

LA-UR-16-20105

Approved for public release; distribution is unlimited.

Title: ISTI Overview

Author(s): Eidenbenz, Stephan Johannes

Intended for: Report

Issued: 2016-01-10

Disclaimer:

Los Alamos National Laboratory, an affirmative action/equal opportunity employer, is operated by the Los Alamos National Security, LLC for the National Nuclear Security Administration of the U.S. Department of Energy under contract DE-AC52-06NA25396. By approving this article, the publisher recognizes that the U.S. Government retains nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or to allow others to do so, for U.S. Government purposes. Los Alamos National Laboratory requests that the publisher identify this article as work performed under the auspices of the U.S. Department of Energy. Los Alamos National Laboratory strongly supports academic freedom and a researcher's right to publish; as an institution, however, the Laboratory does not endorse the viewpoint of a publication or guarantee its technical correctness.



ISTI Overview

Stephan Eidenbenz

November 2015

Information Science & Technology Institute (ISTI): Mission



The Information Science & Technology Institute (ISTI) enables the execution of LANL's institutional IS&T pillar through revitalization of technical IS&T areas, recruiting, and retention of IS&T staff.

ISTI manages, organizes, and/or provides funding for (1) summer schools, (2) university collaborations, (3) workshops, (4) the IS&T seminar series, (5) program development, and (6) the visualization collaboratory at LARP all with a focus on IS&T.

- Recruit, Retain, Revitalize mission-relevant IS&T capabilities and staff
- A LANL-wide IS&T resource cognizant of the diverse IS&T needs and capabilities at LANL's line organizations
- Be a vehicle to foster technical collaboration internally and externally
- Work with Directorates and line organizations to support programmatic goals and to develop capability in strategic science and technology areas



Operated by Los Alamos National Security, LLC for the U.S. Department of Energy's NNSA



UNCLASSIFIED | 2

Overview ISTI Activities

Activities

Summer Schools

- 6-20 summer students focused on a unifying theme
- Results in poster presentations and publications
- About 30% of participants continue at LANL in some form

University Partnerships

- Contracts with high-quality universities, supporting students work in mission-relevant IS&T areas

Seminar Series

- External/internal IS&T speakers: about 25 per year
- New internal IS&T@LANL subseries

Workshops

- Internal/External community building in mission-relevant novel or growing IS&T areas
- Results: Roadmap Reports, Team formation

Capability Building

- Targeted IS&T development funds for proposals, demonstrations, and white papers

FY16



- **10. Cluster School** (C. Connor)
- **6. Codesign School** (B. Bergen, C. Junghans)
- **4. Data Science School** (J. Ahrens)
- **5. Computational Physics School** (S. Runnels)
- **1. Parallel Computing School** (H. Nam, G. Rockefeller, B. Robey)
- **CMU**: Failure at Scale
- **UCD**: Visualization
- **UCSC**: File systems
- **Missouri S&T**: Cyber security
- CoDA: Data Science across DOE
- Physics Informed Machine Learning
- Learning for Material Discovery

ISTI: A Vehicle to Implement the Cross-Cutting IS&T Pillar Strategy



Materials for the Future Pillar

Science of Signatures Pillar

Nuclear and Particle Futures Pillar

IS&T Pillar

Co-Design

Applied Computer Science
Computational Mathematics
Computational Physics
Novel Computing
Simulation Science

Data Science @ Scale

Data Fusion
Image and Signal Processing
Library Science
Machine Learning
Statistics and UQ
Viz and Data Analytics

Complex Networks

Process Modeling
CyberSecurity
Synthetic Cognition
QIS

Underpinning High Performance Computing

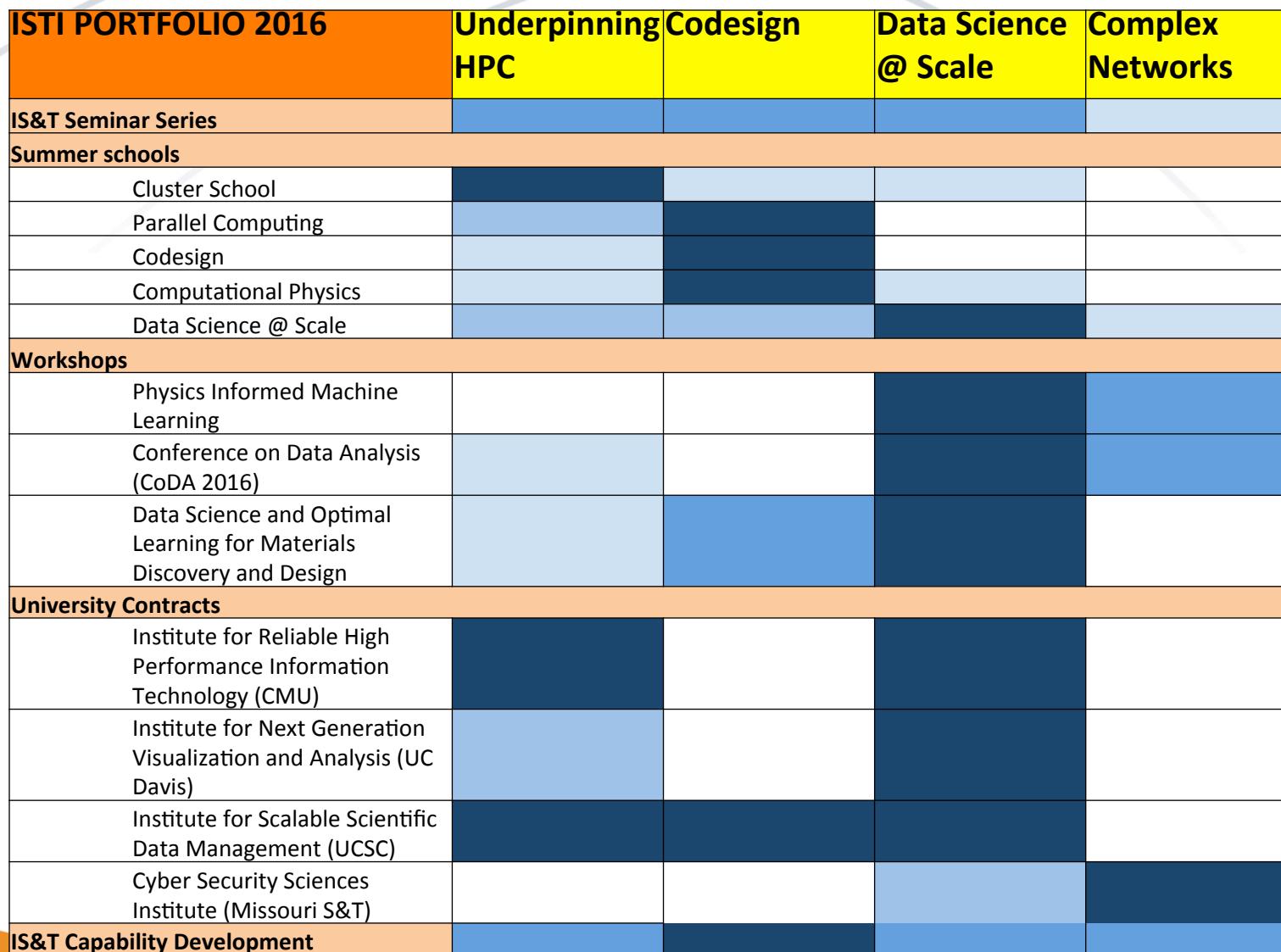


Operated by Los Alamos National Security, LLC for the U.S. Department of Energy's NNSA



UNCLASSIFIED | 4

Alignment of ISTI Activities with IS&T Pillars



Legend

Alignment:

- Core
- Significant
- Medium
- Some
- Minimal



Operated by Los Alamos National Security, LLC for the U.S. Department of Energy's NNSA



UNCLASSIFIED | 5

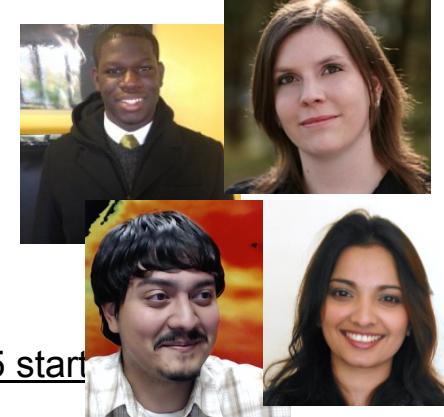
IS&T Data Science at Scale Summer School



Synopsis: Now in its third year, the Information Science and Technology Center's Data Science at Scale School was inaugurated in 2013 to recruit outstanding students to the laboratory to participate in data intensive science projects. Particular focus is placed on using big data technologies to gain insights from science data. Although most students are present at the lab for 12 weeks in the June to August timeframe, the schedule is flexible to meet individual needs.

Demographics:

- 25 students from 13 schools
- 5 returning students and 20 new students
- 2 Undergraduate, 2 Masters and 21 PhD students
- 6 Student Guests
- 6 women and 19 men
- 4 students currently targeted to become Post-Docs ramping up with a Fall '15 start



Fort Valley State University (1 Science Undergraduate Laboratory Internship - SULI)

Johns Hopkins University (3 PhD Students Guests)

Massachusetts Institute of Technology (1 Undergraduate Student)

Purdue University (1 PhD Student)

The Ohio State University (3 PhD Students)

University of Utah (1 PhD Student)

University of California- Davis (4 PhD Students)

University of Delaware (1 PhD Student)

University of Notre Dame (1 PhD Student)

University of Texas- El Paso (1 PhD Student)

University of Vienna (2 Masters Students)

Technical University of Kaiserslautern

(2 PhD Students and 3 PhD Student Guests)

Virginia Tech (1 PhD Student)



Operated by Los Alamos National Security, LLC for the U.S. Department of Energy's NNSA



UNCLASSIFIED | 6

Co-design Summer School

- Los Alamos IS&T Co-Design Summer School
 - For recruiting and advertising LANL's co-design work
 - Small (6), multi-disciplinary team of students
 - 50/50 mix of US/FN
 - Work on co-design problem
 - 2011 & 2012: CoCoMANS
 - 2013: ExMatEx
 - 2014: Adaptive Mesh Refinement (AMR) for Hydrodynamics Simulation
 - 2015: Quantum Molecular Dynamics
 - 2016: Smoothed Particle Hydrodynamics
 - Publish results
 - Open source software
 - Reports, talks, posters
 - Student presentations at conferences
 - SC, SIAM, nVidia GTC, Salishan

Computer System, Cluster, and Networking Summer Institute (CSCNSI)



- **Goal:** Develop critical entry-level skill base through practical skill development in setting up, configuring, administering, testing, monitoring, and scheduling of computer systems
- **Impact:** Recruitment, critical skill development, and staff revitalization through mentoring and lecture opportunities
- **Leveraging:** The SI has been awarded NSF-sponsorship (a 5-year award) beginning in 2011. In addition, the SI typically receives NNSA support under the NNSA SULI and HBCU programs.



Operated by Los Alamos National Security, LLC for the U.S. Department of Energy's NNSA



UNCLASSIFIED | 8

Computer System, Cluster, and Networking Summer Institute (CSCNSI)



- Highly-selective, 9-week program designed for undergraduate CS/CE/EE/... students
 - A collaborative activity: ISTI, NMC, HPC, DCS, ...
 - Students work in small project teams to execute real-world projects on computer clusters that they have assembled and configured.
 - A university instructor provides class instruction
 - Subject matter experts from Los Alamos National Laboratory mentor the team projects which are presented at a technical symposium at the conclusion of the Summer Institute
 - Curriculum includes guest lectures and tours of LANL computing & science facilities
- SI Outreach Goal: Make it Easy
 - Dedicated administrative support for students, mentors, and instructor
 - Mentors focus on technical interaction
 - Full planning and execution of annual Computing & Information Technology Student Mini-Showcase (open to students from all of the LANL computing divisions)



Operated by Los Alamos National Security, LLC for the U.S. Department of Energy's NNSA



UNCLASSIFIED | 9

Computational Physics Workshop/School



- The workshop seeks to bring to LANL a diverse group of exceptional undergraduate and graduate students for informative, enriching lectures and to work with its staff for 10 weeks on interesting, relevant projects that may culminate in articles or conference presentations. Students are organized into groups of 2-3 working under the guidance of one or more mentors
- Topics: e.g.,
 - Exploration of Discrete Ordinates Neutron Transport Methods on Unstructured Meshes
 - Interaction Between Waves and Vortices
 - Mixtures in Warm Dense Matter
- Mentors recruited mainly from XCP, CCS, open call for mentors
- ISTI collaboration with ASC, where ISTI focuses on lecture recording (through Viz Collab) and improving lecture quality



Operated by Los Alamos National Security, LLC for the U.S. Department of Energy's NNSA



UNCLASSIFIED | 10

Parallel Computing Research Internship/ School



The Parallel Computing Summer Research Internship is an intense 10 week program aimed at providing students with a solid foundation in modern high performance computing (HPC) topics integrated with research on real problems encountered in large-scale scientific codes.

Description

During the 10 week program, students will receive training and lectures on modern topics in HPC and software development, including

- parallel programming,
- programming models,
- algorithms,
- hardware architecture and its impact on code design choices,
- high-quality software development in collaborative environments,
- visualization and workflow.

Students will collaborate in teams to identify and investigate different computational problems within the scientific focus area, and implement solutions guided by mentors with scientific and computational expertise.



Operated by Los Alamos National Security, LLC for the U.S. Department of Energy's NNSA



UNCLASSIFIED | 11

Workshops

- **Physics Informed Machine Learning**
 - January 19 – 22, Santa Fe
 - Organizers: Misha Chertkov, Kipton Barros
 - Topics: Energy, Climate, Materials, Images
- **CoDA 2016: Conference on Data Analysis - Exploring Data-Focused Research Across the Department of Energy**
 - March 2 - 4, 2016, Santa Fe
 - Organizer: Kary Myers
 - Topics: Power Grid Data, Subsurface Modeling, Cyber Security, Data Analysis at Exascale, Multisource Data, Really Expensive Data
- **Data Science and Optimal Learning for Materials Discovery and Design**
 - May 16-18, 2016, Santa Fe, New Mexico
 - Organizers: Turab Lookman, Francis J. Alexander, Stephan Eidenbenz
 - Goal: Bring together data scientists, computational physicists, and experimentalists

The NSEC/ISTI Visualization Collaboratory



- Location: LARP Suite 101, capacity 33, looking to increase
- Open visualization Laboratory and video-conferencing center designed to enable collaborative science and technical exchange
- Open 3D visualization capability and facility for researchers to experiment with data intensive methods
- Lecture/talk recording capabilities (*by Jan 2016*)
- Use cases:
 - Scientific discovery through visualization
 - Presentation of movies to external stakeholders/agencies
 - Lectures
 - Training
 - Talks
- Reservations through
Nickole Aguilar Garcia: nagarcia@lanl.gov



Operated by Los Alamos National Security, LLC for the U.S. Department of Energy's NNSA



UNCLASSIFIED | 13

Other ISTI News and Conclusions

- ISTI Science Advisory Council
 - Initial members identified, coordinated with AD and DLs
 - 6-10 active LANL IS&T Scientists
 - Monthly lunch meetings
 - Discuss, identify IS&T R&D trends and impact to ISTI activities
 - Provide feedback on and propose new activities
- NMC funds NM summer students (UNM, NM Tech, NMSU)
 - Brief project description to ISTI and/or NMC
- Thoughts? Comments?