

Advancements in Fuel Spray and Combustion Modeling with High Performance Computing Resources

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Overview

Timeline

Project start: April 1st 2012

Partners

Argonne National Laboratory

Chemical Science and Engineering Mathematics and Computing Science Leadership Computing Facility Advanced Photon Source

Convergent Science Inc. {CRADA} Caterpillar Inc. {CRADA} Cummins Engine Company {CRADA}

Lawrence Livermore National Laboratory Sandia National Laboratory (Engine Combustion Network [ECN]) Advanced Engine Combustion (AEC) 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 13: 500 K FY 14: 500 K FY 15: 525 K

Relevance

> Nozzle flow and Spray research

- □ Fuel spray breakup in the near nozzle region plays a central role in combustion and emission processes
- Improving in-nozzle flow and turbulence predictions is key towards the development of predictive engine models

Combustion modeling using detailed chemistry

- Accurate chemical kinetics for fuel surrogates are key towards developing predictive combustion modeling capability
- □ Large Eddy Simulation (LES) based approaches can provide further insights than simplified Reynolds Averaged Navier Stokes (RANS) calculations

> High-Performance Computing

- Current state-of-the-art for engine simulations in OEMs involve up to 50 processors (approx.) only
- Will be needed in order for OEMs to retain quick turn-around times for engine simulations

Cluster





Super-Computer



Objectives & Approach

In general Engine simulations involve:

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

High-Fidelity Approach:

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

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 of interest

Extensive tuning to match experimental data

Towards Predictive Simulation of the Internal Combustion Engine

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Simulation Approach: Sub-Model Development

Modeling Tool	CONVERGE
	Source code access for spray and HPC Algorithms
Dimensionality and type of grid	3D, structured with Adaptive Mesh Resolution
Spatial discretization approach	2 nd order finite volume
Smallest and largest characteristic grid	Finest grid size simulations:
size(s)	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)
	100 μm for engine (50 million cells)
Turbulence-chemistry interactions model	Direct Integration of detailed chemistry: well-mixed model
	Representative Interactive Flamelet (RIF) Model
Turbulence model(s)	RANS: RNG k-ε; LES: Dynamic Structure
In-nozzle Flow	Homogeneous Relaxation Model (HRM)
Spray models	Lagrangian Models with Multi-component evaporation
	Volume of Fluids (VOF) approach for phase-tracking
	Coupled Eulerian-Eulerian Near Nozzle Model
	"1-way" and "2-way" coupling approaches





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

Milestones, FY 15

Nozzle flow and Spray Research (CRADA with Cummins and CSI)

- Develop SOI and EOI simulation approaches single hole injectors and capture fuel dribbles {100% complete: September 2014}
- Simulate production Cummins injectors with different orifice patterns i.e., with hydrogrinding and conicity {50% complete: March 2015}
- Develop 1-way coupling approach (transition to Lagrangian parcels at the nozzle exit) to capture the influence of nozzle flow on fuel spray and combustion in a Lagrangian framework for Industrial use {50% Complete: July 2015}
- Combustion Modeling with Detailed Chemistry
 - Develop "best practices" for LES Combustion Simulations {100% Complete: December 2014}
 - □ Further reduced n-dodecane mechanism developed and validated against ECN data {100% complete: March 2015}
- High-Performance Computing (Funds-in CRADA with Caterpillar and CSI)
 Identify numerical "best-practices" for open and closed cycle, single-cylinder Caterpillar engine simulations {100% complete: December 2014}

Technical Accomplishments

Full 3D Cummins 9-hole XPI 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_{ini} = 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 this approach for simulating different injector nozzle designs (K-factors and hydro-grindings)







Injector Transients: Profound Influence on Fuel Spray at Low Needle Lifts Mass flow rates with diffe

- Significant shot-to-shot variation from the APS data for needle off-axis motion (wobble)
- Shot-to-shot differences in wobble does not affect global mass flow rates!
- At high lift no cavitation is observed
- Wobble influences the two-phase flow characteristics at low lifts since it influences the stream lines entering each hole
- A nominally designed injector that is not expected to cavitate may still cavitate at low lifts due to needle transients and production tolerances





Mass flow rates with different wobble profiles





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
- Demonstrated an approach to capture shot-to-shot variation in simulations
- Cummins using this approach for their inhouse next generation engine design

Hole-to-Hole Variation Especially @ low-lifts



@ Low-lifts Dribbled Mass Predicted with LES*



- Demonstrated an high-fidelity LES 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

Future work: Predict dribbled mass from the Cummins multi-hole production injector and characterize the influence on spray and combustion characteristics

- * Simulations performed in collaboration with Prof. Battistoni at University of Perugia
- $P_{ini} = 1500 \text{ bar}$ $P_{back} = 1 bar$ EOI @ 2150 µs 2200 µs 2250 µs Dribbles 2300 µs 2395 µs Lig. Volume Fraction

0.00

0.25

0.50

0.75

1.00

Optimized Reduced Mechanisms for Diesel Surrogate



Solid high-T core with highly tunable low-T chemistry

- Prof. T. Lu at University of Connecticut in collaboration with Tsinghua University and Argonne has developed a new approach to more aggressive mechanism reduction for transportation fuel surrogates (n-dodecane)
- The reduced mechanism was developed based on feedback provided by Argonne for many 3D spray-flame simulations at engine-like ambient conditions
- The new reduced 54 species mechanism for n-dodecane performs significantly better than the 106-species mechanism presented by Som in AMR2014 against experimental data from ECN



Optimized mechanism generation approach will provide significant cost-saving to the industry since simulation time scales:
 with N² ~ N³ of number of species
 Linearly with number of reactions

Spray and Combustion Modeling with LES

- Based on reviewer's suggestion from last year, we have started integrating our LES spray modeling approach with the combustion solver in CONVERGE
- ✓ Extensive validation against experimental data from the Engine Combustion Network

Future work: Implementing and testing various turbulence chemistry interaction models for LES





- 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

60

40

with LES

Temperature contours for different min. mesh sizes



Temperature contours for different LES realizations @



20

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

- **Temperature: 2**
- Mixture fraction (Z): 5

Soot: 8



"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

CAT Single Cylinder C15 Engine Simulations: Necessary resolution in ports and need for open cycle

Identified best practices for:

- Grid resolution in ports
 - 0.2 mm min. resolution in intake and exhaust ports
- Number of cycles to wash out initial conditions
 - Spray injection dominates combustion and emission processes
 - Cycle # 2 is globally converged, NOx converged within 6%

Note that for light duty SI engine, due to low injection pressure, injection has low impact and there may not be any convergence at all (Please see Thomas Wallner's presentation {ACE084})





Future Work: Improve memory management in CONVERGE for large simulations since many simulations with more than 20-30 million cells crash due to memory issues

Scaling CONVERGE on HPC Resources

Gasoline Compression Ignition Engine from S. Ciatti

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

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), shown in Som-AMR 2013
- Load balancing the chemical kinetic calculations (>3x)

Load balance chemistry based on equalizing "computational effort per processor" rather than "number of cells per processor" ...and rebalance every timestep!



1000

800

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.

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



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) Caterpillar Inc. (Testing and implementation of HPC tools)

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 "OPTIMA" Active role in Advanced Computing Tech Team (ACTT) by ASCR

Engine Combustion Network Participation & Organization



ANL contributions to other ECN-4 topics by Pei, Wang, Xue, Saha

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- Accelerated the development of models due to the availability of high-fidelity data
- I Motivated experiments to measure parameters that they would not measure otherwise

Response to Previous Year Reviewer Comments

Overall reviewers seemed quite happy with the progress of this project

Comment: Effect of *manufacturing tolerances* of a typical injector

Response: We can account for manufacturing tolerances by using higher resolution calculations, however, the challenge has been to obtain geometrical information with dialed-in manufacturing tolerances. Simulation of ECN Spray B injector is a step towards understanding the manufacturing tolerance effects on simulation results. Comment: Improve code scalability

Response: We have shown good scalability up to 4096 processors on a chosen engine simulation Comment: Needle wobble and its *impacts on combustion*

Response: Developing the 1-way and 2-way coupling approach will allow us to capture the influence on wobble on the spray and then eventually on combustion and emission processes

Comment: Suggested collaboration with a fuel injection system manufacturer

Response: Cummins is an fuel injection system manufacturers. The PI is also had many interactions with Bosch in the past year about possible collaborations

Comment: Focus on gasoline

sprays

Response: The authors have already published two papers on GDI sprays with LES: (1) With FCA on validating GDI sprays against x-ray radiography data (SAE Paper No # 2015-01-0931, (2) With CSI on validation Spray G from ECN (ASME-ICEF2015-1003). Efforts are also underway to develop and validate flashboiling model



Flash boiling calculations of ECN Spray G Injectors from Delphi



Remaining Challenges and Barriers

- <u>Work-flow</u>: 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
- <u>Computing time</u>: 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 FY15 (~20M core hours)
 - Production engine simulations still do not scale well on supercomputers => INCITE awards (scalability on 16K cores) are challenging
- <u>Fuel Properties</u>: Advanced nozzle flow and fuel spray models necessitate better characterization of fuel properties as a function of temperature and mixing rules for multi-component representations. Often these are not available for the temperature exploration range of interest!





Future Work

- 1) <u>1-way coupling</u>: transitioning to Lagrangian parcels at the nozzle exit. Lagrangian resolutions comparable to Eulerian resolutions (~15 μ m)
- 2) <u>2-way coupling</u>: transitioning to Lagrangian parcels downstream of the nozzle exit based on continuous coupling of mass, momentum and energy
- 3) For both the coupling approaches with Cummins XPI:
 - Influence of initial SOI and EOI transients on combustion and emission characteristics
 - Influence of conicity and hydro-grinding on combustion and emissions behavior
- Extend the framework of coupled Nozzle flow and spray modeling from diesel to gasoline fuel that can also capture Flash boiling effects, for the benefit of the automotive industry
- 5) Continue to improve scalability of engine codes on HPC clusters and supercomputers thus enabling high-fidelity engine simulations at reasonable wall-clock times
- 6) 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 Heptamethyl Tri-methyl Tetralin



Summary

Objective

Development of predictive spray, turbulence, and combustion models aided by highperformance 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

- Needle wobble has a profound influence on injector performance @ low-lifts
- > Demonstrated an approach to capture the influence of needle wobble on cyclic variability
- Approach to predicting fuel dribbles from production injectors developed
- Developed "best practices" for LES combustion modeling of spray flames
- Resolution requirements and number of multiple cycles needed for heavy duty engine simulations identified

Collaborations and coordination

- with industry, academia, and national laboratories in US
- through ECN with researchers world-wide

Future Work

- Transition to an Eulerian-Lagrangian approach for comprehensive spray modeling
- Development and validation of realistic diesel surrogate chemical kinetic model
- Identify "best practices" for multi-cylinder simulations with HPC resources

Technical Back-Up Slides

(Note: please include this "separator" slide if you are including back-up technical slides (maximum of five). These back-up technical slides will be available for your presentation and will be included in the DVD and Web PDF files released to the public.)

Eulerian Mixture & Cavitation Model

Mixture Model equations (homogeneous multi-phase model)

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

Momentum: $\frac{\partial \rho \vec{v}}{\partial t} + (\nabla \cdot \rho \vec{v}) \vec{v} = -\nabla p + \nabla \cdot \overline{t} + \rho \vec{f}$
Species: $\frac{\partial \rho Y_i}{\partial t} + (\nabla \cdot \rho Y_i) \vec{v} = \nabla \cdot (\rho D_i \nabla Y_i) + S_i$
inture density: $\rho = \sum_{i=1}^n \alpha_i \rho_i$
volume & mass ai conversed of the second of

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

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

$$\frac{dY_{v}}{dt} = \frac{Y - \overline{Y_{v}}}{\Theta}$$

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

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

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 nearnozzle 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 \tilde{V} 1
 - Mean density is obtained from Favre-averaged liquid mass fraction: $\frac{1}{\bar{\rho}} = \frac{\bar{Y}}{\rho_1} + \frac{1-\bar{Y}}{\bar{\rho}_2}$

☐ The liquid mass fraction is transported with a model for the *turbulent liquid diffusion flux into the gas*: $\frac{\partial \bar{\rho} \tilde{Y}}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_i \tilde{Y}}{\partial m} = -\frac{\partial \bar{\rho} u'_i Y'}{\partial m} - \bar{\rho} \tilde{Y}_{evap}$

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

 $\Box \text{ Void fraction } (\alpha) = \begin{cases} 0 & \text{if the computational cell is filled with pure liquid} \\ 1 & \text{if the computational cell is filled with pure gas} \\ (0,1) & \text{if the computational cell is filled with both liquid and gas} \end{cases}$ * Xue, Som, et al. SAE Journal of Fuel and Lubricants, 2014

EOI Simulation to Capture Dribbled Mass with LES*



- 1500 bar vs. 1 bar
- Diesel fuel properties = f(T)
 - (a) $300 \text{ K} \rightarrow \rho = 848 \text{ kg/m}^3$, $p_{sat} = 1000 \text{ Pa}, \mu = 2.5 \times 10^{-3} \text{ Ns/m}^2$
 - 1.9×10⁹ Pa bulk modulus
 - 1×10⁻⁵ non condensable gas mass fraction



M. Battistoni, Q. Xue, S. Som, "LES of Spray Transients: Start and End of Injection Phenomena," under review Oil and Gas Science Technology 2015

Experimental Conditions 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/		

- Experiments performed under both evaporating and combusting conditions.
- Data available for : Spray penetration, liquid length, vapor penetration, mixture fraction, ignition delay, flame lift-off length, soot distribution , highspeed movies



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
- Vesta: ~ 33,000 core super-computer
- Mira: ~ 758,000 core super-computer

- operated by the Laboratory Computing Resource Center
- operated by the Leadership Computing Facility

Fusion Cluster





