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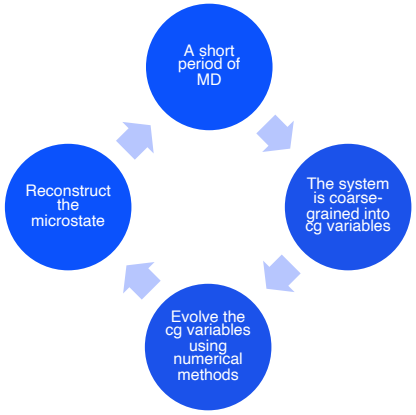
- Conventional Molecular Dynamics(cMD), MetaDynamics and Deductive Multiscale Algorithms(DMA).



- Help experimentalists to understand more details and develop algorithms to accelerate cMD simulations.

- The codes are parallel. Example: spatial decomposition cMD; PETSc is used for DMA development.

- Our research group develops the algorithms based on popular open source MD packages such as Gromacs and OpenMM.

- Some special data structures: MetaDynamics saves the bias potential on a grid; DMA stores cg variables with hierarchical data format.

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The challenges include:

- Compiling source codes on a Cray cluster.
- How to choose the number of nodes and processors.
- How to quickly ‘hack’ open source codes without a detailed developer’s guide provided.

Personally I hope to learn the following content during SDSC 2020 Summer Institute:

- The basic knowledge of GPU computing.
- More details of Open MP.
- How to choose the number of nodes and processors to optimize the performance of supercomputers.