PSAAP (Predictive Science Academic Alliance Program)
21 May 2010

The primary goal of PSAAP (http://sandia.gov/NNSA/ASC/univ/univ.html) is to establish Predictive Science as a major academic and applied research discipline in US universities. Predictive Science is defined as the application of verified and validated large-scale multidisciplinary computational simulations to predict properties and dynamics of complex systems, with quantified uncertainty. Five universities have PSAAP Centers, through which they receive funds from NNSA (currently ~$3.5M/year/campus), and computing allocations on NNSA computers. They are:

Caltech (http://www.psaap.caltech.edu/) Caltech's Center focuses on high-energy-density dynamic response of materials as it arises in hypervelocity normal and oblique impact of metallic projectiles and targets, at velocities up to 10 km/s. Processes can include melting and vaporization, dissociation, ionization, and plasma formation; luminescence and radiative transport, solid-solid phase transitions, high-strain-rate deformation and thermomechanical coupling; fracture, fragmentation, spall and ejecta; deformation instabilities; hydrodynamic instabilities, mixed-phase flows, and mixing. Model-based quantification of uncertainties and margins will drive and closely coordinate the experimental, computational, modeling, software development, verification and validation efforts. PI: Michael Ortiz (Dotty and Dick Hayman Professor of Aeronautics and Mechanical Engineering)

Michigan (http://aoss-research.engin.umich.edu/crash/) The University of Michigan's Center for Radiative Shock Hydrodynamics (CRASH) focuses on radiation hydrodynamics (RH) in the context of a radiative shock wave. CRASH is developing a software framework for RH to serve as a testbed for development, verification and validation of RH modeling elements; developing a system for hierarchically validating the software framework; and extending an existing experimental effort, centered on radiative shocks, to obtain data and quantify uncertainties in the experiments. PI: Paul Drake (Henry S. Carhart Collegiate Professor of Space Sciences, Dept. of Atmospheric, Oceanic and Space Sciences)

Purdue (http://www.purdue.edu/discoverypark/prism/) Purdue's Center for Prediction of Reliability, Integrity and Survivability of Microsystems (PRISM) focuses on micro-electro-mechanical systems (MEMS) technologies for civilian and military applications. The five Center thrusts include contact physics; electro-thermo-mechanical membrane response; multiscale modeling of aerodynamic damping; uncertainty quantification; and the integration of this wide range of models and numerics into a coherent simulation system. PI: Jayathi Murthy (Robert V. Adams Professor of Mechanical Engineering, School of Mechanical Engineering)

Texas (http://pecos.ices.utexas.edu) The University of Texas's Center for Predictive Engineering and COmputational Sciences (PECOS) focuses on reentry of vehicles into the atmosphere. Phenomena include aerothermochemistry, thermal radiation, turbulence and the response of complex materials to extreme conditions. These phenomena arise from the interaction of extremely high temperature gas flows with the vehicle's thermal protection system. The work also includes a systematic, comprehensive treatment of the calibration and validation of the models, as well as the quantification of the uncertainties inherent in such models. PI: Robert Moser (Professor of Mechanical Engineering & Institute for Computational Engineering & Sciences)

Stanford (http://psaap.stanford.edu) The Stanford PSAAP Center focuses on simulation of air-

breathing hypersonic vehicles with a special focus on the prediction of off- design, transient conditions and their associated failure modes. Phenomena include: flow stability for supersonic mixing during combustion; real gas effects, chemically-reacting and dissociated flows, and heat transfer; turbulence, mixing, multi-phase flows, and associated interactions with oblique and intersecting shock waves; moving shocks, unsteady shock/boundary layer interactions and separated flows; transient thermal loads and conjugate heat transfer; flow/ structure interactions; laminar/turbulence transition; and radiative energy transfer and plasma dynamics. In addition, error estimation will be an important part of the complex simulation environment, together with modern methodologies for automatic differentiation and large-scale linear solutions. PI: Parviz Moin (Franklin P. and Caroline M. Johnson Professor of Mechanical Engineering)

Los Alamos contacts for PSAAP Centers – Tri-Lab Sponsor Teams
The Tri-Lab Sponsor Teams (TST) are composed of researchers at the NNSA laboratories. They have the responsibility to act as liaisons with the Centers and facilitate interactions, visits, and collaborations with the NNSA laboratories. The LANL members of the TSTs are:

Caltech Edward M. (Ed) Kober, Apps, phone: 505 663 5623, email: emk@lanl.gov
Mark Anderson, V&V, phone: 505 667 4772, email: mcanderson@lanl.gov
Michigan Donald A. (Don) Haynes, Apps, phone: 505 665 7783, email: dhaynes@lanl.gov
François M. Hemez, V&V, phone: 505 667 4631, email: hemez@lanl.gov
Purdue Tim Germann, Apps, phone: 505 665 9772, email: tcg@lanl.gov
Ryan Maupin, V&V, phone: 505 665 7562, email: maupin@lanl.gov
Stanford John W. Grove, Apps, phone: 505 667 0723, email: jgrove@lanl.gov
David H. Sharp, V&V, phone: 505 667 5266, email: dcso@lanl.gov
Texas Malcolm J. Andrews, Apps, phone: 505 606 1430, email: mandrews@lanl.gov
David M. (Dave) Higdon, V&V, phone: 505 667 2091, email: dhigdon@lanl.gov

Alliance Strategy Team (AST)
The AST helps NNSA headquarters (mainly Thuc Hoang, as program manager) to set policy for and administer PSAAP, including organizing annual external peer reviews. All three NNSA labs have representation on the AST. The members of the AST are:
Thuc Hoang (NNSA, PSAAP program manager)
John Aidun (SNLA)
Nels Hoffman (LANL)
Tina Macaluso (SAIC)
Bob Voigt (SAIC)
Dick Watson (LLNL)

Computer Resources Team (CRT)
The Computer Resource Team (CRT) is established to assist the Centers with usage of the NNSA Laboratories' High Performance Computing (HPC) resources. This includes: scheduling of special runs; handling issues arising with establishing and using accounts; balancing usage across the Centers; conducting a monthly telecon with the Centers to keep them up-to-date with access and scheduling issues and to address any concerns with HPC platforms; collecting and distributing monthly machine usage statistics; providing necessary HPC user documentation and training; visiting the Centers annually to discuss HPC resources and offer technical consultation; etc. The CRT is comprised of a representative from each NNSA Lab who is familiar with his/her Lab computing resources and policies. The following individuals serve on the CRT:
Blaise Barney (LLNL)
Rob Cunningham (LANL)
Barbara Jennings (SNL)