COURSE-GRAINED FORCE FIELD FOR IONIC LIQUIDS

Research Challenge
Ionic liquids have potential applications in energy, healthcare, and nanotechnology. Computational modeling of their behavior, however, is limited by many factors including their slow dynamics, extended range of interactions, and the high computational cost of simulations that are based on all-atom models. The goal of this project was to develop coarse-grained parameters for significantly “cheaper” coarse-grained simulations that could capture complex structure and thermodynamic properties of ionic liquids.

Methods & Codes
Large-scale molecular dynamics simulations were performed using the GROMACS software package. The all-atom model consisted of approximately 100,000 atoms while the coarse-grained model had only 20,000 beads. Coarse-graining was performed using Versatile Object-oriented Toolkit for Coarse-graining Applications making at least 200 iterations for each model to obtain the force fields.

Results & Impact
The team extended the relative entropy coarse-graining method with an additional constraint to the objective function as well as long-range electrostatic interactions considerations. The team applied the improved method to develop coarse-grained parameters that were later used to simulate several imidazolium-based ionic liquids. The team has shown that parameters (force fields) are transferable between different thermodynamic states and alkyl chain lengths. This work can pave the way for more accurate simulation of ionic liquids.

Why Blue Waters
Blue Waters was instrumental to the success of this effort because its enormous computational resources enabled the team to carry out multiple molecular dynamics simulations quickly and efficiently.