APPENDIX

Appendix I: Software used in molecular dynamics simulation.

1. Abalone (classical, implicit water)
2. ABINIT (DFT)
3. ACEMD (running on NVIDIA GPUs: heavily optimized with CUDA)
4. ADUN (classical, P2P database for simulations)
5. AMBER (classical)
6. Ascalaph (classical, GPU accelerated)
7. CASTEP (DFT)
8. CPMD (DFT)
9. CP2K (DFT)
10. CHARMM (classical, the pioneer in MD simulation, extensive analysis tools)
11. COSMOS (classical and hybrid QM/MM, quantum-mechanical atomic charges with BPT)
12. Desmond (classical, parallelization with up to thousands of CPU's)
13. Culgi (classical, OPLS-AA, Dreiding, Nerd, and TraPPE-UA force fields)
14. DL_POLY (classical)
15. ESPResSo (classical, coarse-grained, parallel, extensible)
16. Fireball (tight-binding DFT)
17. GROMACS (classical)
18. GROMOS (classical)
19. GULP (classical)
20. Hippo (classical)
21. Kalypso MD simulation of atomic collisions in solids
22. LAMMPS (classical, large-scale with spatial-decomposition of simulation domain for parallelism)
23. LPMD Las Palmeras Molecular Dynamics: flexible an modular MD.
24. MacroModel (classical)
25. MDynaMix (classical, parallel)
26. MOLDY (classical, parallel) latest release
27. Materials Studio (Forcite MD using COMPASS, Dreiding, Universal, cvff and pcff forcefields in serial or parallel, QMERA (QM+MD), ONESTEP (DFT), etc.)
28. MOSCITO (classical)
29. NAMD (classical, parallelization with up to thousands of CPU's)
30. nano-Material Simulation Toolkit
31. NEWTON-X (ab initio, surface-hopping dynamics)
32. ORAC (classical)
33. ProtoMol (classical, extensible, includes multigrid electrostatics)
34. PWscf (DFT)
35. RedMD (coarse-grained simulations package on GNU licence)
36. S/PHI/nX (DFT)
37. SIESTA (DFT)
38. VASP (DFT)
39. TINKER (classical)
40. YASARA (classical)
41. XMD (classical)

Related software

1. VMD- MD simulation trajectories can be visualized and analyzed.
2. PyMol - Molecular Visualization software written in python
3. Packmol Package for building starting configurations for MD in an automated fashion
4. Sirius - Molecular modeling, analysis and visualization of MD trajectories
5. esra - Lightweight molecular modeling and analysis library (Java/Jython/Mathematica).
6. Molecular Workbench - Interactive molecular dynamics simulations on your desktop
7. BOSS - MC in OPLS
8. Punto is a freely available visualisation tool for particle simulations.

Specialized hardware for MD simulations

1. Anton - A specialized, massively parallel supercomputer designed to execute MD simulations.
2. MDGRAPE - A special purpose system built for molecular dynamics simulations, especially protein structure prediction.

Appendix II : Software used in Homology modeling

Name	Method	Description
LOMETS	Local Meta threading server	Meta-server combining 9 different programs
3D-JIGSAW	Fragment assembly	Automated webserver
Biskit	wraps external programs into automated workflow	BLAST search, T-Coffee alignment, and MODELLER construction
CABS	Reduced modeling tool	Downloadable program
CPHModel	Fragment assembly	Automated webserver
ESyPred3D	Template detection, alignment, 3D modeling	Automated webserver
FoldX	Energy calculations and protein design	Downloadable program
GeneSilico	Consensus template search/fragment assembly	Webserver
Geno3D	Satisfaction of spatial restraints	Automated webserver
HHpred	Template detection, alignment, 3D modeling	Interactive webserver with help facility
LIBRA I	LIght Balance for Remote Analogous proteins, ver. I	Webserver
MODELLER	Satisfaction of spatial restraints	Standalone program in Python
EasyModeller	GUI to MODELLER	Standalone windows executable
Protinfo CM	Comparative modelling of protein structure using minimum perturbation and looop building	Web server
ROBETTA	Rosetta homology modeling and ab initio fragment assembly with Ginzu domain prediction	Webserver
Selvita Protein Modeling Platform	Package of tools for protein modeling	Free demo, interactive webserver and standalone program including: BLAST search, CABS modeling, 3D threading, Psi-Pred secondary structure prediction
SWISS-MODEL	Local similarity/fragment assembly	Automated webserver based on ProModII