

NUMERICAL TECHNIQUES FOR THE SIMULATION AND MODEL REDUCTION OF COMPLEX PHYSICAL SYSTEMS

700 NUMERICAL METHODS AND ALGORITHMS IN SCIENCE AND ENGINEERING

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ABSTRACT

The simulation of complex physical systems for prediction and control requires robust, efficient numerical algorithms, as the time-scales of interest in many applications are typically longer than can be simulated directly. In recent years, a wealth of new techniques and algorithms have been developed to accelerate the accurate simulation of various classes of statistical observable while quantifying the uncertainty of the resulting predictions made. Examples of such techniques include Time Accelerated Dynamics, Hyperdynamics, Coarse-Grained Molecular Dynamics and the Mori-Zwanzig formalism, and find applications in a diverse range of models including molecular systems, crystals, and continuum models [1-4].

In view of the wide range of applicability of these algorithms and the ideas which lie behind them, this minisymposium seeks to bring together both theoreticians and practitioners who study and use numerical simulation for a range of practical scientific problems, aiming to facilitate discussion and two-way dissemination of ideas across disciplinary and topical boundaries.

REFERENCES

- [1] A. Chatterjee, D. Vlachos. “An overview of spatial microscopic and accelerated kinetic Monte Carlo methods”, *Journal of Computer-Aided Materials Design*, Vol. **14**, Issue 2, pp, 253–308, 2007.
- [2] D. Perez, B. Uberuaga, Y. Shim, J. Amar and A. Voter. “Accelerated molecular dynamics methods: introduction and recent developments”, *Annual Reports in Computational Chemistry*, Vol. **5**, pp, 79—98, 2009.

- [3] A. Chorin, O. H. Hald, and R. Kupferman. “Optimal prediction and the Mori-Zwanzig representation of irreversible processes.” *Proceedings of the National Academy of Sciences of the United States of America*, Vol. **97**, pp, 6253--6257, 2000.
- [4] W. E, B. Engquist, X. Li, W. Ren, and E. Vanden-Eijnden. “Heterogeneous multiscale methods: A review.” *Communications in Computational Physics*, Vol. **2**:367--450, 2007.