Molecular dynamics applications (B. Leimkuhler)

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Molecular dynamics and closely related techniques such as smoothed particle hydrodynamics have become important components of modern research in physics, chemistry and biology. With improvements in technology, larger and more complex systems are constantly being analyzed, but there remain many outstanding challenges for simulation. In the past, simplicity rather than accuracy or efficiency has often been the prime factor in the choice of algorithms in macromolecular modeling, but with more ambitious computations and higher expectations for realism, the demands on software and numerical algorithms have changed. The trend now is to combine novel numerical modeling techniques with sophisticated algorithms to yield powerful improvements in computational efficiency.

Many of the algorithmic challenges facing molecular dynamics stem from the difficulty of designing methods which can cope with rapid fluctuations due to chemical bonds, short ranged forces, or the introduction of quantum mechanical effects without excessively limiting the integration time interval. Multiple timescale methods which combine averaging with some type of partitioning of the system offer substantial promise for increased efficiency. Simulations are performed in the context of a statistical mechanical ensemble, which raises additional issues for timestepping.

This minisymposium will survey some exciting new lines of research in molecular dynamics simulation, with emphasis on algorithms issues relevant for the treatment of biomolecules. The speakers will make a special effort to make their research understandable to researchers in scientific computing with limited experience of molecular simulation.