

SIMULATION LABORATORY BIOLOGY

BIOINFORMATICS AND BIOPHYSICS ON HPC SYSTEMS



- Extending timescales of molecular simulations
- New parallel algorithms for biology
- Porting and scaling of life science applications
- Protein folding and interactions
- Molecular networks

Free ProFASi Workshop
 JSC, Sep 24-28, 2018
cecam.org/workshop-1601.html

Know-How

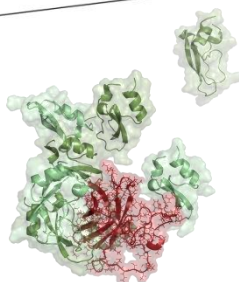
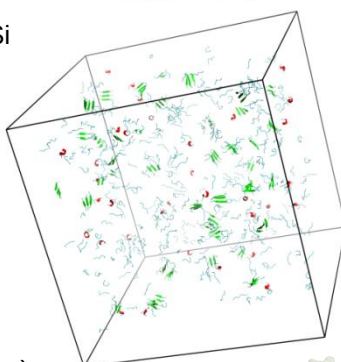
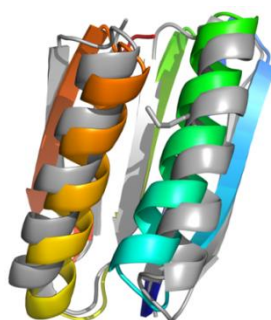
- Bioinformatics data + algorithms
- Simulation of biomolecules
- HPC codes:
 Monte Carlo (ProFASi)
 Local structure prediction (LOCUSTRA)
- Machine Learning

Research

- Peta-Scaling and extending ProFASi
- Protein structure prediction workflow (CASP)
- Protein disorder prediction and simulation
- Computational biology on future HPC architectures

Collaborative Projects

- Disordered proteins (GRS, Barcelona)
- NGS assembly on HPC platforms (Cologne)
- Protein folding and crowding (Lund)
- Multiscale cell simulation (FZJ – IBG1)
- Autom. Workflow optimization (Bonn)
- Large-scale molecular data analysis (Shenzhen, Aachen)



Ab-initio Protein Folding

- 92 residue protein TOP7 (1QYS)
- Largest protein folded *ab-initio* in an all-atom model worldwide, experim. folding time ~ 1 second !
- All-atom model, implicit solvent
- Parallel tempering MCMC (ProFASi)
- $\text{RMSD} \leq 3.5 \text{ \AA}$, 20k CPU-h/folding

Large scale peptide aggregation

- Up to 500 peptide molecules with 6 residues each = 17,500 DOF
- 2048 simulations à $1.5 \cdot 10^6$ sweeps, modified ProFASi, Lund FF, 32 replicas
- Total: $5.4 \cdot 10^{13}$ MC-steps, $\geq 2 \cdot 10^7$ MC-steps/CPU-h
- Aggregate structures show all experimentally known characteristics

Collaborators

