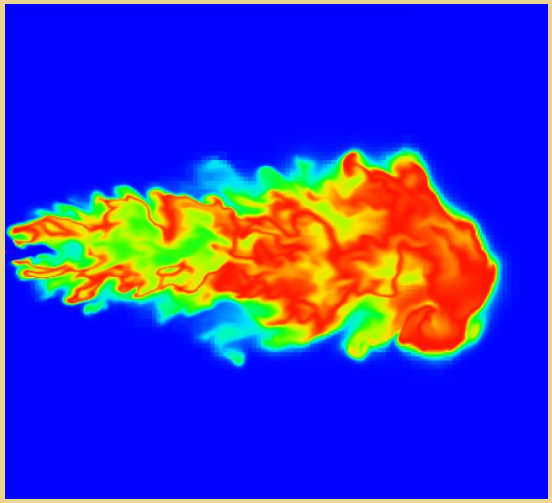
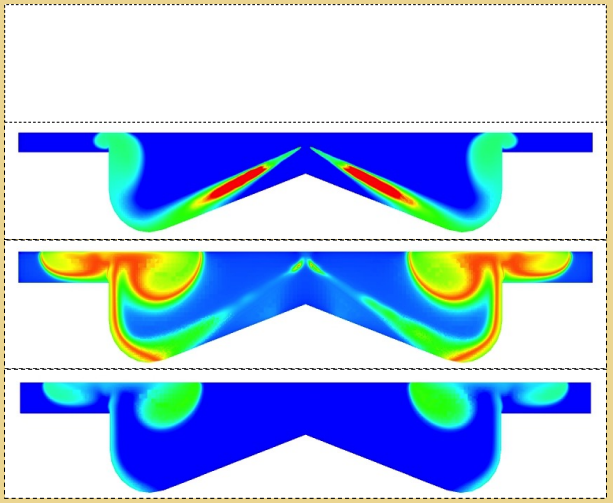
Argonne NATIONAL LABORATORY

# Internal Combustion Engine Simulations: From Desktop - Cluster - Super-Computing



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**Presentation at ATPESC 2015**

August 10th

U.S. DEPARTMENT OF ENERGY

# Acknowledgements

**Sponsors:** U.S. Department of Energy, Office of Vehicle Technology under the management of Gurpreet Singh, Leo Breton, Kevin Stork

**Argonne National Laboratory**

Y. Pei, Z. Wang, **J. Kodavasal**, Q. Xue, K. Saha, M. Ameen, D.E. Longman

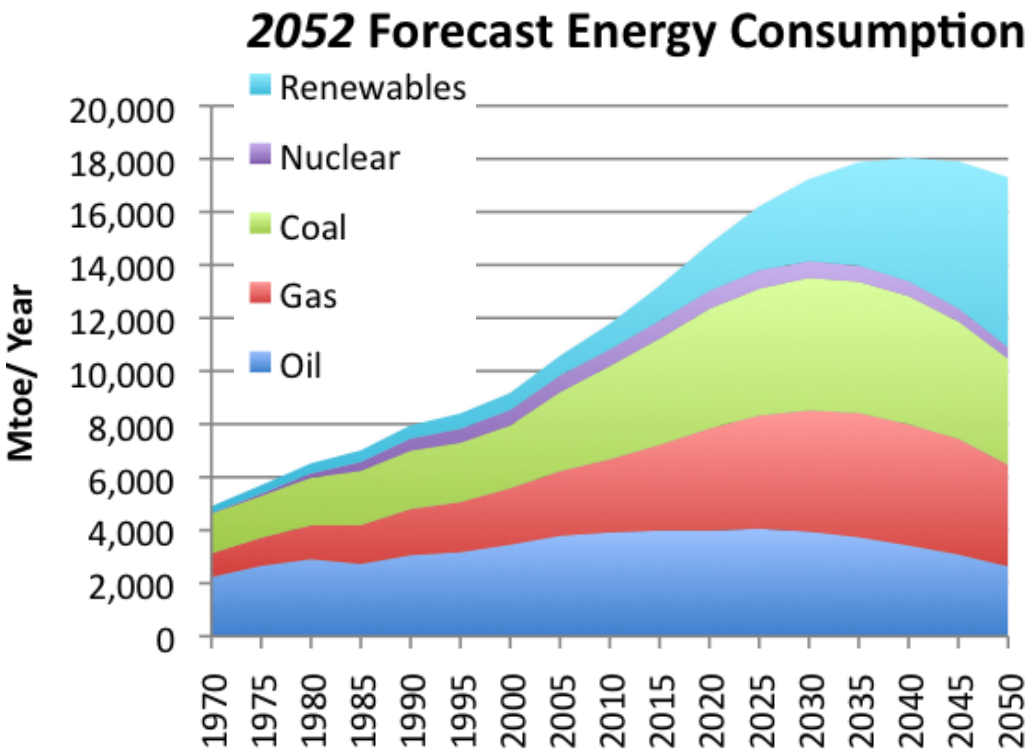
M.J. Davis, R. Sivaramakrishnan, A. Wagner (Chemical Science and Engineering)

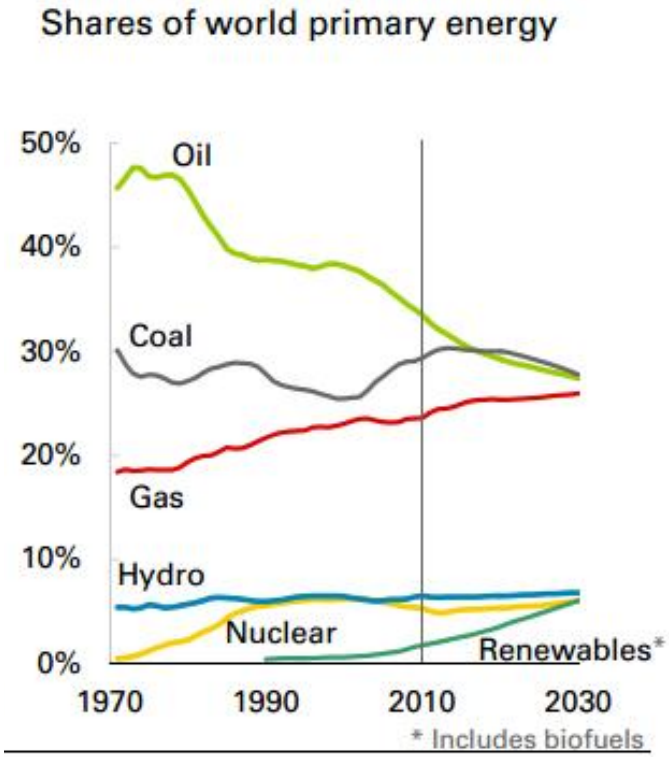
M. Garcia, K .Harms, J. Insley, R. Bair (Leadership Computing Facility)

Prof. M. Battistoni at University of Perugia (visiting researcher at Argonne)

# The Energy Outlook

## Courtesy: International Energy Association 2013

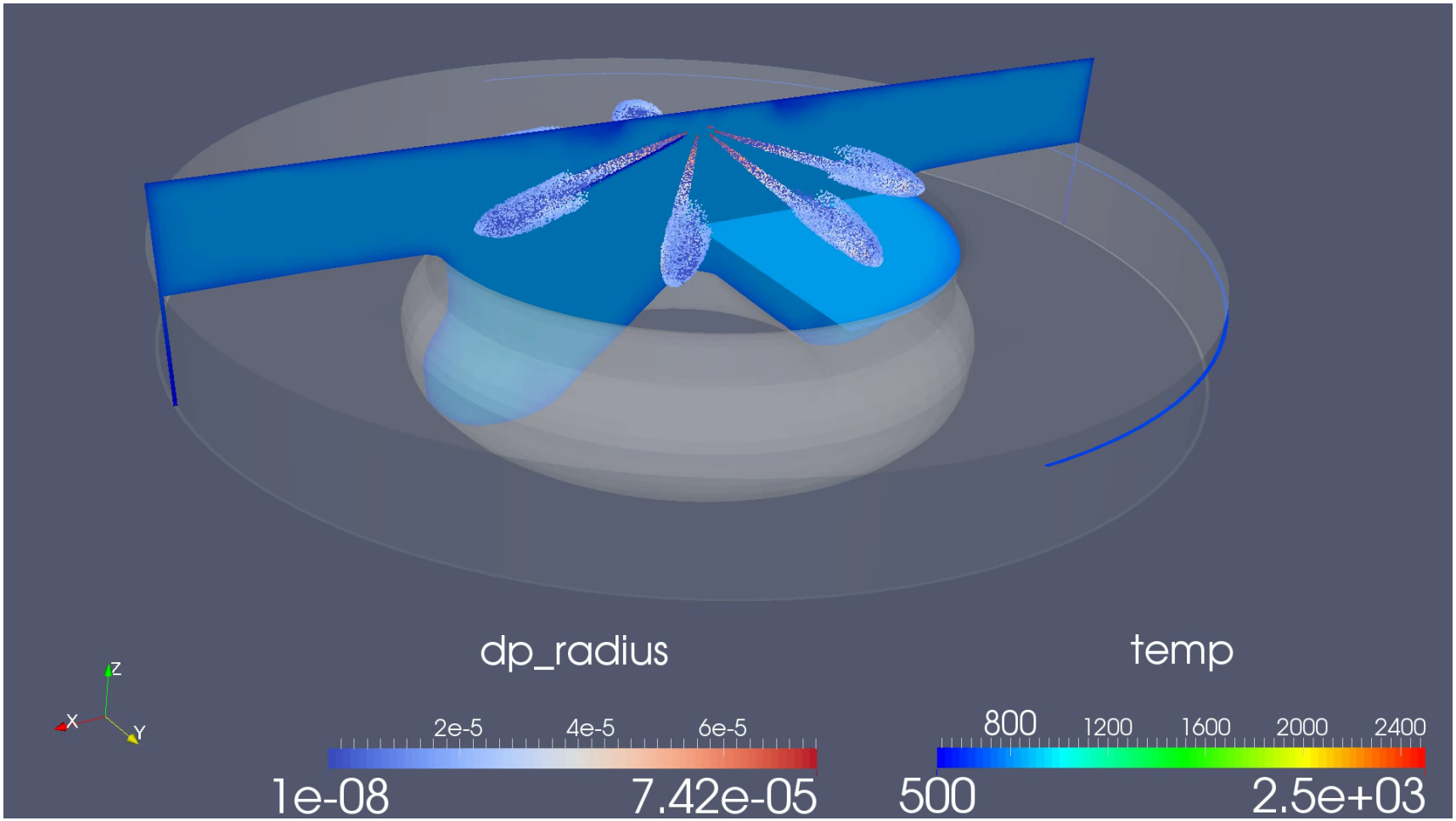



- **The transportation sector relies heavily on Oil and Gas now**
  - Forecasts for 2030 and 2050 show that more than 50% of the world's total energy will still come from Fossil Fuels

**Let us burn these fossils more efficiently and cleanly!!**

# Internal Combustion Engines




**Challenges:** In-nozzle and spray physics, Cyclic variability (need for high-fidelity turbulence models), details of combustion chemistry for different fuels, moving boundaries, grid convergence is challenging, influence on emission predictions, soot modeling, after-treatment, material issues (Conjugate Heat Transfer)…

# Dream

Full *in silico* Engine and Fuel Co-Design with quantified uncertainties that dramatically reduces the need for physical prototyping, allows rapid characterization and testing of novel engine and fuel designs, and reduces design costs and time-to-market of new concepts

# Reality

We can perform simplified simulations on engine and fuel components. The uncertainties are poorly understood.


# Transformation

Exploit emerging computational capabilities through the development of automated, highly parallelized CFD and combustion chemistry codes with fully integrated uncertainty quantification

# DREAM: REVOLUTIONIZE THE CO-DESIGN OF ENGINES AND FUELS

## *Software for Automated Exascale Simulations with Quantified Uncertainties*

According to John Deur, *Director of Engine Research at Cummins Inc.*, the following levels of speedup are needed to significantly impact today's engine development*

Uncertainty Quantification

- [10x] 360 degree cylinder geometry
- [10x] multiple cycle variations
- [10x] more accurate turbulence model (LES)
- [10x] accurate spray dynamics

- [50x] detailed chemical kinetics for real transportation fuels


TOTAL Speedup needs are 500,000 times TODAY'S standard
(today's industry standard is 64 cores with 24 hour turnaround)

**OUR PROBLEM IS EXASCALE => 30 million cores for 24 hour turnaround!**

* DOE Engine Simulation Roadmap Workshop - August 18, 2014

# Reality: Computational Resources

## Clusters

**Fusion Cluster**

- 320 compute nodes
- 2560 compute processors
- 12.5 terabytes memory
- 500 terabytes disk
- 25.9 teraflops peak

**Blues Cluster**

- 310 compute nodes
- 4960 compute processors
- 107.8 teraflops peak

## Super-Computer

PETAFLOPS POWER

48 racks

1,024 nodes per rack

1.6 GHz 16-way core processor

16 GB RAM per node

384 I/O nodes

240 GB/s, 35 PB storage

That's a total of 768K cores, 768 terabytes of RAM, and a peak performance of 10 petaflops.


In 2012, engine codes did not run efficiently on even 100 processors!

**In general Engine simulations involve:**

- Unresolved Nozzle flow
- Simplified combustion models
- Coarse mesh => grid-dependence
- Simplified turbulence models
- Poor load-balancing algorithms

**Reality: Extensive tuning to match experimental data**

**Transformational Approach:**

- Detailed chemistry based combustion models
- Fine mesh => grid-convergence
- High-fidelity turbulence models: LES based
- Two-phase physics based fuel spray model
- In-nozzle-flow models

- Develop tools for High-Performance Computing

**Towards Predictive Simulation of the Internal Combustion Engine**

# CONVERGE is our Current tool since it is preferred by the industry…

| | |
|---|---|
| **Modeling Tool** | **CONVERGE,** almost full source-code access for HPC development |
| Dimensionality and type of grid | 3D, structured with Adaptive Mesh Resolution |
| Spatial discretization approach | 2nd order finite volume |
| **Smallest and largest characteristic grid size(s)** | Finest grid size simulations**:**<br>**2.5 µm for nozzle flow** (31 million peak cell count)<br>**32.5 µm for Spray** (22 million peak cell count)<br>**87.5 µm for engine** (35 million peak cell count) |
| **Total grid number** | **50 millions is the highest cell count run** |
| **Parallelizability** | **Good scalability on up to 4000 processors** |

| | |
|---|---|
| **Turbulence model(s)** | RANS: RNG k-ε; **LES: Smagorinsky, Dynamic Structure** |
| **Spray models** | **Eulerian-Eulerian Near Nozzle Model**<br>Lagrangian Models: |
| **In-nozzle Flow** | **Homogeneous Relaxation Model (HRM)** |
| Time step | Variable based on spray, evaporation, combustion processes |

| | |
|---|---|
| **Turbulence-chemistry interactions model** | Direct Integration of detailed chemistry: well-mixed model<br>**Multi-Flamelet Representative Interactive Flamelet (RIF)** |

**All this work is published in peer-reviewed journals and conference proceedings (http://verifi.anl.gov/publications/)**

# Governing Equations

$$\partial\rho/\partial t+\partial\rho u_i/\partial x_i=s$$

$$\partial\rho u_i/\partial t+\partial\rho u_i u_j/\partial x_j=-\partial P/\partial x_i+\partial\sigma_{ij}/\partial x_j+s_i$$

$$\partial\rho e/\partial t+\partial\rho u_i e/\partial x_i=-P\partial u_i/\partial x_i+\sigma_{ij}\,\partial u_i/\partial x_j+\partial/\partial x_i\,(k\partial T/\partial x_i)+\partial/\partial x_i\,(\rho\sum_m^{\blacksquare}Dh_m\,\partial Y_m/\partial x_i)+S$$

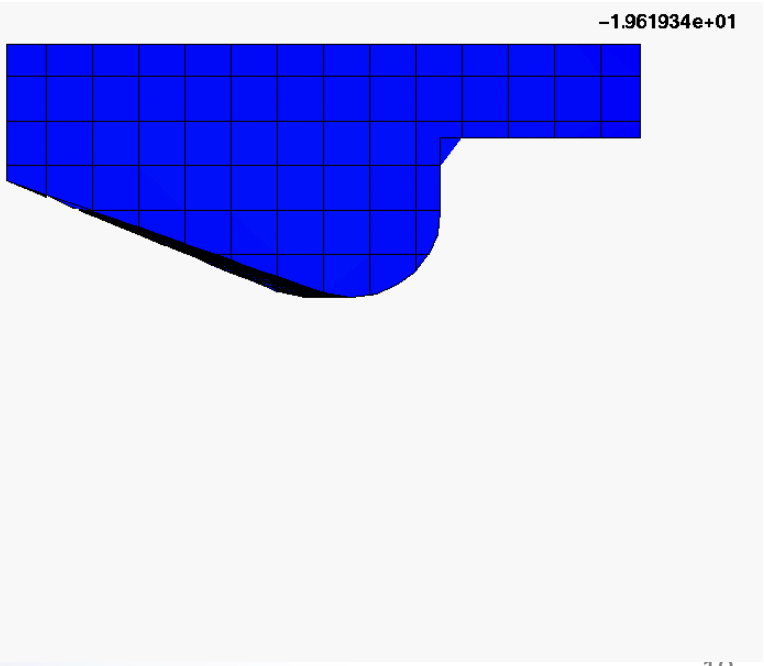
$$\partial\rho_m/\partial t+\partial\rho_m u_i/\partial x_i=\partial/\partial x_i\,(\rho D\partial Y_m/\partial x_i)+s_m$$

Where $\rho$ is the density of the mixture, $\rho_m$ is the density of species $m$, $\sigma_{ij}$ denotes the stress tensor, $k$ stands for the conductivity, $Y_m$ is the mass fraction of species $m$, $D$ is the mass diffusion coefficient, $h_m$ denotes the species enthalpy, $e$ stands for the specific internal energy, and $s$ is the respective source.

Adaptive Meshing:

Boon: Engine Simulations

Bane: High Performance Computing




- AMR enables to provide mesh anywhere in the flow-field as desired
- Load-distribution is extremely challenging with embedding levels higher than 4, especially with moving boundaries (piston, valves, needle, etc.)

# HPC Enabling Simulations that could not be performed in the past ..

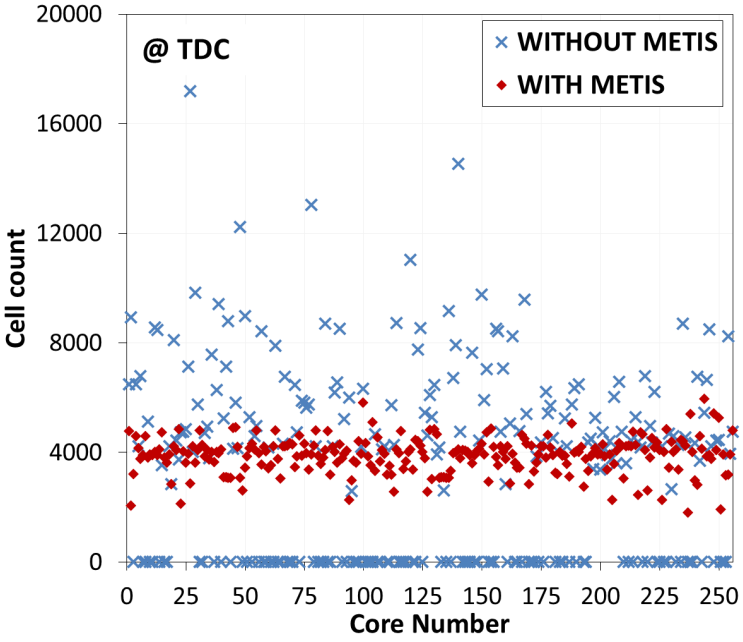
- **Scale-up a single engine simulation to 1000s of processors (Capability Computing)**
  - 30-50 million CFD cells
  - Advanced load-balancing algorithm
  - Resolved I/O issues
  - 2-3 weeks wall-clock time on 1000-5000 cores

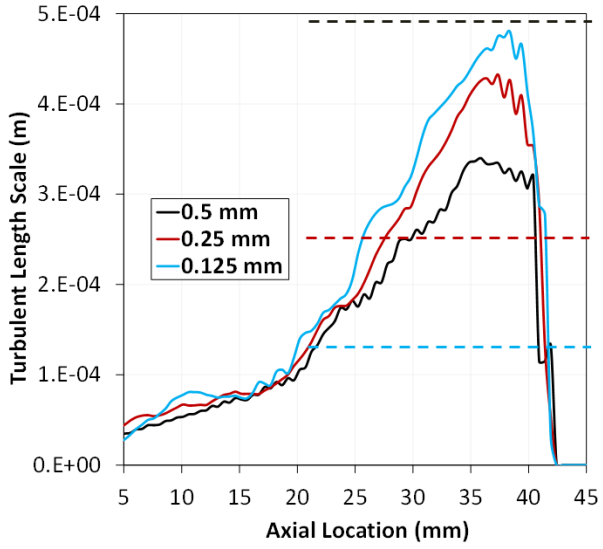


- **Use 1000s of cores for multiple number (10s) of smaller simulations (Capacity Computing)**
  - 1-5 million cells per simulation project
  - 1-3 days wall-clock time on 10-100 cores
  - ❖ **Optimization** of engine operating parameter, e.g., GA optimization
  - ❖ **Uncertainty Quantification** of engine operating parameters and model constants
  - ❖ **Global Sensitivity Analysis** to identify engine relevant chemical kinetics (with BES)
  - ❖ **Multiple LES realizations** to obtain enough statistics
    - LES of Fuel Sprays
    - Nozzle flow simulations with LES



# Enabling Engine Simulations to Use HPC Resources

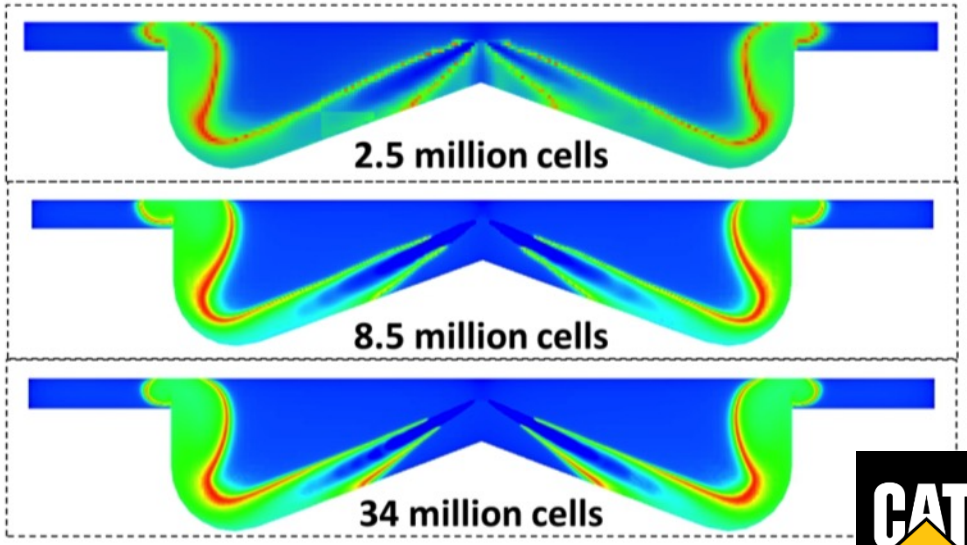


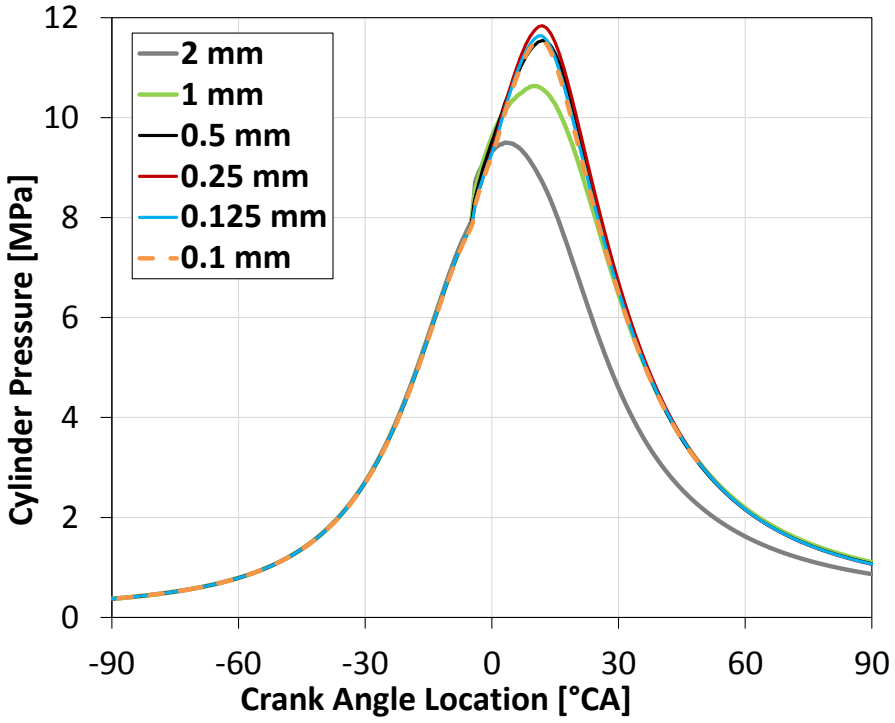

## Scientific Achievements

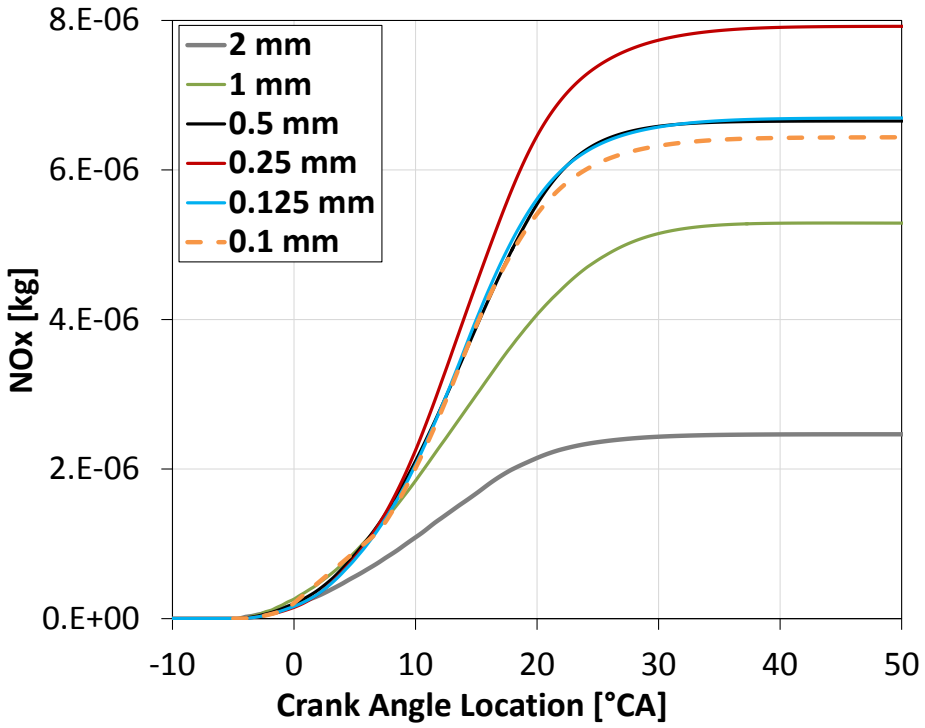
- **High-performance computing enabled due to the implementation of advanced load-balancing algorithms**
- Use of High-spatial and temporal resolution resulting in “grid-convergent” engine results
- Use of detailed chemistry based combustion models
- Largest diesel engine simulation performed

## Cut-plane temperature contours



# Diesel Engine Simulations using HPC Resources




| Minimum cell size (mm) | Peak Cell-count | Wall clock time |
|---|---|---|
| 0.5 | 2.5 million | 14 hours on 64 cores |
| 0.25 | 9 million | 3.5 days on 64 cores |
| 0.125 | 34 million | 13 days on 256 cores |
| 0.1 | 50 million | 14 days on 512 cores |

- Many parameters such as pressure, heat release rate, grid converge at coarse resolutions of 0.5 mm
- NOx emissions grid converge below 0.125mm
- Without HPC, 0.25 mm and lower resolutions would not be possible

Typical engine simulation in industry done on 48-96 processors

# Scaling Engine CFD on Supercomputing Resources

**Gasoline Compression Ignition Engine from S. Ciatti at Argonne**

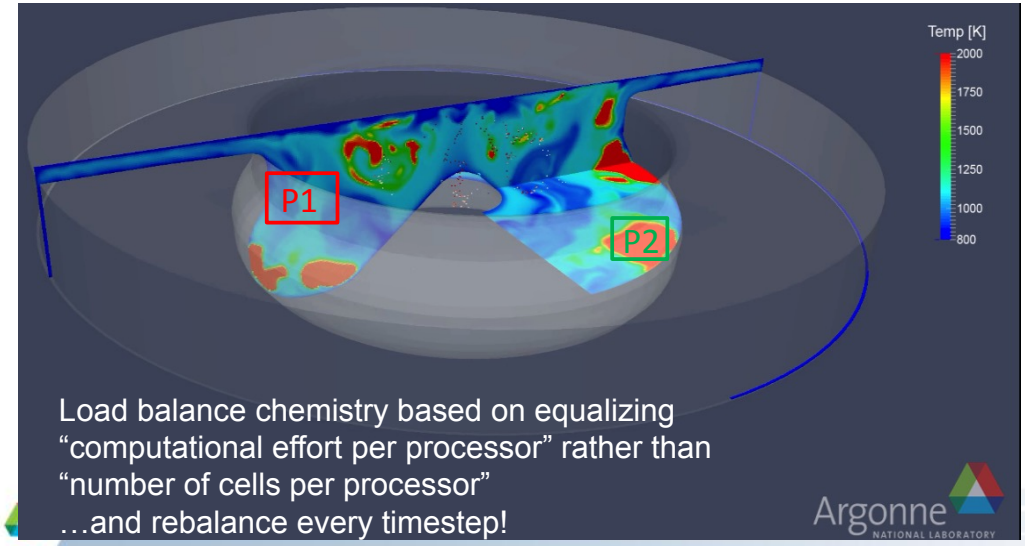
- About 10 million cells @ TDC
- Fixed mesh, no AMR or embedding
- Moving boundaries and DI fuel spray


48 racks
1,024 nodes per rack
1.6 GHz 16-way core processor
16 GB RAM per node
384 I/O nodes
240 GB/s, 35 PB storage

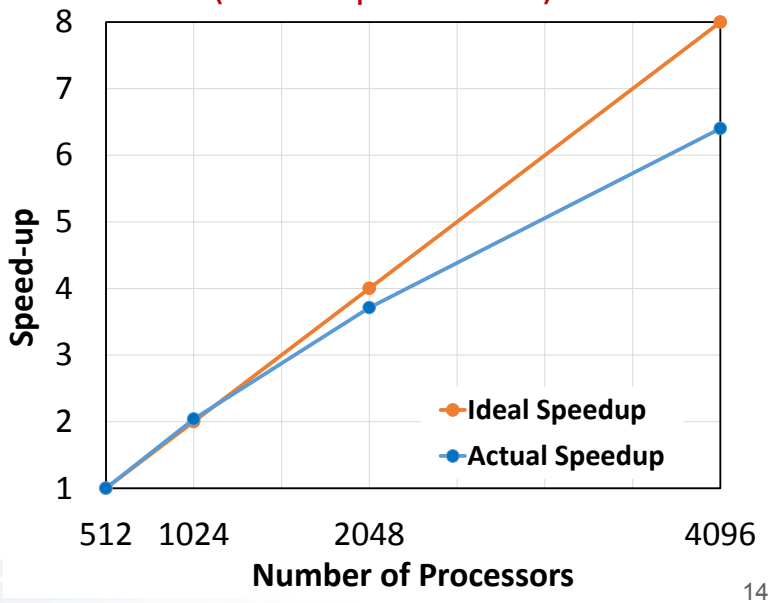
That's a total of 768K cores, 768 terabytes of RAM, and a peak performance of 10 petaflops.

**Optimized to run on MIRA:**

- Speed-up restart (>20x)
- Write restart file (500x)
- Speed-up output and post file writes (1000x)
- Load balancing of cells with METIS (resolved memory constraints)
- Load balancing the chemical kinetic calculations (>3x)



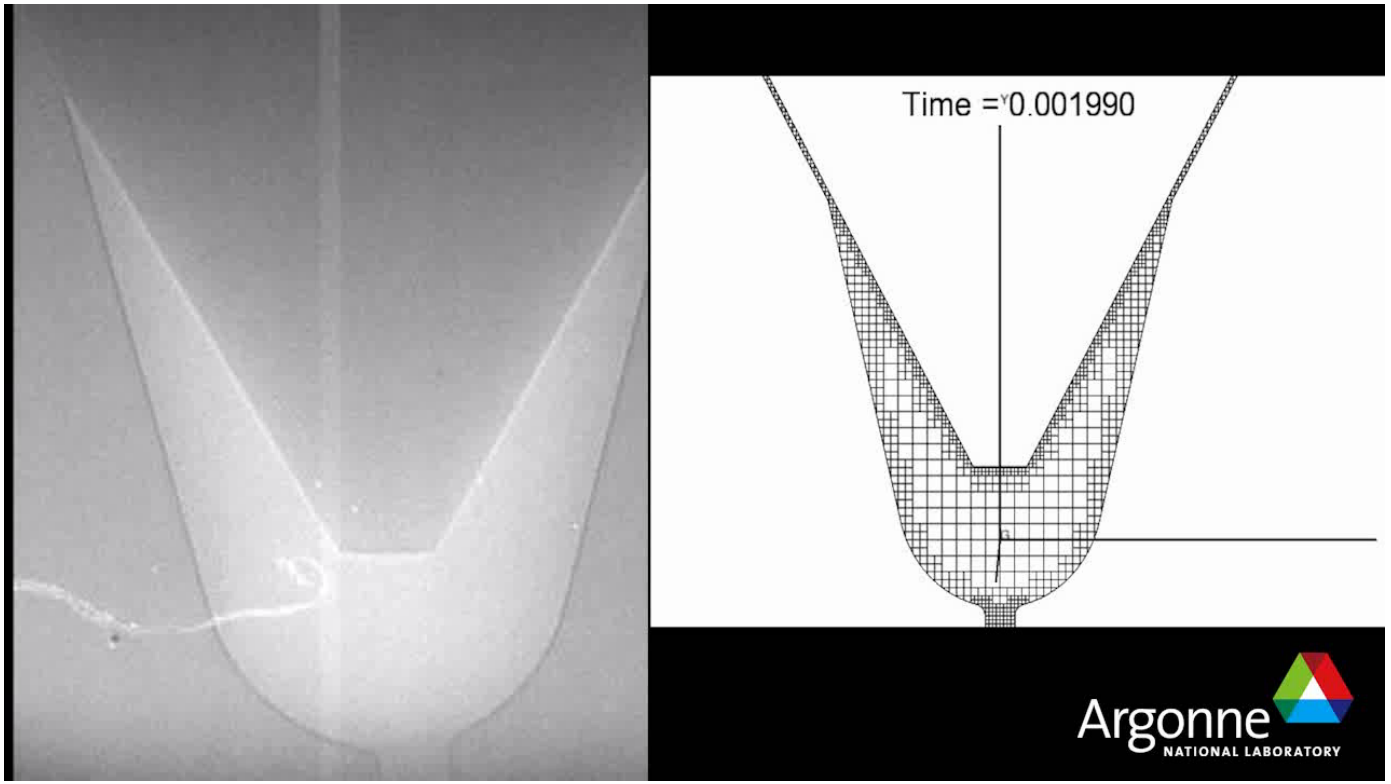

Scaling improvements on MIRA will also benefit smaller jobs run by the industry (24-256 processors)



# In-Nozzle Flows

**X-ray Phase-Contrast Imaging at APS***

**CFD Simulation**



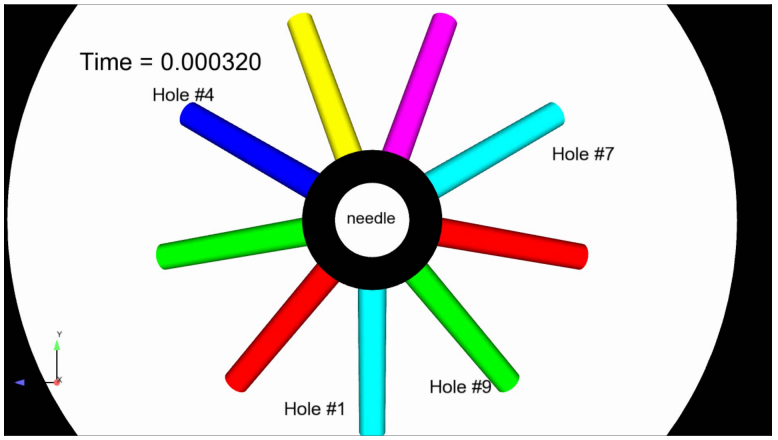

**Project Impact**

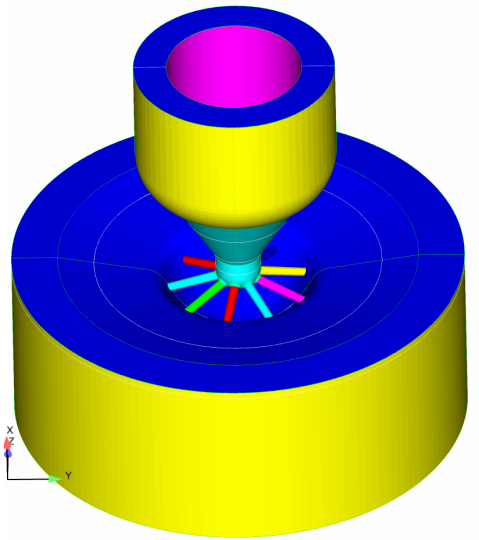
- In-nozzle flow simulations can predict **cavitation inception**
- Needle lift and **off-axis motion** is accounted for in the simulations
- **Influence of nozzle geometry on fuel spray development can now be predicted!**

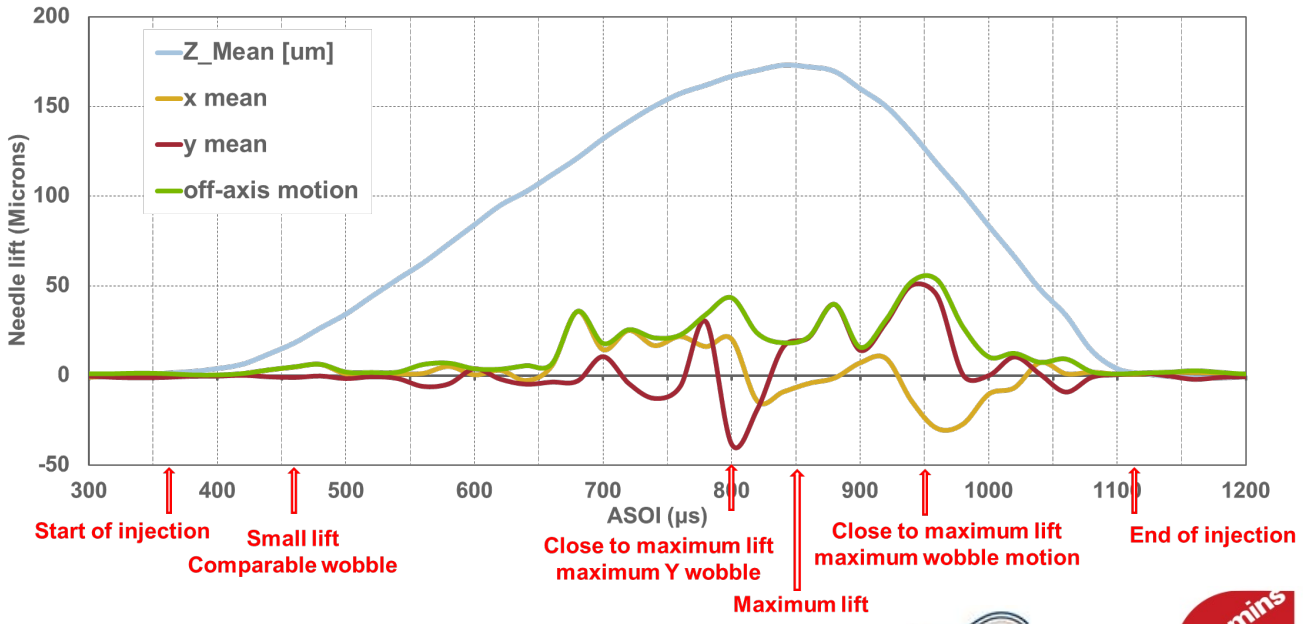
*Data from Chris Powell et al. at the Advanced Photon Source at Argonne

# Full 3D 9-hole Production Injector Simulations

- *First –ever* simulations of a production injector with full needle dynamics (wobble)
  - Min. cell size = 5 µm
  - Max. cell count = 30 - 40 million
- $P_{inj}$ = 2400 bar, $P_{back}$ = 4 bar: Diesel Fuel
- Experimental data for needle lift and wobble obtained from Advanced Photon Source. The plots shown here are for average of 60 shots
- Cummins using *our approach* for simulating different injector nozzle designs (K-factors and hydro-grindings)



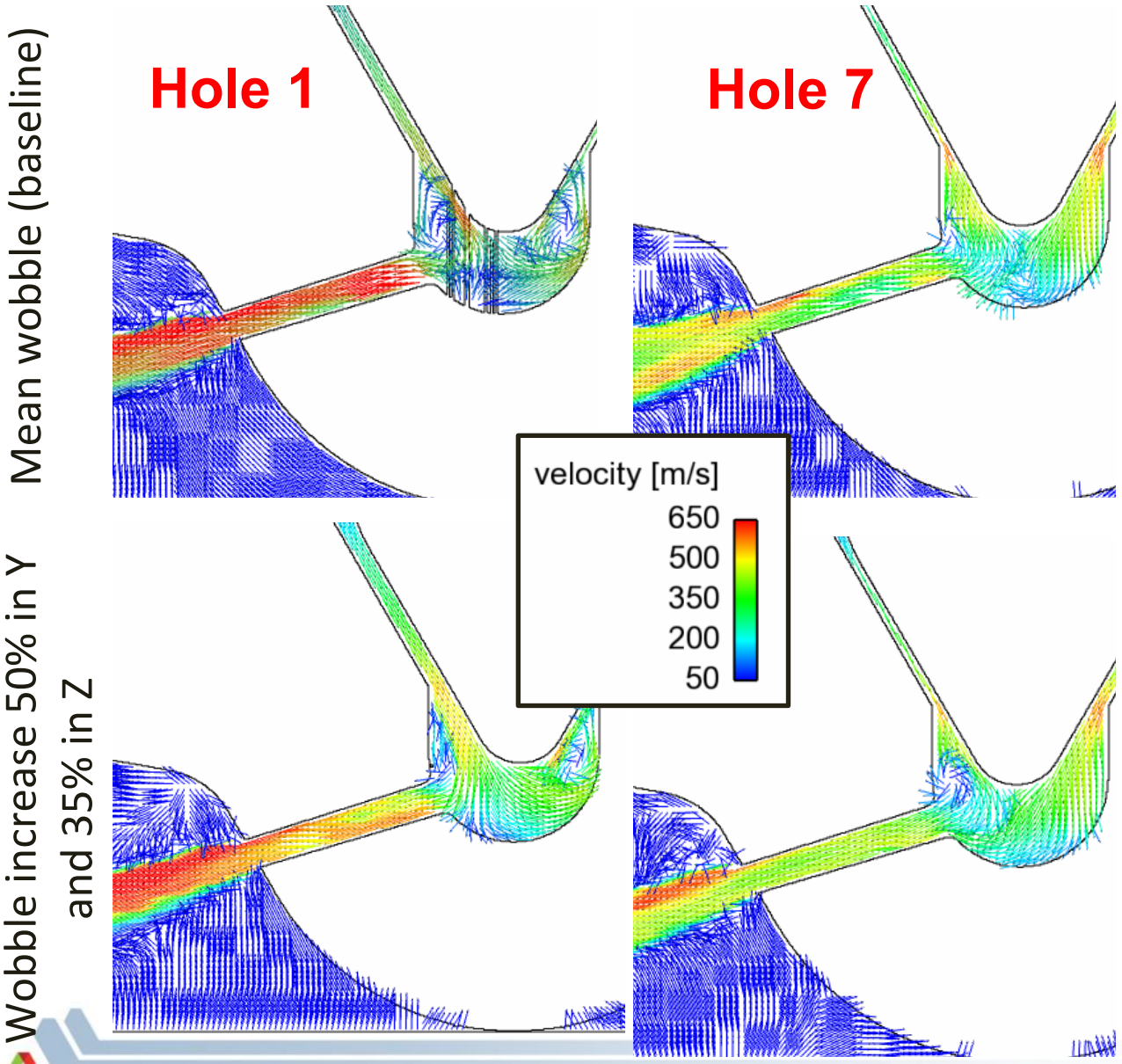






CONVERGENT SCIENCE

Cummins

# Wobble from Shot-to-Shot => Cyclic Variability




- Significant shot-to-shot variation in the APS data for needle off-axis motion (wobble) imposed as boundary condition for each simulation
- Appreciable differences in streamlines and cavitation patterns at many lift profiles
- Simulation of each shot takes about 1 month on 256 processors. HPC allows us to simulate multiple shots
- Demonstrated an approach to capture shot-to-shot variation in simulations
- Cummins using this approach for their in-house next generation engine design

CONVERGENT SCIENCE

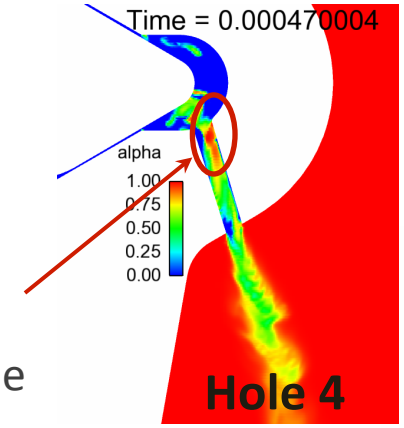
Cummins

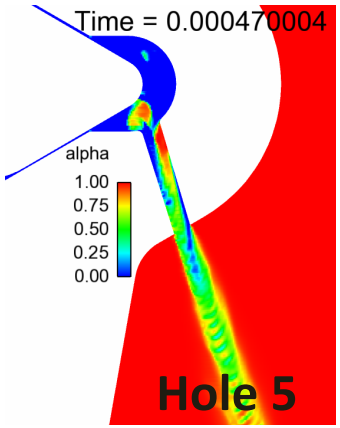
# Hole-to-Hole Variation Especially @ low-lifts

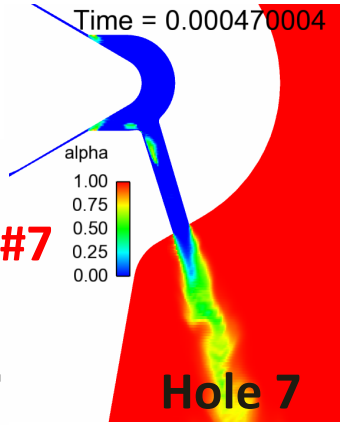
Single-hole or sector simulations cannot capture the necessary physics. HPC allows for multi-hole production injector calculations

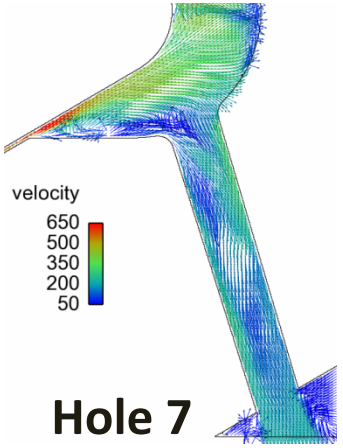
Cavitation more pronounced in the presence of wobble. Without wobble, the extent of cavitation is low and does not reach the nozzle exit

Cavitation contours are observed at the bottom of the orifice due to the flow patterns in the sac due to needle wobble

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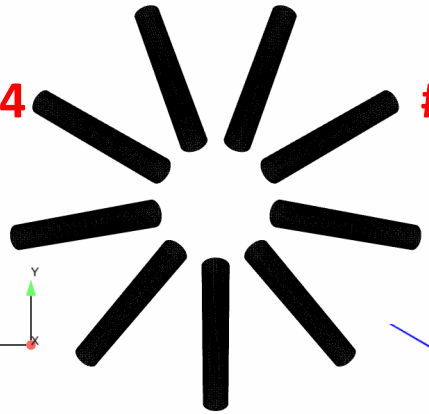

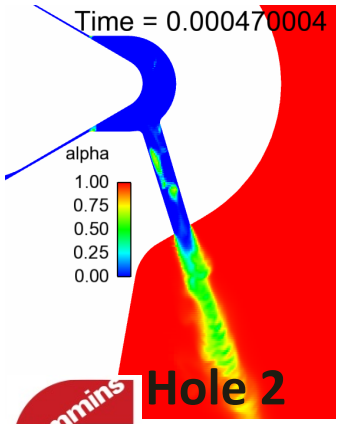


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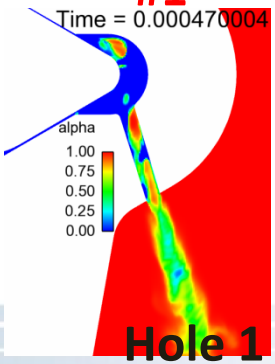
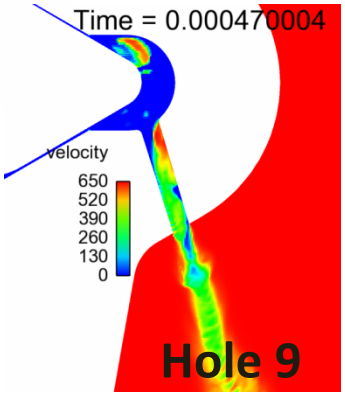
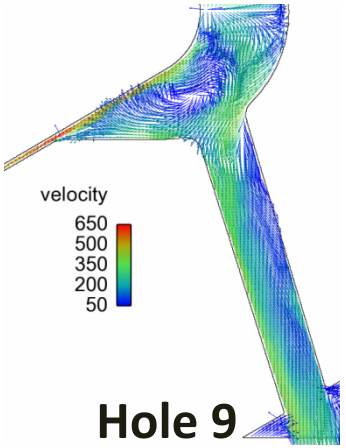
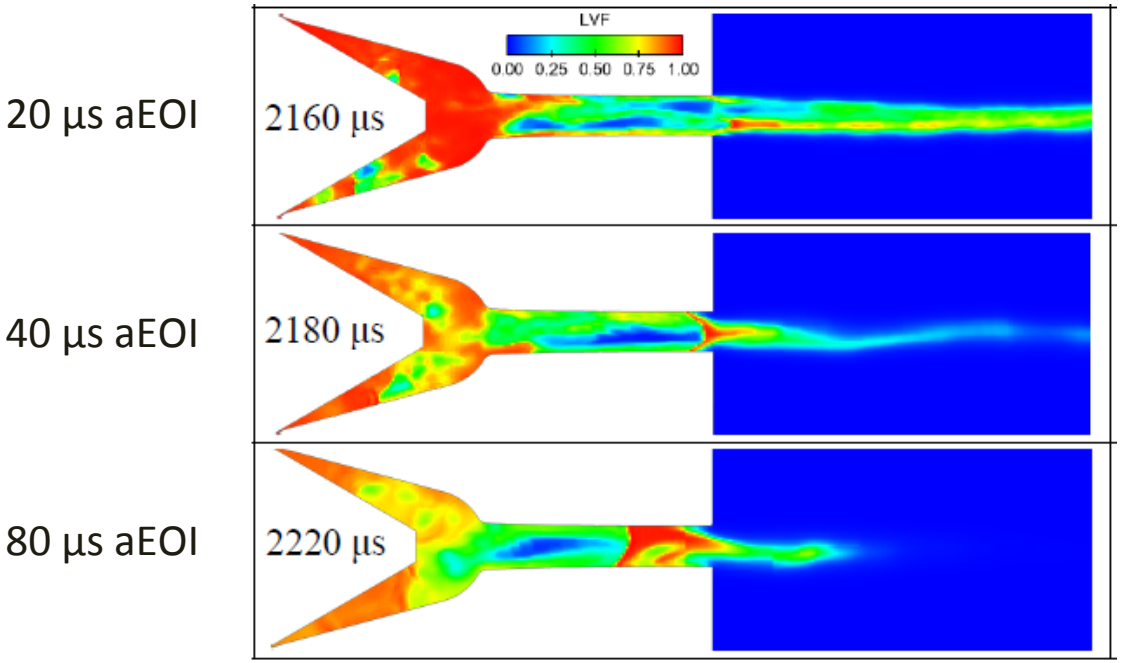


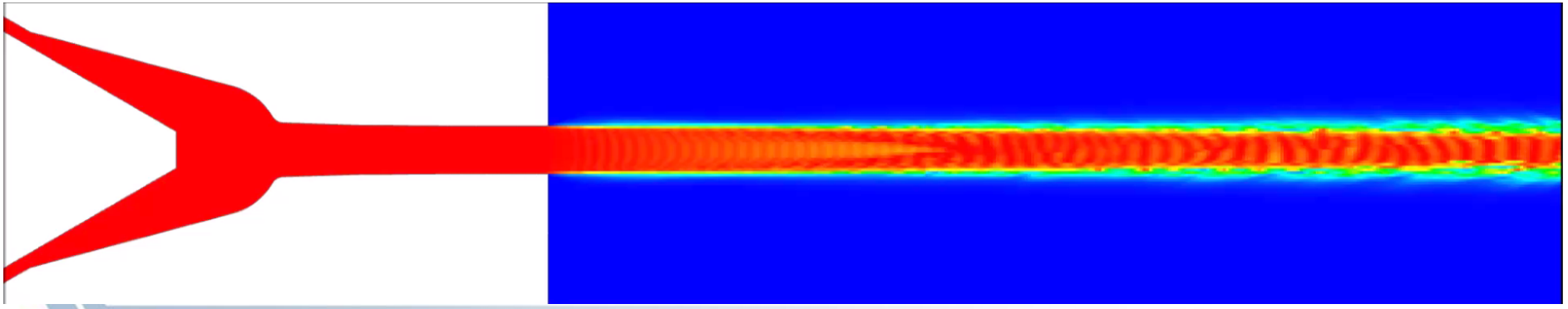



# Fuel Dribble During End-of-Injection

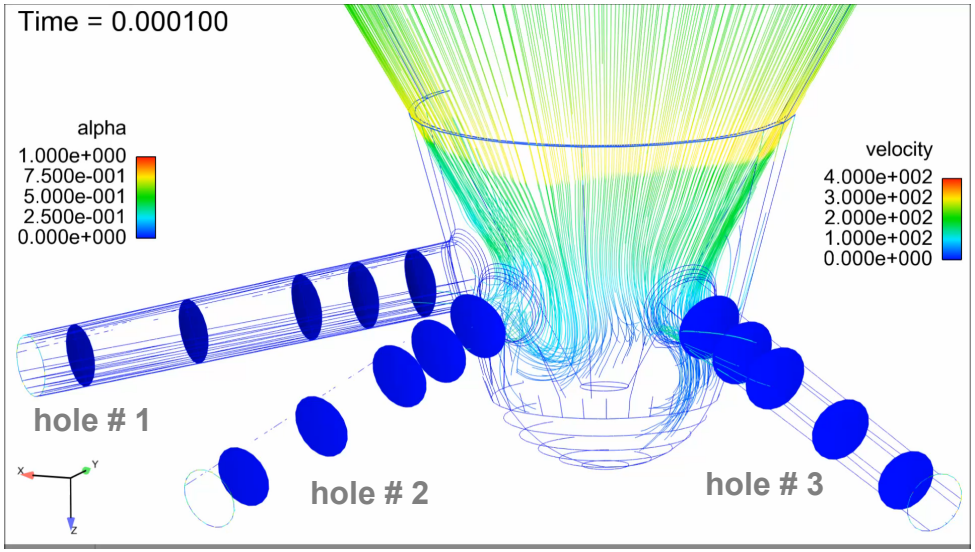
**Large Eddy Simulations capture Fuel Dribble**

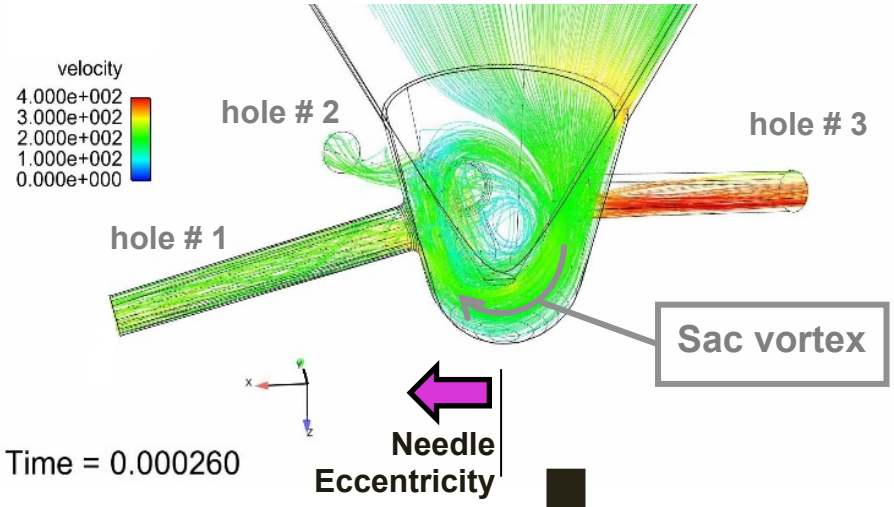


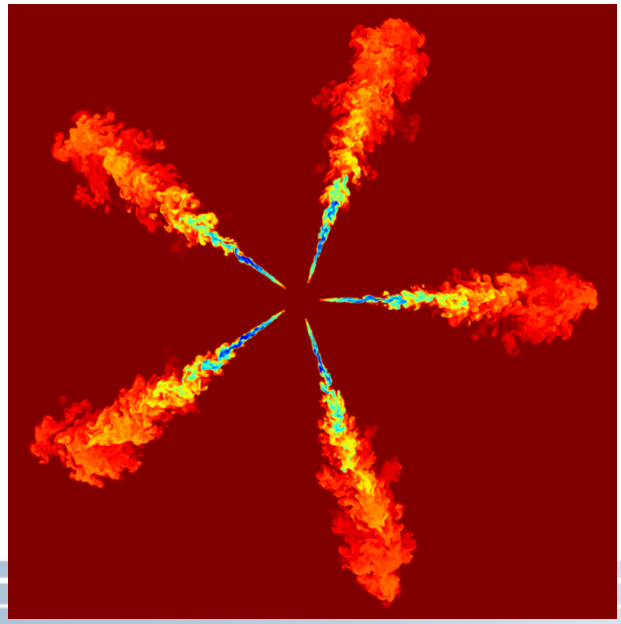

- Dribbled fuel increases emissions as the injected fuel does not burn efficiently
- Extremely difficult to measure the fuel dribbled mass
- Demonstrated an high-fidelity Large Eddy Simulation (LES) turbulence modeling approach to capture the dribbled mass (includes needle wobble) from a single hole injector
- The approach predicts correct sensitivity to injection and back pressure on dribbled mass

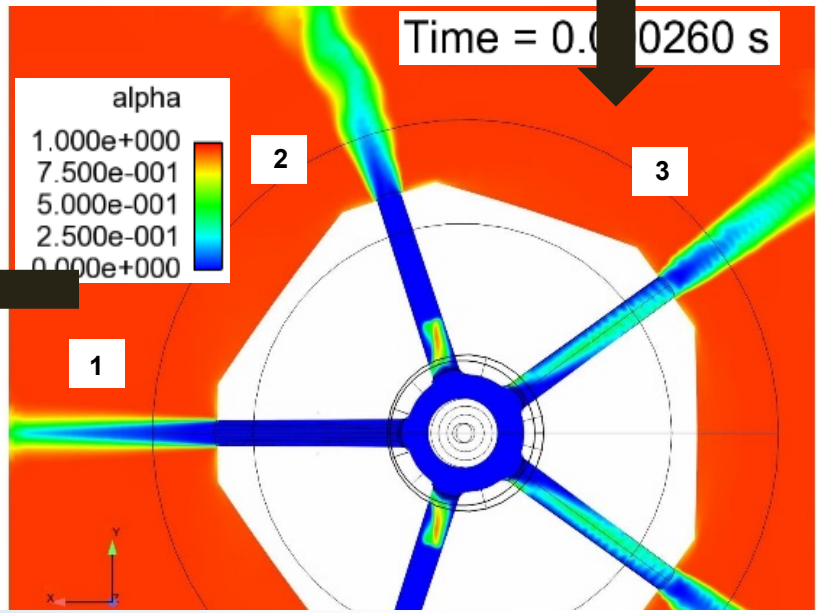


# Plume-to-Plume Variations can now be Captured Due to HPC…



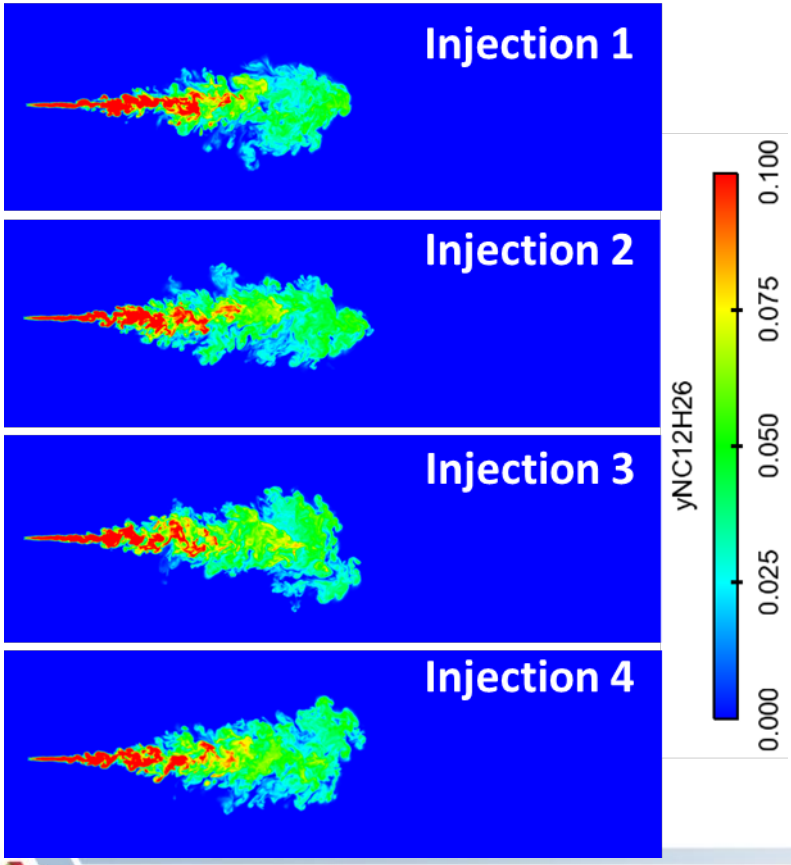



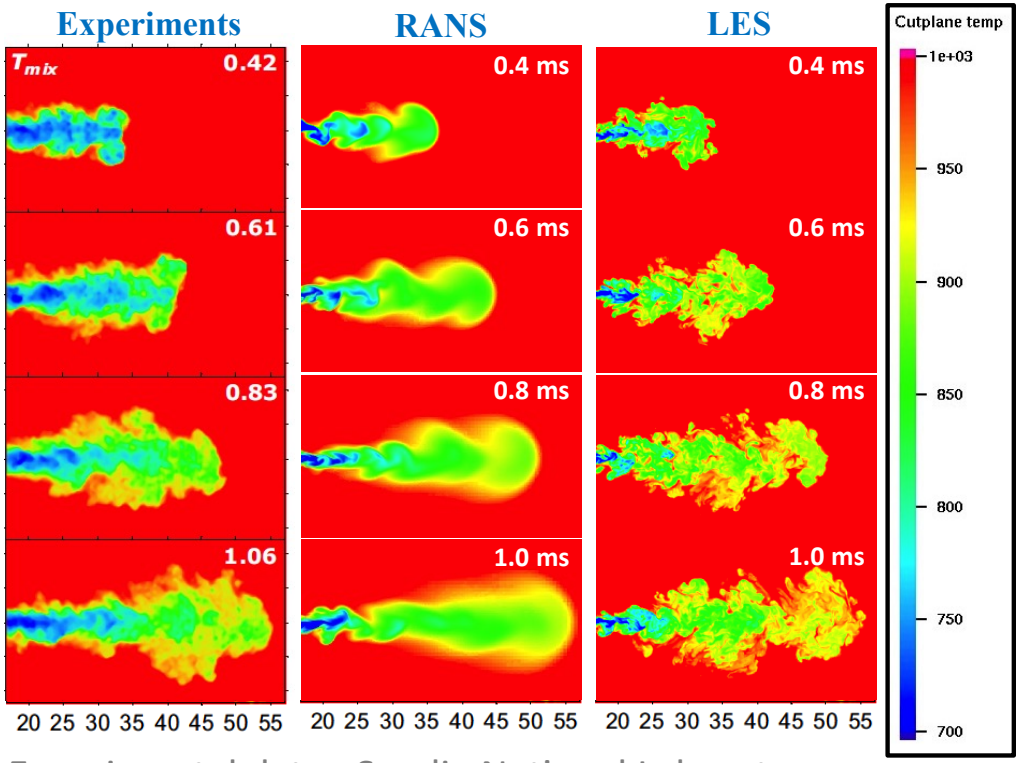


# Turbulence Modeling: Large Eddy Simulations

## Simulation Set-up

- Dynamic structure based LES model developed for engine simulations
- High-temporal and spatial resolutions results in less modeling



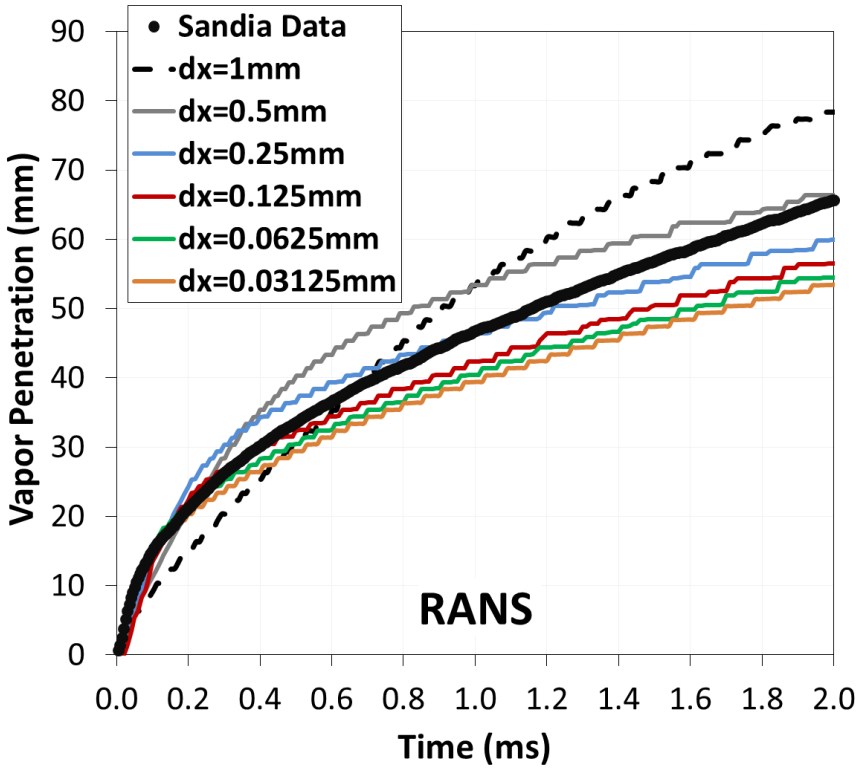



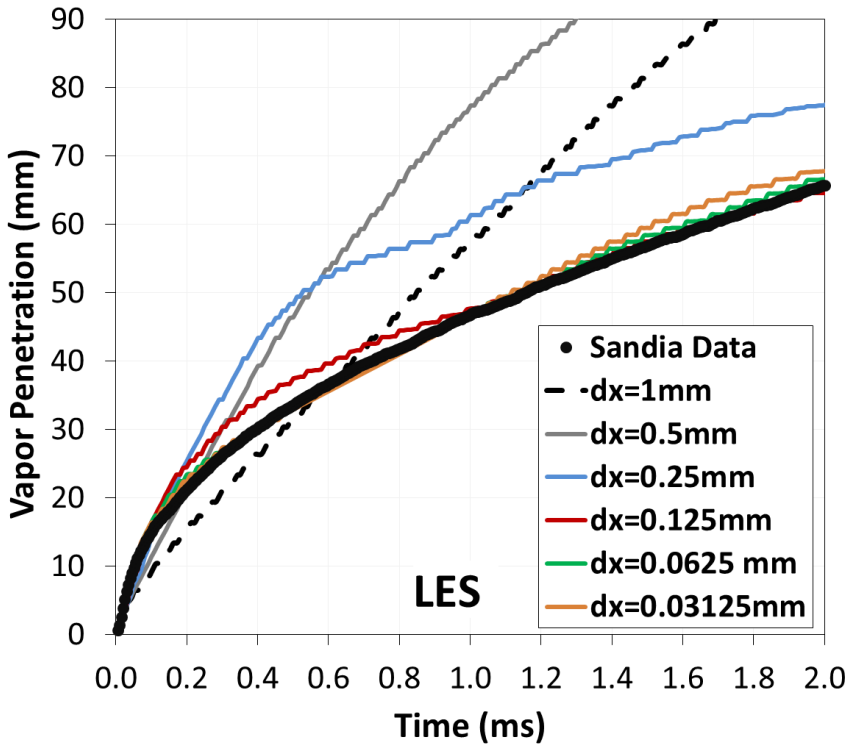

Experimental data : Sandia National Laboratory

## Project Impact

- **LES model can capture flow structures which RANS approach cannot predict**
- LES can also capture **cycle-to-cycle variations**.

# Simplified (RANS) vs. High-fidelity (LES) Turbulence Models

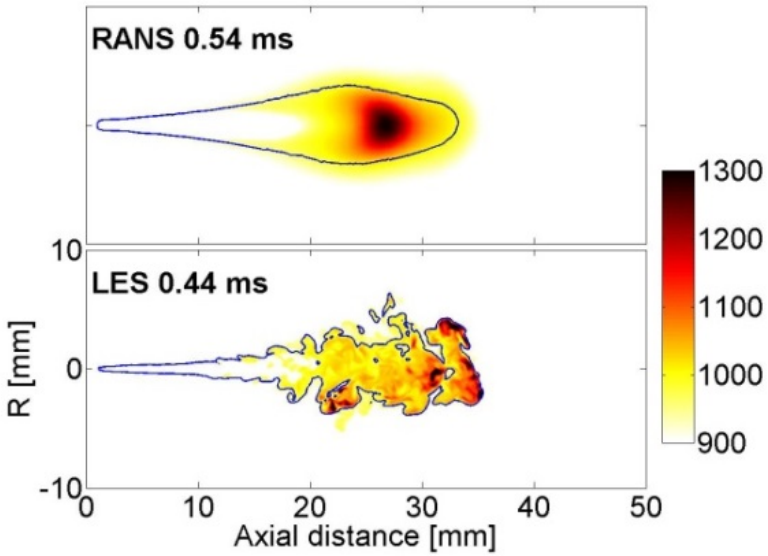



- RANS results though grid-convergent cannot capture the experimental data well
- LES (Dynamic structure model) results can capture the experimental data well
- This is due to the fact that LES resolves more flow structures and hence can predict the fuel-air mixing better
- LES is about 100x more expensive than RANS …

# Spray and Combustion Modeling with LES

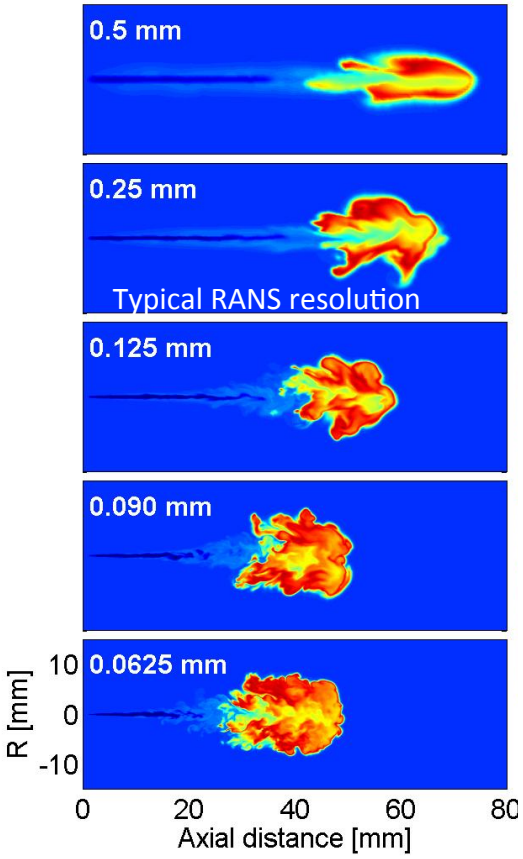
- ➢ Integrating our LES spray modeling approach with the combustion solver in CONVERGE
- ✓ Extensive validation against experimental data from the Engine Combustion Network
- ✓ Multi-cycle engine simulations with LES will follow soon!

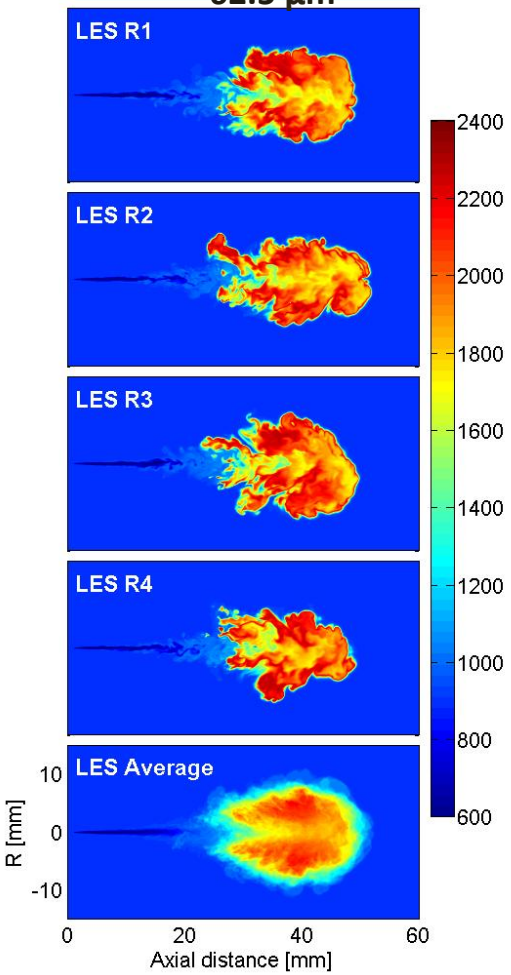

- High-temporal and spatial resolutions with LES results in less modeling
- LES model can capture flow structures which RANS approach cannot predict
- LES captures the phenomenon of volumetric auto-ignition
- LES can also capture cycle-to-cycle variations

# Mesh Resolution and Need for Multiple Realizations with LES

**Temperature contours for different min. mesh sizes**




**Temperature contours for different LES realizations @ 62.5 µm**

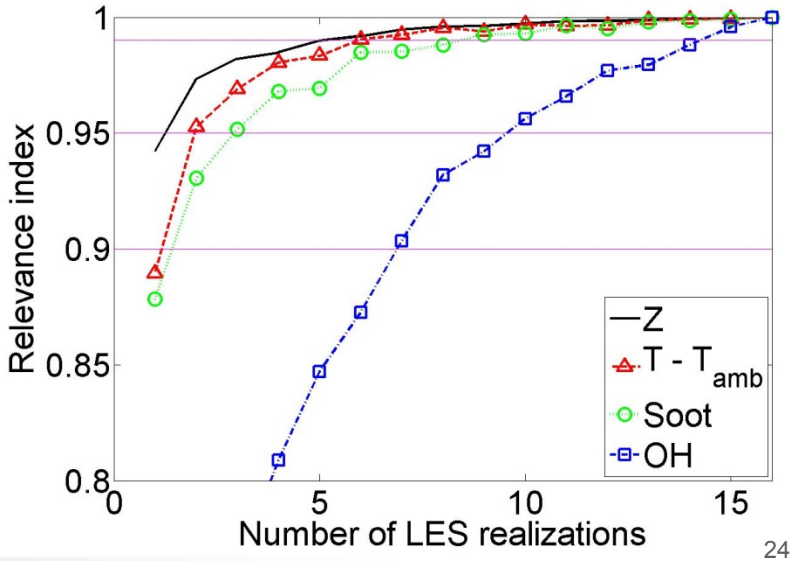



Question from Industry: How many LES realizations are necessary to obtain statistically converged results?

- Temperature: 2
- Mixture fraction (Z): 5
- Soot: 8

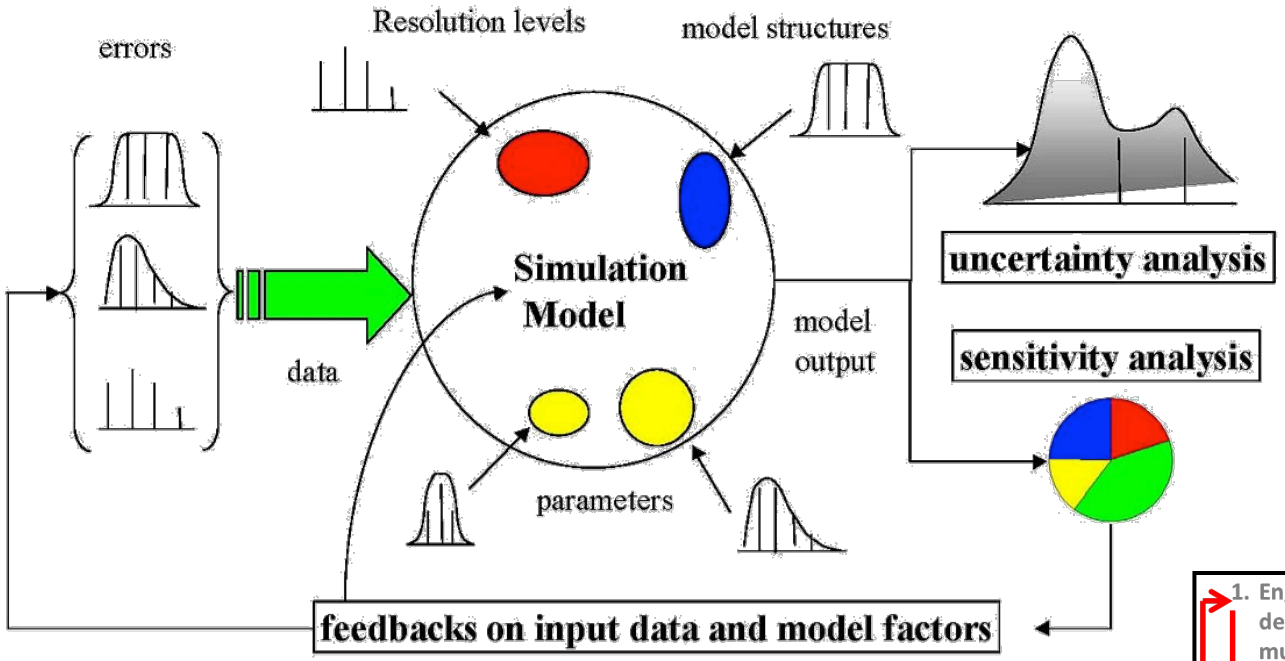
$$\text{Relevance Index } (RI_i) = \frac{\left(\vec{\phi}_i, \vec{\phi}_b\right)}{\| \vec{\phi}_i \| \| \vec{\phi}_b \|}$$

"i" any realization
"b" total number of realizations




- Grid convergence close to 62.5 µm resolution
- Each realization takes about 3 weeks on 200 processors with about 25 million CFD cells

# Introduction: Sensitivity Analysis

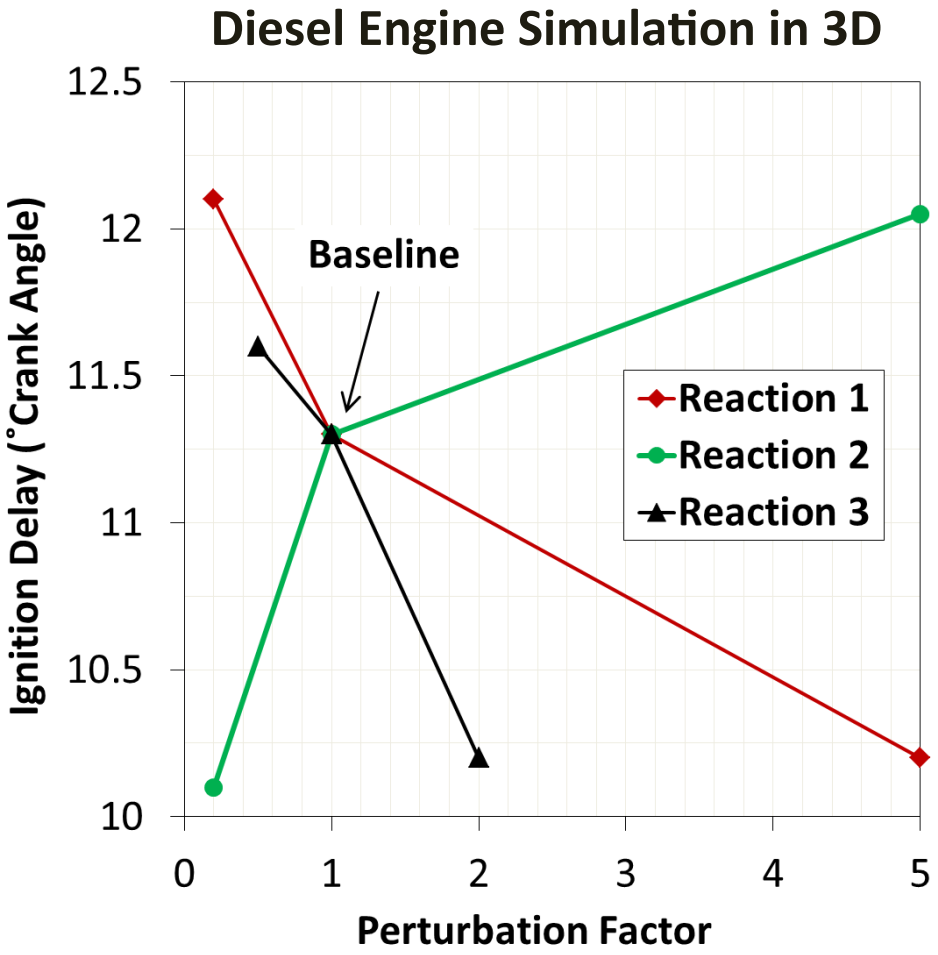



- Uncertainty arising from different sources— e.g., errors in the:
  - Input data
  - Parameter estimation procedure
  - Alternative model structures
- Propagate through the model and result in discrepancies
- Their relative importance is quantified via sensitivity analysis
  - Design the experiments
  - Obtain more accurate predictions
  - Test model robustness in the presence of uncertainty

1. Engine simulations with science-based detailed chemistry run in parallel for multiple initial conditions for physical and operational parameters within their uncertainty ranges
2. Uncertainty quantification analyzes simulation results to produce a physical/operational parameter list ordered by effect on engine performance uncertainties
3. Experimental/theoretical studies to further characterize physical/operational parameters for re-insertion, with reduced uncertainties, into simulations

# Uncertainty in Reaction Rate Parameters in a Kinetic Mechanism

- **Brute Force Sensitivity Analysis** on some reactions:
  1) $nC_7H_{16} + HO_2 = C_7H_{15}$ (isomers) + $H_2O_2$
  2) $HO_2 + HO_2 = O_2 + H_2O_2$
  3) $OH + OH = O + H_2O$
- Based on inputs from ANL-Chemistry group (*funded by BES*), **uncertainty / perturbation factors assigned** for each of these reactions
- The simulations were perturbed based on the new reaction rates




**Reaction Mechanism:** W. Liu, R. Sivaramakrishnan, M.J. Davis, S. Som, D.E. Longman, T. Lu, "Development of a reduced biodiesel surrogate model for compression ignition engine modeling," *34th Proceedings of the Combustion Institute*

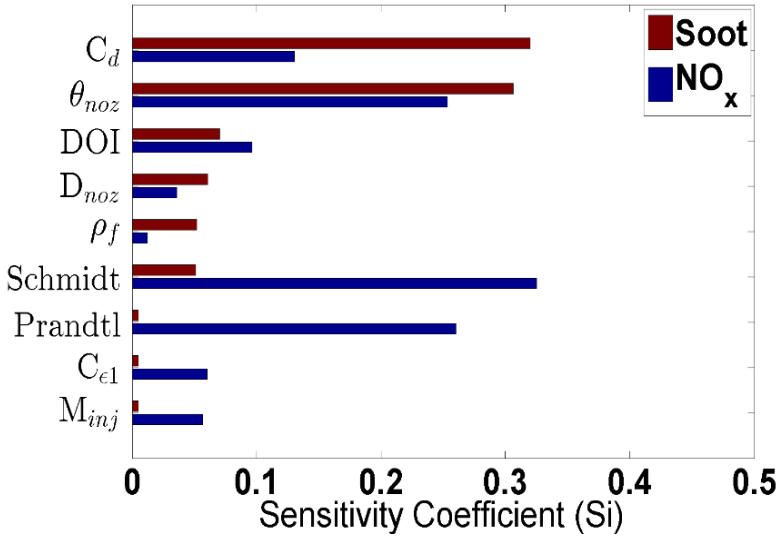
**Perturbations significant to cause engine misfire!**

ALCC award for 60 million core hours for 1 year. Plan to run ~10k simulations on Mira per day to understand kinetic vs. non-kinetic uncertainties

# Uncertainty Analysis on Engine Parameters

- All the uncertain parameters simultaneously and randomly perturbed within the range of uncertainty using Monte-Carlo Sampling
- GSA demonstrated to be a more effective tool compared to brute force sensitivity analysis (perturbing one variable at a time)
  - ✓ Non-linear interactions between variables and their influence on targets can be captured
  - ✓ Computationally efficient
- Closed-cycle simulations of the CAT single cylinder engine. 32 uncertain variables (both experimental and modeling) identified which may influence engine simulation results
  - ✓ 100 simulations per speed-load condition using a sparse method rather than OLS
- **GSA applied to understand the influence of each uncertain parameter (model or engine parameters) towards a target of interest (such as $NO_x$, soot, ignition delay, etc.)**

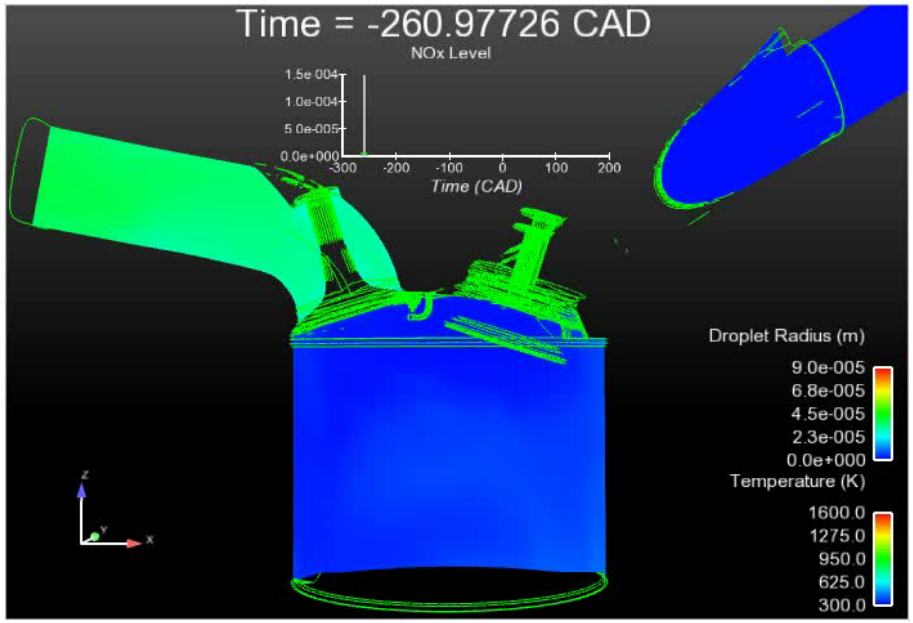
| Variable | Description | Baseline | Min. | Max. |
|---|---|---|---|---|
| $T_{piston}$ | piston wall temperature [K] | 553 | 538 | 568 |
| $T_{cylinder}$ | cylinder wall temperature [K] | 433 | 423 | 443 |
| $T_{head}$ | Cylinder head temperature [K] | 523 | 508 | 538 |
| RPM | engine speed [RPM] | 1500 | 1495 | 1505 |
| SR | Swirl Ratio | 0.98 | 0.95 | 1.00 |
| Schmidt | Schmidt number | 0.78 | 0.70 | 0.90 |
| Prandtl | Prandtl number | 0.9 | 0.8 | 1.0 |
| $I_{tke}$ | initial turbulence intensity [$m^2/s^2$] | 1.6 | 1.0 | 2.0 |
| $L_i$ | initial length scale [mm] | 11.2 | 5.0 | 15.0 |
| $M_{trap}$ | residual mass [mg] | 0.05 | 0.02 | 0.10 |
| $T_{(f,crit)}$ | fuel critical temperature [K] | 657 | 645 | 659 |
| $\rho_f$ | Normalized fuel density | 1.00 | 0.95 | 1.05 |
| $HOV_f$ | Normalized fuel heat of vaporization | 1.0 | 0.9 | 1.1 |
| $VP_f$ | Normalized fuel vapor pressure | 1.0 | 0.9 | 1.1 |

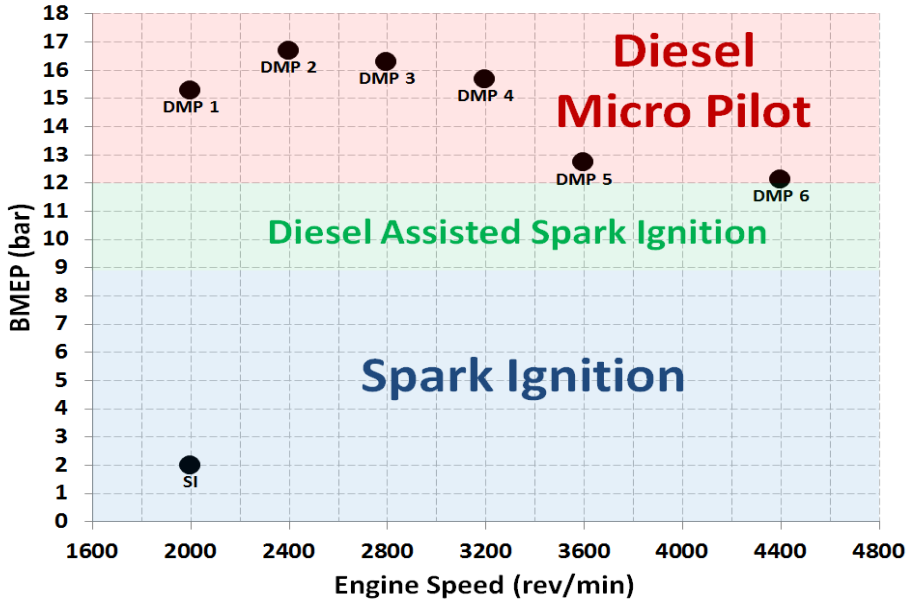


# Dual - Fuel Combustion with Chrysler LLC.

## Project Impact

- Development of a combustion strategy to **smoothly transition** between SI, DASI, and DMP combustion concepts for **Chrysler LLC**.
- **Dual Fuel strategy**: Diesel as a ignition source, gasoline directly injected early for bulk heat release



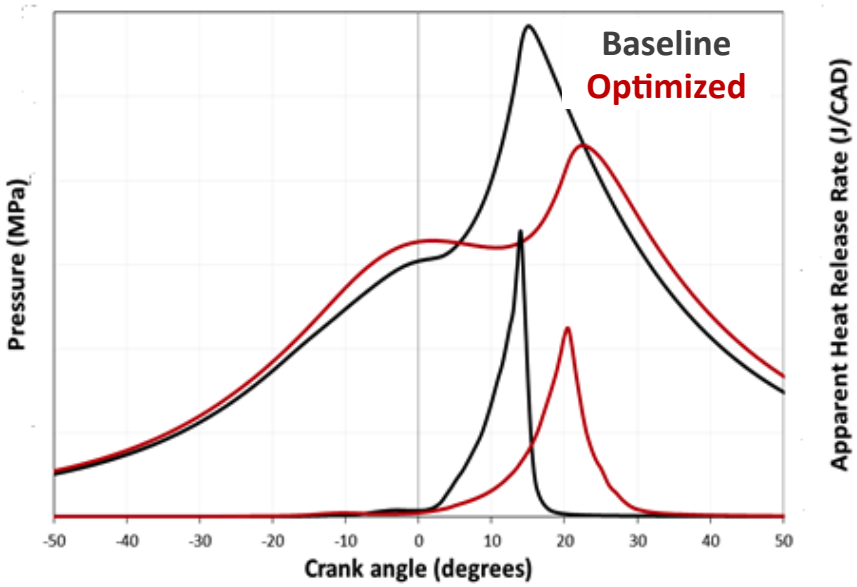



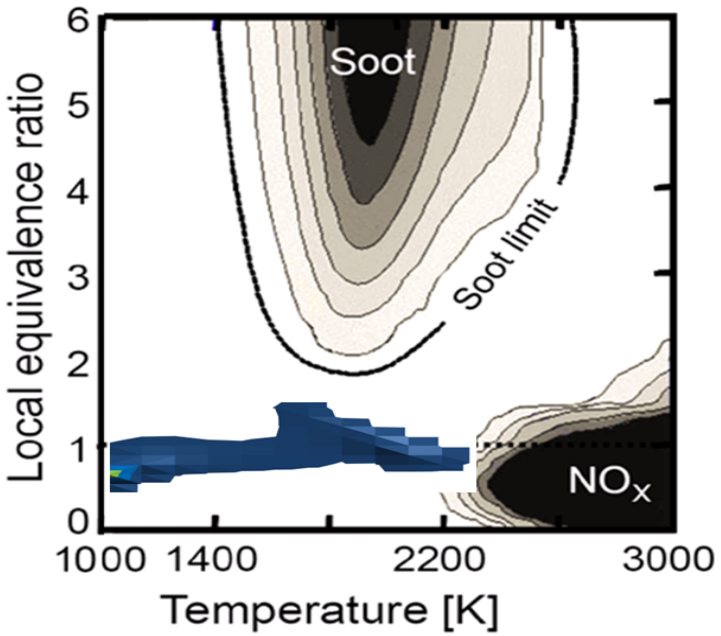

## Scientific Achievements

- Genetic Algorithm based optimization performed to gain **simultaneous performance and emission benefits**
- Simultaneous reduction of both NOx and soot emissions
- Simulations aided experimental studies on finding optimum operating conditions

# CFD based Optimization before Hardware Testing

50 generations (8 simulations each generation): Total 400 cases simulated
40-50 hours for each case simulation on 48 cores
Peak cell count: 3 million




| Parameters | Baseline | Optimized |
|---|---|---|
| EGR ratio (%) | 35.3 | ↓ |
| ICL (° CA ATDC) | 461.8 | ↓ |
| DMP ratio (%) | 13.4 | ↓ |
| Diesel SOI (° CA BTDC) | 19.5 | ↑ |

**Optimization suggests:**

- Higher intake pressure
- Earlier and less DMP injection mass

**And leads to:**

- Retarded combustion phasing
- Longer combustion duration

CHRYSLER

# HPC Enabler for Simulation based Engine Design

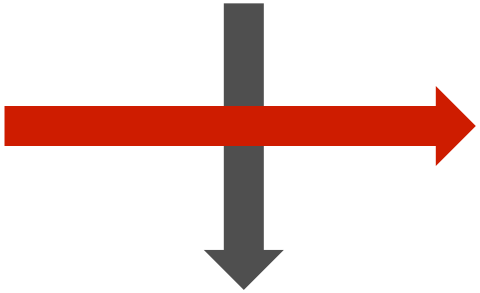
Use of High-spatial and temporal resolution

Robust turbulence models

Use of detailed chemistry based combustion models

Solving “one-of-a-kind” problem

**Cluster**



**Super-Computer**


## Benefits

Unprecedented insights into the combustion process

Grid-convergent results => Increased predictive capability

Modify “best practices” in industry

Enable the use of next-generation computational architectures

# LEAPFROG YOUR COMPETITION: Shrink Your Combustion Engine Development Cycle!

From new fuels
to fuel injection
to combustion
to power
to emissions...


VERIFI's World-Class Chemists Quantify the Effects of Combustion

VERIFI's Supercomputers Do the "Heavy Lifting" of Computation and Visualization

VERIFI's Testing Capabilities Provide Unmatched Experimental Data to Validate Simulation Models

VERIFI's Computational Scientists & Engineers Put It All Together for You

**VERIFI creates design-optimizing simulations that can reduce your financial investment and cut years from your product development cycles.**

**You supply the problem, VERIFI provides the answers!**

# Core Capabilities & Collaborations

## Large variety of engine platforms and fuels

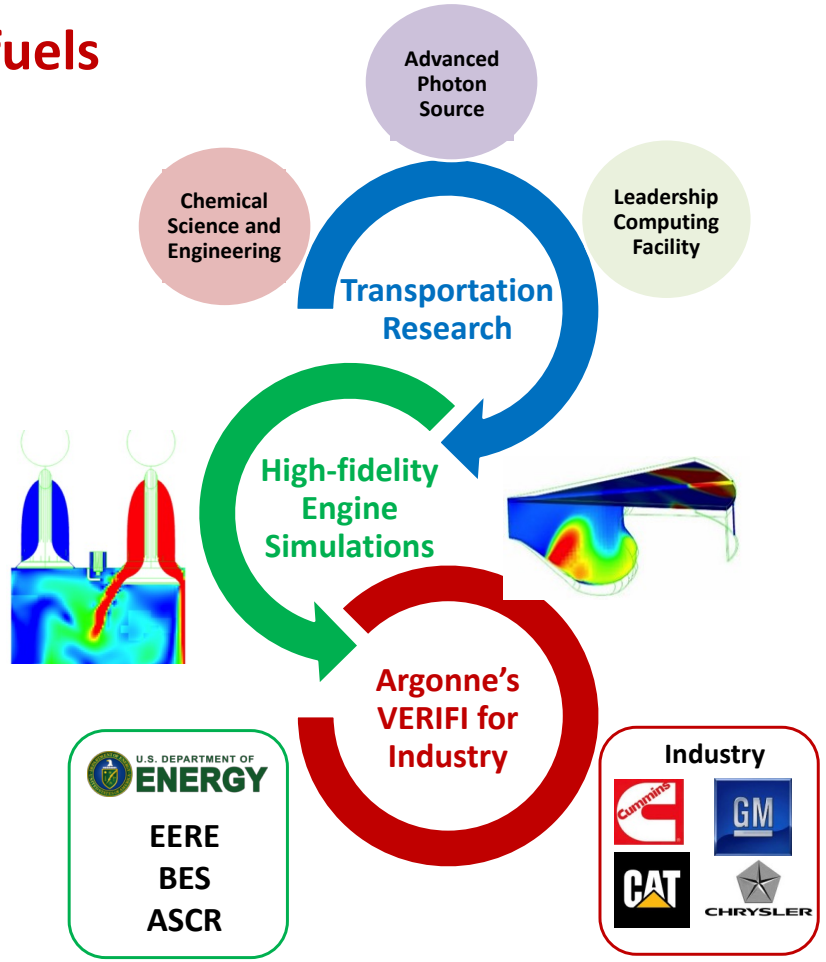
- Light- and heavy-duty engines
- CI – SI – LTC – Dual-fuel
- Gasoline – Diesel – Biofuels
- Gasoline Compression Ignition

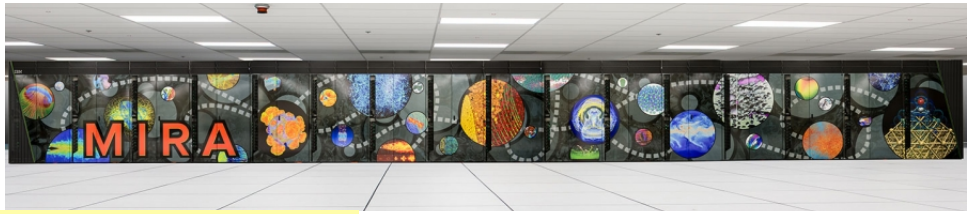
## Model Development

- Nozzle internal flow
- Sprays
  - Lagrangian models
  - Eulerian models
- Detailed chemistry
- Mechanism reduction
- RANS and Large Eddy Simulations
- Cyclic variability
- Turbulence chemistry interaction
- Optimization
- Uncertainty Analysis

## Computational resources

- Clusters and Super-Computer Facility




http://verifi.anl.gov/

# Take Home Message

**Sibendu Som, Ph.D.**
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Computational Fellow – University of Chicago
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## Research Field

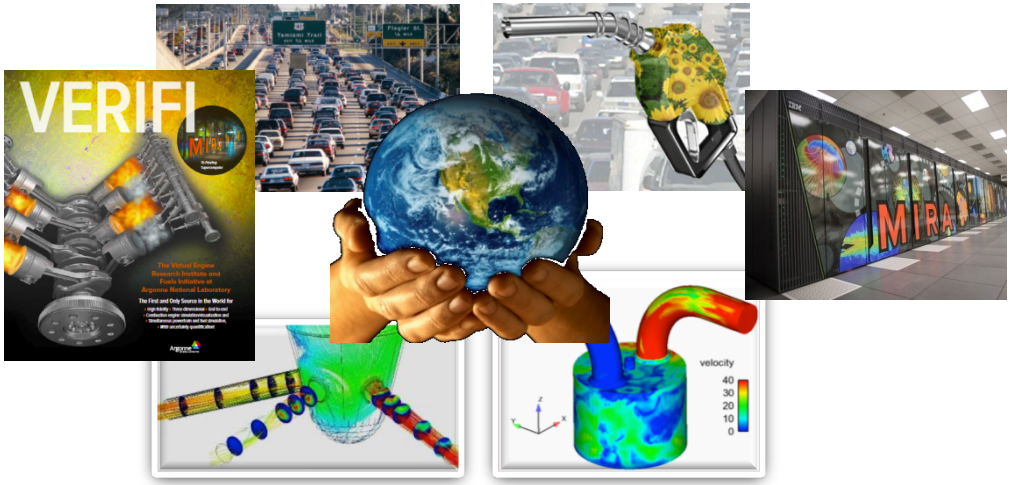
- Improving efficiency and reducing emissions from internal combustion engines (ICEs)
- Expedite the introduction of alternative fuel sources in ICEs

## Research Focus

- Develop high-fidelity computational tools to predict engine behavior prior to testing
- Promote the use of high-performance computing to simulate ICEs

## Research Impact

- Significant cost saving for the industry since predictive computations are cheaper than experiments
- More efficient and cleaner combustion engines




http://www.transportation.anl.gov/engines/multi_dim_model_home.html

http://verifi.anl.gov/

# ALCC Submission on Uncertainty Analysis with HPC


| Case | No. of cores | No. simulations | Total core hours |
|---|---|---|---|
| Engine | ~ 512 | 300 | ~ 38 million |
| Spray | ~ 4000 | 10 | ~ 17 million |

**60 million core hours for 1 year**

Port and Optimize on MIRA

Improve scalability and establish best practices on MIRA

Quantify uncertainties in simulations

Identify the uncertainty range and set-up simulations

Advancing engine simulations with sensitivity analysis and HPC resources

Identify important variables influencing particular engine targets

**PI:** Sibendu Som

**Co-PIs:**

Marta Garcia (ALCF)

Al Wagner (CSE)

P. K. Senecal (Convergent Science Inc.)

Janardhan Kodavasal (ES)

Yuanjiang Pei (ES)

**Plan to run ~10K simulations per day**

# Eulerian Mixture & Cavitation Model

## Mixture Model equations (homogeneous multi-phase model)

Continuity: $\partial\rho/\partial t+\nabla\cdot\rho v=0$

mixture density: $\rho=\sum i=1\uparrow n\blacksquare$

Momentum: $\partial\rho v/\partial t+(\nabla\cdot\rho v)v=-\nabla p+\nabla\cdot\tau+\rho f$

volume & mass fractions: $\alpha\downarrow i\,\rho\downarrow i=Y$

Species: $\partial\rho Y\downarrow i/\partial t+(\nabla\cdot\rho Y\downarrow i)v=\nabla\cdot(\rho D\downarrow i\nabla Y\downarrow i)+S\downarrow i$

void fraction: $\alpha\downarrow g=Y\downarrow g/\rho\downarrow g/\sum\uparrow\blacksquare Y\downarrow i/\rho\downarrow i$

*(plus: Energy, Turbulence)*

## Mass transfer: Homogeneous Relaxation Model (HRM) [1,2]

The model accounts for non-equilibrium heat transfer phenomena, using an empirical correlation

Hypothesis: finite rate of relaxation to equilibrium $dY\downarrow v/dt=Y-Y\downarrow v/\Theta$

Exponential relaxation of the vapor quality $Y$ to the equilibrium table value $Y\downarrow v$ over a timescale $\Theta$.

$Y\downarrow v=h-h\downarrow l/h\downarrow v-h\downarrow l\Theta=\Theta\downarrow 0\,\alpha\uparrow a\varphi\uparrow b$

**Mixture: 1. liquid + 2. vapor + 3. air**


1. Schmidt, D. P., et al., *Int. J. of Multiphase Flow*, 2012
2. Bilicki and Kestin, *Proc. Roy. Soc. Lond. A.*, 1990

# Further Details About Eulerian Mixture Model

- VOF method used to model the internal nozzle two-phase flow with cavitation description closed by the homogeneous relaxation model
- Eulerian single velocity field approach by Vallet et al. (2001) is implemented for near-nozzle spray simulations
  - *Large scale flow features* dominate rather than the small scale structures under the high Reynolds and Weber number conditions
- This approach considers the liquid and gas phases as a complex mixture with a highly variable density to describe the dense spray region
  - Mean density is obtained from Favre-averaged liquid mass fraction: $\frac{1}{\bar{\rho}} = \frac{\tilde{Y}}{\rho_l} + \frac{1-\tilde{Y}}{\bar{\rho}_g}$
- The liquid mass fraction is transported with a model for the *turbulent liquid diffusion flux into the gas*:

$$\frac{\partial \bar{\rho}\tilde{Y}}{\partial t} + \frac{\partial \bar{\rho}\tilde{u}_i\tilde{Y}}{\partial x_i} = -\frac{\partial \widetilde{\bar{\rho}u_i'Y'}}{\partial x_i} - \bar{\rho}\dot{\tilde{Y}}_{evap}$$

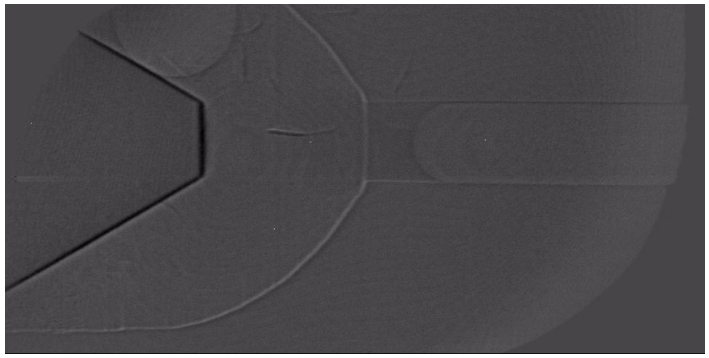
- *Closure for the liquid mass transport is based on a turbulent gradient flux model*:

$$\widetilde{\bar{\rho}u_i'Y'} = \frac{\mu_t}{Sc_t}\frac{\partial \tilde{Y}}{\partial x_i}$$

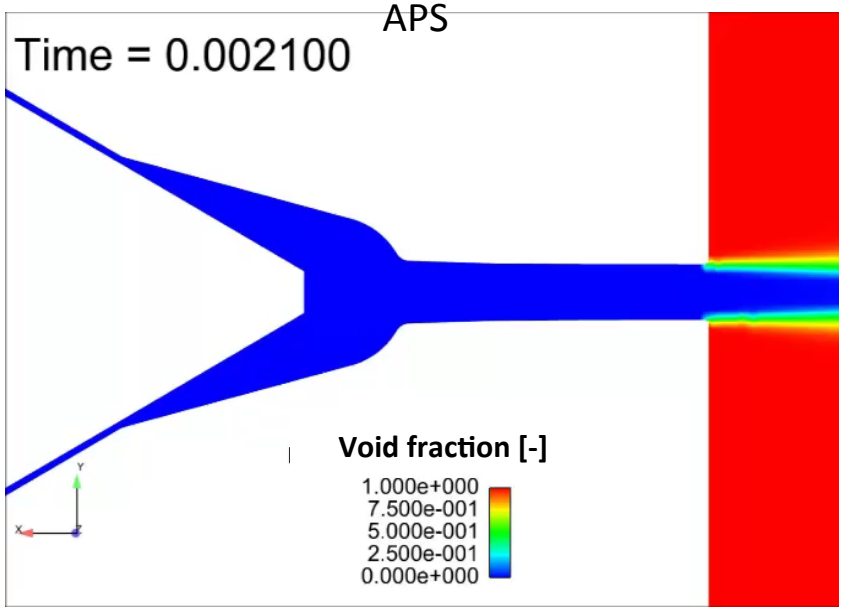
- Void fraction (α) $= \begin{cases} 0 & \text{if the computational cell is filled with pure liquid} \\ 1 & \text{if the computational cell is filled with pure gas} \\ (0,1) & \text{if the computational cell is filled with both liquid and gas} \end{cases}$

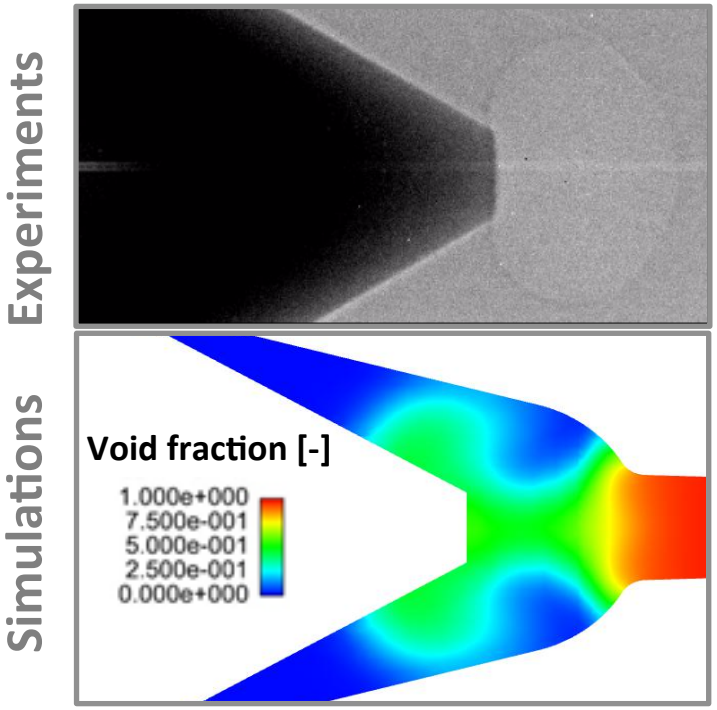
*** Xue, Som, et al. SAE Journal of Fuel and Lubricants, 2014**

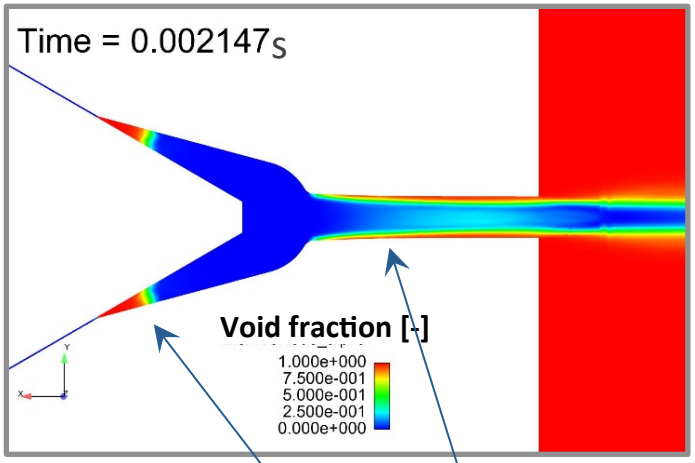
# Needle Transient: End-of-Injection



Movie & Images Courtesy: Dr. Chris Powell from APS




- **High-fidelity "first-of-its kind" simulations**
- Minimum cell size = 5 µm, More than 20 million cells
- Minimum time step size = 1 E-9
- **Simulations explain the physics behind ingested gas in the sac**

# High Performance Computing: Past, Present, and Future!!

**The first CRAY supercomputer**

**IPAD2**


10 Petaflop super-computer @ Argonne

**60 million, IPAD2**

# Methodology for GSA

- Simulations (3D CFD using Converge) varying all variables over uncertainty ranges simultaneously
- **Using an in-house GSA code to f**it the response (ignition delay, liquid length, etc) to the uncertainties

$$t_{ign}(\{u_i\}) = t_0 + \sum A_i(u_i) + \sum\sum B_{ij}(u_i, u_j) + \ldots, u_i\,'s : \text{uncertainties}$$

$$A_i(u_i) = \sum_{k=1}^{2} a_{ik} u_i^k$$

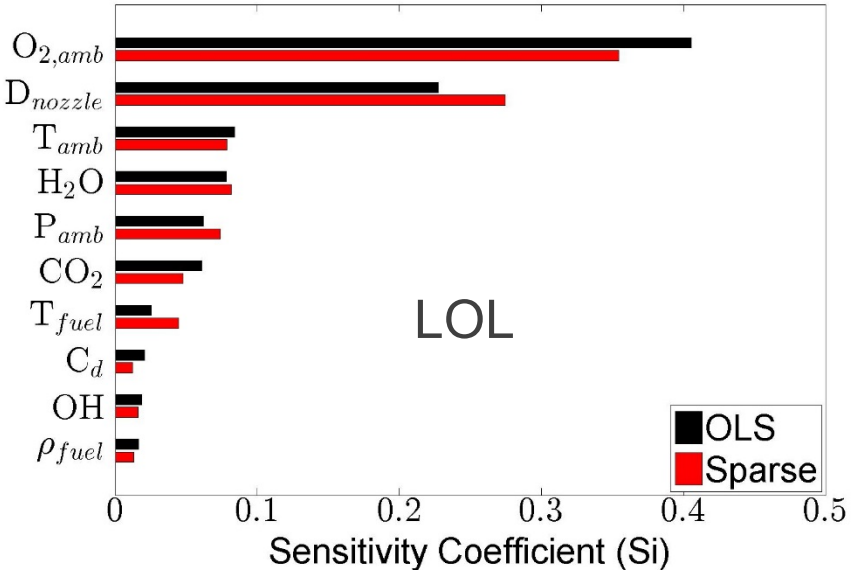
  - The fit of the response to the uncertainties leads to a variance associated with each variable (partial variance: $V_i$)
  - Calculate sensitivity coefficients,

$$S_i = V_i/V,\ \Sigma S_i \cong 1,\ (V\text{: total variance})$$

- Only main effect are considered, cross terms are neglected and will be included in future studies

Y. Pei, R. Shan, S. Som, T. Lu, D. Longman, M.J. Davis, SAE Paper 2014-01-1117, 2014.
D.Y. Zhou, M.J. Davis, R.T. Skodje, The Journal of Physical Chemistry A, pp. 3569-3584, 2013.

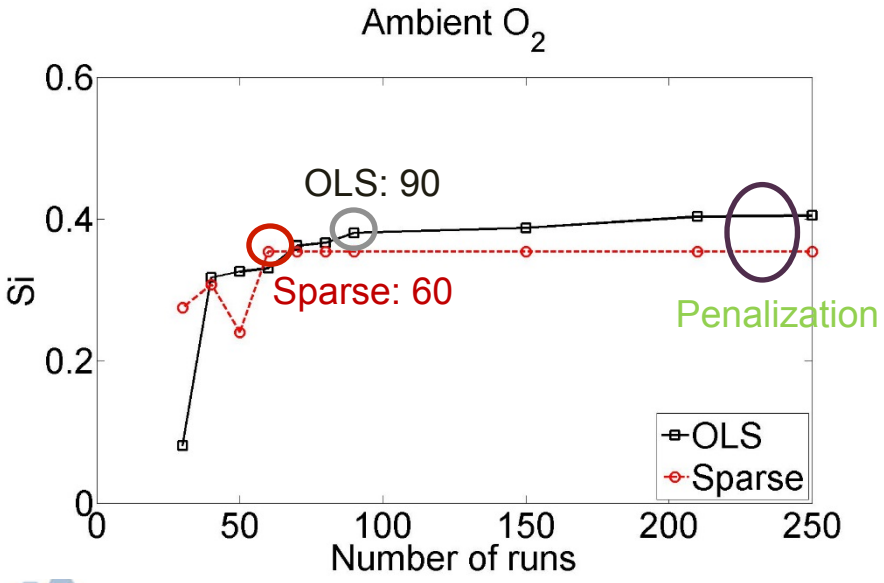
# Number of simulations required: OLS vs. Sparse




- OLS vs. Sparse for LOL:

  (Quadratic)

  - 250 runs analyzed initially
  - The first 10 ranking are shown, the rest 7 have Si less than 0.01.
  - The ordering are essentially the same
  - Some differences for Si
  - Get converged ordering:
    - 80 for OLS vs. 60 for Sparse
    - 30 for Sparse can also get reasonable ordering




- OLS vs. Sparse for ambient $O_2$:
  - Get converged Si:
    - 90~100 for OLS vs. 60 for Sparse
  - OLS is more accurate
  - Sparse can reduce the computational cost by sacrificing some accuracy

# VERIFI's Testing Capabilities Provide Unmatched Experimental Data to Validate Simulation Models

Using Argonne's "big machines" and tools, such as the Advanced Photon Source and Electron Microscopy Center, VERIFI researchers are uniquely able to see what is happening in fuel sprays, combustion and emissions and apply that knowledge to engine simulations. From there, engine researchers can regulate highly configurable test engines at Argonne's Center for Transportation Research facilities to validate simulation results against precise measurements, under a range of well-controlled operating conditions.