Comparison of software for molecular mechanics modeling

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This is a list of computer programs that are predominantly used for **molecular mechanics** calculations.

- GPU – GPU accelerated
- I – Has interface
- Imp – Implicit water
- MC – Monte Carlo
- MD – Molecular dynamics
- Min – Optimization
- QM – Quantum mechanics
- REM – Replica exchange method

Name	View 3D	Model builder	Min	MD	MC	REM	QM	Imp	GPU	Comments	License	Website
Abalone	Yes	Yes	Yes	Yes	Yes	Yes	I	Yes	Yes	Biomolecular simulations, protein folding.	Proprietary, gratis, commercial	Agile Molecule
ADF	Yes	Yes	Yes	Yes	No	No	Yes	Yes	Yes	Modeling suite: ReaxFF, UFF, QM-MM with Amber and Tripos force fields, DFT and semi-empirical methods, conformational analysis with RDKit; partly GPU-accelerated	Proprietary, commercial, gratis trial	SCM
Ascalaph Designer	Yes	Yes	Yes	Yes	Yes	Yes	I	Yes	Yes	Molecular building (DNA, proteins, hydrocarbons, nanotubes), molecular	Mixed: free open source (GNU GPL) & commercial	Ascalaph Project

										dynamics, GPU acceleration		
Avogadro	Yes	Yes	Yes	No	No	No	I	No	No	Molecule building, editing (peptides, small molecules, crystals), conformational analysis, 2D/3D conversion; extensible interfaces to other tools	Free open source GNU GPL	Avogadro
BOSS	No	No	Yes	No	Yes	No	Yes	No	No	OPLS	Proprietary	Yale University
CHARMM	No	Yes	Yes	Yes	Yes	I	I	Yes	Yes	Commercial version with multiple graphical front ends is sold by Accelrys (as CHARMm)	Proprietary, commercial	charmm.org
CHEMKIN	No	No	No	No	No	No	No	No	No	Chemical reaction kinetics.	Proprietary	CHEMKIN
CP2K	No	No	Yes	Yes	Yes	No	Yes	Yes	Yes	CP2K can perform atomistic and molecular simulations of solid state, liquid and biological systems.	Free open source GNU GPLv2 or later	CP2K
Desmond	Yes	Yes	Yes	Yes	No	Yes	No	No	Yes	High performance MD; has comprehensive GUI to build, visualize, and	Proprietary, commercial or	D. E. Shaw Research

											review results and calculation setup up and launch	gratis	Schrödinger
	Discovery Studio	Yes	Yes	Yes	Yes	Yes	No	Yes	Yes	No	Comprehensive life science modeling and simulation suite of applications focused on optimizing drug discovery process: small molecule simulations, QM-MM, pharmacophore modeling, QSAR, protein-ligand docking, protein homology modeling, sequence analysis, protein-protein docking, antibody modeling, etc.	Proprietary, trial available	Dassault Systèmes BIOVIA (formerly Accelrys)
	fold.it	**Y / I**	Yes	Yes	Yes	Yes	Yes	I	No	No	University of Washington and The Baker Labs; structure prediction, protein folding	Proprietary, commercial or gratis	fold.it download page
	FoldX	I	Yes	Yes	No	No	No	No	No	No	Energy calculations, protein design	Proprietary, commercial or gratis	CRG
											High		

GROMACS	No	No	Yes	Yes	No[1]	Yes	I	Yes[2]	Yes	performance MD	Free open source GNU GPL	gromacs.org
GROMOS	No	No	Yes	Yes	Yes	Yes	No	Yes	Yes	Intended for biomolecules	Proprietary, commercial	GROMOS website
HyperChem[3][4][5][6][7]	Yes	Yes	Yes	Yes	Yes	No	Yes	Yes	No	MM+, Ambers, Amber2, Amber3, Amber94, Amber96, Amber99, Bio+83, Bio+85, Charmm-19, Charmm-22, Charmm-27, OPLS, Custom, Extended-Hukel, CNDO, INDO, MINDO3, MNDO, MNDO/d, AM1, PM3, RM1, ZINDO/1, ZINDO/s, TNDO, Hartreee-Fock, MP2, CI, Density Functional Theories, solvent model, conformational sampling, minimizing, MD, MC, Langevin. QM/MM calculations	Proprietary, trial available	Hypercube, Inc.

										can be used. Includes the HyperChem GUI which provides visualizing, molecule building (poly peptide (protein), nucleic acid, poly saccaride, polymer builders), calculation setup, job launch and monitoring, project-level organizing of results, access to a suite of other modelling programs. Developer's kit using HCL, C, C++, Visual Basic, Fortran, Tcl/Tk, DDE.		
	LAMMPS	Yes	Yes	Yes	Yes	Yes	Yes	I	Yes	Yes	Has potentials for soft and solid-state materials and coarse-grain systems	Free open source, GNU GPLv2	Sandia
											OPLS-AA, MMFF, GBSA solvent model, conformational sampling,		

	MacroModel	Yes	Yes	Yes	Yes	Yes	No	I	Yes	No	minimizing, MD. Includes the Maestro GUI which provides visualizing, molecule building, calculation setup, job launch and monitoring, project-level organizing of results, access to a suite of other modelling programs.	Proprietary	Schrödinger
	MAPS [8]	Yes	Yes	Yes	Yes	Yes	Yes	Yes	No	Yes	Building, visualizing, and analysis tools in one user interface, with access to multiple simulation engines	Proprietary, trial available	Scienomics
	Materials Studio	Yes	Yes	Yes	Yes	Yes	No	Yes	Yes	Yes	Environment that brings materials simulation technology to desktop computing, solving key problems in R&D processes	Proprietary, trial available	Dassault Systèmes BIOVIA (formerly Accelrys)
											Standard and reactive		

MBN Explorer[9] + MBN Studio	Yes	Yes	Yes	Yes	Yes	No	No	Yes	Yes	CHARMM force fields; molecular modeler (carbon nanomaterials, biomolecules, nanocrystals); explicit library of examples	Proprietary, free trial available	MBN Research Center
MDynaMix	No	No	No	Yes	No	No	No	No	No	Parallel MD	Free open source GNU GPL	Stockholm University
MOE	Yes	Yes	Yes	Yes	No	No	I	Yes	No	Molecular Operating Environment (MOE)	Proprietary	Chemical Computing Group
Orac	No	No	Yes	Yes	No	Yes	No	Yes	No	Molecular dynamics simulation program to explore free energy surfaces in biomolecular systems at the atomic level	Free open source	Orac download page
NAMD + VMD	Yes	Yes	Yes	Yes	No	Yes	I	Yes	Yes	Fast, parallel MD, CUDA	Proprietary, free academic use, source code	Beckman Institute
NWChem	No	No	Yes	Yes	No	No	Yes	No	No	High-performance computational chemistry software, includes quantum mechanics, molecular dynamics and	Free open source, Educational Community License version 2.0	NWChem

										combined QM-MM methods		
	Protein Local Optimization Program	No	Yes	Yes	Yes	Yes	No	No	No	No	Helix, loop, and side chain optimizing, fast energy minimizing	Proprietary	PLOP wiki
	Q	No	No	No	Yes	No	No	No	No	No	(I) Free energy perturbation (FEP) simulations, (II) empirical valence bond (EVB), calculations of reaction free energies, (III) linear interaction energy (LIE) calculations of receptor-ligand binding affinities	Uppsala Molekylmekaniska HB	Q
	QuantumATK	Yes	Yes	Yes	Yes	Yes	No	Yes	Yes	No	Complete atomistic modeling platform for material science. It includes DFT (Plane-Wave and LCAO), Semi-empirical, and Force Field simulation engines.	Proprietary, commercial	Synopsys QuantumATK
											Computational nanoscience		

	SAMSON	Yes	Yes	Yes	Yes	No	No	Yes	No	No	(life sciences, materials, etc.). Modular architecture, modules termed SAMSON Elements	Proprietary, gratis	SAMSON Connect
	Scigress	Yes	Yes	Yes	Yes	No	No	Yes	Yes	No	MM, DFT, semiempirical methods, parallel MD, conformational analysis, Linear scaling SCF, docking protein-ligand, Batch processing, virtual screening, automated builders (molecular dynamics, proteins, crystals)	Proprietary	SCIGRESS.com
	Spartan	Yes	Yes	Yes	No	Yes	No	Yes	Yes	No	Small molecule (< 2,000 a.m.u.) MM and QM tools to determine conformation, structure, property, spectra, reactivity, and selectivity.	Proprietary, free trial available	Wavefunction, Inc.
											High		

	TeraChem	No	No	Yes	Yes	No	No	Yes	No	Yes	performance GPU-accelerated *ab initio* molecular dynamics and TD/DFT software package for very large molecular or even *nanoscale* systems. Runs on NVIDIA GPUs and 64-bit Linux, has heavily optimized CUDA code.	Proprietary, trial licenses available	PetaChem LLC
	TINKER	I	Yes	Yes	Yes	Yes	I	I	Yes	Yes	Software tools for molecular design-Tinker-OpenMM[10] Software tools for molecular design-Tinker-HP[11]	Proprietary, gratis	Washington University
	Tremolo-X	I	No	Yes	Yes	No	No	No	No	No	Fast, parallel MD	Proprietary	Tremolo-X
	UCSF Chimera	Yes	Yes	Yes	No	No	No	No	No	No	Visually appealing viewer, amino acid rotamers and other building, includes Antechamber and MMTK, Ambertools plugins in	Proprietary, free academic use	University of California

										development.		
YASARA	Yes	Yes	Yes	Yes	No	No	Yes	No	Yes	Molecular graphics, modeling, simulation	Proprietary	YASARA.org

See also [edit]

- Car–Parrinello molecular dynamics
- Comparison of force field implementations
- Comparison of nucleic acid simulation software
- List of molecular graphics systems
- List of protein structure prediction software
- List of quantum chemistry and solid state physics software
- List of software for Monte Carlo molecular modeling
- List of software for nanostructures modeling
- Molecular design software
- Molecular dynamics
- Molecular modeling on GPUs
- Molecule editor

Notes and references [edit]

1. ^ Harrison ET, Weidner T, Castner DG, Interlandi G (2017). "Predicting the orientation of protein G B1 on hydrophobic surfaces using Monte Carlo simulations". *Biointerphases*. **12** (2): 02D401. doi:10.1116/1.4971381. PMC 5148762 . PMID 27923271.
2. ^ Implicit Solvent - Gromacs Archived July 29, 2014, at the Wayback Machine
3. ^ M. Tsuji, K, Shudo, H. Kagechika (2015). "Docking simulations suggest that all-trans retinoic acid could bind retinoid X receptors". *J. Comput. Aided Mol. Des*. **29** (10): 975–988. doi:10.1007/s10822-015-9869-9. PMID 26384496.
4. ^ M. Tsuji (2015). "A ligand-entry surface of the nuclear receptor superfamily consists of the helix H3 of the ligand-binding domain". *J. Mol. Graph. Model*. **62**: 262–275. doi:10.1016/j.jmgm. PMID 26544573.
5. ^ M. Tsuji, K. Shudo, H. Kagechika (2017). "Identifying the receptor subtype selectivity of retinoid X and retinoic acid receptors via quantum mechanics". *FEBS Open Bio*. **7** (3): 391–396. doi:10.1002/2211-5463. PMID 28286734.
6. ^ M. Tsuji (2017). "Antagonist-perturbation mechanism for activation
7. ^ A. Kumer,M. N. Sarker, S. Paul (2019). "The theoretical investigation of HOMO, LUMO, thermophysical properties and QSAR study of some aromatic carboxylic acids using HyperChem programming". *Int. J. Chem. Technol*. **3** (1): 26–37. doi:10.32571/ijct.478179.
8. ^ MAPS
9. ^ I.A. Solov'yov, A.V. Yakubovich, P.V. Nikolaev, I. Volkovets, A.V. Solov'yov (2012). "MesoBioNano Explorer - A universal program for multiscale computer simulations of complex molecular structure and dynamics". *J. Comput. Chem*. **33** (30): 2412–2439. doi:10.1002/jcc.23086. PMID 22965786.
10. ^ M. Harger, D. Li, Z. Wang, K. Dalby, L. Lagardère, J.-P. Piquemal, J. Ponder, P. Ren (2017). "Tinker-OpenMM: Absolute and relative alchemical free energies using AMOEBA on GPUs". *Journal of Computational Chemistry*. **38** (23): 2047–2055. doi:10.1002/jcc.24853. PMC 5539969 . PMID 28600826.
11. ^ L. Lagardère,L.-H. Jolly, F. Lipparini, F. Aviat, B. Stamm, Z. F. Jing, M. Harger, H. Torabifard, G. A. Cisneros, M. J. Schnieders, N. Gresh, Y. Maday, P. Y. Ren, J. W. Ponder, J.-P. Piquemal (2018). "Tinker-HP: a massively parallel molecular dynamics package for multiscale simulations

function-2 fixed motifs: active conformation and docking mode of retinoid X recetor antagonists". *J. Comput. Aided Mol. Des*. **31** (6): 577–585. doi:10.1007/s10822-017-0025-6. PMID 28534193.

of large complex systems with advanced point dipole polarizable force fields". *Chemical Science*. **9** (4): 956–972. doi:10.1039/C7SC04531J. PMC 5909332 . PMID 29732110.

External links [edit]

- SINCRIS
- Linux4Chemistry
- Collaborative Computational Project
- World Index of Molecular Visualization Resources
- Short list of Molecular Modeling resources
- OpenScience
- Biological Magnetic Resonance Data Bank
- Materials modelling and computer simulation codes
- A few tips on molecular dynamics

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