WE START WITH YES.

Argonne NATIONAL LABORATORY

ADVANCEMENTS IN FUEL SPRAY AND COMBUSTION MODELING WITH HIGH PERFORMANCE COMPUTING RESOURCES

Sibendu Som (PI)
J. Kodavasal, K. Saha, M.M Ameen, N. Van Dam, P. Kundu, Y. Pei, Q. Xue
Argonne National Laboratory

Team Leader: Gurpreet Singh
Leo Breton

8th June, 2016

Project ID # ACE075

This presentation does not contain any proprietary, confidential, or otherwise restricted information

OVERVIEW

Timeline

Project start: April 1st 2012

Part of 2017 lab call

Partners

Argonne National Laboratory

Mathematics and Computing Science

Leadership Computing Facility

Advanced Photon Source

Convergent Science Inc. {CRADA}

Cummins Engine Company {CRADA}

General Motors R&D

Lawrence Livermore National Laboratory

Sandia National Laboratory

Advanced Engine Combustion (AEC)

Co-Optima

Advanced Computing Tech Team (ACTT)

University of Connecticut

University of Perugia (Italy)

Barriers

- "Inadequate understanding of stochastics of fuel injection"
- "Improving the predictive nature of spray and combustion models"
- "Incorporating more detailed chemical kinetics into fluid dynamics simulations"
- "Development of High-Performance Computing (HPC) tools to provide unique insights into the spray and combustion processes"

Budget

FY 14: 500 K

FY 15: 525 K

FY16: 490 K

Argonne NATIONAL LABORATORY

OBJECTIVES AND APPROACH

In general Engine simulations involve:

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

Extensive tuning to match experimental data

High-Fidelity Approach:

- Fuel spray and nozzle-flow models
- Detailed chemistry based combustion models
- Fine mesh => grid-convergence
- Improved load-balancing algorithms with METIS
- High-fidelity turbulence models: LES based

+

- High-Performance Computing

Towards Predictive Simulation of the Internal Combustion Engine

Long Term Objective:

- ❖ Develop reliable engine modeling capability with fewer tuning constants
- ❖ Sub-models published in open-literature and available to the industry through software packages
- ❖ Develop "engineering best practices" for industry to use these high-fidelity models

Argonne NATIONAL LABORATORY

RELEVANCE – NEED FOR SPEED AND AVAILABILITY TO OEMS*

- **Nozzle flow and Spray research**
  - In-nozzle flow and fuel spray in the near nozzle region plays a central role in combustion and emission processes
  - *1-way coupling* allows high-fidelity nozzle flow simulations to be effectively coupled with near-nozzle simulations
  - *1-way coupling* approach validated for gasoline and diesel sprays is now available for OEMs through CONVERGE v2.3
- **Combustion modeling using detailed chemistry**
  - Accurate chemical kinetics for fuel surrogates are key for predictive combustion modeling
  - We developed Tabulated Equivalent Strain Flamelet (TESF) model that allows us to include both detailed chemical kinetics and turbulence chemistry interaction in a cost-effective manner
  - TESF model is currently available through UDFs that can be ported to any academic or commercial code
- **High-Performance Computing (HPC)**
  - Current state-of-the-art for engine simulations in OEMs involve up to 50 processors (approx.) only on clusters: high throughput computing allows ~10k such simulations in a matter of weeks for engine design on Mira
  - These HPC advancements are now available for OEMs through CONVERGE v2.3 or custom made executables on Mira

Cluster

Super-Computer

* DOE-VTO workshop to identify roadmap for CFD organized by Leo Breton in 2014

SIMULATION APPROACH: SUB-MODEL DEVELOPMENT

Modeling Tool	CONVERGE Source code access for spray and HPC Algorithms
Smallest and largest characteristic grid size(s)	**Finest grid size simulations:** **2.5 µm for nozzle flow (30 million cells)** **~30 µm for GDI and diesel Sprays (20 million cells)** **~60 µm for spray combustion (30 million cells)**
Turbulence-chemistry interaction (TCI) model	**TESF model accounts for history effects with flamelets and also captures TCI**
Turbulence model(s)	LES: Dynamic Structure sub-grid scale model • **Random number seed perturbations** • **Azimuthal and ensemble averaging techniques**
In-nozzle Flow	**Homogeneous Relaxation Model (HRM)** for diesel and gasoline injectors
Spray models	Volume of Fluids (VOF) approach for phase-tracking **Coupled Eulerian-Eulerian Near Nozzle Model** **1-way coupling approach**
HPC Developments for simulations on MIRA	**Capability Computing: Scalability on 8k processors** **Capacity Computing: ~10k simulations in 1-2 weeks**

Extensive Validation using experimental data from Engine Combustion Network (Courtesy Lyle Pickett et al.) and X-ray data (Courtesy Chris Powell et al.)

Argonne NATIONAL LABORATORY

MILESTONES, FY 16

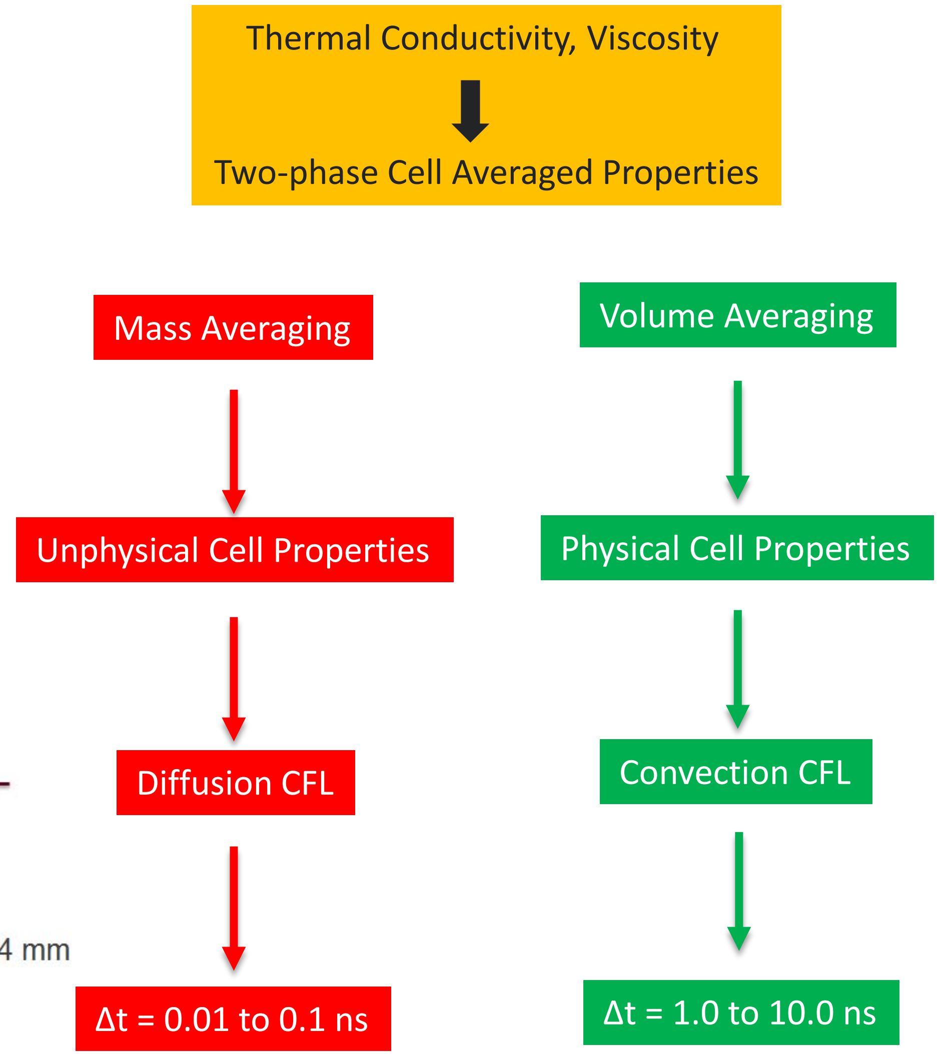
- Nozzle flow and Spray Research (CRADA with Cummins and CSI)
  - Assessment of LES spray models to predict spray variability from experiments {100% complete: January 2016}
  - Develop an integrated approach for modeling diesel and gasoline sprays using *1-way coupling* approach {100% complete: February 2016}
  - Validation of *1-way coupling* approach against diesel and gasoline nozzle flow and spray data {50% complete: June 2016}
- Combustion Modeling with Detailed Chemistry
  - Develop new tabulated flamelet (TESF) model for speeding-up detailed chemistry calculations for multi-component diesel surrogate {80% Complete: May 2016}
  - Validation against experimental data from heavy-duty engine at Sandia and constant volume vessel from ECN {50% complete: September 2016}
- High-Performance Computing
  - Enable high throughput computing on Mira to perform ~10k simulations by integrating with Swift workflow manager {100% complete: April 2016}

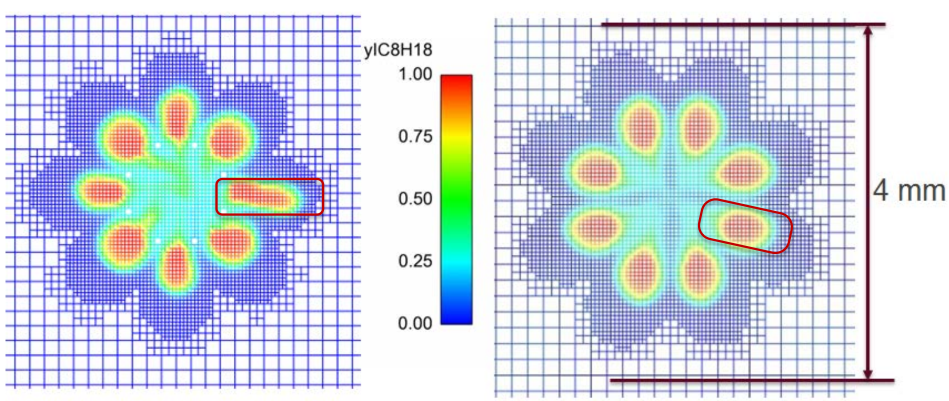
Argonne NATIONAL LABORATORY

TECHNICAL ACCOMPLISHMENTS

DEVELOPING GASOLINE INJECTOR SIMULATION CAPABILITY

- We developed an integrated framework for simulating both diesel and gasoline injectors within the Eulerian simulation approach
  - Assessed Homogeneous relaxation model (HRM) for both diesel and gasoline injector simulations
- Established 'best practices' for flash-boiling simulations based on Spray G injector from the Engine Combustion Network (ECN)
  - Mesh convergence established at 17.5 microns min. resolution
  - Volume averaging instead of mass averaging on cell basis provides more code stability
  - Explored the effect of mesh orientation => Recommendation not to align any plume with the mesh





Not Rotated Rotated

CAPTURE FLASH BOILING FOR GASOLINE INJECTORS

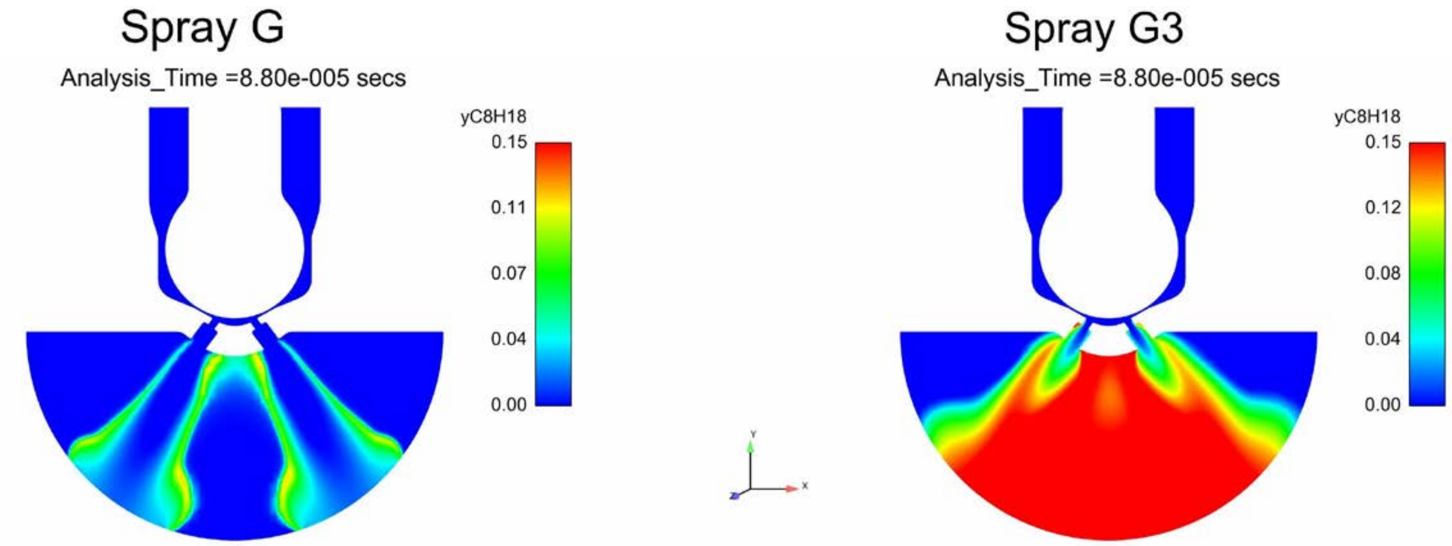
- Based on thermodynamic considerations we can now estimate the propensity of flash boiling in GDI
- 3D-CFD predicts the extent of flashing under different operating conditions
- Flash-boiling (Spray G3) clearly increases spray angle and plume-to-plume interactions

$$R_P = \frac{P_{\mathrm{sat}}(T_{\mathrm{fuel}})}{P_{\mathrm{chamber}}} \qquad Ja = \frac{\rho_l C_P \Delta T}{\rho_v h_{lv}}$$

Available Energy/Latent Heat

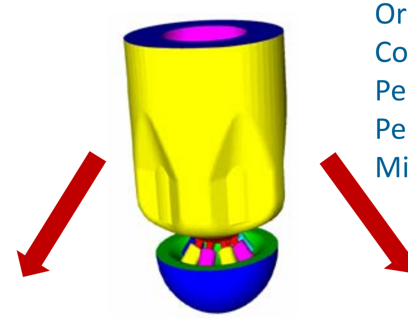
Degree of superheat = $T_{fuel} – T_{sat}$ (P_{ch})

Parameters	Spray G (non-Flashing)	Spray G3 (Flashing)
Injection pressure (Mpa)	20	20
Chamber pressure {P_{ch}} (kPa)	600	100
Fuel injection temperature {T_{fuel}} (K)	363	413
Fuel Saturation temperature at P_{ch}(K)	451	372
Degree of superheat {ΔT} (K)	N/A	40.68
Pressure ratio (R_P)	0.13	2.83
Jacob number (Ja)	N/A	31.29



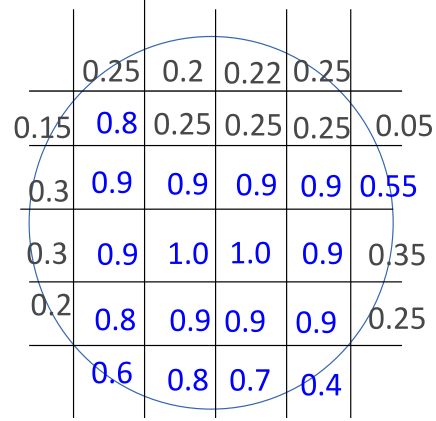
1-WAY COUPLING FOR GDI NOZZLE AND SPRAY SIMULATIONS

- Spray G injector for the ECN
- Rate of Injection (ROI) profile allows us to provide the same mass flow rate at the hole exit for each orifice => plume-to-plume variations cannot be captured
- In-nozzle flow simulations provide information on hole-to-hole variations which can influence plume-to-plume variations and interactions for gasoline injectors
- *1-way coupling* approach allows:
  - Different mass flow rate and discharge coefficient per orifice
  - Parcel injection distribution within an orifice based on extent of phase change
  - Capture effects of backflow of chamber gas into the counter-bore and its influence on the ensuing spray

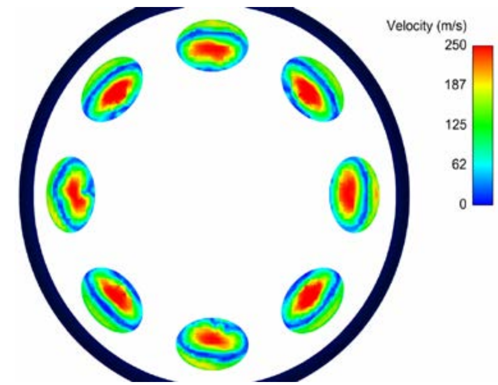


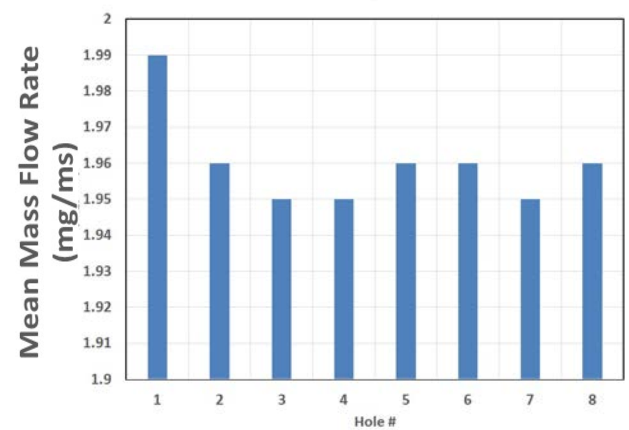
Orifice dia. = 165 µm
Counter-bore dia. = 388 µm
Peak needle lift = 45 µm
Peak cell count ~4.5 millions
Min. cell size = 15 µm

Liquid Volume fraction at counter-bore exit



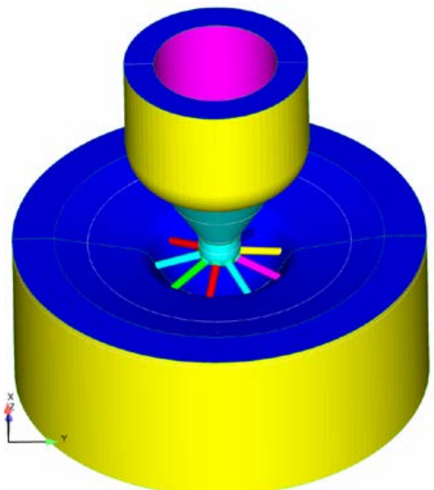
Velocity at counter-bore exit





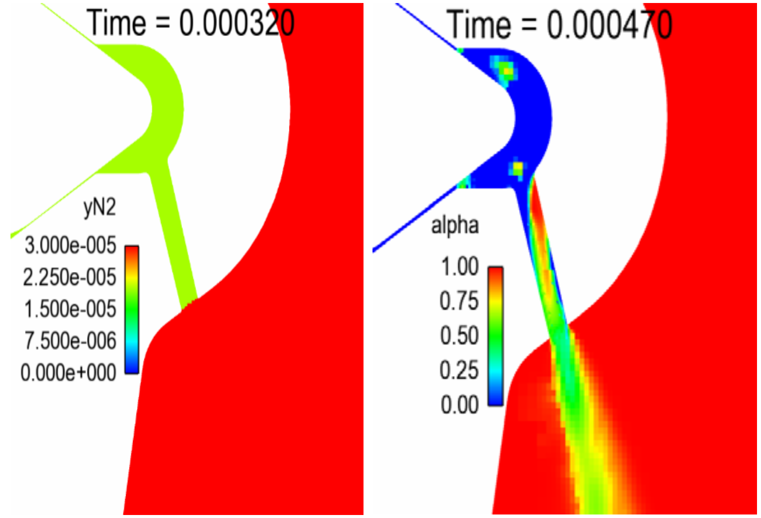
HDD INJECTOR: CAVITATION OR GAS EXPANSION?

Common rail injector	HDD
Nozzle diameter	180 µm
Number of holes	9
Rail pressure (inlet pressure)	240 MPa
Temperature of fuel at injector tip	300 K
Ambient gas	N_2
Ambient temperature	300 K
Ambient pressure	1 MPa

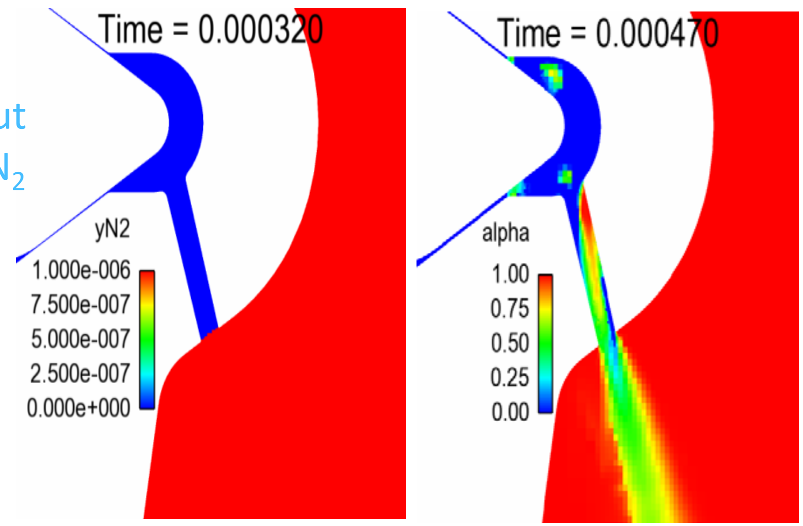


- Som's 2015 AMR presentation showed several results with this injector
- Simulation methodology is now part of Cummins workflow as part of the CRADA

Initialize with dissolved gas N_2

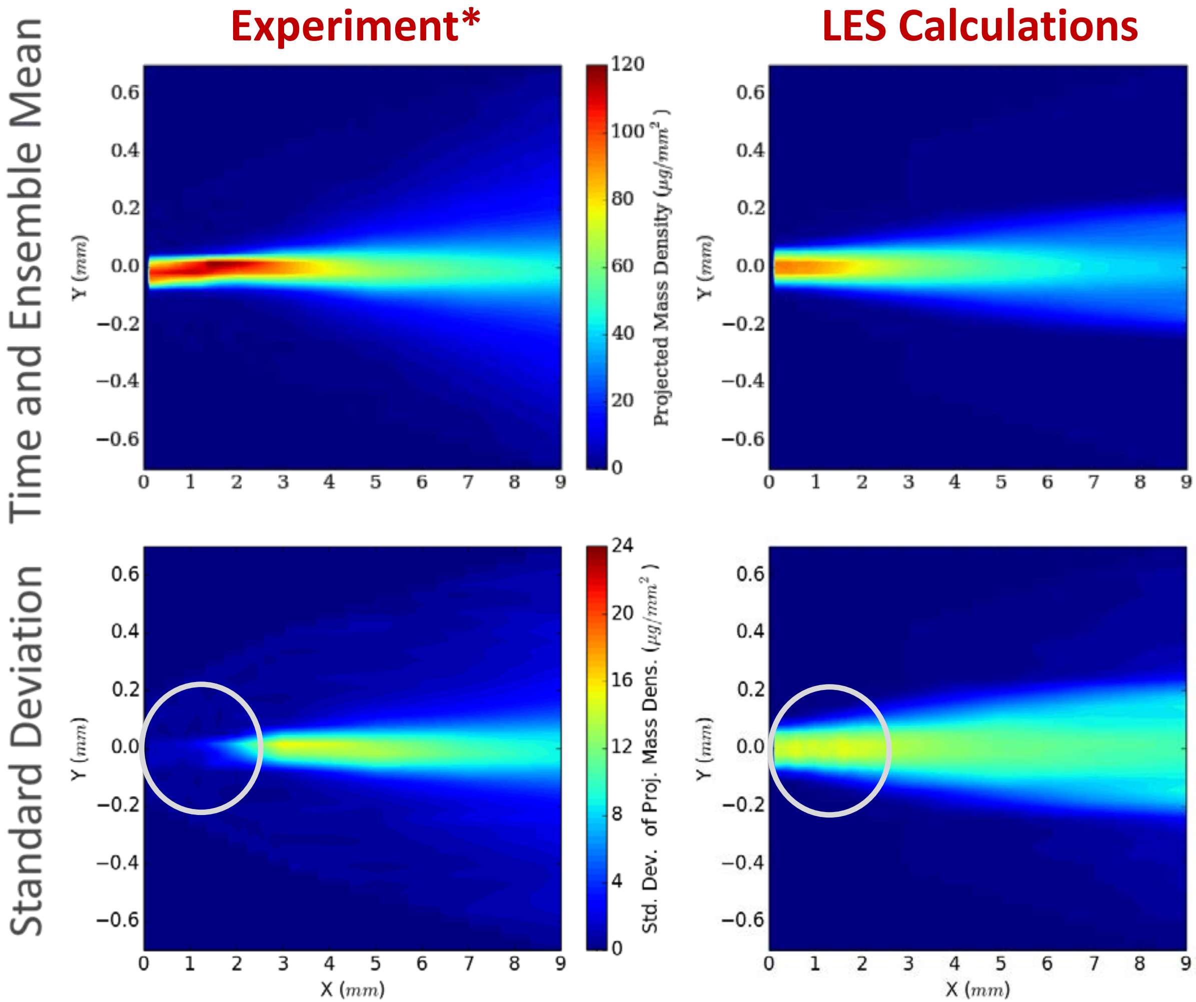


Initialize without dissolved gas N_2



We developed a simulation approach that tracks all gaseous species. This helped us demonstrate that the void fractions at some needle lifts are due to phase change and not due to dissolved gas expansion

SHOT-TO-SHOT VARIATION IN SPRAYS PREDICTED WITH LES



Question from academia and industry: can the random number seed capture the spray variability?

- With LES small perturbations (initial, boundary conditions etc.) are amplified, while RANS dampens them
- RANS do not show any shot-to-shot variation due to random number seed perturbation. LES can capture shot-to-shot variation, but is random number seed a representative way?

- Mean and standard deviation in Projected Mass Density from x-ray experiments is plotted for 32 injection events
- Random seed perturbations in LES enough to capture spray variability in terms of mean and standard deviation downstream
- Near-nozzle LES predicts significant shot-to-shot variation due to the “blob” injection model. Experiments perhaps have a liquid core and do not show any shot-to-shot variability

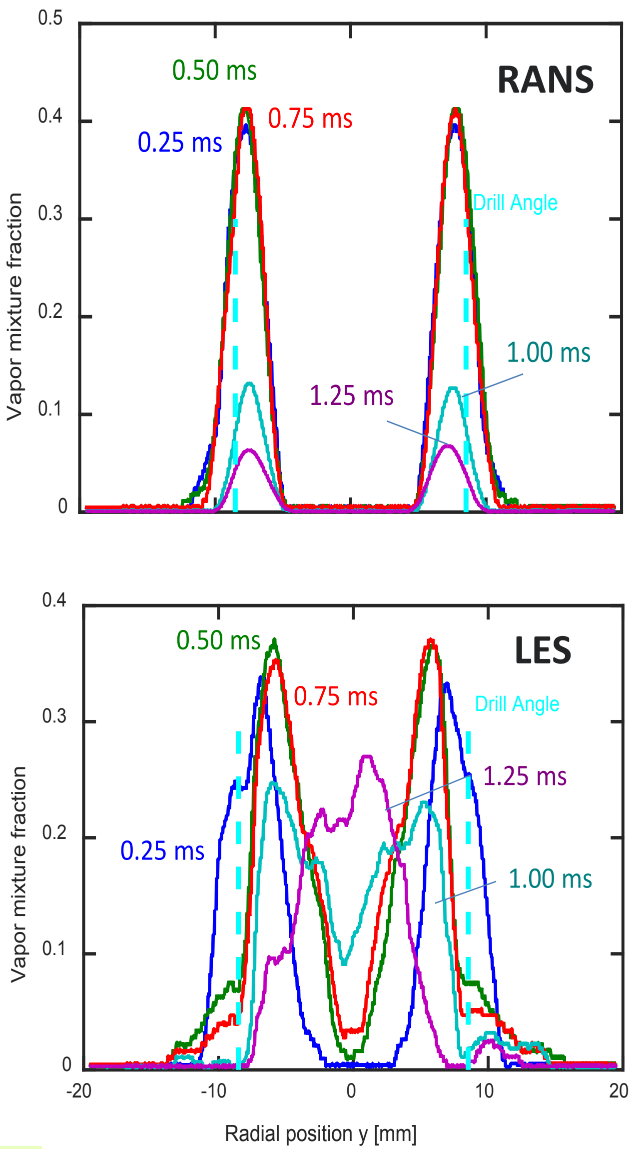
Nozzle Diameter (μm)	118
Injection Pressure (bar)	500
Ambient Pressure (bar)	20
Ambient Temperature (K)	298
Working Fluid	N-dodecane

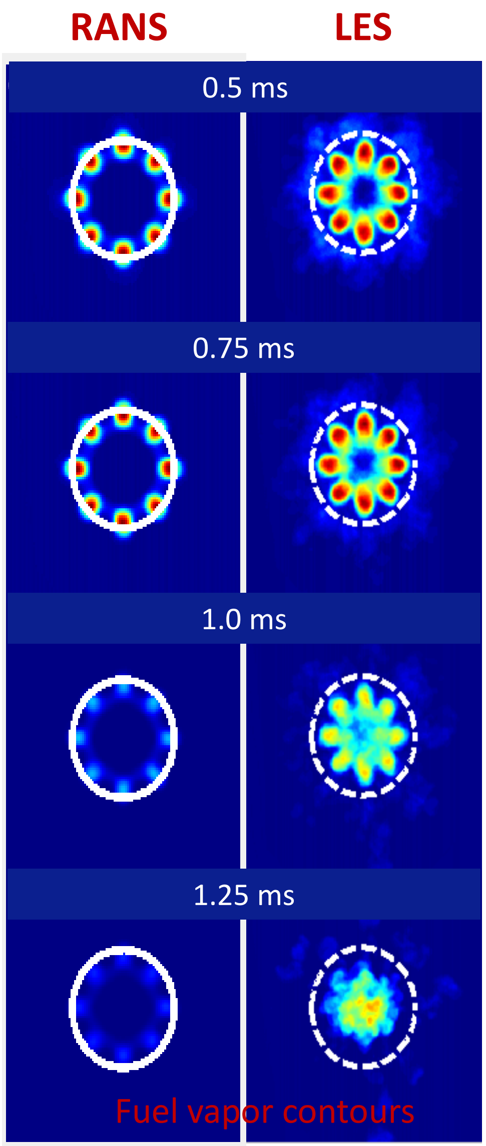
- **10 LES realizations per condition**
- **Each realization is perturbed with a different random number seed**
- **~20 million cells, min. cell size of 62.5 μm, 800k injected parcels**
- **Time-averaged 0.1-2.0 ms ASOI**

* X-ray experimental data shown by C. Powell at AMR 2015 (Swantek et al. SAE 2015-01-1834)

GDI PLUME MERGING CAPTURED WITH LES*

- Spray G experiments at Sandia have shown that GDI plumes merge due to air-entrainment between them
- RANS simulations with mesh converged resolution of 0.25 mm
- LES simulations with mesh converged resolution of 0.09 mm
  - ✓ 20 realization (using Random number seed) per condition run with LES
  - ✓ Each realization takes ~24 hours on 64 processors
- Plume merging is not observed with RANS as air-entrainment is not predicted accurately
- Multi-realization LES captures the plume merging phenomenon very well
- Note that both RANS and LES can capture the global spray characteristics such as liquid and vapor penetration very well





* Data analysis performed by Lyle Pickett (from Sandia) and shown at ECN4 workshop

TESF MODEL FOR REDUCING COMPUTATIONAL COST WITH LARGE KINETIC MECHANISMS

- Salient feature: Incorporate history effects in tabulated combustion models. Current versions of tabulated models do not account for the history effects
- Advantage: High fidelity model with significantly lower computational cost

Multidimensional chemistry tabulation

Flamelet Equation: $$\rho \frac{\partial Y_i}{\partial t} = \rho \frac{\chi}{2} \frac{\partial^2 Y_i}{\partial Z^2} + \dot{\omega}_i$$

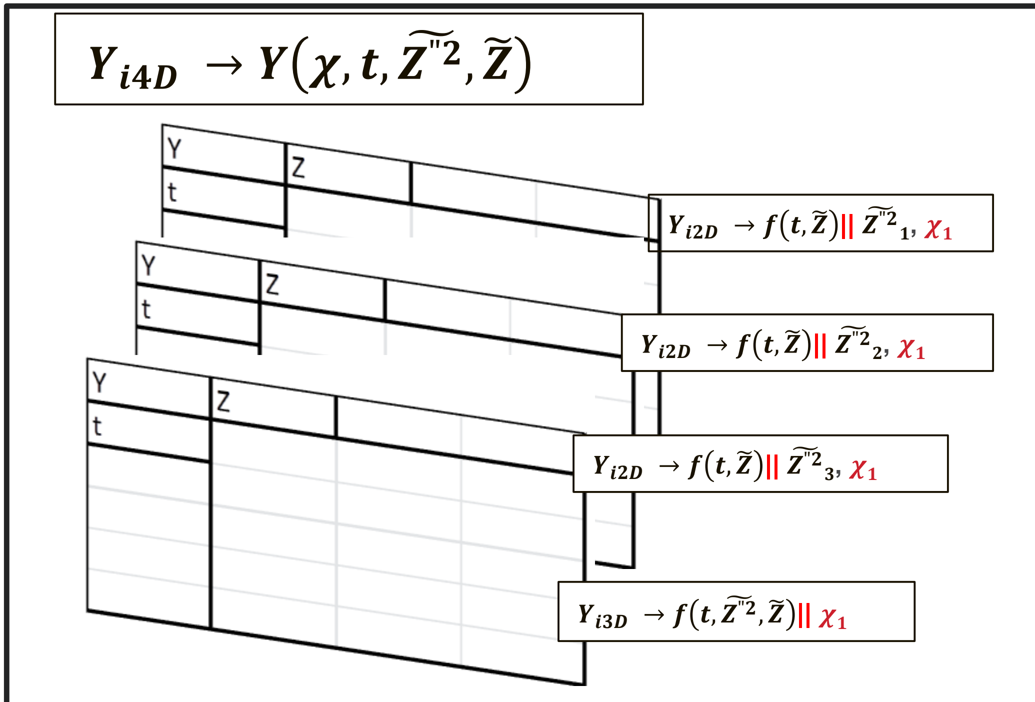
$$Y_i \rightarrow Y\left(\chi, t, \widetilde{Z''^2}, \widetilde{Z}\right)$$

Scalar dissipation rate (TCI term):

$$\widetilde{\chi} = C_\chi \frac{\varepsilon}{k} \widetilde{Z''^2}$$

Tabulation features:

- Multidimensional table generation
- Can be extended to n dimensions
- Each dimension can be calculated independently
- Large scale parallelization with no communication overhead
- **Best speed-ups obtained for large chemistry mechanisms**

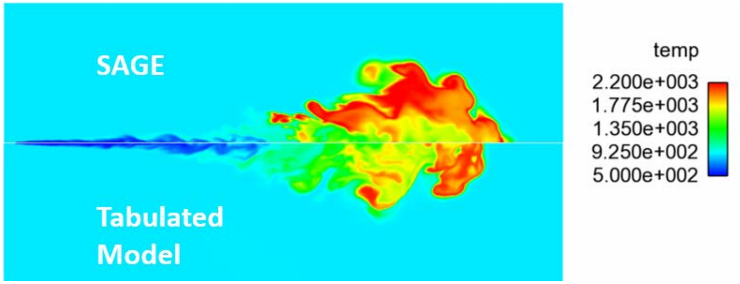


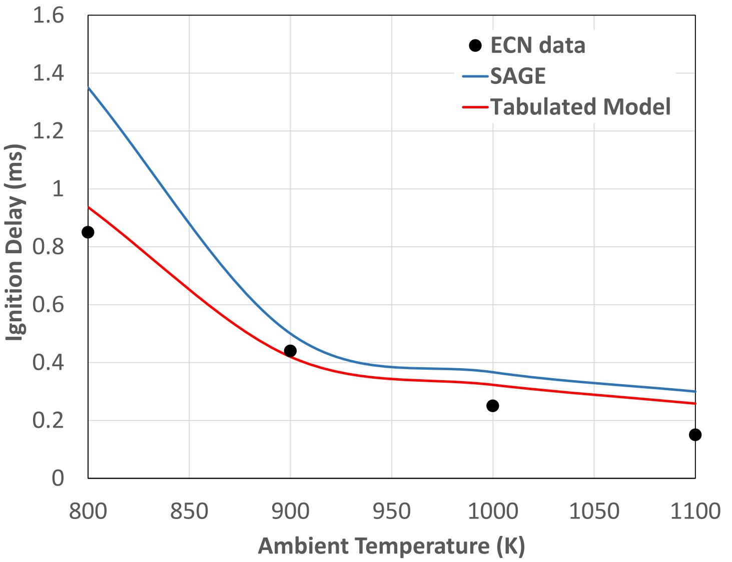
MODELING OF SPRAY FLAMES WITH TESF MODEL

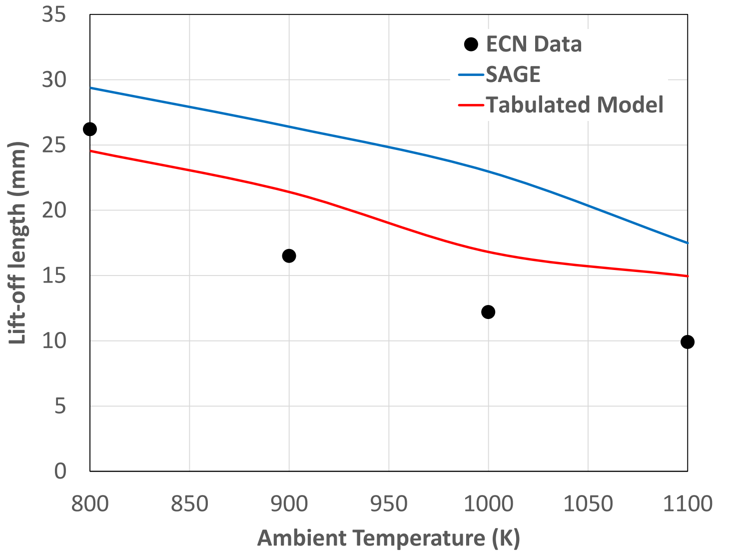
Engine Combustion Network (ECN) Spray A Simulations

Parameter	Description
Fuel	n-dodecane
Nozzle diameter	90 µm
Chemistry Mechanism[1]	103 species,370 reactions (reduced mechanism)
Combustion Model	1) TESF model with reduced mechanism and 20 flamelets (Tabulated model) 2) SAGE with reduced mechanism and multi-zone combustion model (SAGE)
Tabulation	4D table - $(\chi, t, \widetilde{Z''^2}, \tilde{Z})$
Peak cell count	10 million, min. cell size = 90 µm

- TESF model captures the ignition delay and lift-off lengths better than the SAGE model
- We observe **at least a factor of 2 speed-up** with the tabulated model across all conditions (ambient temperature, density, etc.)
- Flame temperatures are lower with the TESF model compared to SAGE which is expected



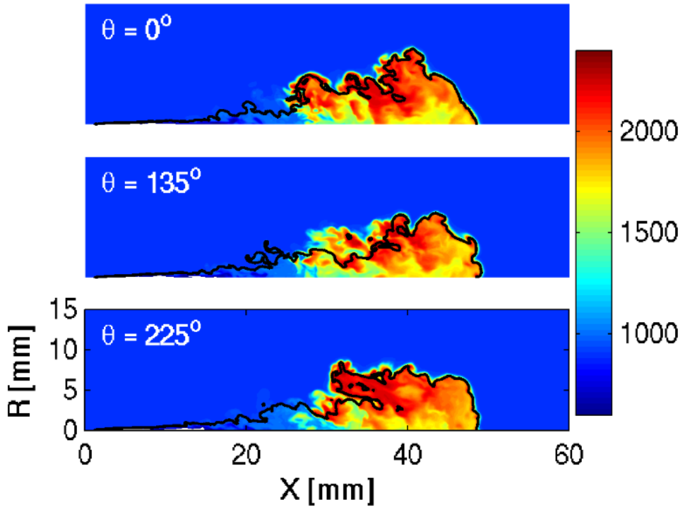




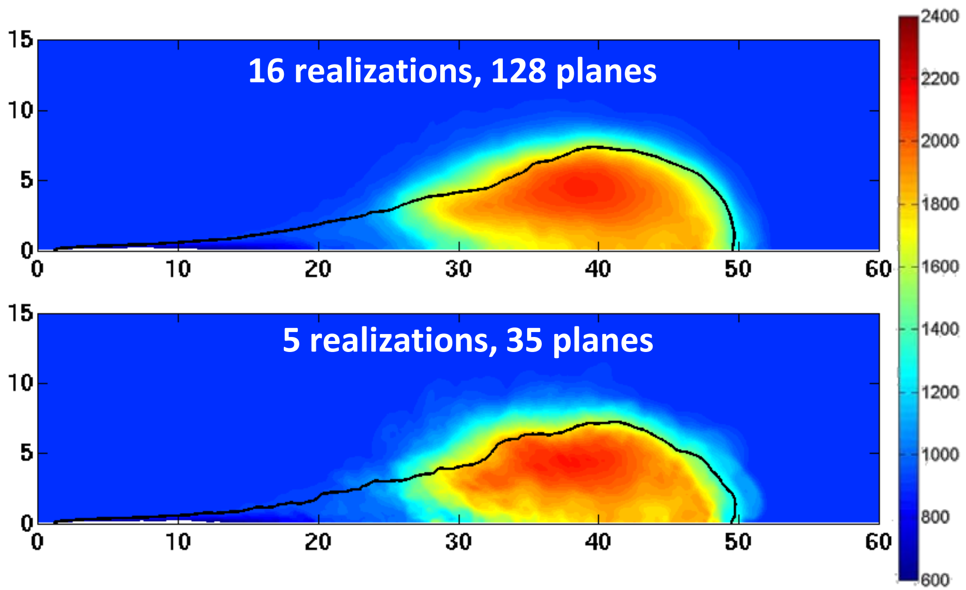
[1]Z. Luo, S. Som, S.M. Sarathy, M. Plomer, W.J. Pitz, D.E. Longman, T. Lu, *Combustion Theory and Modeling*, 2014

AZIMUTHAL AVERAGING TO REDUCE COMPUTATIONAL COST WITH LES COMBUSTION SIMULATIONS

- LES resolves the instantaneous, large scales of the flow. Comparing one LES realization with multi-shot averaged experiments is not reasonable
- Validation of LES requires multiple realizations to compute statistically averaged quantities. 4 different averaging techniques are possible:
  - Ensemble averaging
  - Azimuthal averaging
  - Time averaging during quasi-steady state
  - Combination of ensemble and azimuthal averaging
- Use of the statistical axi-symmetry of the flow to reduce the number of realizations by azimuthal averaging



- Azimuthal averaging over 128 planes are performed for 16 realizations
  - Each realization takes ~2 weeks on 256 processors
- Relevance index analysis is performed to determine
  - Minimum number of realizations
  - Minimum number of planes



Ensemble averaging with 5 realizations followed by azimuthal averaging can reduce computational cost significantly!

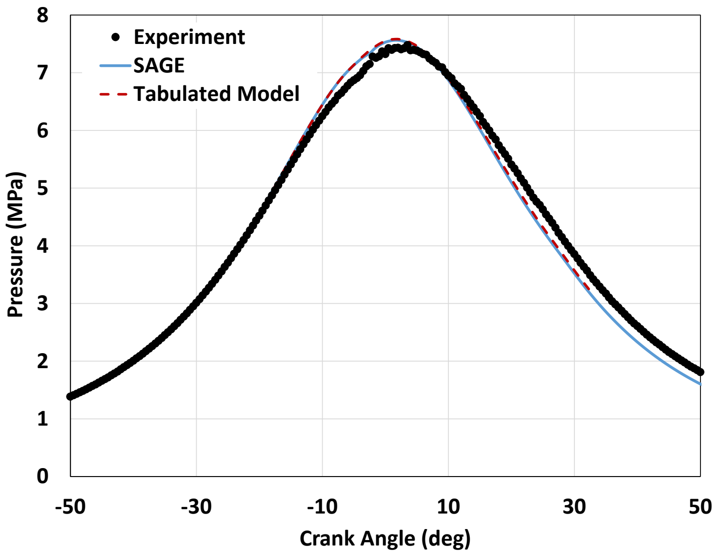
COMPRESSION IGNITION ENGINE SIMULATIONS WITH TESF MODEL

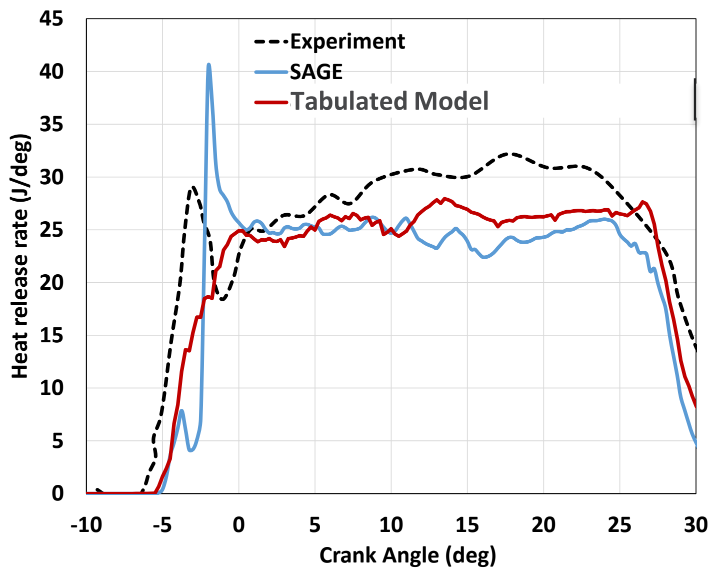
Sandia optical engine data from Charles Mueller et al.[1]

Parameter	Description
Fuel	Methyl Decanoate ($C_{11}H_{22}O_2$)
Reduced Mechanism[2]	115 species,460 reactions
Combustion Model	1) TESF model with reduced mechanism and 40 flamelets (Tabulated model) 2) SAGE with reduced mechanism and multi-zone combustion model (SAGE)
CFD set-up	Current simulations: RANS turbulence model **Future work: Incorporate our LES approach with Dynamic structure model and with ensemble and azimuthal averaging techniques**
Tabulation	5D table - $(P, \chi, t, \widetilde{Z''^2}, \tilde{Z})$
Peak cell count	1 million, 0.25 mm min. cell size

- Pressure and HRR well captured by the 5D TESF model
- We observe at least a **factor of 2 speed-up** with the tabulated model for the engine operating conditions simulated

Future work: Assess the predictive capability of this model with different speed-load conditions, EGR effects, etc.





[1]A.S Cheng, C.E. Dumitrescu, C.J. Mueller, *Energy and Fuels 28*: 7689-7700, 2014
[2]Z. Luo, M. Plomer, T. Lu, S. Som, D.E. Longman, S.M. Sarathy, W.J. Pitz, *Fuel* 99: 143-153, 2012

ENABLING HIGH THROUGHPUT COMPUTING ON MIRA*

Typically engines are designed and operating conditions are optimized based on experimental studies and engineer's intuition → All design space may not be explored and engineering intuition may not work for a completely new concept being designed from scratch → Goal: Develop capabilities to use leadership class machines (e.g., Mira) for high throughput computing to run ~10k simulations in two weeks

Approach

- Import engine simulation code (CONVERGE) on Mira
- Profile the code to identify computational bottlenecks and remove them
- Incorporate advanced load-balancing schemes
- Improve inter-processor communication
- Improve I/O with MPI

768k cores on Mira allow for Thousands of high-fidelity simulations set-up

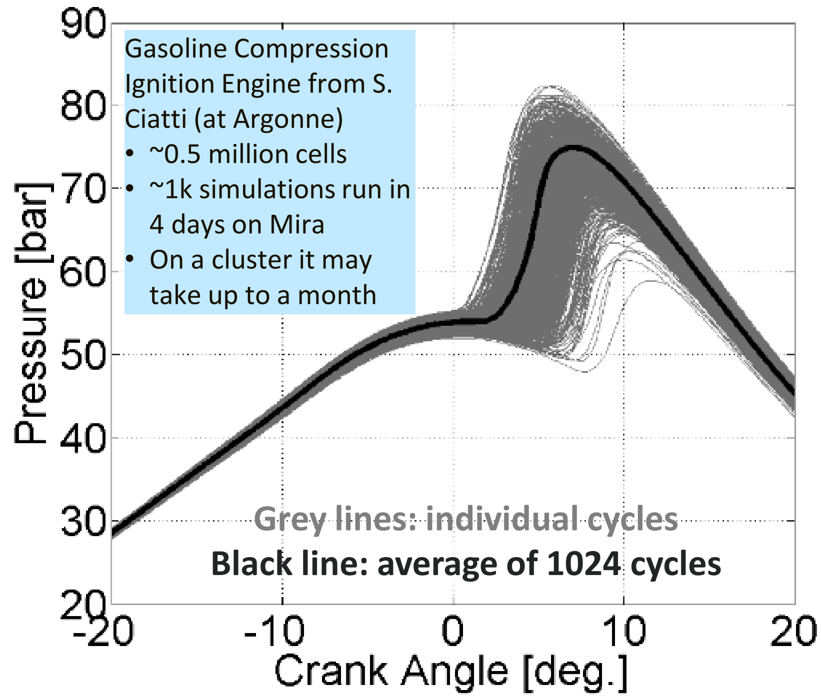
case 1

case 2

case 10,000

→ **workflow manager (Swift)** →

- ✓ Job launching scripts for optimum throughput
- ✓ Automated restarts
- ✓ Error handling
- ✓ Pre/post processing



*** ~60 Million core hours provided through the ALCC program of ASCR**

COLLABORATIONS

Argonne National Laboratory

Engine and Emissions Group: (Provide data for model validation)
Chemical Science and Engineering Group: (Mechanism development and reduction)
Leadership Computing Facility (Improving Scalability of CONVERGE, HPC resources)
Mathematics and Computing Science: (HPC resources)

Convergent Science Inc. (Algorithm and code development in CONVERGE)

Cummins (Provide experimental data, alpha testing of new models)

GM R&D (In-nozzle flow and spray simulations for GDI injectors) => new collaboration

Sandia National Laboratory (Provide experimental data through the ECN)

Lawrence Livermore National Laboratory (Mechanism development)

University of Connecticut (Mechanism Reduction)

University of Perugia (In-nozzle Flow Simulations)

Presentations at Advanced Engine Combustion (AEC) Working group
Toolkit Development in “Co-Optima”
Active role in Advanced Computing Tech Team (ACTT) by ASCR

Engine Combustion Network (4) Participation and Organization

- Topic 2 (Near nozzle flow and sprays): Som (leader)
- ANL contributions to other ECN-4 topics by Pei, Wang, Xue, Saha
- Accelerated the development of models due to the availability of high-fidelity data
- Motivated experiments to measure parameters that they would not measure otherwise

COLLABORATIONS THROUGH VERIFI

Based on the capabilities developed under this program, we have established the Virtual Engine Research Institute and Fuels Initiative (VERIFI)

VERIFI is designed to provide HPC solution for industrial problems of interest using either clusters of leadership class supercomputer such as Mira

CONVERGENT SCIENCE

DENSO

NAVISTAR®

aramco

GT Gamma Technologies

FCA FIAT CHRYSLER AUTOMOBILES

GE

CAT

Cummins®

achates POWER

2nd workshop on June 22nd and 23rd 2016

The Role of HPC in co-optimizing engines and fuels

RESPONSE TO PREVIOUS YEAR REVIEWER COMMENTS

Overall the reviewers were positive about the progress of this project

Comment: HPC cannot be considered as a tool today to design tomorrow's engine. Maybe the engines of day after tomorrow can be designed with HPC

Response: Author agrees that capability computing (i.e., running one simulation on ~10k processors) may not be able to aid in the design of tomorrow's engine. However, the high throughput computing (capacity computing) that we have demonstrated can definitely be used to explore the design space thoroughly. 768k processors on Mira allow us to run ~10k simulations in matter of weeks and explore/optimize engine design

Comment: The computing time is a challenge even with supercomputers

Response: Yes, the simulations with detailed chemical kinetics are still too expensive for incorporating into an engine design process. The TESF model is at least a factor of 2 faster. This model can be further optimized and then coupled with the solver enhancements at LLNL. Such an approach will bring more robust chemistry into the engine design process

Comment: More gasoline sprays should be modeled

Response: This year we have simulated the flow inside gasoline injectors with RANS and LES, captured flash boiling phenomenon, developed 1-way coupling and performed LES spray simulations for GDI applications. The main accomplishments have been shown in this presentation. Publications are listed in "reviewer only" slides

Comment: Collaborate more with LD automotive applications since US automotive fleet consists of 96-97% gasoline engines

Response: We have initiated a new collaboration with GM R&D on GDI nozzle flow simulations. We are open to collaboration with other LD OEMs as well

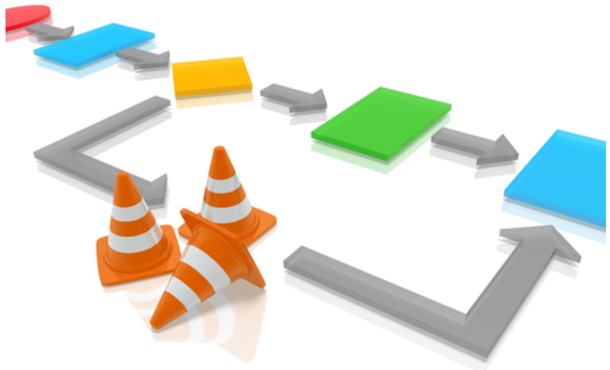
Comment: LES tools have not been applied to engine yet. Recommend applying to selective engine cases to assess the significance of LES on emissions

Response: Agreed. We are in the process of simulating Charles Mueller's (from Sandia) with high-fidelity LES and detailed kinetics (for 5-component diesel surrogate) from LLNL. The tabulated combustion model development is a key step towards this project

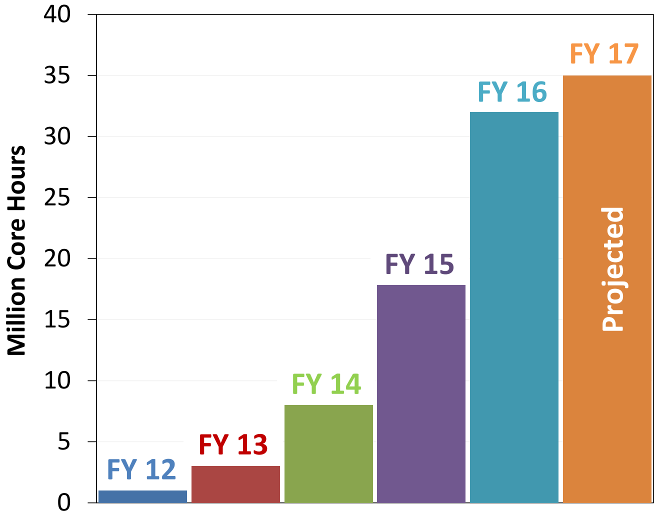
Argonne NATIONAL LABORATORY

REMAINING CHALLENGES AND BARRIERS

- Work-flow: More efficient "workflow" to ensure that code improvements and model developments reach industrial partners in a more timely fashion
  - Model development and validation time-scale is usually 6-9 months
  - Commercial code releases are usually once a year



- Computing time: High-fidelity calculations that need to be performed to develop 'best practices' for industry are expensive. The need for multi-cycle realizations with LES also increase simulation time extensively
  - Our computing needs have grown from FY12 (1-2M core hours) to FY16 (~30M core hours)
  - Computing time from ASCR is not guaranteed since ALCC and INCITE awards are extremely competitive



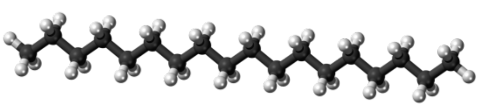
- High-fidelity experimental engine data: We not only need experimental data for boundary conditions from our experimental collaborators but we need uncertainty in these boundary conditions and measured data. Note that the simulations calculate results based on some averaged inputs from experiments and do not account for the experimental uncertainties that can be significant

Argonne NATIONAL LABORATORY

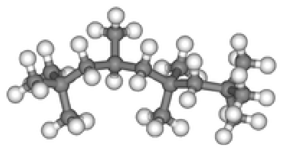
FUTURE WORK

1) Extend the framework of coupled Nozzle flow and spray modeling from diesel to gasoline fuel which can also capture Flash boiling effects: some validation data will be available through the x-ray measurements
2) Extend the *1-way coupling* approach and couple with existing combustion solver in CONVERGE to predict the influence of nozzle flow on combustion and emissions
3) CRADA project with Cummins and CSI (FY16-FY18)
   - Develop cavitation erosion model for diesel injectors: validation against published data in literature
   - Development of fluid structure interaction model to predict needle transients: validation against x-ray measurements of needle lift and wobble
   - Develop "engineering best-practices" to enable industry use these high-fidelity models
4) Continue to improve scalability of engine codes on HPC clusters and supercomputers thus enabling high-fidelity engine simulations at reasonable wall-clock times
   - Scale the expensive coupled nozzle flow and spray simulations on Mira to reduce runtime
5) The quest for better and more representative chemical kinetic models will require the use of five-component mixture for diesel fuel => continue collaborative research with LLNL and Sandia (TESF model a key step to increase fidelity and reduce computational cost with large mechanisms)

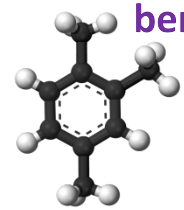
N-Octadecane



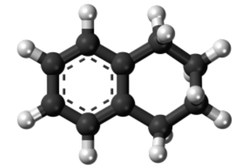
Heptamethyl nonane



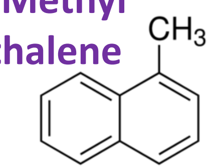
Tri-methyl benzene



Tetralin



Alpha Methyl Naphthalene



Argonne NATIONAL LABORATORY

SUMMARY

- **Objective**
  - Development of predictive spray, turbulence, and combustion models aided by high-performance computing tools and comprehensive validation
- **Approach**
  - Coupling expertise from DOE Office of Science on fundamental chemical kinetics, industrial partners, and HPC resources for development of robust engine models
- **Technical Accomplishment**
  - Developed an integrated approach for simulating diesel and gasoline nozzle flow and sprays using the same code structure and models
  - Demonstrated that LES can mimic shot-to-shot variability in sprays. Proposed an approach for averaging LES realization to reduce computational cost
  - Developed and implemented a new tabulated flamelet (TESF) model which is shown to be more accurate and is at least faster by a factor of 2 compared to existing model for the conditions investigated
  - Ported engine code on Mira supercomputer and integrated with a workflow manager to enable high throughput computing (~1k simulations in days). Mira now available for engine design
- **Collaborations and coordination**
  - with industry, academia, and national laboratories
  - through ECN with researchers world-wide
  - through VERIFI collaborations with light-duty, heavy-duty, and energy companies
- **Future Work**
  - Continue making advancements towards developing high-fidelity models. Propose “engineering best practices” for the industry to use these models in their engine design process by coupling with HPC tools and resources

Technical Back-Up Slides

EULERIAN MIXTURE & CAVITATION MODEL

Mixture Model equations (homogeneous multi-phase model)

Continuity: $\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \vec{v} = 0$

Momentum: $\frac{\partial \rho \vec{v}}{\partial t} + (\nabla \cdot \rho \vec{v})\vec{v} = -\nabla p + \nabla \cdot \bar{\bar{\tau}} + \rho \vec{f}$

Species: $\frac{\partial \rho Y_i}{\partial t} + (\nabla \cdot \rho Y_i)\vec{v} = \nabla \cdot (\rho D_i \nabla Y_i) + S_i$

(plus: Energy, Turbulence)

mixture density: $\rho = \sum_{i=1}^{n} \alpha_i \rho_i$

volume & mass fractions: $\alpha_i \rho_i = Y_i \rho$

void fraction: $\alpha_g = \frac{Y_g/\rho_g}{\sum Y_i/\rho_i}$

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

$$\frac{dY_v}{dt} = \frac{Y - \overline{Y_v}}{\Theta}$$

Exponential relaxation of the vapor quality Y to the equilibrium table value $\overline{Y_v}$ over a timescale Θ.

$$\overline{Y_v} = \frac{h - h_l}{h_v - h_l} \qquad \Theta = \Theta_0 \alpha^a \psi^b \qquad \psi = \left| \frac{p_{sat} - p}{p_{crit} - p_{sat}} \right|$$

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

Argonne NATIONAL LABORATORY

EXPERIMENTAL CONDITIONS FOR COMBUSTION SIMULATIONS

Spray flame experiments from ECN

Parameter	Quantity
Fuel	n-dodecane
Nozzle outlet diameter	90 µm
Nozzle K-factor	1.5
Nozzle shaping	Hydro-eroded
Discharge coefficient	0.86
Fuel injection pressure	150 MPa
Fuel temperature	363 K
Injection duration	1.5 ms
Injected fuel mass	3.5 mg
Injection rate shape	Square
Ambient temperature	800 - 1200 K
Ambient gas density	22.8 Kg/m^3
Ambient O_2 Concentration	15 %

http://www.sandia.gov/ecn/

Heavy duty optical engine experiments

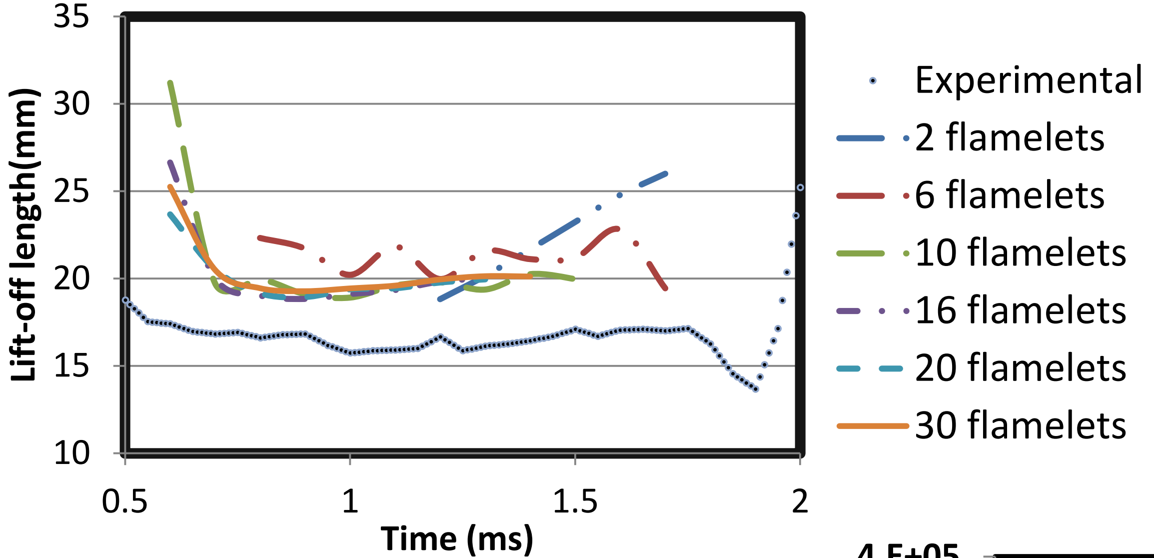
Parameter	Quantity
Cycle	4-stroke CIDI
Valves per cylinder	4
Bore	125 mm
Stroke	140 mm
Connecting rod length	225 mm
Piston bowl diameter	90 mm
Piston-bowl depth	16.4 mm
Swirl ratio	0.59
Squish height	1.5 mm
Displacement	1.72 L
Injector	Cat CR 350
Compression ratio	12.3:1

A.S Cheng, C.E. Dumitrescu, C.J. Mueller,
***Energy and Fuels 28*: 7689-7700, 2014**

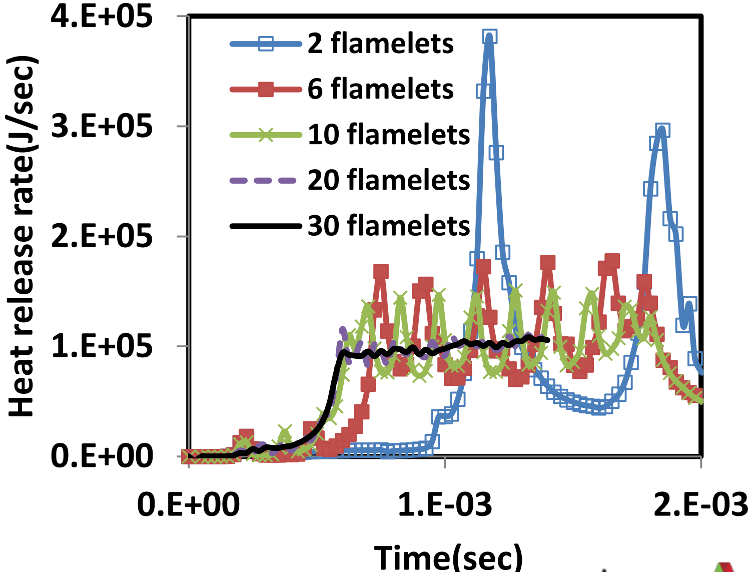
Argonne NATIONAL LABORATORY

TESF MODEL WITH MULTIPLE FLAMELETS

- Lift-off lengths for different number of flamelets for Spray A 900K conditions
- A minimum of 20 flamelets are required to predict the lift-off length correctly for the Spray A baseline conditions

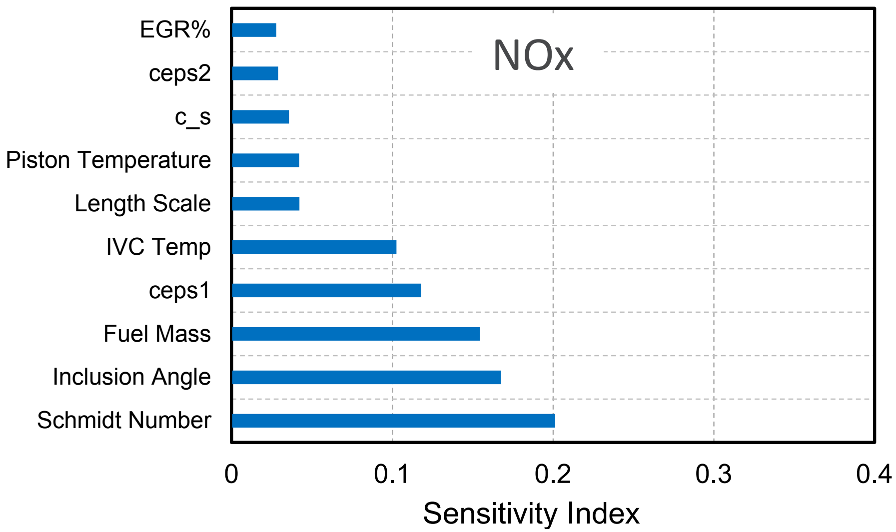


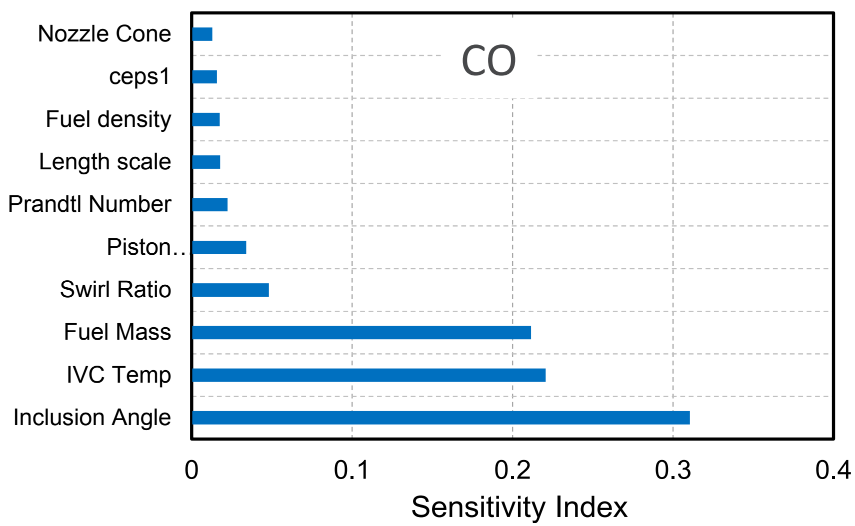
- HRR curve stabilizes as we increase the number of flamelets
- This type of convergence should decide the number of flamelets for the RIF model
- We need at least 20 flamelets



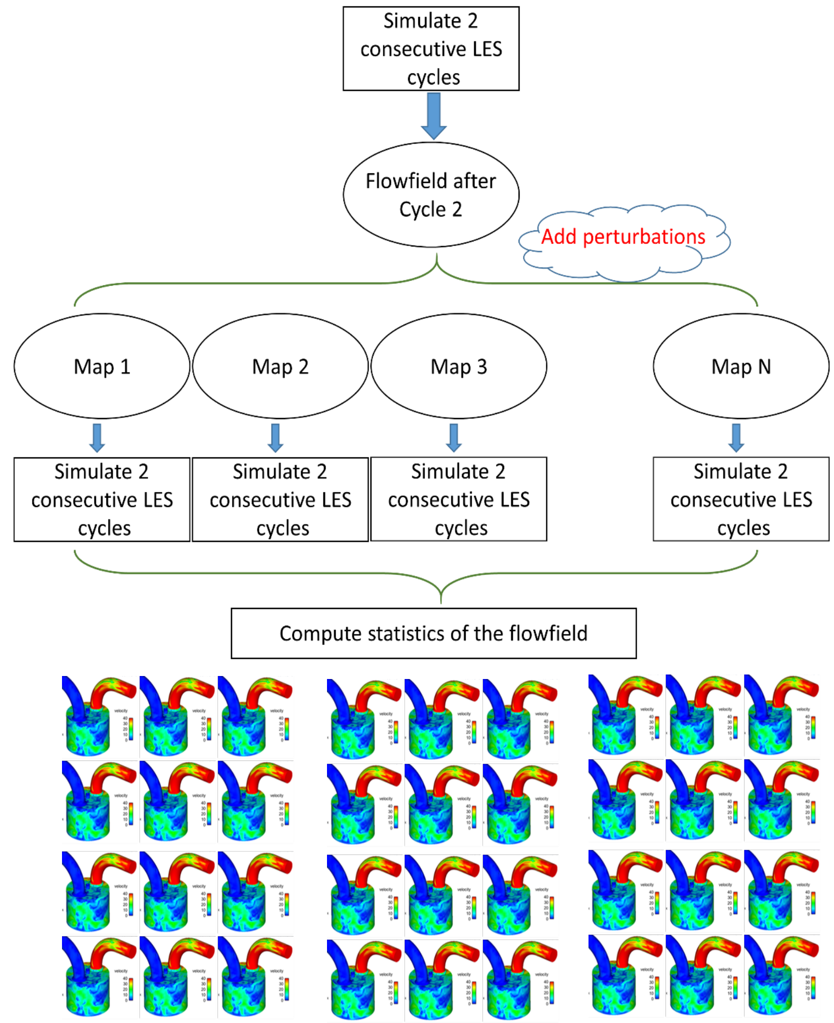
IMPACT OF HIGH THROUGHPUT COMPUTING ON MIRA

Perform uncertainty quantification by perturbing ~1000s of engine simulation input parameters and determine which parameters effect NOx and soot predictions





Perform ~1000s of parallel simulations to capture cyclic variability in SI engines (TCC engine simulations performed on Mira in collaboration with GM R&D)



COMPUTATIONAL RESOURCES

We gratefully acknowledge the computing resources provided at Argonne National Laboratory

- Fusion: ~ 2,500 - core computing cluster
- Blues: ~ 5,000 - core computing cluster

} operated by the Laboratory Computing Resource Center

- Vesta: ~ 33,000 – core super-computer
- Mira: ~ 786,000 – core super-computer

} operated by the Leadership Computing Facility

Fusion Cluster

MIRA Super-Computer

We gratefully acknowledge the computing resources provided by the ASCR Leadership Computing Challenge (ALCC) award of 60 million core-hours on Mira supercomputer at the ALCF at Argonne National Laboratory

Argonne NATIONAL LABORATORY