Requirements

To apply to the summer school, you must:

- Be enrolled in a PhD program at an accredited university in a relevant field of study
- Be available to live and work in Los Alamos, New Mexico for 10 weeks, sometime from mid-May through early September of 2015 (exact dates TBD)

Desired Disciplines

Domain Science
- Quantum Chemistry
- Material Science
- Molecular Biology

Applied Mathematics
- Discrete Mathematics
- Graph Theory
- Linear Solvers

Computer Science
- Programming Models
- Task and Data Parallelism

Students will be chosen based both on their qualifications and on the alignment of their skills and interests with the focus area of the summer school. Broadly speaking, we will attempt to create a balanced team with an even distribution of students from the disciplines of physics, applied mathematics and computer science.

Sponsorship

The Co-Design Summer School is an institutionally sponsored project funded by the Los Alamos Information Science & Technology Institutue (IS&T). The IS&T Institute provides a connection to program management for capability needs and provides IS&T integration and support for mission-critical centers and activities, such as MaRIE (matter-radiation interactions in extremes) and the new Bio-Security and Energy Security centers.

http://codesign.lanl.gov/summer-school

To apply for the 2015 summer school, please visit our website:

http://codesign.lanl.gov/summer-school

Erin Carrier
2014 University of Illinois

Students will work with some of the leading experts in their respective fields of study to solve cutting edge problems in predictive science, using the most advanced resources available at the institution that invented supercomputing.

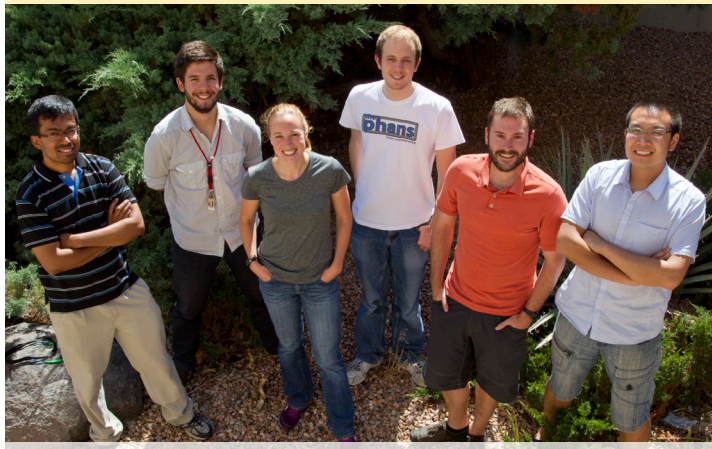
In addition to great science, Los Alamos also offers lots of sunny weather for outdoor activities like hiking, biking, rock climbing and running. After you exercise your brain, you will have plenty of time to enjoy the beauty of Northern New Mexico!

Robert Bird
2014 University of Warwick

Los Alamos
NATIONAL LABORATORY
EST. 1943

Los Alamos 2015 IS&T Co-Design Summer School

"This is an experience that is guaranteed to change your life!"



2012 School: Karthik Murthy (Rice), Emmanuel Cieren (LaBRI, France), Colleen McCarthy (NC State), Nicolas Feltman (CMU), Chris Leibs (CU Boulder), Yijie Wang (University of South Florida)

http://codesign.lanl.gov/summer-school

What is the Co-Design Summer School?

The Los Alamos IS&T Co-Design Summer School was created to train future scientists to work on the kinds of interdisciplinary teams that are demanded by today's challenges. Launched in 2011, the summer school recruits top candidates in a range of fields spanning domain science, applied mathematics, computational and computer science, and computer architecture. Participants work together to solve a focused problem that is designed to build the skills needed to tackle the grand challenges of the future. Foremost among the skills upon which we focus, is the ability of students to work across disciplines with other team members, while employing their own unique expertise. This is the heart of Co-Design.

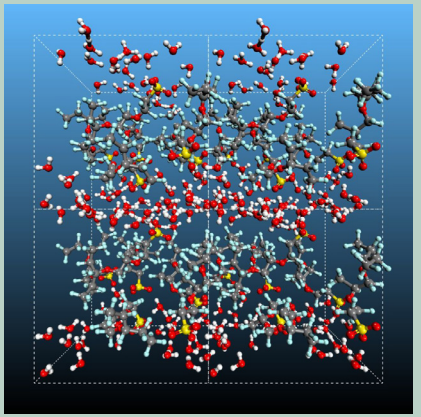
What exactly is Co-Design?

Co-Design is the social and technical equivalent of a multiple-constraint optimization problem. The rapid evolution of computing architectures, and the expanding space between specializations in domain science and computer architecture means that it is impossible for a single individual to cover all of the skills needed to solve current-day computational science challenges. Co-Design bridges this space through interactions between members of an interdisciplinary team. With the right amount of overlap, team members can communicate with each other effectively to solve a problem.

2015 Co-Design Summer School Focus: Quantum Molecular Dynamics (QMD)

In molecular dynamics (MD) simulations, the relative positions of atoms evolve over a series of time steps according to the force acting upon each atom. MD is employed in materials science, chemistry, and biology to study structures, defects, and equilibrium and non-equilibrium phenomena. Quantum-based models capture the making and breaking of covalent bonds, charge transfer between species of differing electronegativities, and long-range electrostatic interactions.

This year's summer school will work on advancing the second order spectral projection method (SP2). This is a new QMD method that reduces the computational costs associated with assembly of the density matrix by introducing a recursive, matrix-matrix expansion (*D* in the figure below) of the Fermi operator. This method is well-suited to modern architectures because it can be parallelized through the partitioning of a graph representation of the matrix expansion. Requiring expertise in physics, applied mathematics and computer science, the domain science and computational aspects of this problem will provide an excellent challenge for our students!



The SP2 method reduces computational complexity and allows greater parallelism...

$$D = \theta\left(\mu I - H\right) = \lim_{n\to\infty} f_n\left(f_{n-1}\left(\ldots f_0\left(H\right)\ldots\right)\right)$$

$$f_n(H) = X \pm \left(X - X^2\right)$$

Graph Equivalence