



# Final Reports

From the 2012

## Los Alamos National Laboratory Computational Physics Student Summer Workshop

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Scientific Computing Program

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# Background

## Philosophy of the Workshop

The two primary purposes of LANL's Computational Physics Student Summer Workshop are (1) To educate graduate and exceptional undergraduate students in the challenges and applications of computational physics of interest to LANL, and (2) Entice their interest toward those challenges. Computational physics is emerging as a discipline in its own right, combining expertise in mathematics, physics, and computer science. The mathematical aspects focus on numerical methods for solving equations on the computer as well as developing test problems with analytical solutions. The physics aspects are very broad, ranging from low-temperature material modeling to extremely high temperature plasma physics, radiation transport and neutron transport. The computer science issues are concerned with matching numerical algorithms to emerging architectures and maintaining the quality of extremely large codes built to achieve multi-physics calculations. Although graduate programs associated with computational physics are emerging, it is apparent that the pool of U.S. citizens in this multi-disciplinary field is relatively small and is typically not focused on the aspects that are of primary interest to LANL. Furthermore, more structured foundations for LANL interaction with universities in computational physics is needed; currently interactions rely almost solely on individuals' personalities and personal contacts. Thus a tertiary purpose of the Summer Workshop is to build an educational network of LANL researchers, university professors, and emerging students to advance the field and LANL's involvement in it.

This was the second year for the Summer Workshop. Like the previous year, the workshop's goals were achieved by bringing into LANL a select group of students recruited from across the United States and immersing them for ten weeks in lectures and interesting research projects. The lectures provided an overview of the computational physics topics of interest this year along with some detailed instruction while the projects gave the students a positive experience accomplishing technical goals. Each team consisted of two students working under one or more mentors from LANL on specific research projects associated with predefined topics. This year, the topics were on verification of simulations in plasma and radiation-hydrodynamics codes, hypervelocity material deformation, plasma physics, graphical processor unit ("GPU") programming, multi-material mixing, turbulence modeling, computational material science, and electromagnetic pulse simulations.

The students' growth was furthered by their participation on teams where their teammates were sometimes of different academic rank. It also developed them by requiring them to produce written and oral reports that they presented to peers, mentors, and management.

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## Funding and Participation Profile

### LANL Staff

The Advanced Scientific Computing (ASC) Program at Los Alamos National Laboratory, under charge code JPDJ, sponsors the Summer Workshop by funding the workshop coordinator, paying for the lease at the University of New Mexico – Los Alamos campus, and also funding twelve of the eighteen students. The remaining six students were funded by various projects (some of them under ASC and some not), as shown below. This year, there were nine mentors, up from six the previous year. Also, while last year's mentors were almost solely in XCP, participation this year spread to include mentors from XTD, T, and CCS. This broad participation is welcome and it is hoped that it continues in future years. The details of the funding and divisional participation are summarized below.

#### Charge Code JPDJ (ASC Sponsoring Code):

Capturing Material Discontinuities and GPU Programming (Robey, XCP-2)  
Development of ICF Mix Code (Vold, XCP-2)  
Rad-Hydro Verification Test Problems (Ramsey, XCP-8)  
Methods Supporting Multi-Material Cell Calculations (Shashkov, XCP-4)  
Grain Boundary Formation Simulation (Reichhardt, T-1)  
Verification Study of Planar Shocks in Dense Plasmas (Masser, CCS-2)

#### Charge Code J466:

Electromagnetic Pulse Simulations (Tierney, XCP-6)

#### Charge Code J444:

Turbulent Mixing (Gore, XTD-6)

#### Charge Code X96H:

Advanced Cell-Centered Hydro Methods (Morgan, XCP-8)

### Students

Forty-one students applied for admission to the workshop, all eligible U.S. citizens with the breakdown shown in the chart below. The eighteen that ultimately were selected and participated were from the following schools: Caltech, San Diego State, Notre Dame, University of Toledo, Florida State, University of Michigan, University of New Hampshire, Stony Brook State University of New York, University of Washington, RPI, MIT, University of Toledo, UCLA, University of Maryland, and Middle Tennessee State. Their rank breakdown is also shown in the chart below.

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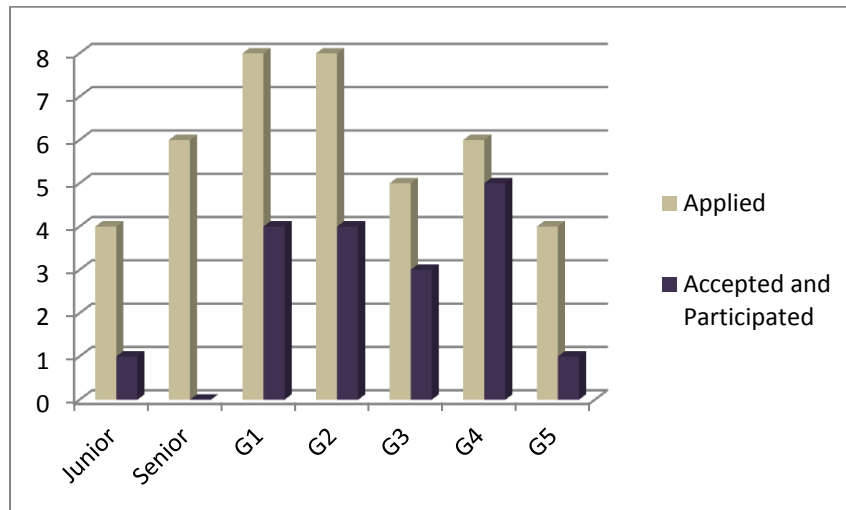


Chart showing the academic rank breakdown of the applicant pool and the ultimate participants. G1 means “1<sup>st</sup> year graduate student.” G2 means “2<sup>nd</sup> year graduate student,” and so on.

## Lecture Schedule

The workshop coordinator and participants greatly appreciated the contributions made by several lecturers, including some from outside LANL. The lectures were scheduled so the students could obtain the most benefit from them. Specifically, they were most frequent in the beginning of the workshop, when the students’ research was just getting started and they needed the most background information. Then, their frequency dropped dramatically and finally to no lectures towards the end so the students could complete their research without interruption. The lectures given and an image of the lecture schedule follow on the next two pages.

Name	Affiliation	Topic	Length in hours
Scott Runnels	LANL	Intro. to C++	2
		Intro. to Grid Data Structures	1
		Intro. to Hydro Terminology	1
		Diffusion on Two Grids	1
		Intro. to Artificial Viscosity	1
Erik Vold	LANL	Computational Transport	2
Bob Robey	LANL	Parallelism: MPI & GPUs	1
Nathaniel Morgan	LANL	Intro. to Lagrange Hydro	1
		Lagrange SGH in r-z	1
		Intro. to ALE	1
		Intro. to CCH Hydro	1
		Test-Driven Hydrocode Development	1
Misha Shashkov	LANL	Interface Reconstruction	1
		Remapping	1
Jim Kamm	Sandia	Verification	3
Greg Weirs	Sandia	Verification	2
Scott Ramsey	LANL	Verification	2
Rob Gore	LANL	Turbulence Modeling	8
Tom Masser	LANL	Shocks in Simple Plasmas	1
Cynthia Reichhardt	LANL	Material Modeling	1
Bill Rider	Sandia	History of Hydrocodes	4
Chris Simmons	UT-Austin	Software Quality	1
Nick Malaya	UT-Austin	Verification w/ Manufactured Sol'ns	1
Bhuvana Srinivasan	LANL	Multi-Fluid Plasmas	1
Ben Bergen	LANL	Computational Sciences	1
Heidi Tierney	LANL	EMP	1

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# Student Reports

The reports that follow are assembled from separate PDF files. The table of contents at the beginning of this document uses page numbers in this fully assembled PDF file. In other words, it is recommended that the reader use the page indicator in the PDF viewer as the page number when navigating this combined document.

**Capturing Material Discontinuities  
and GPU Programming**

**(Bob Robey, mentor)**

**Methods Supporting Multi-Material  
Cell Calculations**

**(Misha Shashkov, mentor)**

**Advanced Cell-Centered Hydro  
Methods**

**(Nathaniel Morgan, mentor)**

**Rad-Hydro Verification**  
**(Scott Ramsey, mentor)**

**EMP Simulations**  
**(Heidi Tierney, mentor)**

**Grain Boundary Formation  
Simulation**  
**(Cynthia Reichhardt, mentor)**

**Turbulent Mixing**  
**(Rob Gore, mentor)**



**Development of an ICF Mix Code**

**(Erik Vold, mentor)**

**Verification of Shocks in Plasmas**

**(Tom Masser, mentor)**

