Introduction to Computer Simulations in Condensed Matter Systems

Outline

1. **Introduction to classical simulation** ($\sim$ 3 weeks, Martin Weigel)
   - basic statistical mechanics
   - basic molecular dynamics, ergodicity
   - Markov chains and the Monte Carlo method
2. **Electronic systems** ($\sim$ 3 weeks, Thomas Gruhn)
   - numerical integration of the Schrödinger equation
   - Born-Oppenheimer approximation and Hartree-Fock theory
   - introduction to density-functional theory
3. **MC and MD simulations** ($\sim$ 2 weeks, Martin Weigel)
   - Monte Carlo algorithms, cluster updates
   - reweighting and umbrella sampling
   - molecular dynamics and symplectic integrators
   - error analysis, autocorrelations, jackknifing
4. **Quantum molecular dynamics** ($\sim$ 2 weeks, Thomas Gruhn)
   - the Car-Parinello approach
   - othonormalization
   - case studies
5. **Advanced topics** ($\sim$ 3 weeks)
   - optimization problems
   - quantum Monte Carlo
   - parallelization
   - current research
   - ...