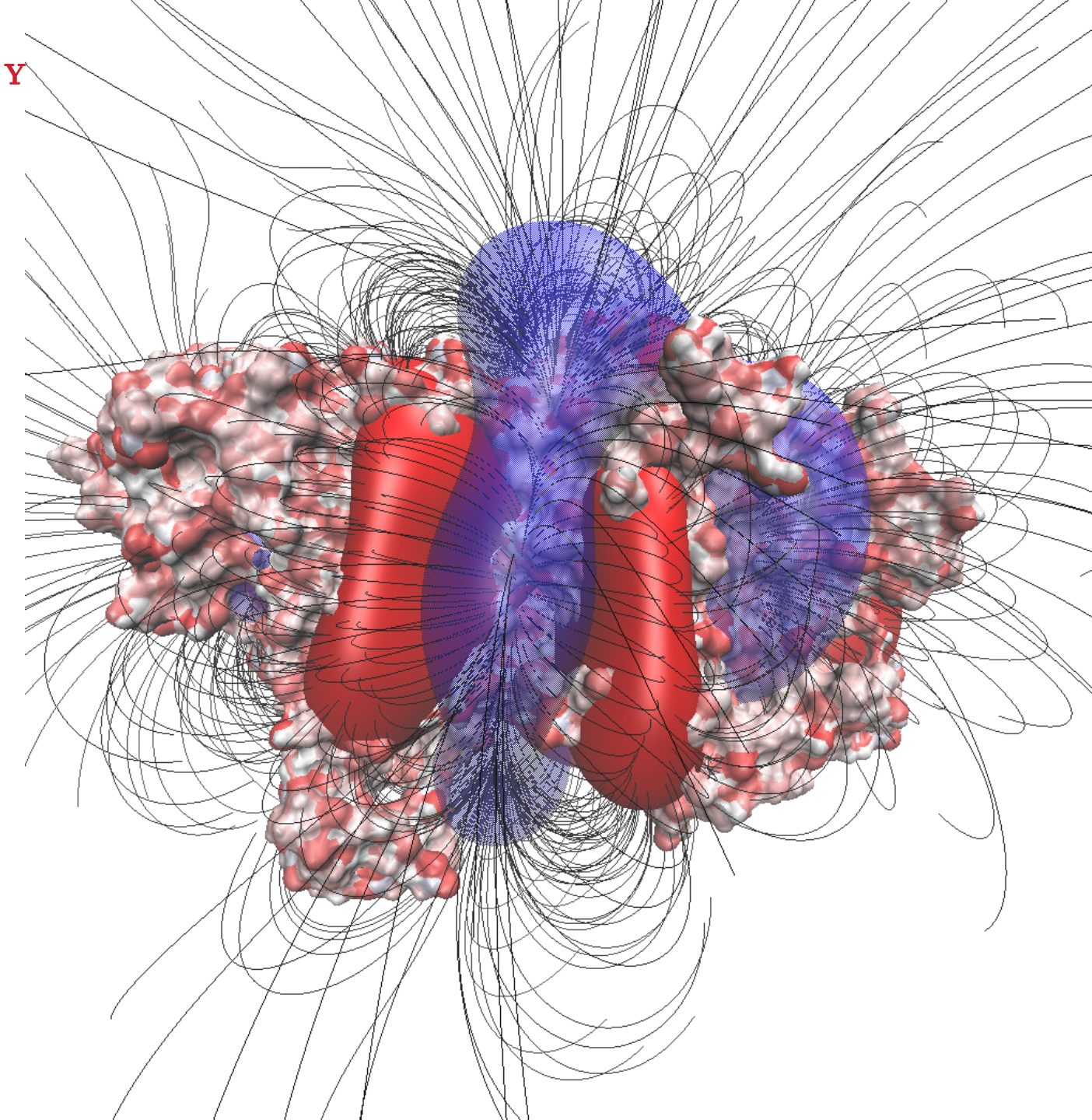
CSUN
CALIFORNIA STATE UNIVERSITY NORTHRIDGE

Acceleration of the 3-D Reference Interaction Site Model Via a Multi-Grid Solver



Garrett Limon
Dr. Tyler Luchko

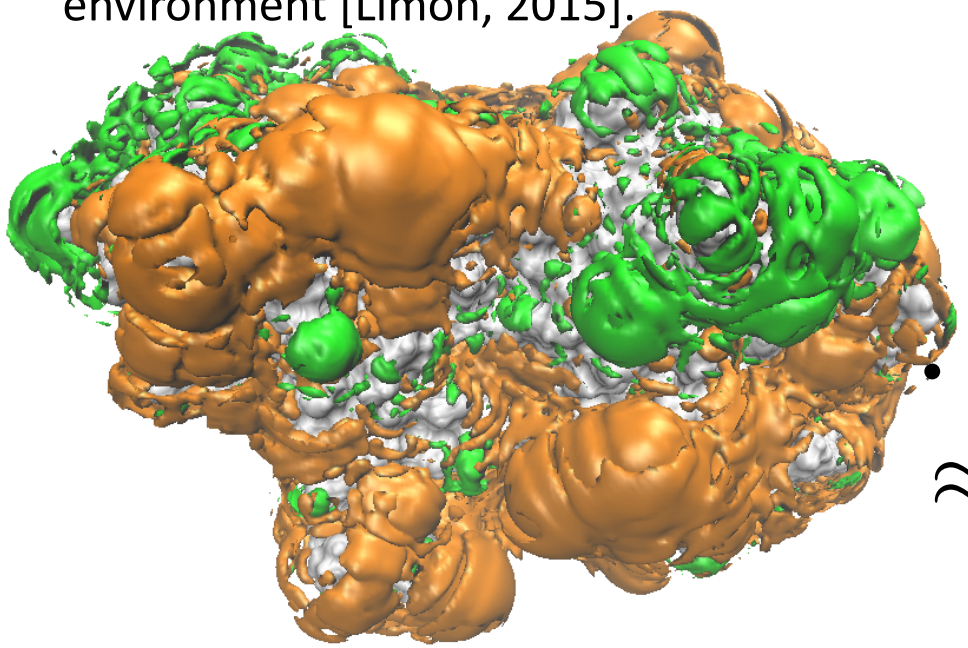
Abstract

In our research, we are developing and implementing a multigrid method for the 3-dimensional reference interaction site model (3D-RISM) theory of solvation which is distributed as part of the AmberTools molecular modeling suite. 3D-RISM works by modeling biomolecular systems via their solvent distributions, rather than treating each individual atom separately. Currently, solving the 3D-RISM integral equations is computationally expensive and a method of speeding up these calculations is sought out to reduce the computational costs while maintaining the desired level of accuracy in the calculations. Researchers have shown that a multigrid approach to the 3D-RISM integral equations drastically helps to speed up calculations on just a single processor. Our algorithm will be implemented into the 3D-RISM source code, optimized for efficiency, and then parallelized to be compatible with the AmberTools MPI infrastructure. The results of this work can reasonably be assumed to provide a significant speed-up in calculations, resulting in the ability to model larger biomolecular systems using 3D-RISM.

3D-RISM

Background

- The Three-Dimensional Reference Interaction Site Model calculates equilibrium solvent (water and ions) density distributions around a solute (molecule) [Kovelenko, 2004; Luchko, 2010].
- Using 3D-RISM, we can obtain many thermodynamic properties of these molecules and their local environment [Limon, 2015].



Integral Equations

$$h_\gamma^{\mathrm{UV}}(\mathbf{r}) = \sum_\alpha \int \mathbf{r}' c_\alpha^{\mathrm{UV}}(\mathbf{r}-\mathbf{r}')\chi_{\alpha\gamma}^{\mathrm{VV}}(r')$$

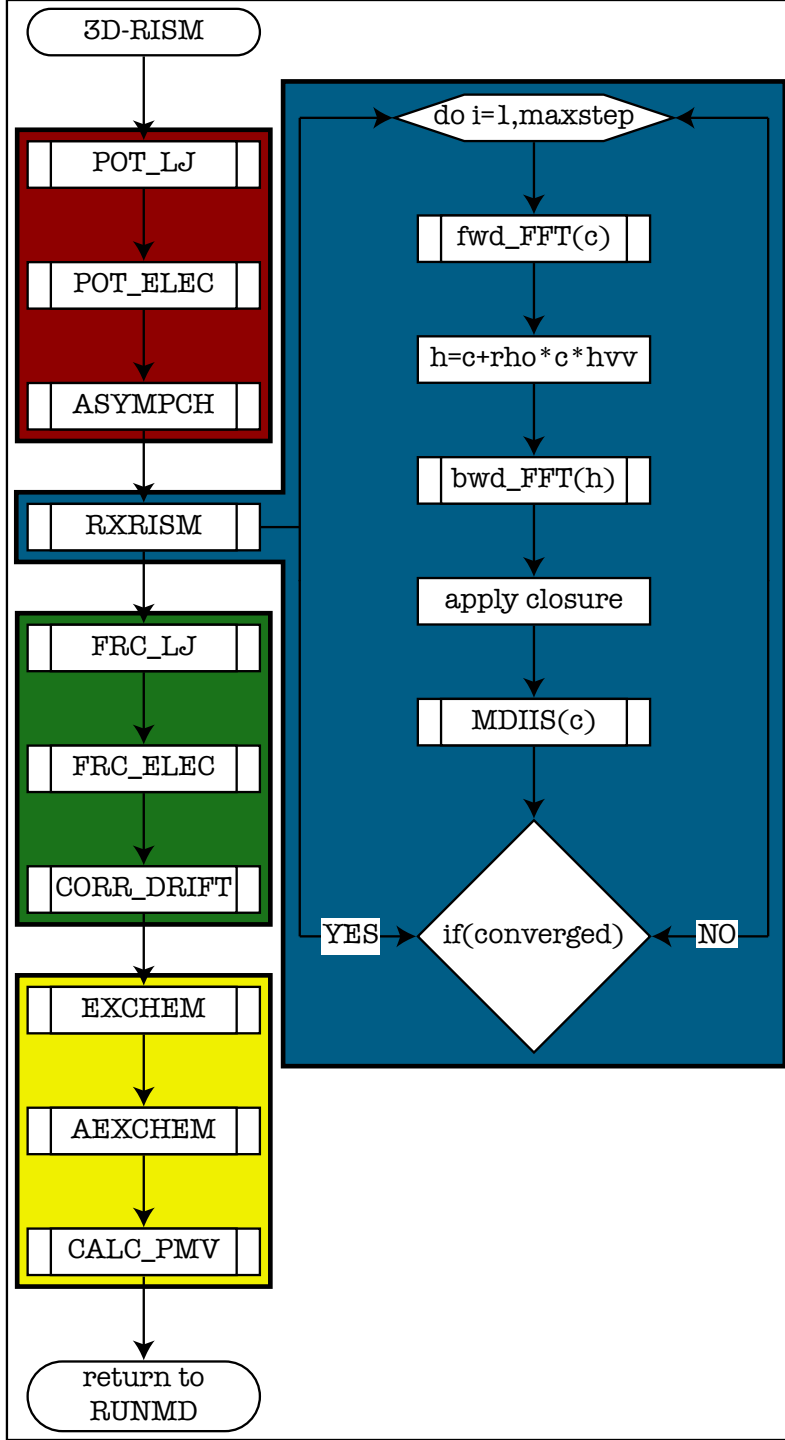
$$h(\mathbf{r}) = \exp\big[-\beta U(\mathbf{r}) + h(\mathbf{r}) - c(\mathbf{r}) + b(\mathbf{r})\big] - 1$$

Numerical Methods

- Currently, the integral equations are solved on DISCRETE grids using the Modified Direct Inverse in the Iterative Subspace (MDIIS) method.
- This scales as

$$\approx D * N_x * N_y * N_z$$

where D is constant.

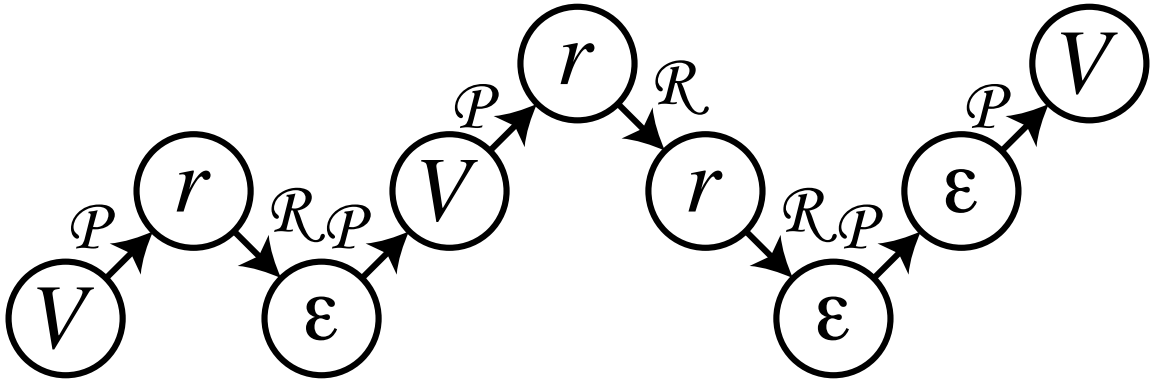


Multi-Grid

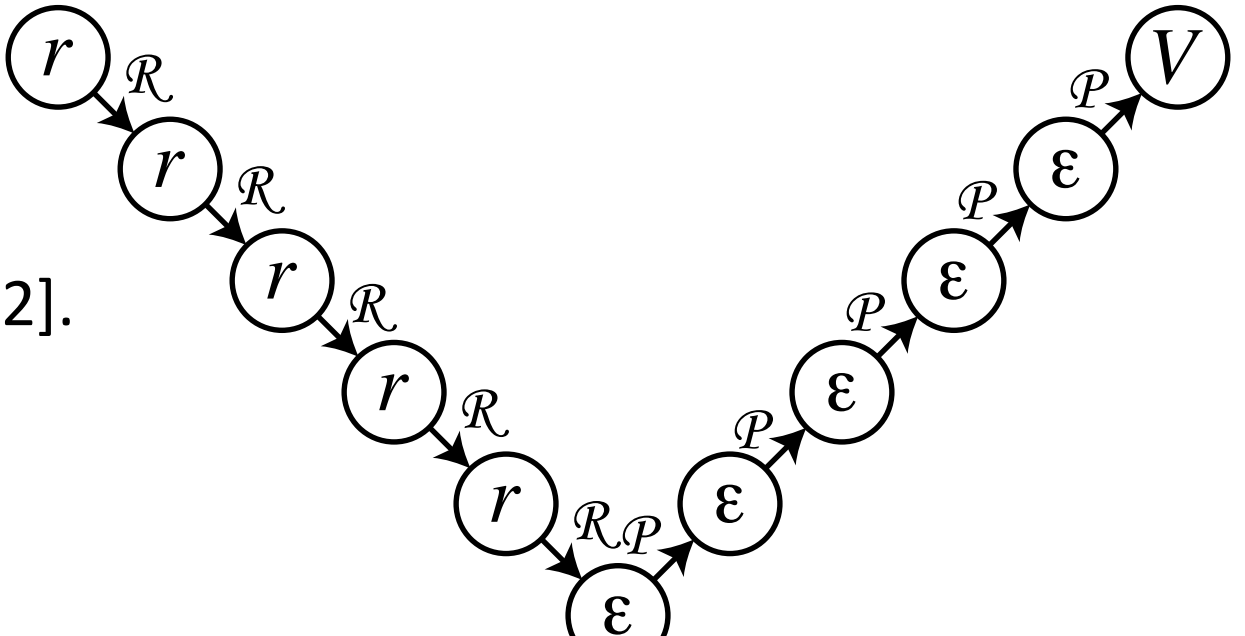
- A Multi-Grid algorithm is used in many numerical solver applications where discrete grids are computationally expensive [Hackbaucsh, 1985].
- Makes use of ’fine’ and ‘coarse’ grids, referred to as a multi-level solver.
- We require mapping operators which can transform solutions from fine grids to coarse grids (restriction) and vice versa (prolongation). *Difficult to parallelize*
- The Multi-Grid method has already been shown to improve convergence speeds on integral equations, including the 3D-RISM equations [Fedorov, 2008; Sergiievskyi, 2012].
- Scales as $\approx C * \left[N_x * N_y * N_z\right]_{\text{fine}}$

  where C is significantly less than D and less overall calculation points are needed.

Full Multigrid



V-Cycle Multigrid



Parallelization

- 3D-RISM is currently parallelized using MPI.
- Certain parts of the 3D-RISM code are more efficiently parallelized than others.
- Efficiently parallelizing the Multi-Grid solver will be a significant contribution to the overall speed-up as well as the most challenging phase of this project.
- The International HPC Summer School will provide necessary skills I will need in order to complete this project.