

# Developing transferable force fields for specialized hardware

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Anton, a specialized supercomputer for performing molecular dynamics simulations, has enabled atomistic simulations on the millisecond timescale. The ability to sample on this timescale puts increased emphasis on the question of the accuracy of current force fields, not only for biomolecules but also for pharmaceutically relevant small molecules that cover broad sections of chemical space.

To address these issues, we are taking a multi-pronged approach—including improved physical models, better algorithms, and higher accuracy quantum chemical reference data—to the force-field development process. I will describe how these components have come together in the development of polarizable force fields that take advantage of Anton’s capabilities, and how what we have learned is influencing our next generation of models.