

ANNOUNCEMENT

The next issue of the *Journal of Computational Physics* will be a special issue on computational molecular biophysics. The *Journal*, in response to recent rapid advances in computational methods and experimental data on biological polymers, invited Professor Tamar Schlick, an applied mathematician at the Courant Institute and Chemistry Department of New York University, to organize this special issue. The focus of the special issue, in keeping with the general aims of the *Journal*, is on computational methods that contribute to the solution of scientific problems. Professor Schlick, who is a member of the Editorial Board of the *Journal*, has chosen articles and contributors to create a representative and lively issue that will be of interest to specialists as well as members of the wider scientific computing community.

The Special Issue will appear May 1, 1999 (Vol. 151, No. 1), and will represent advances in the following areas:

- Molecular dynamics simulations:
 - integration methods
 - fast electrostatic summation
 - treatments for various canonical ensembles
- Quantum-mechanical and quantum-classical simulations
- Conformational sampling techniques and analyses:
 - hybrid Monte Carlo
 - essential dynamics descriptions
 - potential reconstruction for analyses of single-molecule biochemical experiments
- Simulation program design for advanced computing platforms
- Biomolecular applications, all of which require modeling and simulation ingenuity:
 - carcinogen/DNA complexes
 - protein/DNA complexes
 - membrane supramolecular assemblies—protein folding

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