

CV

TOREY ELIZABETH BATTELLE

(a.k.a. Torey Semi)

CONTACT INFORMATION

Torey Battelle
3930 Osceola St. Denver, CO 80212

Cell: 303.396.3731
Email: toreliza@gmail.com

OBJECTIVE: To obtain a leadership position with a university research computing group, a national laboratory, or in academia, at which I can apply my experience in high performance computing, computational research and management, to make and support fundamental, innovative contributions to technological challenges of national importance.

EDUCATION

Ph.D. Applied Physics
Department of Physics, Colorado School of Mines, Golden CO
B.A. Physics
Department of Physics, Middlebury College, Middlebury VT
Graduated cum laude

INTERESTS, GOALS AND SKILLS

Professional Goals: Optimize the role of HPC and RC in scientific research
Develop strengths of diverse RC support team individuals to create innovative, effective whole
Simplify access to RC infrastructure to increase exposure to non-traditional research groups
Promote and encourage use of RC services to non-traditional research groups
Augment RC outreach programs to promote cutting edge developments in RC support
Lead a team that develops, tests and implements novel approaches to RC support

Environment Skills: Excellent leadership and management skills
Visionary approach to research with focus on producing results
Excellent ability to work in isolation
Exceptional skills as collaborator with members of research and computing teams
Superior writing skills and ability to deliver publishable material

Computing Skills: *Hardware:* 656-node, 154 Tflop, 17.4 Tbyte Hybrid IBM BlueGeneQ- iDataPlex HPC;
5508-core and growing shared-resource HPC with cpu, GPU, Phi node configurations;
Power8 nodes, x86 servers, routers, gateways; *Filesystems:* Lustre, GPFS
Networking/Middleware: Ethernet, Infiniband, MPI, OpenMP, OpenACC, NVLink, CUDA,
MPI (MPICH, MVAPICH/MVAPICH2, OpenMPI, IBM MPI);
Software:
OS: UNIX, Linux, MacOSX;
Computational, Scientific Codes: **BUILDING and RUNNING:**
Abinit, AtomPAW, VASP, Siesta, RSPt, MaterialsStudio DMol3,
QuantumEspresso, QChem, GROMACS, RGWBS
Programming: Fortran90+, MPI, C, C++, L^AT_EX, Mathematica, Matlab
Libraries: Blas, Lapack, Scalapack, MKL, ESSL, FFTW, many more;
Debugging: Alinea DDT, *Profiling:* gprof, Alinea MAP;
Other: BASH, Python and other scripting languages, XCrySDen, Vesta, Elk, APE,
Code optimization

TOREY BATTELLE

MANAGEMENT, RESEARCH, HPC EXPERIENCE: COLORADO SCHOOL OF MINES

DATES

Assistant Director of Research Computing

High Performance Computing Group

Mar 2019- Present

Oversee all HPC operations

Increase productivity of Mines' Research Groups

Represent Research Computing for Mines' research partnership expansions

Engage in external Research Computing advocacy and advancement groups

Computational and Research Support Scientist

High Performance Computing Group

June 2015- Current

Increase productivity of Mines' Research Groups

Use extensive troubleshooting capabilities to solve HPC-related research challenges

Acquire new HPC platform with all involved

HPC Support Specialist

High Performance Computing Group

September 2013- June 2015

Provide support for users of BlueM (combined BlueGeneQ and iDataPlex)

Manage and respond to help tickets

Work with schedulers: PBS, Slurm, LoadLeveler

Continue to build, install, test programs

Provide user guidance for optimizing code performance

Liaise among group leader, system administrator, applications personnel

Graduate Research Assistant

High Performance Computing Group

Summer 2013

Prepared BlueM for professor and student use

Ported and troubleshot codes from old HPC (Ra) to new HPC (BlueM)

Performed benchmarking and testing on codes

Thesis Work: Department of Physics

Jan 2012 - May 2013

Computational Analysis of the Structural Preferences of the CaAl_2Si_2 Class Ternary Semiconductor

Worked toward making general statement on structural preferences of ternary compounds

Created pseudopotentials, performed calculations with Abinit, ELK, APE electronic structure codes

Developed new structural description for CaAl_2Si_2 to enhance properties for thermoelectric apps

Additional Research: Department of Physics

Computational Analysis of Defect Transport in Uranium Dioxide

Fall 2008 - Fall 2011

Modeled (DFT) **motion of fission products** (Kr atoms) in bulk UO_2

Modeled **vacancy cluster (bubble) formation** in bulk UO_2

Simulated **defect diffusion** and its role in fuel expansion

Performed calculations with VASP, Materials Studio, RSPt

PT Symmetric Hamiltonians and Quantum Information Research

Fall 2007 - Summer 2008

Modeling of extensions to Weyl equation in context of quantum computing

Study of quantum lattice gas algorithms and type-II quantum computers

Neutron Detection Research

Summer 2007

Study of exotic nuclei, programming in C language, calculations performed using Géant

TOREY BATTELLE

RESEARCH AND HPC EXPERIENCE

DATES

Sandia National Laboratories and Los Alamos National Laboratory

Development, implementation and use of relativistic module

for existing electronic structure code (RSPT)

Spring 2010 - Fall 2011

Collaboration with national laboratory scientists

Coding and compiling: C, Fortran90; analysis, interpretation of results, updating of code

Comparison of output: non-relativistic, SRA, Dirac equation

Expansion of knowledge and experience with actinides: emphasis on Pu, U

Idaho National Laboratory

Faculty-Student Research Team:

Characterization and modeling of irradiated fuels from ATR

Summer 2009

Collaboration with experimentalists to improve upon methods of analysis

Development of ability to communicate effectively in diverse group of researchers

Competent usage of HPC Icestorm at INL, and requisite electronic structure codes

Expansion of knowledge of and experience with irradiated materials and the ATR

Troubleshooting, analysis and dissemination of results

Solar Energy Research Institute:

Lab Technician: Growth of Si-Ge Superlattices for Solar Cell Application

1985 - 1987

Design and construction of thin-film solar cell deposition system

Deposition and analysis of Si-Ge thin-film solar cells

Improvement of deposition process

SELECTED PUBLICATIONS

Daniel A. Rehn, John.M. Wills, **Torey E. Battelle**, Ann E. Mattson, "The Dirac Equation and its Implications for Density Functional Theory-based Calculations of Materials Containing Heavy Elements", - *Phys. Rev. B.101.085114.2020*

J.Ma, **Torey Battelle**, et. al., "Ask.Cyberinfrastructure.org: Creating a Platform for Self-Service Learning and Collaboration in the Rapidly Changing Environment of Research Computing", *J. Comp. Sci. Ed.2.37.2021*

T. Semi, M.T. Lusk, T.J. Bartel, "The Influence of Lattice Strain on Single Vacancy and Krypton Atom Diffusion in Uranium Dioxide", *MRS Proceedings April 2011*

Mark W. Coffey, Ron Deiotte, **T. Semi**, "Comment on 'Universal quantum circuit for two-qubit transformations with three controlled-NOT gates' and 'Recognizing small-circuit structure in two-qubit operators'", *Phys. Rev A.77.066301.2008*

T. Semi, D.M. Wood, "The Mechanism Behind the CaAl₂Si₂ Ternary Structural Preference and the Origin of Its Semimetal Behavior", - *to be submitted to Phys. Rev. B*

CONFERENCE PRESENTATIONS

Oral Presentations:

T. Semi "Parallel Implementation of Quantum Espresso as Instance of Optimization of Electronic Structure Code on IBM BlueGeneQ", *SC14 - November 2014, New Orleans, LA.*

K. Shaheen, **T. Semi** T.J. Bartel, L. Zhang, R. Dingreville "Integrating Mesoscale Models of Microstructural Evolution of Uranium Dioxide Fuel within Continuum-scale Models of Thermo-mechanical Behaviour of Nuclear Fuel Elements", *NuMat 2010, The Nuclear Materials Conference, October 2010, Karlsruhe, Germany.*

TOREY BATTELLE

J.M. Wills, **T. Semi** "Implementation of Dirac Bases in RSPt (a FP-LMTO Electronic Structure Code)", *RSPt Conference - October 2010, Uppsala, Sweden.*

T. Semi, M.T. Lusk, T.J Bartel "The Effect of Strain on Vacancy and Gas Dynamics in UO₂", *Multiscale Modeling and Simulation of Nuclear Materials Conference - October 2009, Albuquerque, NM.*

T. Semi, M.T. Lusk, T.J Bartel "The Influence of of Lattice Strain on Single Vacancy and Krypton Atom Diffusion in UO₂", *2011 Materials Research Society Spring Meeting - April 2011, San Francisco, CA.*

Poster Presentations:

T. Semi, J.M. Wills, A.E. Mattsson "The Effects of Relativity on First-Principles Calculations", *17th Int'l Conference of APS Topical Group on Shock Compression of Condensed Matter - June 2011, Chicago, IL.*

T. Semi, D.M. Wood "Thermoelectrics, CaAl₂Si₂ and Zintl Compounds", *Supercomputing 2012 Conference - October 2012, Salt Lake City, UT*

COMMUNITY LEADERSHIP AND INVOLVEMENT

ACCESS/MATCH program contributor (Affinity Groups) 2022

XSEDE Campus Champion Leadership Team (2019-current)

XSEDE Campus Champion since 2017

Program co-manager of Ask.CI website (Q&A site for research computing): 2018-current

RMACC Executive Board member and Symposium Committee member, 2019-current

Technical Program Editor SC20, SC21

Co-presenter of Campus Champions workshop: SC19, SC20, SC21

Host of Emotional Intelligence workshop (SIYLI) at Mines, 2019

Co-director of Mines booth production and coordination: SC15, SC16, SC17, SC18, SC19

Active participant in SC (SC12- SC21) and PEARC conferences

EDUCAUSE: ECAR Research Computing Committee Member, 2016-2017

PROFESSIONAL HONORS, AWARDS, AND MEMBERSHIPS

Member of Women in HPC: RMACC Chapter, current

Recipient of completion award for Academic Management Institute, 2018

Winner of Internet2 Global Summit Gender Diversity Scholarship, 2016

Middlebury College, Middlebury, VT: B.A. with Honors in Physics, cum laude, 1985

American Physical Society

American Association for the Advancement of Science

Association for Computing Machinery

TEACHING EXPERIENCE

Teaching Assistant, Department of Physics, Colorado School of Mines:

DATES

2006 - 2011

Grading and Availability to Students

Field Session 2012 Computing Section Classroom Instruction

Linux, Mathematica, L^AT_EX, Inkscape

Physics 200 Undergraduate Electricity and Magnetism

Physics 324 Undergraduate Astronomy and Astrophysics

Physics 507 Graduate Electricity and Magnetism

Physics 511 Mathematical Physics

Physics 520 Graduate Quantum Mechanics I

Physics 521 Graduate Quantum Mechanics II

Physics 530 Graduate Statistical Mechanics