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MADRNA: Coarse Graining RNA Force Fields via Machine Learning

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In Protein structure prediction there have been massive improvements recently with the help of machine learning. In RNA structure prediction however the situation is less ideal due too much sparser experimental data. In principle, molecular dynamics (MD) can provide access to structural dynamics, but the relevant time scales are often out of reach due to prohibitive computational expenses.

A promising approach to scale MD to larger molecules and time scales is machine learning (ML)-based coarse graining.
It combines (i) systematic coarse graining, where the degrees of freedom (DOFs) of a molecular system are systematically reduced, and (ii) ML potentials that model the interaction of the new coarse-grained degrees of freedom.

Our approach is based on variational force matching, i.e., we generate trajectories of RNA using classical all-atom simulations, project them down to a coarse-grained level, and train a ML potential to minimize the discrepancy between predicted forces and the forces obtained in simulations.
Due to crucial stabilizing effects such as base pairing and stacking, special care is needed when specifying the coarse graining.
Our ML potential is built upon the graph neural network SchNet, which enables learning the many-body interactions that govern RNA dynamics.

Preliminary results on a set of tetraloops indicate that our method is able to capture the behavior of RNA correctly. At the same time, it reduces the number of simulated atoms by 2 orders of magnitude and allows for a step size twice as large during simulation, compared to the all-atom setting.

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