

ORAC

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- Input and Output files

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ORAC: A molecular dynamics program to simulate solvated biomolecules

<http://www.chim.unifi.it/orac>

ORAC is a program for running classical simulations of biomolecules.

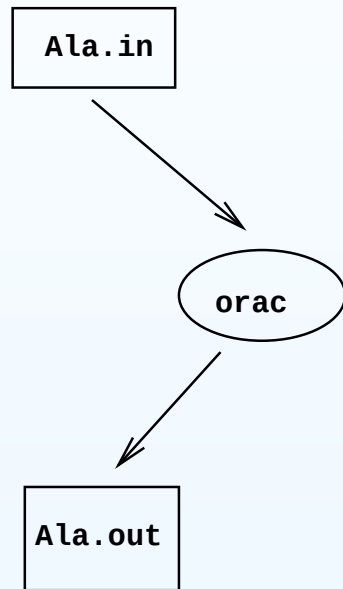
- Simulations can be carried out in the NVE, NPT, NHP, and NVT thermodynamic ensembles.
- The integration of the equations of motion in any ensemble can be carried out with the r-RESPA multiple time step integrator
- electrostatic interactions can be handled with the Smooth Particle Mesh Ewald method
- by Massimo Marchi (CEA Saclay, Paris FR) and P. Procacci (Dip. Chimica, Florence University I)

Input and Output files

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- Standard input and standard output:



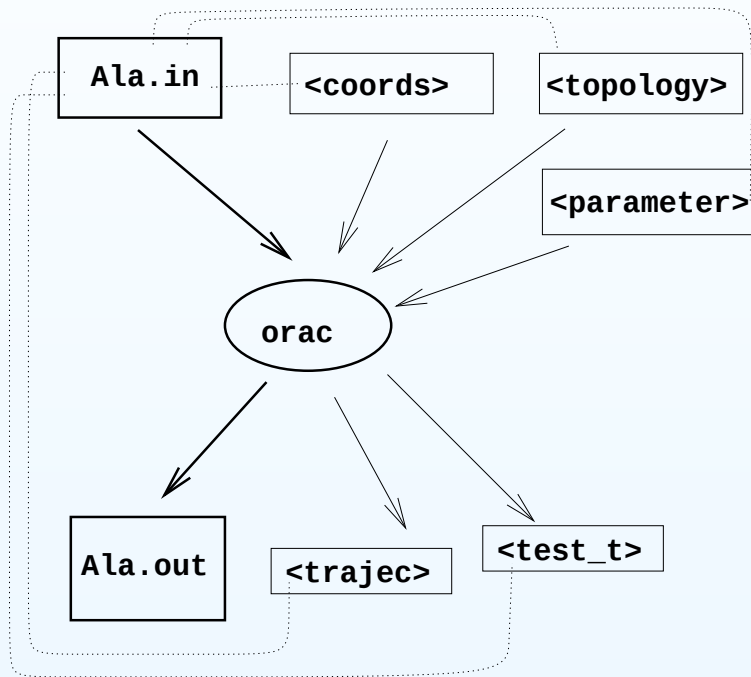
orac < Ala.in > Ala.out

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- Auxiliary files whose names are defined in main input:



orac < Ala.in > Ala.out