Introduction of CONVERGE v2.3 and Future Plan for CONVERGE

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Introducing Version 2.3

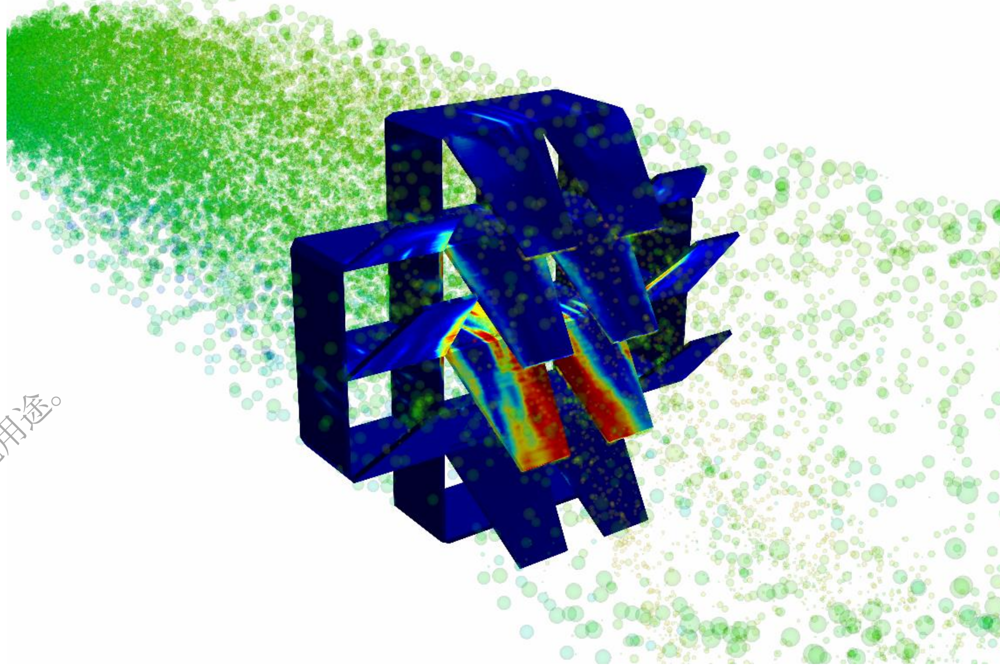
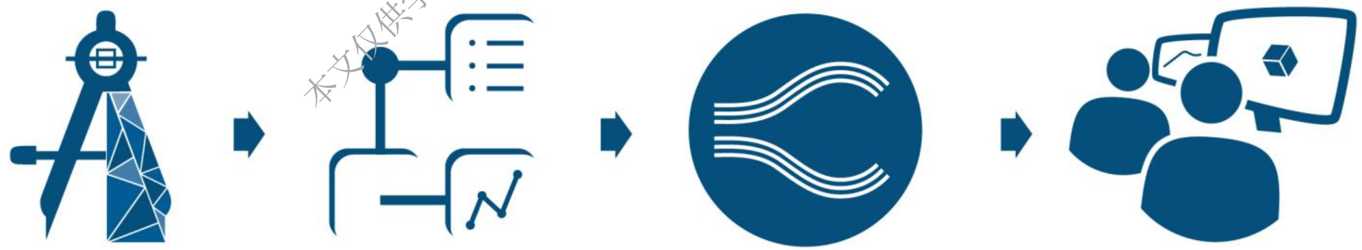


Image courtesy of SWRI

- CONVERGE v2.3 offers you more user-friendly, powerful, and flexible tools that allow you to gain insight into complex physical problems
  - Advanced new surface preparation tools
  - Additional models and more user-controlled options
  - A more efficient and robust solver
  - Enhanced post-processing tools



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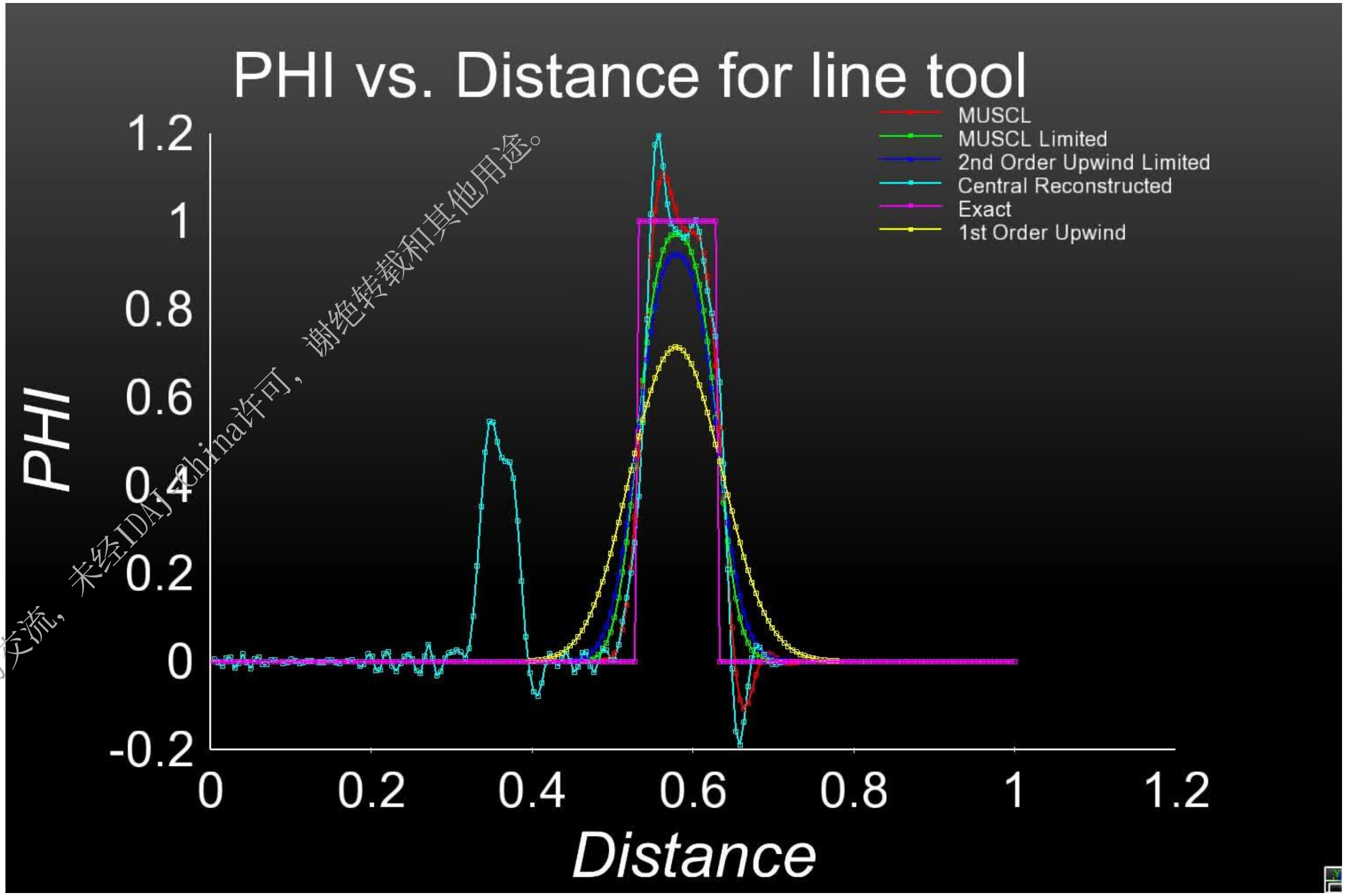
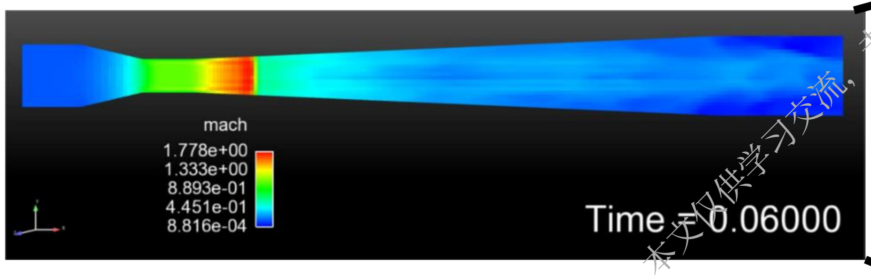
Solver (1/5)

- **MUSCL scheme and flux limiters**: MUSCL is a third-order method for convective terms that, when combined with flux limiters to ensure stability, yields solutions with less numerical viscosity and more spatial accuracy

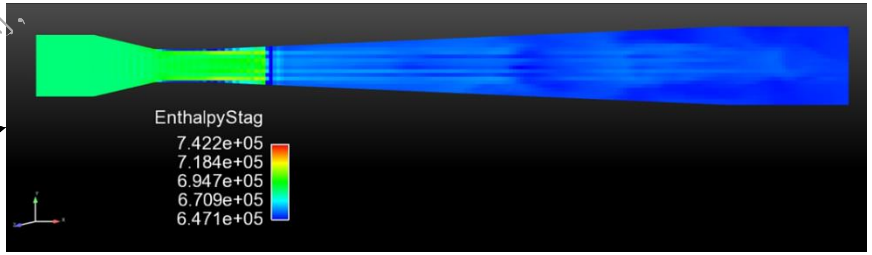


Solver (2/5)

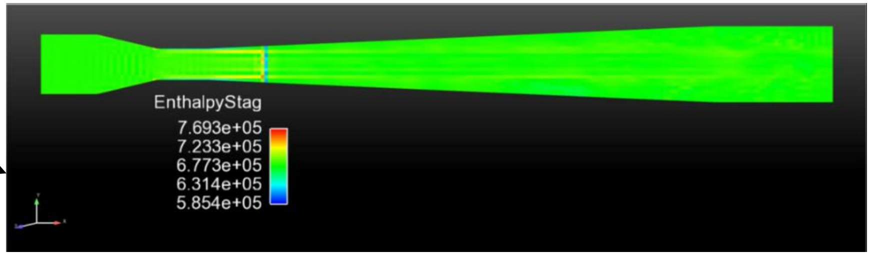
- **Total energy solver**: Simulating high-speed flows that include discontinuities may prevent energy conservation if you choose to solve only for specific internal energy, but the v2.3 total energy solver conserves total energy



With total energy solver turned OFF

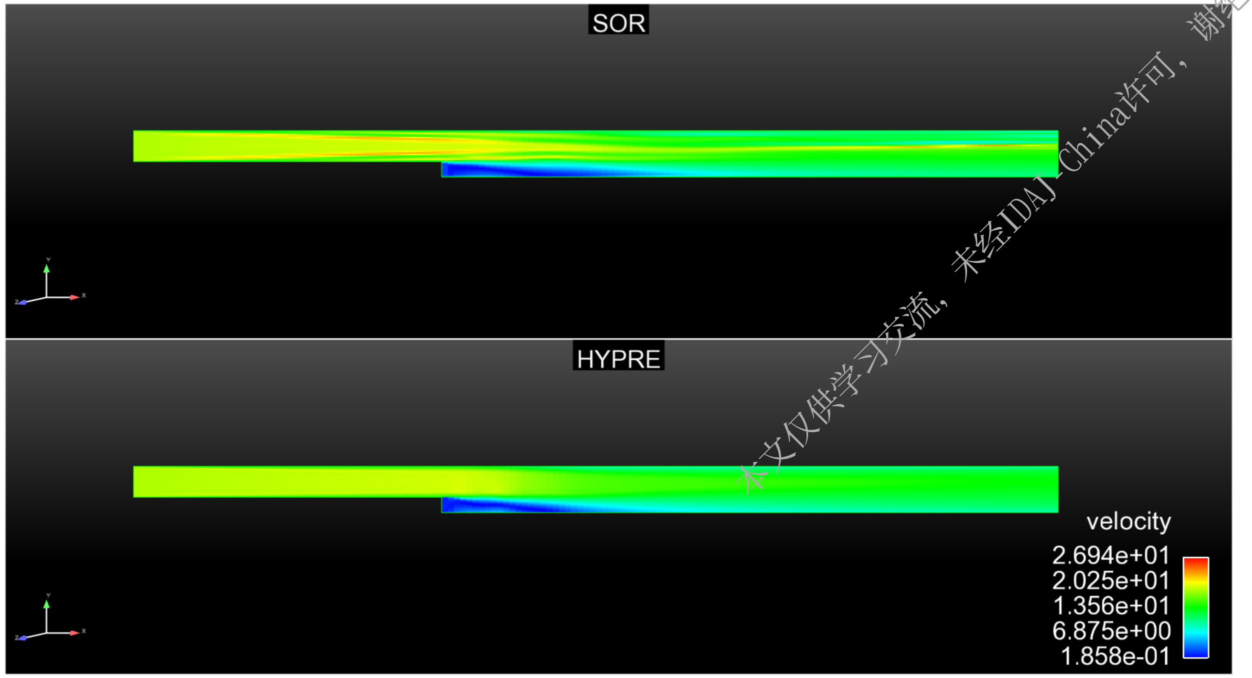


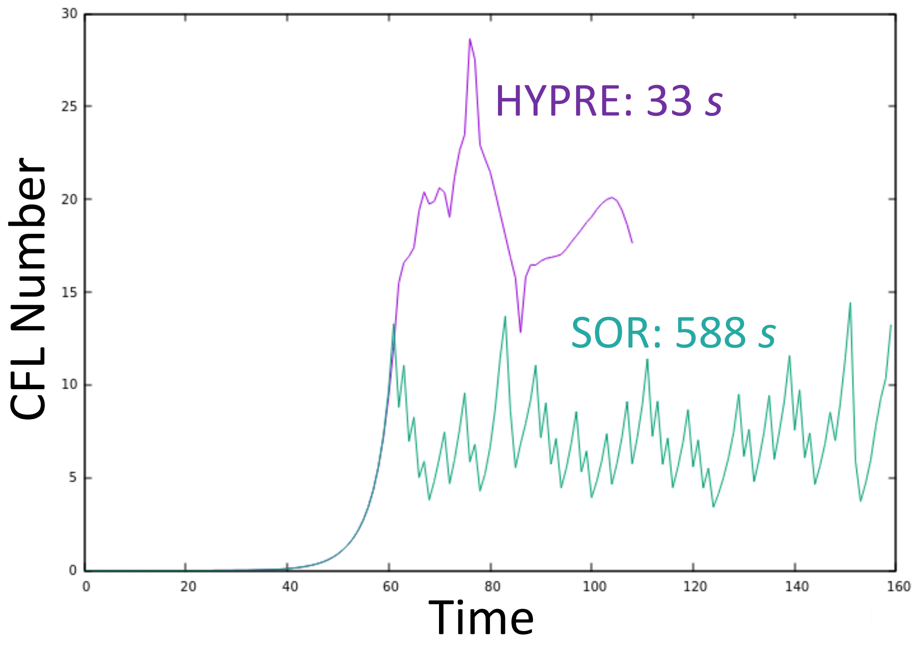
With total energy solver turned ON



Solver (3/5)

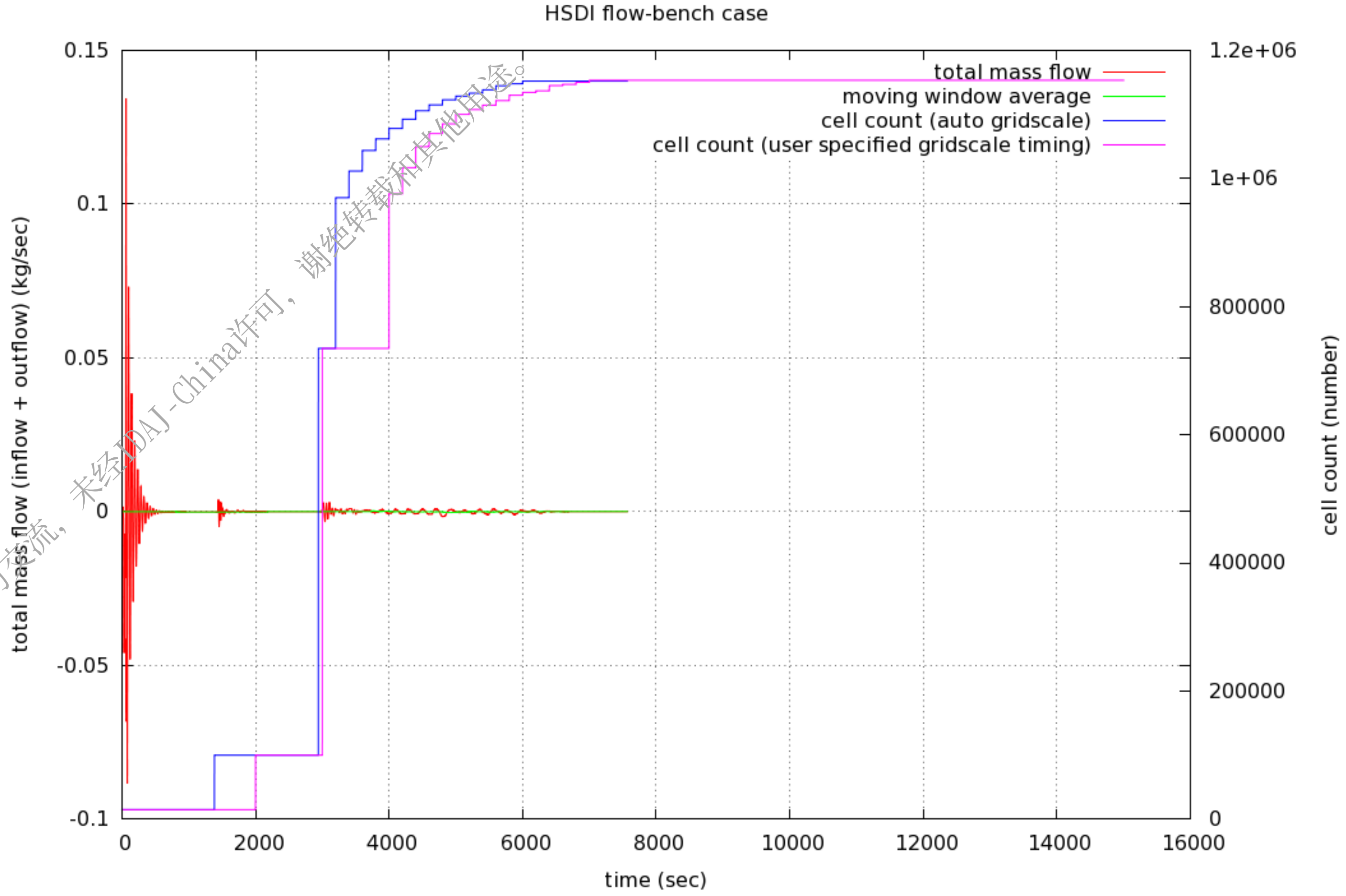
- **Linear solver options**: New linear solvers for all of the transport equations obtain fast, stable convergence on systems that SOR struggles to solve





Solver (4/5)

- **Steady-state convergence criteria selection capability**: Monitor multiple variables to determine the convergence of a steady-state simulation
  - Set up this feature via *monitor_steady_state.in*



Solver (5/5)

- **Mixture-averaged diffusion model**: Calculate the diffusion coefficient with a species-dependent, mixture-averaged option

$$\int \frac{\partial \rho_i}{\partial t} dV + \int \rho_i u \cdot n dA = \int \rho D_m \frac{\partial Y_i}{\partial x} dA + \int S \, dV$$

OLD species transport equation

$$\int \frac{\partial \rho_i}{\partial t} dV + \int \rho_i u \cdot n dA = \int \rho (D_{i,m} \frac{\partial Y_i}{\partial x} - V_c) dA + \int S \, dV$$

NEW species transport equation

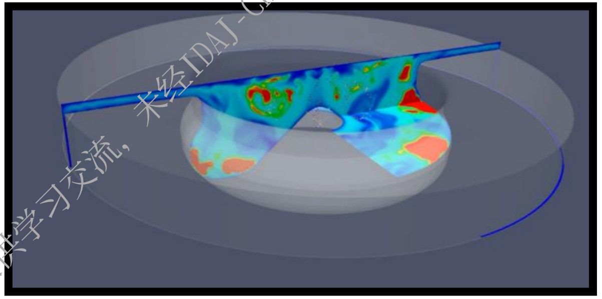
$$V_c = (\sum D_{i,m} \frac{\partial Y_i}{\partial x}) \cdot Y_m \qquad D_{i,m} = \frac{1 - Y_i}{\sum_{j,j \neq i} X_j / D_{ij}}$$

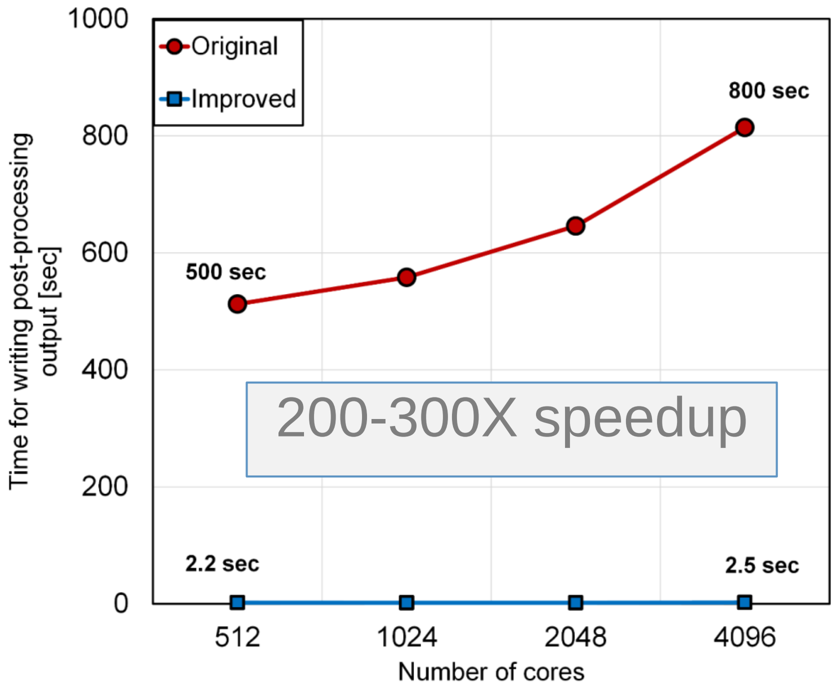
D_{ij} is tabulated

Efficiency (1/4)

- **Parallel I/O**: Write *post*.out* files and read *restart*.rst* files faster
  - Especially for large files on a large number of CPU cores

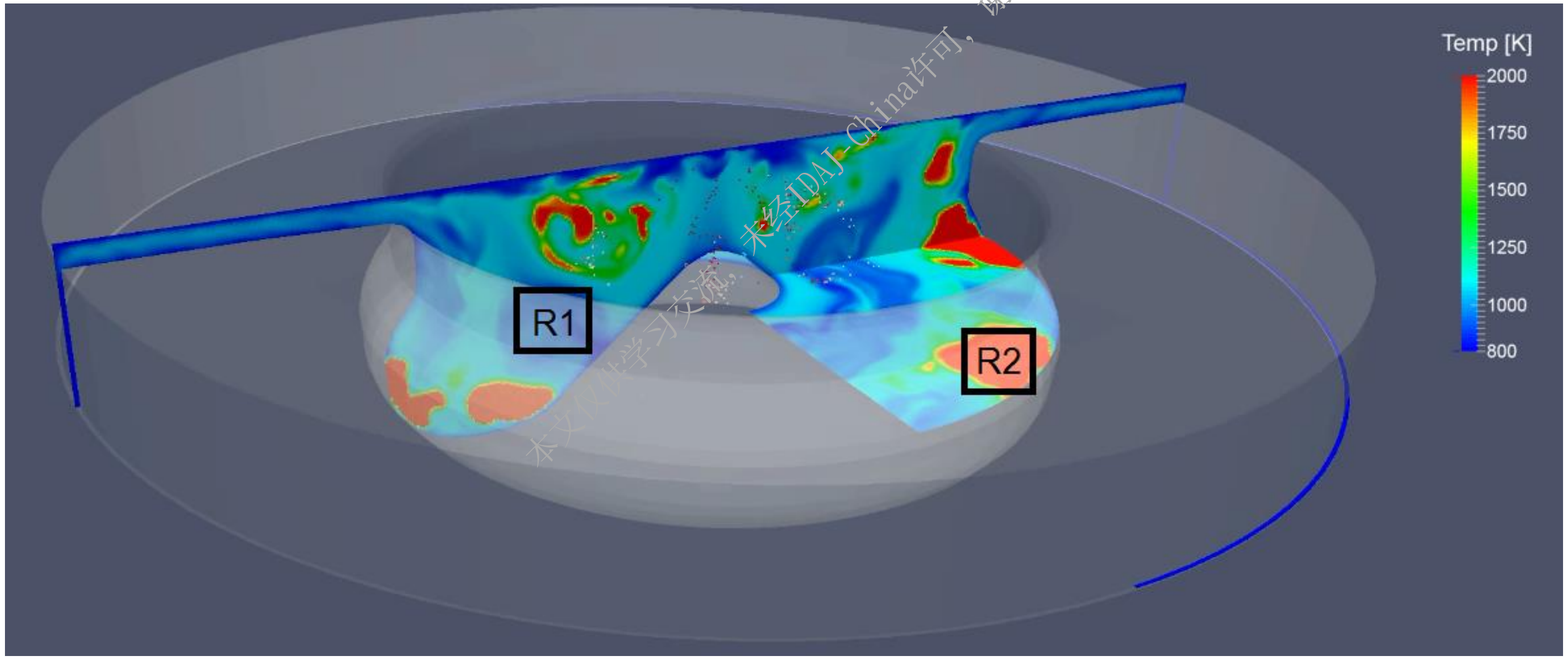
Base mesh (up to SOI)	0.60 *mm*
Embedding/AMR (up to SOI)	2 levels on vel. and temp.
Minimum cell size (up to SOI)	0.15 *mm*
Fixed mesh from SOI (using gridscale)	0.15 *mm*
Cells (TDC)	9 million
Peak cell count	30 million
Combustion model	SAGE in every cell
Turbulence Model	LES (Dynamic Structure)





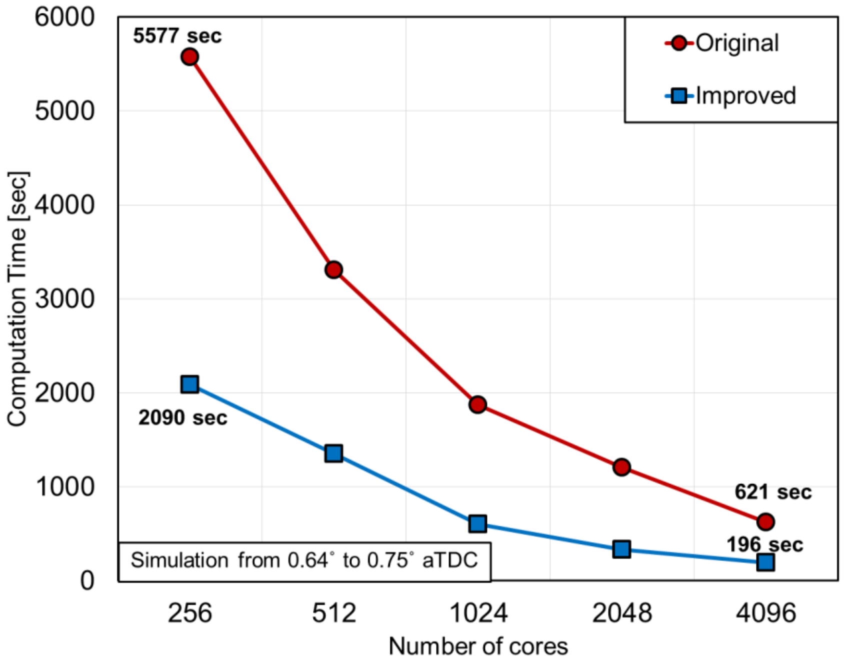
Efficiency (2/4)

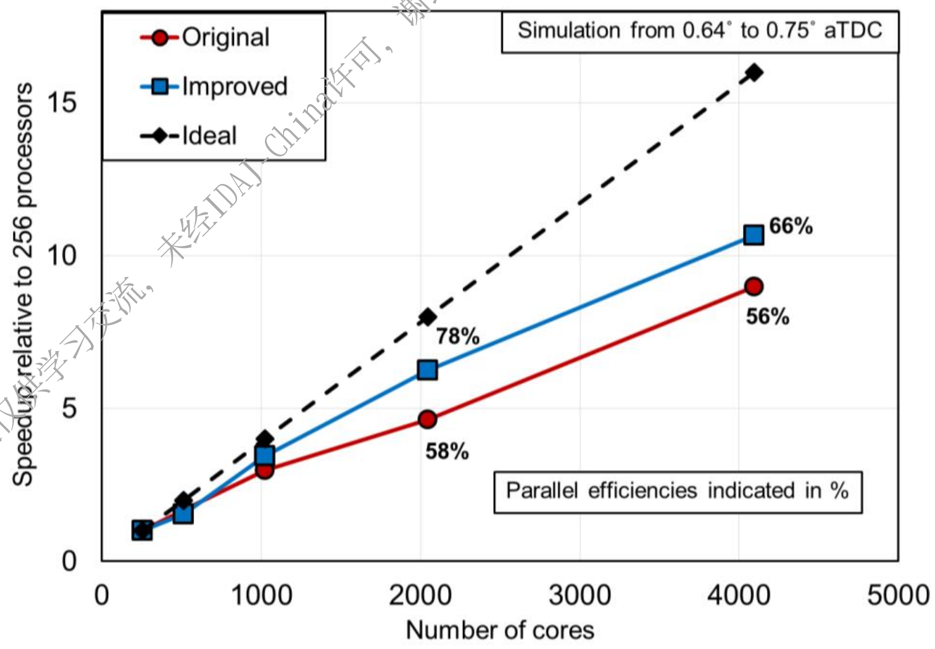
- **Chemistry load balance**
  - Original load balance for chemistry was based on number of cells
  - Not all cells need the same amount of computational effort for chemistry
  - New approach balances the total computational effort



Efficiency (3/4)

- **Chemisty load balance**: Parallel scalability for detailed chemistry has been significantly improved

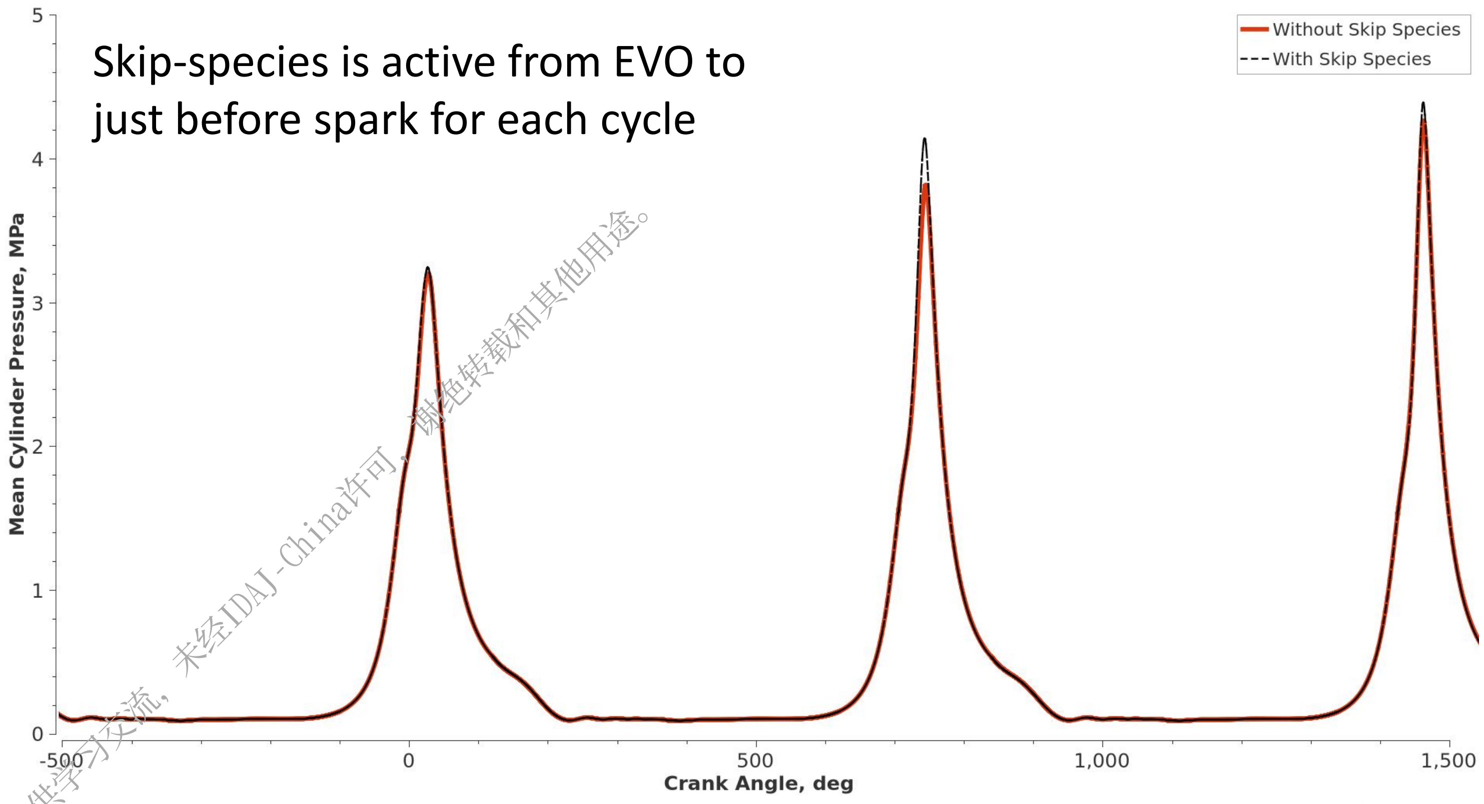




- Over 3X speedup in compute time on 4096 cores
- 78% scaling efficiency on 2048 cores, 66% scaling efficiency on 4096 cores

Efficiency (4/4)

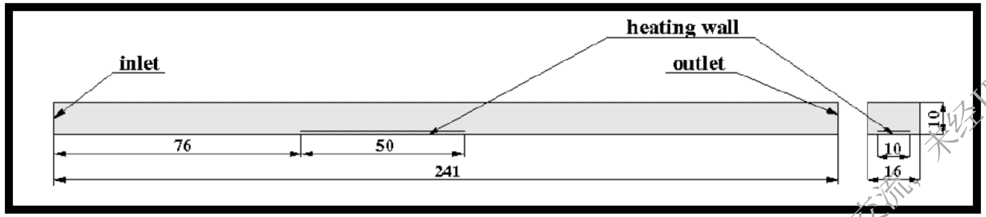
- **Reduced species**: Include only major species in calculations at specific times when the minor species can be ignored (*e.g.*, during the intake and exhaust stages of an engine simulation)
    - Provides good speedup, especially for multiple cycle engine simulations



Runtime (16 processors: 3.5GHz, 32GB)		
without Skip Species	203 hrs	58% speedup
with Skip Species	86 hrs	

Boundary (1/2)

- **Nucleate boiling**: Account for the additional heat transfer due to nucleate boiling by computing the heat flux through a wall at high temperatures and in contact with liquid
  - There is no phase change involved

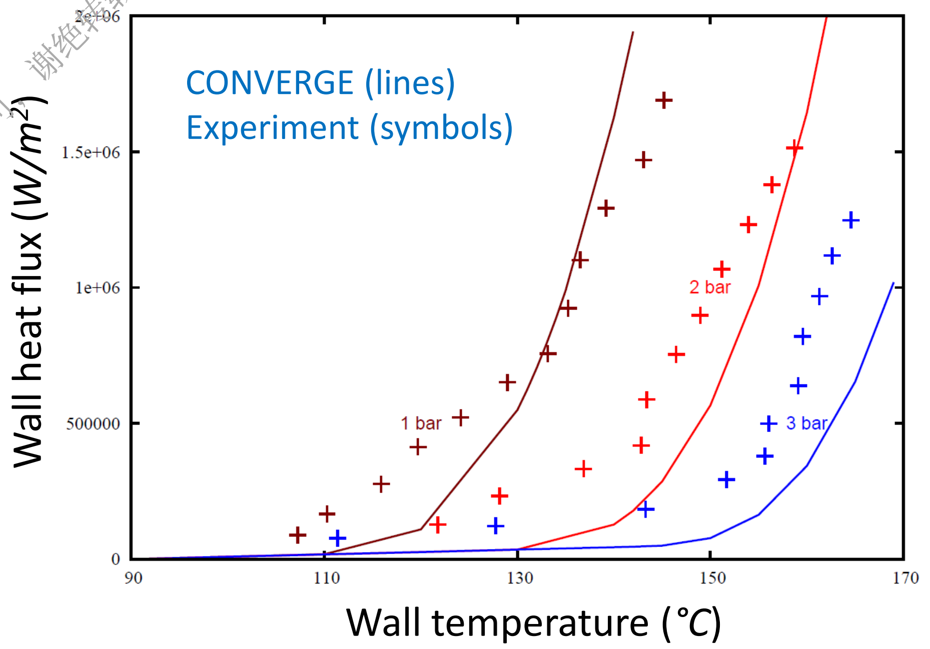


<u>Inlet BC</u>

Temperature = 90^oC

Pressurae = 1, 2, 3 *bar*

Velocity = 0.15 *m/s*



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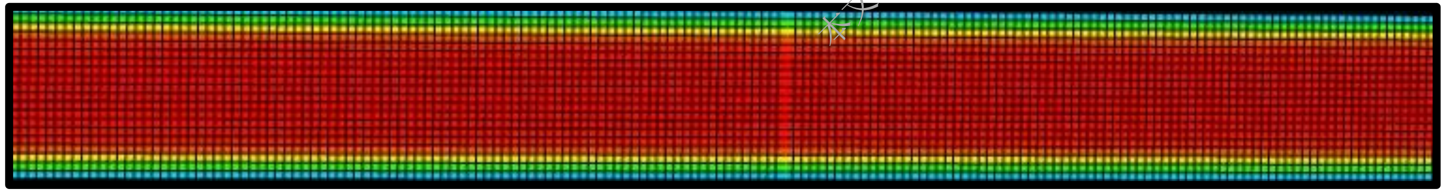
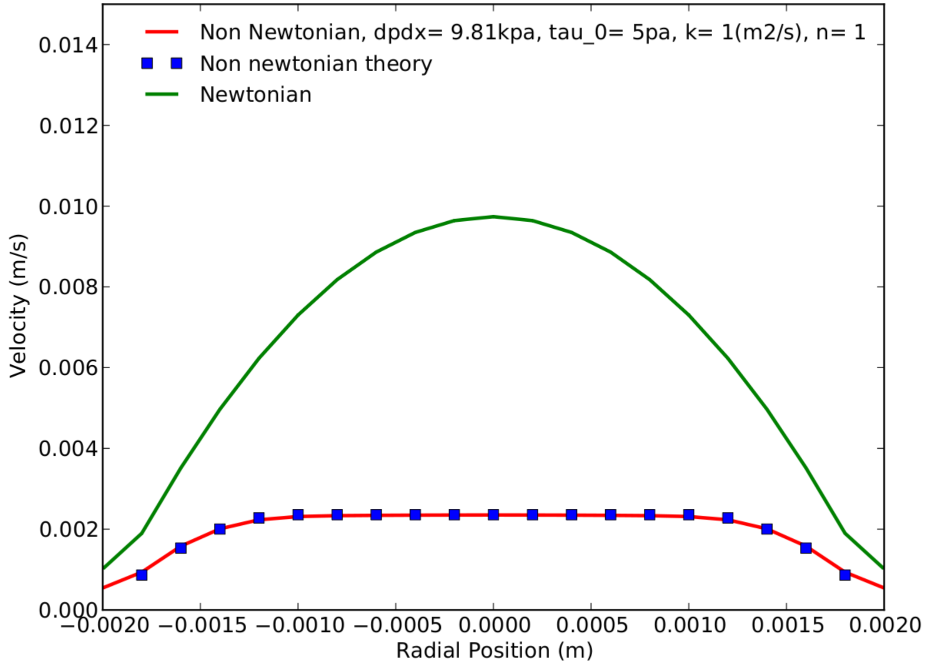
Boundary (2/2)

- AMR can be restricted on walls to not go below a user-specified y+ value
  - Law-of-the-wall is not valid when cells near the wall are too small
- Transonic INFLOW boundaries
  - In earlier versions of CONVERGE, INFLOW boundaries had to be either supersonic or subsonic all the time, now they can transition
- Automatic velocity profile for INFLOW boundaries
  - When using a specified velocity or mass flow at an inlet, the INFLOW boundary will no longer force a flat profile across the boundary
- 1D Conjugate Heat Transfer (described later in the presentation)

Materials

- **Non-Newtonian flow**: CONVERGE contains the Herschel-Bulkley model, which considers yield stresses (Bingham-type fluids) and shear thinning and thickening behavior
- New Non-Newtonian applications
  - Blood flow (bio-medical industry)
  - Drill coolant flow (oil and gas industry)
  - Flow/mixing of oils and batter (food industry)

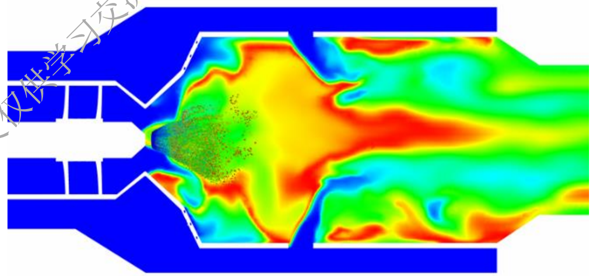


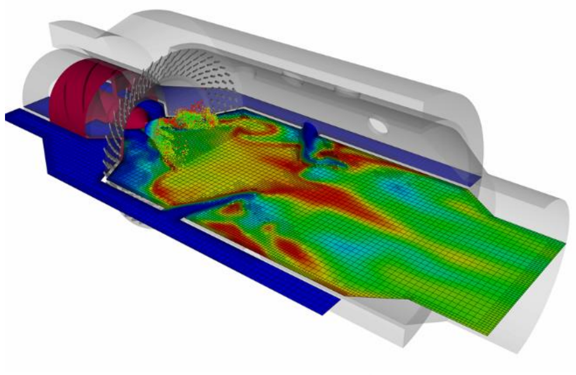


Quickly simulate steady combustion in flow-dominated systems

Combustion (1/3)

- **Flamelet Generated Manifold model**: Capture turbulent flame dynamics with precomputed lower dimensional flamelet solutions
  - Fast and simple evaluations of fluid, thermodynamic, and chemical properties, which are constrained to the manifold generated by the flamelet solutions
  - Can have manifolds generated from 0D auto-igniting flamelets, 1D premixed flamelets, or 1D non-premixed flamelets





Combustion (2/3)

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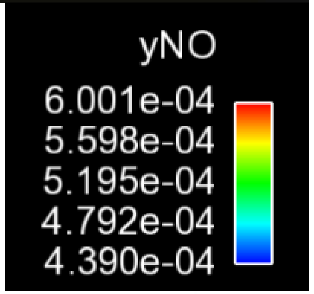
ifp Energies nouvelles

- **Improvement to ECFM3Z/ECFM**: CSI has been working with IFPEN on ECFM3Z/ECFM model improvement and development since early 2015--new features will be available in future intermediate Converge v2.3 releases
- Improvement on auto-ignition delay prediction
  - Fully automatic generation of Tabulated Kinetics of Ignition (TKI) table by using a Python tool
  - Ignition delay and reaction rate on progress variable are tabulated in HDF5 format
- Improvement on flame tracking
  - Added unburned enthalpy transport equation for more accurate prediction on laminar flame speed
  - Improved Intermittent Turbulent Net Flame Stretch (ITNFS) model for chemistry and turbulence interaction(TCI)
- Improvement on spark modeling
  - Implementing the Imposed Stretch Spark Ignition Model (ISSIM)

Combustion (3/3)

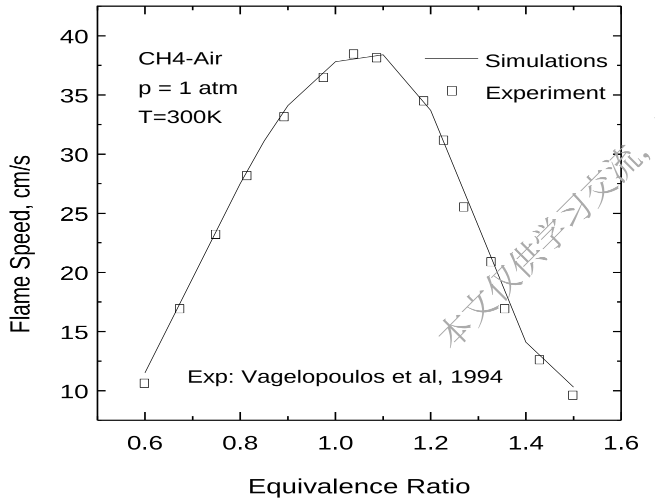
- **Surface chemistry**: Model surface chemistry between a solid surface and gas phase species
  - Can be activated on stationary wall boundaries or in porous regions

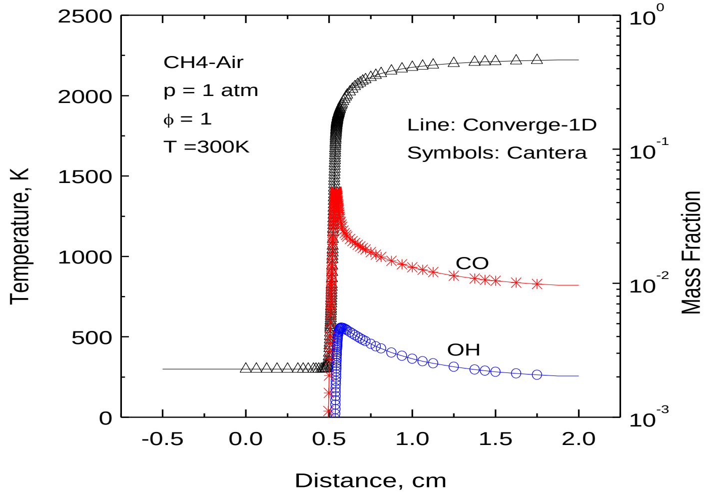


NOx reduction in SCR using surface chemistry

Combustion Utilities (1/3)

- **One-dimensional laminar flamespeed solver**: Compute species and temperature profiles in steady-state, freely propagating, premixed laminar flames
  - Account for finite-rate chemical kinetics and mixture-averaged molecular transport
  - Calculate the laminar premixed flamespeed, which is an important fuel property





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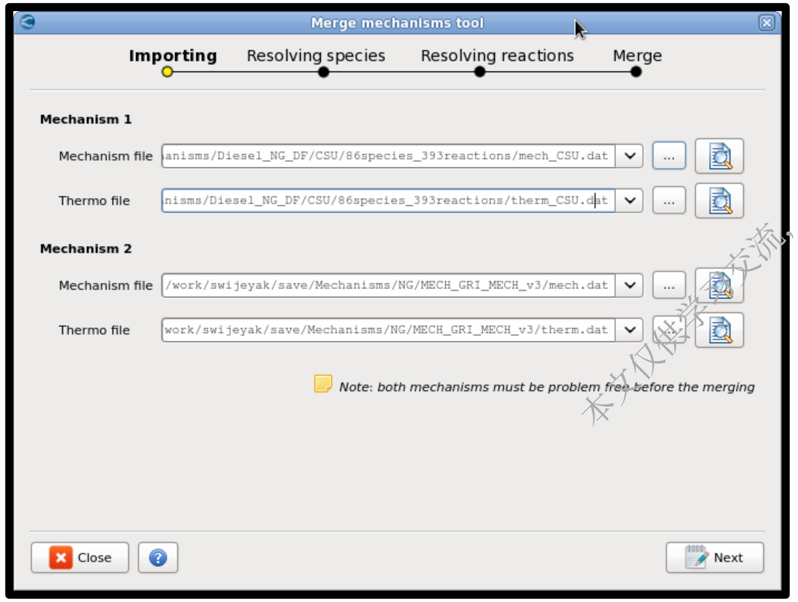
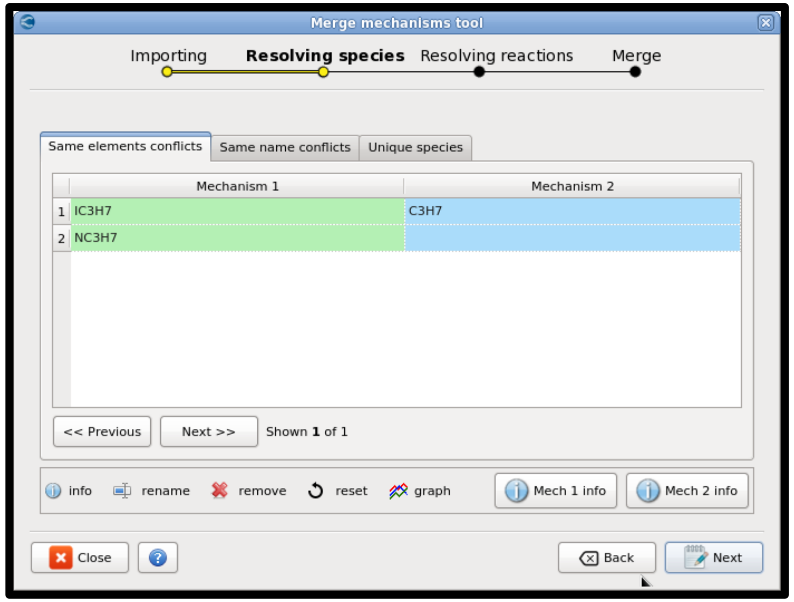
Combustion Utilities (2/3)

- **Mechanism merge**: Merge two mechanisms via a three-step process that incorporates user-specified information on species, thermodynamics, and reaction conflicts
  - Can also insert new species and their reactions from one mechanism into another





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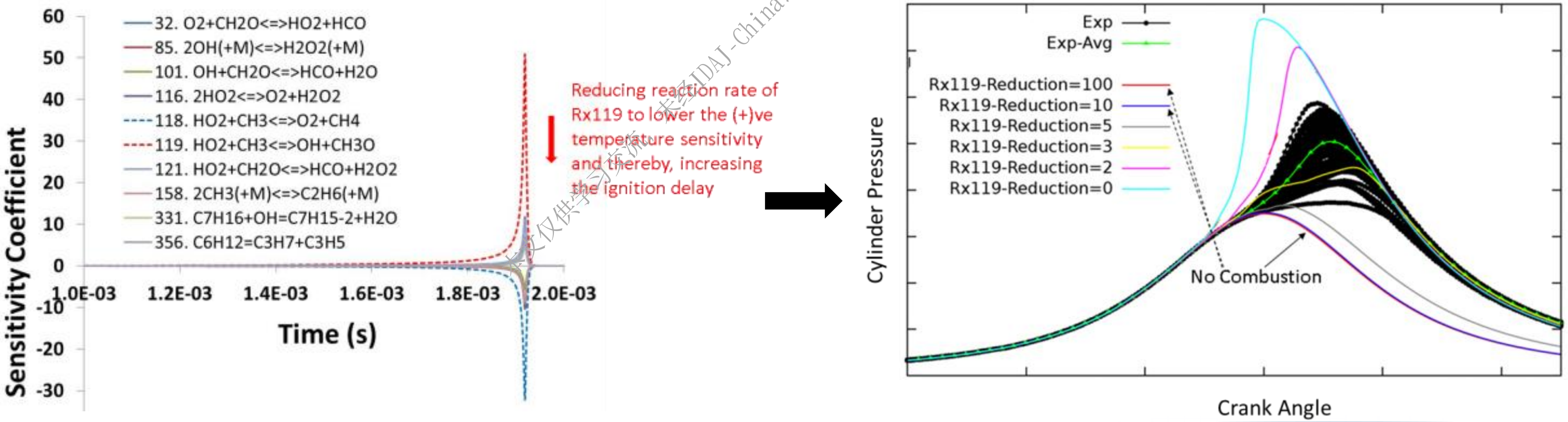
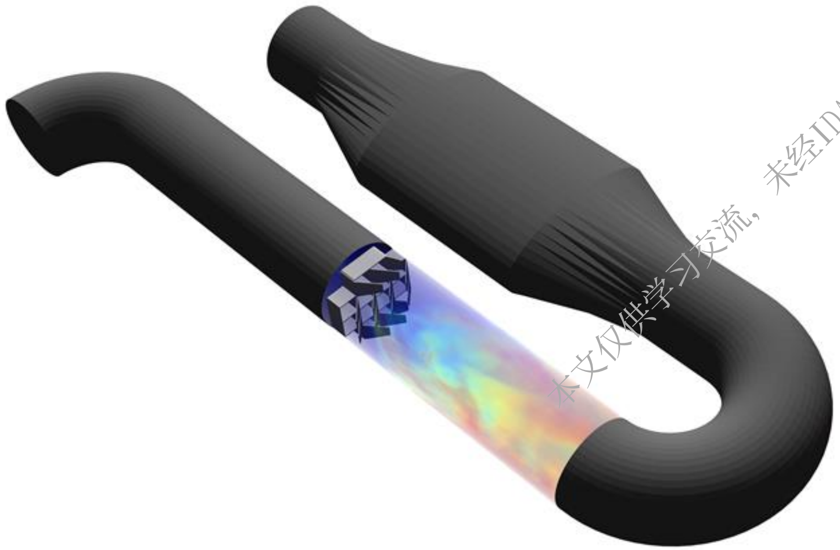
Combustion Utilities (3/3)

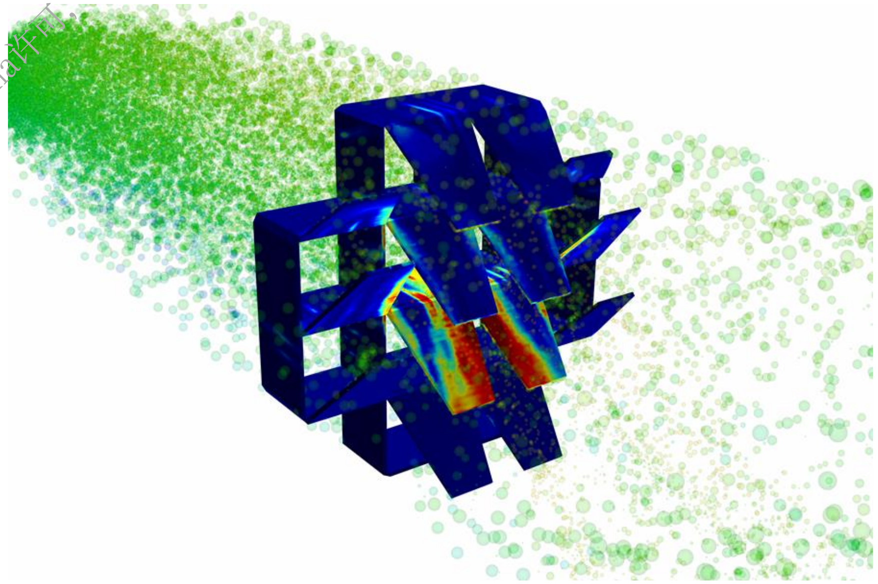
- **Zero-dimensional sensitivity analysis**: Calculate normalized sensitivity coefficients of temperature and species on each reaction in a mechanism
    - Determine which reaction contributes most to the temperature rise or destruction or formation of species either in a constant pressure or constant volume simulation



Spray

- **Molten solid urea depletion**: Calculate urea-water solution depletion in sprays and wall films
  - Water evaporates while urea decomposes using an Arrhenius formula.



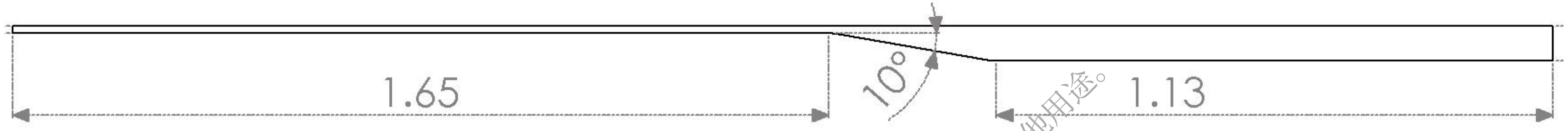


Turbulence (1/2)

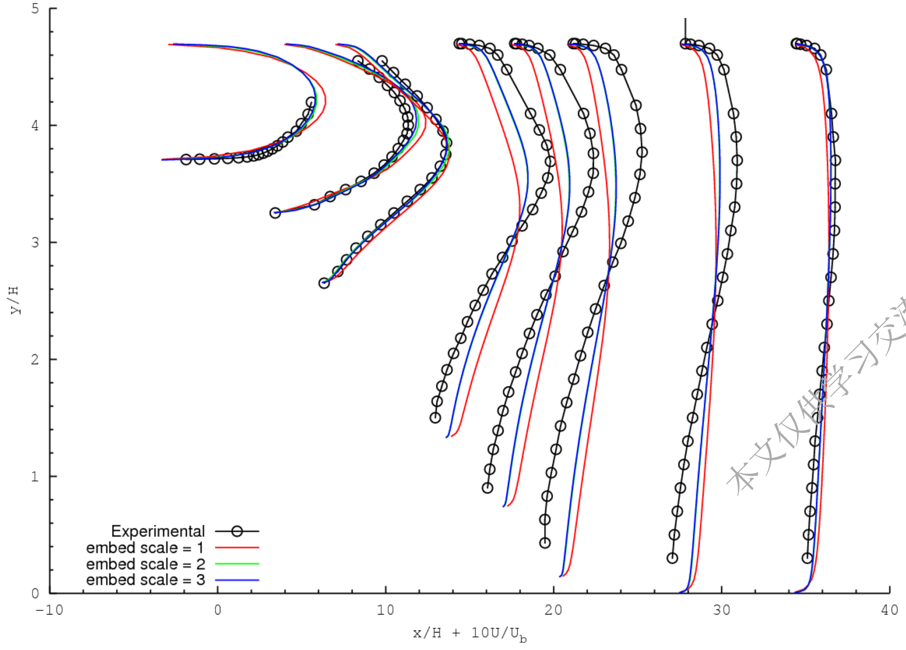
- **k-ω turbulence models**: CONVERGE now contains the standard k-ω model (1998 and 2006 implementations) and the shear stress transport (SST) k-ω model
  - These models are especially good for cases with external flows and boundary layers
- **k-ε turbulence models**: CONVERGE now contains the realizable k-ε model, which is for rotational flows such as the flow within a gas turbine

Turbulence (2/2)

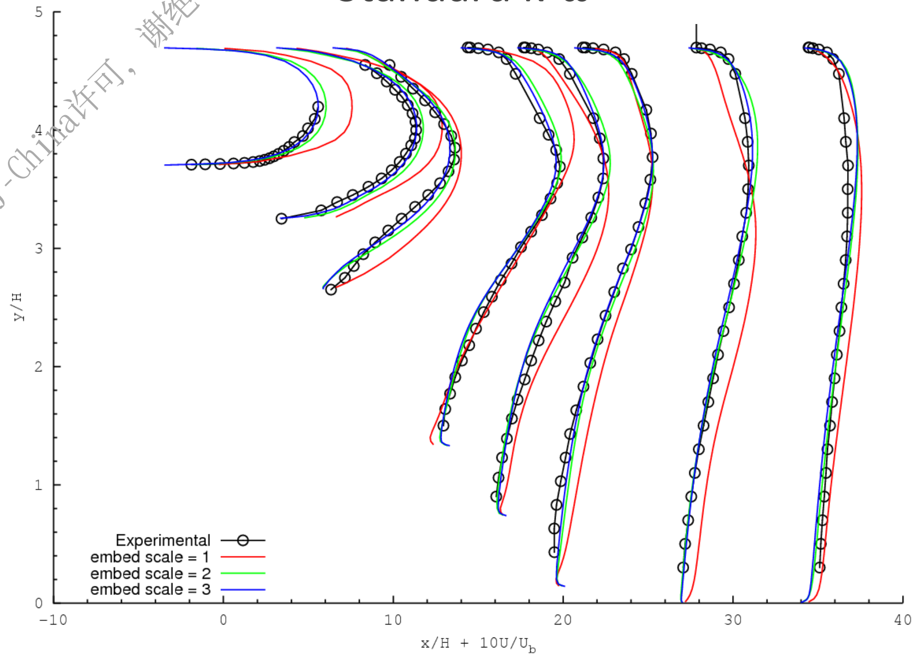
For a simple diffuser, k-ω does a much better job predicting the velocity profile



Standard k- ε

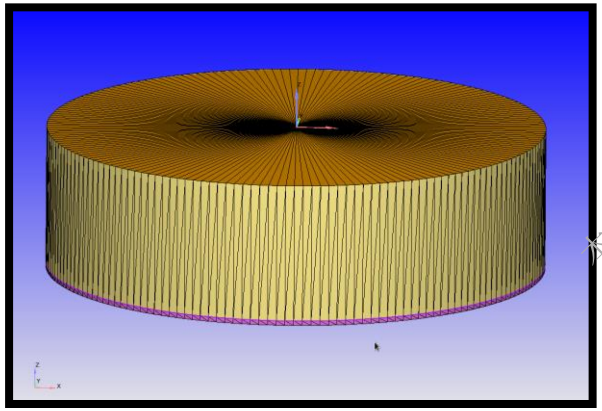


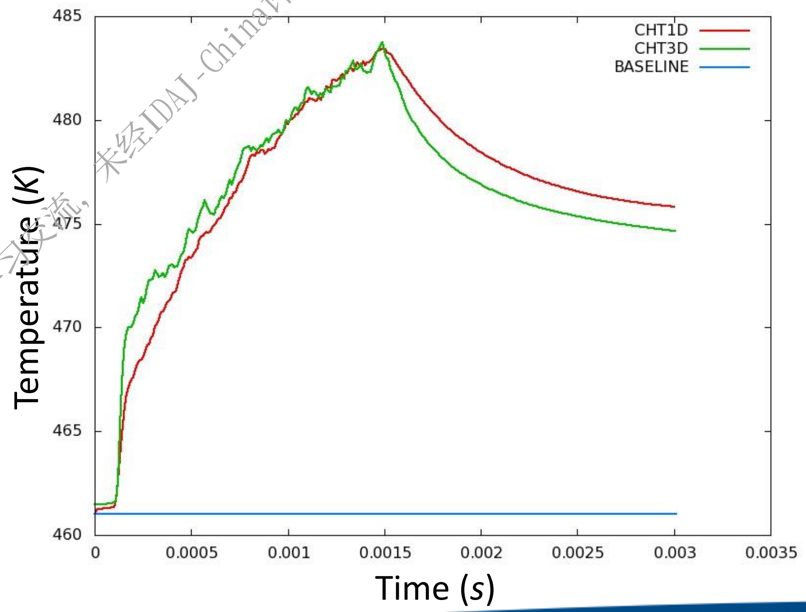
Standard k-ω



Conjugate Heat Transfer (1/2)

- **One-dimensional conjugate heat transfer model**: 1D CHT model allows the wall temperature to change due to the heat convection between the fluid phase and the wall
  - Divide the solid wall into layers with different properties
  - Example: spray bomb case





- Plot: wall temperature at center of fluid-solid interface
- Baseline case does not have any CHT and thus has a constant wall temperature

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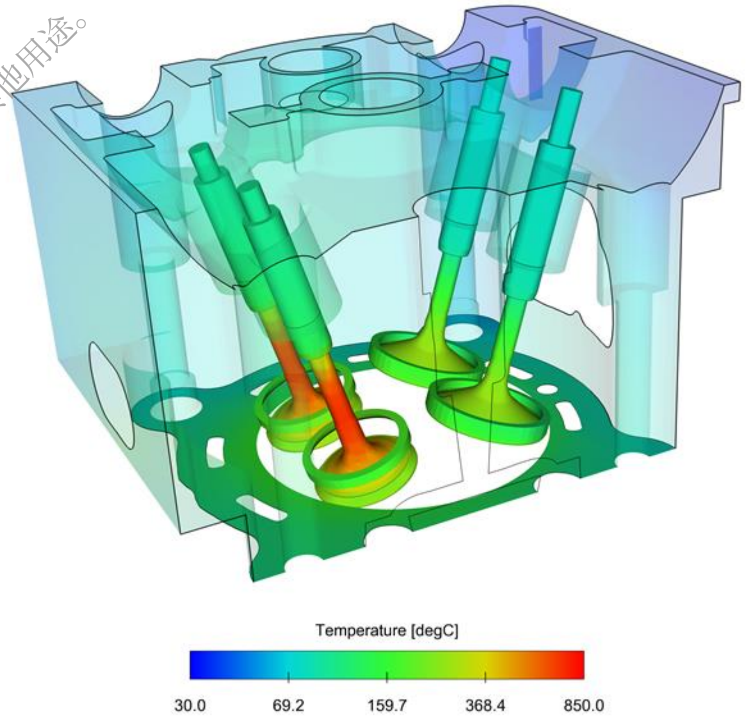
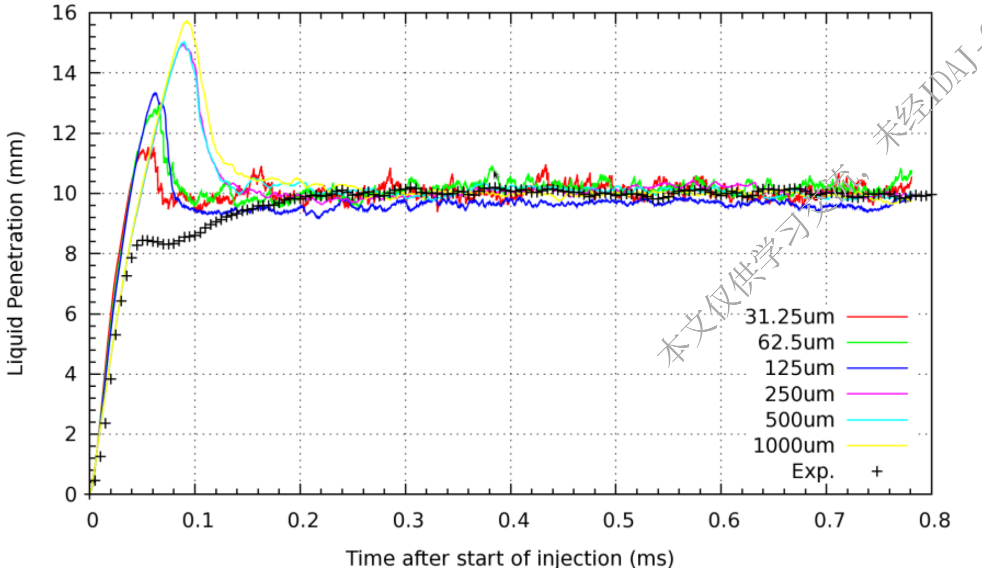
Conjugate Heat Transfer (2/2)

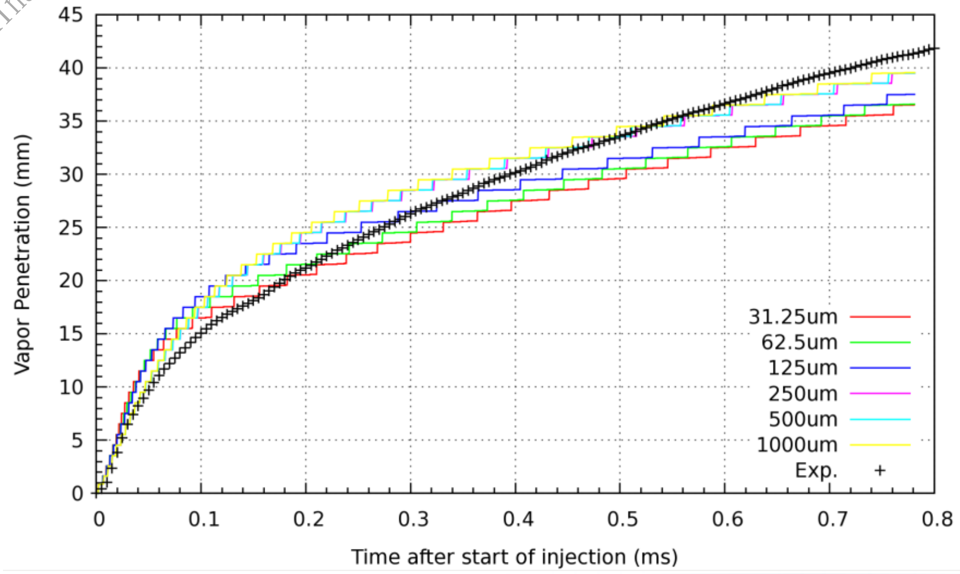
- **Contact resistance**: Model contact resistance between fluids and solids
- **Contact resistance in small gaps**: Model heat transfer in small gaps such as the gap between a closed valve and the valve seat in an engine
    - Define the contact resistance values used in this approach through a user-defined function



Volume of Fluid

- **VOF-spray one-way coupling**: CONVERGE now uses detailed fluid flow information near the nozzle exit during VOF simulations to inject parcels for Lagrangian spray calculations
- Example case: ECN Spray A (evaporating)





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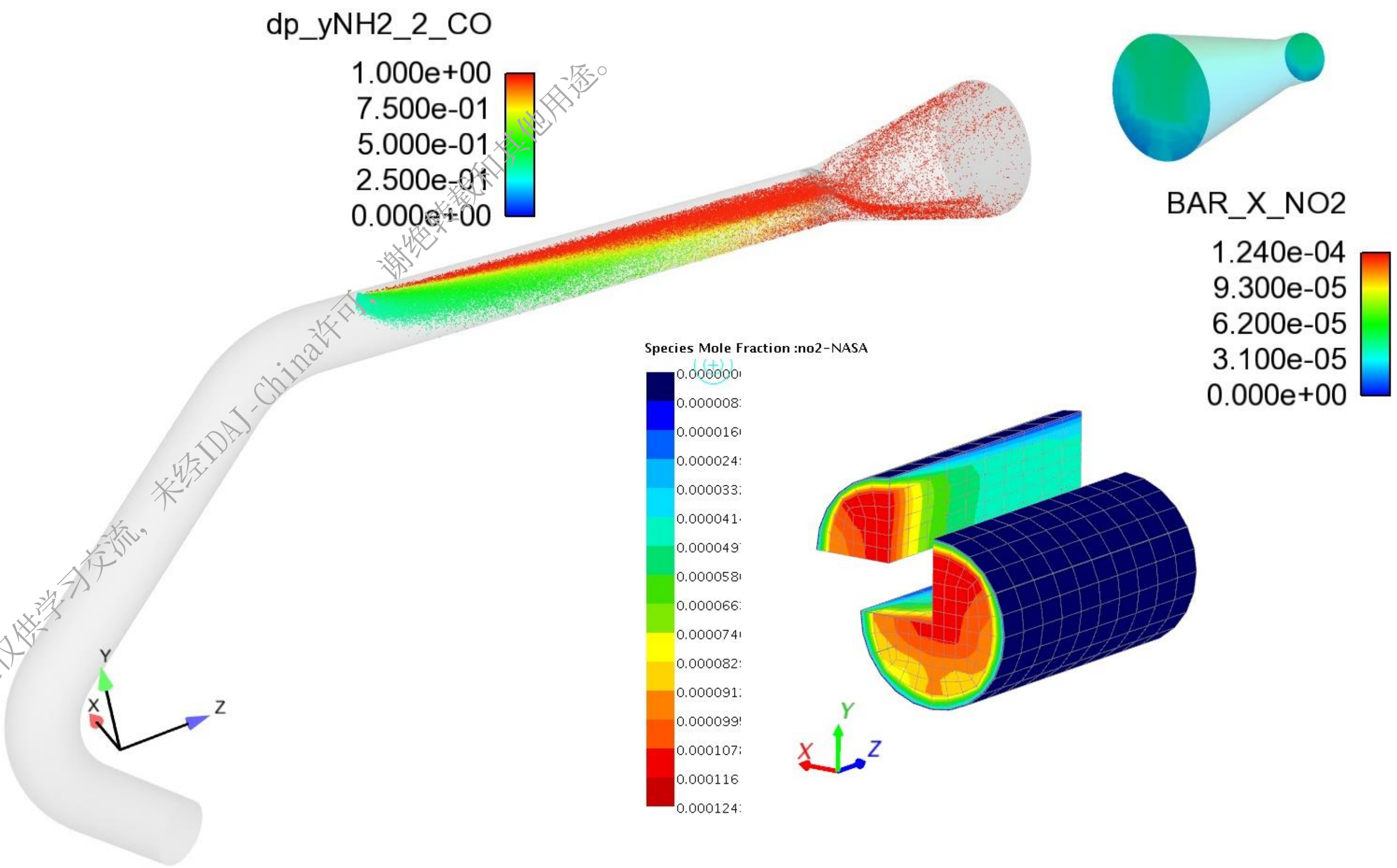
CONVERGE – GT-SUITE Coupling (1/2)

- **Two-dimensional coupling**: Couple to GT-SUITE via two-dimensional coupling
  - Thus you can couple a CONVERGE simulation to a GT-POWER simulation that includes an aftertreatment device



CONVERGE – GT-SUITE Coupling (2/2)

- **GT-POWER/FSI coupling**: CONVERGE can now couple its fluid-structure interaction (FSI) model with GT-SUITE
  - You can use GT-SUITE's approach to rigid bodies subjected to constraints and external forces defined in GT-POWER and fluid forces provided by CONVERGE
    - GT: Complete hydro-mechanical injector
    - CONVERGE: High resolution 3D flow inside the injector

Movie showing velocity magnitude in the injector and pressure on the surface

Output File Changes

- **Memory usage**: CONVERGE can output memory usage to an output file
  - This is helpful for transient simulations to monitor memory usage during the simulation
  - Useful for troubleshooting possible problems with the setup
- **Residual output**: CONVERGE can output iteration residual to an output file
  - Helpful for monitoring convergence without having to parse the screen output or logfile

Current Development Features

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Current Development Items (1/3)

- 1D flamespeed solver
  - Integrate the flamespeed solver more tightly with CONVERGE
  - Develop new convergence methods for faster solutions
- Surface Chemistry
  - Add the ability to solve multiple chemical mechanisms in both gas and surface phase
- MRF/RRF
  - Will offer significant speed enhancement for pumps and rotating compressors
- Steady Solver Enhancements
- Multiple solvers
  - Allow for solving incompressible and compressible portions of the domain simultaneously
  - Necessary for simulating in-cylinder combustion and water jacket cooling at the same time
- GPU Combustion Solver
  - Currently available as a UDF, but still working to make the GPU speedup useful

Current Development Items (2/2)

- HPC Enhancements
  - Surface subdivided onto each core
    - Lower memory
    - Better scaling
  - Adding OpenMP capability
    - More efficiently use hybrid parallel architectures
  - New load balance implementation
    - ParMETIS
    - Cell-based instead of block-based
    - No inputs required from the user
    - Better load balance, even when scaling to thousands of cores
  - Parallel post file writing in portable cgns format
    - Prevents the need for a post file converter

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THANK YOU!

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