What to Expect in CONVERGE Version 3.0

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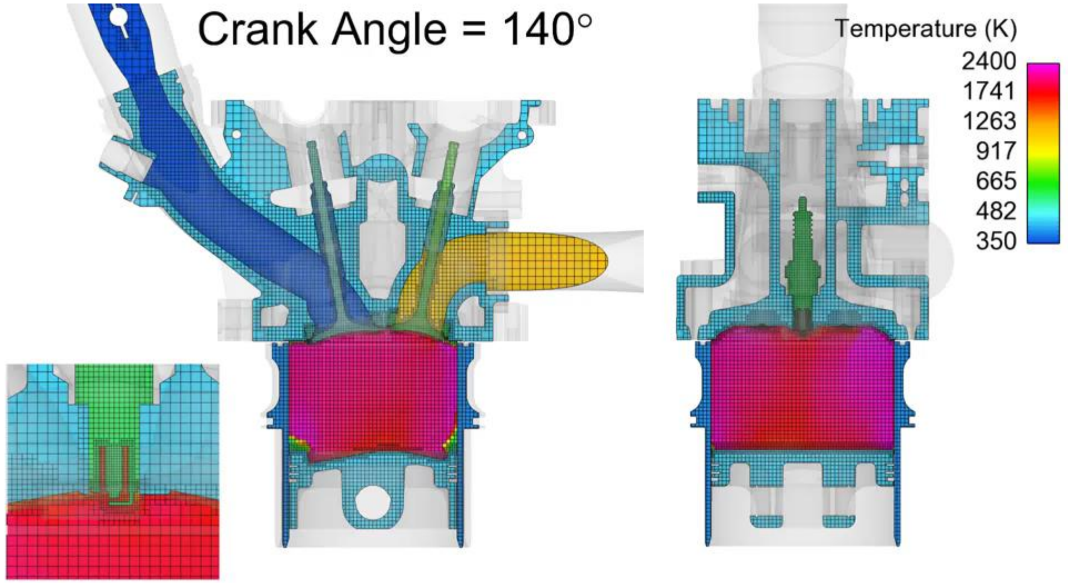
Overview

- New combustion models and utilities (version 2.4+)
- Major 3.0 new features
  - Boundary layer meshes
  - General periodic boundaries
  - Enhanced solvers
  - YAML input files
- Version 3.0 code restructuring
  - Memory reduction
  - Load balance
  - Data structures
  - Post processing files



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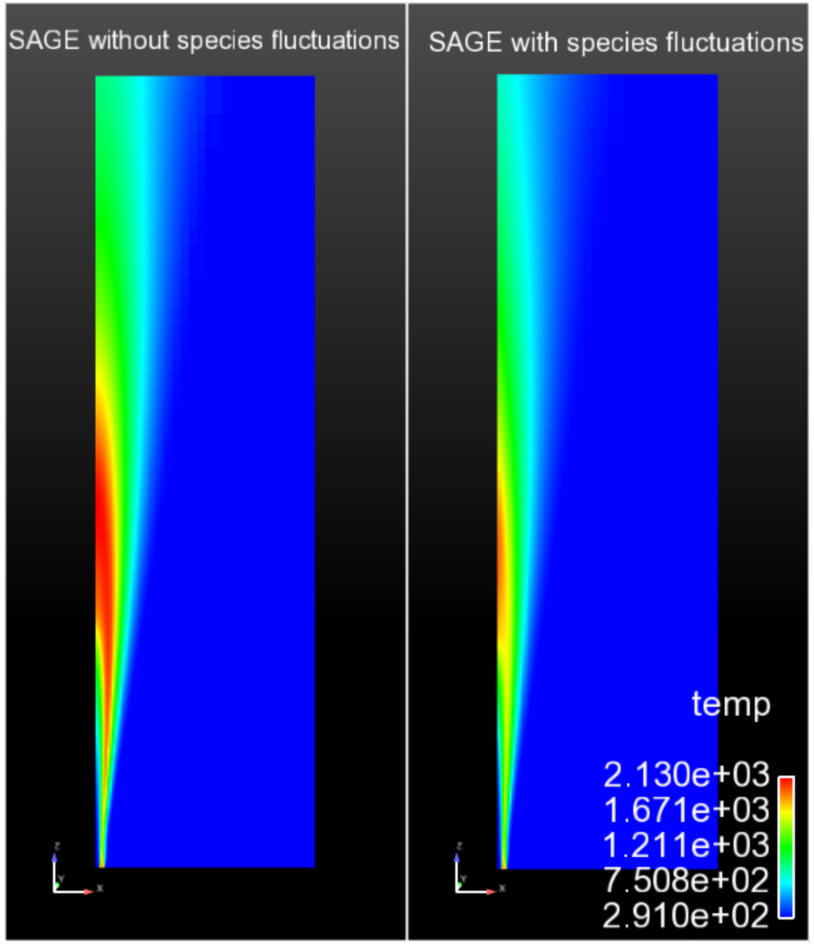
New Combustion Models (V2.4+)

SAGE with Species and Temperature Fluctuations (1/2)

- In RANS, the species and temperature fluctuations effects can be considered during chemical source evaluation.
- A three-point PDF is proposed for both diffusion flame and premixed flame.

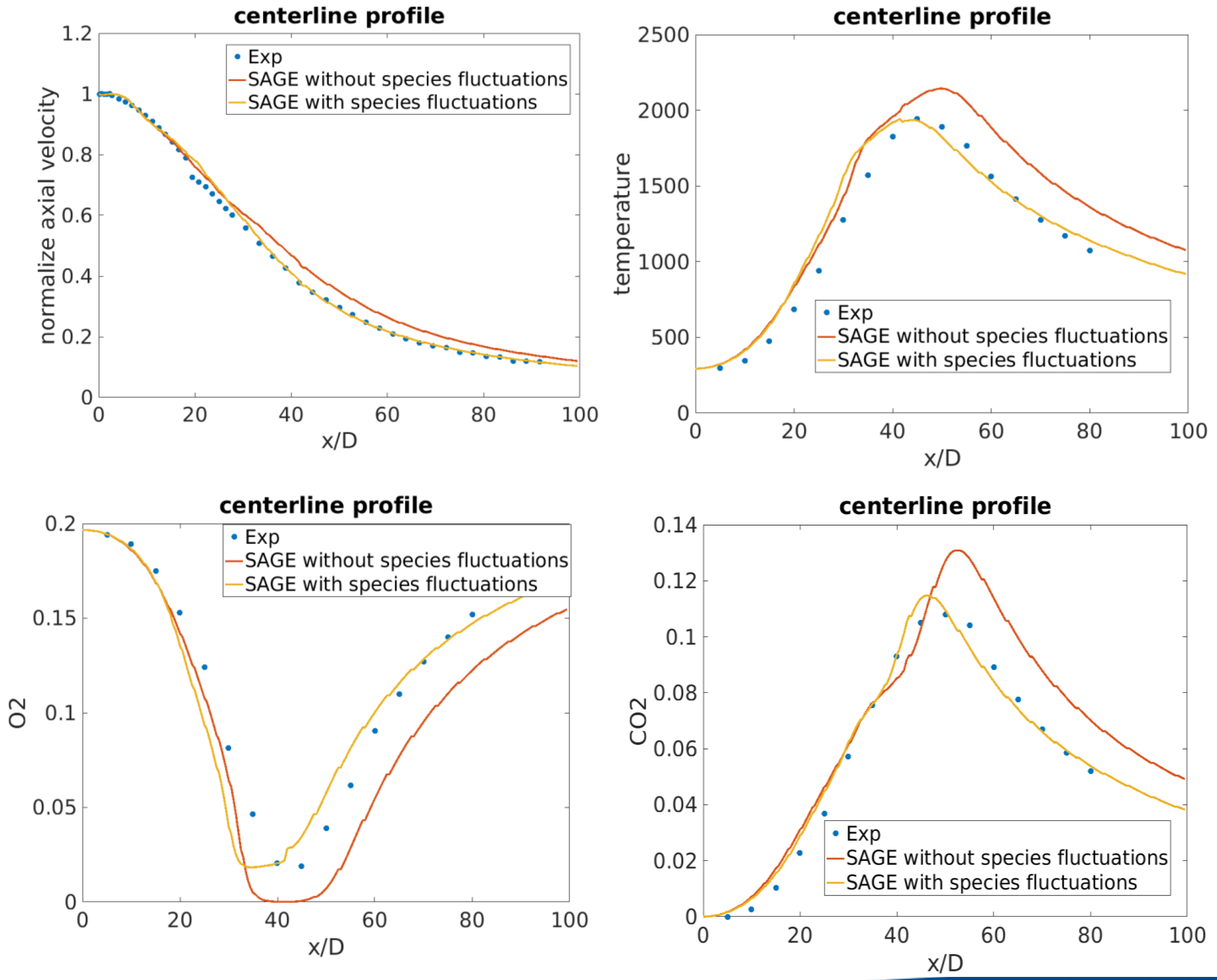
$$\frac{\partial \rho Y_i^k}{\partial t} + \frac{\partial \rho u_j Y_i^k}{\partial x_j} = \frac{\partial}{\partial x_j}(\rho(D_t + D)\frac{\partial Y_i^k}{\partial x_j}) + \omega_i^k, (k = 1, 2, 3)$$

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



Flame D

SAGE with Species and Temperature Fluctuations (2/2)

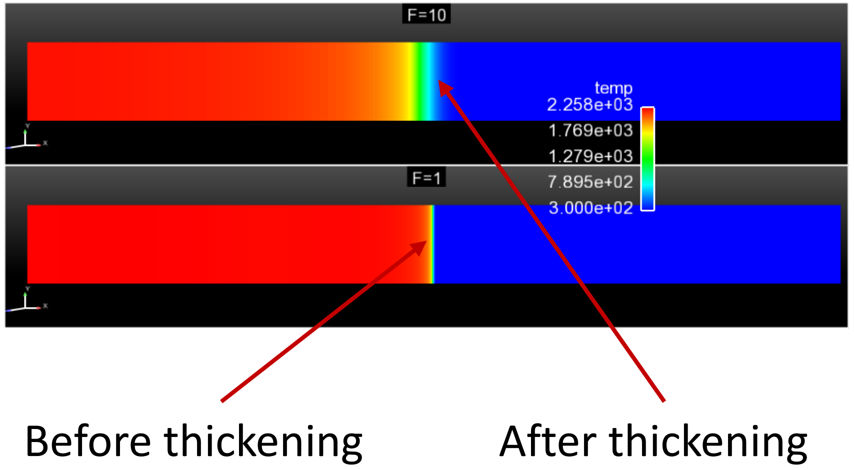


Results with species fluctuations are more consistent with the experimental measurements.

Thickened Flame Model

- The thickened flame model is an effective premix combustion model for LES
- Very popular among gas turbine applications
- Can give reasonable results with relative coarse grid for turbulent premixed flames
- Can be easily coupled with detailed chemistry/emission

1D Laminar Flame Temperature Contour



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Species Based ECFM/ECFM3Z Model

- Original ECFM approach uses a passive based progress variable
  - Incoherence in transport/diffusion of species and passives
  - Need to use first order upwind
  - Progress variable not zero in unburned gases before combustion

$$\tilde{c} = 1 - \frac{\tilde{Y}_F}{\tilde{Y}_{FT}}$$

- Species based progress variable
  - Solves the issues above
  - Allows the detailed chemistry/emission coupling
  - Allows multi-component fuel

$$\tilde{c} = \frac{\sum_i \tilde{Y}_i^b}{\sum_i \tilde{Y}_i^u + \sum_i \tilde{Y}_i^b}$$

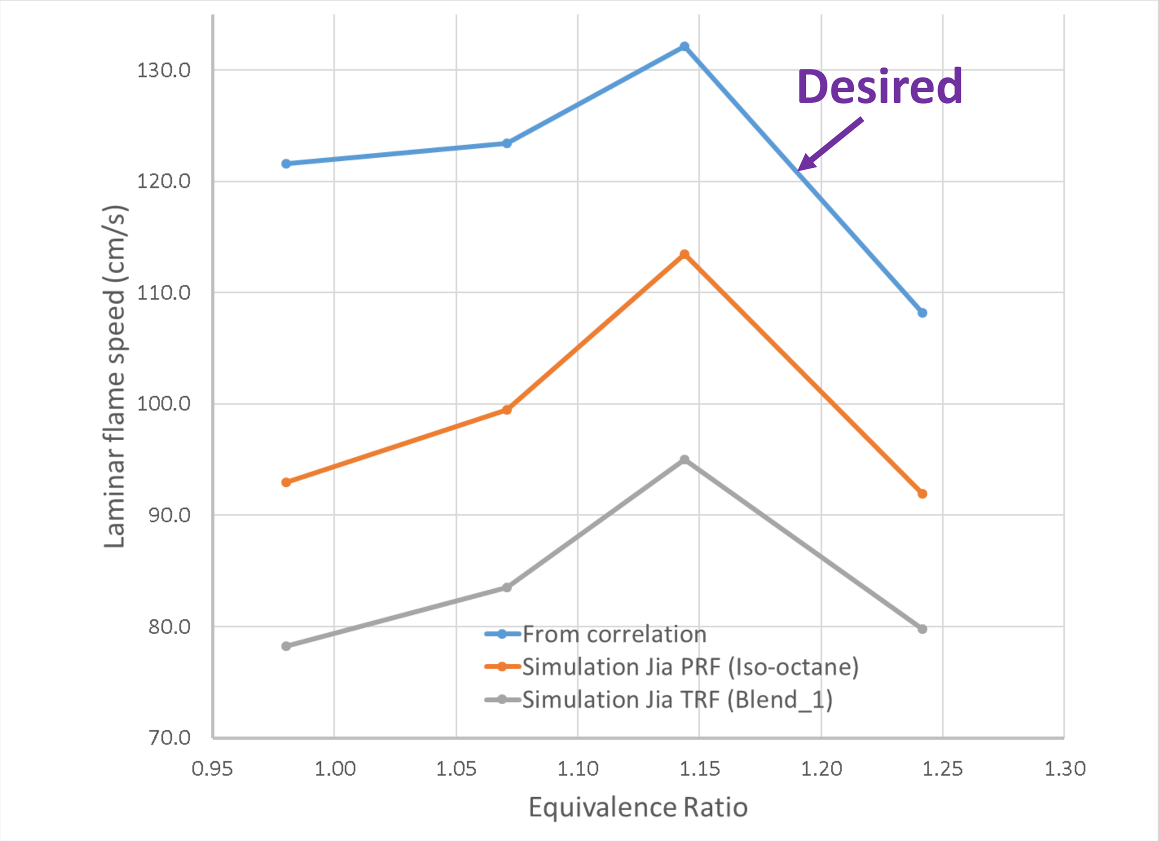
New Combustion Utilities (V2.4+)

Mechanism Optimization (1/3)

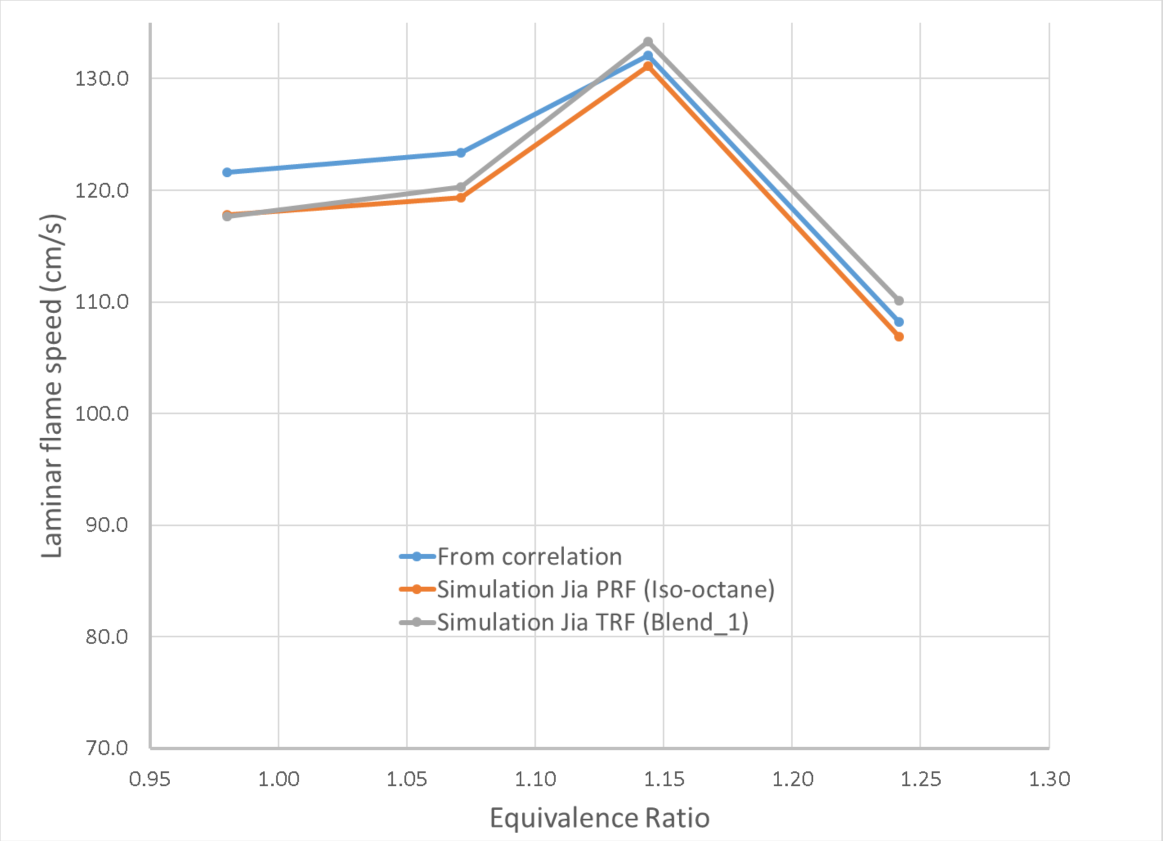
- Reducing from the detailed mechanisms will introduce errors
  - Reduction is often based on ignition delays only
  - Reduced conditions may not cover all the conditions in a real IC engine
- Mechanisms optimization is an option to improve the accuracy
  - Without increasing the mechanism size or computational cost
  - Optimization can be performed on:
    - ignition delay (0D)
    - laminar flame speed (1D)
    - 3D results
- Implemented by coupling of CONVERGE chemistry utilities and Congo (GA)

Mechanism Optimization (2/3)

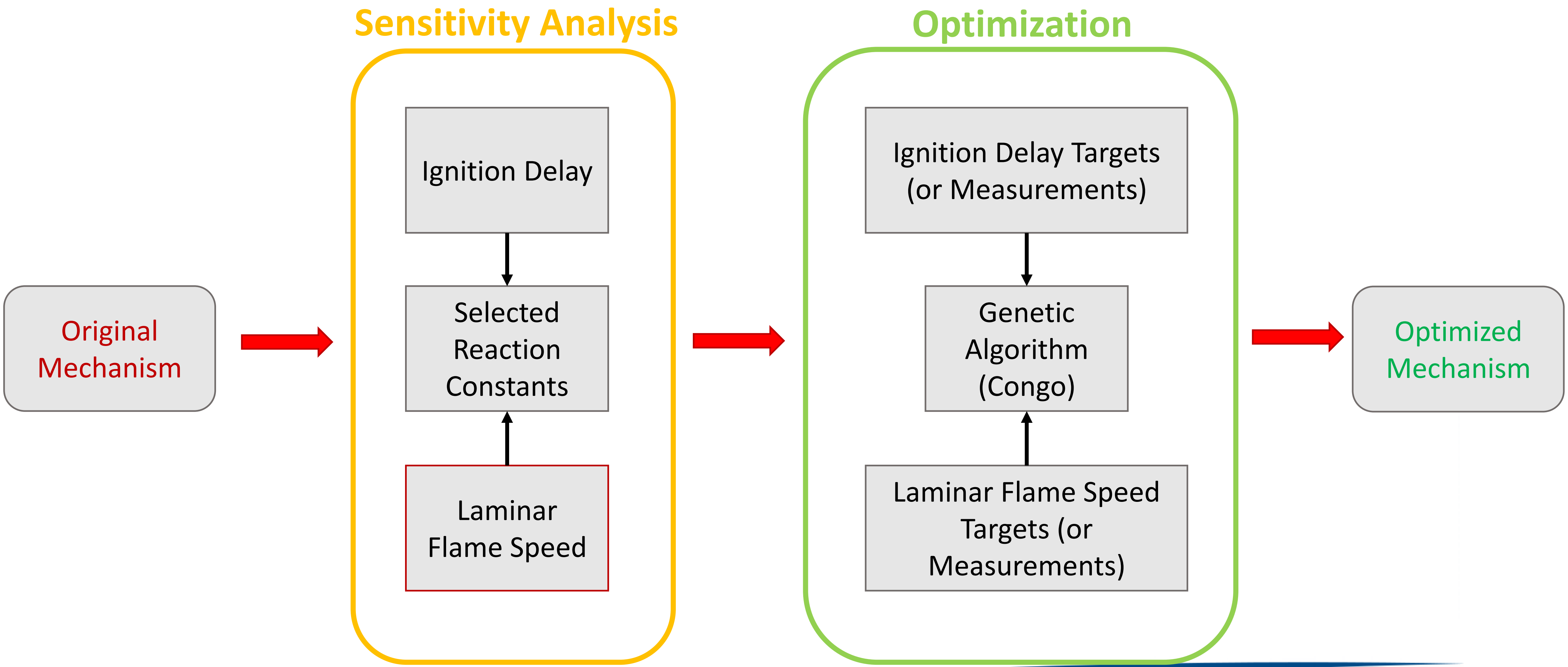
Before



After



Mechanism Optimization (3/3)



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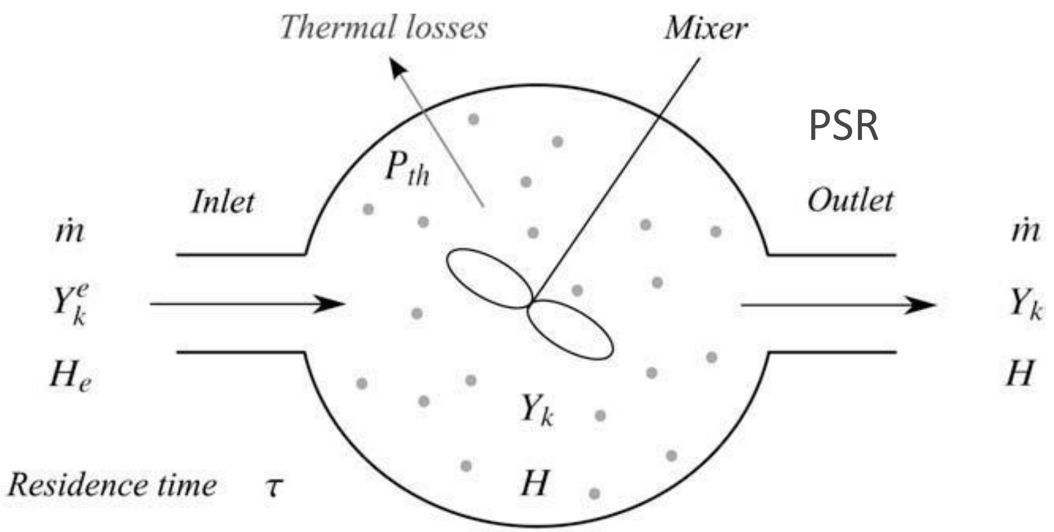
Chemistry Tools/Utilities (1/2)

- A variety of 0D and 1D chemistry tools will be available for mechanism optimization and validation
  - Perfect stirred reactor (PSR)
  - Plug flow reactor (PFR)
  - Jet stirred reactors (JSR)
  - Rapid compression machine (RCM)
  - 0D engine
  - Opposed flow diffusion flame
  - Improved 1D laminar flame speed solver for large mechanisms and engine conditions



- New license policy on 0D and 1D tools
  - Allows running of an **unlimited** number of 0D and 1D cases with a single valid license

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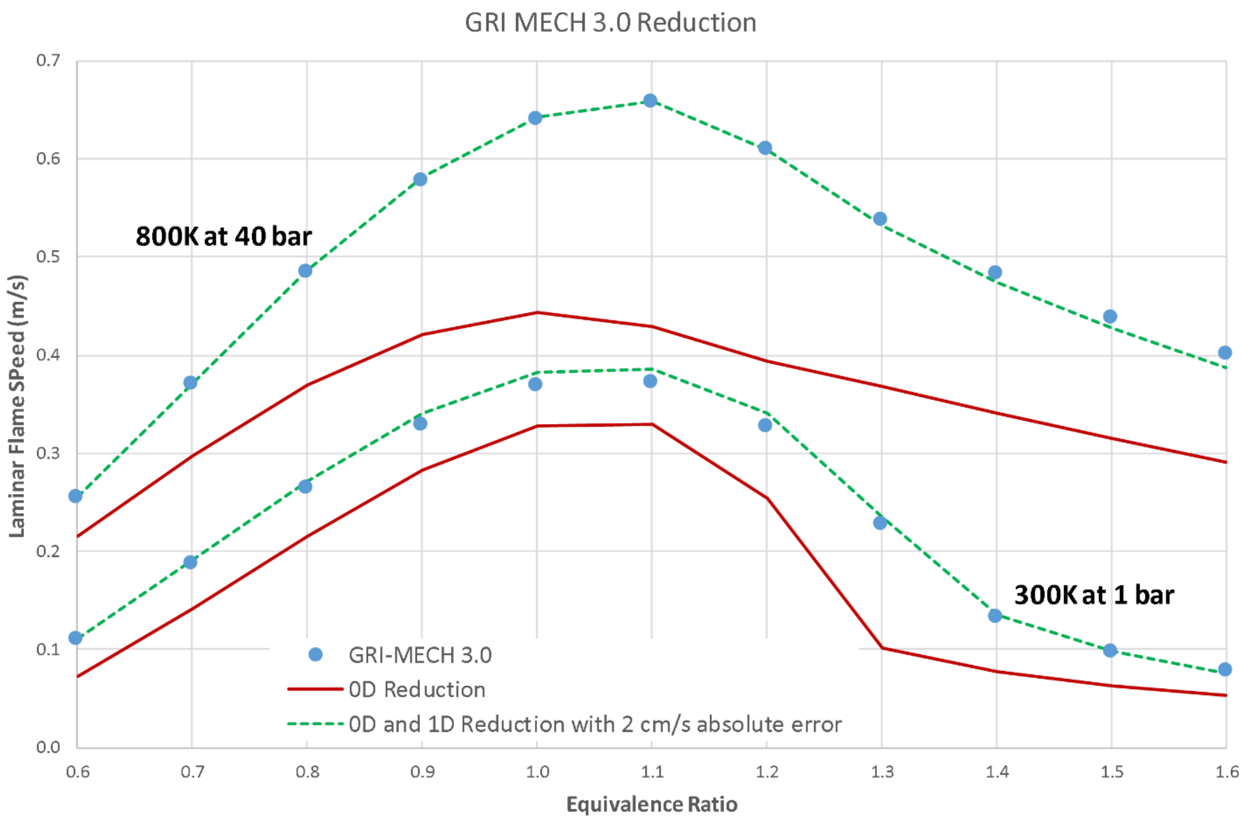
Chemistry Tools/Utilities (2/2)

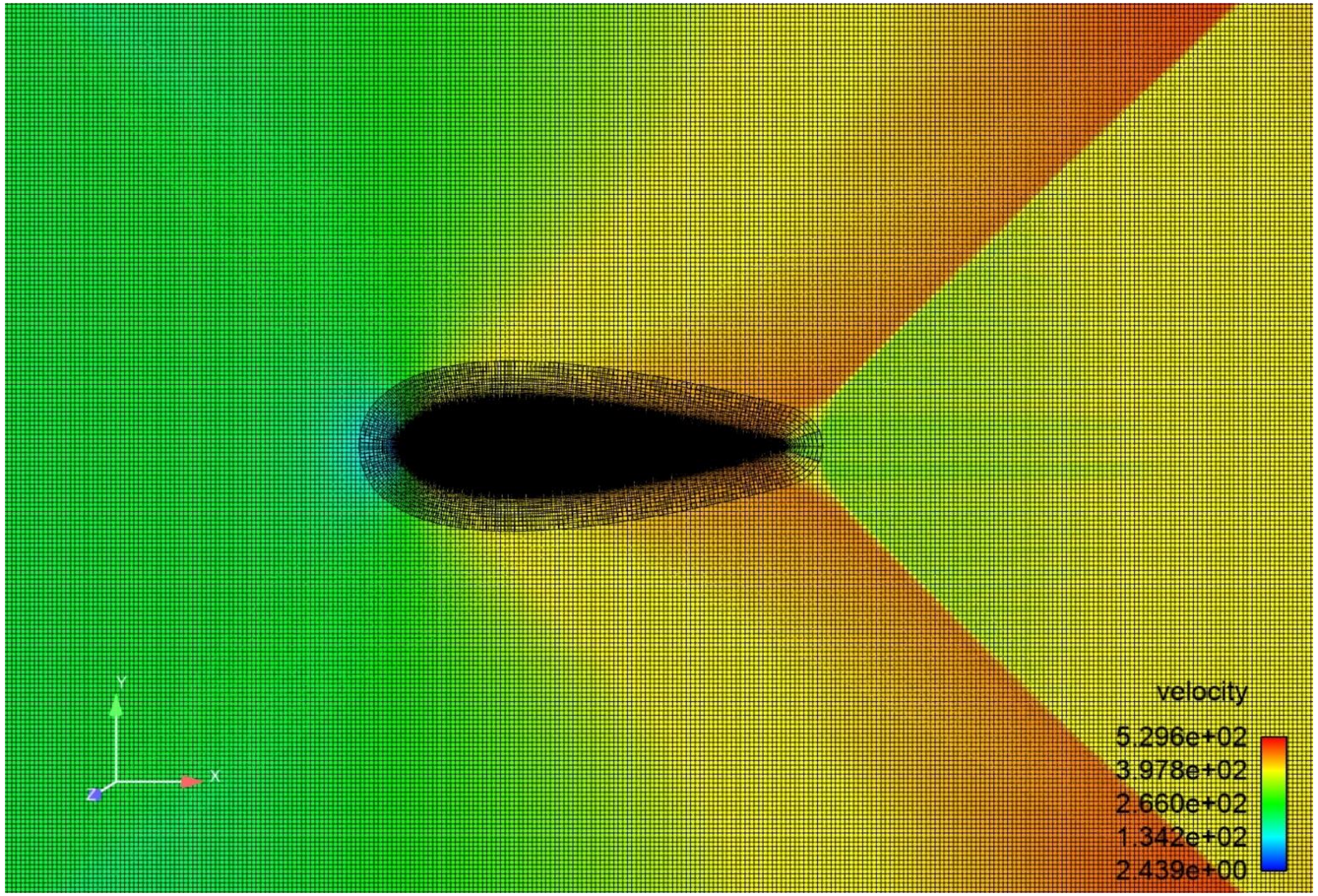
- Improved mechanism reduction
  - Mechanism reduction can include laminar flame speed
- Automated flame speed table generation
  - HDF5 flame-speed database file
  - Supports dual fuel
  - can be coupled with G-equation, ECFM, and FGM



Boundary Layer Meshes

Boundary Layer Meshes (1/2)

- Boundary layer implementation will take advantage of existing CONVERGE functionality to more easily implement the feature
  - Cell pairing
  - Partial children
  - FLOW THROUGH interfaces
- Boundary layer mesh setup to be automatically created at runtime in the solver
- User to specify resolution and adaption parameters through inputs
- NOT an overset approach—cells will naturally transition at interface to orthogonal mesh



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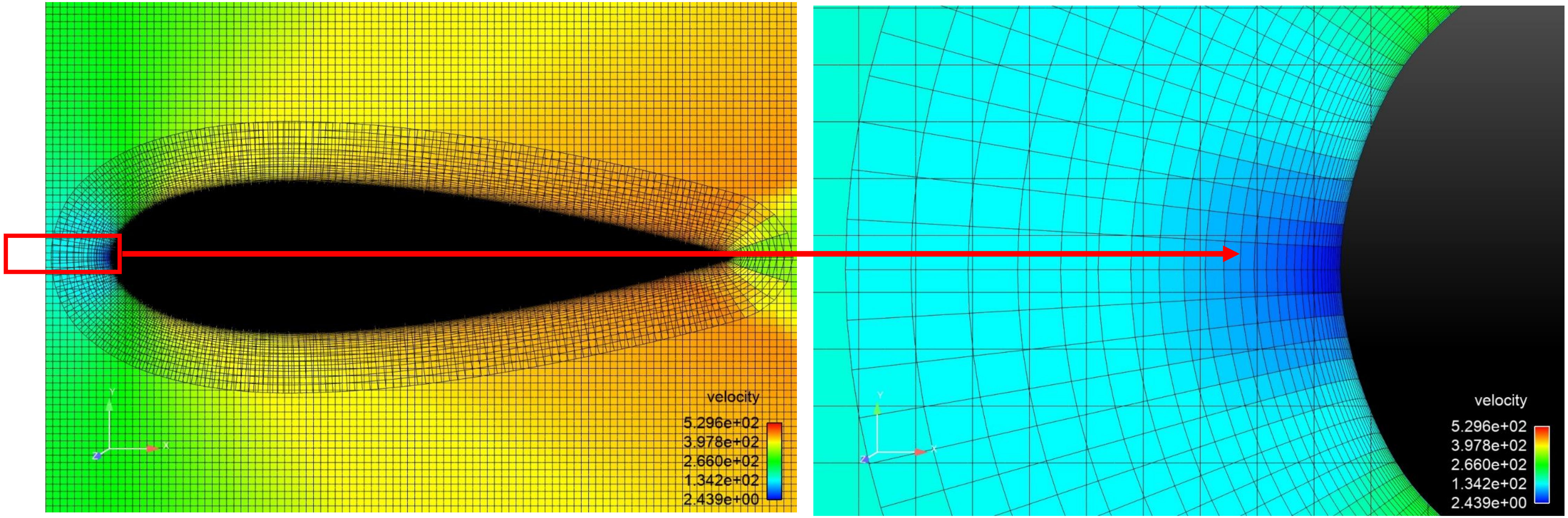
Boundary Layer Meshes (2/2)

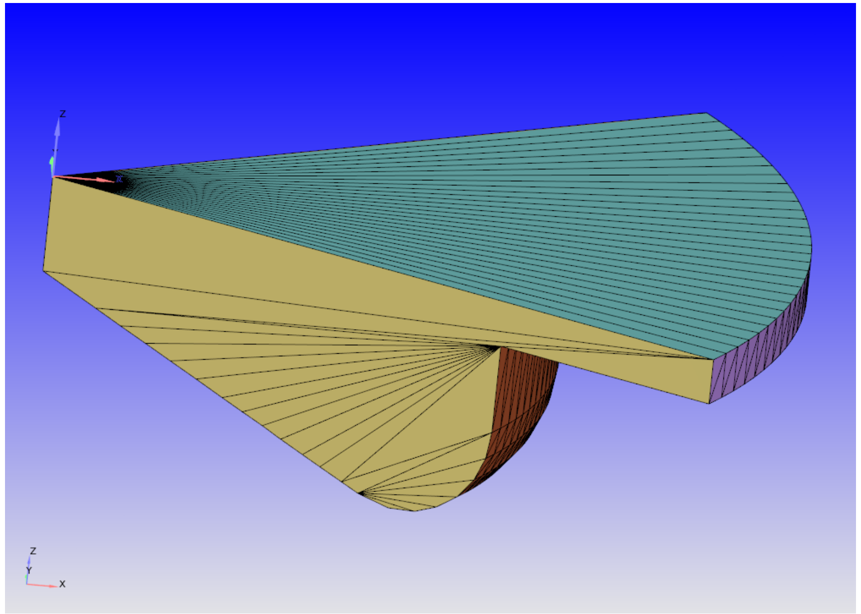
Velocity field in a flow over airfoil



General Periodic Boundaries

General Periodic Boundaries

- Current periodic boundaries are very restricted
  - Can only have a single transformation matrix for all boundaries
  - Must be planar
  - Must be symmetric about the x-z plane
- New implementation much more flexible
  - Boundary faces need not be planar
  - Can be intersected by parts (e.g. gas turbine blades)
  - Any orientation
  - Any number of periodic faces and transformations
- CONVERGE will be able to solve the hard problem of flow in a box



Enhanced Solvers

Rainbow SOR (1/2)

- Solver results will not change even if you change the number of threads/processors
- Facilitates threading
- 3D non-uniform graph variation on Red/Black SOR
  - Color graph in parallel (order n)
  - Reorder solved nodes by color
- Each color is solved in parallel thus maintaining Gauss-Seidel [no Jacobi on processor boundaries]

Acceleration of Pressure SOR using Optimal Omega

- Maximum Eigenvalue is estimated from the rate of convergence
- Optimal omega is estimated from the max Eigenvalue estimate
- For problems requiring lots of pressure iterations, can reduce the total number of iterations by an order of magnitude

$$\lambda_{max} = \lim \left(\frac{\left\| \delta^{(k)} \right\|}{\left\| \delta^{(k-1)} \right\|} \right)$$

Check after 10 SOR iterations

$$\omega_0 = \frac{2}{1 + \sqrt{1 - \frac{(\lambda_{max} + \omega - 1)}{\lambda_{max}\omega^2}}}$$

$$\omega = \omega_0 - \frac{2 - \omega_0}{4}$$

Optimal Omega updated after every 10 SOR iterations

YAML Formatted Input Files

YAML Formatted Input Files

- Standardized format
- Easily manipulated with scripting languages such as Python
- Simplifies backwards compatibility between versions
- More flexible parsing to handle missing features that are turned off


```yaml
version: 3.0
filename: inputs
---
surface_filename:                     surface.dat
mechanism_filename:                   mech.dat
thermodynamic_filename:               therm.dat
simulation_control:
   crank_flag:                        false
   start_time:                        -490.0
   end_time:                          180.0
   restart_flag:                      false
   restart_number:                    0
   map_flag:                          false
   check_grid_motion_flag:            0
   parallel_scale:                    -4
   load_cyc:                          100
   reread_input:                      true
   random_seed:                       0
output_control:
   twrite:
      post:
         interval:                    99999
      transfer:
         interval:                    10.0
      files:
         interval:                    0.0001
      restart:
         interval:                    99999
   screen_print_level:                0
   num_restart_files:                 1
   write_map_flag:                    0
   wall_output_flag:                  0
   transfer_flag:                     0
   mixing_output_flag:                1
   species_output_flag:               1
   region_flow_flag:                  2
```

Version 3.0 Code Restructuring

High Performance Computing Challenges

- Lower RAM per core
  - Case setup must be completely scalable
- Slower clock speeds
  - Performance on supercomputers is typically measured in FLOPS per watt
- I/O on limited number of nodes
- Low tolerance for out-of-order instructions
  - Vectorization is important again

Titan supercomputer at Oak Ridge National Laboratory

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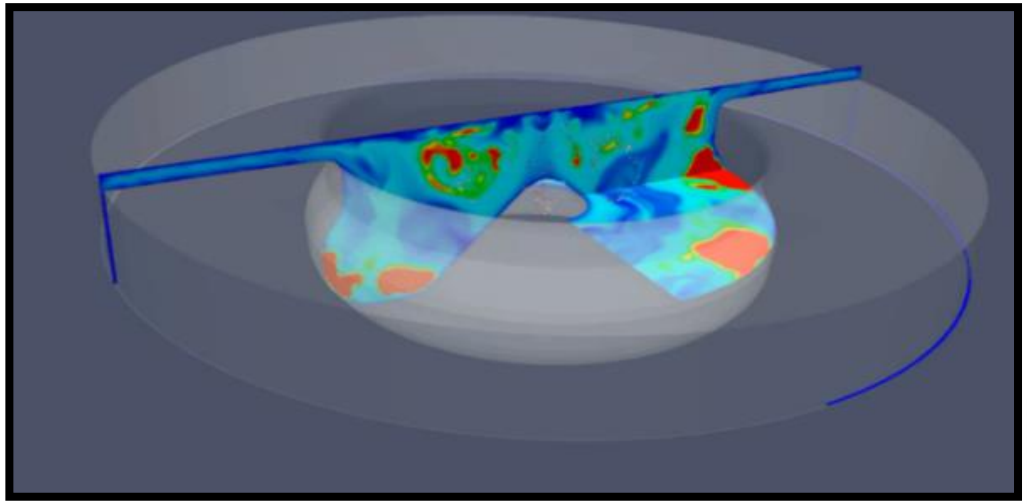
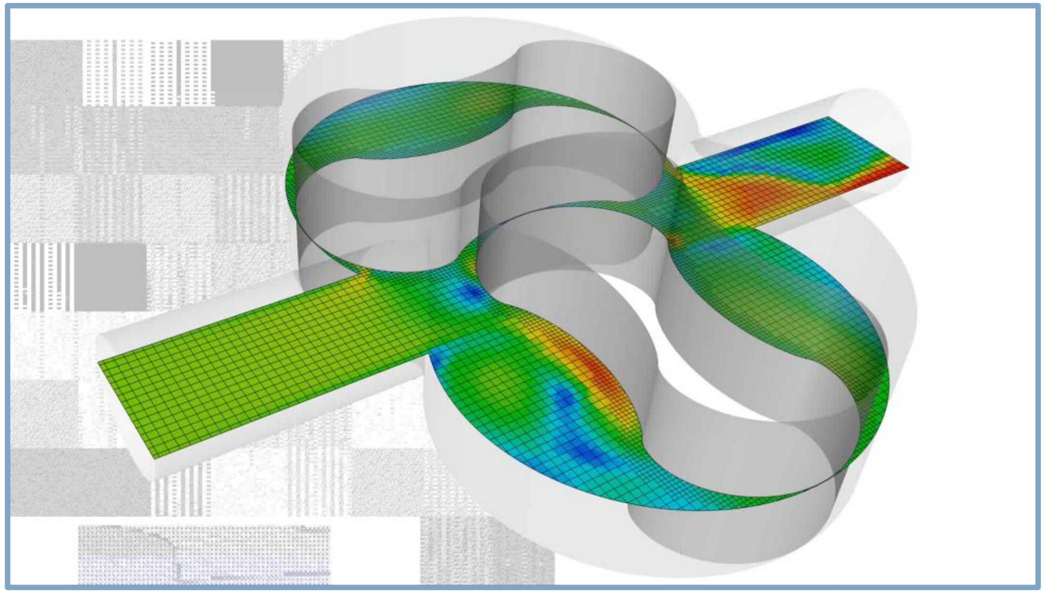
Collaborators on 3.0 Development

- Argonne National Lab
- Oak Ridge National Lab
- Lawrence Livermore National Lab
- IFPEN
- Intel
- NVIDIA



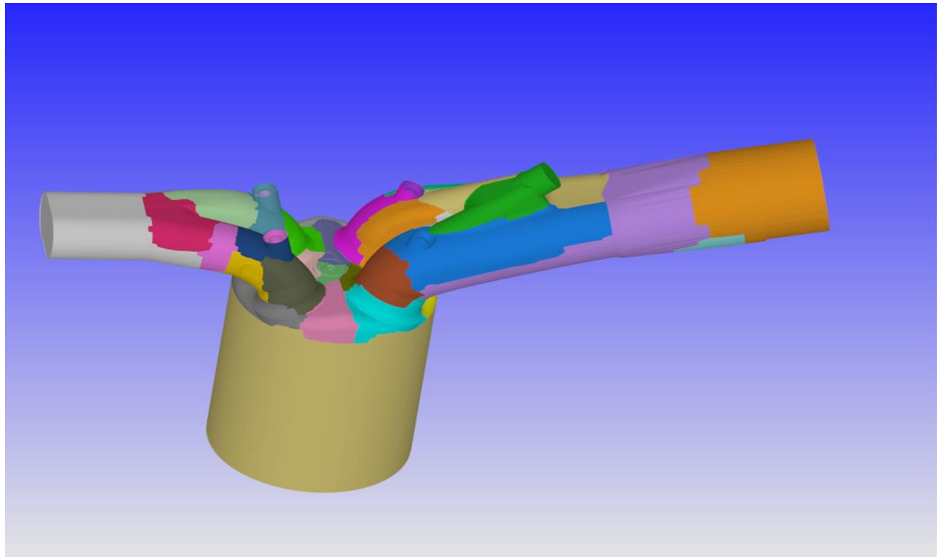
Current Memory Constraints

- Current CONVERGE stores the surface and parallel map on all processors
  - These portions represent a fixed memory cost on all processors
  - Cases with a large number of cores typically require more parallel blocks, thus requiring a larger fixed memory cost on each core
- For 100’s of cores, the fixed memory is not a major issue
- For 1000’s of cores, the memory is a deal-breaker
- These issues addressed in version 3.0

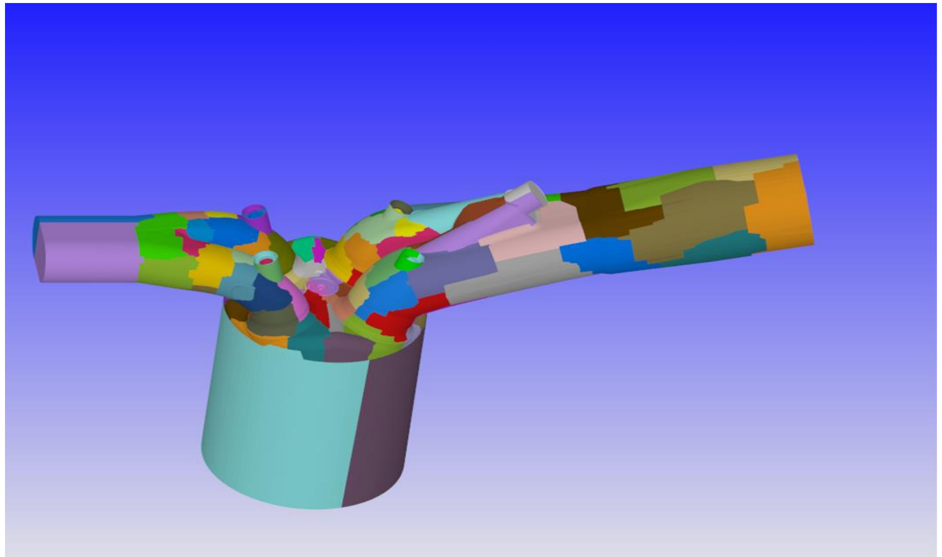


Distributed Surface

- Distributing the surface allow for proper scaling of memory required for the geometry



48 Partitions



128 Partitions

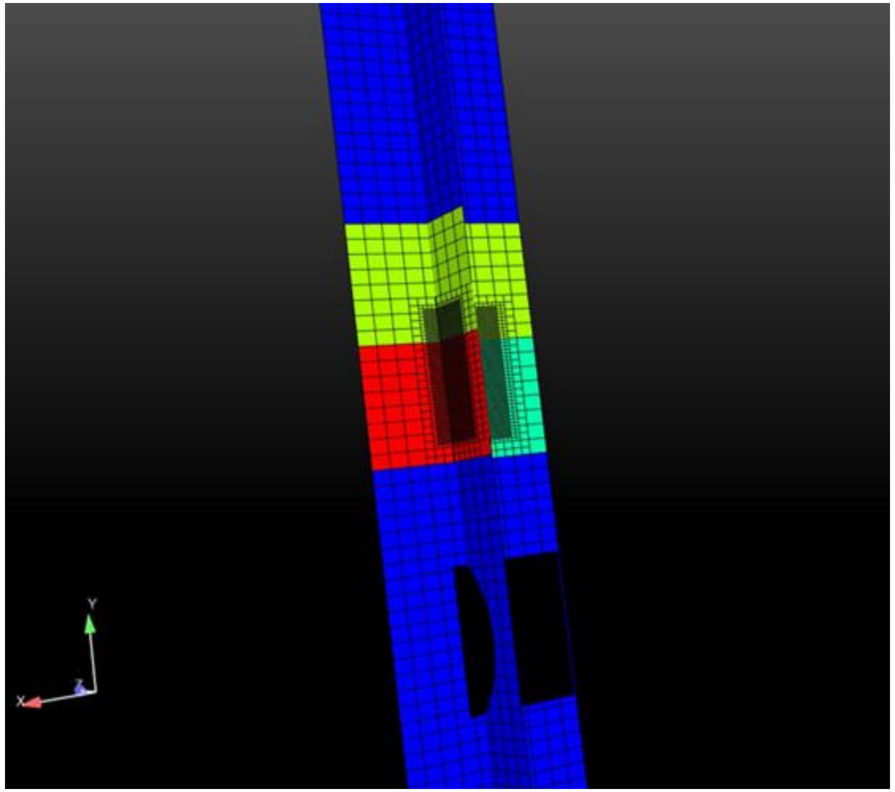
Cell Based Load Balance (1/2)

- In current CONVERGE, 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 will be 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

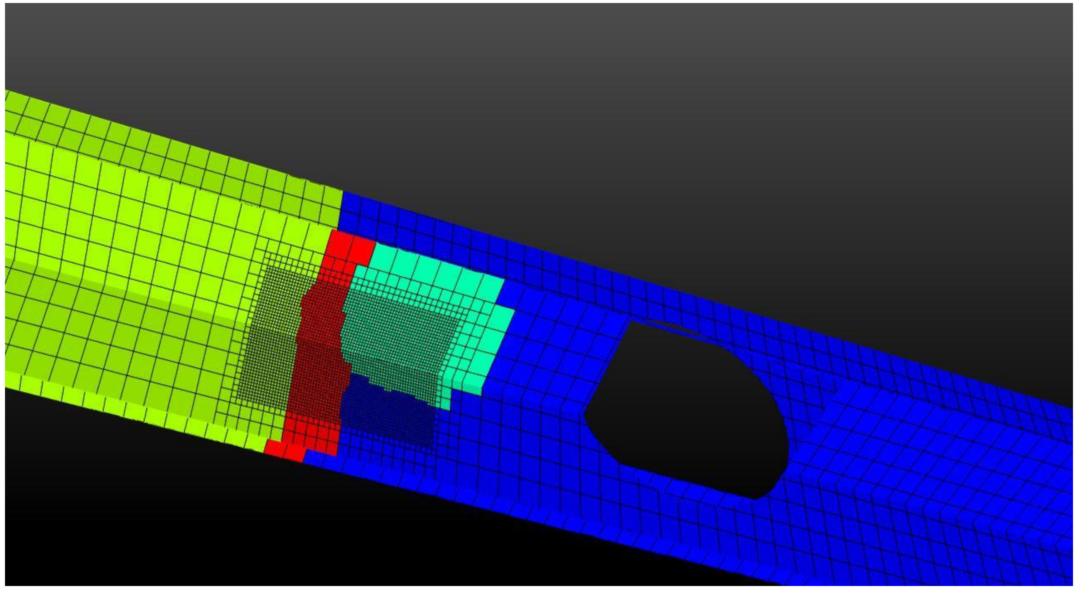
Cell Based Load Balance (2/2)

Processor	Block-based partitioning	Cell-based partitioning
1	11346	25684
2	46874	24542
3	25057	26332
4	19951	24094

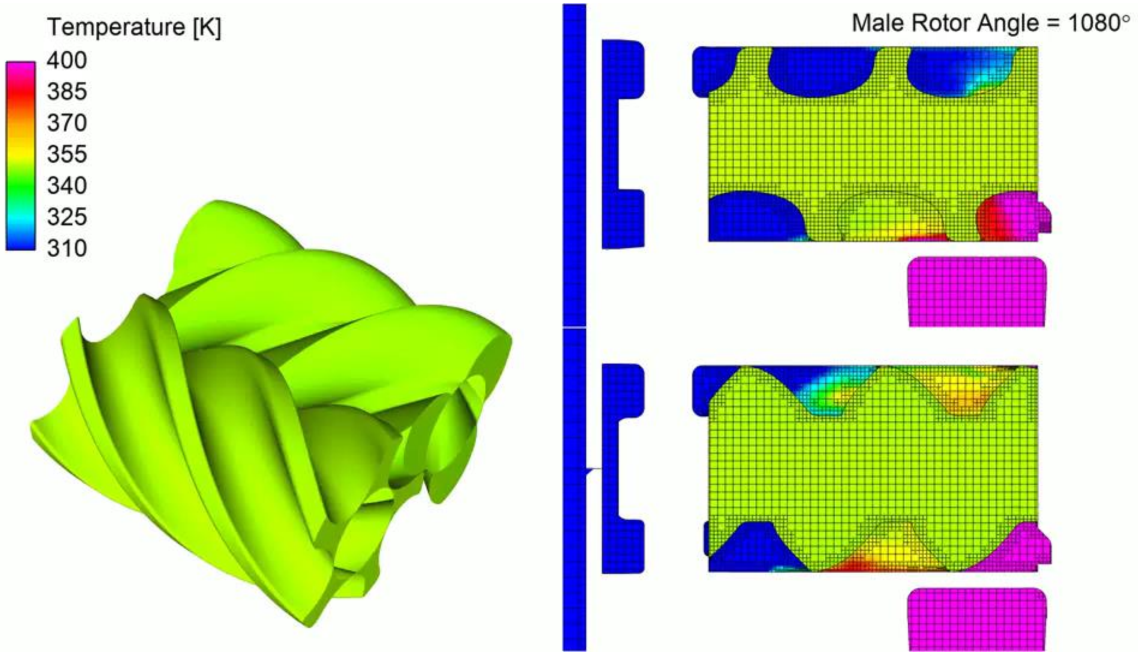
Block-based



Cell-based

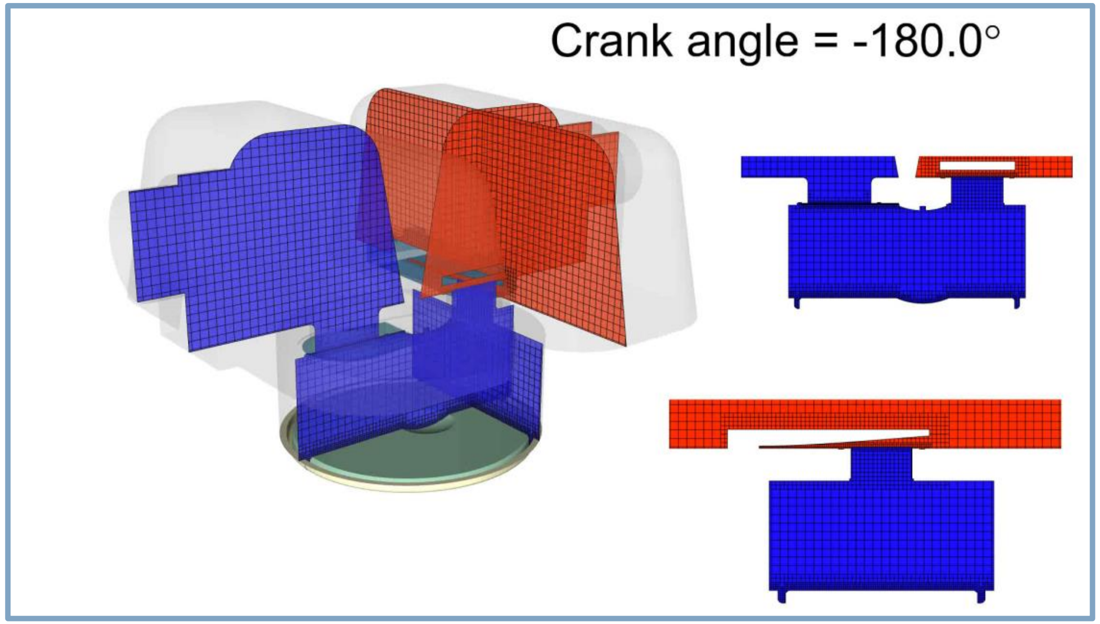


Data Structure Redesign



- Object oriented focus
- Improved scalability
- Hybrid MPI/Threading support
- Smaller memory footprint
- Vectorized operators
- Added flexibility for quicker/dependable feature delivery
- Easier-to-use UDF's

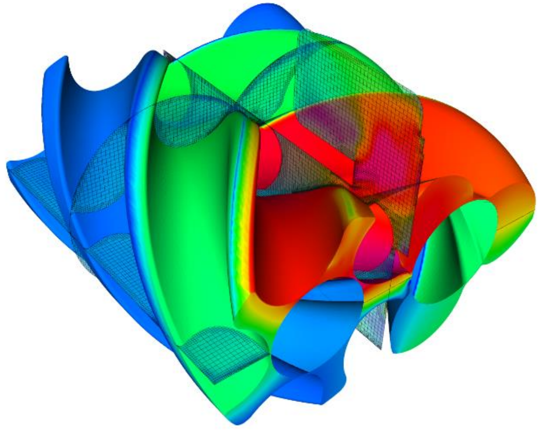
Improved User Experience

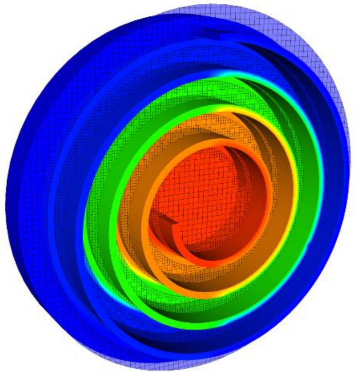


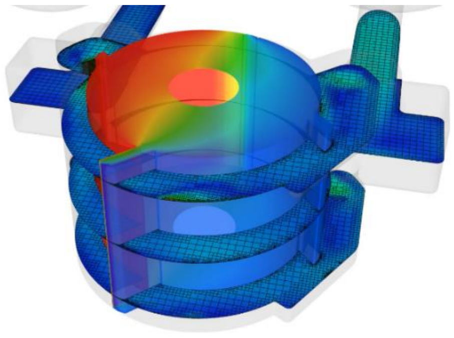
- Complete UDF API overhaul
- Simplified Object Oriented API
- Improved documentation utilizing Doxygen standard
- Improved sample code readability
- Improved compatibility (fewer rebuilds required)
- Seamless optimized data structures and operators
- Support for a variety of programming languages (Fortran, python)

Large Output Files

- Post, restart, and map files to be written in HDF5 format
- HPC industry standard with proven performance/scalability track record
- View/Edit binary output files (map/restart/post) files using standard HDF5 tools
- No post_convert step for most post processors
- Easily fine tune your machine's performance using MPI I/O hints







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When Will Version 3.0 Be Released?

June 2018

Convergent Science: Company Status

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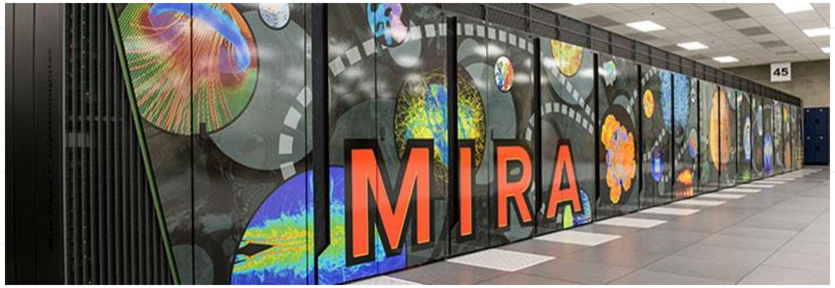

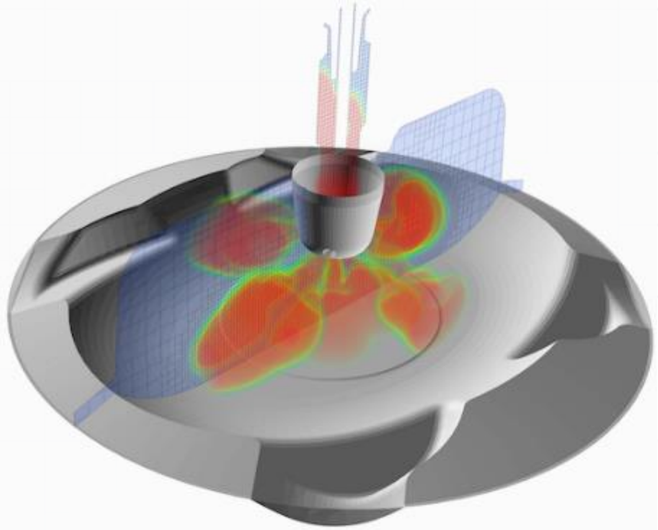

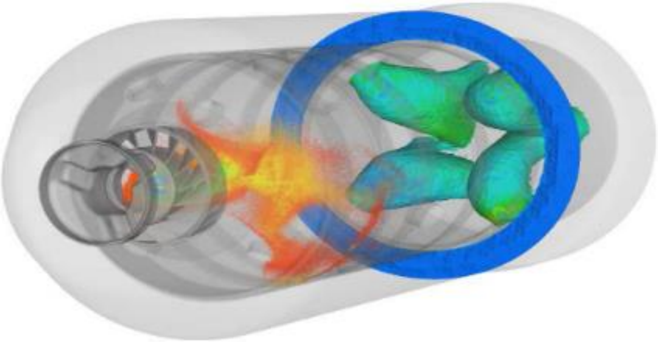

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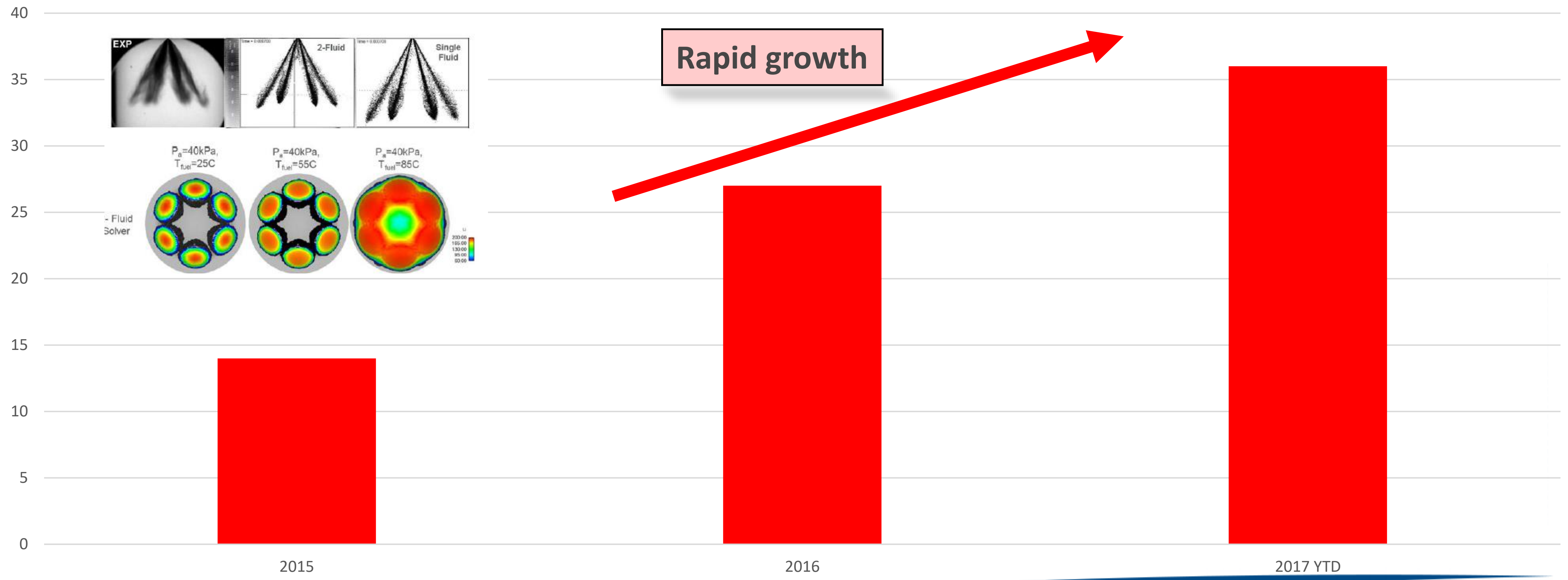
European IC engine market growth

Total number of IC Engine customers in Europe 2015-2017



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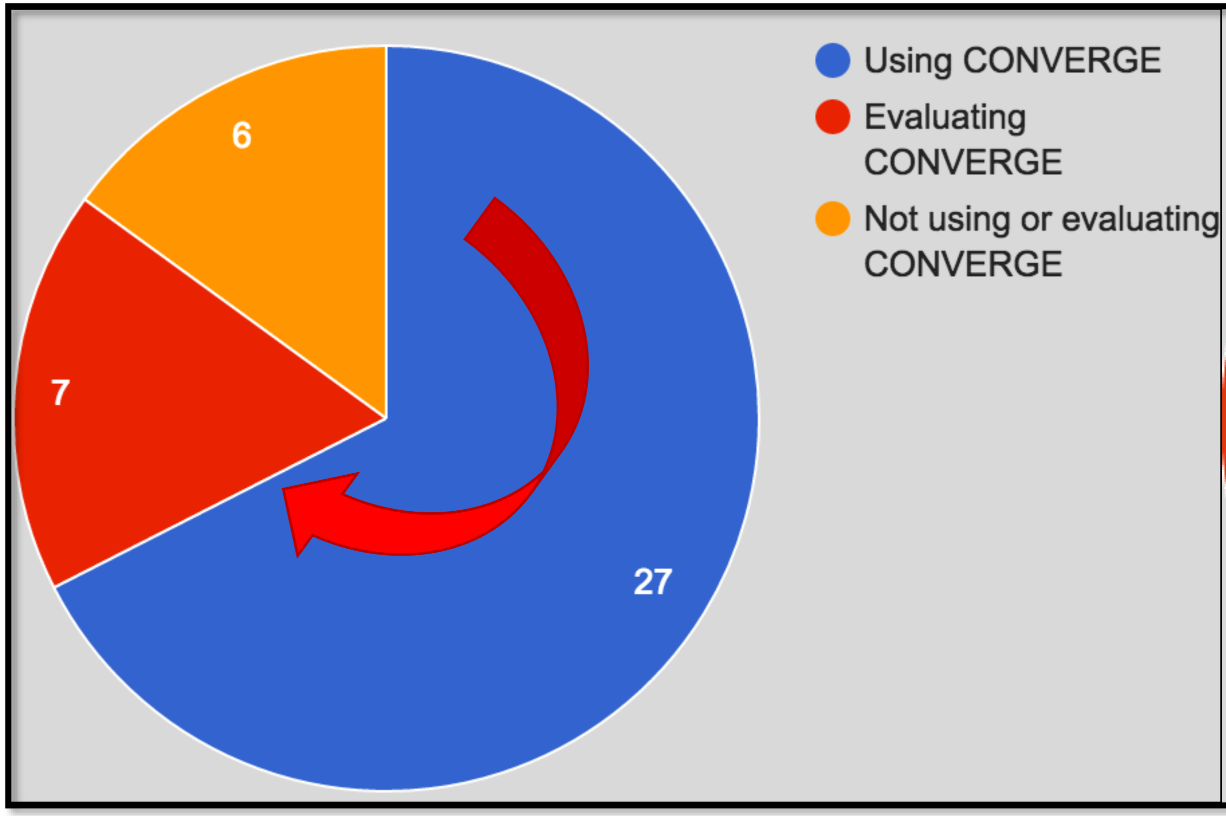
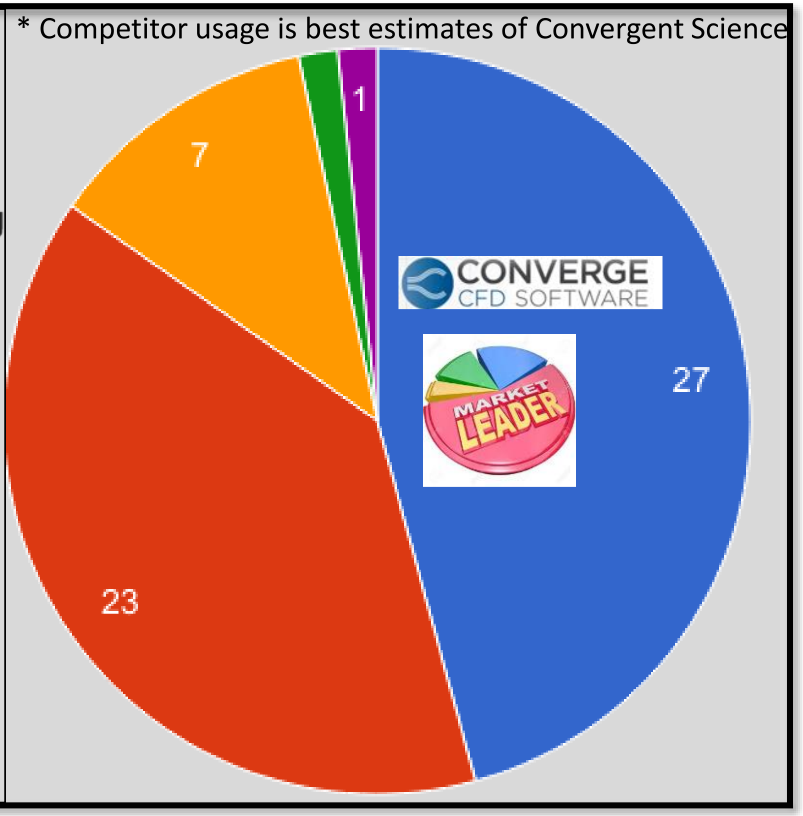
European IC Engine Market Share





- 34 of 40 (85%) of Euro engine makers use CONVERGE
- CONVERGE is most widely used CFD code for IC engine modeling in this region

Note: The sum on the right chart reflects that some companies use more than one CFD code for IC engine modeling

CONVERGE CFD SOFTWARE

Europen User's Conference

1st CONVERGE User Conference in Europe

- 106 Participants
- Keynote speakers:
  - DR. Christian Angelberger
    Expert Engine Combustion Modeling IFP Energies Nouvelles
  - DR. Sibendu Som
    Lead Computational Scientist Argonne National Laboratory
- 27 technical presentation
- Introductory and Advanced training courses
- 34 industrial partner
- 22 universities

Soot modeling by PSM model : Validation on Renault Diesel engine

Bore : 80 mm
Stroke : 80 mm
Single cylinder displacement : 0.4 l
Compression ratio : 15,5
Injection pressure : 1600 bar
Swirl number : 2.5

Combustion simulation in SI engine

Knocking analysis for combustion chamber optimizing

RENAULT NISSAN

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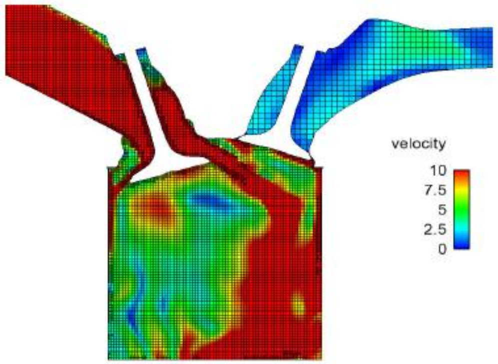
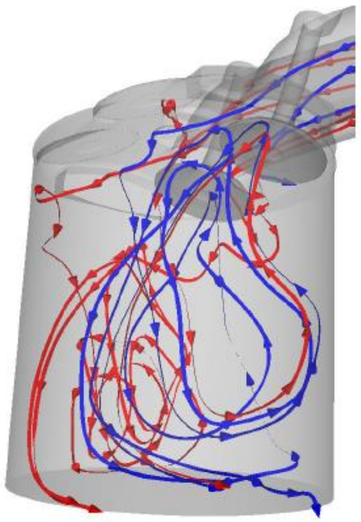
PSA



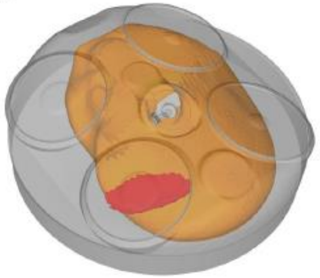


SI ENGINE SIMULATION USING ECFM-ISSIM

VALIDATION ON EB2DT ENGINE

Stephane Chevillard[1], Olivier Colin[1], Julien Bohbot[1], Clément Dumand[2]

Time = 33 CAD

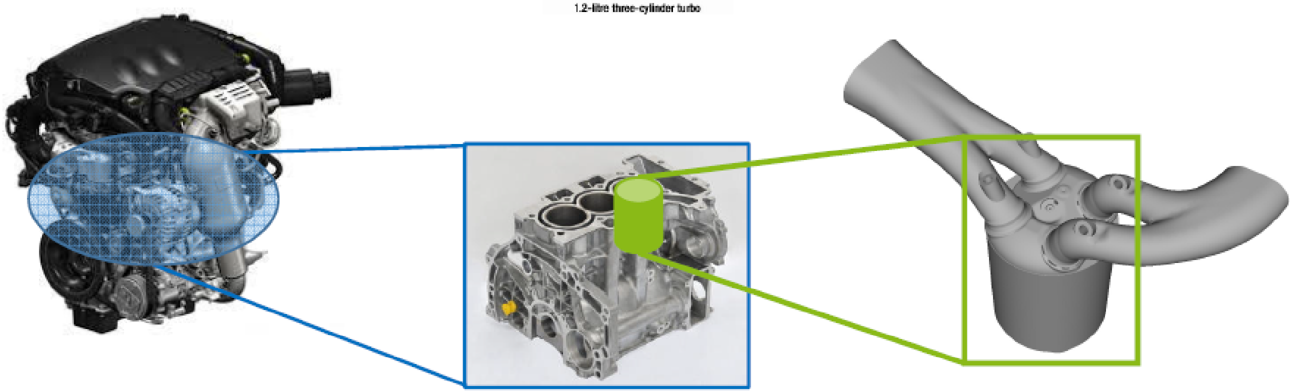


[2] PSA GROUPE

[1] IFP Energies nouvelles

PSA GROUPE ENGINE : 1.2L PURE TECH EB2DT

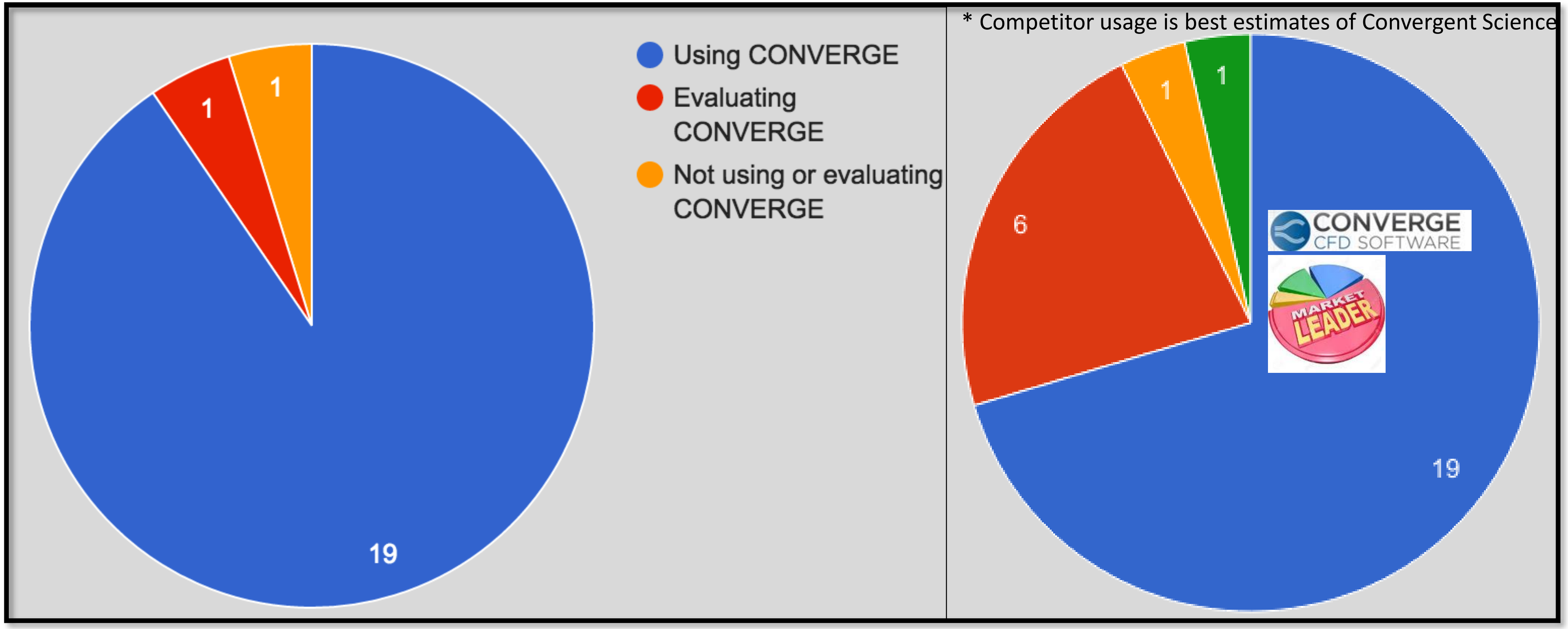
- A real industrial engine configuration
- All following results are normalized
- Only one of the three cylinders is simulated with CONVERGE



Engine capacity	400 cm^3
Compression rate	10,3
Fuel	SP95-E10
DATA base	
High load / RPM	5500rpm / 23 bar
Load variation @ 1750rpm	12 bar and 23 bar IMEP
FAER variation @ 3500rpm/23bar	ϕ_m=1 , ϕ_m=1.1 and ϕ_m=1.3
Load variation @ 4000rpm	13 and 23 bar IMEP

Complex fuel has to be taken into account
Detailed in Vienna presentation

US IC Engine Market Share

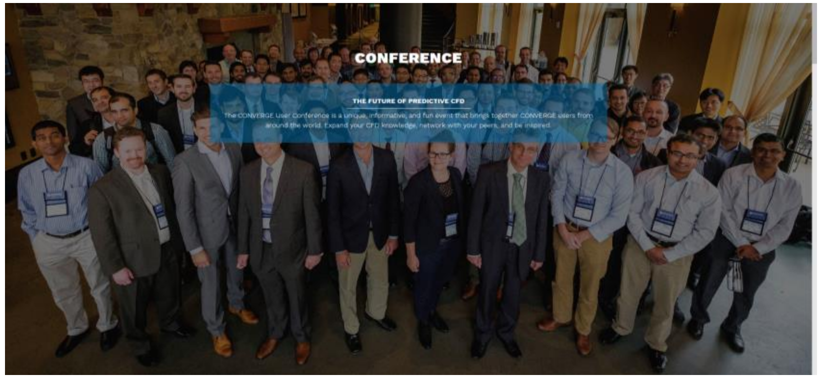


- 20 of 21 (95%) US engine makers use CONVERGE
- CONVERGE is most widely used CFD code for IC engine modeling in this region

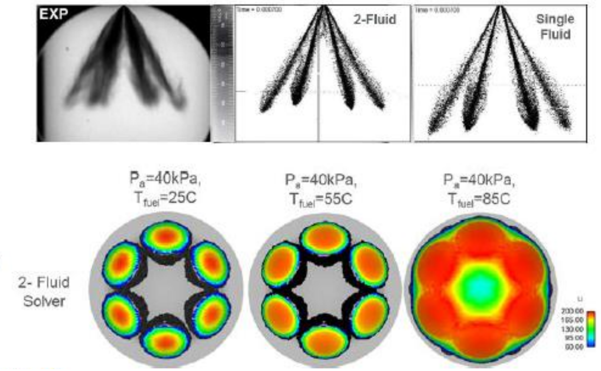
Note: The sum on the right chart reflects that some companies use more than one CFD code for IC engine modeling

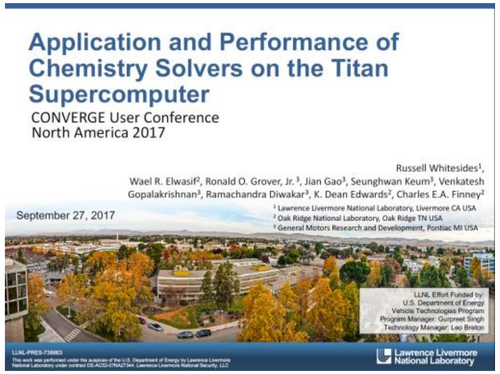
2017 N.A. User's Conference

- Convergent Science had a very productive user conference in Fall of 2017
- Presentations showing CONVERGE work at Renault, Isuzu, Fiat Chrysler, Argonne National Lab, Aramco, Caterpillar, General Motors, Sandia National Lab, IFPEN, SwRI, Oak Ridge National Lab, Navistar, Gamma Technologies
- Topics include Diesel modeling, knock modeling, supercomputing, SCR/urea modeling, conjugate heat transfer, emissions modeling, spray modeling



CONVERGE
USER CONFERENCE
— NORTH AMERICA 2017 —





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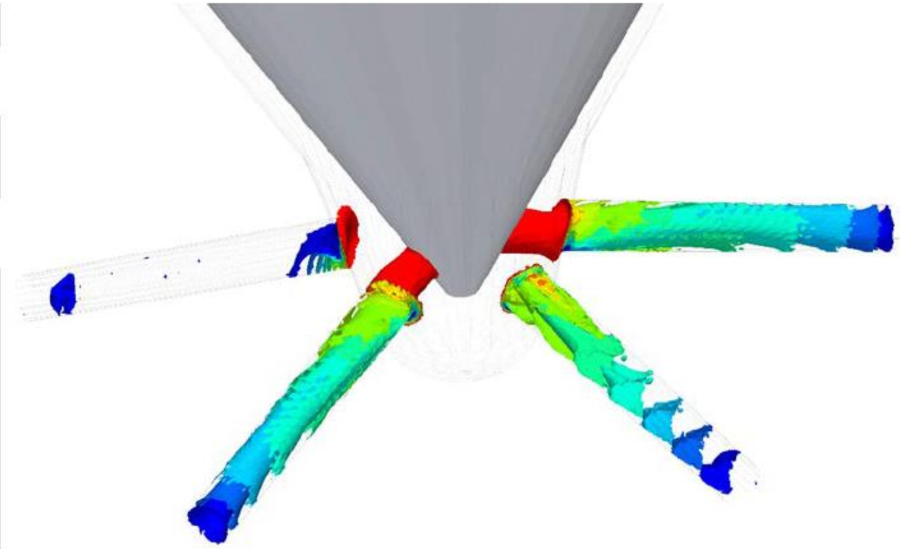
RECENT PROGRESS IN NOZZLE FLOW AND SPRAY MODELING AT ARGONNE



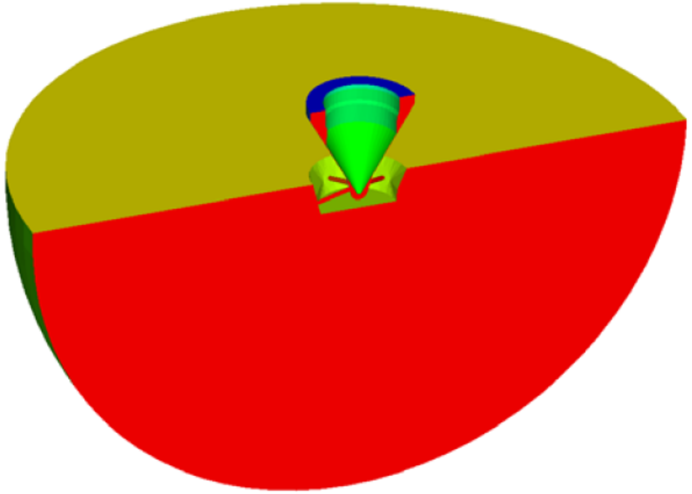
<u>ROBERTO TORELLI</u>, KAUSHIK SAHA, SIBENDU SOM

Argonne National Laboratory
Lemont, IL - USA

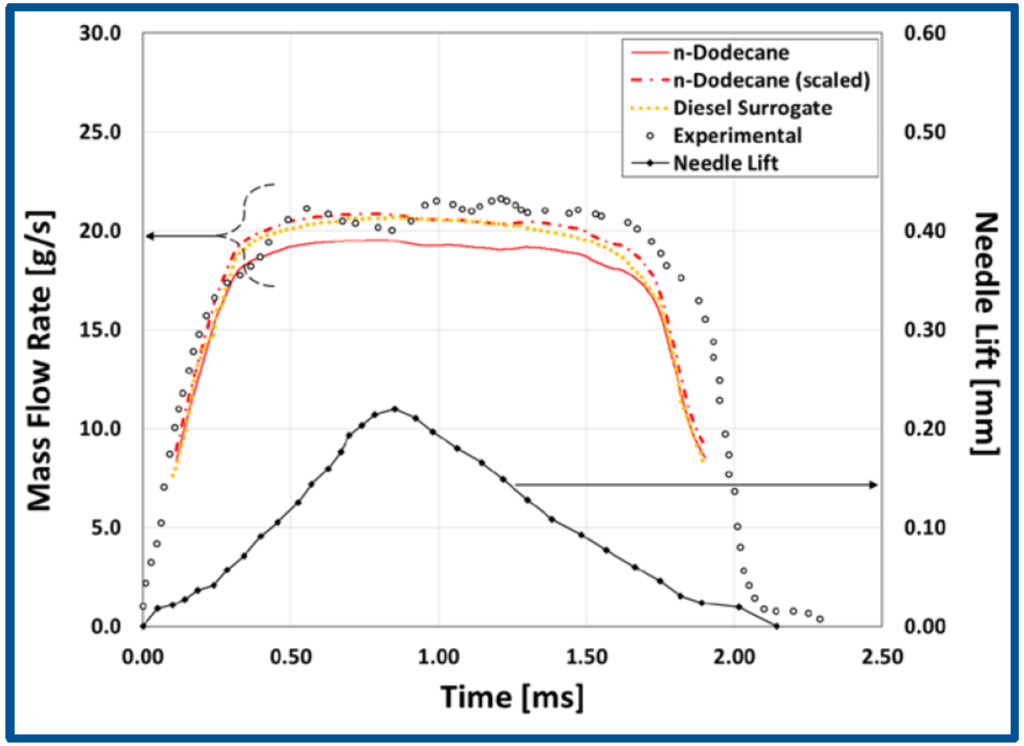
Tuesday September 26, 2017
Converge User Conference – The Dearborn Inn, Detroit, MI

CFD MODELING FRAMEWORK

Mesh strategy



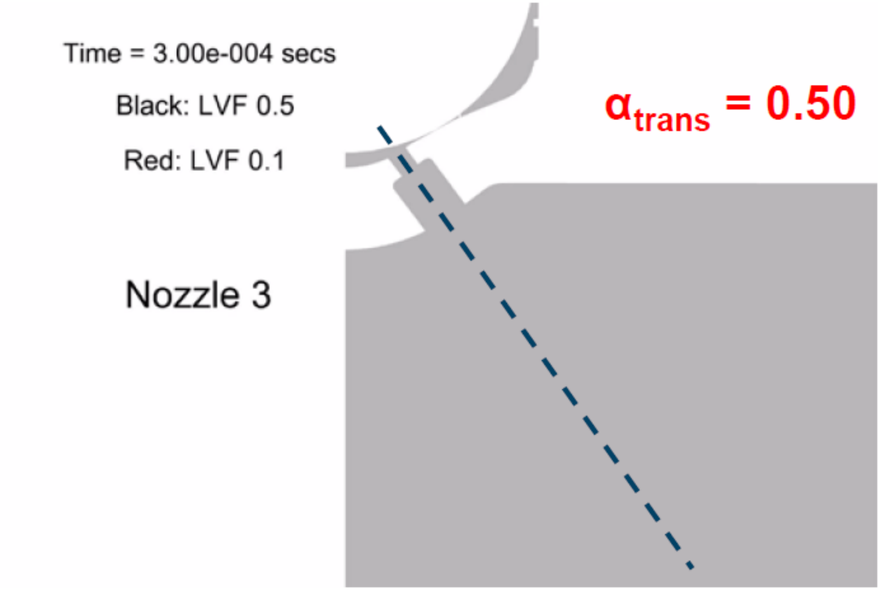
	Data	Units
Base mesh size	160	[µm]
Max refinement level	4	[-]
Min mesh size	10	[µm]
Maximum CFL	0.8 (variable)	[-]
Average time step	8-10 E-09	[s]
Peak cell count	0.55 M	[cells]
Number of cores	16	[procs]
Run Time (best case)	350	[h]

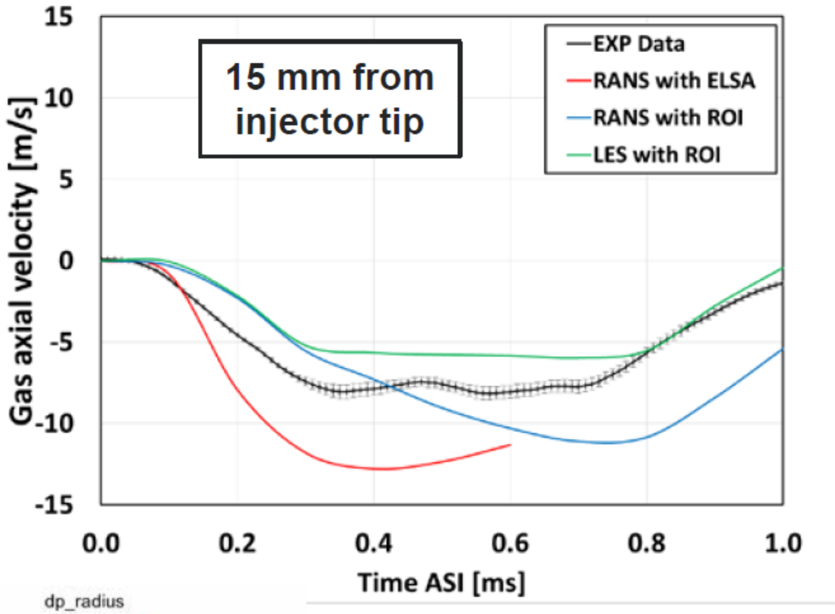


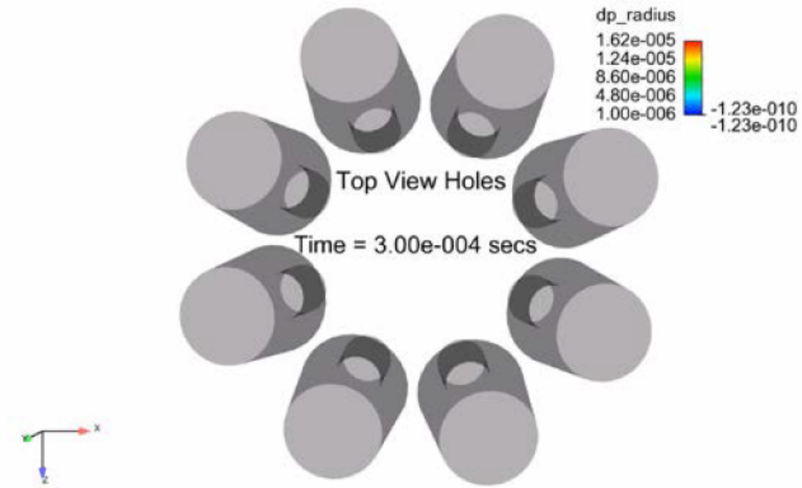
Torelli, R., Som, S., Pei, Y., Zhang, Y. et al., "Comparison of In-Nozzle Flow Characteristics of Naphtha and N-Dodecane Fuels," *SAE Technical Paper 2017-01-0853*, 2017.

SPRAY G ELSA (ONGOING ACTIVITY)

Liquid-gas coupling and gas axial velocity



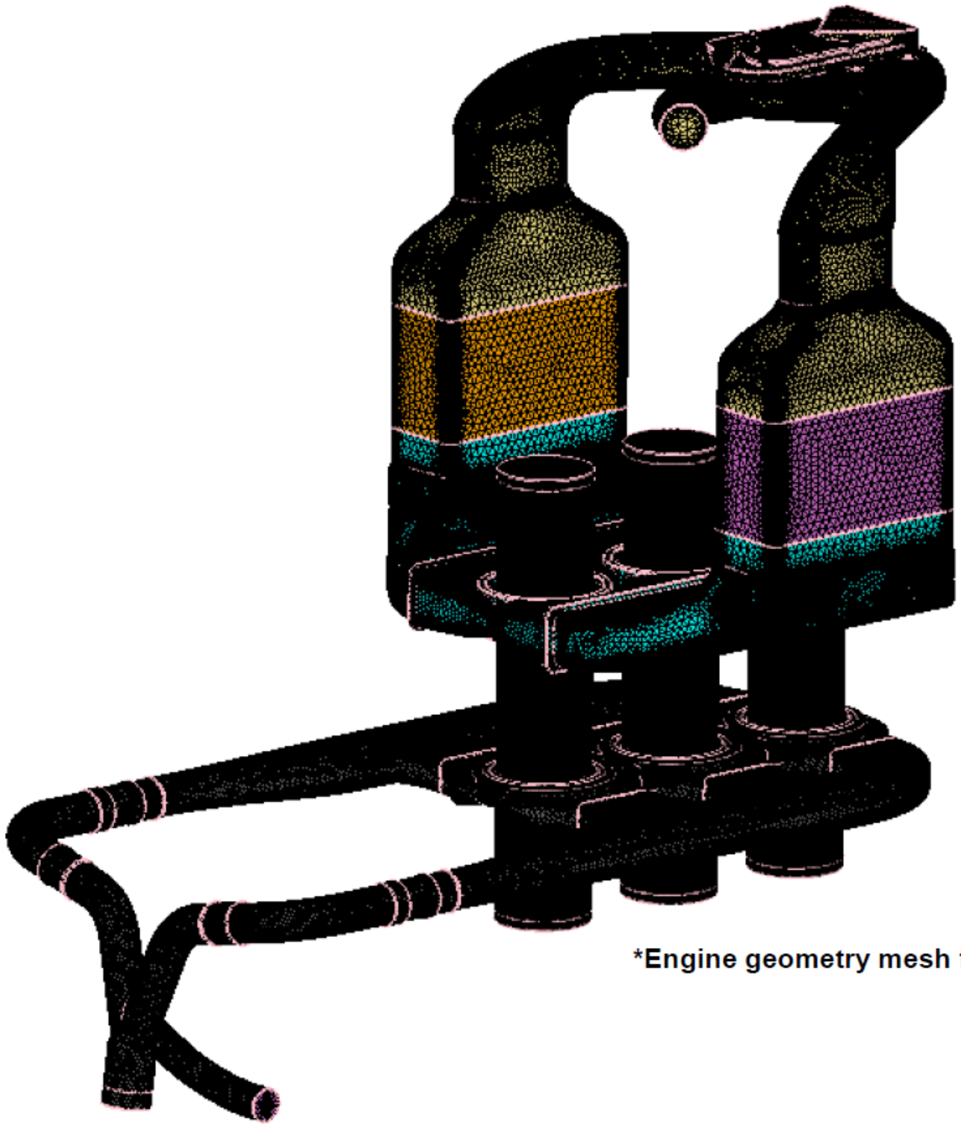




Argonne NATIONAL LABORATORY

Open Cycle Process

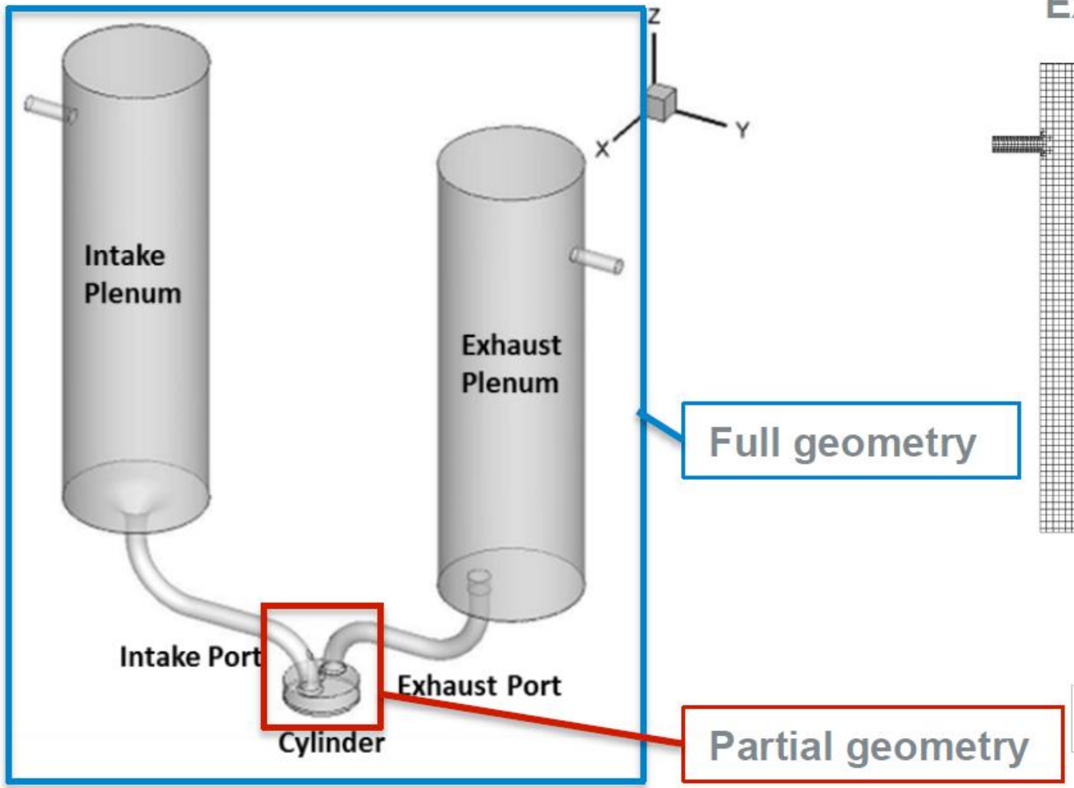
- Up to 6 cylinder geometry
  - With intake and exhaust ports that are cover and uncovered by the piston skirts
- Entire engine cycle
  - Combustion is represented by a pressure trace from GT-Power or measurements
  - Transient pressure boundary conditions obtained from GT-Power simulations or high speed measurements
- User Define Function (UDF)
- Closed couple coolers simulated as porous media

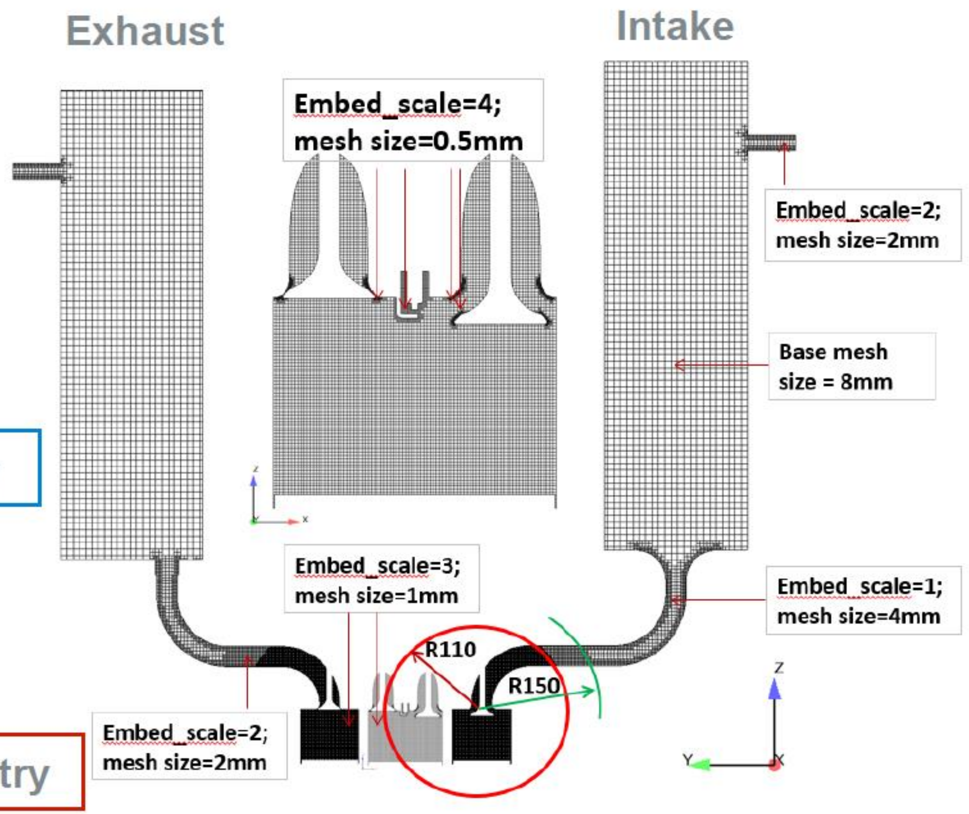


*Engine geometry mesh for Converge

achatesPOWER™

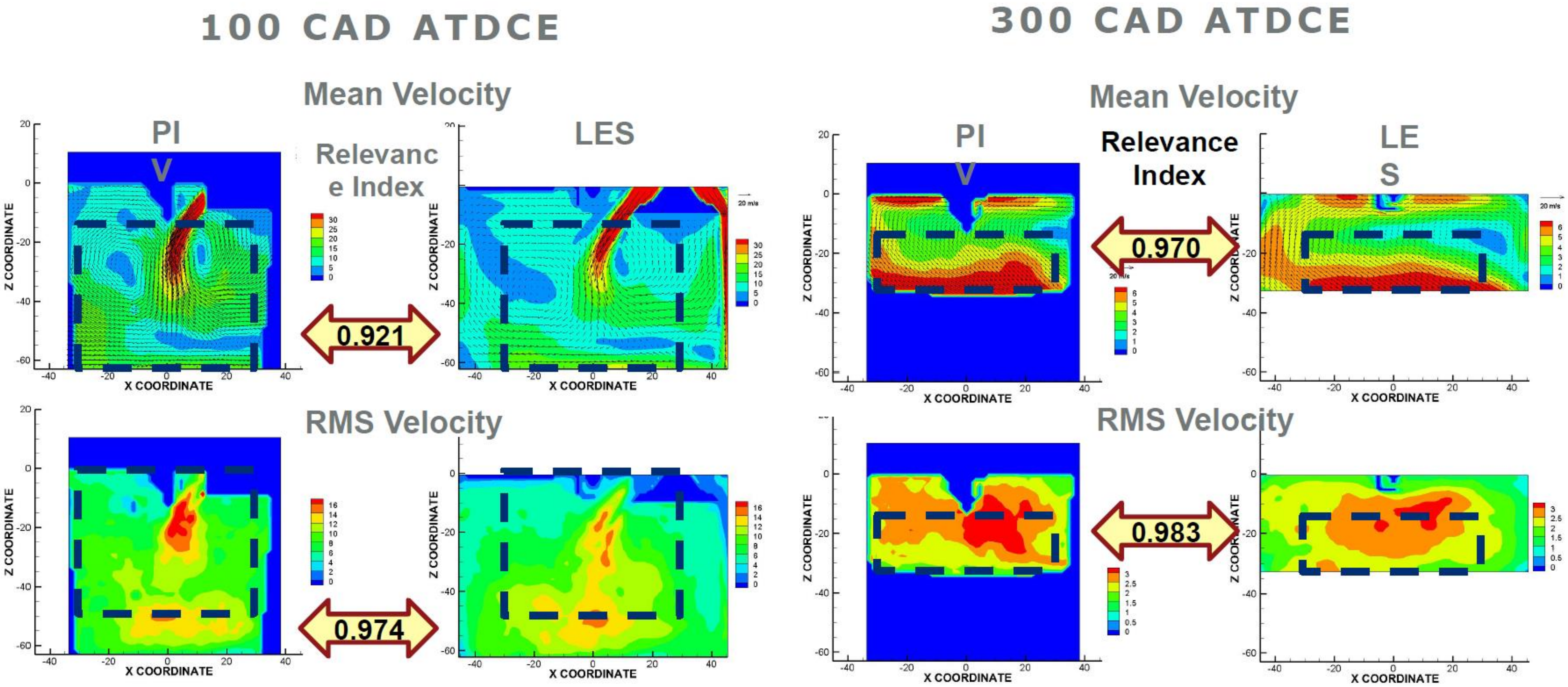
3D COMPUTATIONAL DOMAIN AND MESHING





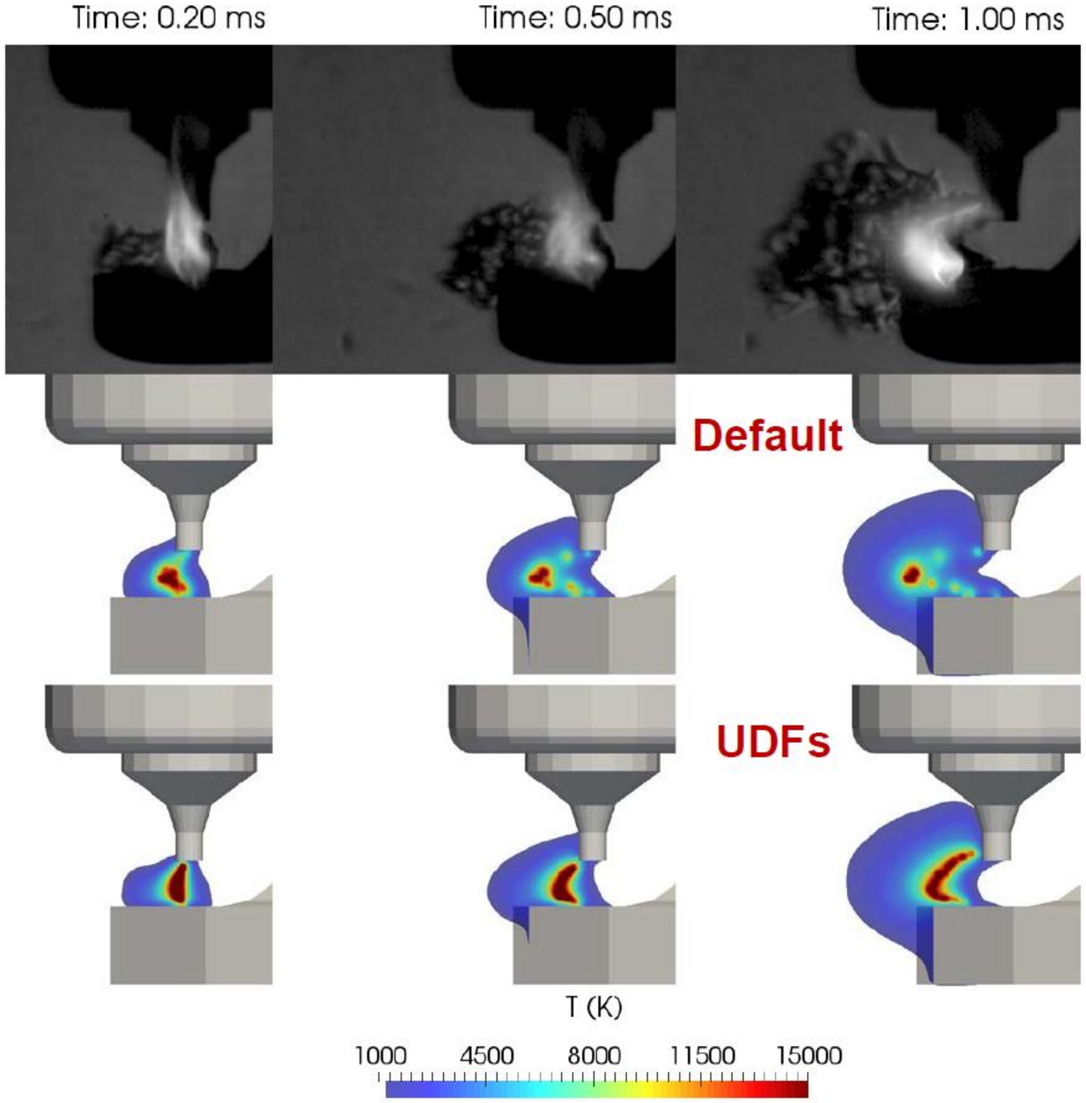
- Mesh arrangement with in-cylinder mesh size of 1 mm
- GT-Power modeling results are used to define boundary conditions for 3D CFD simulation

56-CYCLE AVERAGE, TCC 800RPM 95KPA



T. Kuo, X. Yang, V. Gopalakrishnan, Z. Chen, "**LES FOR IC ENGINE FLOWS**", Oil & Gas Science and Technology-Revue d IFP Energies nouvelles, Vol. 69(2014), No.1, pp.61-81

Spark ignition Model Development at ANL



Modified model behavior:

- More realistic channel shape in the flow field
- Energy is deposited evenly along the channel
- End points keep moving along the electrodes
- Channel is not centered with respect to the flame
- Flame propagation is slow
- Flow-field from simulations might not be accurate
- Combustion model and kinetic mechanism (GRI Mech 3.0) were not investigated

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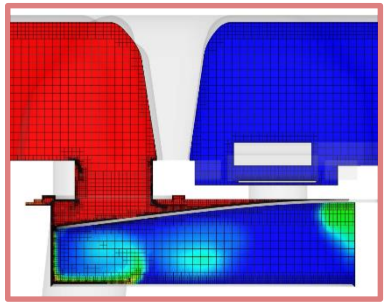
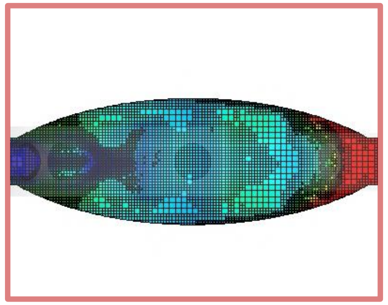
Argonne

Compressors and Pumps: Classification

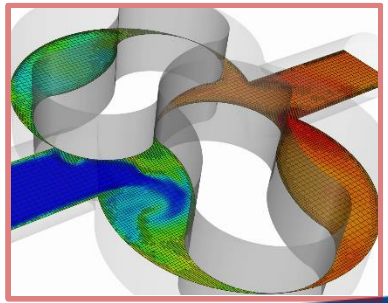
- **Compressors and Pumps**
  - **Positive Displacement**
    - **Reciprocating**
      - **Piston**



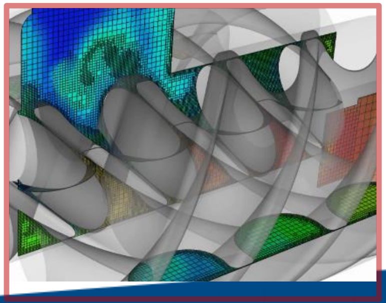
      - **Diaphragm**



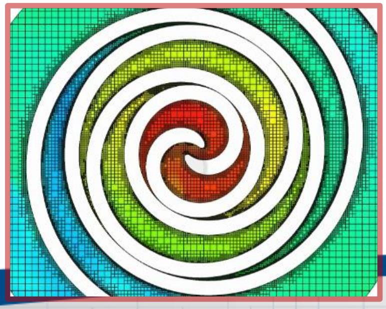
    - **Rotating**
      - **Lobe**



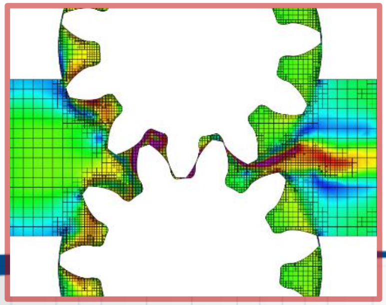
      - **Screw**



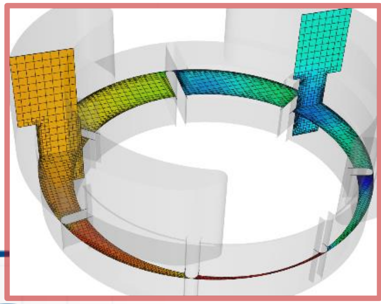
      - **Scroll**



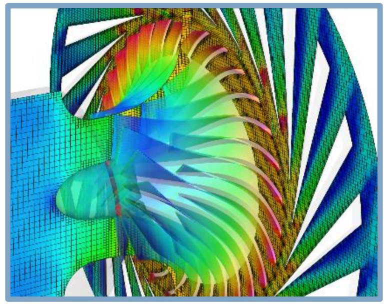
      - **Gear**



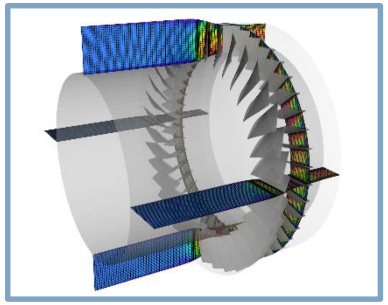
      - **Vane**



  - **Dynamic**
    - **Centrifugal**



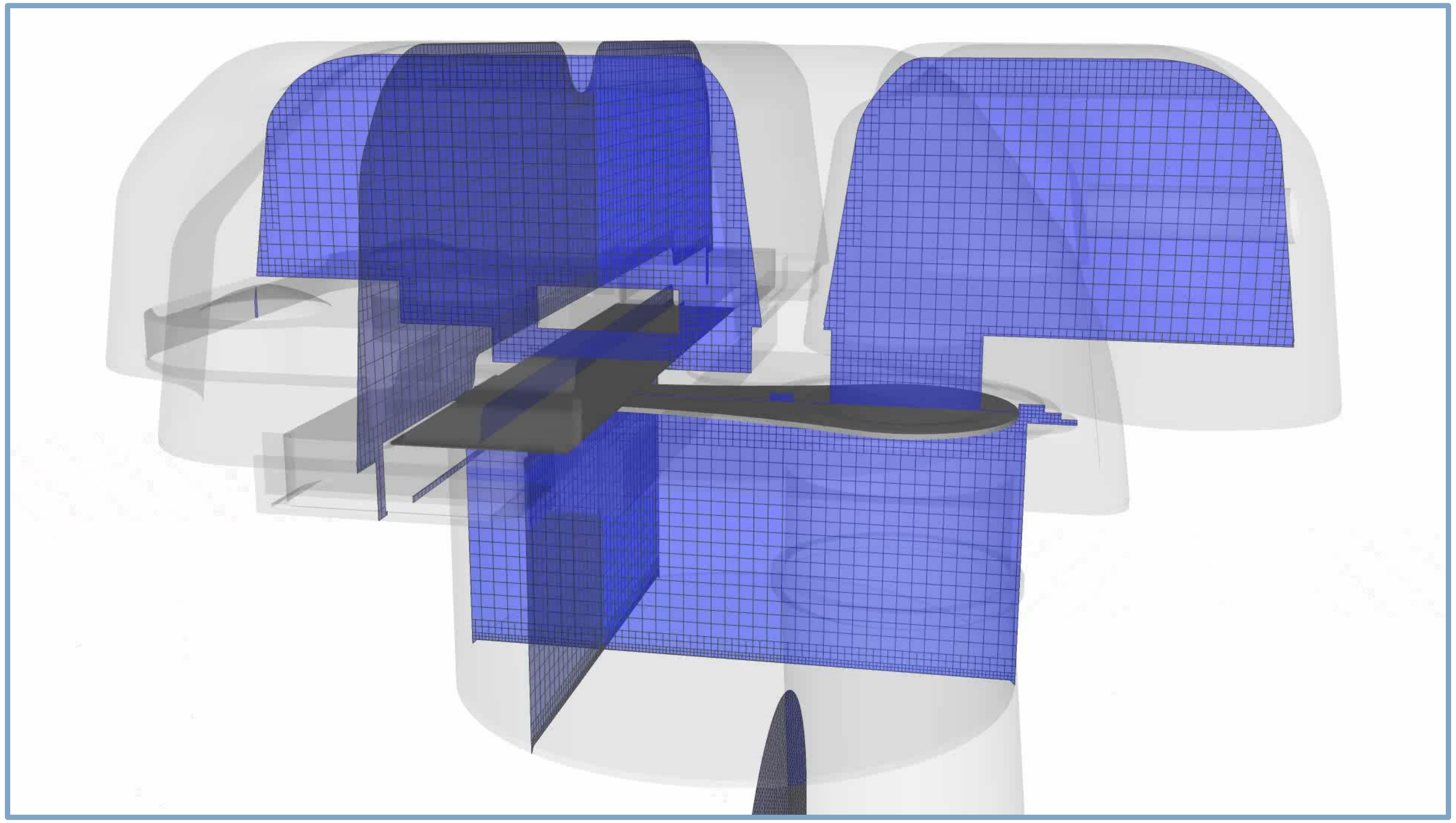
    - **Axial**



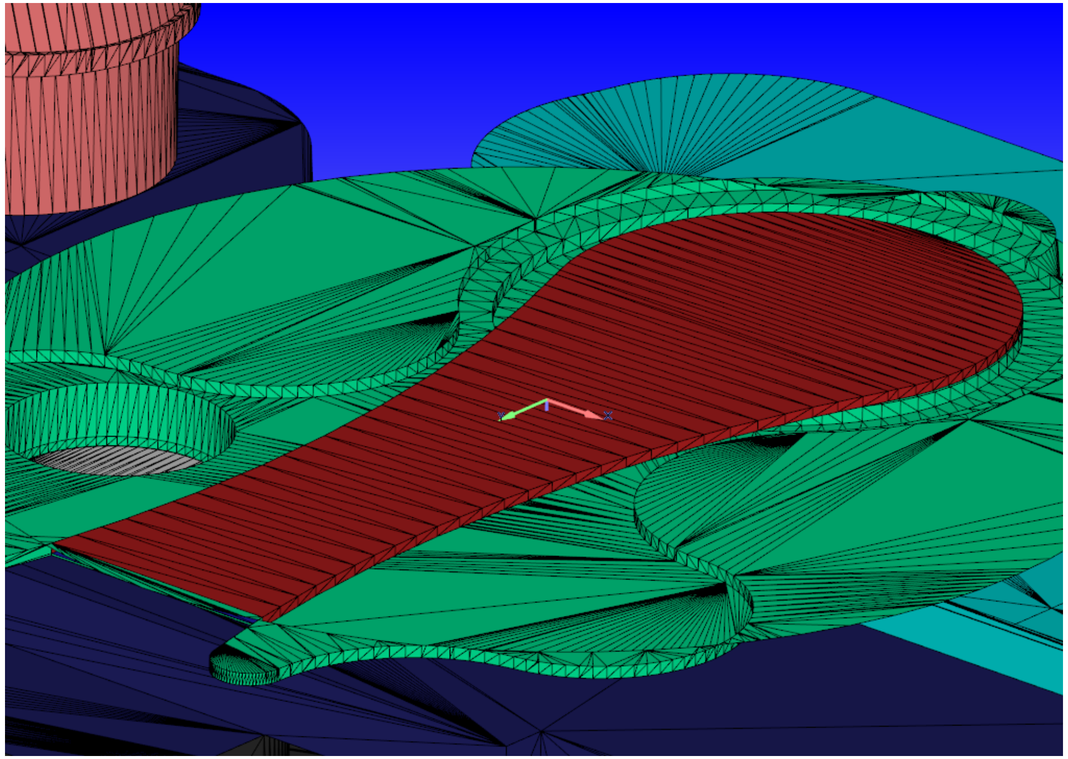
Reciprocating Compressors: Reed Valves

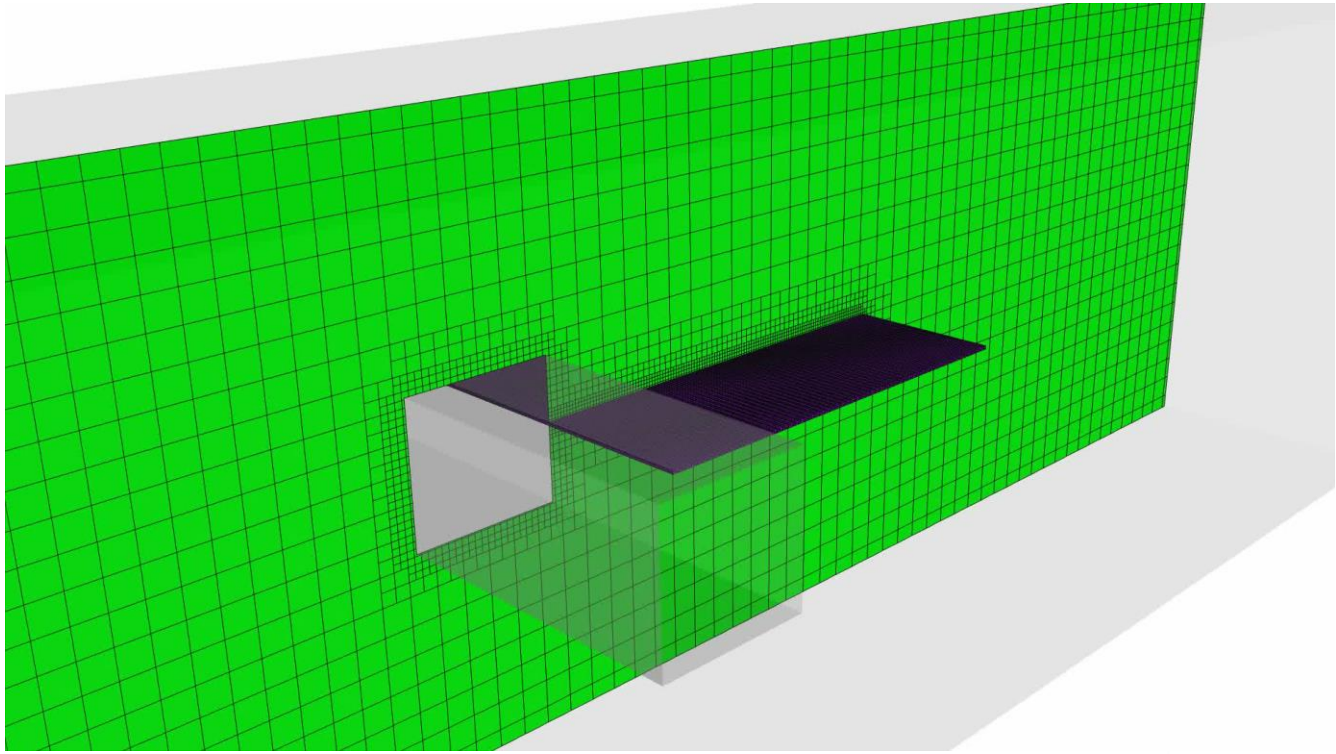
Key Modeling Challenges

- Piston motion
- Small clearances
- Valve dynamics
- Complex geometries (mufflers)
- Gas properties
- Multiphase: oil, condensation
- Pressure waves
- Leakage losses



Reciprocating Compressors: Reed Valves





Beams are modeled with 1D Euler beam equation

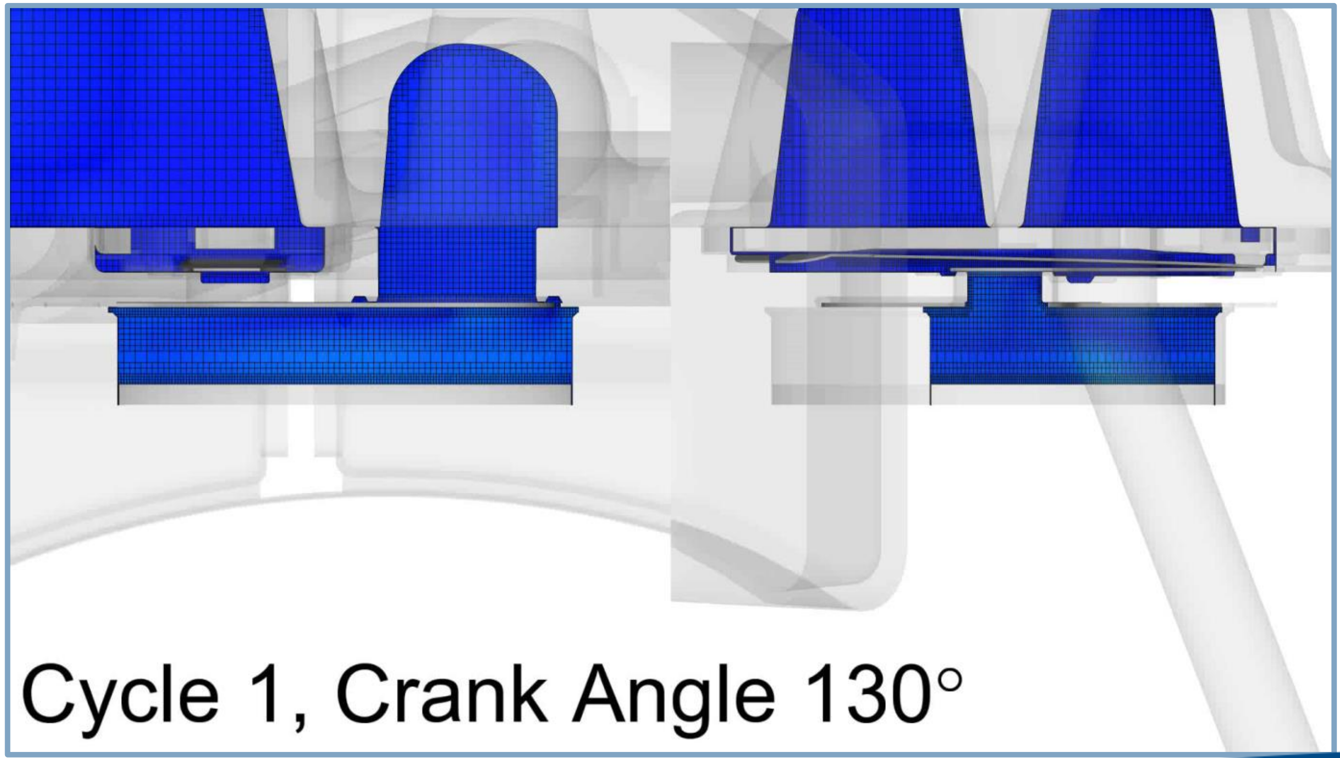
Implemented through user_motion UDF

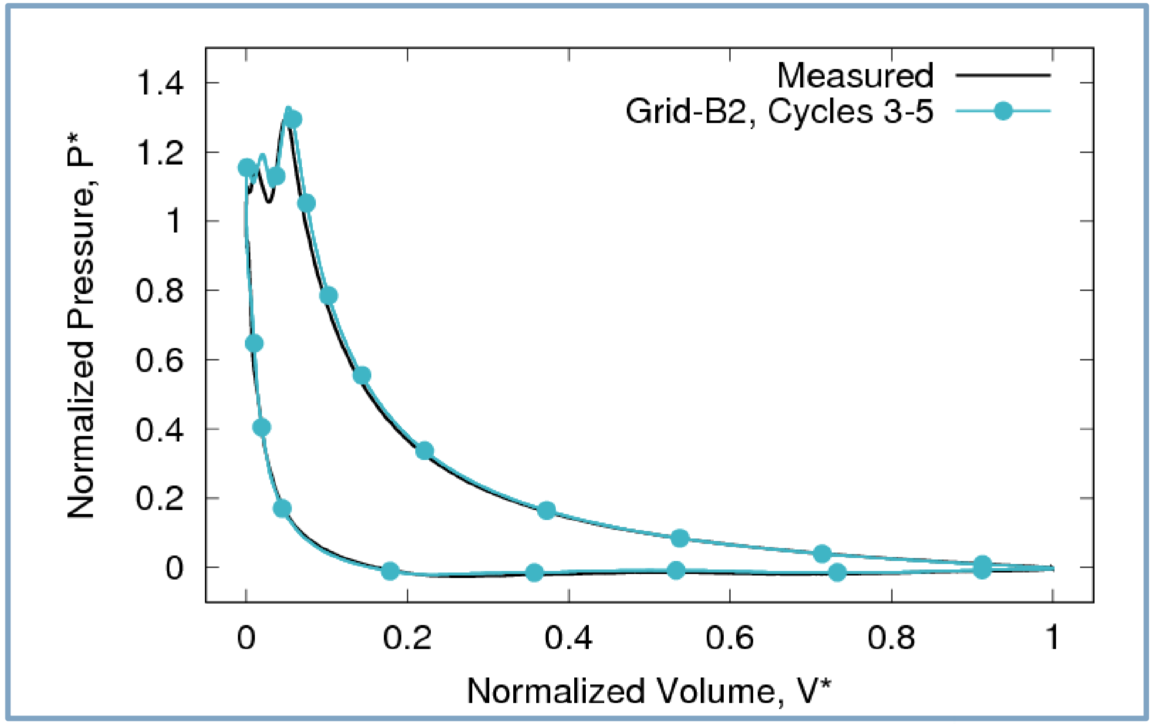
Custom events to trigger valve seating and opening

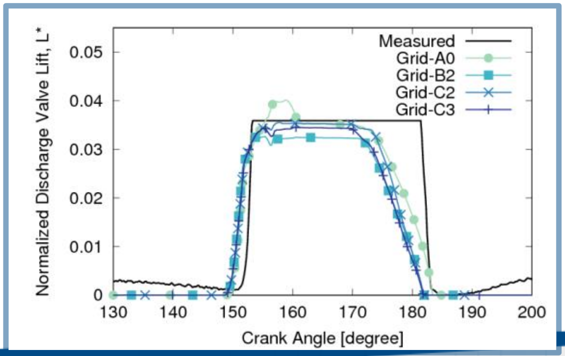
Reciprocating Compressors: Reed Valves

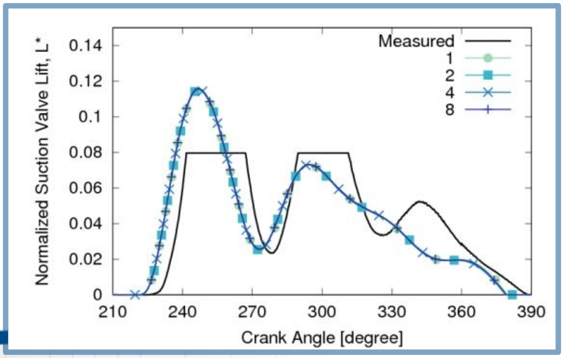
Validation case: R-134a refrigeration compressor

Measurements of valve lift and cylinder pressure





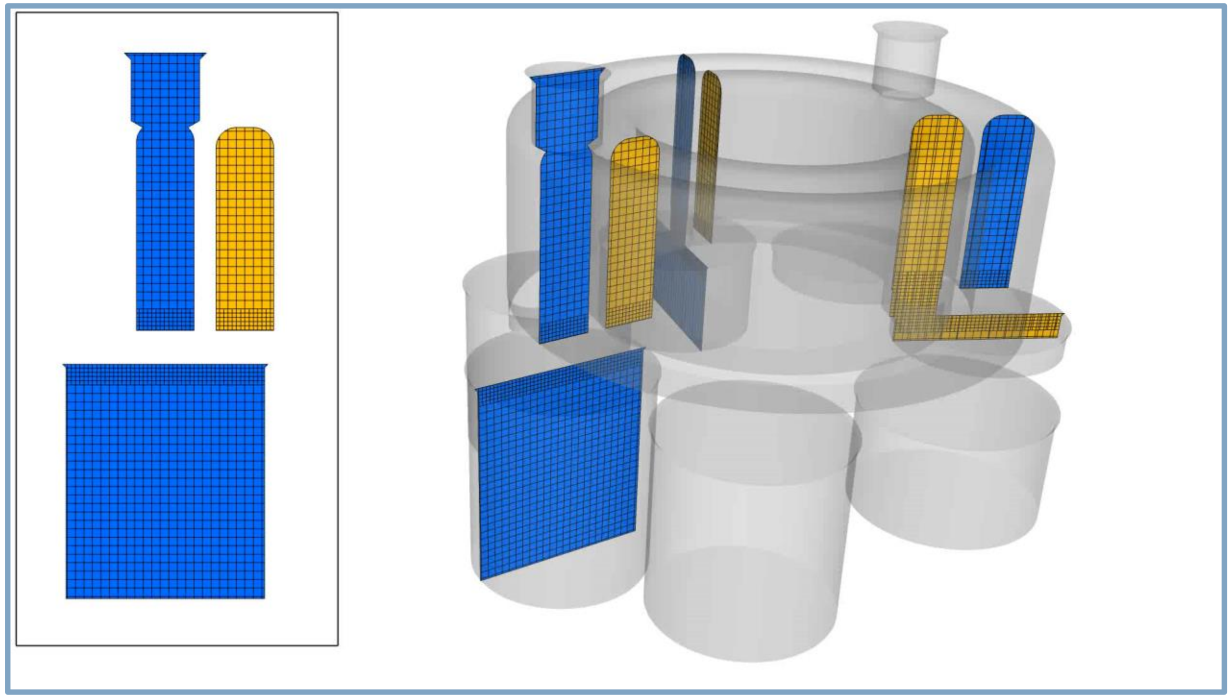




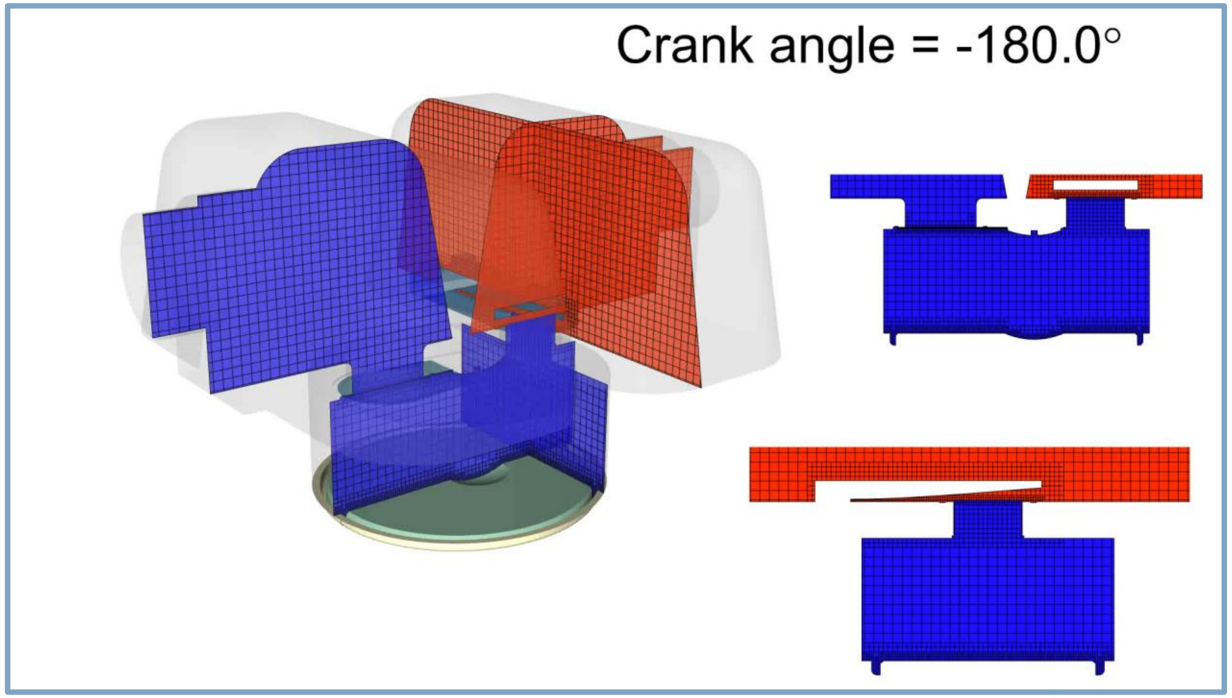
Reciprocating Compressors: Reed Valves

Related Applications

Swashplate Automotive AC Compressor



Wobbling Piston Medical Pump



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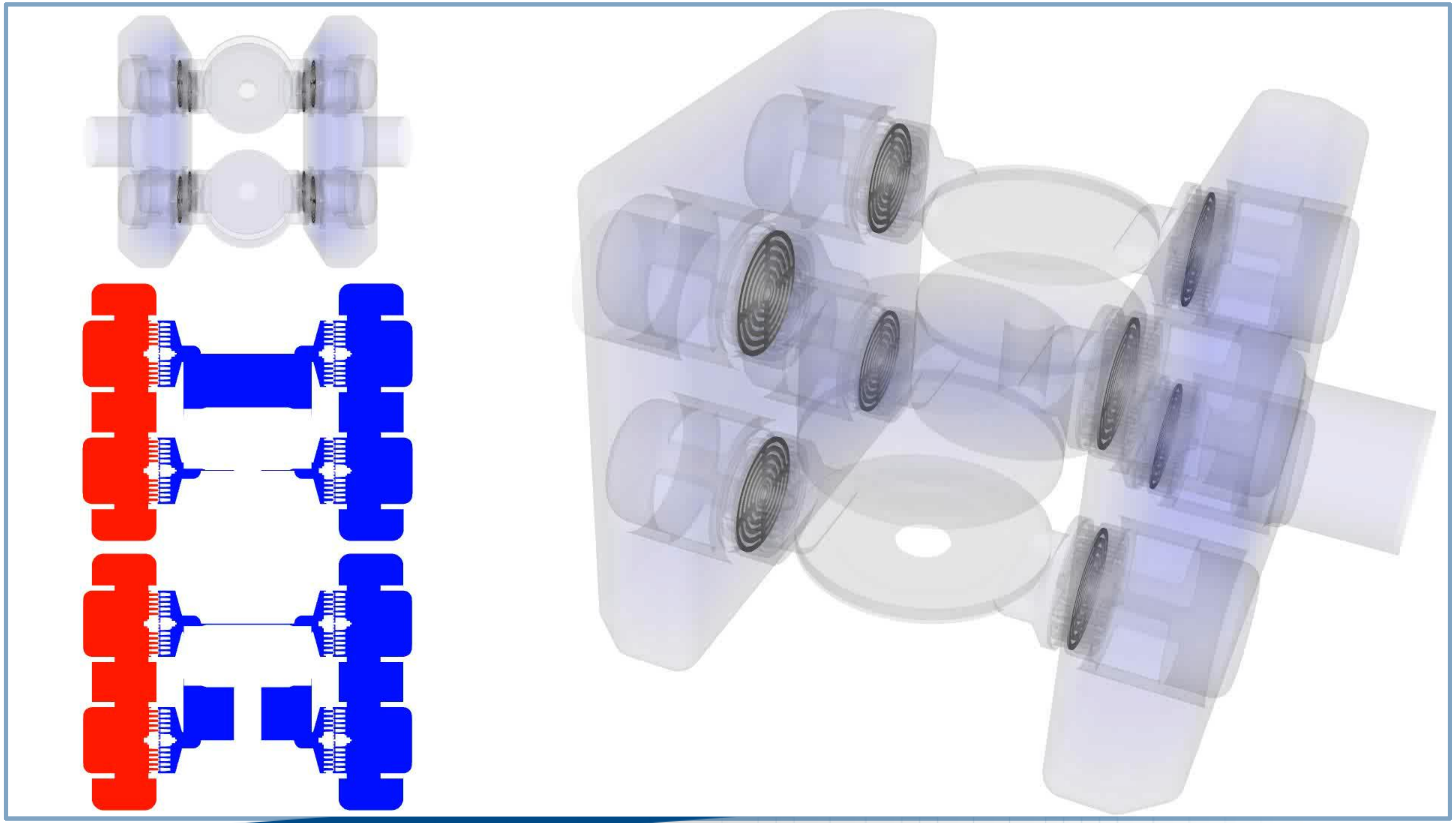
Reciprocating Compressors: Plate Valves

Industrial gas processing compressors (air, natural gas, CO2, ammonia, etc.) utilize larger, slower compressors with plate valve, poppet valves, or other similar valve types.

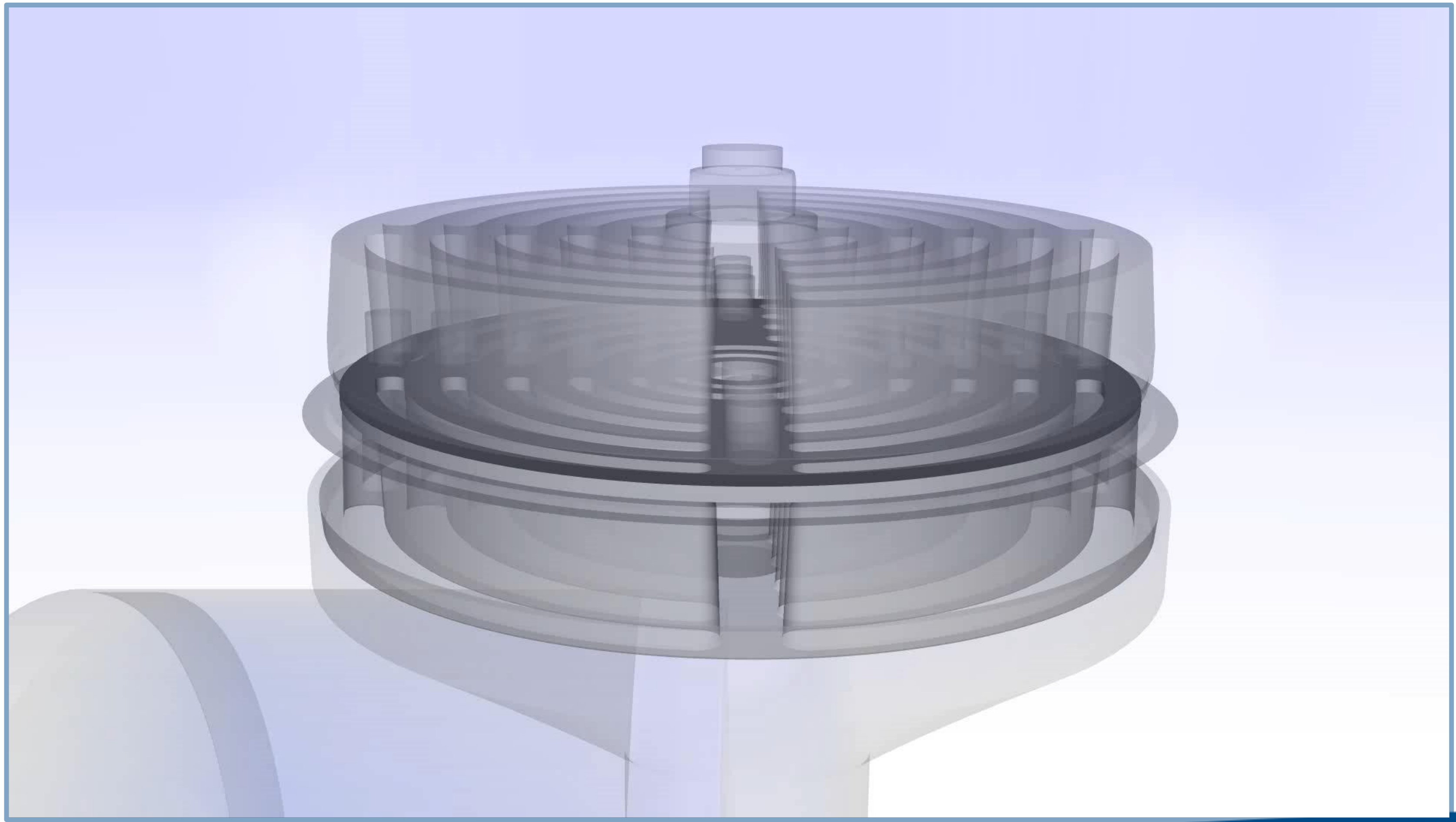
Predicting the pressure pulsations, temperature distribution, and valve dynamics are of key importance.

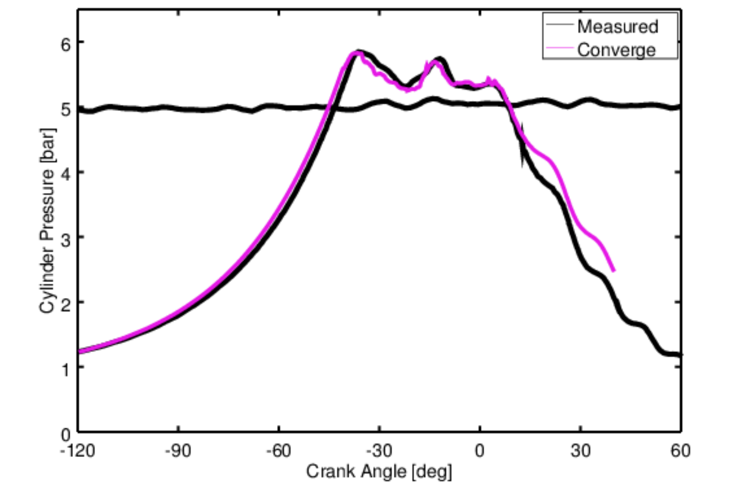


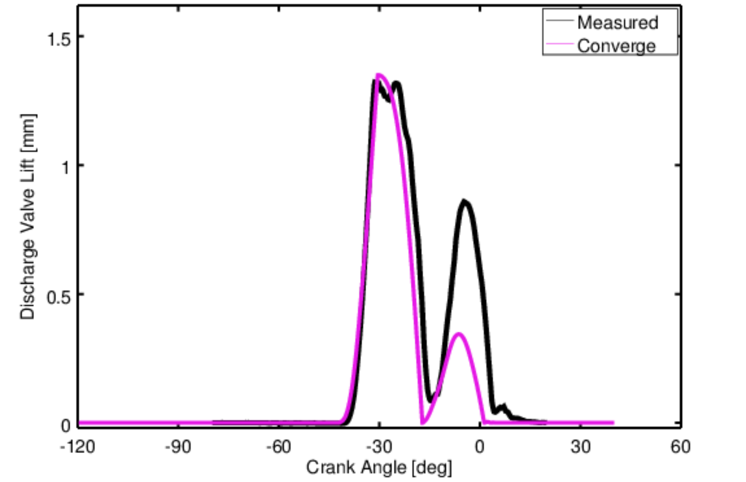
Reciprocating Compressors: Plate Valves

Validation case is a 0.22 bore, 700 rpm double-acting air compressor

Measured cylinder and muffler pressures and valve lifts







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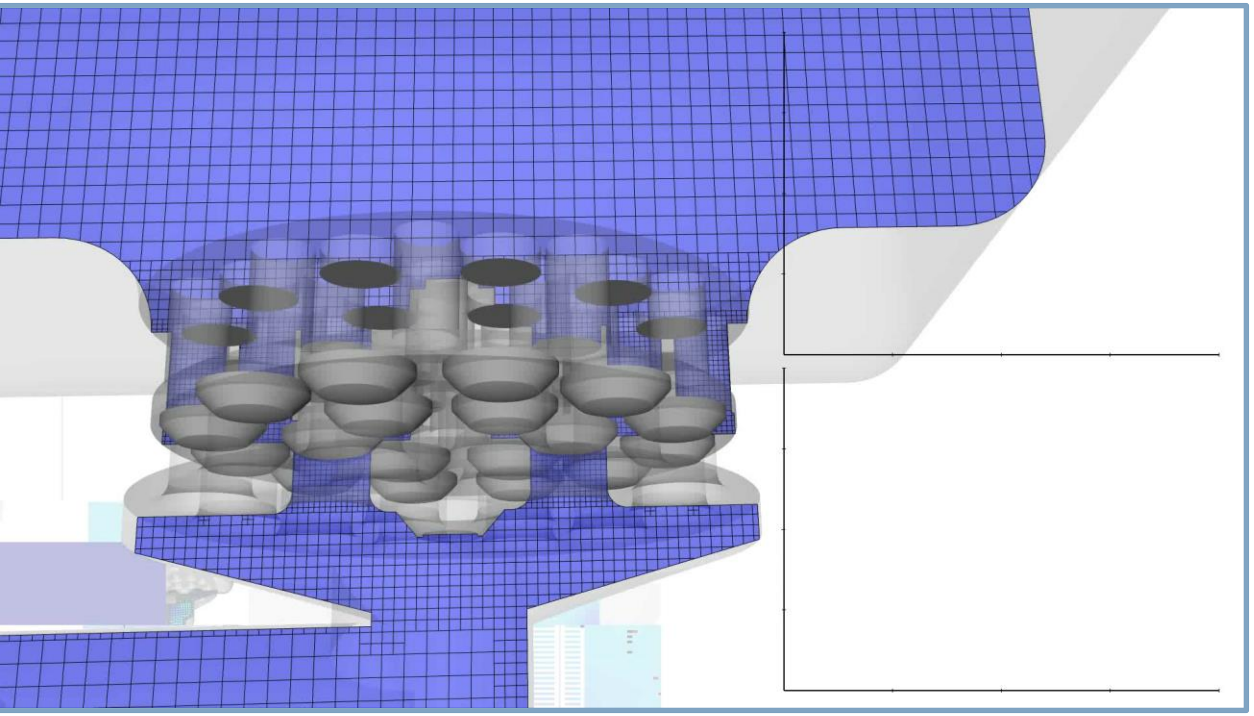
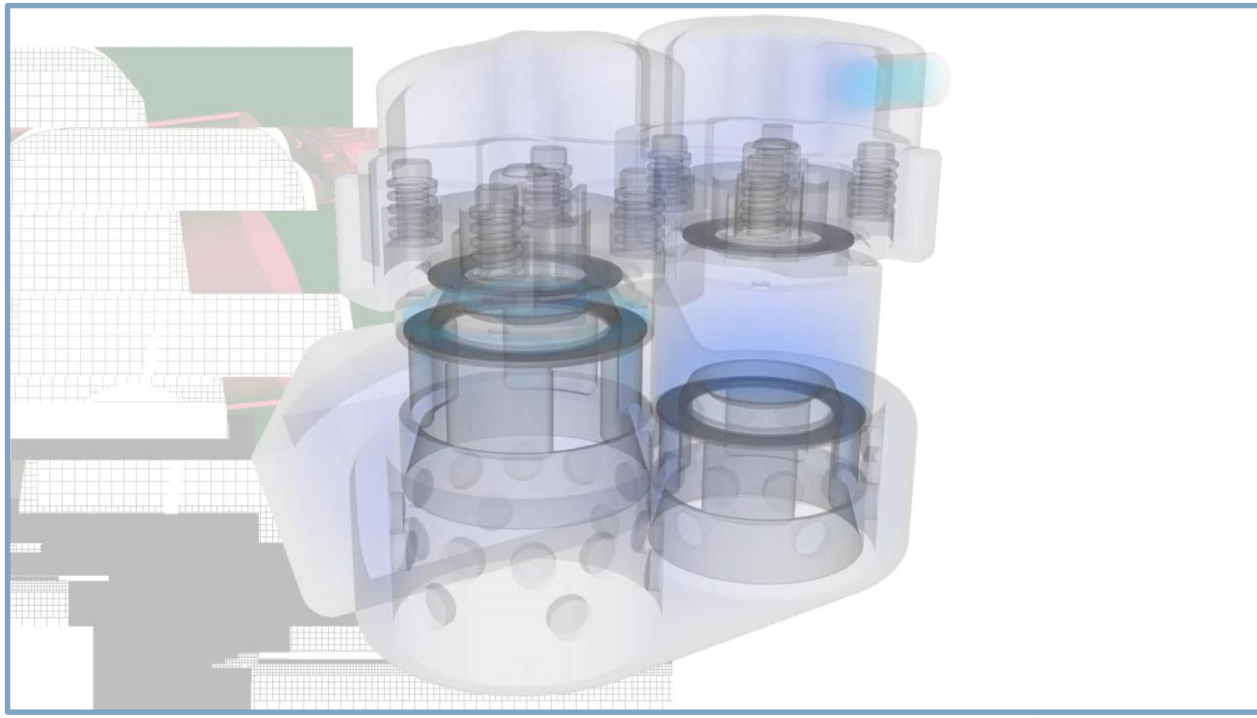
Reciprocating Compressors: Plate Valves

Related Applications

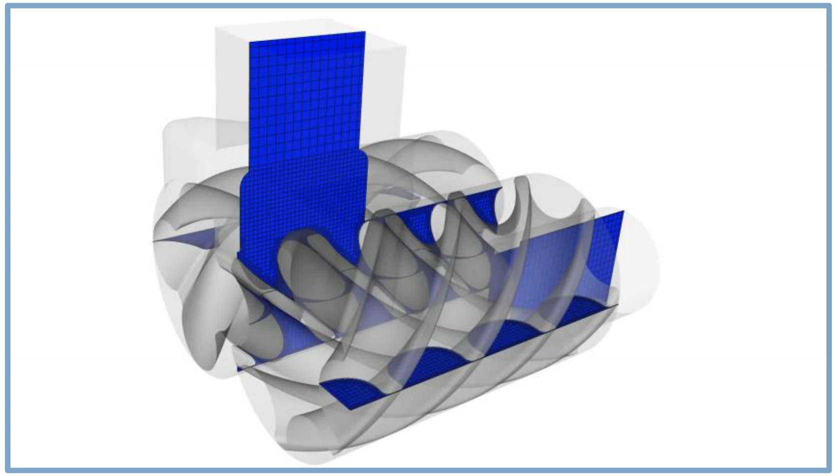
Poppet Valve Arrays

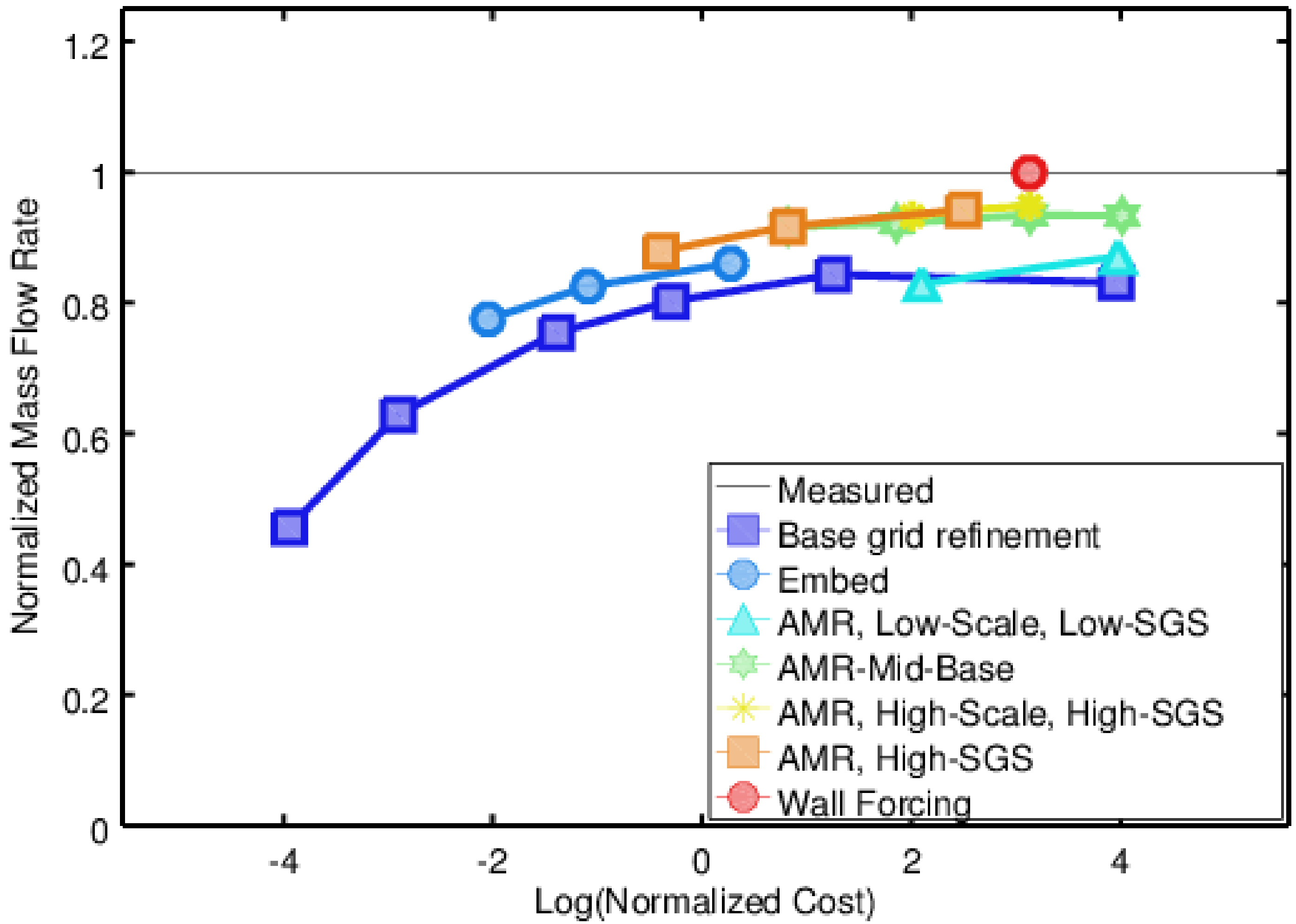


Ring Valves



Screw Compressors: Twin Screw Supercharger





Some key modeling issues on screw compressors:

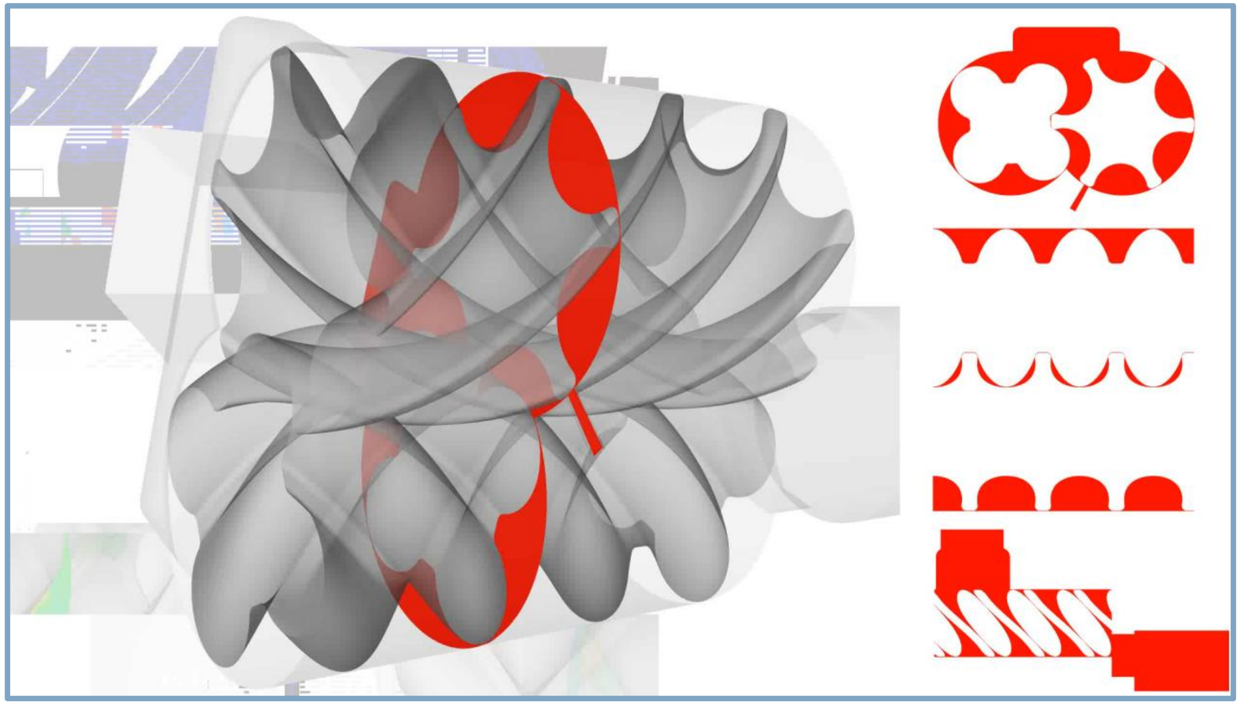
complex motion grid generation (not a problem for CONVERGE)

Resolving or modeling flow through small clearances

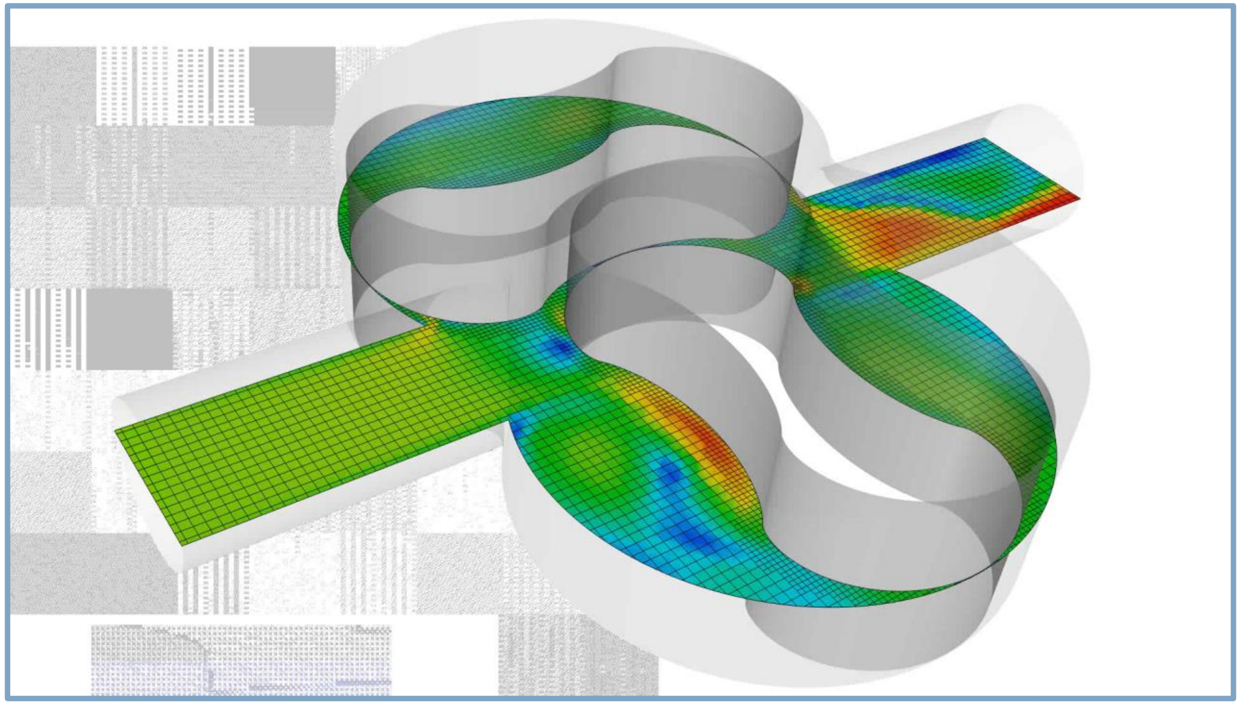
Screw Compressors: Twin Screw Supercharger

Related Applications

Liquid Flooded Screw Compressor



Roots Blower Supercharger



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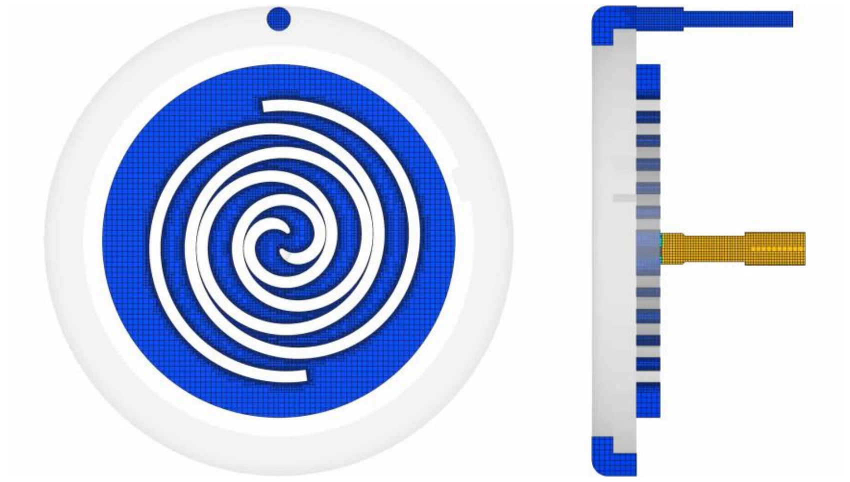
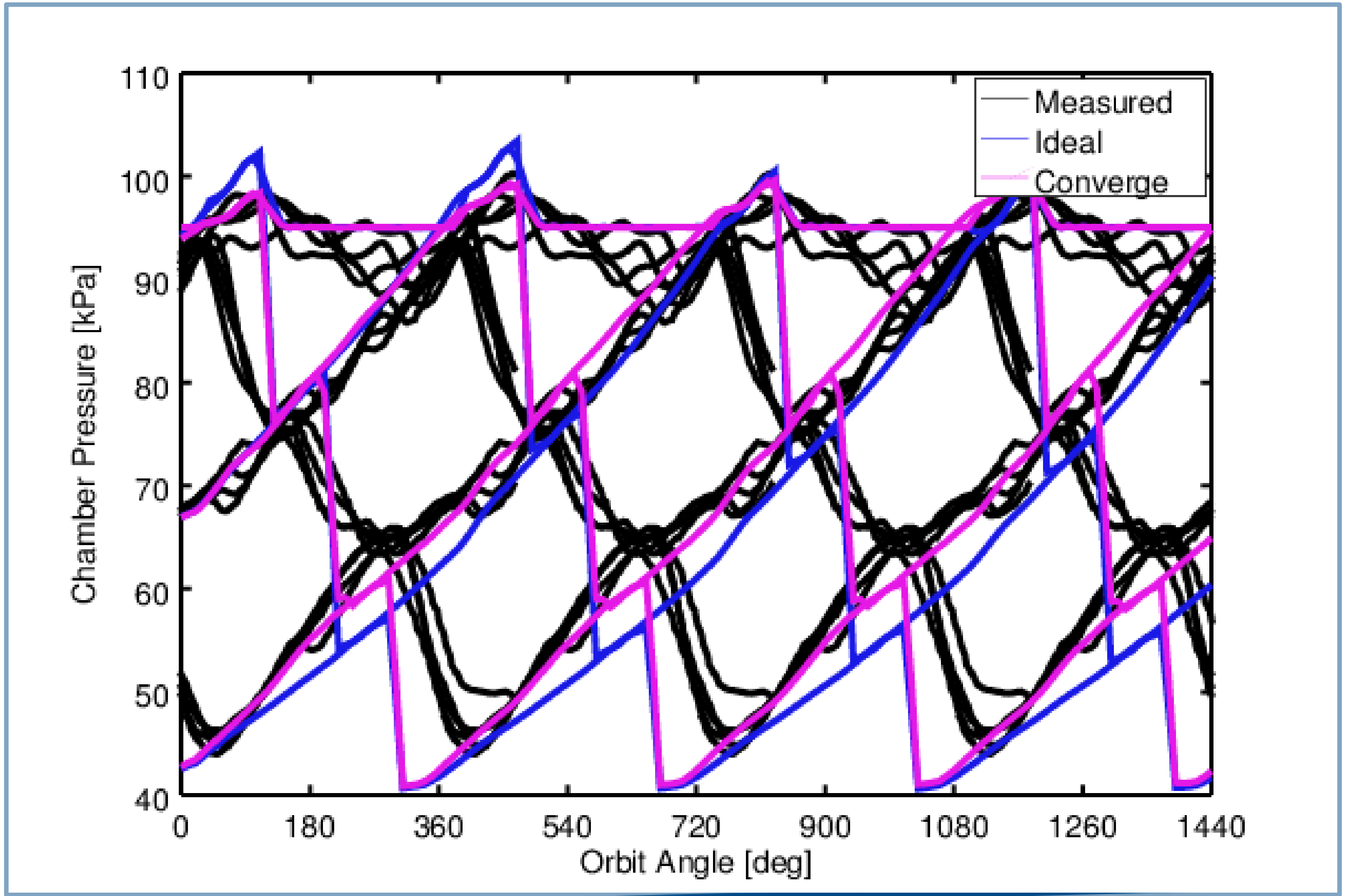
Scroll Compressors: Dry Scroll Vacuum Pump

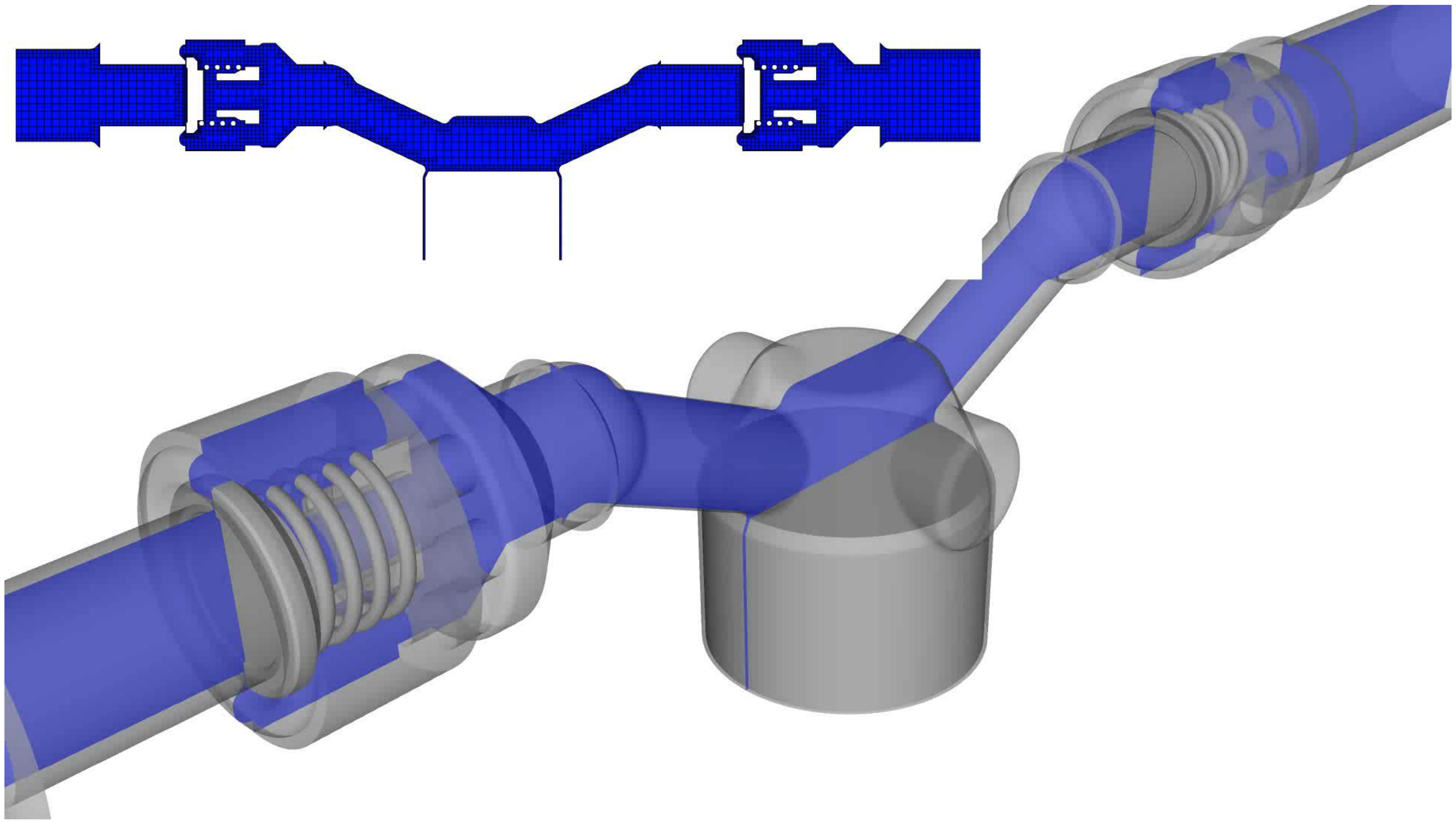


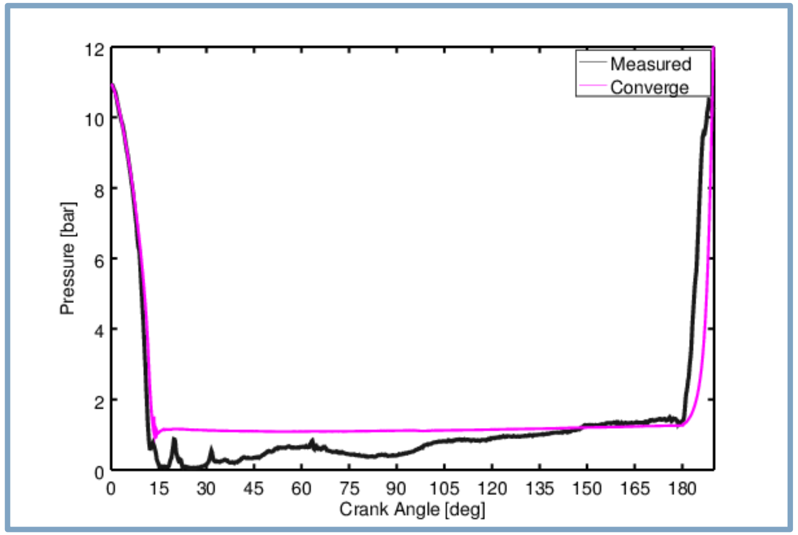


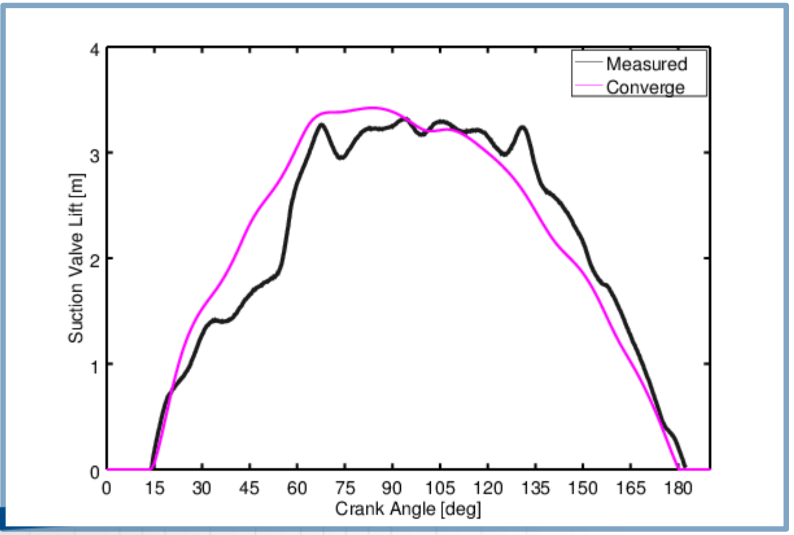
Scroll compressor validation case is a dry scroll vacuum pump operating between 17 kPa and 95 kPa

Modeling the clearance flow is critical to obtaining the non-ideal performance curves.

Reciprocating Pumps: High Pressure Fuel Pump







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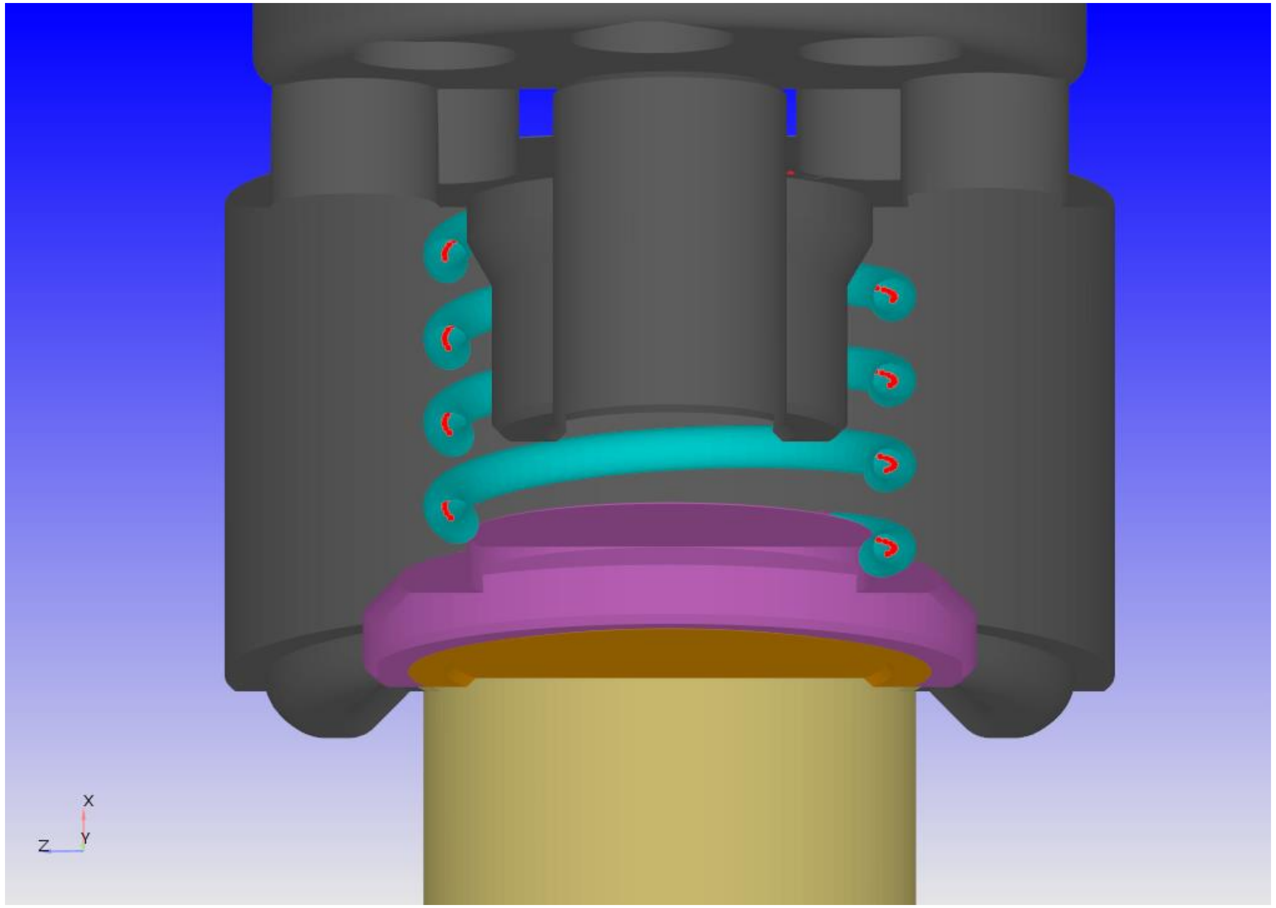
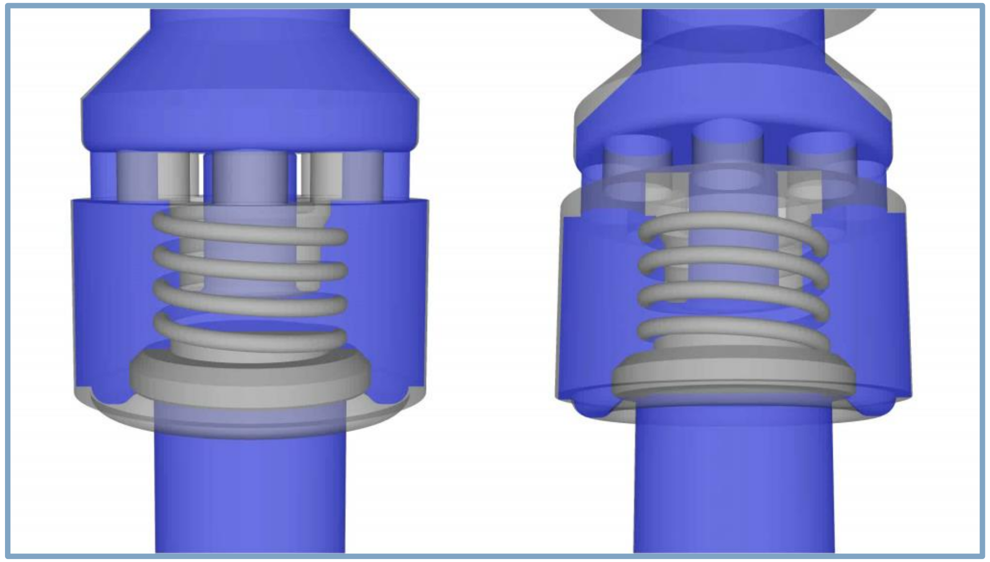
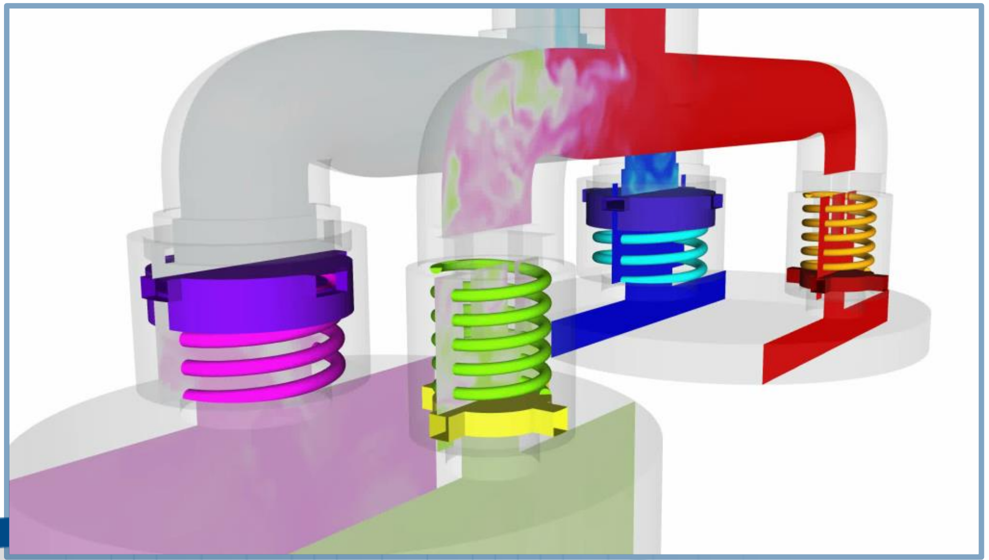
Reciprocating Pumps: High Pressure Fuel Pump

New volume-conserving spring motion function:



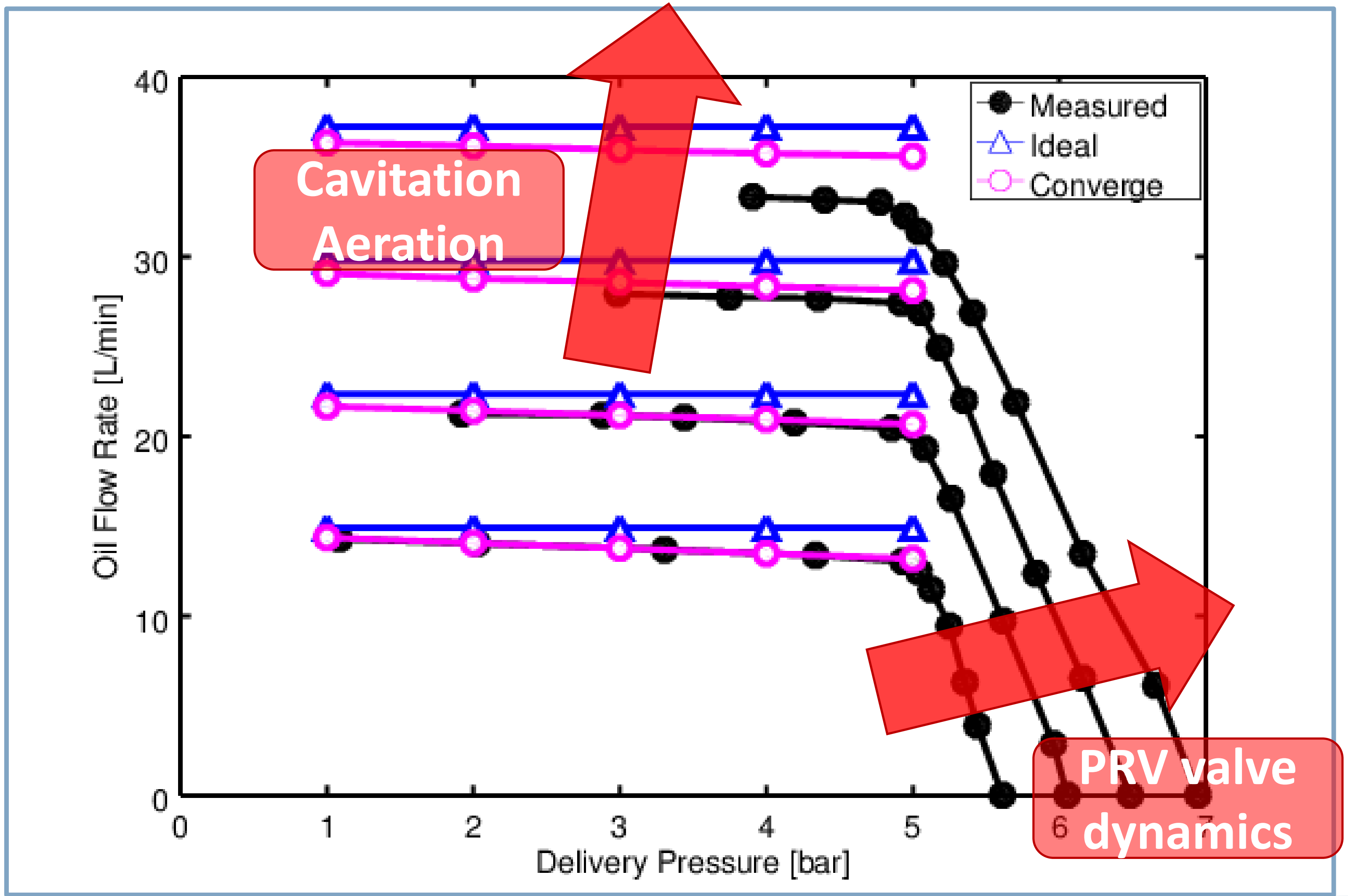


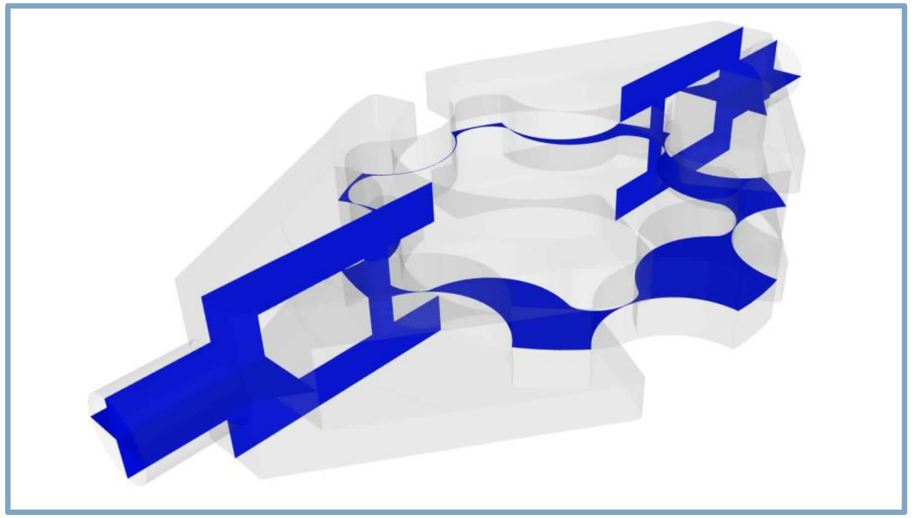


Helix centers and cross sections automatically detected

Volume-conserving mappings applied based on position

Gear Pumps: Gerotor Oil Pump





Gerotor validation case:

Proper clearance flows are required to obtain differences from ideal capacity

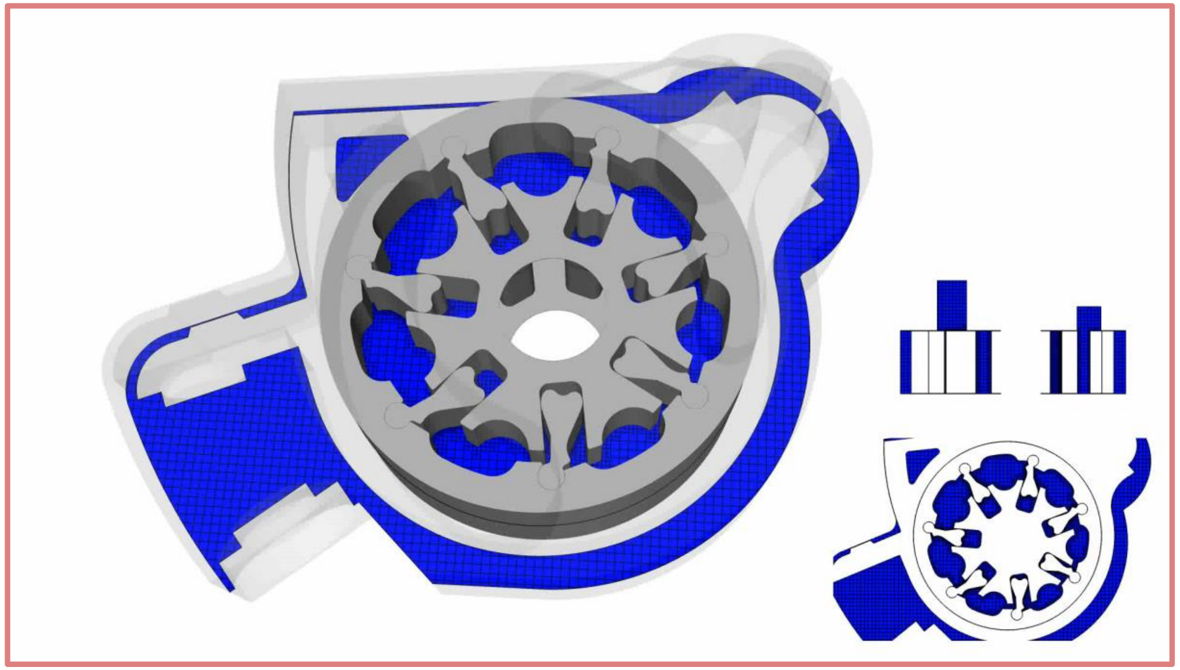
Cavitation and aeration more important at higher flow rates

PRV dynamics (not in current model) necessary for higher pressures

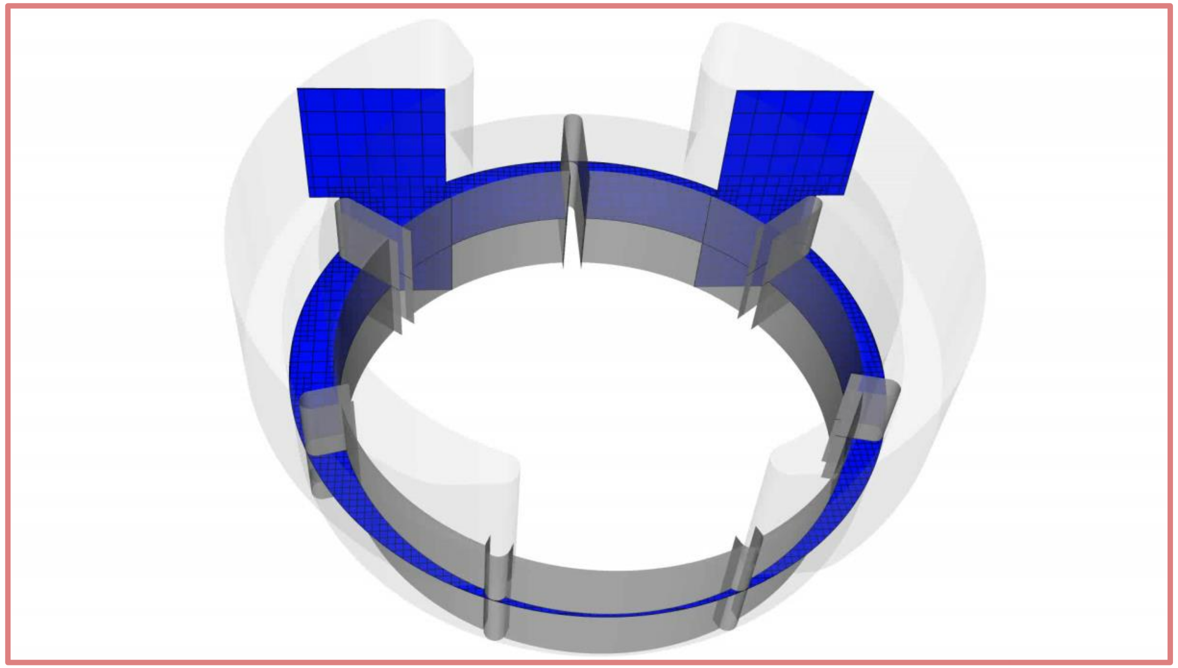
Gear Pumps: Gerotor Oil Pump

Related Applications

Pendulum Slider Oil Pump



Vane Oil Pump



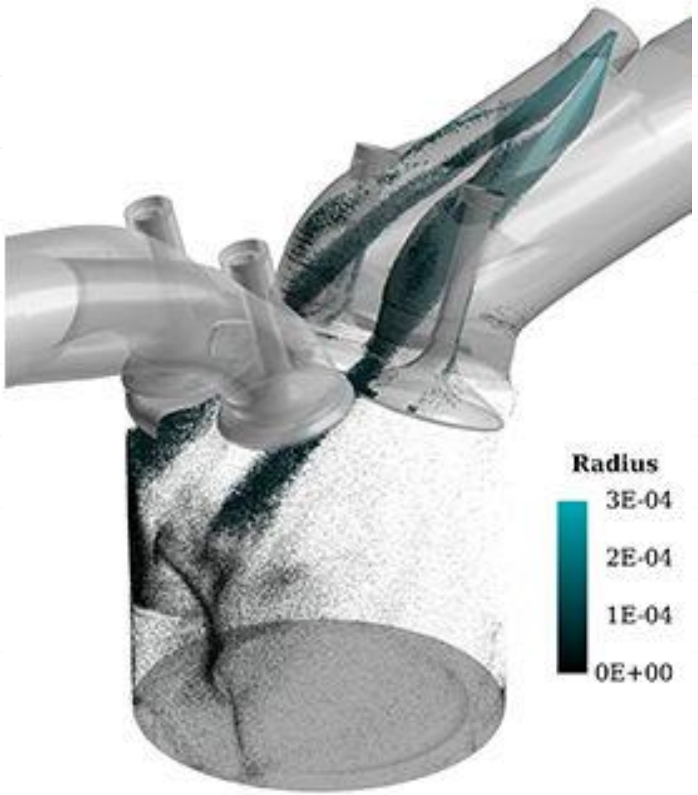
Giving our customers a competitive advantage through cutting edge IC Engine modeling technology will continue to be the top priority of Convergent Science

Our goal is to maximize the value to our existing customers by solving more problems (adjacent markets such as CHT and under-hood)

We will also continue to push into new markets where synergies can be leveraged

THANK YOU!

CONVERGECFD.COM



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