Simulation of Internal Combustion Engines with High-Performance Computing Tools

Final CRADA Report

Energy Systems

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Non Proprietary Final CRADA Report

Date: 12/21/2016

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CRADA Title: Simulation of Internal Combustion Engines with High-Performance Computing Tools

CRADA Start/End Date: 01/29/14 to 08/08/15

Argonne Dollars: \$50,000

Participant Dollars: \$135,000

Argonne PI: Sibendu Som

Participant(s):

<u>Caterpillar Inc.</u>	<u>\$135,000</u>
Name	Participant Dollars

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<u>Convergent Science Inc.</u>	<u>\$0</u>
Name	Participant Dollars

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<u>N/A</u>	<u>\$</u>
Name	Participant Dollars

Complete Address

DOE Program Gurpreet Singh

Manager:

Summary of Major Accomplishments:

Traditional Lagrangian spray modeling approaches for internal combustion engines are highly grid-dependent due to insufficient resolution in the near nozzle region. This is primarily because of inherent restrictions of volume fraction with the Lagrangian assumption together with high computational costs associated with small grid sizes. A state-of-the-art grid-convergent spray modeling approach was developed and implemented by Senecal et al. (ASME-ICEF2012-92043) in the CONVERGE software. The key features of the methodology include Adaptive Mesh Refinement (AMR), advanced liquid-gas momentum coupling, and improved distribution of the liquid phase, which enables use of cell sizes

Summary of Major Accomplishments:

smaller than the nozzle diameter. This modeling approach was rigorously validated against non-evaporating, evaporating, and reacting data from the literature. The current numerical study focusses on further demonstration of the grid-convergent modeling approach for simulating a single-cylinder Cat® compression ignition engine. The simulated injector is characterized with a nominal nozzle exit diameter of 259 μm . Simulations using various minimum grid sizes (ranging from 125 μm to 1000 μm) are compared for engine performance and emissions parameters of interest such as pressure, heat release rate, ignition delay, NO_x, HC, and soot emissions. The peak cell-count for the highest resolution simulation was on the order of 34 million. These computationally expensive simulations were facilitated at a high-performance computing facility at Argonne National Laboratory. METIS load-balancing algorithm was developed and implemented in Converge code for the simulations. Scaling studies were also performed. The validity of previously recommended grid settings (ASME-ICEF2012-92043) for accuracy/runtime trade-off is further assessed. Efficacy of a simplified combustion model is also compared against a detailed chemical kinetics based combustion model.

Summary of Technology Transfer Benefits to Industry:

The workflow developed for high-fidelity engine simulations became part of "best practices" for Caterpillar Inc. internally. Convergent Science benefitted with the implementation of the advanced load-balancing algorithm.

Other Information/Results: (Papers, Inventions, Software, etc.)

The results were presented at an SAE paper (S. Som, D.E. Longman, S.M. Aithal, R. Bair, M. Garcia, S. 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). APT # 74721

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