**Description of Code**

The following describes the functions of an in-house grand canonical Monte Carlo (GCMC) code that can simulate both a confined and bulk, aqueous electrolyte system, where, currently, the electrolyte is NaCl. This code closely follows the algorithms described by Moucka et al. with an exception in regards to the solvent.1 Individual translations of molecules are handled using the Metropolis method, while the insertion/deletion of the solvent molecules, water, is handled using the grand canonical ensemble as opposed to the osmotic ensemble.2 Insertions/deletions of ions are handled differently. The solute is added, or removed, as an ion pair to maintain charge neutrality of the system. Furthermore, the process of adding or removing an ion pair consists of the utilization of fractional states, meaning the solute must go through stages before it is fully added or removed from the system.1 A biasing potential is implemented to facilitate the process, since the addition or removal of an ion pair is statistically unlikely and therefore would be nearly impossible to see this occur during a simulation.

In addition, the code also contains additional functions that provide useful information about the systems being studied. Of significance are functions utilized in the calculations of radial distributions and pressure tensors. The pressure tensors are calculated via volume perturbation method where small test volume-scaling moves are performed in the forwards and backwards directions and subsequently averaged. This code is still under development and will include more functions in the future.

**Reference**

1. Moucka, F.; Lisal, M.; Skvor, J.; Jirsak, J.; Nezbeda, I.; Smith, W. Molecular Simulation of Aqueous Electrolyte Solubility. 2. Osmotic Ensemble Monte Carlo Methodology for Free Energy and Solubility Calculations and Application to NaCl. *J. Phys. Chem. B*. **2011**, 115, 7849-7861.
2. Moucka,F.; Bratko, D.; Luzar, A. Electrolyte pore/solution partitioning by expanded grand canonical ensemble Monte Carlo simulation. *J. Phys. Chem.* **2015**, 142, 124705.