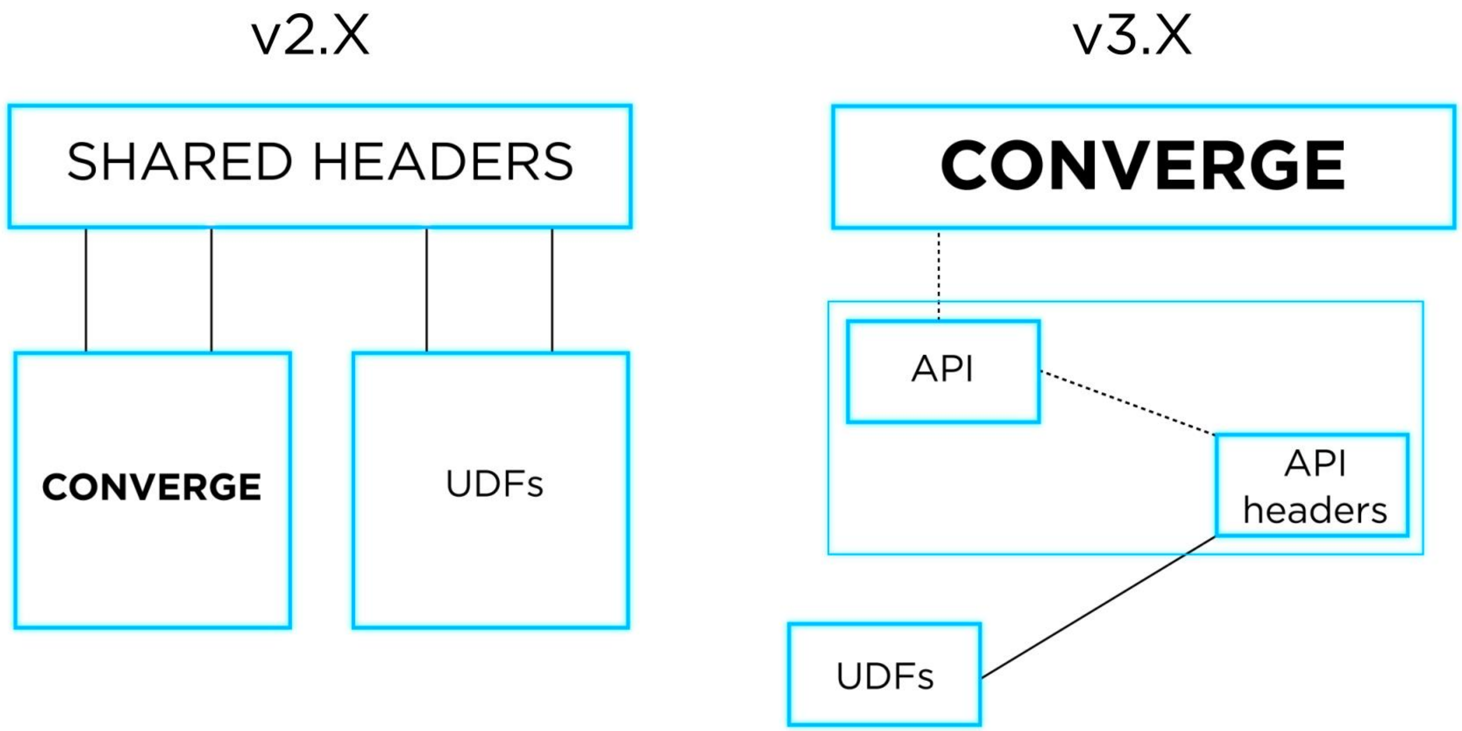
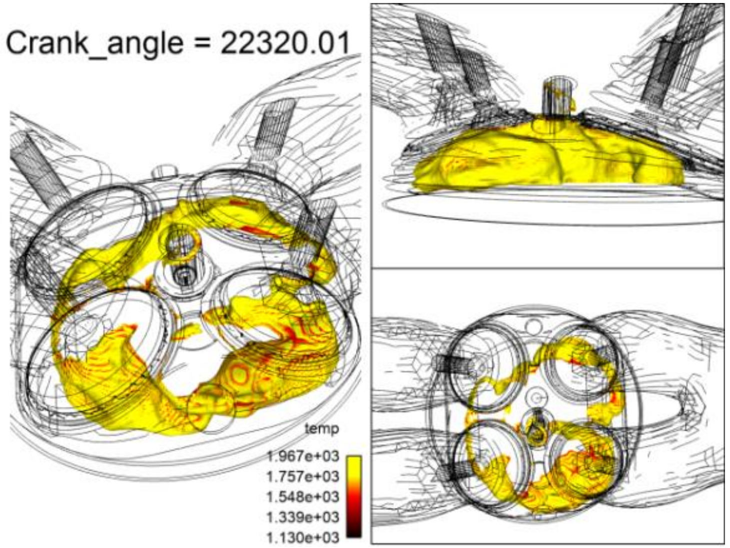
User-Defined Functions



Combustion Improvements

Combustion Enhancements in v3.0

- SAGE speed improvements
- Added speed and stability to 0D and 1D chemistry tools
- New combustion models
  - LES models
    - TFM-LES with flamefront AMR
    - ECFM-LES
  - Species-based FGM
  - SAGE PDF (RANS)



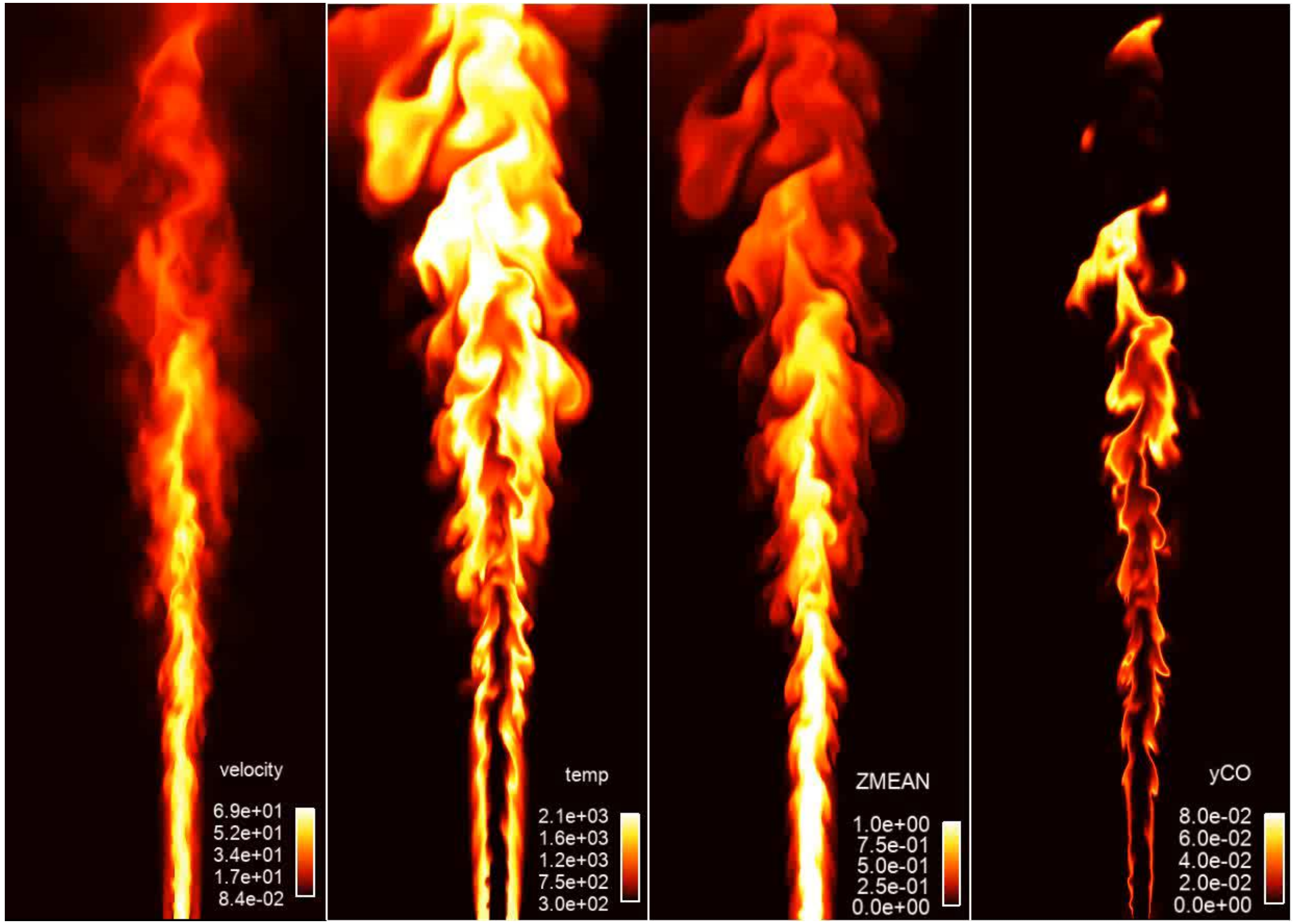
$$\frac{\partial \rho Y_i^k}{\partial t} + \frac{\partial \rho u_j Y_i^k}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\rho(D_t + D)\frac{\partial Y_i^k}{\partial x_j}\right) + \omega_i^k, (k = 1, 2, 3)$$

$$\frac{\partial \rho Y_i}{\partial t} + \frac{\partial \rho u_j Y_i}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\rho(D_t + D)\frac{\partial Y_i}{\partial x_j}\right) + P_1\omega_i^1 + P_2\omega_i^2 + P_3\omega_i^3$$

Considering species or energy variations.

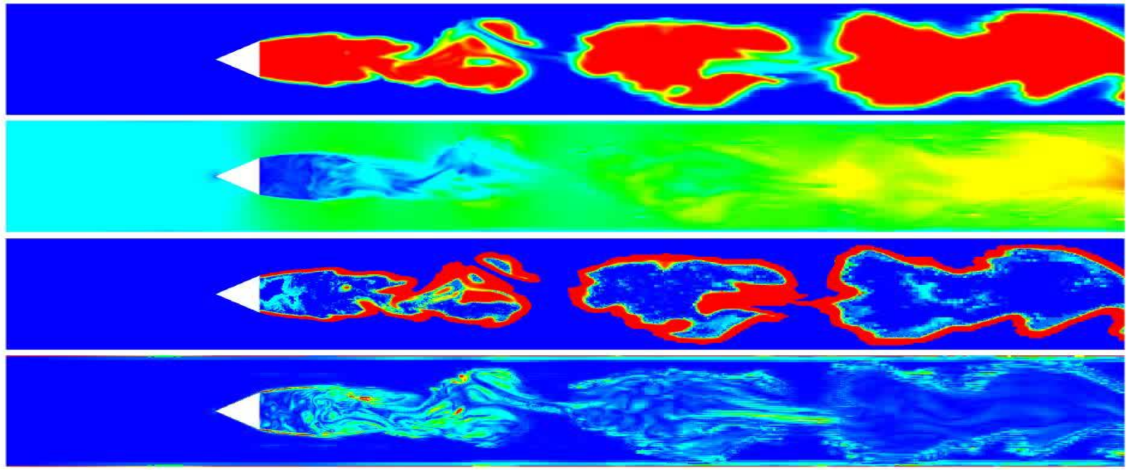
SAGE Speed-up

- Optimized rate calculations
  - Moderate speedups achieved for smaller mechanisms
  - Constant overhead
  - Depends linearly on size of mechanism
- Sparse matrix Jacobian assembly
  - Benefit for large mechanisms
- Customized preconditioner
  - Significantly faster than SuperLU option

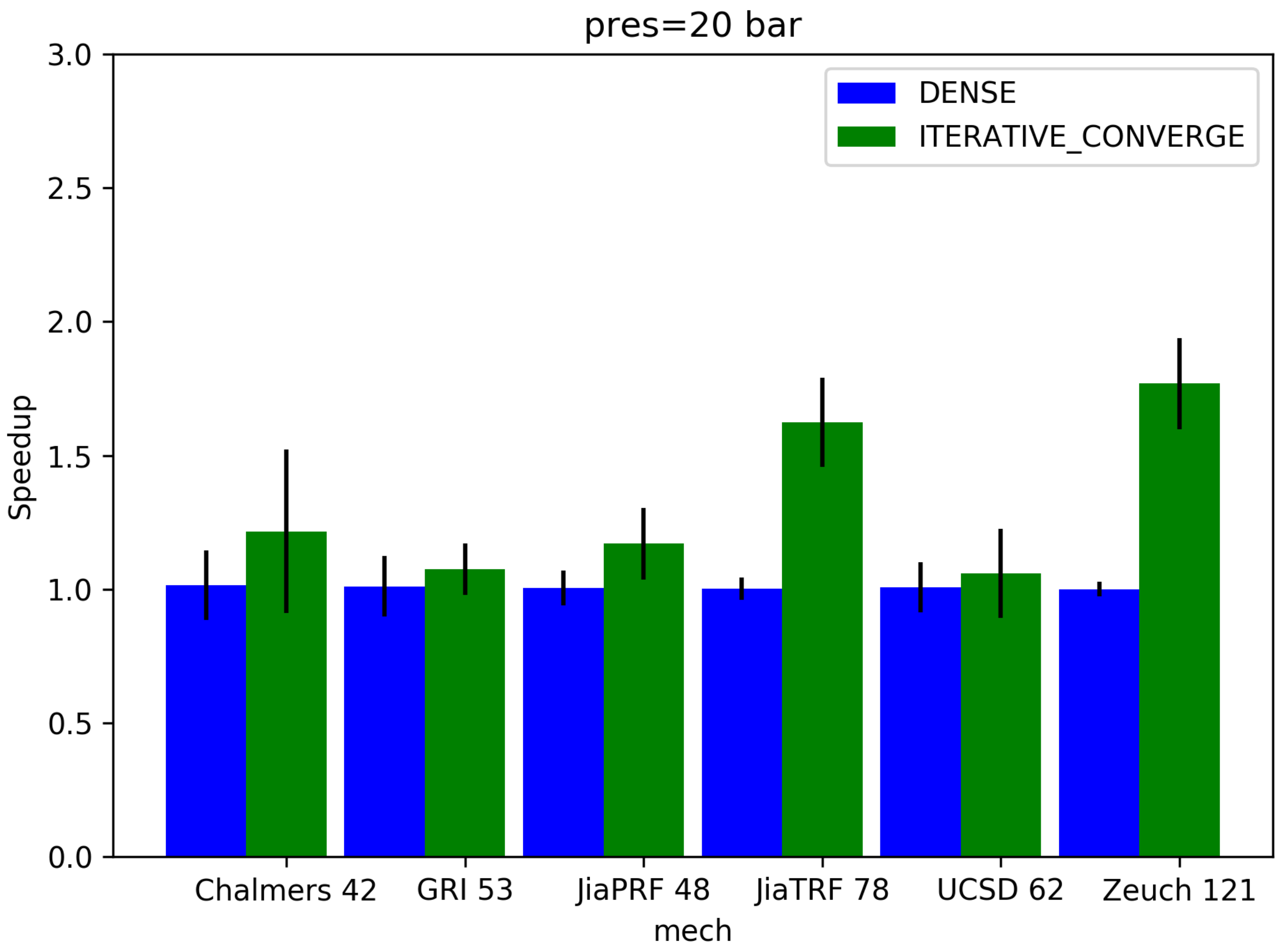


SAGE vs. Improved SAGE Comparisons

- Single cell cases
  - 20 bar pressure
  - 9 different conditions and each condition is repeated 3 times
  - solve_temp = 0
  - rel tol: 1.e-4 and abs_tol: 1.e-14



Small mechanisms (<150 species)



Chalmers (chlmr)	[42 species, 168 reactions]
GRI	[53 species, 325 reactions]
Jia PRF	[48 species, 153 reactions]
Jia TRF	[78 species, 217 reactions]
UCSD mechanism	[62 species, 316 reactions]
Zeuch mechanism	[121 species, 593 reactions]

DENSE solver is best option for small mechanisms in v2.4/v3.0

ITERATIVE_CONVERGE is part of improved sage

Speedup comes primarily because of optimized rate calculations

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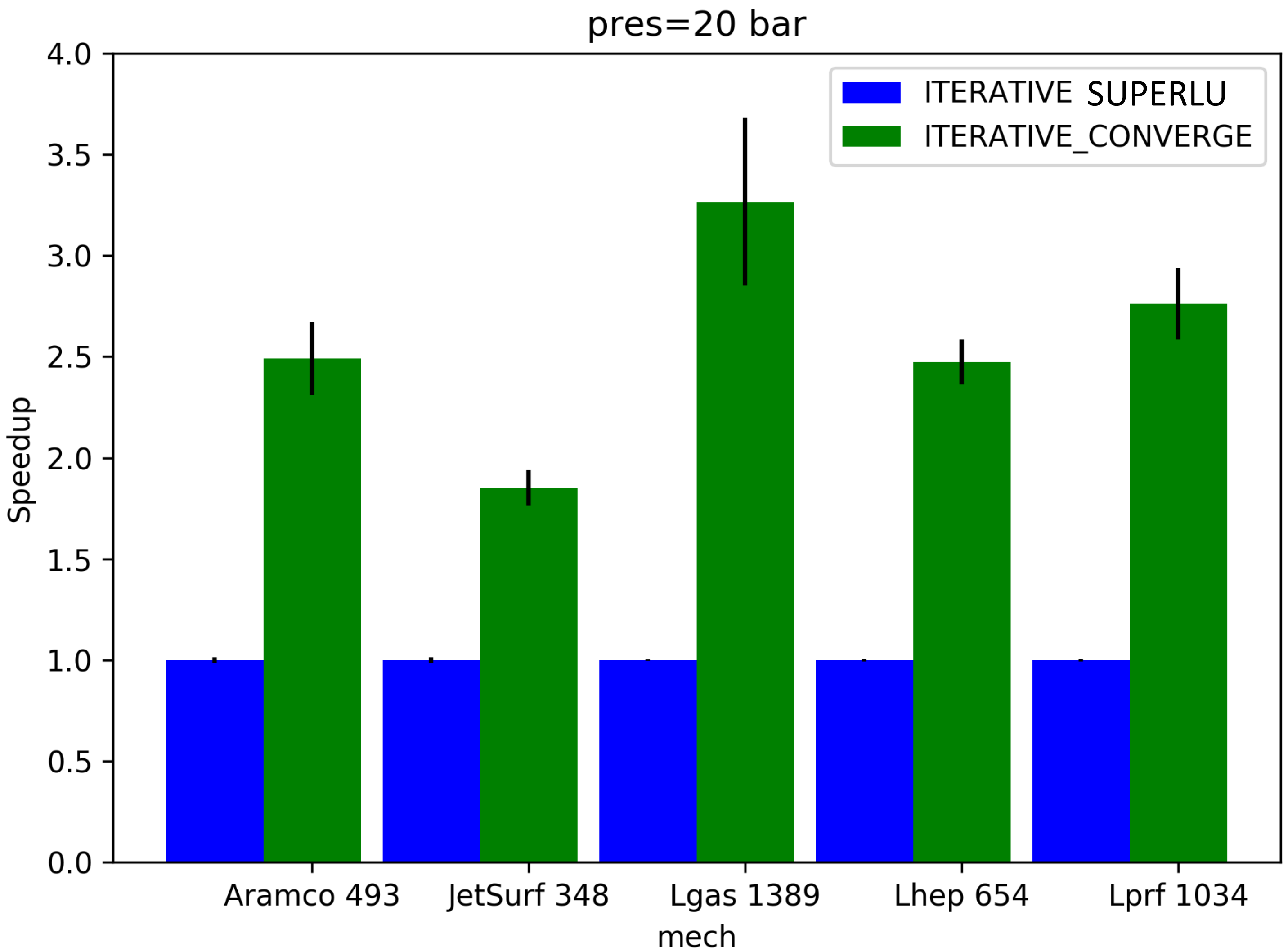
Larger Mechanisms (>150 species)



Aramco (armc)	[492 species, 2716 reactions]
Jet Surf	[348 species, 2168 reactions]
LLNL gasoline (Lgas)	[1389 species, 5935 reactions]
LLNL n-heptane	[654 species, 2827 reactions]
LLNL PRF (Lprf)	[1034 species, 4236 reactions]

ITERATIVE_SUPERLU was the best available fast option in v2.4/v3.0 for large mechanisms

ITERATIVE_CONVERGE is part of improved sage

Speedup comes primarily due to improved preconditioner

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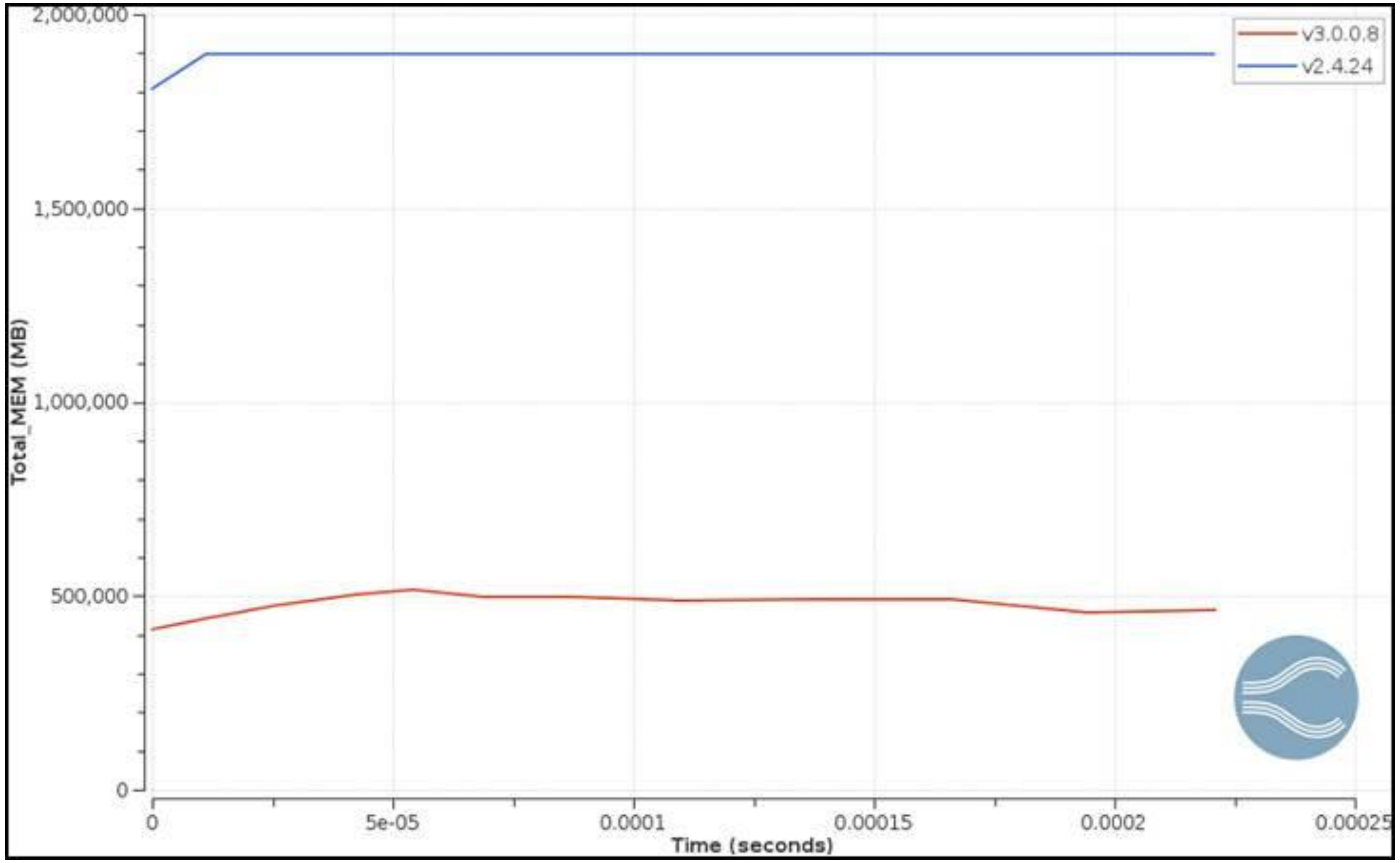
Memory Reduction

Sample Memory Reduction

- Simple spray and combustion in a box
  - Removes any improvement from surface storage
- 50 million cells
- 264 cores



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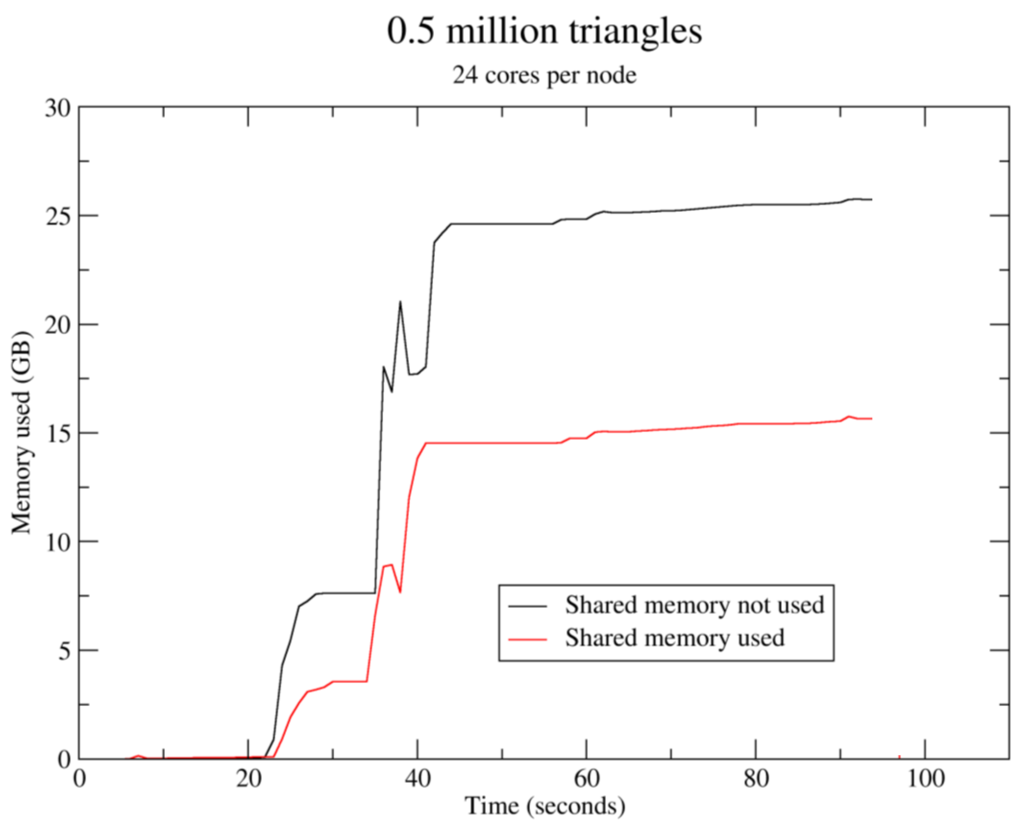
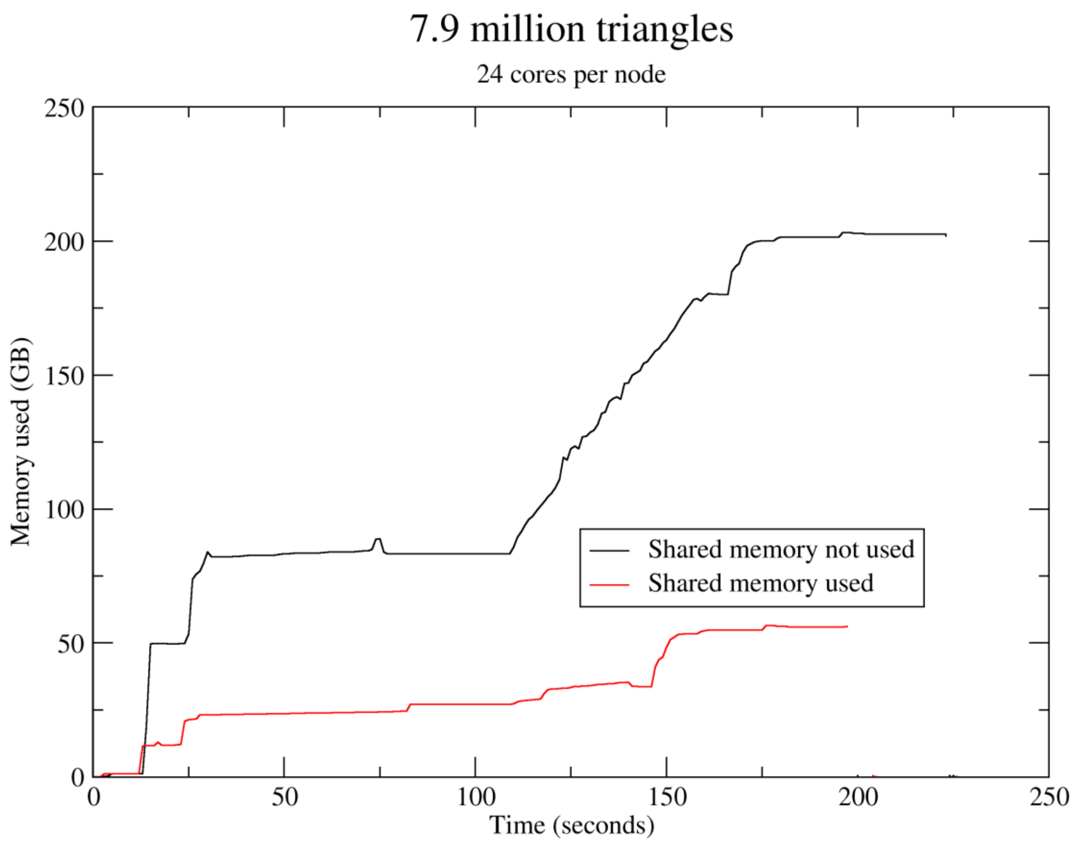
Reduced Surface Memory Footprint

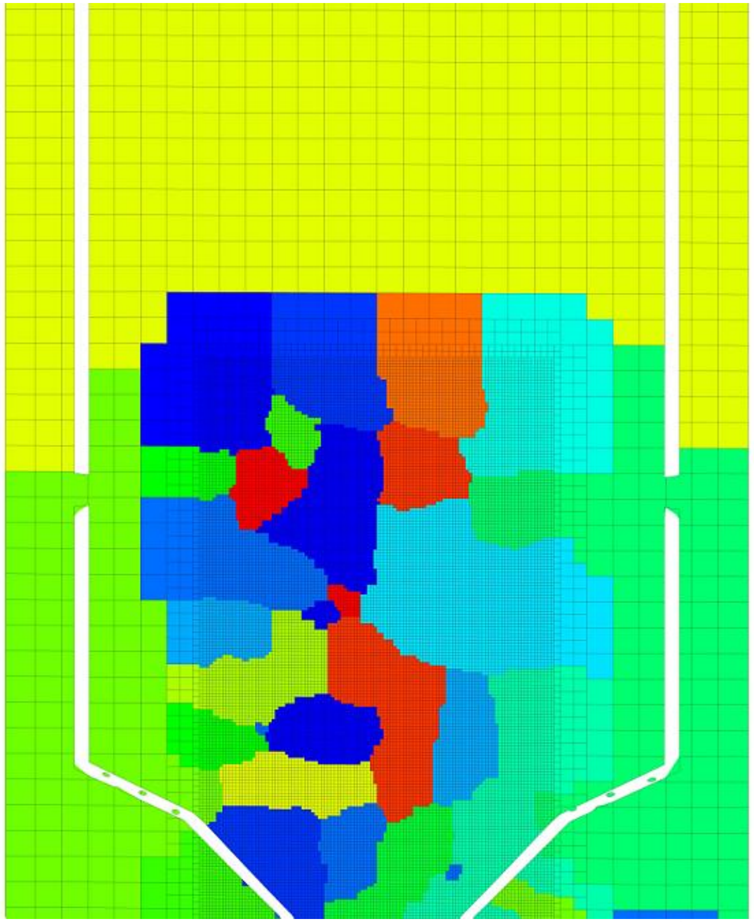




Scaling

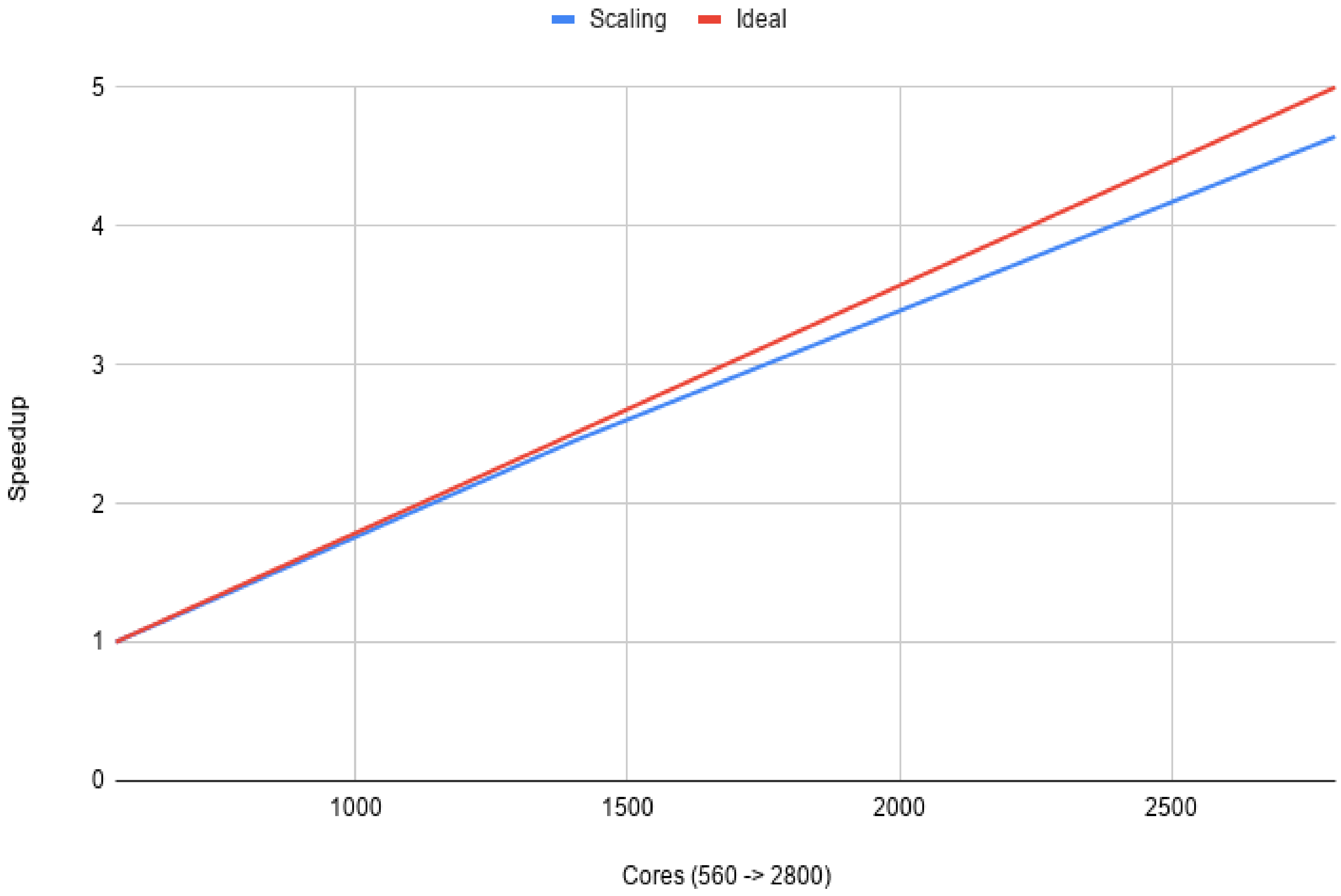
Cell Based Load Balance

- In CONVERGE 2.x, domain partitioning is done on blocks coarser than the solution grid
  - This can cause poor distribution of workload in cases with high embed scales
- Starting with CONVERGE 3.0 the solution grid is partitioned directly
  - This allows us to get a good load balance for all solution meshes, even with lots of embedding and/or AMR
- No parallel map is stored on each processor
  - No fixed memory cost
- Automatic detection of need for load balance
  - No user parameters need to be specified for load balance



Flame D Scaling

- 48 million cells
- Nodes were 28 core Haswell (2 processors per node)
- Infiniband interconnect
- 17K cells per core at 2800 cores



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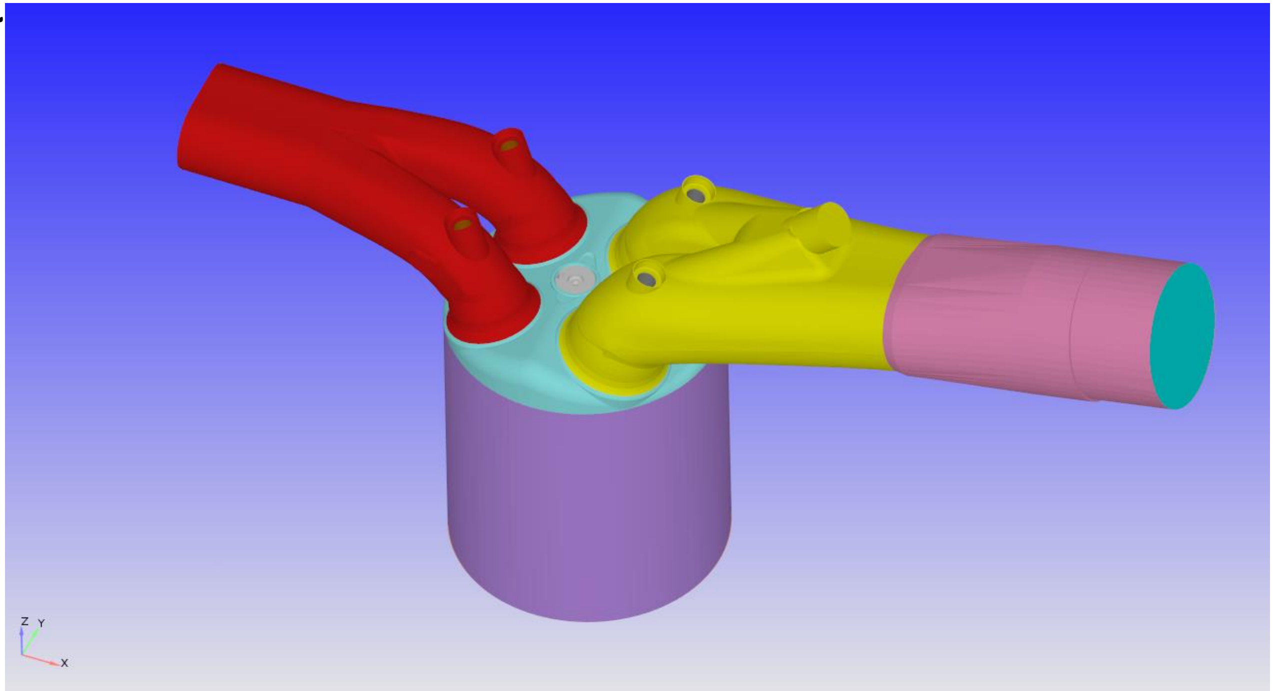
SI8 PFI Sage Scaling Study

- Standard example case run without modification
  - spray, combustion, AMR, and moving geometry are all part of the simulation
  - restart files written every 5CA
  - post files written as normal
  - max cell count is 1.3M, minimum is 230K
- Run on our internal cluster
  - 28 core 3.1 GHz Intel Skylake
  - single processor nodes
  - 100GB Infiniband interconnect
  - local attached SSD storage



V3.0 SI8 Scaling

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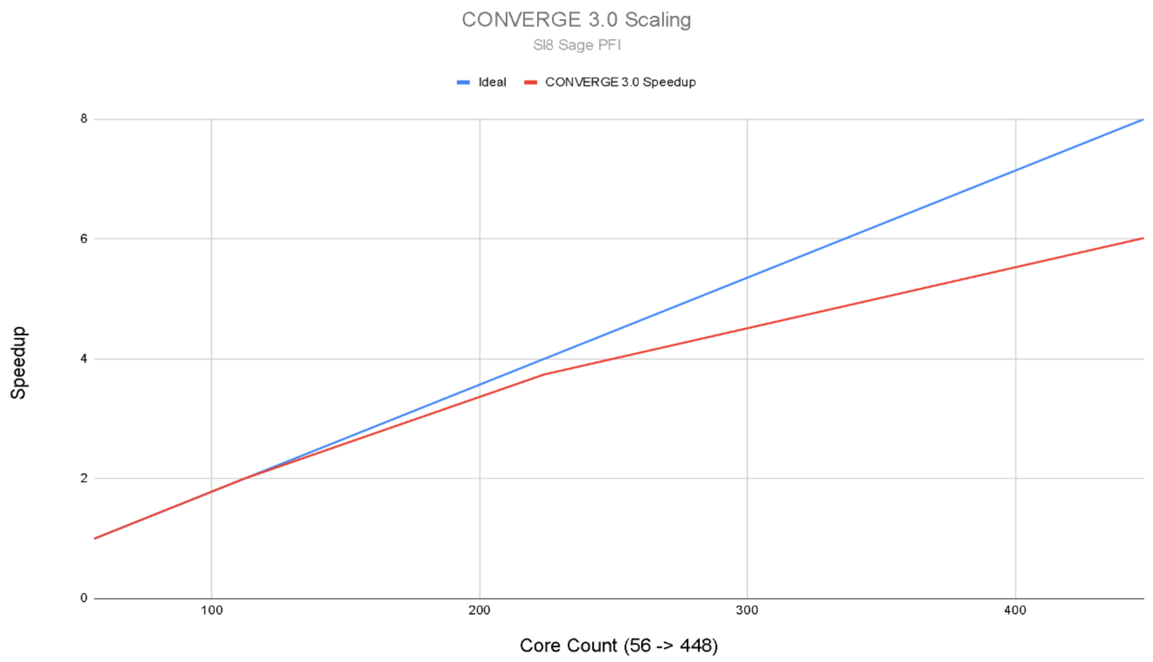
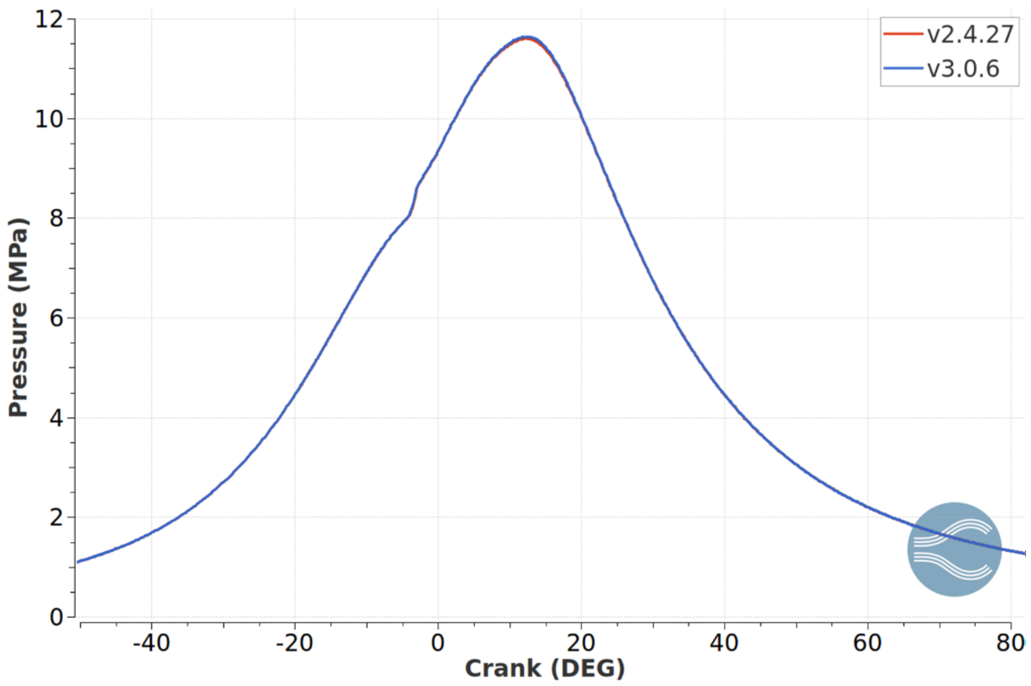


Cores	Time(h)	Speedup	Efficiency	Cells/core	Engine Cycles/day
56	11.51	1	100%	12,500	2.1
112	5.75	2.00	100%	6,200	4.2
224	3.08	3.74	93%	3,100	7.8
448	1.91	6.67	75%	1,600	12.5

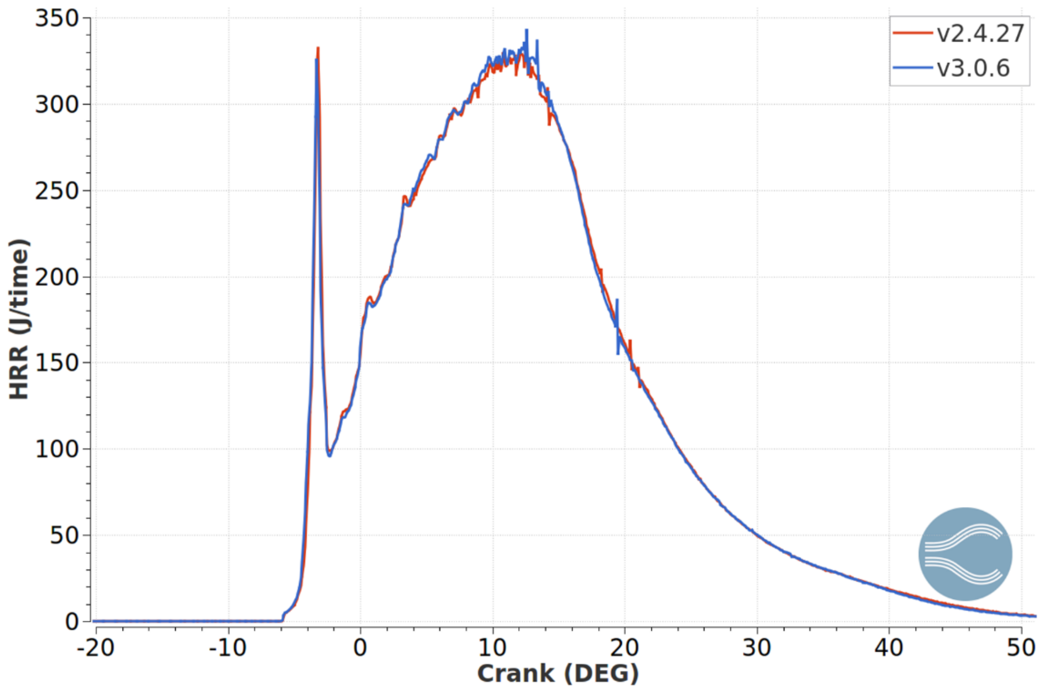
Engine Results Comparison (2.4 vs. 3.0)

Cat 3400 Comparison

Pressure



Heat Release



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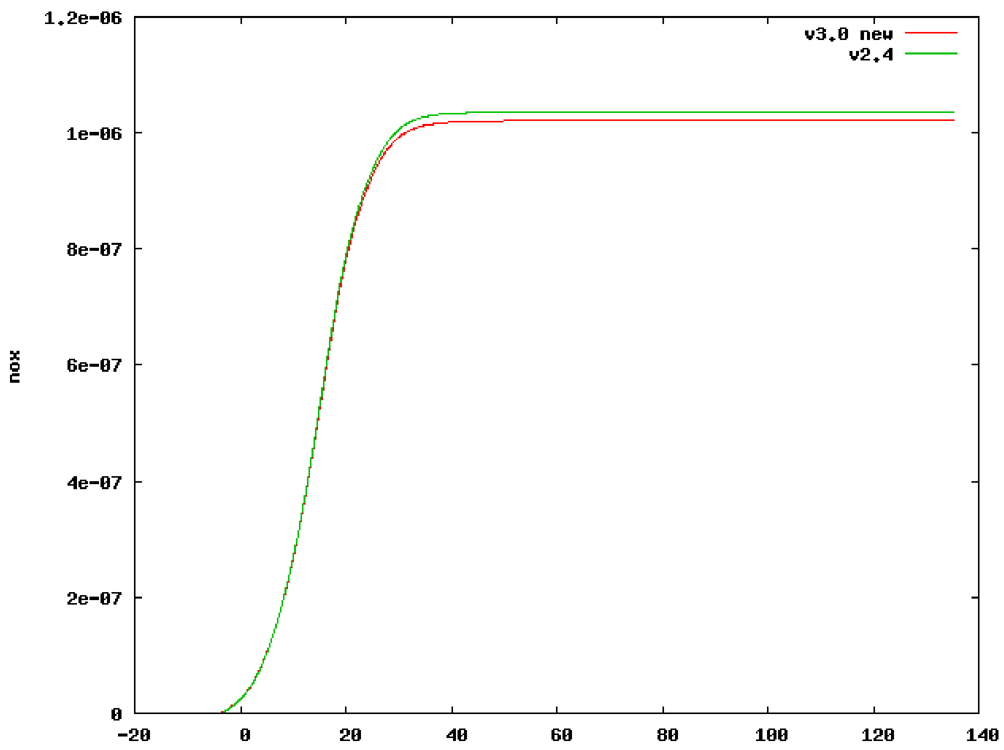
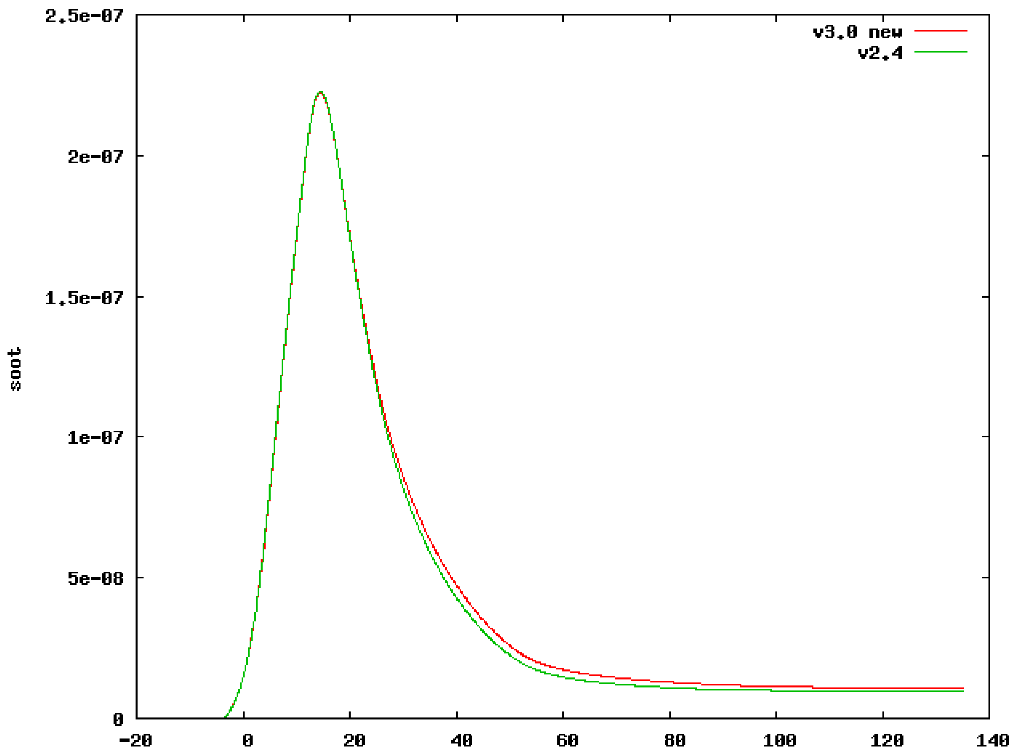
Cat 3400 Comparison

NOx

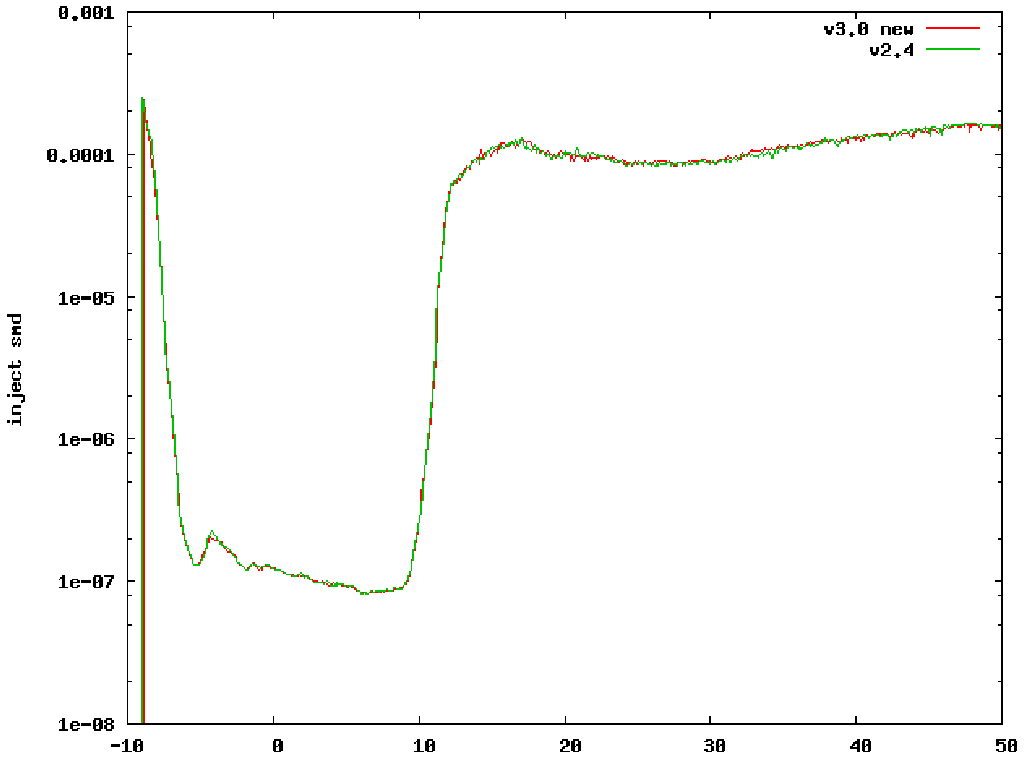


Soot

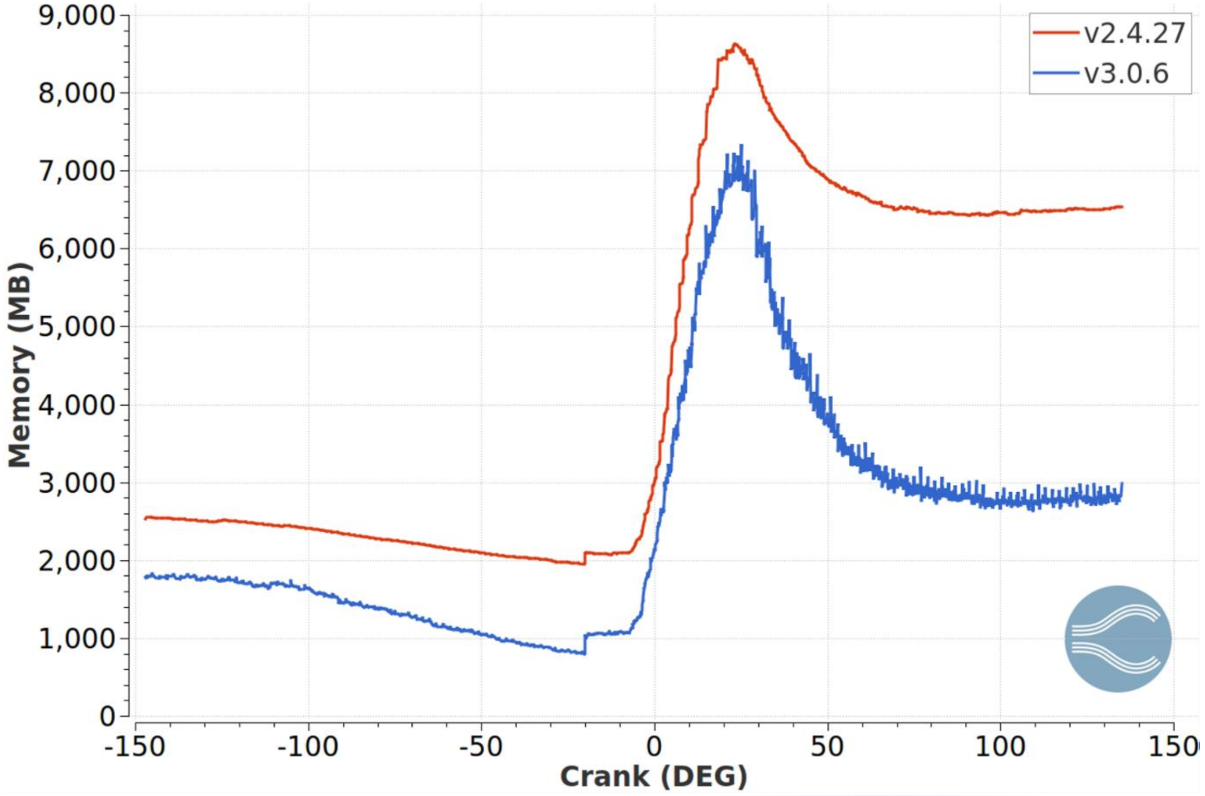


Cat 3400 Comparison

SMD



Memory



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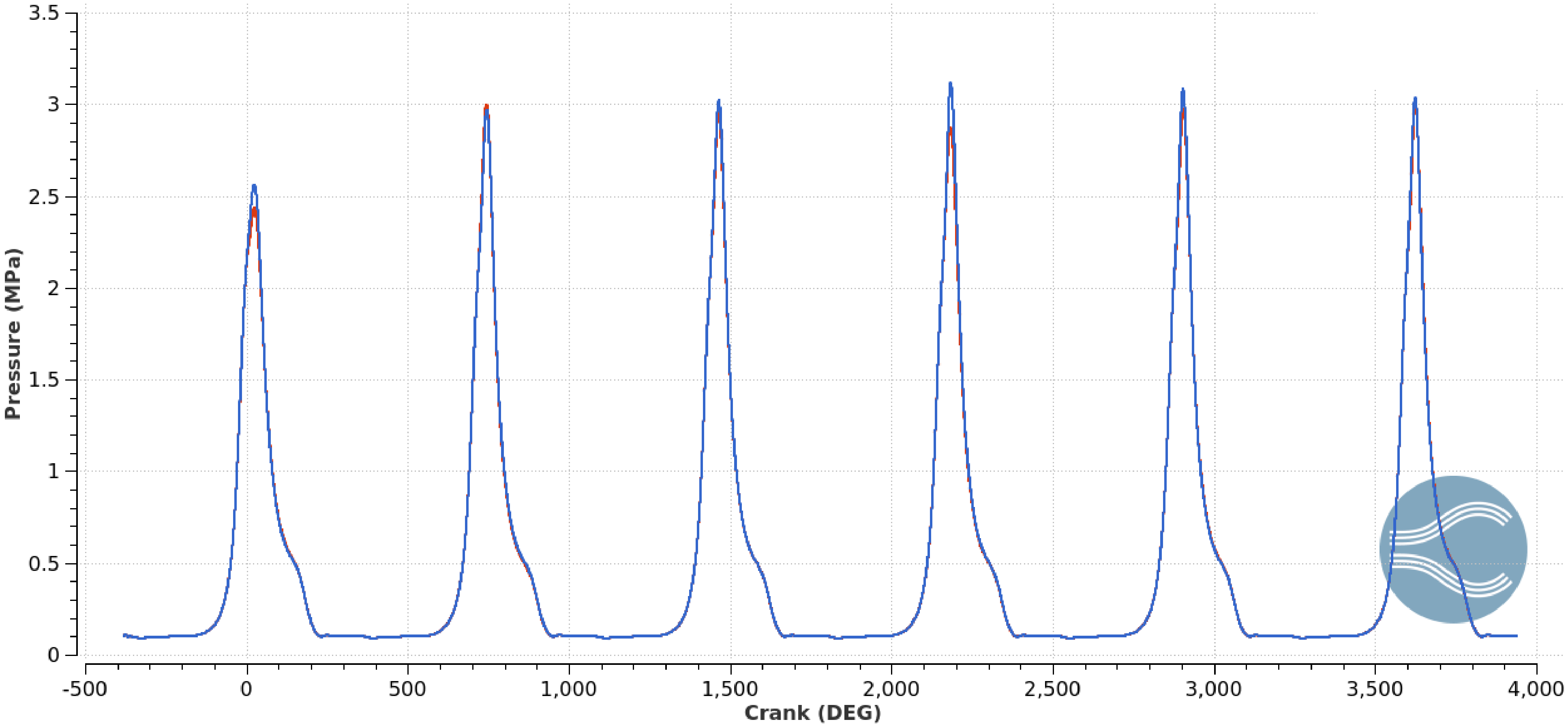
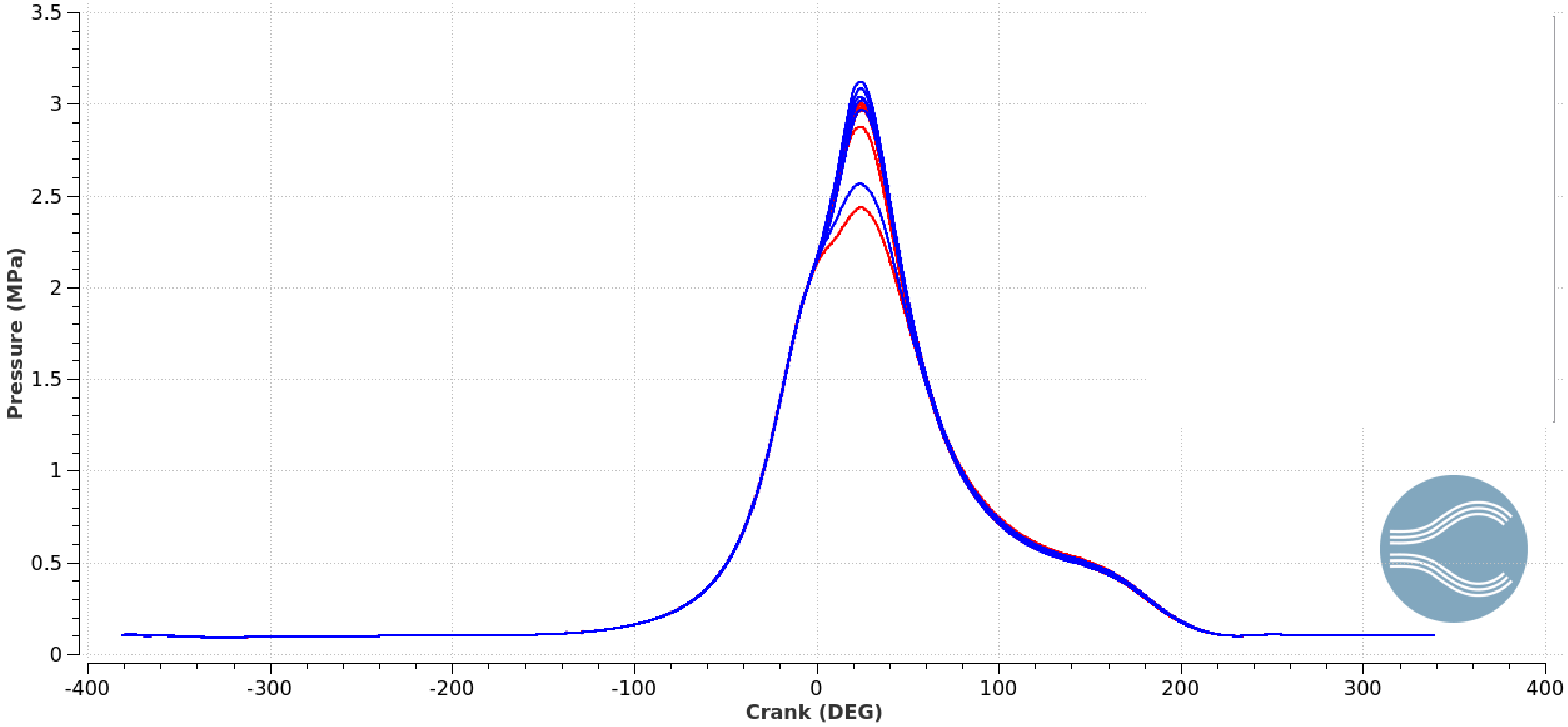
Tumble GDI Pressure Comparison



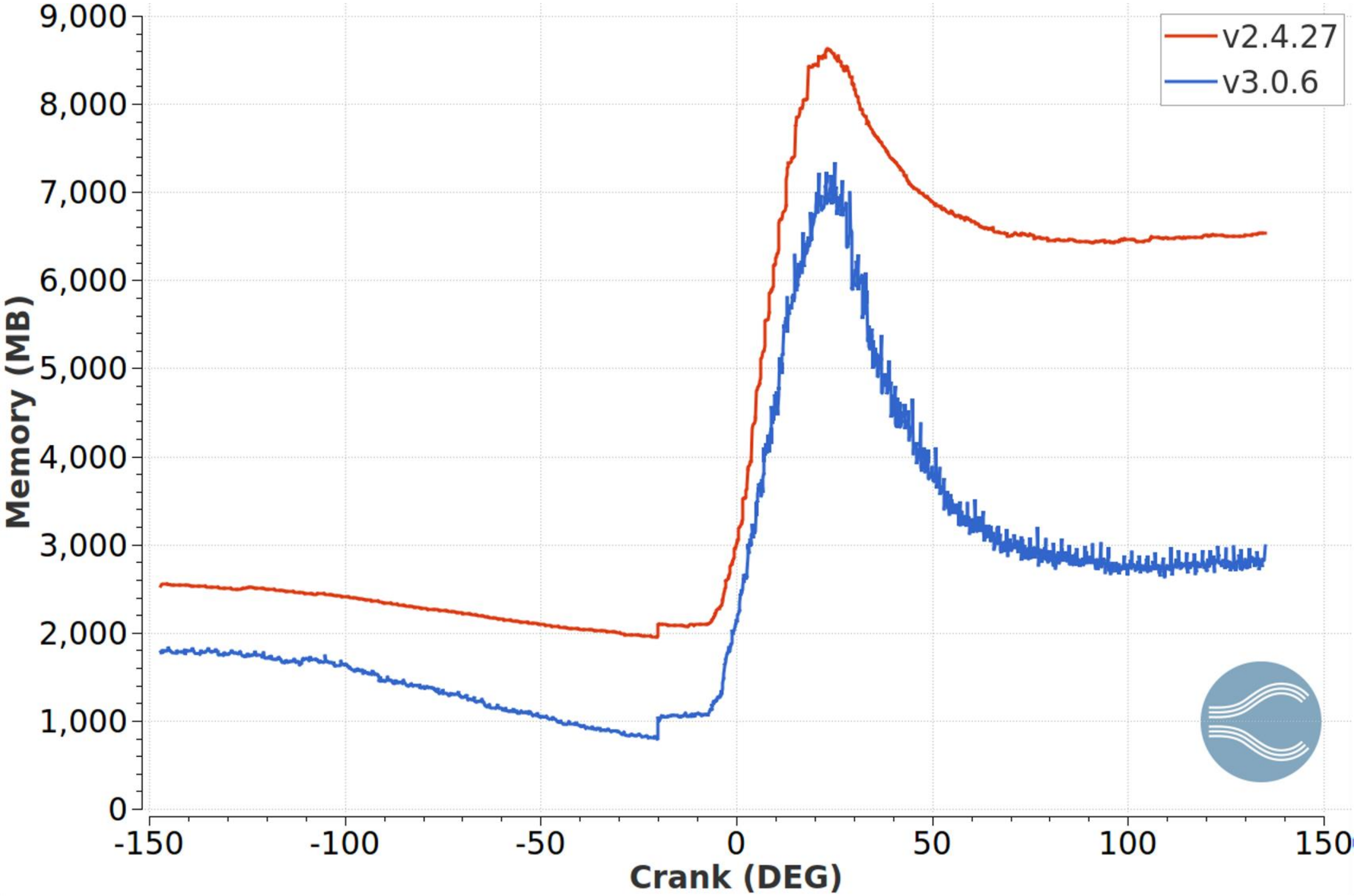
Red = 2.4.26 Blue = 3.0.6

Tumble GDI Pressure Comparison



Red = 2.4.26 Blue = 3.0.6

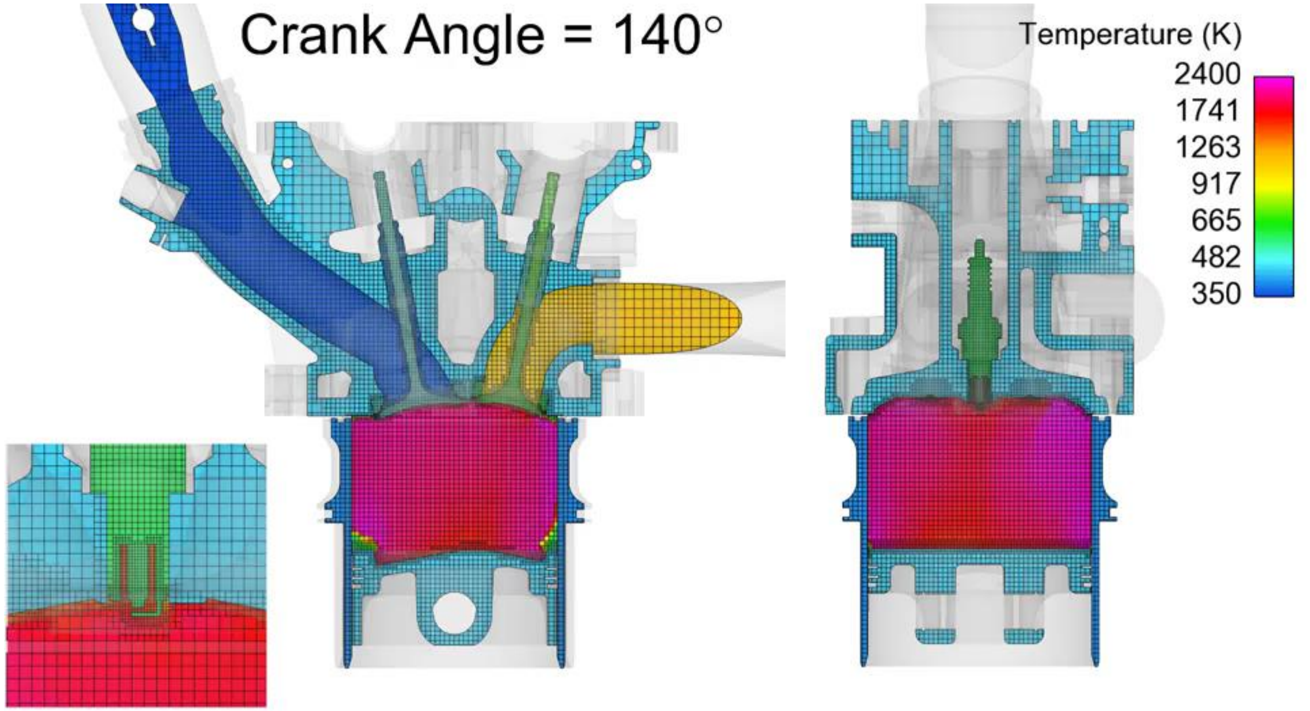
Tumble GDI Memory Comparison



3.1

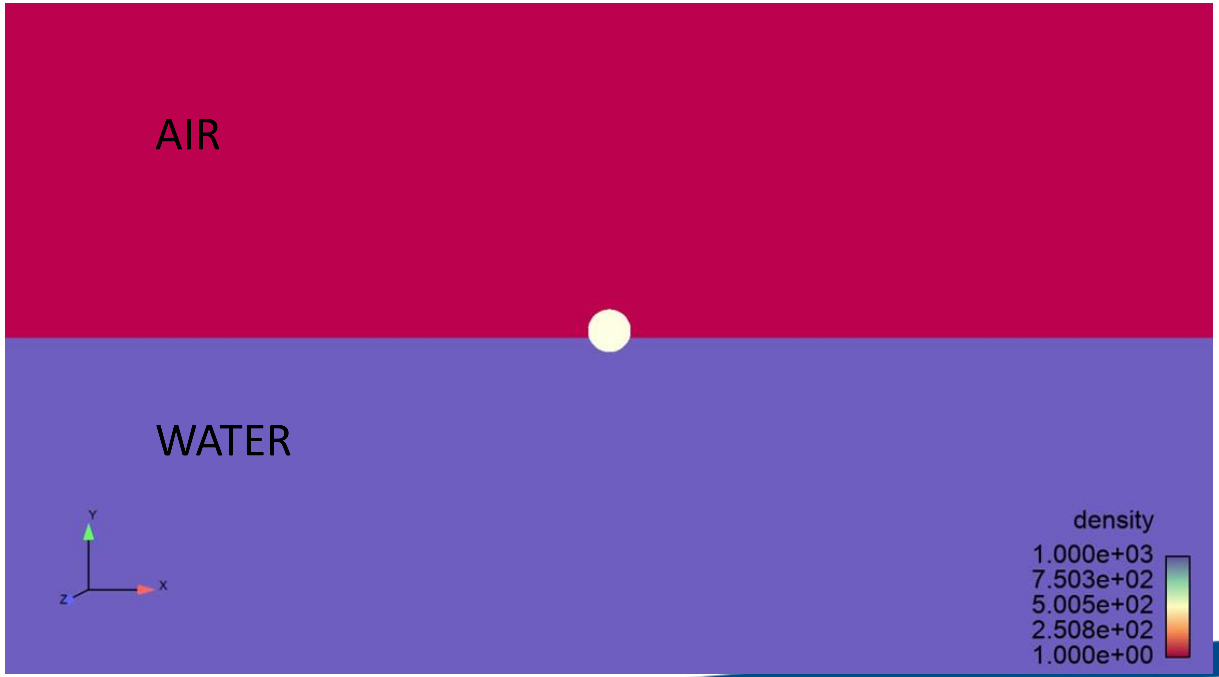
Coming in v3.1 -- Solver

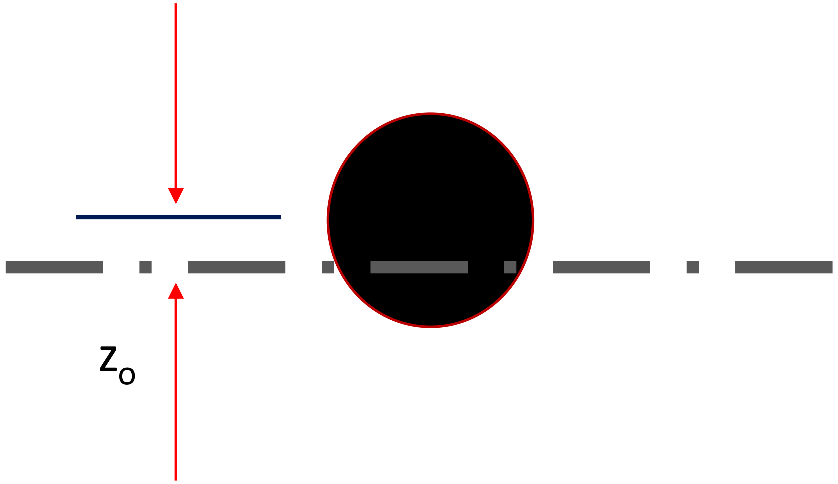
- Further speed/scaling enhancements
  - Vectorization
  - Architecture-specific optimization
- Multiple solvers for multiple streams
- Implicit fluid-structure interaction
- Adjoint Solver
- VOF for multiple liquids
- Coupling with JMAG for energy deposition



Implicit FSI Example --Heaving Cylinder

- Cylinder floating at an air water interface
- Sphere has a density of 500 Kg/m^3





Initial height z_o = 0.0254m
Radius of sphere, a = 0.0762m

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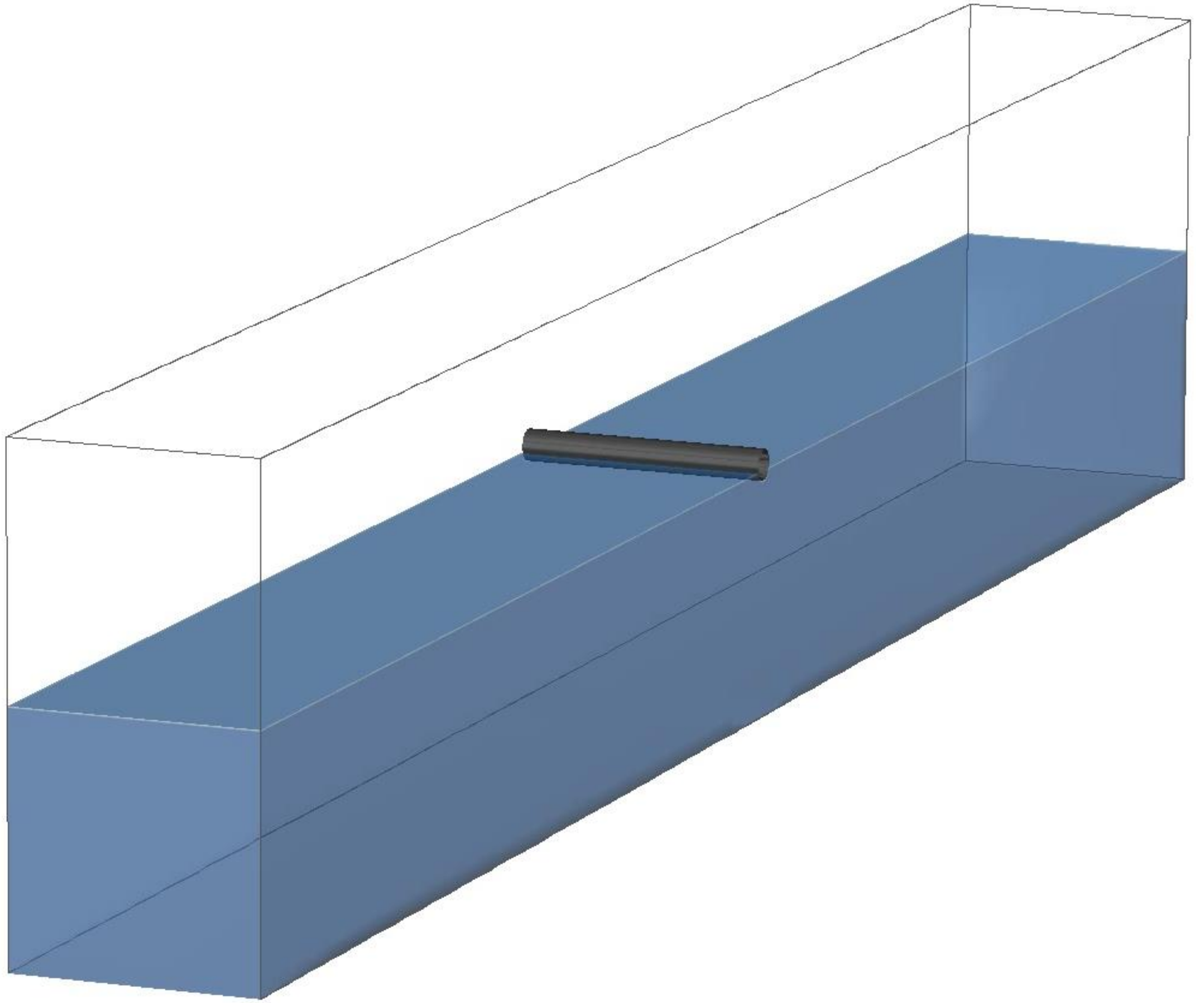
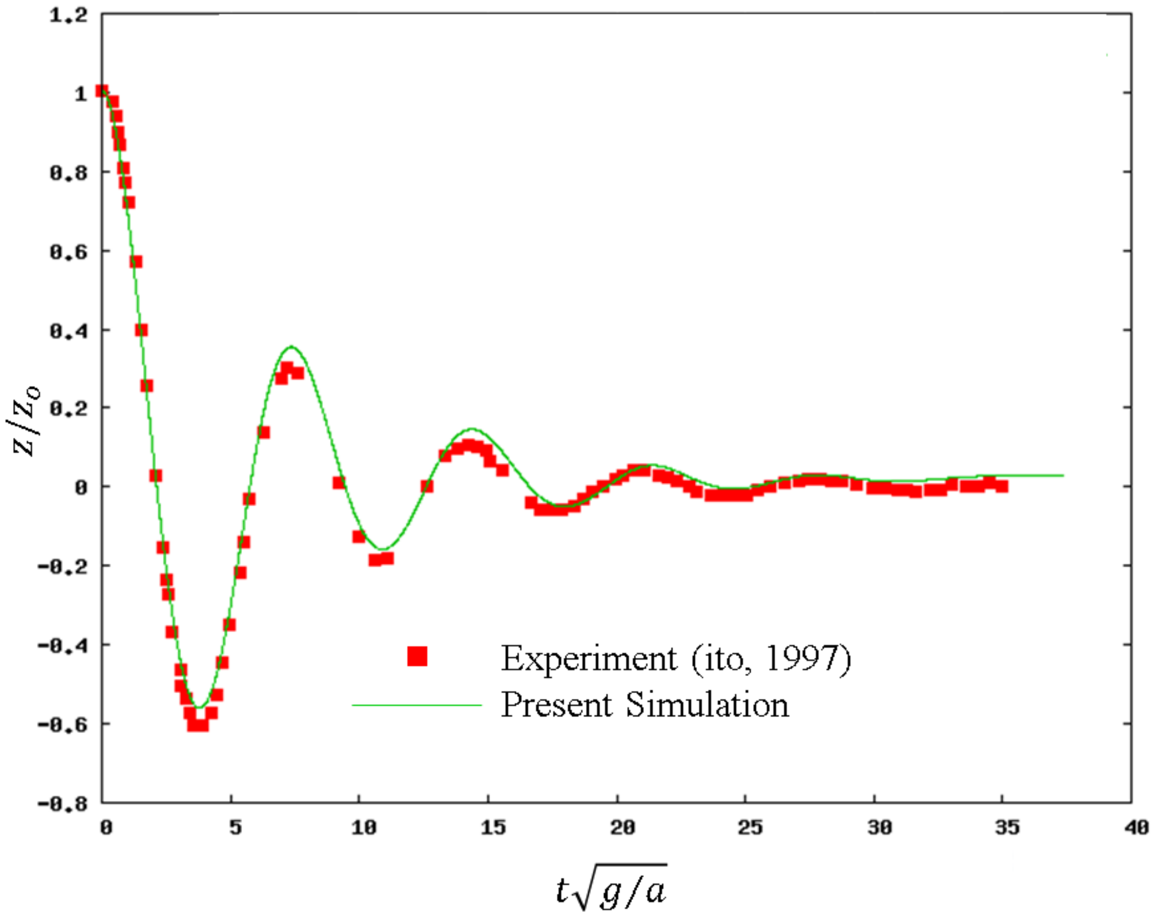
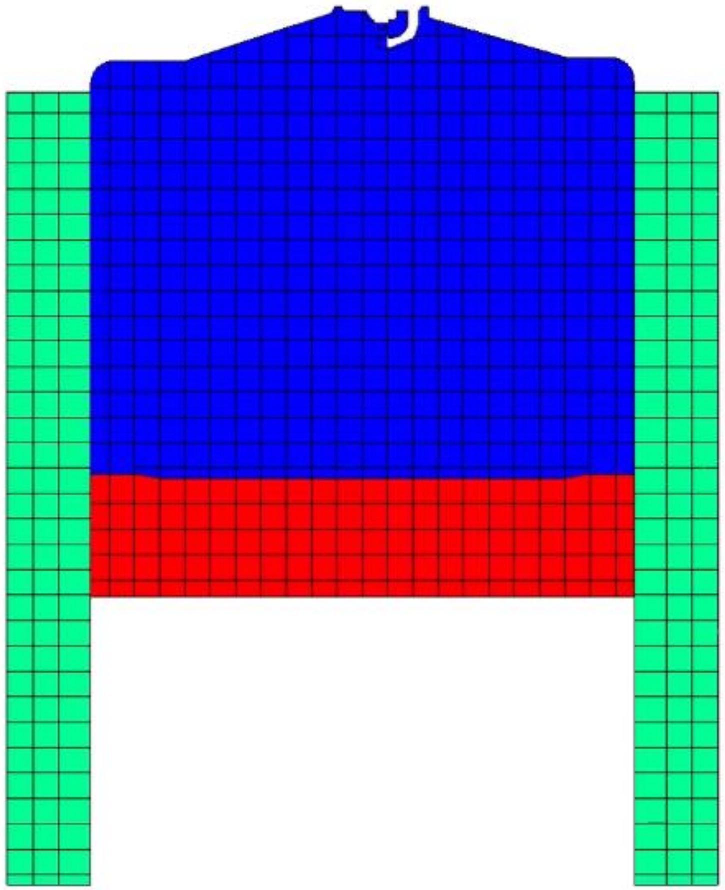
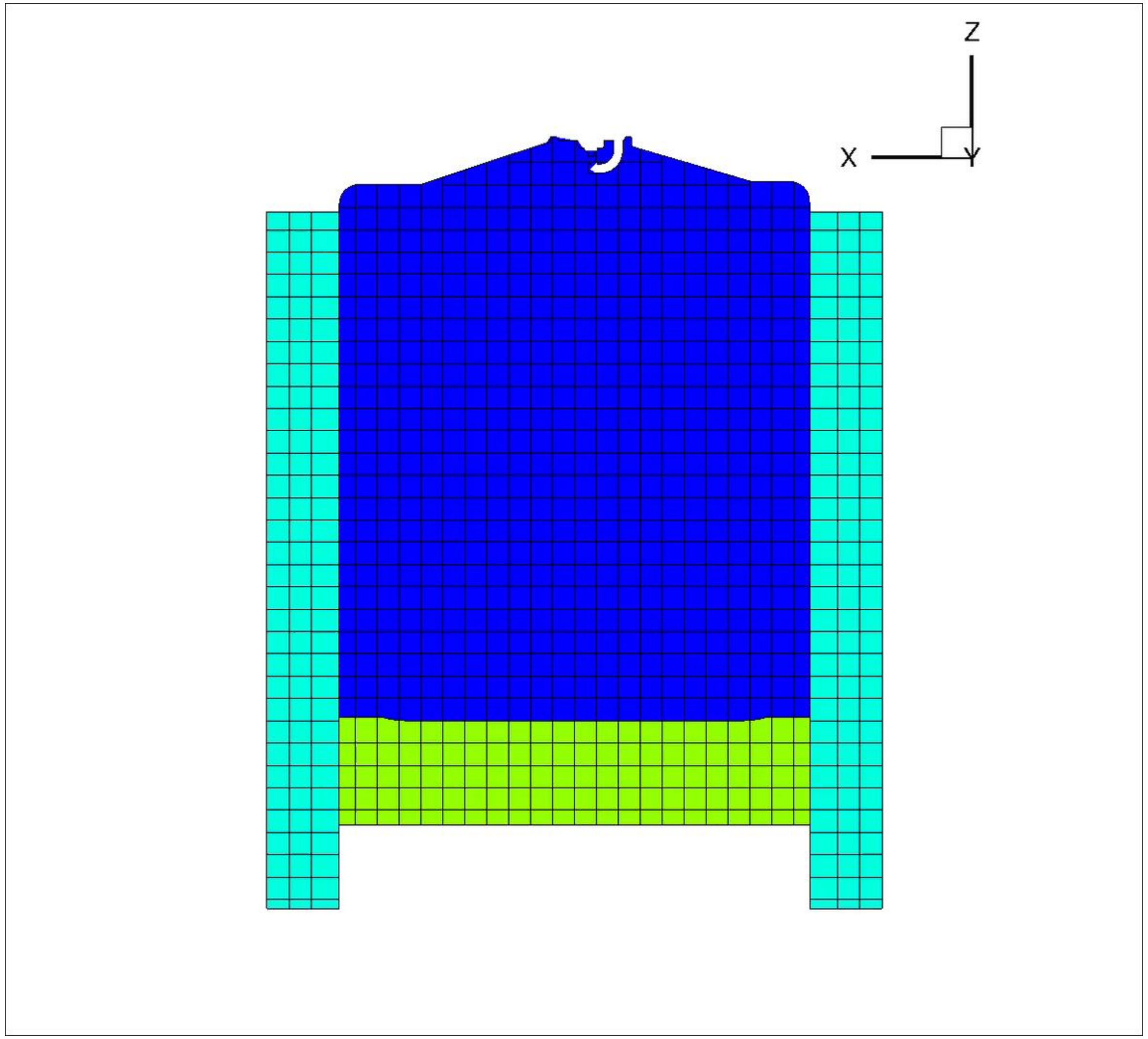



1.2
1
0.8
0.6
0.4
0.2
0
-0.2
-0.4
-0.6
-0.8
0
5
10
15
20
25
30
35
40
z/z_o
$t\sqrt{g/a}$
Experiment (ito, 1997)
Present Simulation

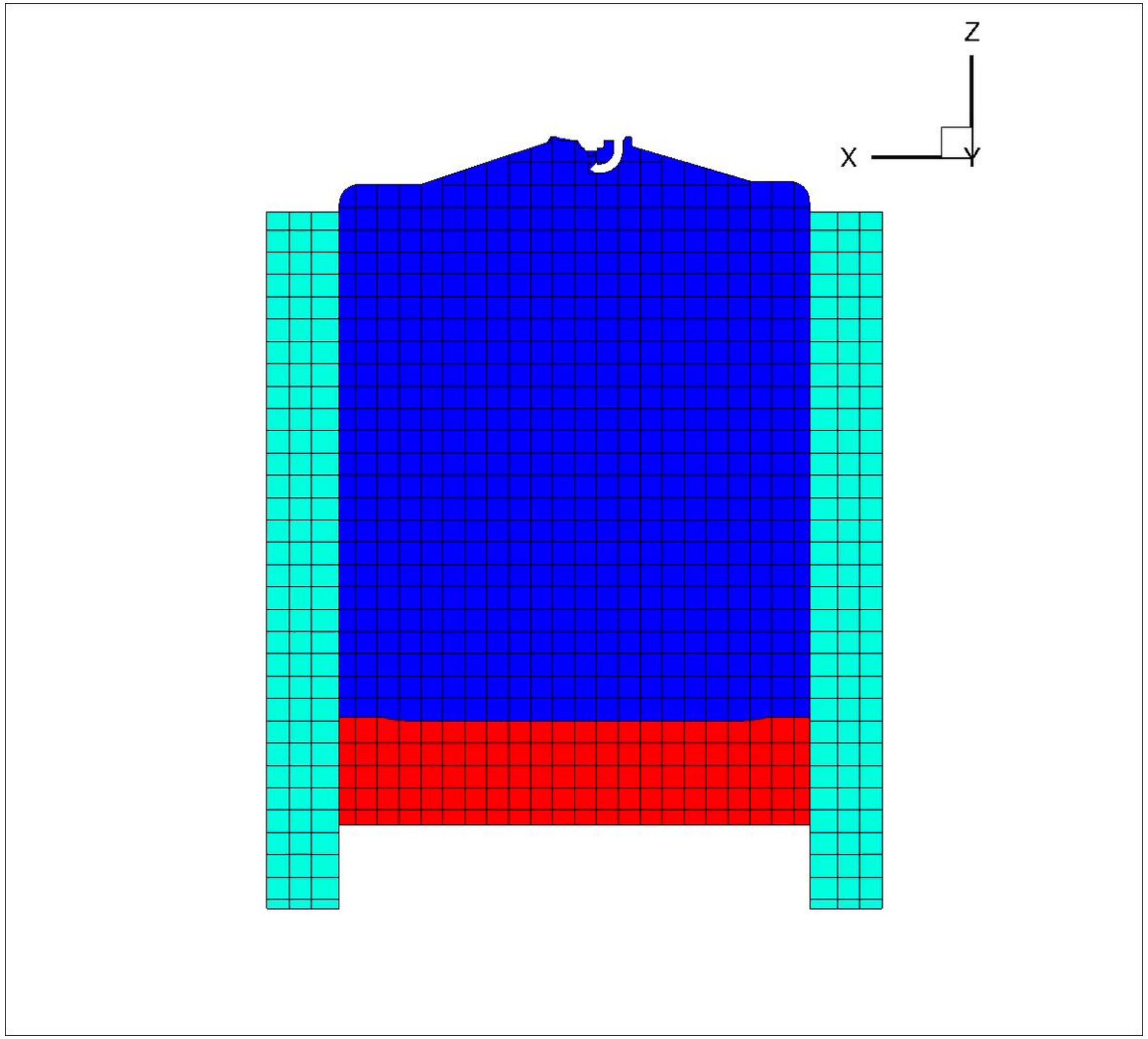
Coming in v3.1 – Grid Enhancements

- Better inlaid grid surface tools
- AMR for inlaid grids
- Moving inlaid grids
- Different meshes for different streams
  - Allows for moving streams to have an unchanging mesh





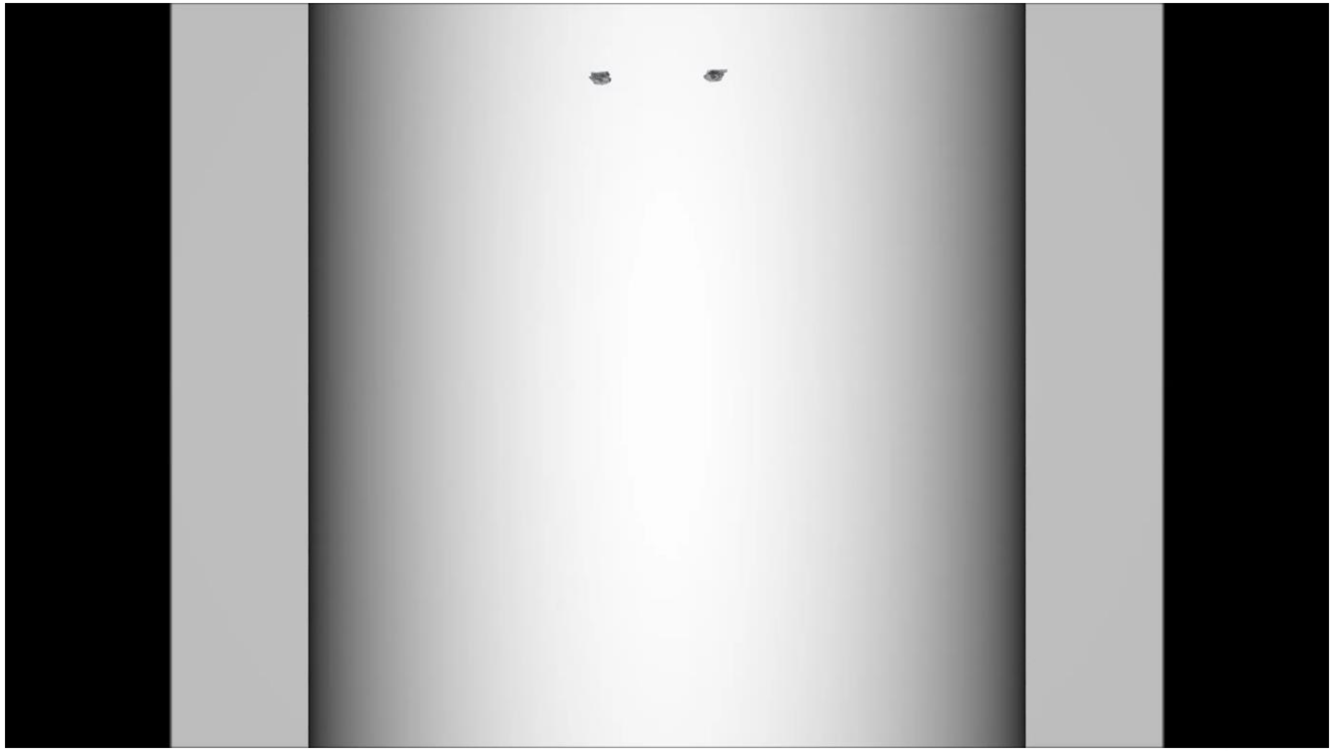
3.0



3.1

Coming in v3.1 – Spray and Combustion

- Support for multiple gas and surface mechanisms
- Stream/region based combustion models
- ECFM coupling with SAGE and detailed soot
- Solid particle simulation



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