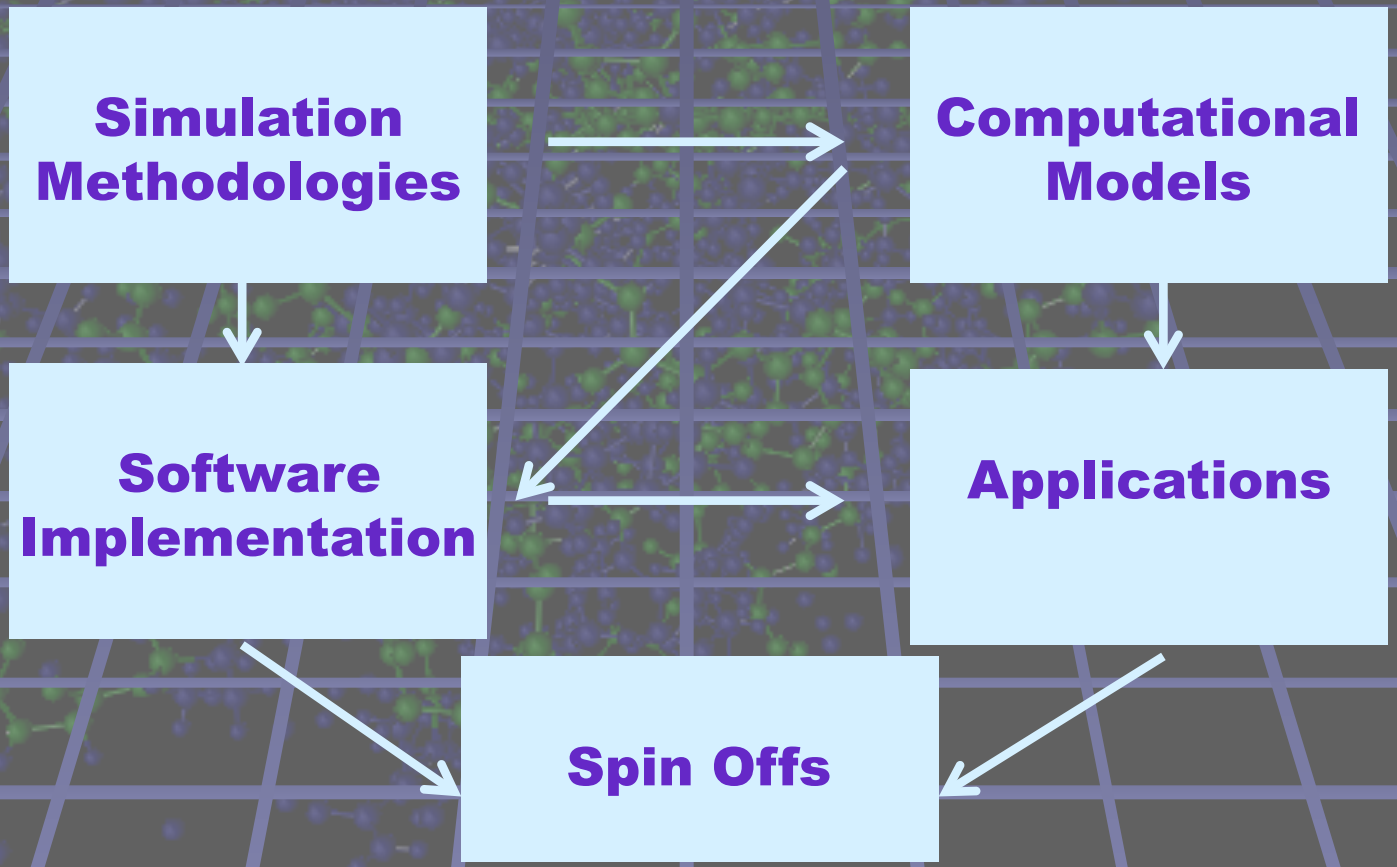
Molecular simulation in BCAM

Overview

Our objective is to enable efficient detailed simulations of extremely large and complex systems which are not possible with conventional simulation methods

Areas of involvement



Current research projects

- Hybrid Monte Carlo methods for simulation of complex systems (BCAM – University of Potsdam, Germany)
- Dynamical modelling of morphology development in multiphase latex particles (BCAM – POLYMAT, Basque Country)
- Large scale simulation of transferrin-Aluminium complex (BCAM – UPV/EHU, Basque Country)
- Computational study of polymorphism in drugs (BCAM – UPV/EHU – University of St. Andrews, UK
- Numerical algorithms and their implementation in semiclassical CAM analysis of numerical scattering data (BCAM – UPV/EHU)
- High performance computing for geophysics applications (BCAM – INRIA – UFGRS – UNAM)
- Reliable computational methods for infinite dimensional problems (BCAM)