A MASSIVELY PARALLEL ALGORITHM FOR THE SOLUTION OF CONSTRAINED EQUATIONS OF MOTION WITH APPLICATIONS TO LARGE-SCALE, LONG-TIME MOLECULAR DYNAMICS SIMULATIONS Amir Fijany, Jet Propulsion Laboratory, Pasadena, CA 91109; William A. Goddard, III, California Institute of Technology, Pasadena, CA 91125

Successful molecular dynamics (MD) simulation of large systems (> million atoms) for long times (> nanoseconds) requires the integration of constrained equations of motion (CEOM). Constraints are used to eliminate high frequency degrees of freedom (DOF) and to allow the use of rigid bodies. Solving the CEOM allows for larger integration timesteps and helps focus the simulation on the important collective dynamics of chemical, biological, and materials systems. We explore advances in multibody dynamics which have resulted in O(N) algorithms for propagating the CEOM. However, because of their strictly sequential nature, the computational time required by these algorithms does not scale down with increased numbers of processors. We then present the new constraint force algorithm for solving the CEOM and show that this algorithm is fully parallelizable, leading to a computational cost of O(N/P+logP) for N DOF on P processors.

ABSTRACT. Please be BRIEF—150 words maximum if possible. Title of paper should be ALL CAPS; author(s) listed by first name, middle initial, last name; indicate address with zip code. Presenting author's name should be underlined. SINGLE SPACE, BLACK INK.