

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 91 109; 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.

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D. AUTHORS

Principal Author:

Last Name First Name MI

Fijany Amir

Presenting Author (if different):

Co-authors: Tahir Cagin, California Institute of Technology

Terry R. Coley, Virtual Chemistry, Inc.

William A. Goddard, HI, California Institute of Technology

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E. Principal Author's Business Mailing Address Including Zip Code

Jet Propulsion Laboratory  
MS 303-310  
Pasadena, CA 91109

F. Principal Author's Telephone, Fax Number, and E-mail Address

8183066491

8183066912

Amir.Fijany@jpl.nasa.gov

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