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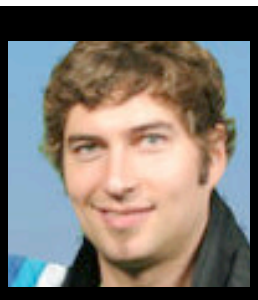
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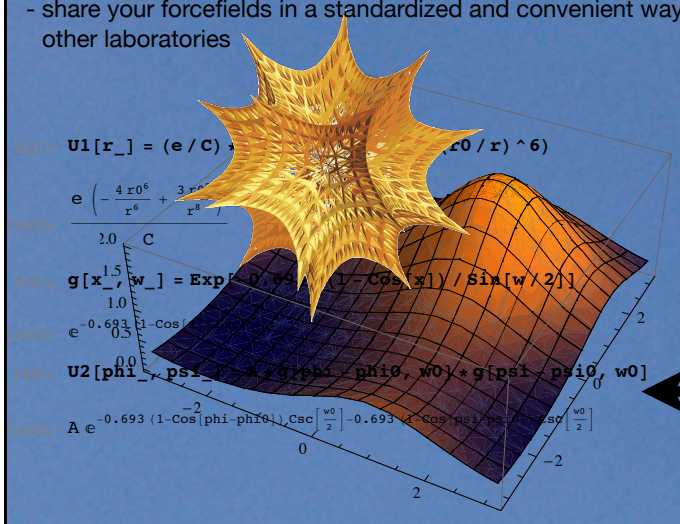
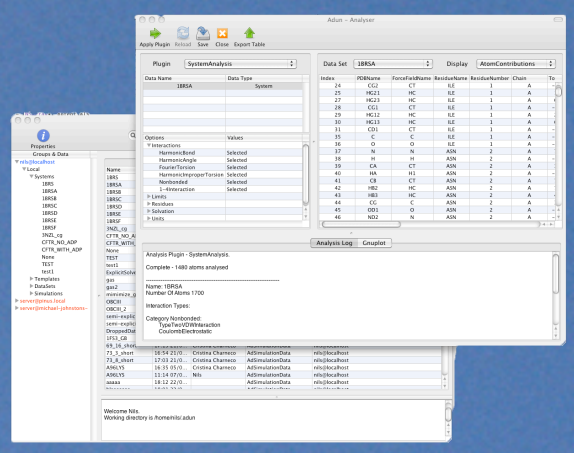
VPH conference 2010

Implementation of a multiscale model for molecular dynamics simulations of protein folding and aggregation in **ADUN**

FORCEFIELD META LANGUAGE

- easily create new forcefields without programming skills
- import equations directly from Mathematica
- share your forcefields in a standardized and convenient way with other laboratories



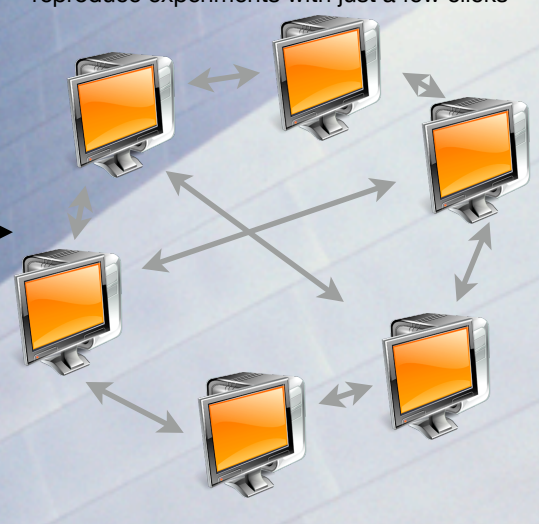


ADUN GUI

- control simulations, either remote or local
- import and export from and to various formats
- apply a multitude of plugins on your data like Essential Dynamics, RMSD calculations, hierarchical clustering...
- create your own powerful scripts with a built-in Smalltalk engine

PEER TO PEER NETWORKING

- share your trajectories and structures with other laboratories worldwide or locally
- easily stream data from collaborators
- reproduce experiments with just a few clicks

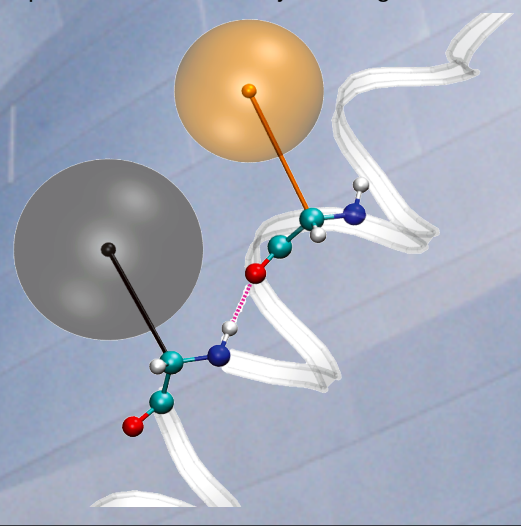


SIMULATE

- make use of an ever growing number of forcefields and forcefield terms, like: AMBER, CHARMM, ENZYMIX, Warshel's CG, Generalized Born, Semi-Explicit-Assembly, statistical potentials for RNA simulation...
- perform your simulations in parallel with Replica Exchange

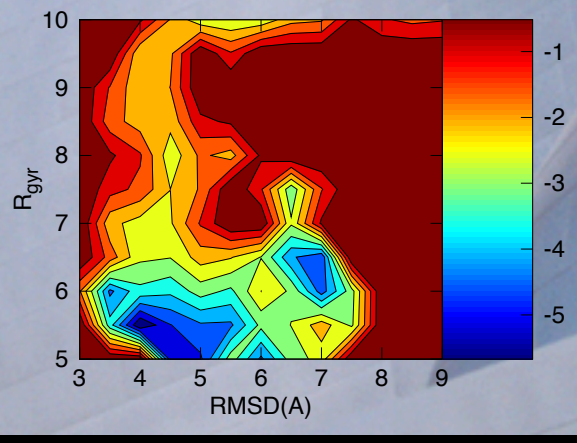
MULTISCALE MD

- perform simulations rapidly using a coarse-grained potential
- swap to all-atom potentials and use free energy perturbation to correct your energies



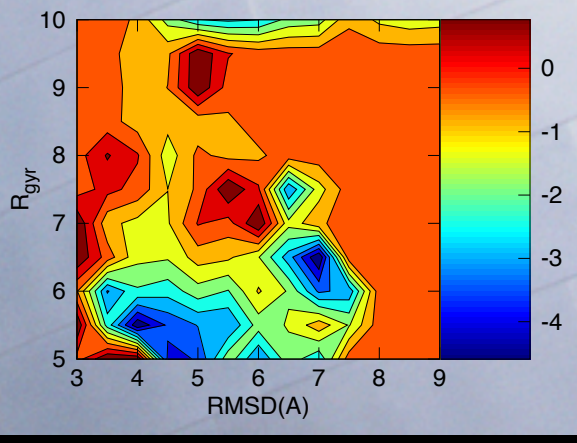
COARSE-GRAINED FEL

- the Free Energy Landscape of a 15-residue all alanin alpha-helix
- derived from a 20ns simulation using Warshel's coarse-grained potential



CORRECTED FEL

- the coarse-grained Free Energy Landscape was corrected by a FEP approach
- in this approach, the difference in free energy of moving from the coarse-grained potential to an all-atom potential (ENZYMIX) was calculated
- this calculation was performed using Free Energy Perturbation
- the coarse-grained FEL was then corrected using the derived free energy differences



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