JÜLICH Forschungszentrum | JÜLICH SUPERCOMPUTING CENTRE

SIMULATION AND DATA 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**

Know-How

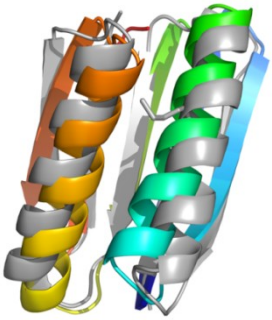
- Bioinformatics data + algorithms
- Simulation of biomolecules
- Machine learning
- SDL Biology HPC codes:
  Monte Carlo (ProFASi)
  Local structure prediction (LOCUSTRA)

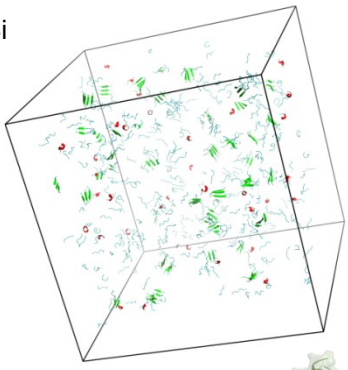
Research

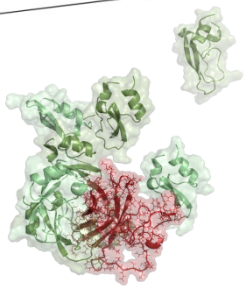
- Peta-Scaling and extending ProFASi
- Protein structure prediction (CASP)
- Protein disorder prediction and simulation
- Computational biology on future HPC architectures

Collaborative Projects

- Intrinsically disordered proteins (GRS, CSIC Barcelona)
- Protein folding and crowding (U. Lund)
- Multiscale cell simulation (FZJ – IBG1)
- HPC Proteomics (FZJ - ZEA3)
- Large-scale molecular data analysis (Siat Shenzhen, RWTH Aachen)
- DNA/RNA simulation (RWTH Aachen)
- Computational medicine (EU: Sano)







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)
- RMSD ≤ 3.5 Å, 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, ≥ $2 \cdot 10^7$ MC-steps/CPU-h
- Aggregate structures show all experimentally known characteristics

Collaborators

CSIC Consejo Superior de Investigaciones Científicas

UNIKLINIK RWTH AACHEN

sano

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