Tsogbayar Tsednee (PhD) California State University, Northridge

My previous research work: theoretical investigations on scattering for few-electron atomic and molecular systems in the field of atomic, molecular and optical physics. Main numerical/mathematical method is a *pseudospectral* method by which a differential equations describing a physical natures of a nature are solved numerically.

- did not use any supercomputing, parallel codes etc.,
- use mostly own written codes (*Fortran (77,90)*; matlab, maple, etc.,)
- no experiences on data analysis;

Current research work: in general, lab's research work is mostly focused on simulations of (drug) biomolecules, such as, DNA, etc.,

- research uses an integral equation (IE) theory in study of classical liquids.
- previously own developed a codes based on 1D and 3D reference interaction site model (3D-RISM) (Fortran (90,95), C++; Python, etc.,)
- has in-house small cluster (metropolis.csun.edu)

My role since June 2017: theoretical study on IE theory; solve the equation by developing (new) different mathematical approach and apply it for atomic and molecular fluids using own written codes (*Fortran* & matlab).

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What I hope to learn at the Summer Institute:

- how to use super computing clusters, such as, Comet etc.,
- understand how it works
- understand what a high-performance computation, CPU and GPU are.
- understand what a code parallelization, MPI and OpenMP, etc., are.
- get acquainted with data science

In future:

- I will employ such a kind of computational cluster, such as, Comet in my research of simulation of large biomolecules.
- I will try to use a parallelization of codes if applicable