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(54) Title: METHOD FOR ANALYTICAL JACOBIAN COMPUTATION IN MOLECULAR MODELING

(57) Abstract: A method for obtaining analytic Jacobians used in implicit integration methods in the computations for the dynamics of a physical system. With this method, the Jacobian with at least twice the number of digits of accuracy as a numerical Jacobian can be computed. This also results in the implicit integration method being more efficient because a smaller number of iterations are required to solve the nonlinear stage equations of the equations of motion, as well as the ability to take larger timesteps. This speedup in computation is very useful in molecular modeling.