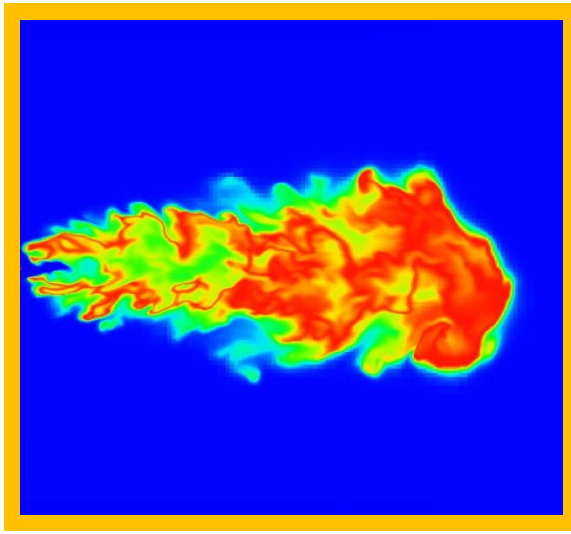
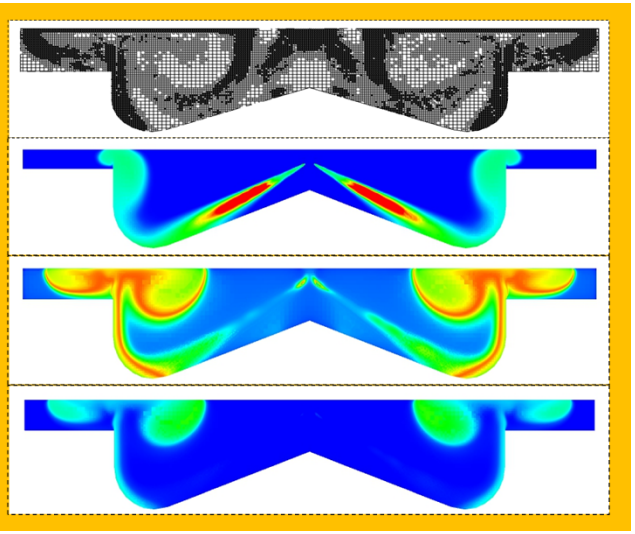
HPC Enabling a Paradigm Shift in IC Engine CFD





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VERIFI Workshop

November 12th, 2014

Acknowledgements

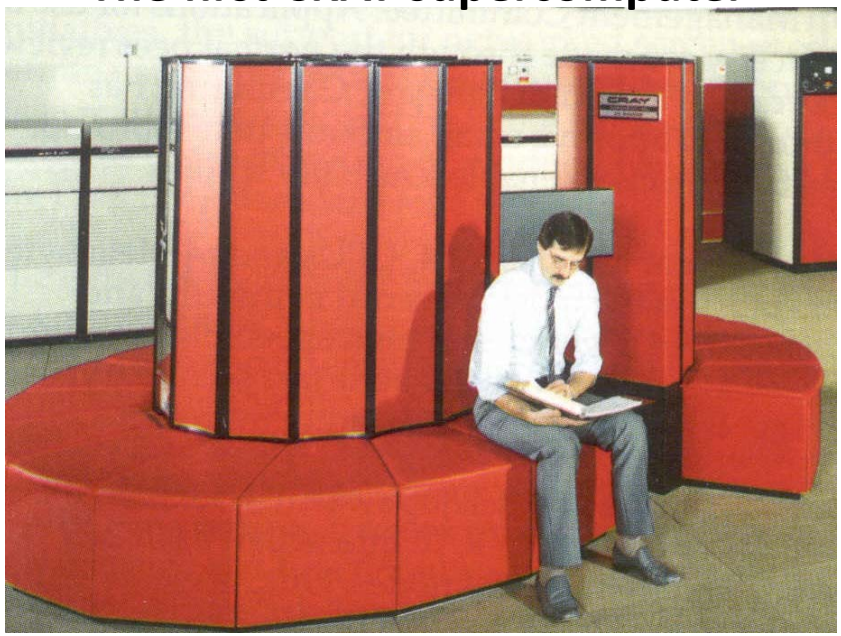
Sponsors: U.S. Department of Energy, Office of Vehicle Technology under the management of Gurpreet Singh, Leo Breton, Ken Howden

Argonne National Laboratory
Y. Pei, Z. Wang, J. Kodavasal, P. Kundu, Q. Xue, K. Saha, D.E. Longman
M.J. Davis, R. Sivaramakrishnan (Chemical Science and Engineering)
M. Garcia, R. Bair (Leadership Computing Facility)

Prof. M. Battistoni at University of Perugia (visiting researcher at Argonne in FY2013)

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

The first CRAY supercomputer



IPAD2

60 million, IPAD2

10 Petaflops super-computer @ Argonne

In general Engine simulations involve:

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

Extensive tuning to match experimental data

High-Fidelity 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

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!

Approach

Modeling Tool	**CONVERGE** Source code access for Spray, Combustion, and High Performance Computing Algorithms
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**:** **5 µm for nozzle flow** (31 million peak cell count) **32.5 µm for Spray** (22 million peak cell count) **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 1000 processors**

Turbulence model(s)	RANS: RNG k-ε; **LES: Smagorinsky, Dynamic Structure**
Spray models	**Eulerian-Eulerian Near Nozzle Model** 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 **Multi-Flamelet Representative Interactive Flamelet (RIF)**

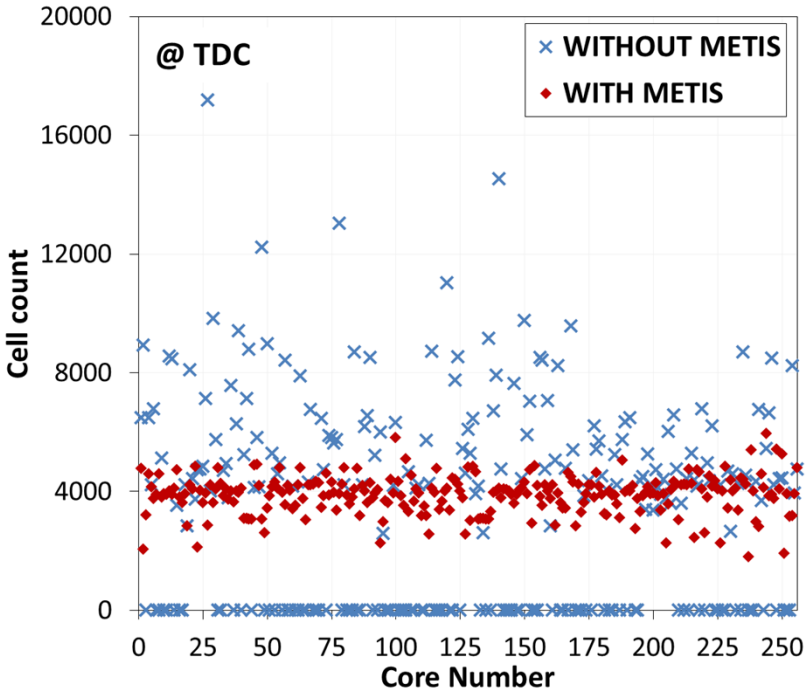
All this work is published in peer-reviewed journals and conference proceedings (http://verifi.anl.gov/publications/)

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

- **Scale-up a single engine simulation to 1000s of processors**
  - 30-50 million CFD cells
  - Advanced load-balancing algorithm
  - Resolved I/O issues
  - 2-3 weeks wall-clock time on 500-1000 cores

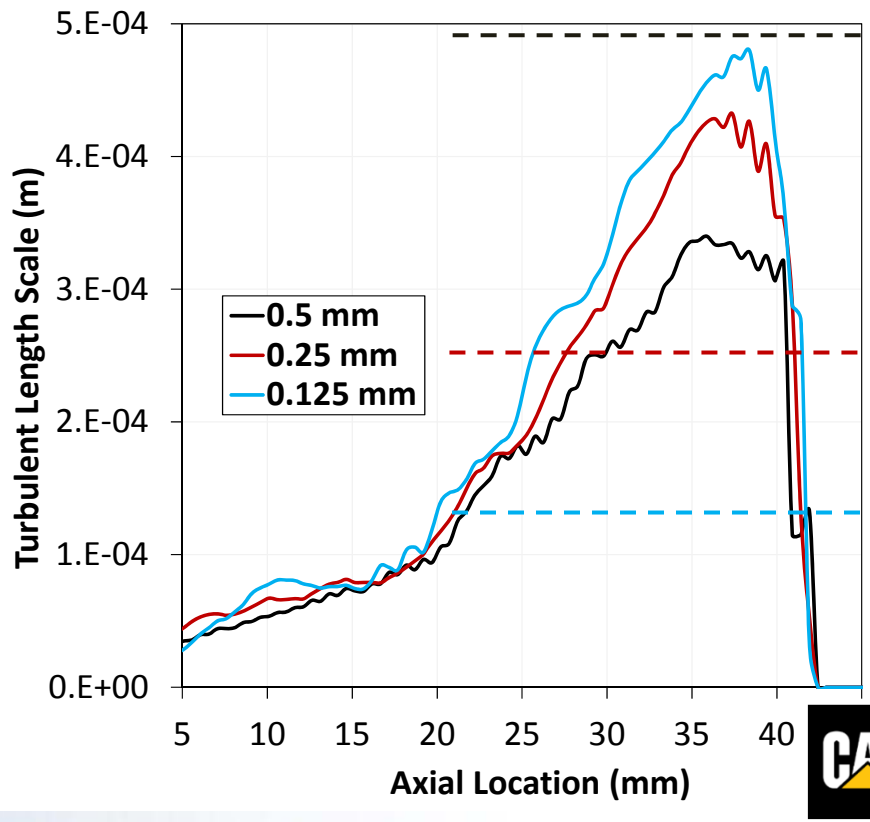
- **Use 1000s of cores for multiple number (10s) of smaller simulations**
  - 1-5 million cells per simulation project
  - 1-3 days wall-clock time on 10-100 cores
  - ❖ **Optimization** of engine operating parameter, e.g., GA optimization
  - ❖ **Uncertainty Quantification** of engine operating parameters 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

Load-balancing with METIS



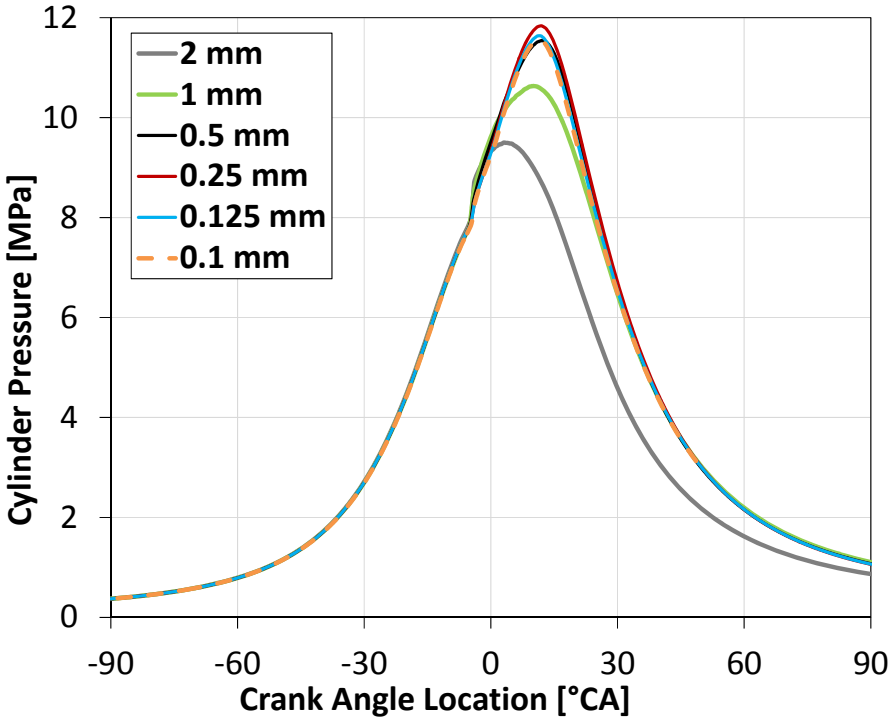
Scientific Achievements

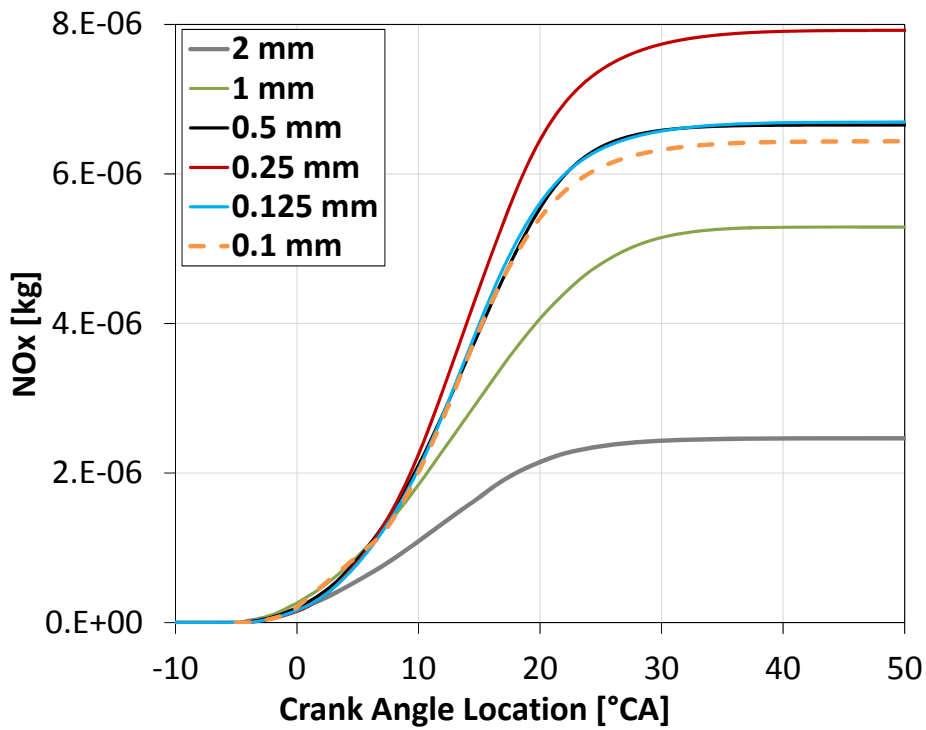
- Engine simulations are generally memory intensive
- **High-performance computing enabled due to the implementation of advanced load-balancing algorithms**



- **METIS** is a load-balancing algorithm originally developed at University of Minnesota
- @ TDC the maximum number of CFD cells on a single processor without METIS is 22136, whereas the minimum value is 0. The corresponding values with METIS are 5953 and 1805 respectively

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

- Single cylinder Caterpillar Engine simulated
- Many parameters such as pressure, heat release rate, grid converge at coarse resolutions of 0.5 mm
- NOx emissions grid converge below 0.125mm

Largest diesel engine simulation performed!!

Typical engine simulation in industry done on 24-64 processors

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

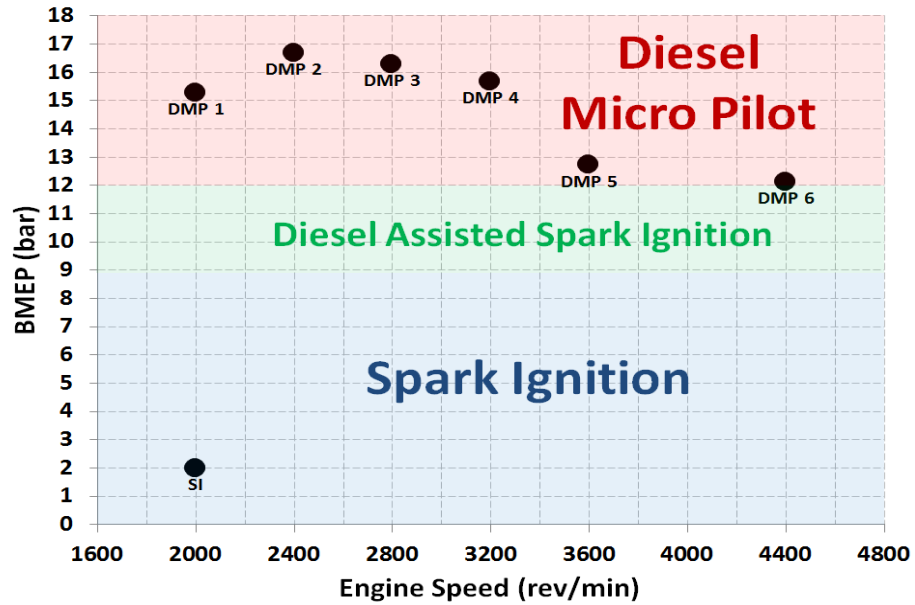
S. Som, D.E. Longman, S.M. Aithal, R. Bair, M. Garcia, S.P. Quan, K.J. Richards, P.K. Senecal, T. Shethaji, M. Weber, "A numerical investigation on scalability and grid convergence of internal combustion engine simulations," SAE Paper No. 2013-01-1095, *SAE 2013 World Congress,* Detroit, MI, April 2013

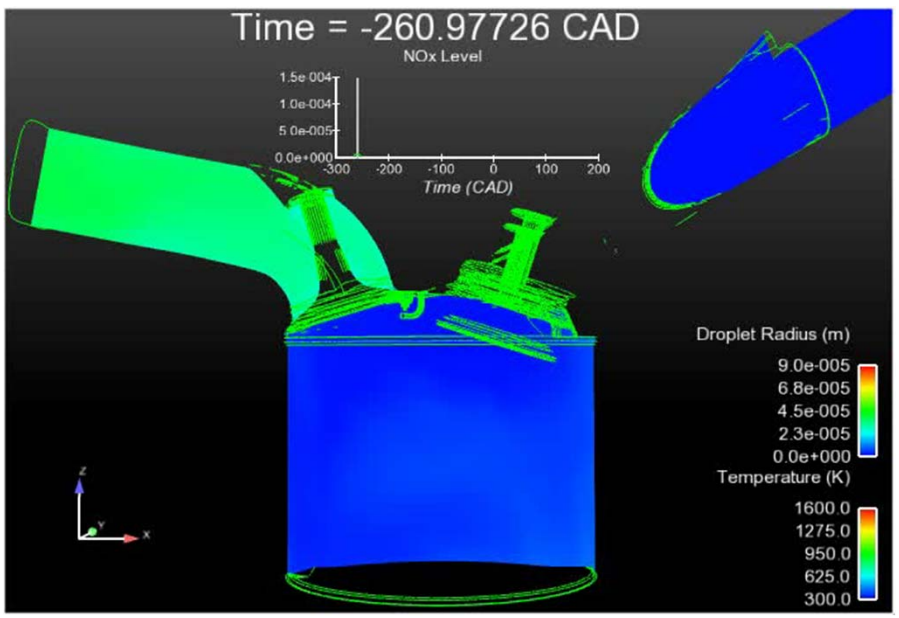
Use 1000s of cores for multiple number (10s) of smaller simulations

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

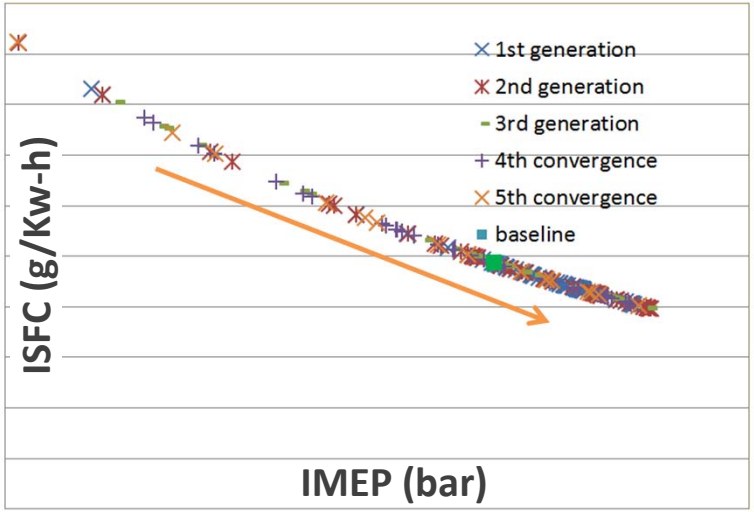
- Genetic Algorithm based optimization performed to gain **simultaneous performance and emission benefits**
- Simultaneous reduction of both NOx and soot emissions
- Simulations aided experimental studies on finding optimum operating conditions

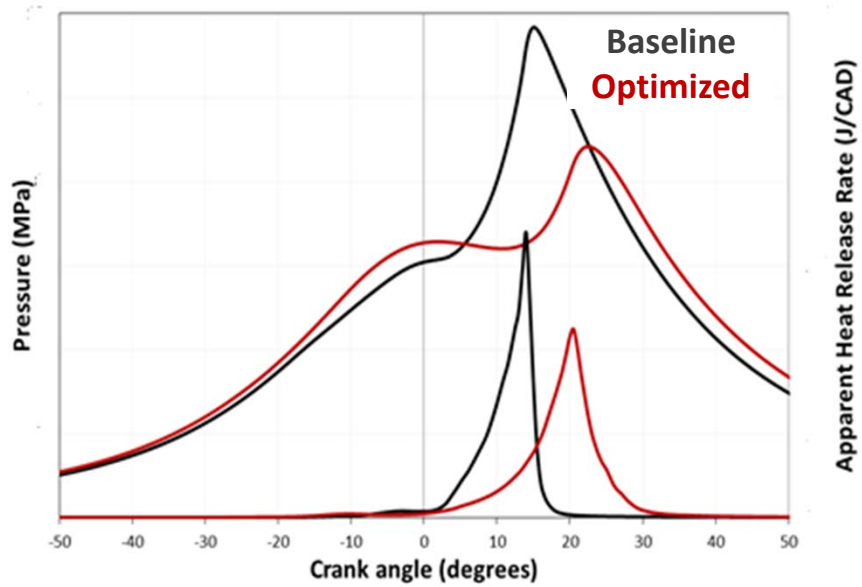
CHRYSLER

Z. Wang, R. Scarcelli, S. Som, S.S. McConnell, N. Salman, Y. Zhu, K. Freeman, K. Hardman, R.A. Reese, P.K. Senecal, M. Raju, S.D. Gilver, SAE Paper No. 2013-01-1091

Optimized Chrysler Dual-Fuel Engine

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

Merit = ISFC_target/ISFC - constraints (IMEP, knock index, COV_indicators)

knock index : maximum amplitude pressure oscillation for a CA window

COV_indicators : average of TKE, stdev of ϕ

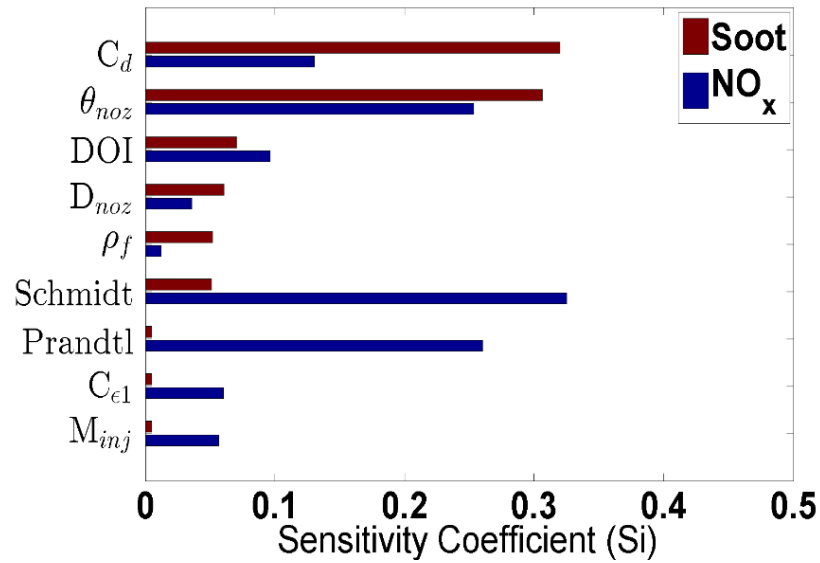
CHRYSLER

Uncertainty Quantification on Engine Parameters

- **32 uncertain variables** (both experimental and modeling) identified which may influence engine simulation results
- All the variables **simultaneously and randomly** perturbed within the range of uncertainty using **Monte-Carlo Sampling**
- **Global sensitivity analysis (GSA)** applied to understand the influence of each uncertain parameter towards a target of interest
- GSA code provided by Dr. M.J. Davis in CSE group at Argonne

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
ρ_f	Normalized fuel density	1.00	0.95	1.05
HOV_f	Normalized fuel heat of vaporization	1.0	0.9	1.1

- 100 simulations per speed-load conditions to get statistically converged results
  - Each simulation takes about 40-50 hours on 48 processors
  - Peak cell count: 2 millions (0.25 mm min. cell size)
- GSA demonstrated to be a more effective tool compared to brute force sensitivity analysis by perturbing one variable at a time
  - ✓ Non-linear interactions between variables and their influence on targets can be captured
  - ✓ Computationally efficient



Y. Pei, R. Shan, S. Som, T. Lu, D.E. Longman, M.J. Davis, "Global sensitivity analysis of a diesel engine simulation with multi-target functions," SAE Paper No. 2014-01-1117, *SAE 2014 World Congress,* Detroit, MI, April 2014

GSA to Identify Engine Relevant Chemical Kinetics

- Based on inputs from ANL-Chemistry group, **uncertainty factor assigned** for a chemical kinetic mechanism for biodiesel fuel combustion
- All reactions were **simultaneously and randomly perturbed within the uncertainty range** to obtain a series of reaction mechanisms
- **GSA** on 0D homogeneous ignition delay calculations predicts certain reactions to be important
- **GSA** on 3D engine simulations can now be used to develop reaction mechanisms
  - The uncertainty on these reactions need to be reduced asap
- **HPC can enable engine simulations which guide the development of accurate chemistry**

Reaction	3-D Rank*
$C_7H_{15}O_2$-2 = $C_7H_{14}OOH_2$-4 (-)	1
$PC_4H_9O_2$ = $C_4H_8OOH_1$-3 (-)	2
NC_7H_{16}+OH = C_7H_{15}-3+H_2O (-)	3
C_4H_8OOH1-3O_2 = NC_4KET_{13}+OH (-)	4
$C_7H_{15}O_2$-4 = $C_7H_{14}OOH_4$-2 (-)	5
$C_7H_{14}OOH_2$-4O_2 = NC_7KET_{24}+OH (-)	6
PC_4H_9 = C_2H_5+C_2H_4 (+)	7
$PC_4H_9O_2$ = PC_4H_9+O_2 (+)	8
NC_7H_{16}+HO_2 = C_7H_{15}-3+H_2O_2 (-)	9
OH+OH(+M) = H_2O_2(+M) (-)	10
$C_7H_{15}O_2$-3 = $C_7H_{14}OOH_3$-5 (-)	11
$C_7H_{14}OOH_4$-2O_2 = NC_7KET_{42}+OH (-)	12
HO_2+HO_2 = O_2+H_2O_2 (+)	13

"Low-Temp chemistry" in 3D simulations

S. Som, W. Liu, D.Y. Zhou, G.M. Magnotti, R. Sivaramakrishnan, D.E. Longman, R.T. Skodje, M.J. Davis, "Quantum tunneling affects engine performance," *Journal of Physical Chemistry letters* 4: 2021-2025, 2013
(145 species and ~ 900 reactions)

800 3-D engine runs:

- Caterpillar engine sector simulations
- 40 to 60 hours on 24 processors for each
- RNG k-ε turbulence model
- 0.25 mm minimum cell size, peak cell count of ~ 1 million

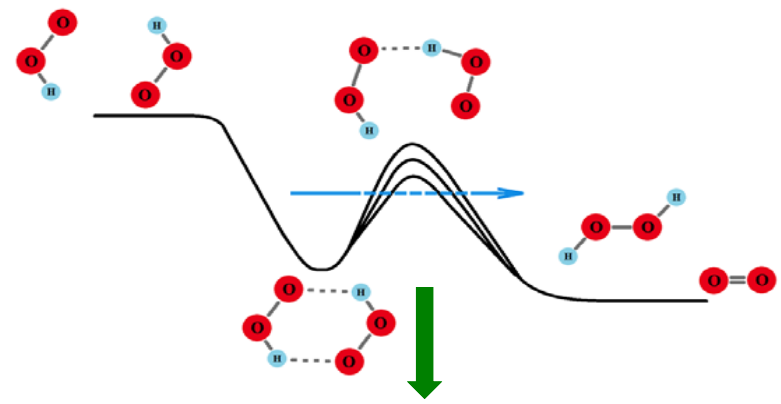
Quantum Tunneling Affects Engine Performance

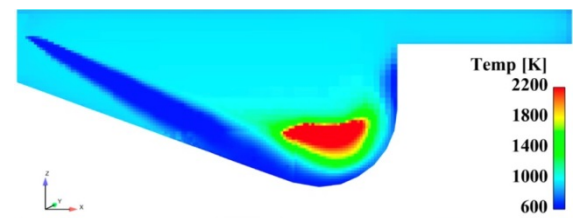
Project Impact

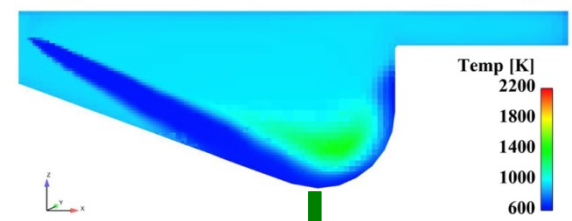
- ✓ Move **seamlessly from quantum chemistry to engine modeling**
- ✓ Motivate **new fundamental studies to address deficiencies in knowledge of the chemistry** that occurs at engine-relevant conditions

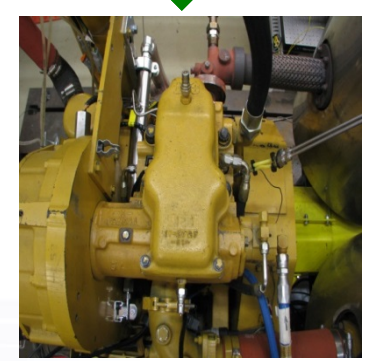
Scientific Achievement

- ❖ Demonstrated that the performance of **advanced engines** is increasingly tied to the details of the **fuel combustion chemistry**
- ❖ **Quantum mechanical effects** are shown to have an influence in a classical sense for **engine simulations**!





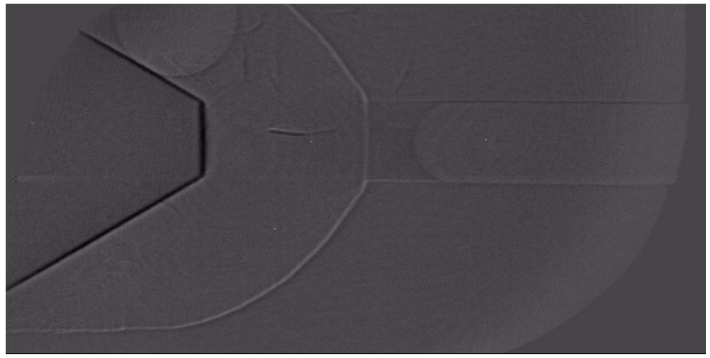




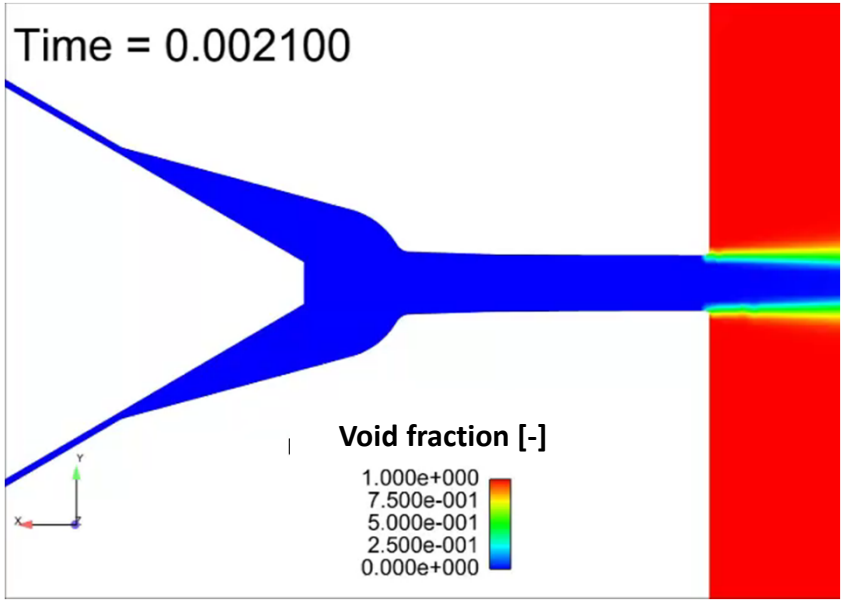
S. Som, W. Liu, D.Y. Zhou, G.M. Magnotti, R. Sivaramakrishnan, D.E. Longman, R.T. Skodje, M.J. Davis, "Quantum tunneling affects engine performance," *Journal of Physical Chemistry letters* 4: 2021-2025, 2013

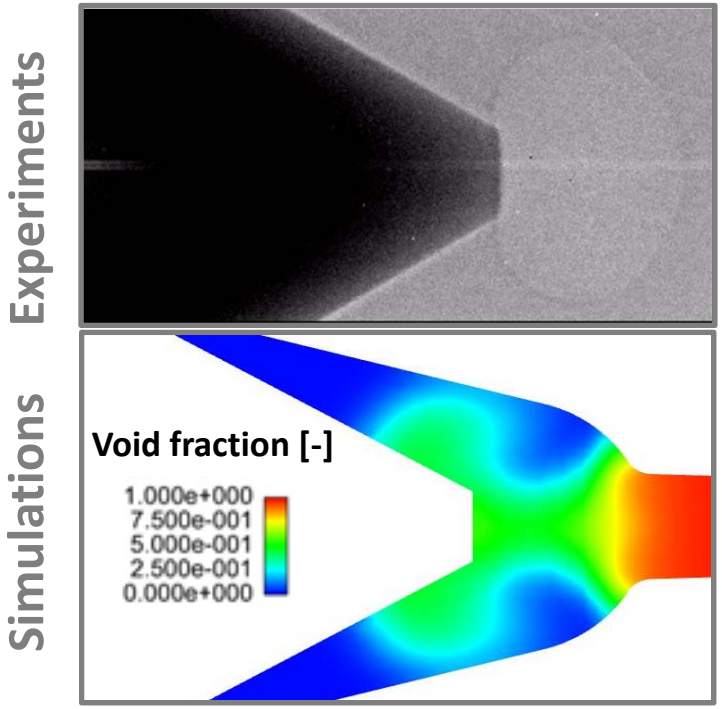
Nozzle Flow and Spray Simulations

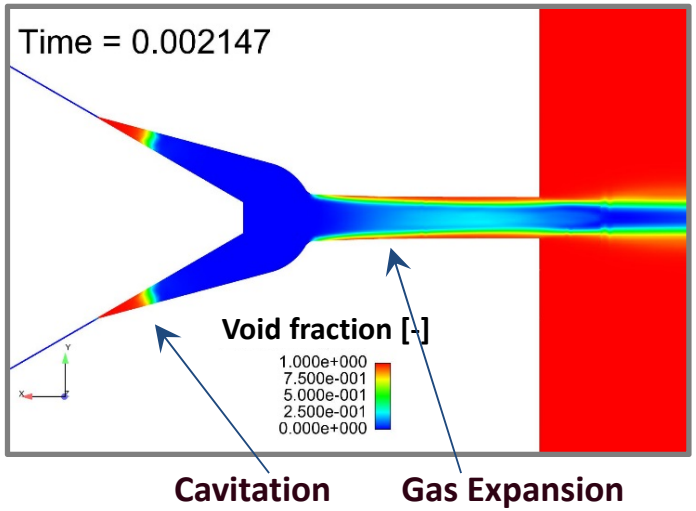
Needle Transient: End-of-Injection



Movie Courtesy: C. Powell, A. Kastengren at Argonne



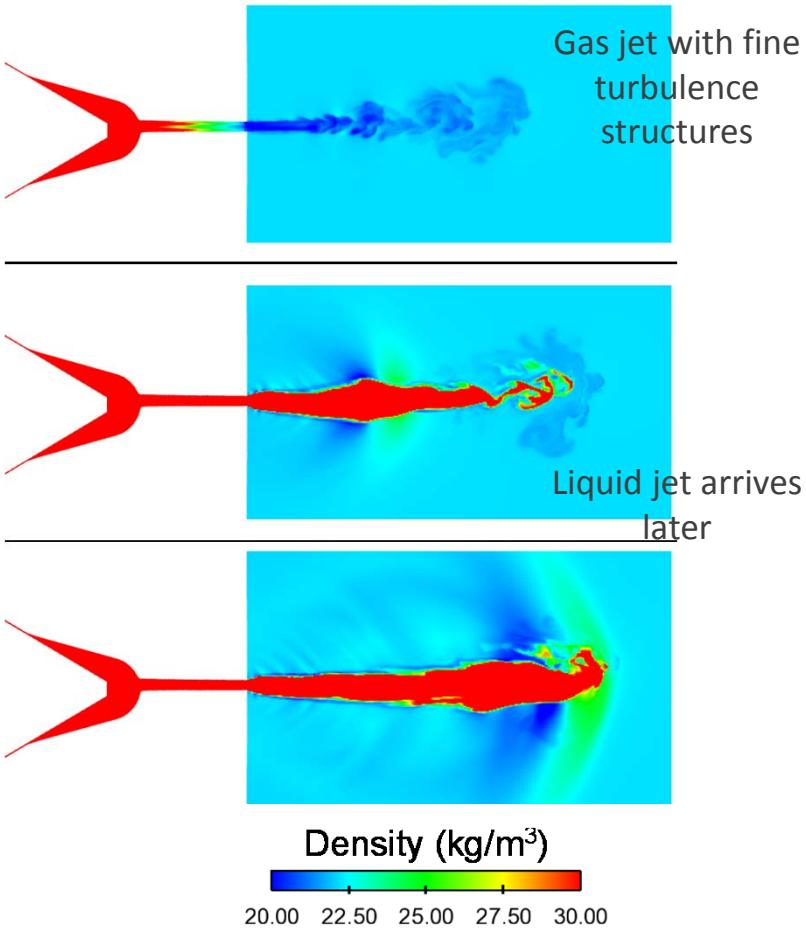




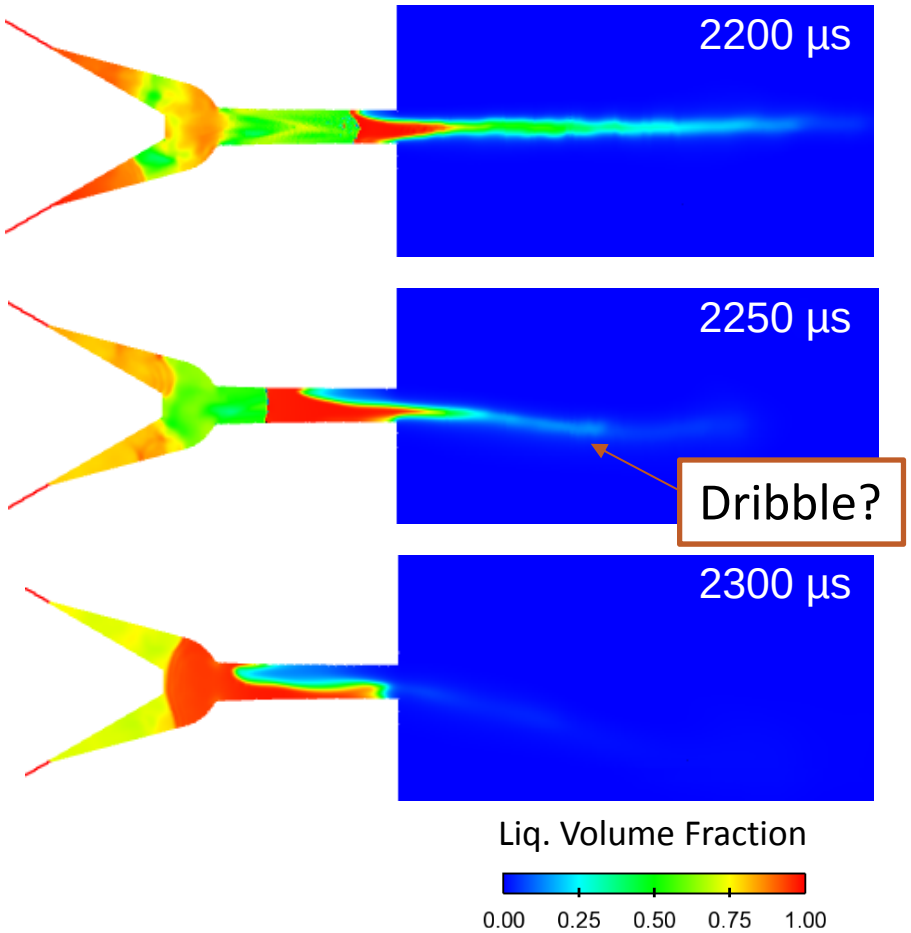
- **"First-of-its kind" simulations**
- Minimum cell size = 5 µm, More than 20 million cells
- Minimum time step size = 1 E-9
- **Simulations explain the physics behind ingested gas in the sac**

Injection Transient Predicted with LES

Start-of-Injection



End-of-Injection

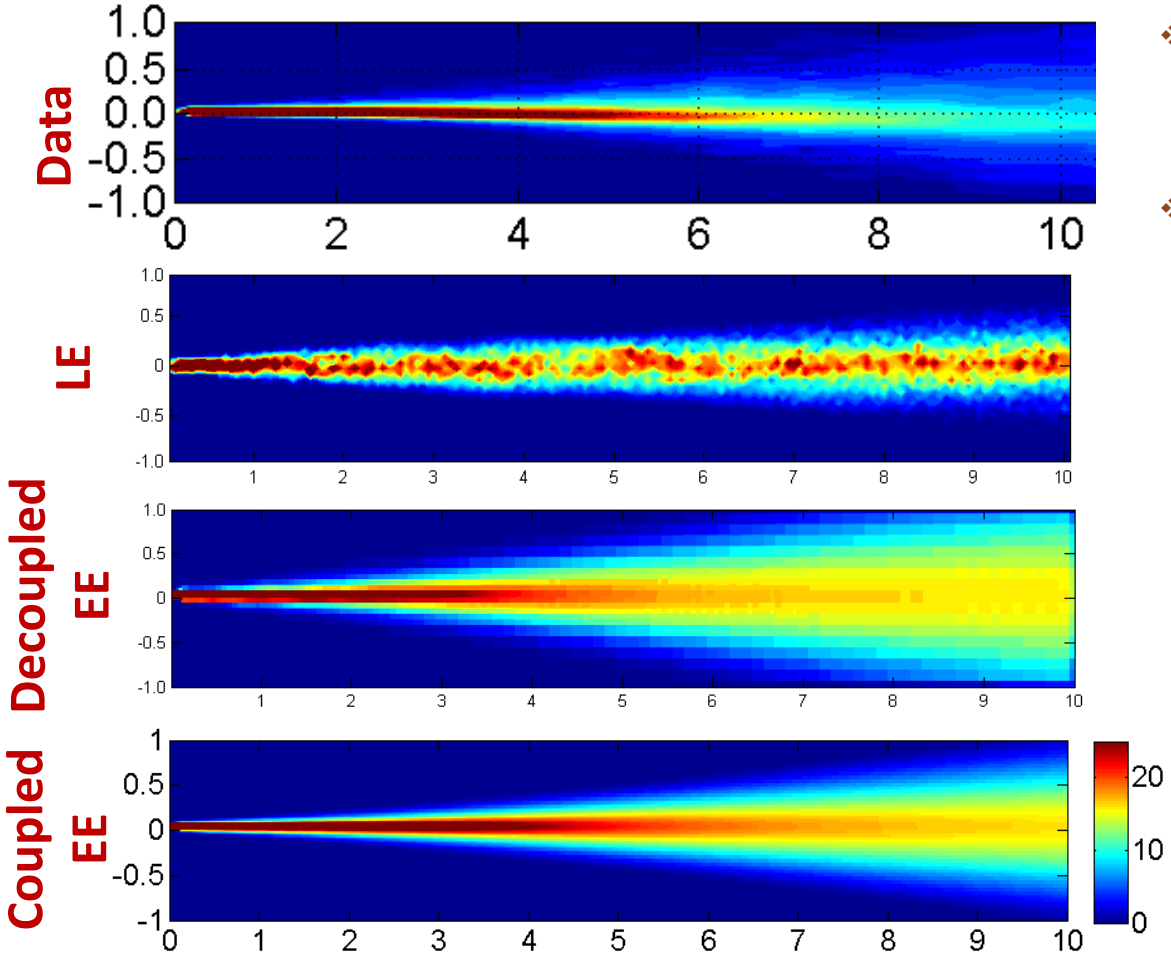


Simulation take 3-4 weeks on 100 processors

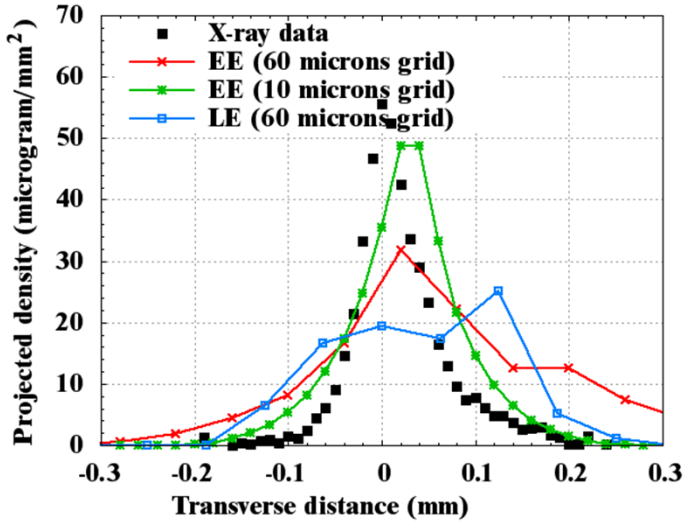
M. Battistoni, A.L. Kastengren, C.F. Powell, S. Som, "Fluid Dynamics modeling of End-of-Injection Process," *26th ILASS Americas,* Portland, OR, May 2014

Comparison of Eulerian and Lagrangian Approaches

Projected Density at 0.51 ms (µg/mm²)



- Coupled EE model is 3 times more expensive than decoupled EE model
- Coupled EE model is about 5 times more expensive than the LE model for the same resolution

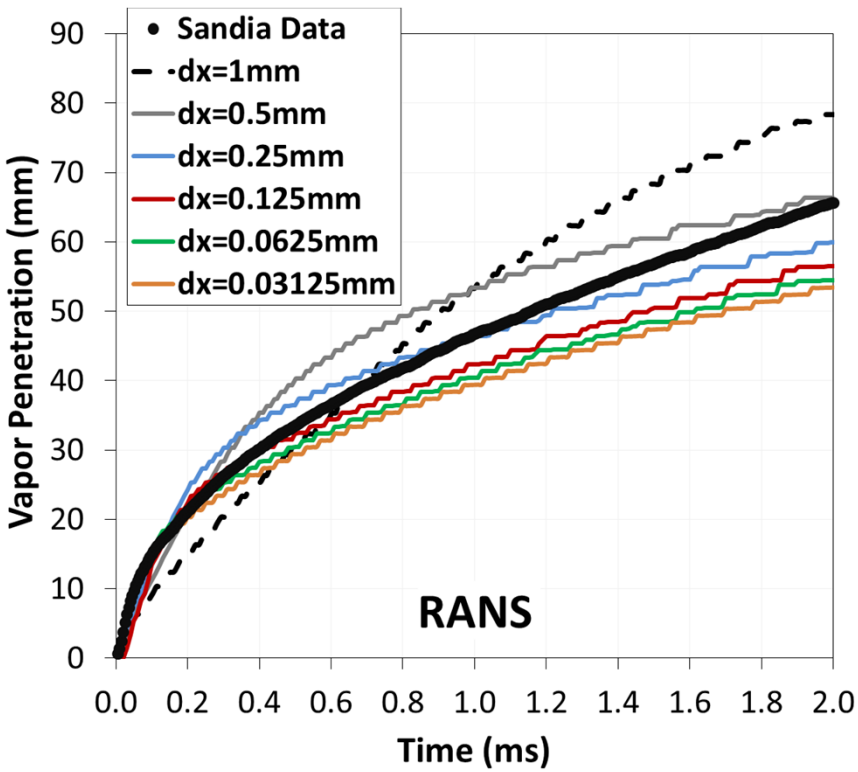


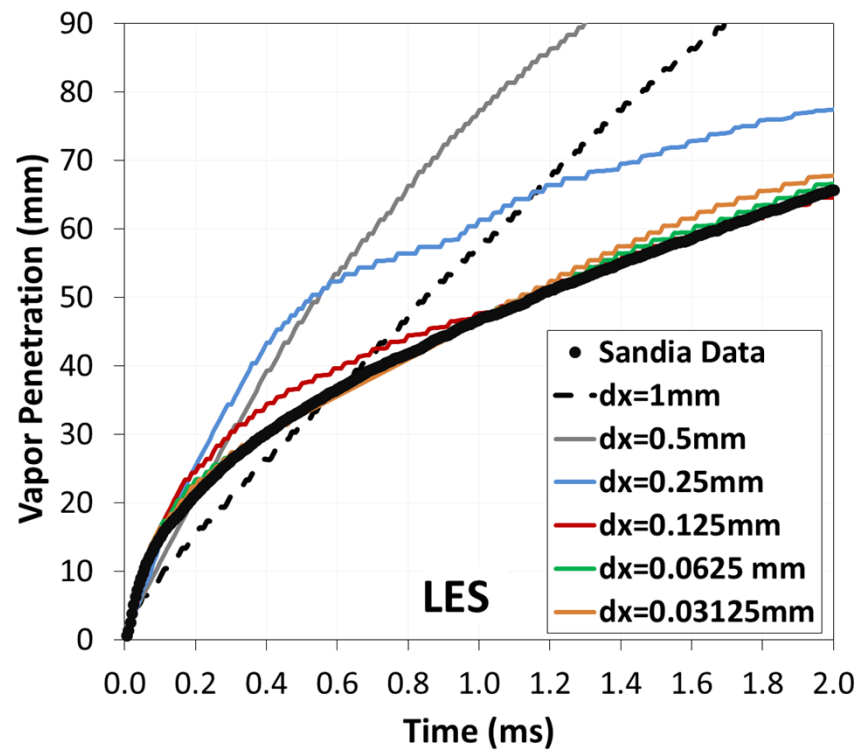
- Eulerian (EE) model is better than traditional Lagrangian (LE) approach in the near nozzle region
- Lagrangian simulations: 62.5µm minimum resolution; blob injection model; 300K parcels
- Decoupled EE simulations perform as well as coupled EE model for this case. This shows that if the Rate of injection is reliable, perhaps decoupled EE model is sufficient.

Data: Kastengren , Powell et al., Atomization and Sprays (2014)

CONVERGENT SCIENCE

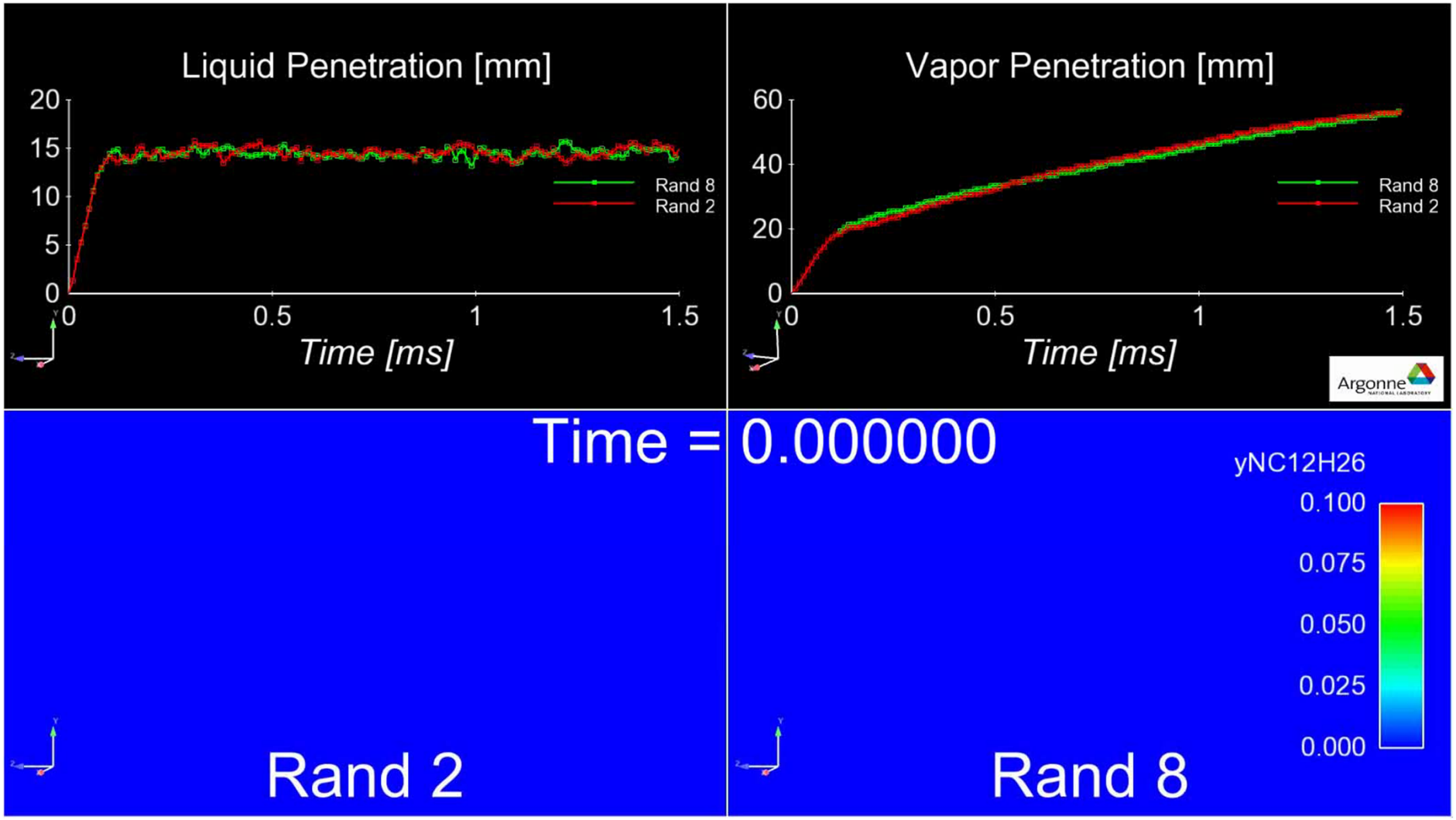
Simplified (RANS) vs. High-fidelity (LES) Turbulence Models





- 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
- Experimental data for Spray A from Sandia National Laboratory through ECN

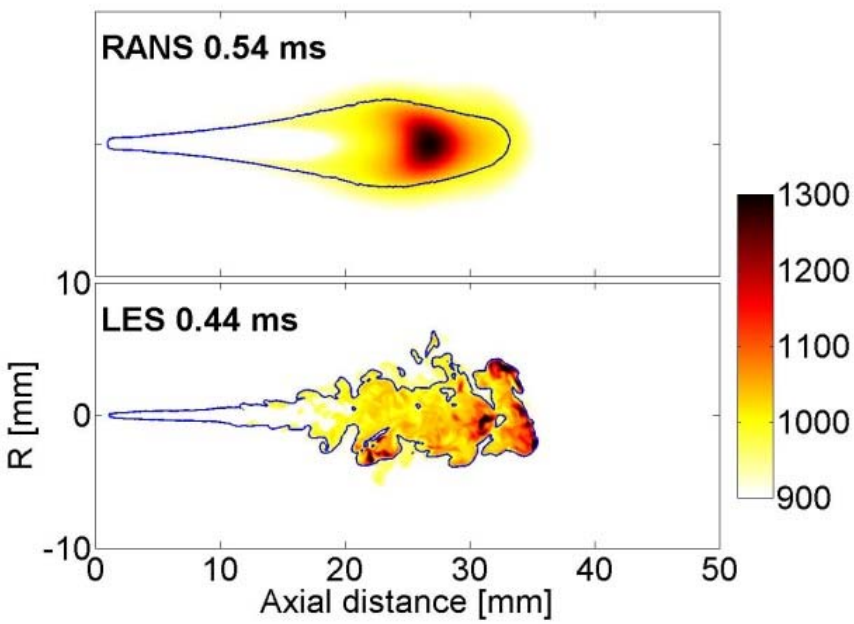
Variations in Spray Structure for different Realizations*



* Xue, Som, et al., Atomization and Sprays, 2013

LES Spray-Combustion Calculations

- No sub-grid scale Turbulence Chemistry Interaction model
- Each simulation is perturbed in the spray similar to the non-combusting work
- ECN data (from Pickett et al. @ Sandia) for validation



- 0.0625 mm calculation with 20-22 million cells takes about 14 days on 256 cores
- Non-combusting sprays grid-converged at 0.0625 mm resolution, not yet sure about the combusting cases
- **HPC provides opportunity to further tune TCI models for coarse mesh simulations** based on fine (grid-converged) mesh resolutions

Evolution of Engine Simulations

Clusters

Fusion Cluster

- 320 compute nodes
- 2560 processors
- 12.5 TB memo
- 500 terabytes
- 25.9 teraflops

Blues Cluster

- 310 compute nodes
- 4960 processors
- 107.8 teraflops peak

VERIFI

Argonne NATIONAL LABORATORY

The Virtual Engine Research Institute and Fuels Initiative at Argonne National Laboratory

Super-Computer

PETAFLOPS POWER

48 racks

ack

re processor

de

240 GB/s, 35 PB storage

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

2008

2015

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

The Argonne Leadership Computing Facility (ALCF) is home to unparalleled computing resources:

- Mira, a 10-petaflop IBM Blue Gene/Q system, one of the fastest supercomputers in the world
- Tukey, a visualization cluster that converts computational data into intuitive, high-resolution displays that enable engineers to instantly grasp the impact of design changes
- Fusion, a Linux-based machine that runs commercial simulation packages

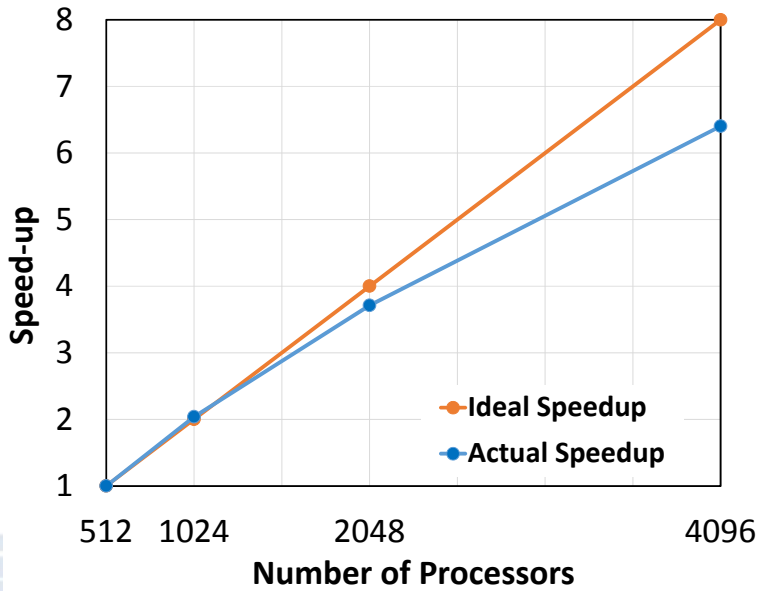
PETAFLOPS POWER

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.

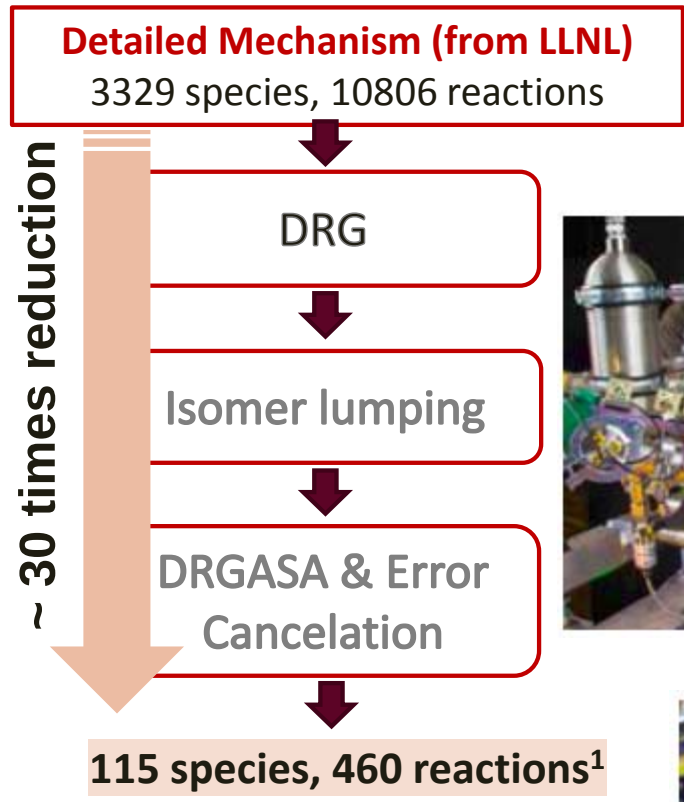
The system is capable of carrying out 10 quadrillion floating-point operations per second.

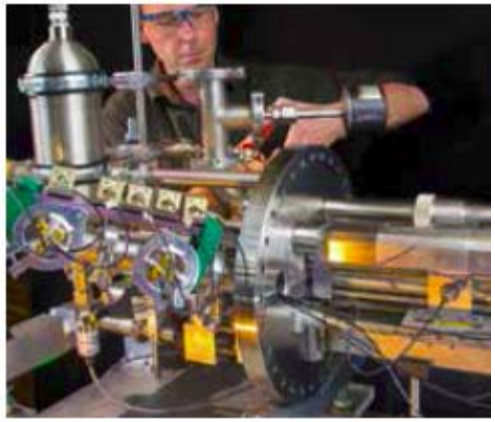
Profiling and improving file read, writes, and kinetic load balancing results in scale-up to 4096 processors on MIRA

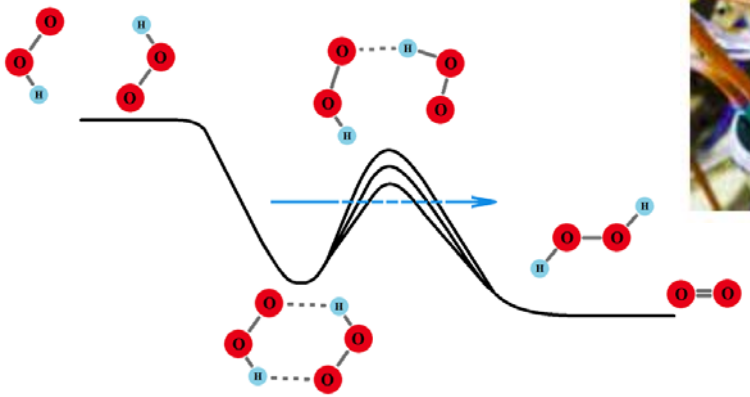


VERIFI's World-Class Chemists Quantify the Effects of Combustion

Argonne's world-class theoretical and experimental combustion chemists build models from first principles and validate them with uncertainty quantification. They work to understand and characterize the web of chemical reactions that takes place in the combustion process for a variety of fuels over a wide range of temperatures and pressures. Using state-of-the-art shock tube, flow tube and rapid compression machine laboratories, they study combustion-like explosions and quantify their flow and chemical effects. The resulting chemical models are incorporated into computer simulations to predict and optimize the performance of combustion engines.

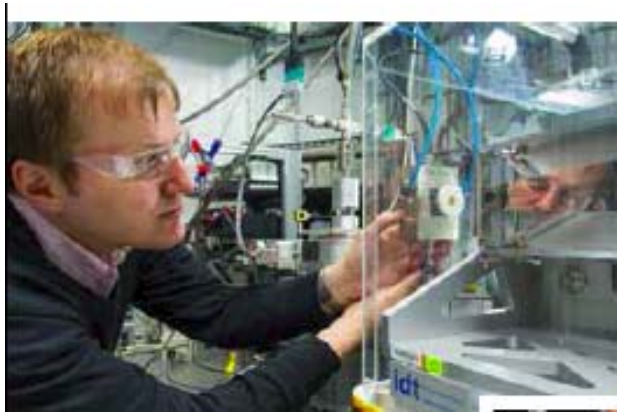


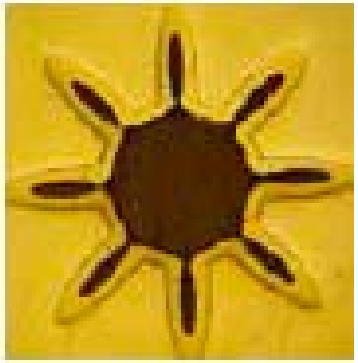


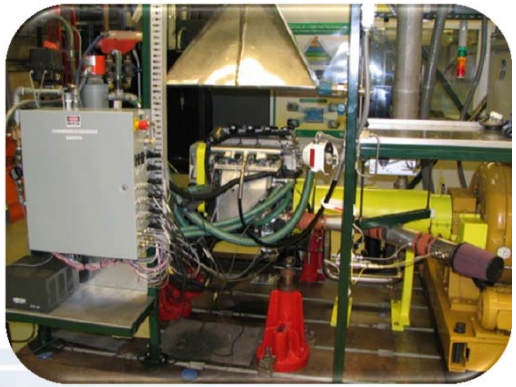


VERIFI's Testing Capabilities Provide Unmatched Experimental Data to Validate Simulation Models

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.







Summary

- **HPC enabling simulations which were not possible even 5 years back**
  - Envision a *paradigm shift* in engine simulation approaches in the near-future
- **Simulation projects with about a million core hours (on cluster based computing) are routine and can provide unique results. Some examples were demonstrated:**
  - Optimization, Uncertainty Quantification
  - Multiple cycle simulations, especially with LES
  - Nozzle flow simulations with LES
- **The simulations are not faster than doing experiments, but depending on the application, they can provide information that you cannot get from experiments. For e.g., Sensitivity Analysis/Uncertainty Quantification**
- **We have modified the "best practices" for performing engine simulations for our industrial partners**
- **In order to utilize the next generation of computational architecture (peta-scale and beyond), it is critical to scale-up engine simulations to run efficiently beyond 1000s of cores**
  - This necessitates high temporal and spatial resolution, advanced turbulence, turbulent combustion models, together with detailed chemistry and robust multi-phase flow models!
  - These simulations are generating "big data" which need to be efficiently data-mined to aid the development of simpler "engineering" level models

Thank You!

Any Questions??

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http://verifi.anl.gov/

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