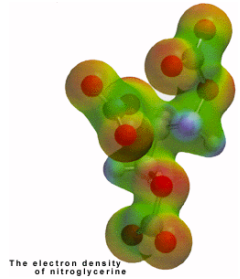
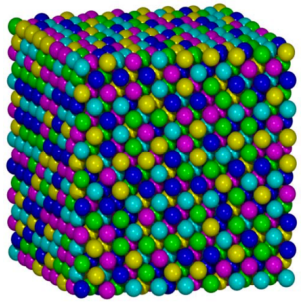
Yanqing Su, Postdoctoral Scholar
Department of Mechanical Engineering
University of California, Santa Barbara

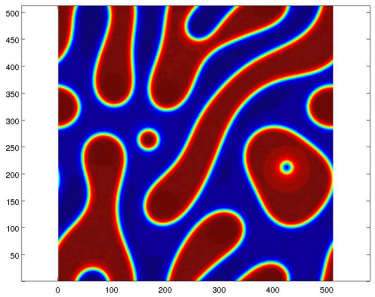
My research centers around dynamics of defects in metallic materials at the nano/micro scales



- Density functional theory (subatomic scale)
  - Theory: A series of approximated Schrödinger equations
  - An MPI-equipped academic code:Vienna Ab initio Simulation Package (VASP)
- Atomistic simulations (atomic/submicro scales)
  - Theory: Newton's second law with interatomic interactions
  - An MPI-equipped open source code: Large-scale Atomic/ Molecular Massively Parallel Simulator (LAMMPS)



- Phase-field method (submicro/micro scales)
  - Theory: Diffusion equation with energy functional of "phases"
  - An in-house phase-field dislocation modeling code, written in C and parallelized with MPI



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Challenges in my research

- Density functional theory
  - Large memory usage and low parallel efficiency with large # of cores
- Phase-field method
  - Currently, the simulation cell is divided into slices along one direction
  - Full 3D parallelization will be more efficient

Learning goals at the Summer Institute

- Learn the computational tools, especially VisIt, GPU, and OpenMP
- Be a better programmer and improve the efficiency of the in-house phase-field modeling code