2018
Stewardship Science
Academic Programs Annual

♦ Stewardship Science Academic Alliances
  ♦ High Energy Density Laboratory Plasmas
    ♦ National Laser Users’ Facility
  ♦ Predictive Science Academic Alliance Program II
Predictive Science Academic Alliance Program II
Overview

Predictive Science Academic Alliance Program (PSAAP) II is a five-year program established in 2014 by the Advanced Simulation and Computing (ASC) program of the National Nuclear Security Administration to demonstrate predictive science in an extreme-scale computing environment. Each of the following centers is using a multi-scale and multiphysics application as a focus for their research, and is applying state-of-the-art verification and validation techniques in order to undertake predictive science with uncertainty quantification. Three of the sites are Multidisciplinary Simulation Centers (MSCs) and three are Single-Discipline Centers (SDCs) funded at approximately $4 million and $2 million, respectively.

- University of Florida, “Center for Compressible Multiphase Turbulence”
- University of Illinois-Urbana-Champaign, “Center for Exascale Simulation of Plasma-Coupled Combustion”
- University of Notre Dame, “Center for Shock Wave-processing of Advanced Reactive Materials”
- Stanford University, “Predictive Simulations of Particle-laden Turbulence in a Radiation Environment”
- Texas A&M University, “Center for Exascale Radiation Transport”
- University of Utah, “The Carbon-Capture Multidisciplinary Simulation Center”

Due to the complexity of the applications, predictive science can only be done on the most powerful computers available. Thus, the intent is to develop and demonstrate technologies and methodologies to support effective extreme computing leading to exascale by focusing on these science and engineering applications. Each center is utilizing a different computing environment to support the simulation of their application and provide the necessary data for validation and uncertainty quantification. These simulations are being performed on a variety of systems made available by the ASC at the NNSA national laboratories and by the Office of Science at Argonne National Laboratory and Oak Ridge National Laboratory.

One of the unique characteristics of the program is that every student supported with PSAAP II funds must spend an internship of at least 10 weeks at one of the NNSA national laboratories. The program is in its fourth year and, to date, over 100 students have taken advantage of the opportunity. These internships provide the laboratories with access to students who are exposed to the complexity of conducting research on multi-disciplinary problems in a high performance computing environment. This exposure has led to the hiring of over 20 students following completion of their PhD degrees.

Each of the six Centers is briefly discussed on the following pages.
The Center for Shock Wave-processing of Advanced Reactive Materials (C-SWARM) is dedicated to developing predictive computational tools for multiscale modeling of heterogeneous materials under extreme conditions that will execute effectively on future Exascale platforms. Through adaptive simulations, C-SWARM’s goals are to predict conditions for the synthesis of novel materials and provide prognoses of non-equilibrium structures that will form under shock wave-processing. Using this approach, researchers at C-SWARM plan to identify conditions under which they can synthesize cubic boron nitride (c-BN). They will then duplicate the conditions in the laboratory in order to demonstrate the effectiveness of their predicted conditions. c-BN has many applications since its hardness is similar to that of diamond, but its thermal and chemical stability is superior.

C-SWARM scientists employ adaptive multiscale and multi-time computational schemes to model reactive powder materials that are used during shock wave-processing. Moreover, the C-SWARM team is developing novel numerical techniques such as the adaptive wavelet method, and the parallel generalized finite element solver (PGFem3D). Students and research staff benefit greatly from working on a difficult problem that requires an interdisciplinary approach involving teams of researchers in conjunction with high-performance computing.

The modeling of high-energy reactive materials requires complex constitutive equations. The computational physics team has proposed a new continuum theory for powders that couples pressure sensitivity and rate dependence of cold compacted materials, and has performed large parallel thermo-mechanical simulations on NNSA computing platforms (see Figure 1). After detailed calibration, verification, and validation, such complex simulations are used for design and analysis of computer experiments. In particular, the computational physics team performs predictive simulations and optimizes the design conditions to increase the pressure, density, and temperature conditions during gas gun experiments.

Based on the computational design, the experiments are performed to confirm the validity of the predictions. Once fully completed, C-SWARM’s collaborative and interdisciplinary framework can be the basis for Virtual Materials Testing standards and aid in the development of new material formulations. An advanced asynchronous multi-tasking runtime system and advanced software libraries support the C-SWARM software applications. The modular implementation of the multi-tasking runtime system (HPX-Lite) enables both performance and productivity. Moreover, to separate scientific applications from details of the runtime system, C-SWARM researchers are developing a Domain Specific Embedded Language and Active System Libraries that are based on the concepts of generic and meta-programming techniques to effectively eliminate the penalty that frequently arises from abstractions. The researchers from the computer science team are focusing on the development of Matrix and Tensor Template Libraries (MTL/TTL), Photon networking, multiscale graph scheduling, adaptive wavelet multi-processing, and Exascale architectures.

The integrated V&V/UQ program provides a platform for verification, validation, and propagation of uncertainties. The emphasis of C-SWARM is on quantifying the predictive ability of the multiscale simulations in an efficient manner. The key component is a series of carefully co-designed experiments and data-driven simulations (with quantified uncertainties) to enable meaningful and rigorous comparisons of simulation predictions with experimental results.

Figure 1. Simulations using a new continuum theory for powders with comparison to experimental data.