The Molecular Sciences Software Institute

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What is the MolSSI?

- Designed to **serve** and **enhance** the software development efforts of the broad field of computational molecular science.
- Launched August 1st, 2016, funded by the National Science Foundation.
- Collaborative effort by Virginia Tech (TDC), Rice U. (C. Clementi), Stony Brook U. (R. Harrison), U.C. Berkeley (T. Head-Gordon), Stanford U. (V. Pande), Rutgers U. (S. Jha), U. Southern California (A. Krylov), and Iowa State U (T. Windus).
- Part of the NSF's commitment to the White House's National Strategic Computing Initiative (NSCI).
- A total of 26 Software Workshops held 2016-2019 in both the U.S. and Europe.
- Dozens of educational workshops/summer schools held so far, another dozen planned for 2020.
- Currently supporting 27 Software Fellows – graduate students and postdocs across the U.S. – with 60 supported over the life of the program.

MolSSI Community Code Partners So Far...

- ACESIII
- ADF
- Amber
- APBS
- BOSS
- CFOUR
- CHARMM
- Columbus
- Dalton
- Tiger-CI
- Dirac
- DL_POLY
- ELSI
- FHI-aims
- GAMESS
- Gaussian
- Gromacs
- LAMMPS
- Molcas
- Turbomole
- Molpro
- MPQC
- MRChem
- NAMD
- NWChem
- NWChemEx
- ONETEP
- OpenMM
- Orca
- VASP
- PARSEC
- PCMSolver
- PLUMED
- PQS
- PSI4
- Q-Chem
- QBox
- QMworks
- Quantum ESPRESSO
- Schrödinger

MolSSI Software Infrastructure Projects

- MolSSI Integral Reference Project (MIRP) – provides both reference data and reference implementations of common integrals found in computational chemistry;

- MolSSI QCArchive – open, community-driven, multi-use quantum chemistry databases of benchmarks, force-field-related datasets, and other information for data mining and other machine learning initiatives

- MolSSI QM Schema – a JSON-based standard for common data to enable more complex workflows among quantum chemistry codes;
- MolSSI/EMSL Basis-Set Exchange – an overhaul and expansion of the well-known basis-set exchange originally developed by Pacific Northwest National Labs with more than 40,000 unique visitors per month;
- MolSSI Driver Interface – provides a standardized API for fast, on-the-fly communication between computational chemistry codes;

- MolSSI SEAMM (Simulation Environment for Atomistic and Molecular Modeling) – a user-friendly computational environment for creating and running simulations of molecular, crystalline, amorphous, and fluid systems that are described at the level of atoms;

MolSSI Software Scientists

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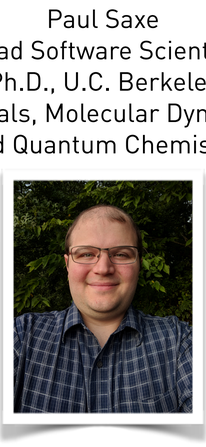

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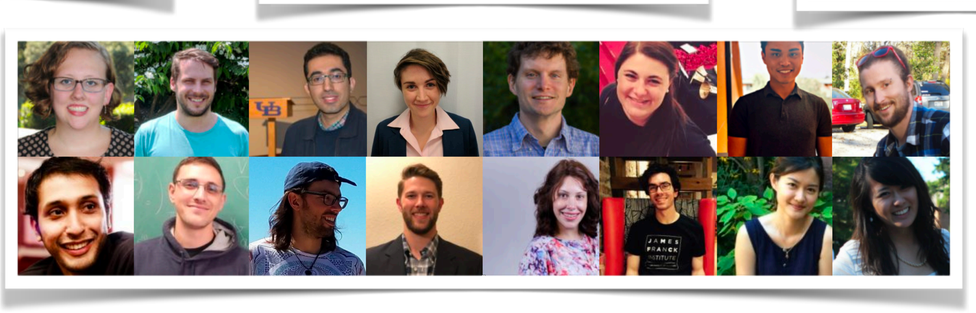
MolSSI Software Fellows

- We currently support 27 Fellows simultaneously for a total of 60 funded over the lifetime of the program.
- MolSSI Software Fellows report 32 publications, 54 presentations, and 46 source code repositories arising from their projects so far.



Watch molssi.org for the latest information!

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