Advances in Time-Integration

Time-integration algorithms have experienced notable progress in the last decade, especially with the formulation of geometric integrators. However, significant open challenges remain in the accurate integration of systems with multiple time scales. For example, in the simulation of macromolecules the time-scales associated with covalent bonds and long-range elecrostatic forces can differ by orders of magnitude. Similarly, in three-dimensional structural dynamics or elastodynamics a widespread distribution of time-scales is often found depending on the mesh, the geometry of the domain and the material properties. In all of these situations, accurately integrating the solution over a long time-scale can become a formidable challenge.

The organizers welcome contributions in the following two related areas:

1. Construction and analysis of integration algorithms for elastodynamics, molecular dynamics and structural dynamics. For example, issues of interests are: stability and accuracy of multi-time-step integrators, especially related to algorithmic resonances; algorithms that (nearly) conserve certain quantities of interest for very long times, for example energy.
2. Novel ideas and advances in the formulation of coarse-grained models aimed at reaching longer time scales while preserving or accurately computing quantities of interest. For example, issues of interest are: computation of appropriate coarse-grained variables, their associated reduced dynamics and measurements of their performance (uncertainty); stochastic models, such as generalized Langevin dynamics or Markov chain models.