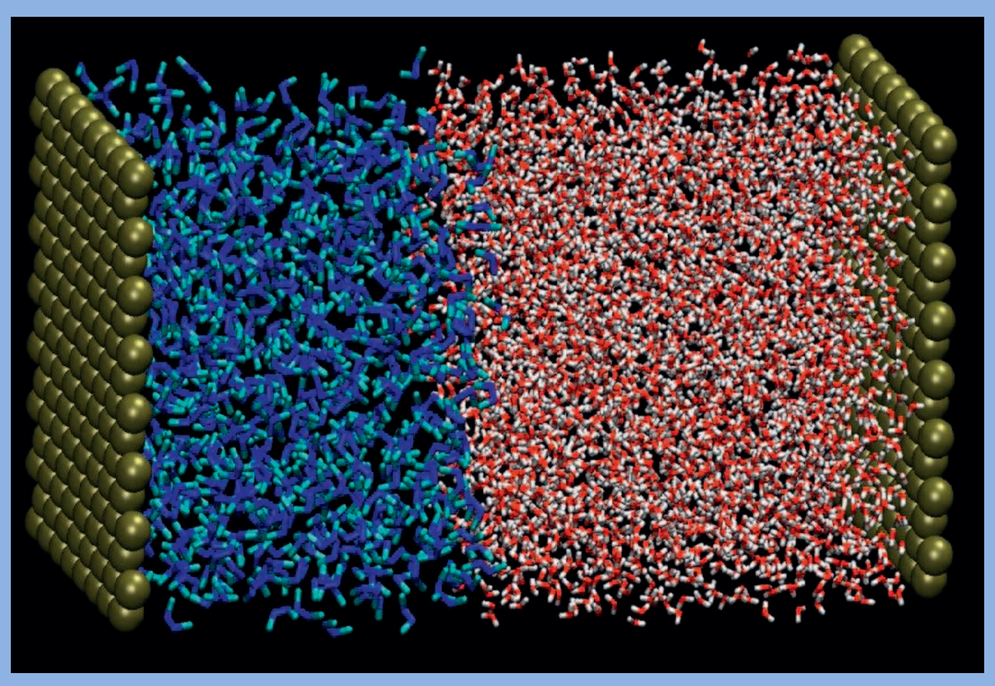
JÜLICH Forschungszentrum | JÜLICH SUPERCOMPUTING CENTRE

SIMLAB MOLECULAR SYSTEMS

HPC-SUPPORT AND DEVELOPMENT: FROM AB-INITIO TO MESO-SCALE



Water-Ammonia interface between two rigid walls

Research and Development

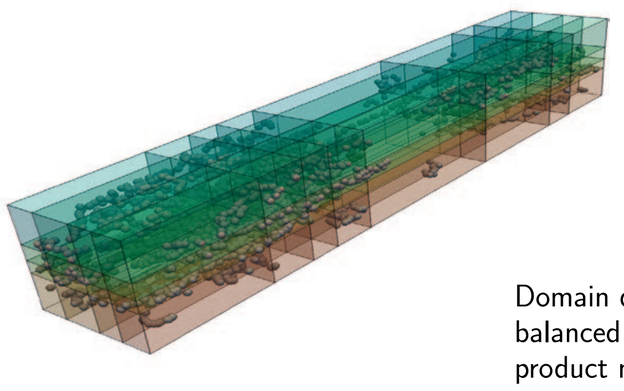
- Parallel algorithms for particle simulations
- Multiscale methods
- Parallel ab-initio methods

Support in Scientific Computing

- Algorithm and scalability analysis and improvement
- Extension of code functionality
- Support in proposal preparation for cpu-grant applications

Parallel Algorithms

- Load balancing
- Hybrid parallelization (MPI+threads)
- Hyperscaling (High-Q club)



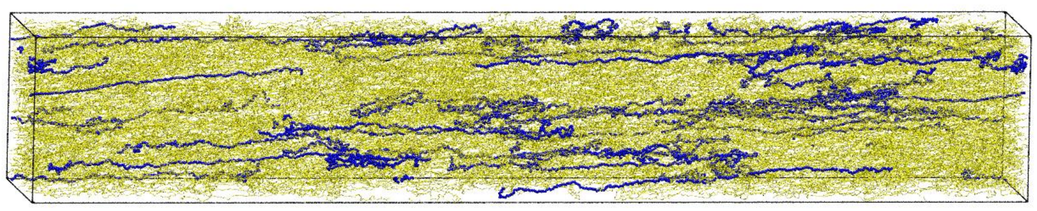
Domain distribution in a load-balanced system based on a tensor product method

Long-Range Interactions

- Scalable Fast Coulomb Solvers (ScaFaCos)
- Multigrid techniques
- Optimized particle-mesh transfer

Mesoscopic Particle Dynamics

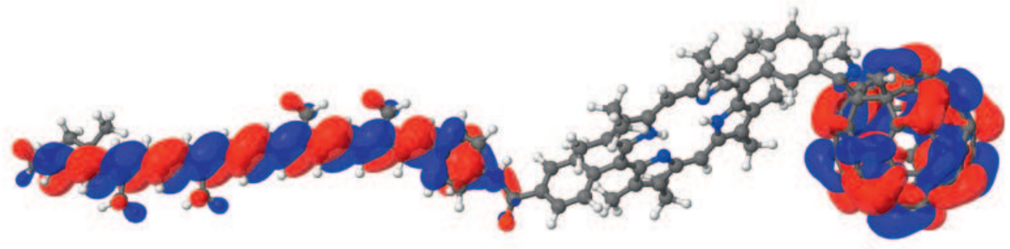
- Massively parallel multi-particle collision dynamics code (MP2C)
- Multiscale particle coupling (MD/MP2C)
- MPMD for multi-level simulations



Semi-diluted polymer system in shear flow simulated with an MPC liquid coupled to MD. Blue polymers highlighted for clarity.

Parallel Ab-Initio Methods

- Multi-reference configuration interaction (MR-SDCI, Spin-Orbit MR-SDCI)
- Density functional theory (RI-DFT)



HOMO and LUMO of a light-harvesting model system: donor(polyene)-spacer(porphyrine)-acceptor(fullerene)

Ab-Initio Code Development/Toolkits

- Turbomole (DFT)
- Columbus (MR-SDCI, SO-MR-SDCI)
- Columbus-OpenMolcas/Molcas Link

Collaborations and Projects

- Theoretical soft matter and biophysics
- CECAM
- European Soft Matter Infrastructure (EUSMI)
- Center of Excellence E-CAM

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