Reversible Multiple-Scale Methods with Molecular Dynamics Applications

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The reversible averaging method [L. Reich, J. Comput. Phys. 171, 2001] provides an efficient resonance-free integrator for large time-step simulation of conservative systems. The method has been found to be effective for gravitational N-body problems. In this talk, I will outline the method, demonstrate its remarkable stability property, and consider applications to molecular systems, including constant temperature and pressure dynamics and quantum mechanics models based on Feynmann Path Integrals.