

# Workshop on the Role of High-Performance Computing in Engines and Fuels Co-Optimization

Hosted by

**The Virtual Engine Research Institute and Fuels Initiative (VERIFI)**

Advanced Photon Source (APS) Conference Center, Argonne National Laboratory

June 22–23, 2016

## Wednesday, June 22, 2016

- 7:00-7:45 a.m.      *Breakfast buffet (Guest House) {Sponsor: Parallel Works}*
- 7:45 a.m.            Transportation by bus to conference site (APS Auditorium)
- 8:00-8:30 a.m.      Registration
- 8:30-8:45 a.m.      Peter Littlewood: Laboratory Director of Argonne National Laboratory  
**Welcome to Argonne**
- 8:45-9:15 a.m.      Leo Breton: Technology Development Manager at US DOE  
**Title**
- 9:15-9:45 a.m.      David Cleary: Research Center Leader at Aramco Services Company  
**INNOVATION TO DEMONSTRATION – Enabling a Sustainable Mobility Solution**
- 9:45-10:00 a.m.    *Coffee break (APS Auditorium) {Sponsor: Convergent Science Inc.}*
- 10:00-10:15 a.m.    Sibendu Som: Principal Mechanical Engineer at Argonne National Laboratory  
**Workshop Objectives and Mechanics**
- 10:15-10:45 a.m.    Anthony Dean: Professor and Dean of Chemical and Biological Engineering at  
Colorado School of Mines  
**Impact of Fuel Structure on Pyrolysis Kinetics: Implications for Combustion**
- 10:45-11:15 a.m.    Hui Xu: Technical Advisor at Cummins Engine Company  
**Application of Fuel Combustion Chemistry in Gaseous Fueled Spark Ignited  
Engine Analysis**
- 11:15 -11:45 a.m.    William H. Green: Professor at Massachusetts Institute of Technology  
**A Priori Methods for Predicting the Performance of Fuels**
- 11:45 a.m.            Transportation by bus to Guest House
- 12:00-1:15 p.m.    *Lunch (Guest House) {Sponsored by Intel}*
- 1:15 p.m.            Transportation by Bus to Conference site (APS auditorium)
- 1:30-2:00 p.m.      Gaurav Bansal: Senior HPC Application Engineer at Intel  
**High Performance Optimizations of CFD Codes on Current and Next  
Generation Intel Platforms**

- 2:00-2:30 p.m. Tianfeng Lu: Professor at University of Connecticut  
**Development of Efficient Reduced Models and Chemistry Solvers for Engine Simulations**
- 2:30-3:00 p.m. Stephen Klippenstein: Distinguished Scientist at Argonne National Laboratory  
**Theoretical Chemical Kinetics as a Tool for Fuel Chemistry Modeling**
- 3:00-3:15 p.m. *Coffee break (APS Auditorium) {Sponsor: Convergent Science Inc.}*
- 3:30-5:30 p.m. **Three tours for everyone (buses leave from the APS Auditorium)**
- Engine facilities and Rapid Compression Machine
  - Advanced Photon Source
  - Argonne Leadership Computing Facility and Visualization Lab
- Buses back to the Guest House**
- 6:00-7:00 p.m. *Reception (Guest House Dining Room) {Sponsored by Convergent Science Inc.}*
- 7:00-8:00 p.m. *Dinner (Guest House Dining Room) {Sponsored by Convergent Science Inc.}*
- 7:30-8:00 p.m. Diane Hart: Manager, Sponsored Research Office, Argonne National Laboratory  
**Working with Argonne**

### ***Tour Descriptions***

#### **Engine Facilities and Rapid Compression Machine**

Argonne's engine testing capability spans from light duty to heavy duty, with engines ranging in size from 0.5L up to 19L. Argonne's facilities include state-of-the-art instrumentation for in-cylinder visualization and regulated and un-regulated emissions characterization (gaseous and particulate). These experiments generate high-quality data for validation of VERIFI simulations. Argonne is also the only national laboratory with a rapid-compression machine for generating very controlled, engine-like conditions for studying fuel ignition and combustion properties.

#### **Advanced Photon Source**

The Advanced Photon Source (APS) is a user facility at Argonne, which produces the brightest x-ray beams in the Western hemisphere, enabling multi-disciplinary research that advances science. A dedicated hutch at APS allows VERIFI researchers to gain fundamental understanding of fuel injection and spray phenomena (such as cavitation and jet interactions) and aid advanced model developments.

#### **Argonne Leadership Computing Facility**

The Argonne Leadership Computing Facility is a user facility at Argonne that provides the computational science community with a world-class computing capability dedicated to breakthrough science and engineering. The tour will include a visit to Argonne's 10-petaflop MIRA supercomputer. The VERIFI team uses these facilities and collaborates extensively with ALCF scientists to scale up engine calculations.

**Thursday, June 23, 2016**

- 7:00-7:45 a.m.      *Breakfast buffet (Guest House) {Sponsored by CRAY}*
- 7:45-8:00 a.m.      Transportation by bus to conference site (APS Auditorium)
- 8:00-8:15 a.m.      Registration
- 8:15-8:45 a.m.      Jackie Chen: Distinguished Member of the Technical Staff at Sandia National Laboratories  
**Direct Numerical Simulation of Turbulent Flames with Low-Temperature Ignition**
- 8:45-9:15 a.m.      Michael Martin: AAAS Science & Technology Policy Fellow, ASCR, US DOE  
**Exploring the Role of High-Performance Computing across Clean Energy Technologies**
- 9:15-9:30 a.m.      *Coffee break (APS Auditorium) {Sponsor: Convergent Science Inc.}*
- 9:30-10:00 a.m.      Janardhan Kodavasal: Mechanical Engineer at Argonne National Laboratory  
**Capacity and Capability Computing for Engine Simulations at Argonne**
- 10:00-10:30 a.m.      Tang-Wei Kuo: Lab Group Manager at GM Global R&D Center  
**Leveraging National Laboratory Computing Resources to Improve IC Engine Simulation**
- 10:30-11:00 a.m.      Dr. Syed Wahiduzzaman: Vice President at Gamma Technologies  
**On the Pursuit of a Physically Grounded Quasi-Dimensional CCV Model using LES**
- 11:00-11:30 a.m.      Federico Piscalia: Associate Professor at Politecnico di Milano  
**Time-Resolved Simulations of Moving Boundary Problems in OpenFOAM: Application to Cavitating Sprays and In-Cylinder Flows**
- 11:30 a.m.              Transportation by bus to Guest House
- 11:45-1:00 p.m.      *Lunch (Guest House) {Sponsored by CRAY}*
- 1:00 p.m.              Transportation by bus to conference site (APS Auditorium)
- 1:15-1:45 p.m.      Dave Strenski, Application Analyst  
**CAE in a Petascale Computing World**
- 1:45-2:15 p.m.      Paul Fischer: Professor at University of Illinois at Urbana  
**VERIFI 2.0 Perspective for NEK5000**
- 2:15-2:20 p.m.      Doug Longman: Section Manager at Argonne National Laboratory  
**Thank You**
- 2:20 p.m.              **Buses leave from the APS Auditorium for Building 240 for parallel sessions**

2:45-5:45 p.m. **Two parallel sessions at Building 240**

- “Hands-on” (Room 1404/1405)
- “One-on-One” (The VERIFI team will email room information to individuals who signed up for this session)

### ***Parallel Sessions***

#### **Hands-on Session**

Experience firsthand the tremendous power of a supercomputer applied to a practical engine simulation problem. This one-of-a-kind immersive session is for engineers in the automotive industry, and does not require any prior knowledge of specific software or operating systems. Each participant will run hundreds of production-type simulations using CONVERGE on 8000 cores of Mira. VERIFI researchers will guide you through the process of logging on to Mira and launching these simulations. During the session, you will learn about the technical advances Argonne has made to enable such a large-scale simulation campaign to run in a highly automated fashion.

#### **One-on-One Session**

VERIFI experts will be available for discussions with industry representatives to understand their computing needs and provide guidance on how VERIFI projects could help them design and optimize next-generation engines and fuels. Argonne will provide a list of VERIFI experts available for discussion.