Bioinformatika és genomanalízis az orvostudományban

Molekula-modellezés alapjai

Cserző Miklós

2020

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A mai előadás

- A térszerkezet jelentősége
- A térszerkezet meghatározása
- A molekula-mechanika elve
- Az MM erőtér
- Molekula dinamika
- Szimulációk futtatása és kiértékelése
- Mit lehet modellezni és mit nem

A térszerkezet

- A biokémia dogmája: a szerkezet és funkció összefügg
- Azért van szerkezet, hogy működhessen
- A szerkezet hiánya is egyfajta funkció
- A szerkezet dinamikusan és nem statikusan értelmezendő
- Ez áll fehérjékre és RNS-re is

Szerkezetmeghatározás

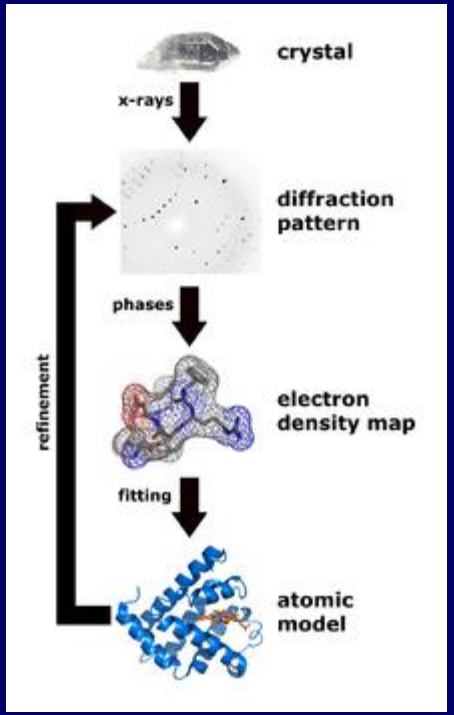
- A szerkezet kisérletesen meghatározható
- Két gyakori módszer: Röntgen-krisztallográfia, NMR
- Tisztított anyagon folyik a mérés
  - Kritályos formában
  - Vizes oldatban

Krisztallográfia

- Elve: a Röntgen-sugár szóródik az elektronokon
- Egy elektronon a szóródás igen gyenge
- A kristályszerkezet miatt a szóródás sokszorosára erősödik
- A diffrakciós mintázatból kiszámolható az elektronsűrűség
- Ez adja a térszerkezetet
  - Példa: autóparkoló feltérképezése teniszlabda-ágyúval

Az eljárás menete

- A számítás ciklusokban
- Fourier és inverz-Fourier transzformációk
- Durva modell – finomított modell
- Nehéz atomokat könnyebb megtalálni
- A hidrogént nagyon nehéz



NMR

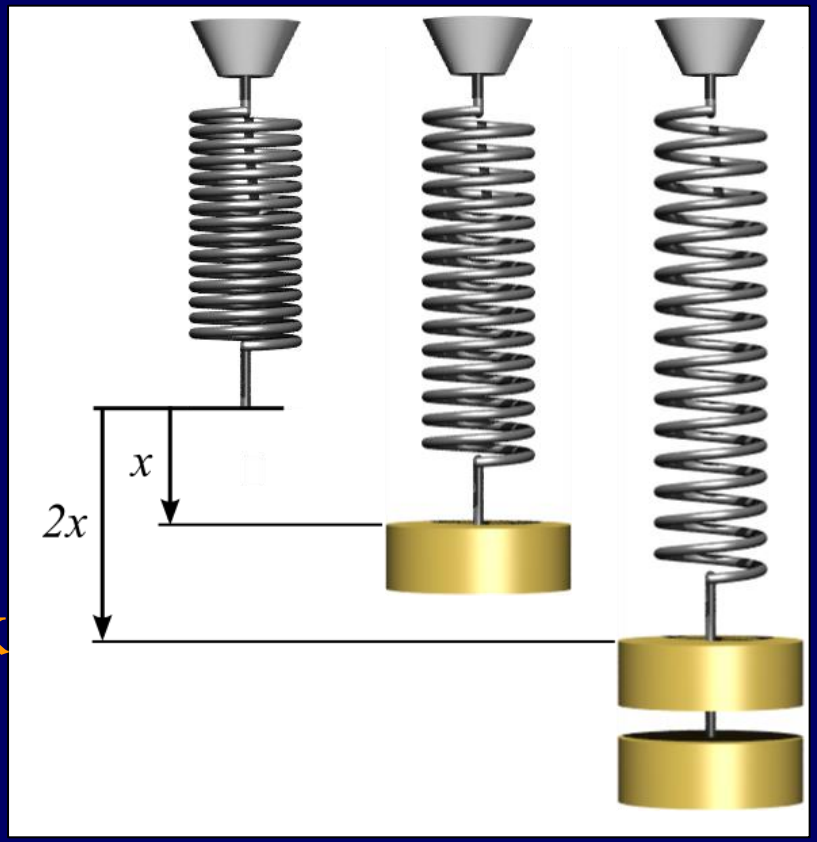
- Bizonyos atommagok kölcsönhatnak a külső mágneses térrel
- Szomszédos atommagok terével is kölcsönhatnak
- A kölcsönhatás ereje $1/x^6$ szerint változik a távolsággal
- A mágneses térben gerjesztett minta radiófrekvenciás spektrtuma a méresi adat

A mérés

- ^{13}C, ^{15}N és ^{31}P megfelelő a mérésre
- Csak azok az atommagok adnak jelet, amelyek elég közel vannak egymáshoz (6 Å)
- A rendszer dinamikus – a távolság nem egy adott érték, hanem egy tartomány
- A mérés az egymáshoz közel eső atomok listáját adja meg – "constrain list"
- De hogy lesz ebből térszerkezet?

Molekula mechanika

- Newtoni-elven működő modell
- Rugón rögzített test
  - Rugóállandó
  - A test tömege
- Az atommagok a testek
- A kémiai kötések a rugók
- A kötések nem szakadnak fel



Az erőtér

- Az atommagok tömege ismert
- Ehhez már csak a megfelelő rugóállandókat kell megkeresni
- Ez minden atomra más
- Sőt, minden atompárra más
- Még sőt, egy atomra más kordináció esetén más
- Legsőt, számítanak a további kapcsolódó atomok

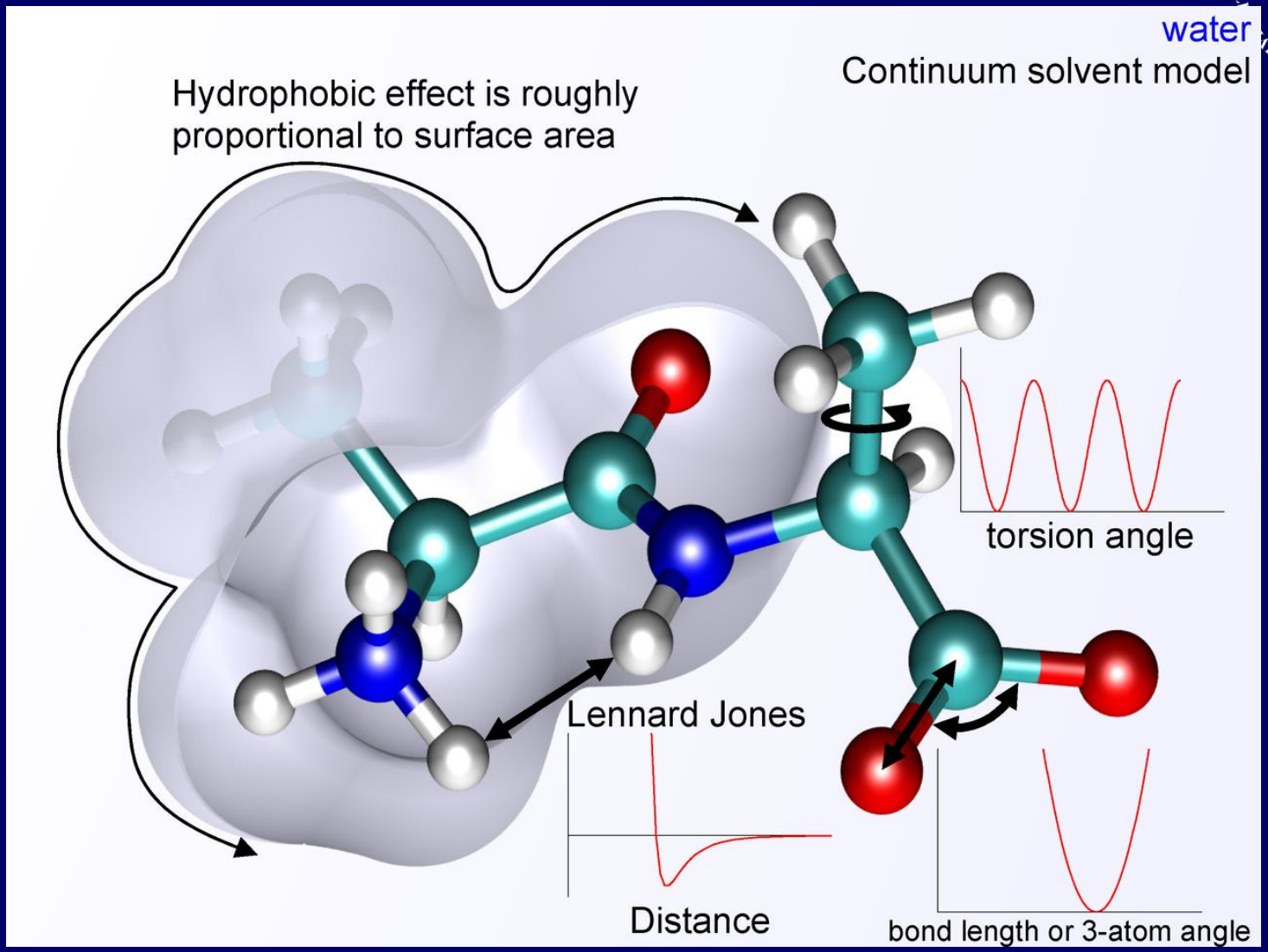
Pl. H – C kötés esetén

- H – N
- H – C
- H – C – N
- H – C – C
- H – C = C
- H – C – O
- H – C – P
- .....

- A “H - C” kötés rugóállandójára minden esetben más értéket kapunk
- A megfelelő állandókat kvantumkémiai számítással kapjuk meg

Az energia függvény

- $E = E_{kovalens} + E_{nem\text{-}kovalens}$
- $E_{kovalens} = E_{kötés} + E_{szög} + E_{térszög}$
- $E_{nem\text{-}kovalens} = E_{elektrosztat.} + E_{VdW}$
- Ezt kell kiszámolni minden atom-párra
- Összegezni – ez lesz a rendszert jellemző összes energia


water
Continuum solvent model
Hydrophobic effect is roughly
proportional to surface area
torsion angle
Lennard Jones
Distance
bond length or 3-atom angle

Megfontolások, következmények

- A párkölcsönhatások száma n^2-tel arányos
- Ez nagyon sok lehet már közepes méretű fehérjék esetén is
- Nagy CPU igény – párhuzamos megoldás
- Nem lehetne egyszerűsíteni egy kicsit?
- Csak óvatosan, az MM már eleve közelítő megoldás!!!

Lehetőségek

- Oldószerrel vagy oldószer nélkül
- Egyesített atomokkal
- "Periódikus doboz" megközelítés
- Mekkora távolságig érdemes elmenni?
- Ha már levágás, hogyan érdemes?

Molekula dinamika

- MM: a rendszer jellemezhető egy látszólagos energiával
- A rendszer két konformációja közül kiválasztható a kedvezőbb
- A két állapot közti átmenet során az atomokra erő hat
- Tehát gyorsulni fognak, lendületük lesz
- A rendszer konformációinak időbeli sorozatát kapjuk

MM, MD és NMR

- Az NMR mérésből megkapjuk a közeli atomok listáját
- A szerkezet meghatározásához MM/MD szimuláció kell
- "Kérek egy szerkezetet, ami részleteiben olyan mint a fehérjék általában, de a következő atomok legyenek közel egymáshoz: ……"

MM, MD és krisztallográfia

- Finomítási eljárás: több ciklusban
- Ha előre helyesen kitalálom az atomok helyét kevesebb ciklusra van szükség
- Generáljuk a hiányzó atomok helyét molekula modellezéssel
- A végső modell minőségellenőrzésére szintén alkalmas a MM/MD

Elérhető eszközök

- Integrált alkalmazások:
  - Open source:
    - VMD/NAMD: http://www.ks.uiuc.edu/Research/vmd/
    - Chimera: https://www.cgl.ucsf.edu/chimera/
  - Kereskedelmi:
    - YASARA: http://www.yasara.org/index.html
    - Biograf: http://www.biograf.ch/index.php?id=software
- CUDA: https://www.nvidia.com/en-us/gpu-accelerated-applications/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NEW: YASARA for Android brings the most feature-complete molecular modeling environment to selected smartphones and tablets, including interactive molecular dynamics simulations.
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Yet Another Scientific Artificial Reality Application
About YASARA - Watching Nature@Work
YASARA is a molecular-graphics, -modeling and -simulation program for Windows, Linux, Mac OS X and Android developed since 1993, that finally makes it really easy to answer your questions. With an intuitive user interface, photorealistic graphics and support for affordable shutter glasses, autostereoscopic displays and input devices, YASARA creates a new level of interaction with the 'artificial reality', that allows you to focus on your goal and forget about the details of the program.
YASARA is powered by PVL (Portable Vector Language), a new development framework that provides performance way above traditional software. PVL allows you to visualize even the largest proteins and enables true interactive real-time simulations with highly accurate force fields on standard PCs (see benchmarks). You
structure of the day 2014/12/08


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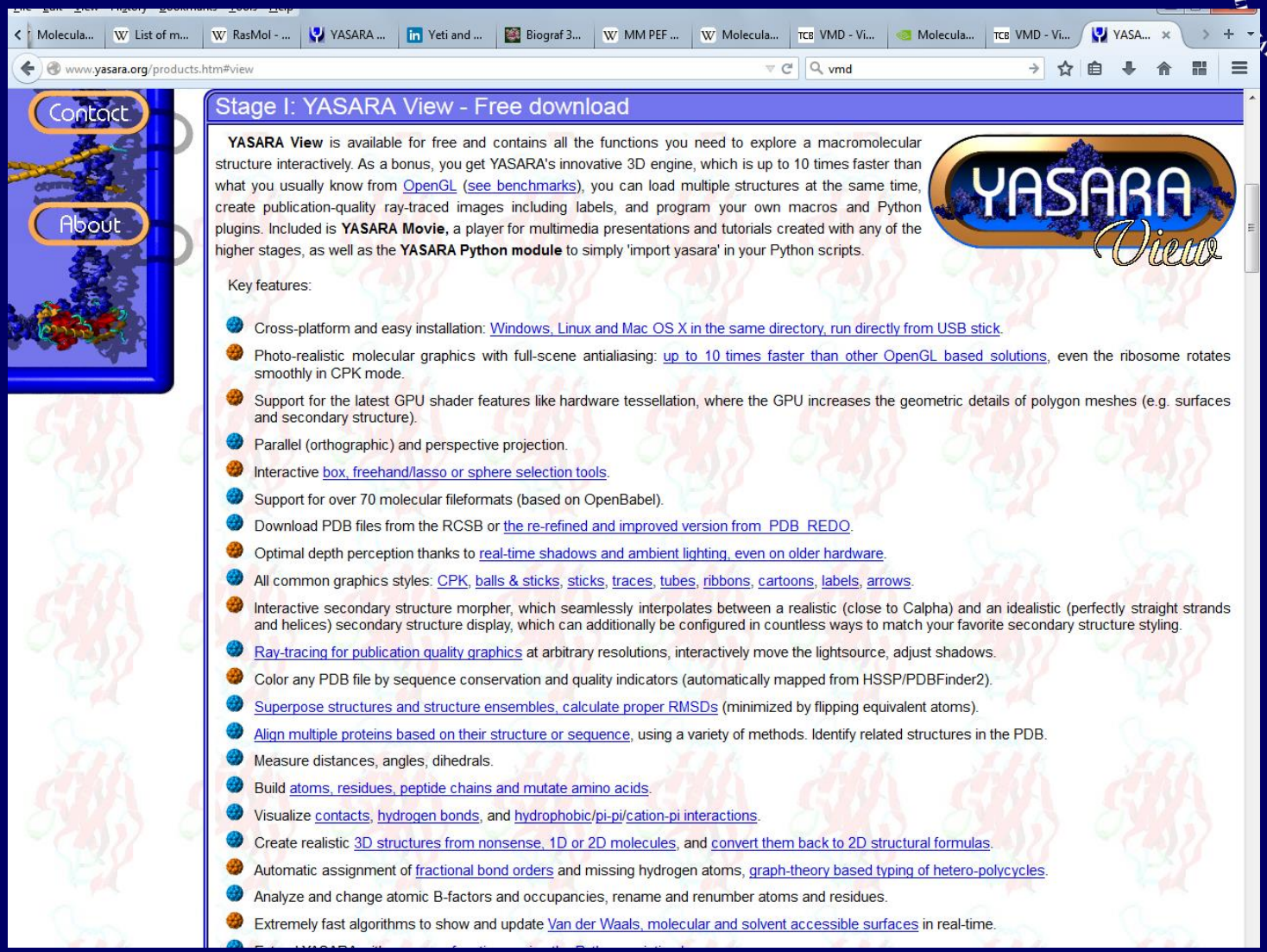
There are four different stages of YASARA for Linux, Windows, Mac OS X and Android, aimed at increasingly complicated fields of application. A certain stage contains the features of all the previous stages, plus a number of additional functions to tackle a wider range of scientific questions. Features with unique properties which you will not find in other programs are marked with orange buckyballs below.
YASARA View - Molecular graphics and analysis, freely download now.
YASARA Model - Everything above, plus molecular modeling
YASARA Dynamics - Everything above, plus molecular simulations
YASARA Structure - Everything above, plus structure prediction and validation, docking, knowledge-based potentials
YASARA NMR Module - NMR structure determination
YASARA/WHAT IF Twinset - Extensive structure validation (PDBReports) and WHAT IF functions
Android tablets and smartphones that can run interactive MD simulations starting at 175 EUR.
A stereoscopic molecular modeling lab for 250 EUR, and a cave for 700 EUR.
Read more about the philosophy behind YASARA.
System requirements: None, please download the free YASARA View to verify that YASARA runs on your computer (and please contact us if you encounter problems).
Stage I: YASARA View - Free download
YASARA View is available for free and contains all the functions you need to explore a macromolecular structure interactively. As a bonus, you get YASARA's innovative 3D engine, which is up to 10 times faster than what you usually know from OpenGL (see benchmarks), you can load multiple structures at the same time, create publication-quality ray-traced images including labels, and program your own macros and Python plugins. Included is YASARA Movie, a player for multimedia presentations and tutorials created with any of the higher stages, as well as the YASARA Python module to simply 'import yasara' in your Python scripts
YASARA View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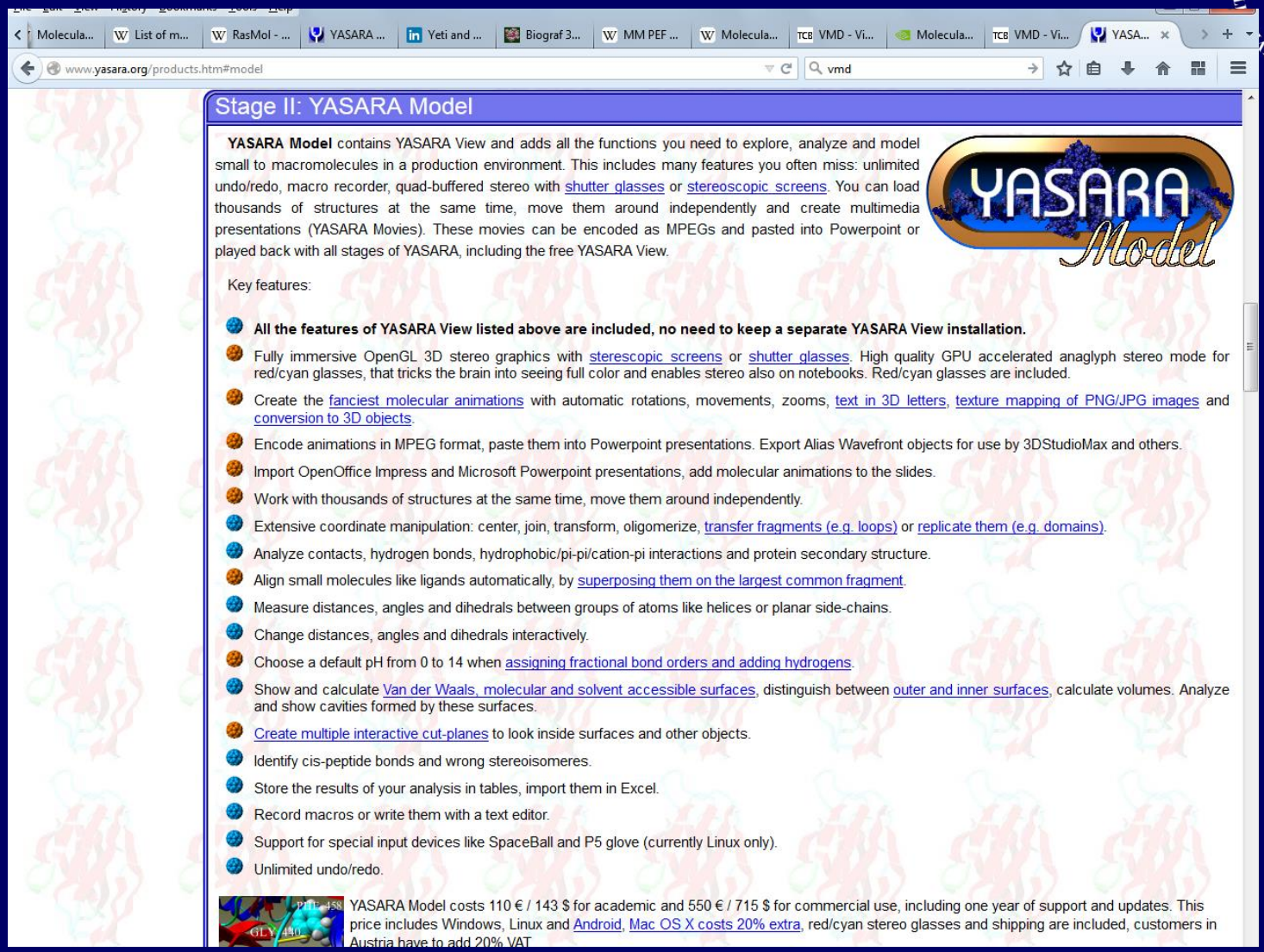
YASARA View
Key features:
Cross-platform and easy installation: Windows, Linux and Mac OS X in the same directory, run directly from USB stick.
Photo-realistic molecular graphics with full-scene antialiasing: up to 10 times faster than other OpenGL based solutions, even the ribosome rotates smoothly in CPK mode.
Support for the latest GPU shader features like hardware tessellation, where the GPU increases the geometric details of polygon meshes (e.g. surfaces and secondary structure).
Parallel (orthographic) and perspective projection.
Interactive box, freehand/lasso or sphere selection tools.
Support for over 70 molecular fileformats (based on OpenBabel).
Download PDB files from the RCSB or the re-refined and improved version from PDB_REDO.
Optimal depth perception thanks to real-time shadows and ambient lighting, even on older hardware.
All common graphics styles: CPK, balls & sticks, sticks, traces, tubes, ribbons, cartoons, labels, arrows.
Interactive secondary structure morpher, which seamlessly interpolates between a realistic (close to Calpha) and an idealistic (perfectly straight strands and helices) secondary structure display, which can additionally be configured in countless ways to match your favorite secondary structure styling.
Ray-tracing for publication quality graphics at arbitrary resolutions, interactively move the lightsource, adjust shadows.
Color any PDB file by sequence conservation and quality indicators (automatically mapped from HSSP/PDBFinder2).
Superpose structures and structure ensembles, calculate proper RMSDs (minimized by flipping equivalent atoms).
Align multiple proteins based on their structure or sequence, using a variety of methods. Identify related structures in the PDB.
Measure distances, angles, dihedrals.
Build atoms, residues, peptide chains and mutate amino acids.
Visualize contacts, hydrogen bonds, and hydrophobic/pi-pi/cation-pi interactions.
Create realistic 3D structures from nonsense, 1D or 2D molecules, and convert them back to 2D structural formulas.
Automatic assignment of fractional bond orders and missing hydrogen atoms, graph-theory based typing of hetero-polycycles.
Analyze and change atomic B-factors and occupancies, rename and renumber atoms and residues.
Extremely fast algorithms to show and update Van der Waals, molecular and solvent accessible surfaces in real-time.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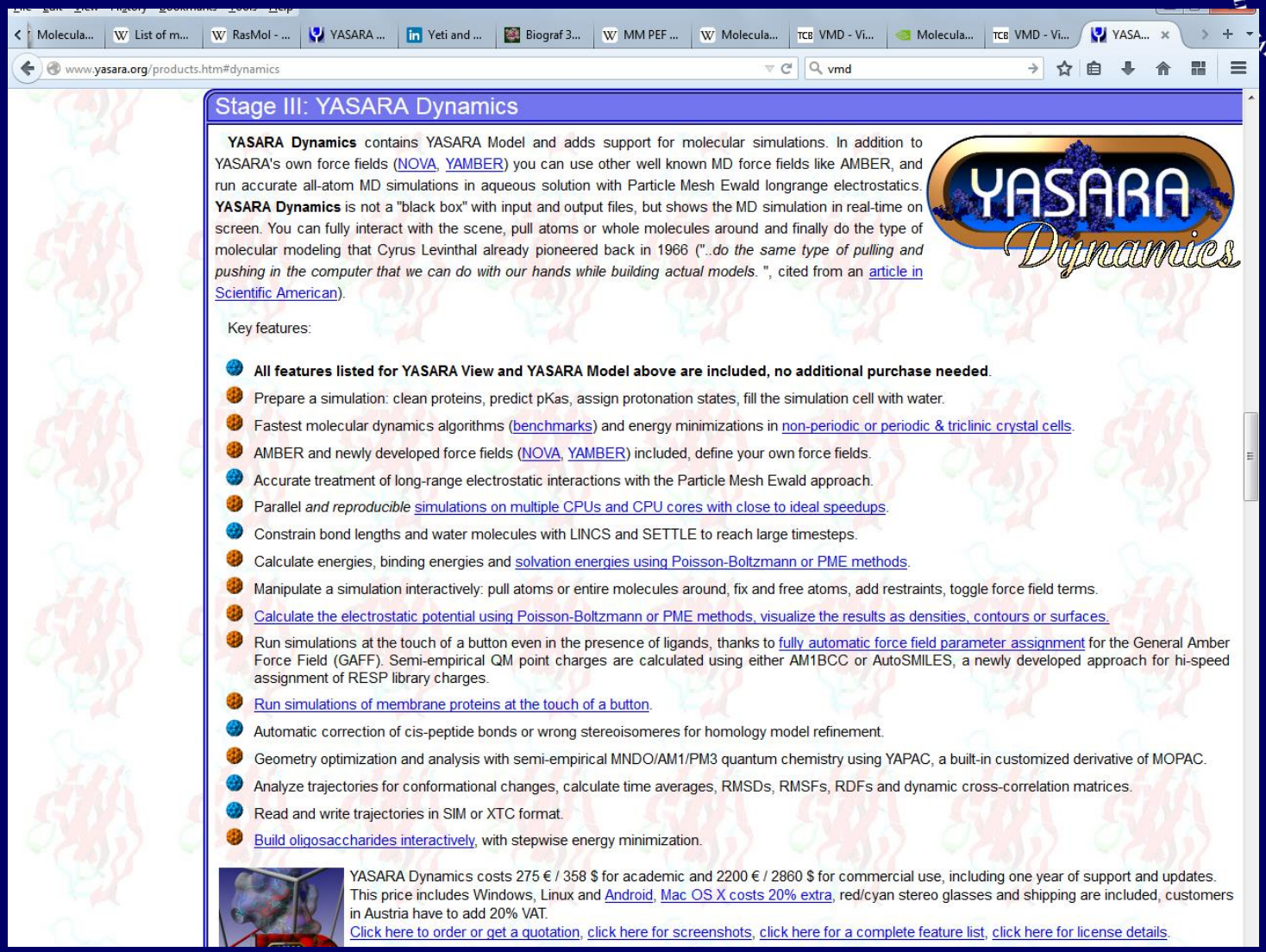
Stage II: YASARA Model
YASARA Model contains YASARA View and adds all the functions you need to explore, analyze and model small to macromolecules in a production environment. This includes many features you often miss: unlimited undo/redo, macro recorder, quad-buffered stereo with shutter glasses or stereoscopic screens. You can load thousands of structures at the same time, move them around independently and create multimedia presentations (YASARA Movies). These movies can be encoded as MPEGs and pasted into Powerpoint or played back with all stages of YASARA, including the free YASARA View.
YASARA Model
Key features:
All the features of YASARA View listed above are included, no need to keep a separate YASARA View installation.
Fully immersive OpenGL 3D stereo graphics with sterescopic screens or shutter glasses. High quality GPU accelerated anaglyph stereo mode for red/cyan glasses, that tricks the brain into seeing full color and enables stereo also on notebooks. Red/cyan glasses are included.
Create the fanciest molecular animations with automatic rotations, movements, zooms, text in 3D letters, texture mapping of PNG/JPG images and conversion to 3D objects.
Encode animations in MPEG format, paste them into Powerpoint presentations. Export Alias Wavefront objects for use by 3DStudioMax and others.
Import OpenOffice Impress and Microsoft Powerpoint presentations, add molecular animations to the slides.
Work with thousands of structures at the same time, move them around independently.
Extensive coordinate manipulation: center, join, transform, oligomerize, transfer fragments (e.g. loops) or replicate them (e.g. domains).
Analyze contacts, hydrogen bonds, hydrophobic/pi-pi/cation-pi interactions and protein secondary structure.
Align small molecules like ligands automatically, by superposing them on the largest common fragment.
Measure distances, angles and dihedrals between groups of atoms like helices or planar side-chains.
Change distances, angles and dihedrals interactively.
Choose a default pH from 0 to 14 when assigning fractional bond orders and adding hydrogens.
Show and calculate Van der Waals, molecular and solvent accessible surfaces, distinguish between outer and inner surfaces, calculate volumes. Analyze and show cavities formed by these surfaces.
Create multiple interactive cut-planes to look inside surfaces and other objects.
Identify cis-peptide bonds and wrong stereoisomeres.
Store the results of your analysis in tables, import them in Excel.
Record macros or write them with a text editor.
Support for special input devices like SpaceBall and P5 glove (currently Linux only).
Unlimited undo/redo.
YASARA Model costs 110 € / 143 $ for academic and 550 € / 715 $ for commercial use, including one year of support and updates. This price includes Windows, Linux and Android, Mac OS X costs 20% extra, red/cyan stereo glasses and shipping are included, customers in Austria have to add 20% VAT.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Stage III: YASARA Dynamics
YASARA Dynamics contains YASARA Model and adds support for molecular simulations. In addition to YASARA's own force fields (NOVA, YAMBER) you can use other well known MD force fields like AMBER, and run accurate all-atom MD simulations in aqueous solution with Particle Mesh Ewald longrange electrostatics. YASARA Dynamics is not a "black box" with input and output files, but shows the MD simulation in real-time on screen. You can fully interact with the scene, pull atoms or whole molecules around and finally do the type of molecular modeling that Cyrus Levinthal already pioneered back in 1966 ("..do the same type of pulling and pushing in the computer that we can do with our hands while building actual models. ", cited from an article in Scientific American).
YASARA Dynamics
Key features:
All features listed for YASARA View and YASARA Model above are included, no additional purchase needed.
Prepare a simulation: clean proteins, predict pKas, assign protonation states, fill the simulation cell with water.
Fastest molecular dynamics algorithms (benchmarks) and energy minimizations in non-periodic or periodic & triclinic crystal cells.
AMBER and newly developed force fields (NOVA, YAMBER) included, define your own force fields.
Accurate treatment of long-range electrostatic interactions with the Particle Mesh Ewald approach.
Parallel and reproducible simulations on multiple CPUs and CPU cores with close to ideal speedups.
Constrain bond lengths and water molecules with LINCS and SETTLE to reach large timesteps.
Calculate energies, binding energies and solvation energies using Poisson-Boltzmann or PME methods.
Manipulate a simulation interactively: pull atoms or entire molecules around, fix and free atoms, add restraints, toggle force field terms.
Calculate the electrostatic potential using Poisson-Boltzmann or PME methods, visualize the results as densities, contours or surfaces.
Run simulations at the touch of a button even in the presence of ligands, thanks to fully automatic force field parameter assignment for the General Amber Force Field (GAFF). Semi-empirical QM point charges are calculated using either AM1BCC or AutoSMILES, a newly developed approach for hi-speed assignment of RESP library charges.
Run simulations of membrane proteins at the touch of a button.
Automatic correction of cis-peptide bonds or wrong stereoisomers for homology model refinement.
Geometry optimization and analysis with semi-empirical MNDO/AM1/PM3 quantum chemistry using YAPAC, a built-in customized derivative of MOPAC.
Analyze trajectories for conformational changes, calculate time averages, RMSDs, RMSFs, RDFs and dynamic cross-correlation matrices.
Read and write trajectories in SIM or XTC format.
Build oligosaccharides interactively, with stepwise energy minimization.
YASARA Dynamics costs 275 € / 358 $ for academic and 2200 € / 2860 $ for commercial use, including one year of support and updates. This price includes Windows, Linux and Android, Mac OS X costs 20% extra, red/cyan stereo glasses and shipping are included, customers in Austria have to add 20% VAT.
Click here to order or get a quotation, click here for screenshots, click here for a complete feature list, click here for license details.

Stage IV: YASARA Structure

YASARA Structure contains YASARA Dynamics and adds all the functions needed to predict and validate macromolecular structures, including ligand docking and highly accurate force fields with knowledge-based potentials. If you already own one of the other YASARA stages, you can upgrade easily, just contact us for a quote.

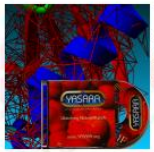
Key features:

- **All features listed for YASARA View, YASARA Model and YASARA Dynamics above are included, no additional purchase needed.**
- Small-molecule docking at the touch of a button, using tuned versions of AutoDock and VINA with automatic setup, receptor flexibility and multi-CPU support. Additional support for Fleksy, an induced fit docking program based on FlexX, developed at Organon/Schering-Plough.
- Side-chain rotamer prediction combining graph-theory and dead-end elimination with accurate treatment of electrostatics, solvation and subtle packing effects.
- Knowledge-based loop modeler with a compressed index of the PDB, peptide segments spanning selected anchor residues can be located within a fraction of a second, while considering sequence and secondary structure preferences. Loops can be optimized together with surrounding side-chains, considering all energy components including solvation.
- New force fields (YASARA and YASARA2) with multi-dimensional knowledge-based components for highly accurate refinement simulations to aid protein structure determination and prediction.
- Homology modeling at the touch of a button: select the target sequence and get a homology model, combined from multiple templates, refined in explicit solvent, as well as a detailed scientific report describing how the model was built, including extensive validation with figures and quality plots. Check the CASP results.
- pH dependent hydrogen bonding network optimizer, that automatically considers ligands and determines ambiguities in X-ray density.
- Built-in BLAST and PSI-BLAST, with automatically updated SwissProt, UniRef90, PDB and PDBC sequence databases, the latter augmented with WHAT_CHECK/ PDBFinder2 validation data to rank PDB structures sharing the same sequence.
- Secondary structure prediction with PsiPred and DSC.
- Extensive structure validation to judge the quality of experimental structures and models, based on a new combination of force field energies and Z-scores, that yields results not only for proteins, but for all organic molecules. This allows to validate for example protein-ligands interactions, an important aspect in drug design.
- Perform twisted structural alignments, where the protein is bent and wound to maximize the number of structurally aligned residues, for example to create sequence profiles for homology modeling
- Prediction and visualization of ion binding sites using valence scanning.

YASARA Structure costs 375 € / 488 $ for academic and 3300 € / 4290 $ for commercial use, including one year of support and updates. This price includes Windows and Linux, Mac OS X costs 20% extra, red/cyan stereo glasses and shipping are included, customers in Austria have to add 20% VAT.
Click here to order or get a quotation, click here for screenshots, click here for a complete feature list, click here for license details.

YASARA NMR Module

The YASARA NMR Module solves protein structures at the touch of a button, based on the protein sequence and distance- & dihedral-angle restraints. Input files are compatible with X-PLOR, folding and refinement are visualized in real-time on screen, allowing to identify problematic restraints. Floating assignments are supported, all the details are described here.



The YASARA NMR Module is an add-on for YASARA Structure and costs 50 € / 65 $ for academic and 500 € / 650 $ for commercial use, including one year of support and updates. This price includes Windows and Linux, Mac OS X costs 20% extra, customers in Austria have to add 20% VAT. If you do not have YASARA Structure yet, click here to order or get a quotation and click here for license details, otherwise contact us directly.

The WHAT IF / YASARA Twinset

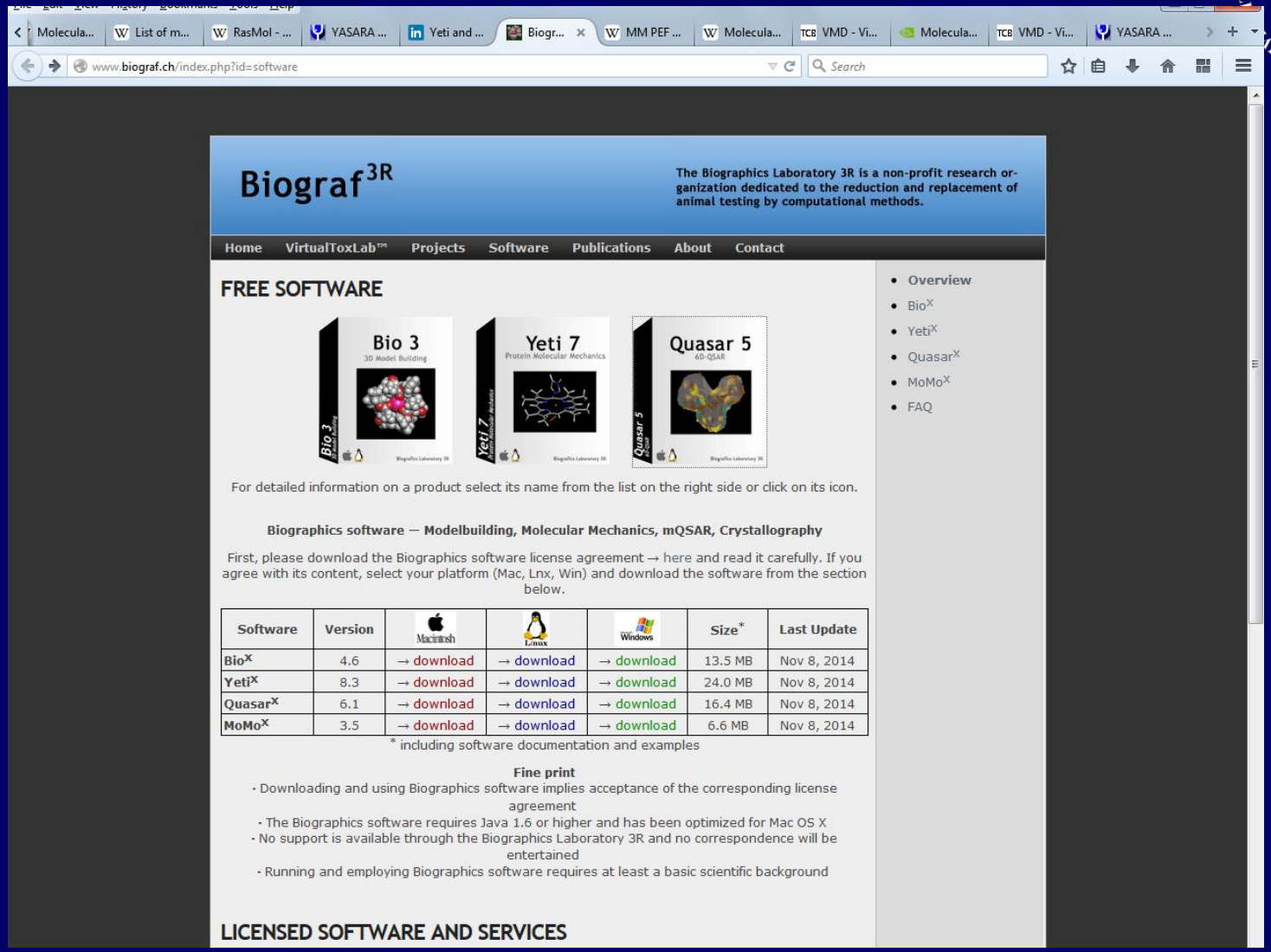
The Twinset is a customized joint-distribution of WHAT IF and YASARA Dynamics (Linux and Windows, not MacOSX) or YASARA Structure (Linux only). With over 2000 citations, WHAT IF is a widely used program for structure validation and modeling. In the Twinset, WHAT IF inherits YASARA's user interface, graphics engine, macro language, unlimited undo/redo etc, so that WHAT IF functions become easily accessible.

The Twinset is freely available for academic use and costs 1500 € / 1950 $ for unlimited commercial use per building (this fee is waived if you own a group leader license of YASARA Dynamics or Structure). **In addition, you need** 512MB RAM, 1GB of swap space and **licenses for YASARA Dynamics or Structure and also WHAT IF**. Click here for WHAT IF license details, and note that the academic WHAT IF version is now shareware. Customers in Austria have to add 20% VAT.

To order the Twinset, just place a normal order for YASARA Dynamics or YASARA Structure and then request the Twinset upgrade from support@yasara.org, telling us your WHAT IF license number. If you already own YASARA, email us your YASARA serial number and WHAT IF license number.

Molecular modeling on Android for 175 EUR

Since April 2013, YASARA is available for selected Android smartphones and tablets, providing today's most feature-complete mobile molecular modeling environment, including interactive MD simulations. Tablet prices start at 175 EUR, two videos and all the details are available here.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www.biograf.ch/index.php?id=software&subid=bio

Biograf 3R

The Biographics Laboratory 3R is a non-profit research organization dedicated to the reduction and replacement of animal testing by computational methods.

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SOFTWARE

BIO X

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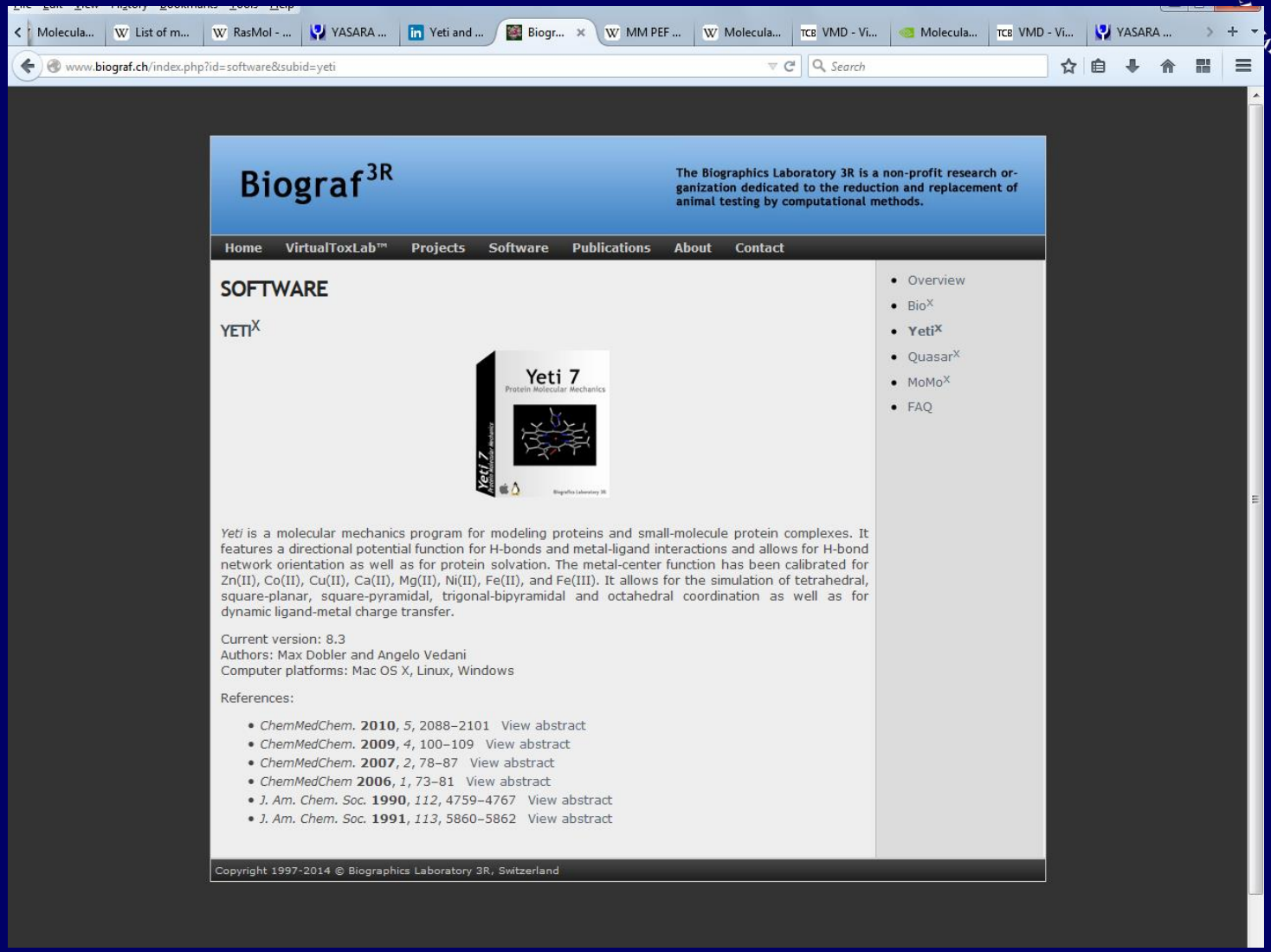
The molecular-modeling software *Bio* is a versatile tool for constructing, analyzing and minimizing molecular structures. The implemented minimizer is based on a directional force field for hydrogen bonds and metal-ligand interactions. The software includes functional-group templates and user-expandable databases for organic molecules, carbohydrates, peptides, and nucleic acids. *Bio* allows for H-bond network orientation, full, zone or constrained refinement, ligand superposition (best fit), visual bump check during docking, dynamic torsion-angle manipulation, and mutation/completion of amino-acid residues.

Current Version: 4.6
Author: Max Dobler
Computer platforms: Mac OS X, Linux, Windows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YASARA ...
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Yeti is a molecular mechanics program for modeling proteins and small-molecule protein complexes. It features a directional potential function for H-bonds and metal-ligand interactions and allows for H-bond network orientation as well as for protein solvation. The metal-center function has been calibrated for Zn(II), Co(II), Cu(II), Ca(II), Mg(II), Ni(II), Fe(II), and Fe(III). It allows for the simulation of tetrahedral, square-planar, square-pyramidal, trigonal-bipyramidal and octahedral coordination as well as for dynamic ligand-metal charge transfer.
Current version: 8.3
Authors: Max Dobler and Angelo Vedani
Computer platforms: Mac OS X, Linux, Windows
References:
ChemMedChem. 2010, 5, 2088–2101 View abstract
ChemMedChem. 2009, 4, 100–109 View abstract
ChemMedChem. 2007, 2, 78–87 View abstract
ChemMedChem 2006, 1, 73–81 View abstract
J. Am. Chem. Soc. 1990, 112, 4759–4767 View abstract
J. Am. Chem. Soc. 1991, 113, 5860–5862 View abstract
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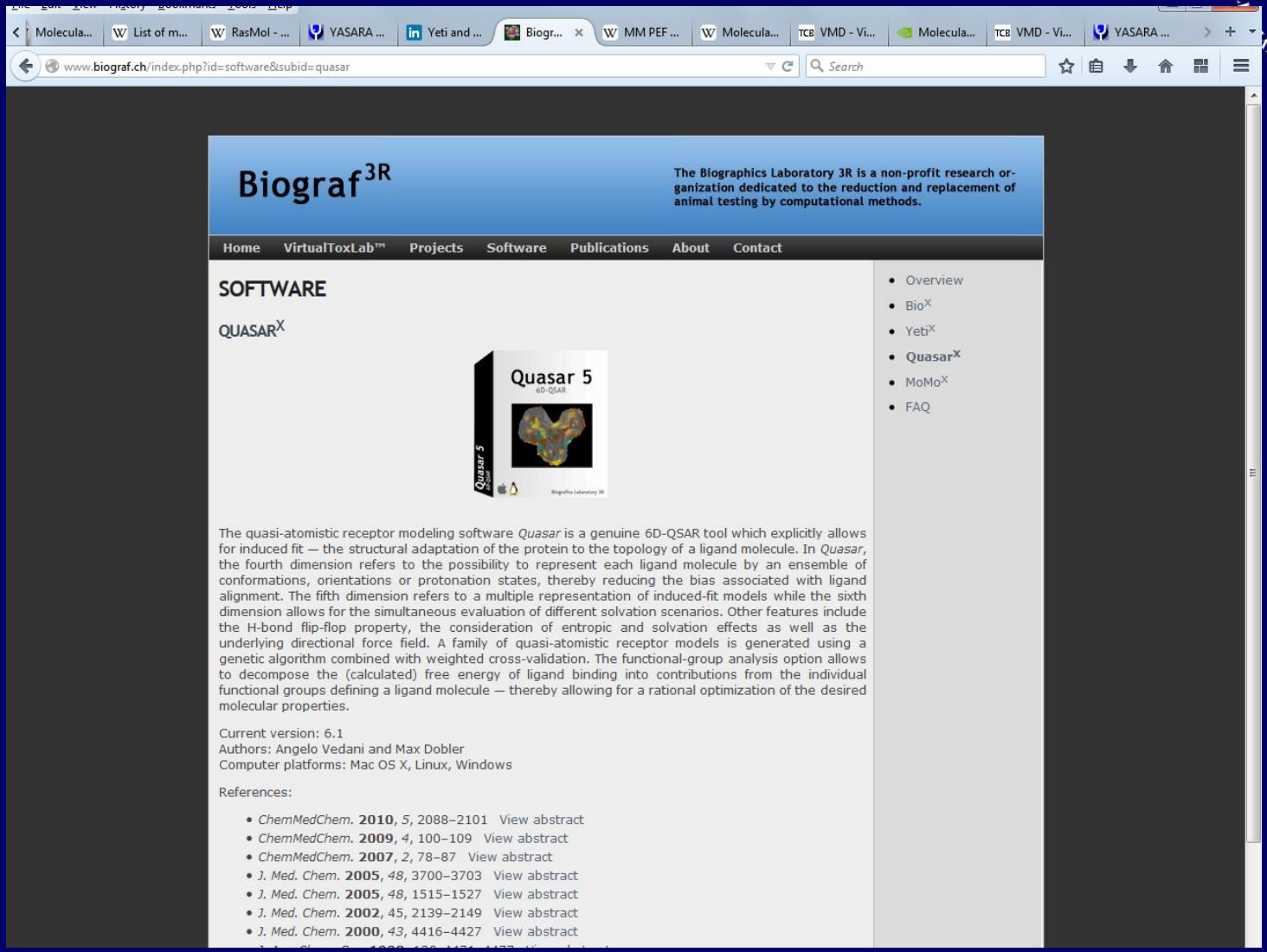
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The quasi-atomistic receptor modeling software Quasar is a genuine 6D-QSAR tool which explicitly allows for induced fit — the structural adaptation of the protein to the topology of a ligand molecule. In Quasar, the fourth dimension refers to the possibility to represent each ligand molecule by an ensemble of conformations, orientations or protonation states, thereby reducing the bias associated with ligand alignment. The fifth dimension refers to a multiple representation of induced-fit models while the sixth dimension allows for the simultaneous evaluation of different solvation scenarios. Other features include the H-bond flip-flop property, the consideration of entropic and solvation effects as well as the underlying directional force field. A family of quasi-atomistic receptor models is generated using a genetic algorithm combined with weighted cross-validation. The functional-group analysis option allows to decompose the (calculated) free energy of ligand binding into contributions from the individual functional groups defining a ligand molecule — thereby allowing for a rational optimization of the desired molecular properties.
Current version: 6.1
Authors: Angelo Vedani and Max Dobler
Computer platforms: Mac OS X, Linux, Windows
References:
ChemMedChem. 2010, 5, 2088–2101 View abstract
ChemMedChem. 2009, 4, 100–109 View abstract
ChemMedChem. 2007, 2, 78–87 View abstract
J. Med. Chem. 2005, 48, 3700–3703 View abstract
J. Med. Chem. 2005, 48, 1515–1527 View abstract
J. Med. Chem. 2002, 45, 2139–2149 View abstract
J. Med. Chem. 2000, 43, 4416–4427 View abstract

www.ks.uiuc.edu/Research/vmd/

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  - NAMD Molecular Dynamics Simulator
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VMD Mailing List

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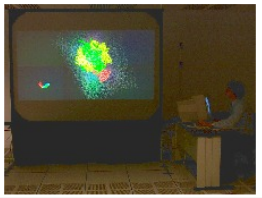
VMD
Visual Molecular Dynamics

VMD is a molecular visualization program for displaying, animating, and analyzing large biomolecular systems using 3-D graphics and built-in scripting. VMD supports computers running MacOS X, Unix, or Windows, is distributed free of charge, and includes source code.
(more details...)

Spotlight

VMD can be used with tiled displays and cluster-based rendering systems for relatively low-cost, high resolution display of molecular geometry. This feature is particularly attractive for institutions with tiled display systems used for auditoriums, or other large-format presentation rooms. The image at the right shows a six projector tiled display at NCSA, running VMD.

Other Spotlights



Overview

Molecular representations
Molecular file formats
GPU-accelerated computing
Interactive molecular dynamics
Programs that use VMD
VMD research publications
How to cite VMD
VMD citation list, (12,743 as of May'14)

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VMD 1.9.1 (MacOS X, Unix, Windows)
VMD plugin library
VMD script library
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Documentation and Support

User and installation guides
Quick help

News and Announcements

Visualization of Energy Conversion Processes in a Light Harvesting Organelle at Atomic Detail, **Winner SC'14 Visualization and Data Analytics Showcase** NEW
Petascale Tcl with NAMD, VMD, and Swift/T NEW
VMD 1.9.2 beta 1 posted for download NEW
Optimizing VMD on GPU-accelerated ARM platforms NEW
GPU-Accelerated Analysis and Visualization of Large Structures Solved by Molecular Dynamics Flexible Fitting, FD169, 2014. NEW
Methodologies for the Analysis of Instantaneous Lipid Diffusion in MD Simulations of Large Membrane Systems, FD169, 2014. NEW
Webinar: GPU-Supercharged Molecular Visualization / Analysis with VMD
2014 VMD Calendar
GPU-accelerated molecular visualization on petascale supercomputing platforms, UltraVis'13
Early Experiences Scaling VMD Molecular Visualization and Analysis Jobs on Blue Waters, Proc. XSCALE, 2013.
Rapid parameterization of small molecules using ffTK, JCC, 2013.
Most cited since 2008: "GPU-Accelerated Molecular Modeling Coming of Age"
VMD QuickSurf rendering of HIV-1 capsid on cover of Nature 497 (7451), 2013.
Lattice microbes: High-performance stochastic simulation method for the reaction-diffusion master equation, J. Comp. Chem, 2013.
Force Field Toolkit (FFTK) tutorial screencasts
Fast Visualization of Gaussian Density Surfaces for Molecular Dynamics and Particle System Trajectories, EuroVis 2012.
Immersive out-of-core visualization of large-size and long-timescale molecular dynamics trajectories, LNCS, 2011.
Past announcements

www.ks.uiuc.edu/Research/namd/

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Download NAMD

Download VMD

Parallel Programming Laboratory

NAMD Scalable Molecular Dynamics

NAMD, recipient of a **2002 Gordon Bell Award** and a **2012 Sidney Fernbach Award**, is a parallel molecular dynamics code designed for high-performance simulation of large biomolecular systems. Based on **Charm++ parallel objects**, NAMD **scales** to hundreds of cores for typical simulations and **beyond 200,000 cores** for the largest simulations. NAMD uses the popular molecular graphics program **VMD** for simulation setup and trajectory analysis, but is also file-compatible with AMBER, CHARMM, and X-PLOR. NAMD is distributed **free of charge** with source code. You can **build** NAMD yourself or download **binaries** for a wide variety of platforms. Our **tutorials** show you how to use NAMD and **VMD** for biomolecular modeling.

The 2005 reference paper **Scalable molecular dynamics with NAMD** has over **4000 citations** as of September 2014.

Wit, grit and a supercomputer yield chemical structure of HIV capsid (article referring to NAMD simulations on **Blue Waters** reported in **Zhao *et al.*, *Nature*, 497:643-646, 2013.**)

Rapid parameterization of small molecules using the force field toolkit, JCC, 2013.

HPCwire Editors' Choice Award: Best use of HPC in life sciences

NAMD Powers *Molecules by Theodore Gray* App for iPhone and iPad NEW

Search all NAMD resources: Search NAMD web site and tutorials Google

Spotlight: Waste into Fuel (Sept 2014)

Other Spotlights

Biofuels are a well-known alternative to the largely used fossil-derived fuels, however the competition with food production is an ethical dilemma. Fortunately a solution is offered by second-generation biofuels, which can be produced from agricultural waste, or more specifically, from plant cell wall polysaccharides. Using the strategy of microorganisms, several enzymes are employed in the production of this advanced biofuel. However the biofuel industry faces problems such as the loss of efficiency of the enzymes that arises over time due to intermittent high concentration of non-suitable substrates. Simulations can guide biochemical experiments aimed at investigating the mechanism that makes the enzymes vulnerable to such substrates, helping the development of more efficient and, thereby, less costly enzymes. A **recent study**, based on molecular modeling with **NAMD**, reported that reduction of efficiency in an important enzyme, know as Man5B, is associated with a loss of the enzyme's flexibility. Molecular dynamis simulations showed that a poor substrate slows down a crucial opening and closing movement of the enzyme's catalytic cleft while a good substrate keeps the movement almost intact. The insight is of crucial importance since it suggests mutations to enzymes presently employed in second-generation biofuel production that need to be replaced less often and, thereby, rendering the production more cost-effective. Read more on our **biofuels website**.

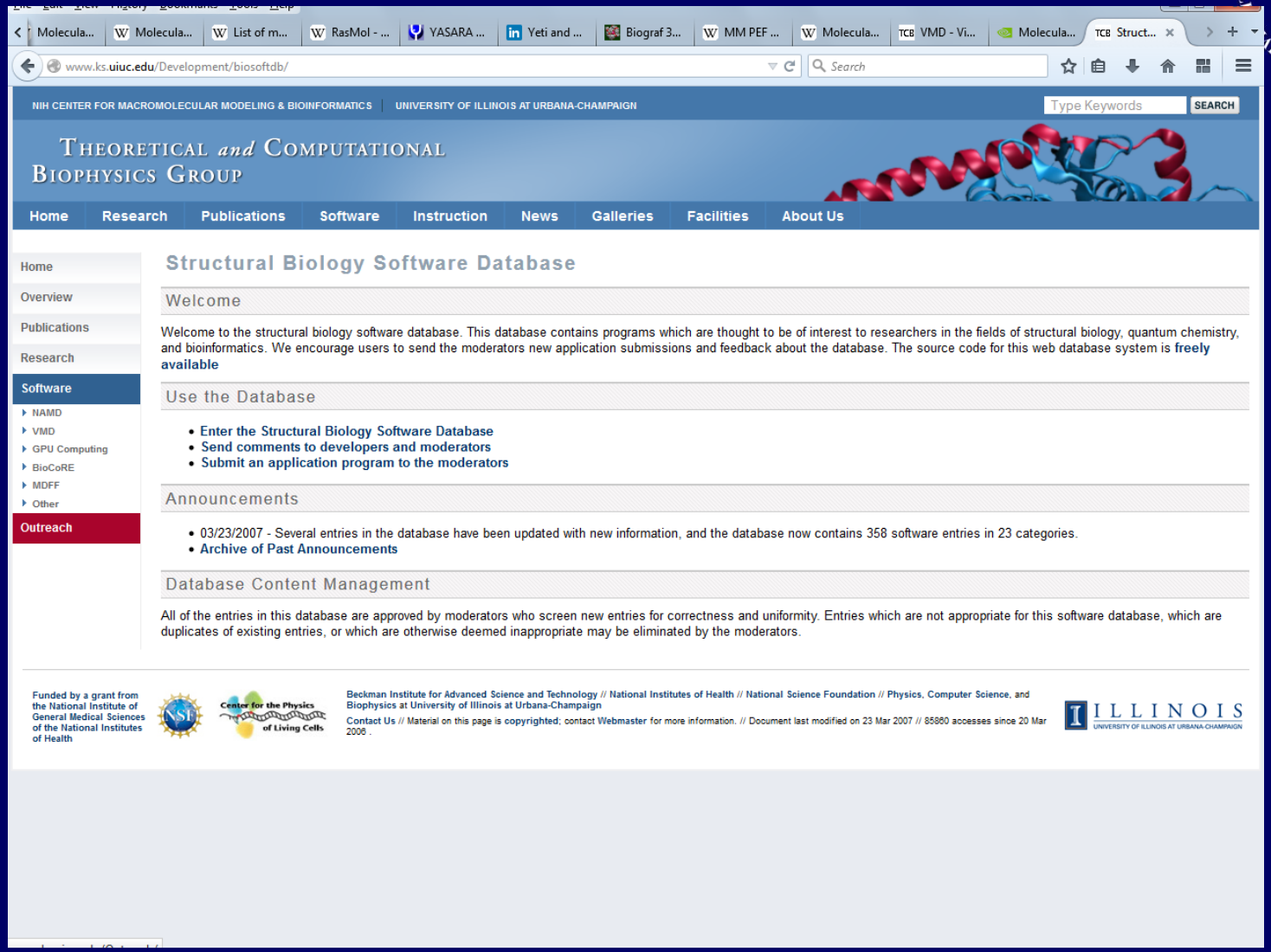
image size: 620.6KB

Overview

Having Problems with NAMD?
Why NAMD? (in pictures)
Molecular Dynamics Flexible Fitting

Announcements

NAMD 2.10 New Features NEW
NAMD 2.10b2 (Nov 2014) NEW
NAMD 2.10b1 (Aug 2014)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Structural Biology Software Database
Welcome
Welcome to the structural biology software database. This database contains programs which are thought to be of interest to researchers in the fields of structural biology, quantum chemistry, and bioinformatics. We encourage users to send the moderators new application submissions and feedback about the database. The source code for this web database system is freely available
Use the Database
Enter the Structural Biology Software Database
Send comments to developers and moderators
Submit an application program to the moderators
Announcements
03/23/2007 - Several entries in the database have been updated with new information, and the database now contains 358 software entries in 23 categories.
Archive of Past Announcements
Database Content Management
All of the entries in this database are approved by moderators who screen new entries for correctness and uniformity. Entries which are not appropriate for this software database, which are duplicates of existing entries, or which are otherwise deemed inappropriate may be eliminated by the moderators.
Funded by a grant from the National Institute of General Medical Sciences of the National Institutes of Health
Center for the Physics of Living Cells
Beckman Institute for Advanced Science and Technology // National Institutes of Health // National Science Foundation // Physics, Computer Science, and Biophysics at University of Illinois at Urbana-Champaign
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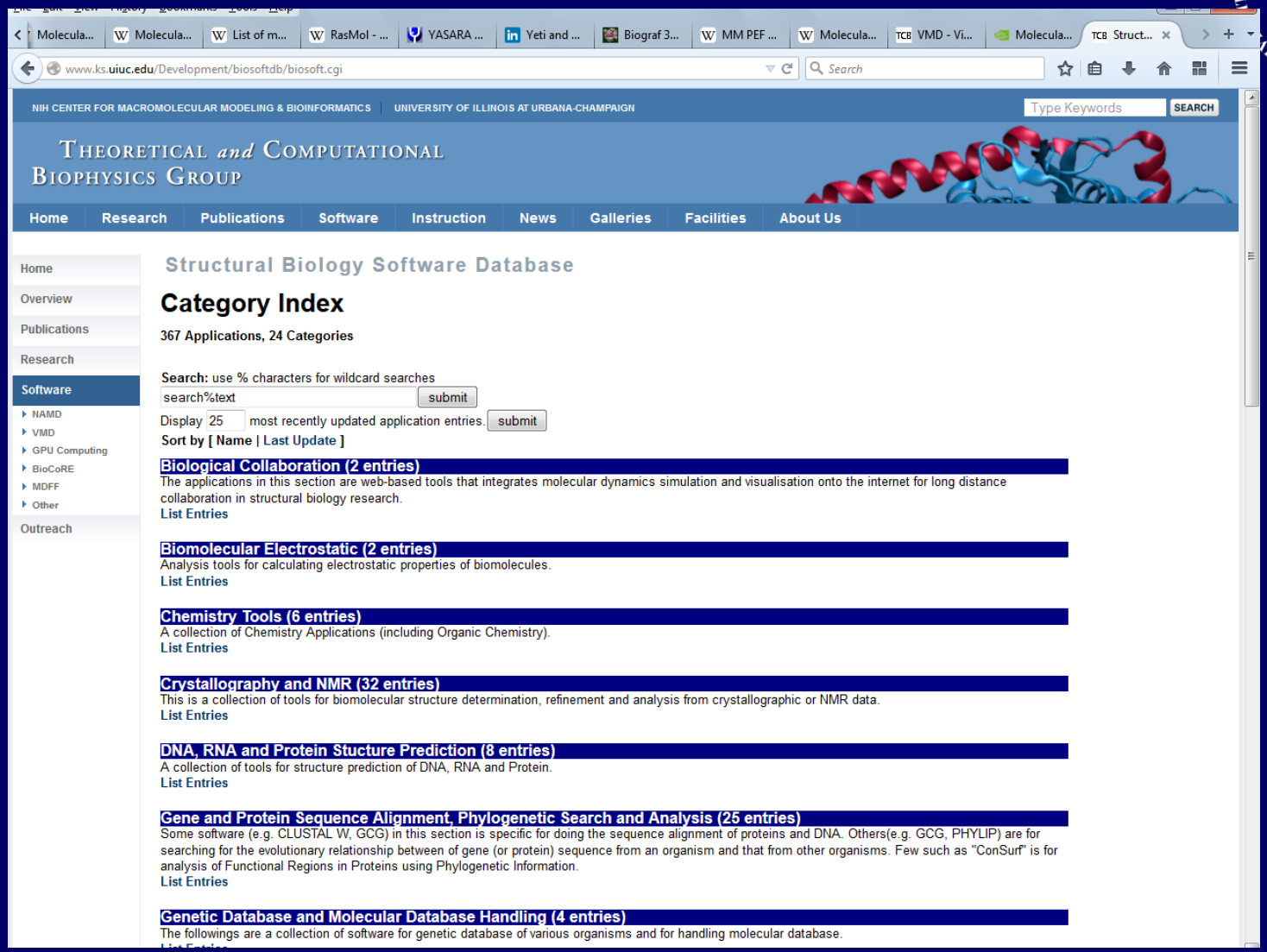
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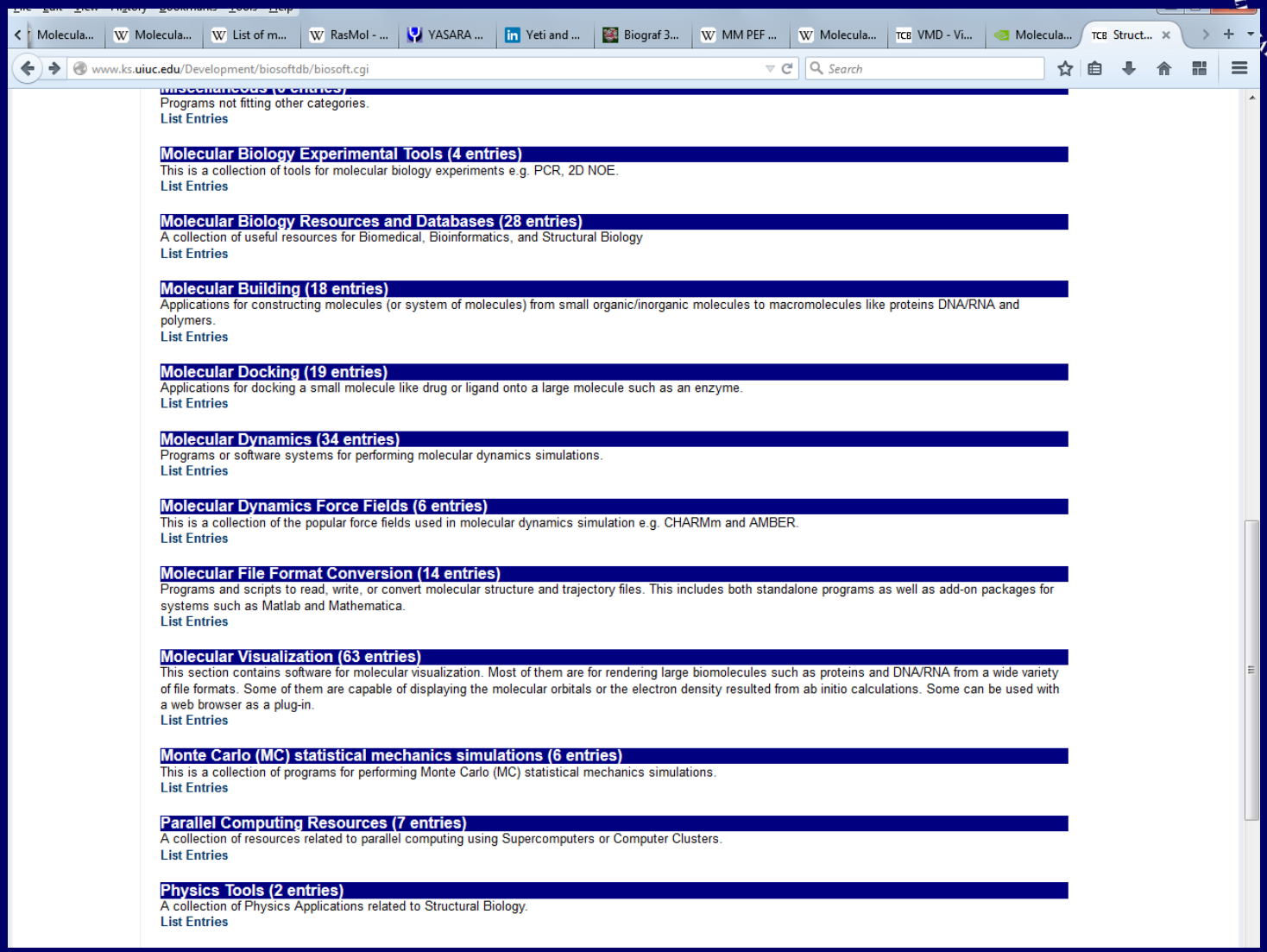
Category Index
367 Applications, 24 Categories
Search: use % characters for wildcard searches
search%text
submit
Display 25 most recently updated application entries.
submit
Sort by [Name | Last Update]
Biological Collaboration (2 entries)
The applications in this section are web-based tools that integrates molecular dynamics simulation and visualisation onto the internet for long distance collaboration in structural biology research.
List Entries
Biomolecular Electrostatic (2 entries)
Analysis tools for calculating electrostatic properties of biomolecules.
List Entries
Chemistry Tools (6 entries)
A collection of Chemistry Applications (including Organic Chemistry).
List Entries
Crystallography and NMR (32 entries)
This is a collection of tools for biomolecular structure determination, refinement and analysis from crystallographic or NMR data.
List Entries
DNA, RNA and Protein Stucture Prediction (8 entries)
A collection of tools for structure prediction of DNA, RNA and Protein.
List Entries
Gene and Protein Sequence Alignment, Phylogenetic Search and Analysis (25 entries)
Some software (e.g. CLUSTAL W, GCG) in this section is specific for doing the sequence alignment of proteins and DNA. Others(e.g. GCG, PHYLIP) are for searching for the evolutionary relationship between of gene (or protein) sequence from an organism and that from other organisms. Few such as "ConSurf" is for analysis of Functional Regions in Proteins using Phylogenetic Information.
List Entries
Genetic Database and Molecular Database Handling (4 entries)
The followings are a collection of software for genetic database of various organisms and for handling molecular database.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VMD - Vi...
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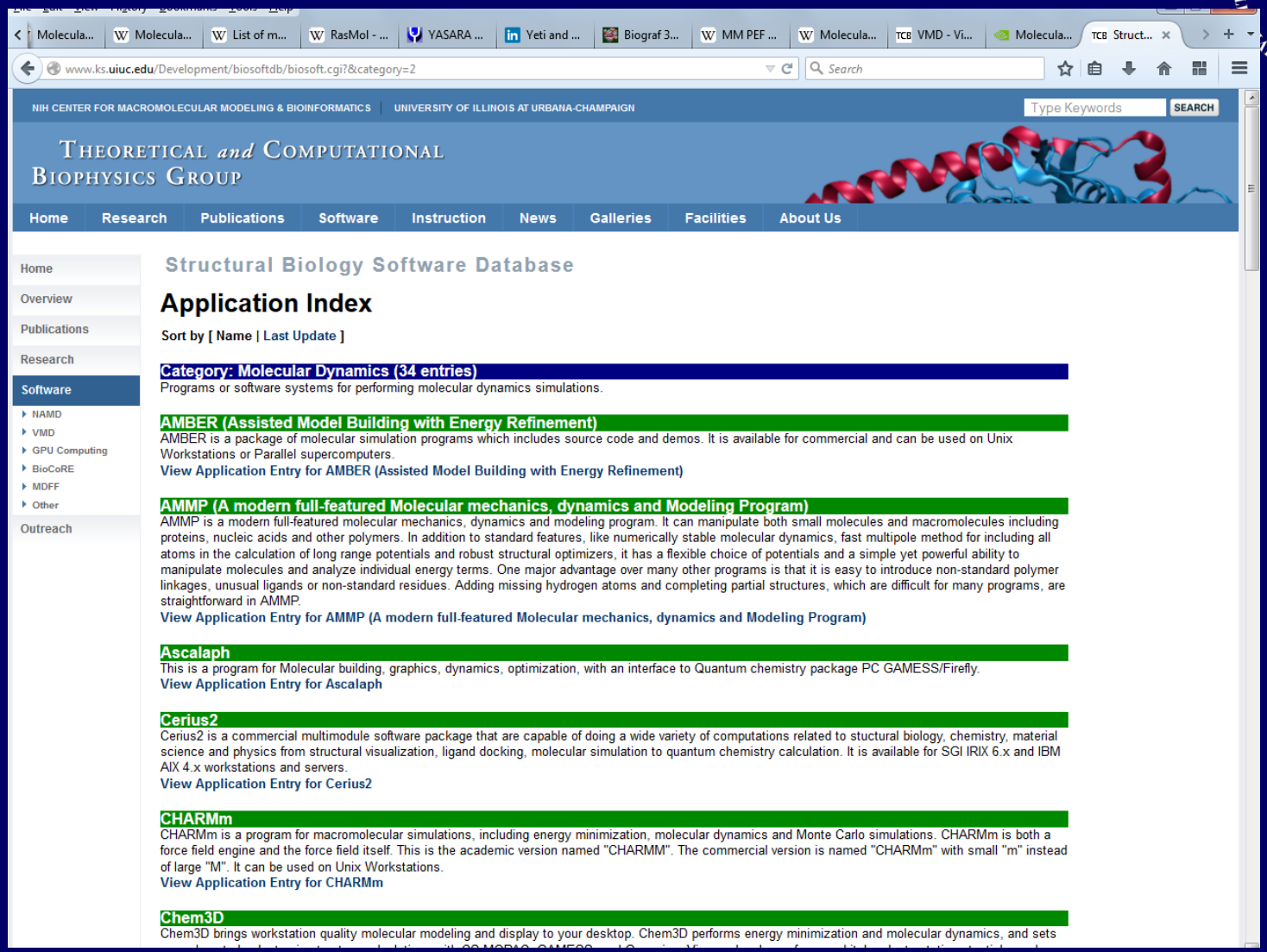
www.ks.uiuc.edu/Development/biosoftdb/biosoft.cgi
Search
Programs not fitting other categories.
List Entries
Molecular Biology Experimental Tools (4 entries)
This is a collection of tools for molecular biology experiments e.g. PCR, 2D NOE.
List Entries
Molecular Biology Resources and Databases (28 entries)
A collection of useful resources for Biomedical, Bioinformatics, and Structural Biology
List Entries
Molecular Building (18 entries)
Applications for constructing molecules (or system of molecules) from small organic/inorganic molecules to macromolecules like proteins DNA/RNA and polymers.
List Entries
Molecular Docking (19 entries)
Applications for docking a small molecule like drug or ligand onto a large molecule such as an enzyme.
List Entries
Molecular Dynamics (34 entries)
Programs or software systems for performing molecular dynamics simulations.
List Entries
Molecular Dynamics Force Fields (6 entries)
This is a collection of the popular force fields used in molecular dynamics simulation e.g. CHARMm and AMBER.
List Entries
Molecular File Format Conversion (14 entries)
Programs and scripts to read, write, or convert molecular structure and trajectory files. This includes both standalone programs as well as add-on packages for systems such as Matlab and Mathematica.
List Entries
Molecular Visualization (63 entries)
This section contains software for molecular visualization. Most of them are for rendering large biomolecules such as proteins and DNA/RNA from a wide variety of file formats. Some of them are capable of displaying the molecular orbitals or the electron density resulted from ab initio calculations. Some can be used with a web browser as a plug-in.
List Entries
Monte Carlo (MC) statistical mechanics simulations (6 entries)
This is a collection of programs for performing Monte Carlo (MC) statistical mechanics simulations.
List Entries
Parallel Computing Resources (7 entries)
A collection of resources related to parallel computing using Supercomputers or Computer Clusters.
List Entries
Physics Tools (2 entries)
A collection of Physics Applications related to Structural Biology.
List Entries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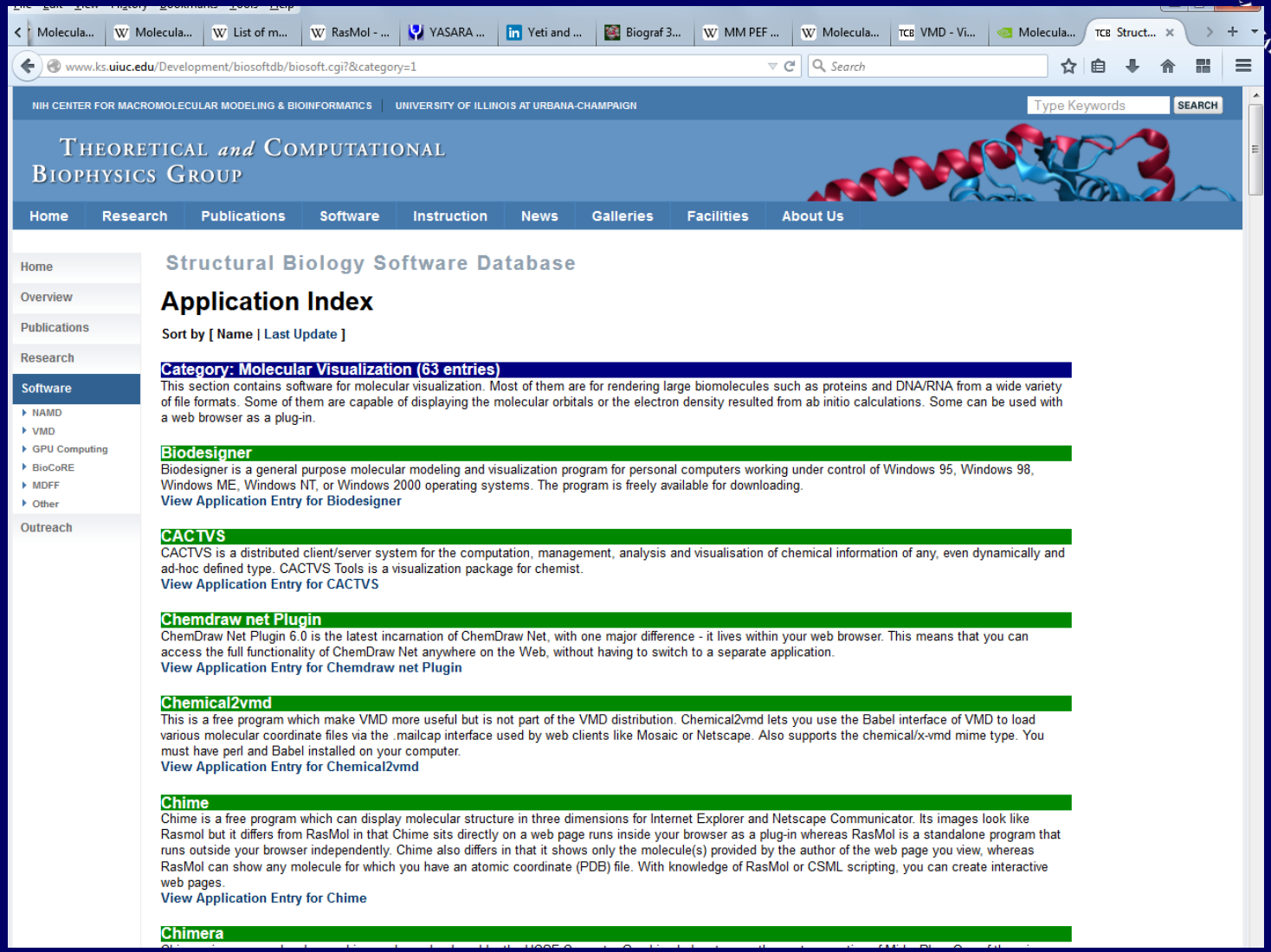
Application Index
Sort by [Name | Last Update]
Category: Molecular Dynamics (34 entries)
Programs or software systems for performing molecular dynamics simulations.
AMBER (Assisted Model Building with Energy Refinement)
AMBER is a package of molecular simulation programs which includes source code and demos. It is available for commercial and can be used on Unix Workstations or Parallel supercomputers.
View Application Entry for AMBER (Assisted Model Building with Energy Refinement)
AMMP (A modern full-featured Molecular mechanics, dynamics and Modeling Program)
AMMP is a modern full-featured molecular mechanics, dynamics and modeling program. It can manipulate both small molecules and macromolecules including proteins, nucleic acids and other polymers. In addition to standard features, like numerically stable molecular dynamics, fast multipole method for including all atoms in the calculation of long range potentials and robust structural optimizers, it has a flexible choice of potentials and a simple yet powerful ability to manipulate molecules and analyze individual energy terms. One major advantage over many other programs is that it is easy to introduce non-standard polymer linkages, unusual ligands or non-standard residues. Adding missing hydrogen atoms and completing partial structures, which are difficult for many programs, are straightforward in AMMP.
View Application Entry for AMMP (A modern full-featured Molecular mechanics, dynamics and Modeling Program)
Ascalaph
This is a program for Molecular building, graphics, dynamics, optimization, with an interface to Quantum chemistry package PC GAMESS/Firefly.
View Application Entry for Ascalaph
Cerius2
Cerius2 is a commercial multimodule software package that are capable of doing a wide variety of computations related to stuctural biology, chemistry, material science and physics from structural visualization, ligand docking, molecular simulation to quantum chemistry calculation. It is available for SGI IRIX 6.x and IBM AIX 4.x workstations and servers.
View Application Entry for Cerius2
CHARMm
CHARMm is a program for macromolecular simulations, including energy minimization, molecular dynamics and Monte Carlo simulations. CHARMm is both a force field engine and the force field itself. This is the academic version named "CHARMM". The commercial version is named "CHARMm" with small "m" instead of large "M". It can be used on Unix Workstations.
View Application Entry for CHARMm
Chem3D
Chem3D brings workstation quality molecular modeling and display to your desktop. Chem3D performs energy minimization and molecular dynamics, and sets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Biodesigner
Biodesigner is a general purpose molecular modeling and visualization program for personal computers working under control of Windows 95, Windows 98, Windows ME, Windows NT, or Windows 2000 operating systems. The program is freely available for downloading.
View Application Entry for Biodesigner
CACTVS
CACTVS is a distributed client/server system for the computation, management, analysis and visualisation of chemical information of any, even dynamically and ad-hoc defined type. CACTVS Tools is a visualization package for chemist.
View Application Entry for CACTVS
Chemdraw net Plugin
ChemDraw Net Plugin 6.0 is the latest incarnation of ChemDraw Net, with one major difference - it lives within your web browser. This means that you can access the full functionality of ChemDraw Net anywhere on the Web, without having to switch to a separate application.
View Application Entry for Chemdraw net Plugin
Chemical2vmd
This is a free program which make VMD more useful but is not part of the VMD distribution. Chemical2vmd lets you use the Babel interface of VMD to load various molecular coordinate files via the .mailcap interface used by web clients like Mosaic or Netscape. Also supports the chemical/x-vmd mime type. You must have perl and Babel installed on your computer.
View Application Entry for Chemical2vmd
Chime
Chime is a free program which can display molecular structure in three dimensions for Internet Explorer and Netscape Communicator. Its images look like Rasmol but it differs from RasMol in that Chime sits directly on a web page runs inside your browser as a plug-in whereas RasMol is a standalone program that runs outside your browser independently. Chime also differs in that it shows only the molecule(s) provided by the author of the web page you view, whereas RasMol can show any molecule for which you have an atomic coordinate (PDB) file. With knowledge of RasMol or CSML scripting, you can create interactive web pages.
View Application Entry for Chime
Chimera

VMD - Visual Molecular Dy... | YASARA - Yet Another Scie... | Biograf 3R - Computational Alt... | Computational Chemistry |... | UCSF Chimera Home Page

https://www.cgl.ucsf.edu/chimera/

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UCSF CHIMERA

an Extensible Molecular Modeling System

UCSF Chimera is a highly extensible program for interactive visualization and analysis of molecular structures and related data, including density maps, supramolecular assemblies, sequence alignments, docking results, trajectories, and conformational ensembles. High-quality images and animations can be generated. Chimera includes complete documentation and several tutorials, and can be downloaded free of charge for academic, government, non-profit, and personal use. Chimera is developed by the Resource for Biocomputing, Visualization, and Informatics, funded by the National Institutes of Health (NIGMS P41-GM103311).

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Recent Citations

Dynamical features of the *Plasmodium falciparum* ribosome during translation. Sun M, Li W *et al. Nucleic Acids Res.* 2015 Dec 2;43(21):10515-24.

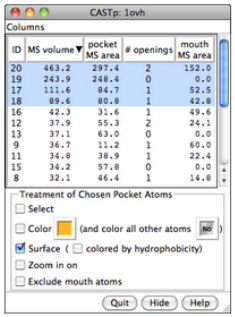
Gating machinery of InsP3R channels revealed by electron cryomicroscopy. Fan G, Baker ML *et al. Nature.* 2015 Nov 19;527(7578):336-41.

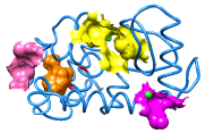
Structural insights into the reaction mechanism of S-adenosyl-L-homocysteine hydrolase. Kusakabe Y, Ishihara M *et al. Sci Rep.* 2015 Nov 17;5:16641.

The molecular architecture of the Dam1 kinetochore complex is defined by cross-linking based structural modelling. Zelter A, Bonomi M *et al. Nat Commun.* 2015 Nov 12;6:8673.

Structure of an RNA polymerase II preinitiation complex. Murakami K, Tsai KL *et al. Proc Natl Acad Sci*

Feature Highlight





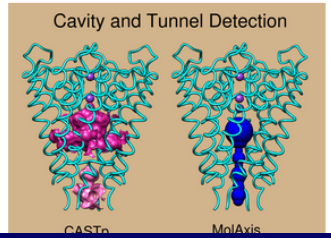
CASTp Pocket Data

Structures and their pocket measurements can be fetched directly from the Computed Atlas of Surface Topography of proteins (CASTp) database or read from local files previously returned by the CASTp server. In Chimera, the pockets are shown in a pocket list. Choosing rows in the list performs actions such as zooming in on pockets and selecting the surrounding atoms.

The figure shows the four largest pockets by volume identified by CASTp for PDB entry 1ovh (a cavity mutant of T4 lysozyme), shown in yellow, orange, pink, and magenta in order of decreasing volume. The largest is lysozyme's active site, with two openings. The second largest is the engineered cavity. Mutated positions are shown in red. Green balls are Cl^- ions.

(More features...)

Gallery Sample



Cavity and Tunnel Detection

Side-by-side views of a potassium channel structure (Protein Data Bank entry 1bl8) showing different approaches to cavity detection. On the left are molecular surface patches corresponding to the structure's two largest pockets by MS volume in the Computed Atlas of Surface Topography of proteins (CASTp) database. On the right is a tunnel in blue identified by the MolAxis server. Simple editing converted MolAxis output into a BILD file for display in Chimera. (More samples...)

Chimera Search

Go

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News

July 23, 2015

Chimera production release 1.10.2 is now available. Fixes include code signing for Mac OS X installation. The 1.10 series will be the last to support OS X 10.6 and 10.7. See the release notes for details.

January 9, 2015

Chimera production release 1.10.1 is now available. 64-bit builds are recommended for all capable platforms, and the 1.10 series will be the last to support OS X 10.6 and 10.7. See the release notes for details.

November 5, 2014

Chimera production release 1.10 is now available. 64-bit builds are recommended for all capable platforms, and v1.10 will be the last to support OS X 10.6 and 10.7. See the release notes for what's new.

(Previous news...)

Upcoming Events

VMD - Visual Molecular Dy... | YASARA - Yet Another Scie... | Biograf 3R - Computational Alt... | Computational Chemistry |... | Getting Started with UCSF ...

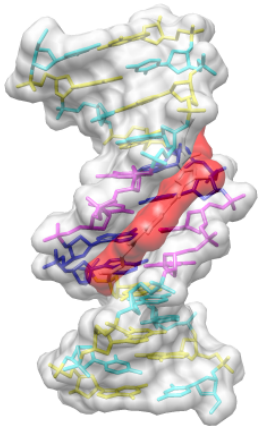
https://www.cgl.ucsf.edu/Outreach/Tutorials/GettingStarted.html

UCSF Chimera - Getting Started

This tutorial provides an overview of basic features in Chimera. You can interact with Chimera using menus and/or commands. The basic features of Chimera are available either way, but not all command functions are available in menus or graphical interfaces, and not all menu or graphical interface functions are available in commands. Thus, it is useful to become familiar with both ways of interacting with Chimera.

The **Working with menus** and **Working with commands** sections are independent of each other and (for the most part) cover identical operations, accomplished in different ways. If you go through both sections, you can skip portions that cover issues you already understand. You can also go back and forth between the sections to see the correspondence between menu and command operations.

Outline:



DNA helix with bound netropsin

Typographical Conventions

Item	Example	Description
Keyboard key	Ctrl	The control key
Mouse key	Btn1	Mouse button 1 (left button)
Menu action	File→Open	File Menu bar pulldown, followed by Open

Working with Menus, Part 1 - Manipulation, Selection, and Chains

← Getting started

VMD - Visual Molecular Dy... | YASARA - Yet Another Scie... | Biograf 3R - Computational Alt... | Computational Chemistry |... | UCSF Chimera Tutorials

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UCSF CHIMERA

an Extensible Molecular Modeling System

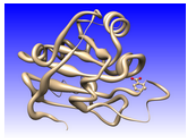
Chimera Tutorials

A set of tutorials is included in the Chimera User's Guide.

The expanded "Getting Started" tutorial is more suitable for printing (more self-contained rather than hyperlinked) than the above.

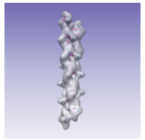
Video tutorials and tutorials from past Chimera workshops are also available.

This page contains still more tutorials.

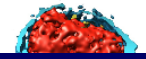


Mapping sequence conservation onto structures, with several example situations and data files. First presented in Fall 2014.

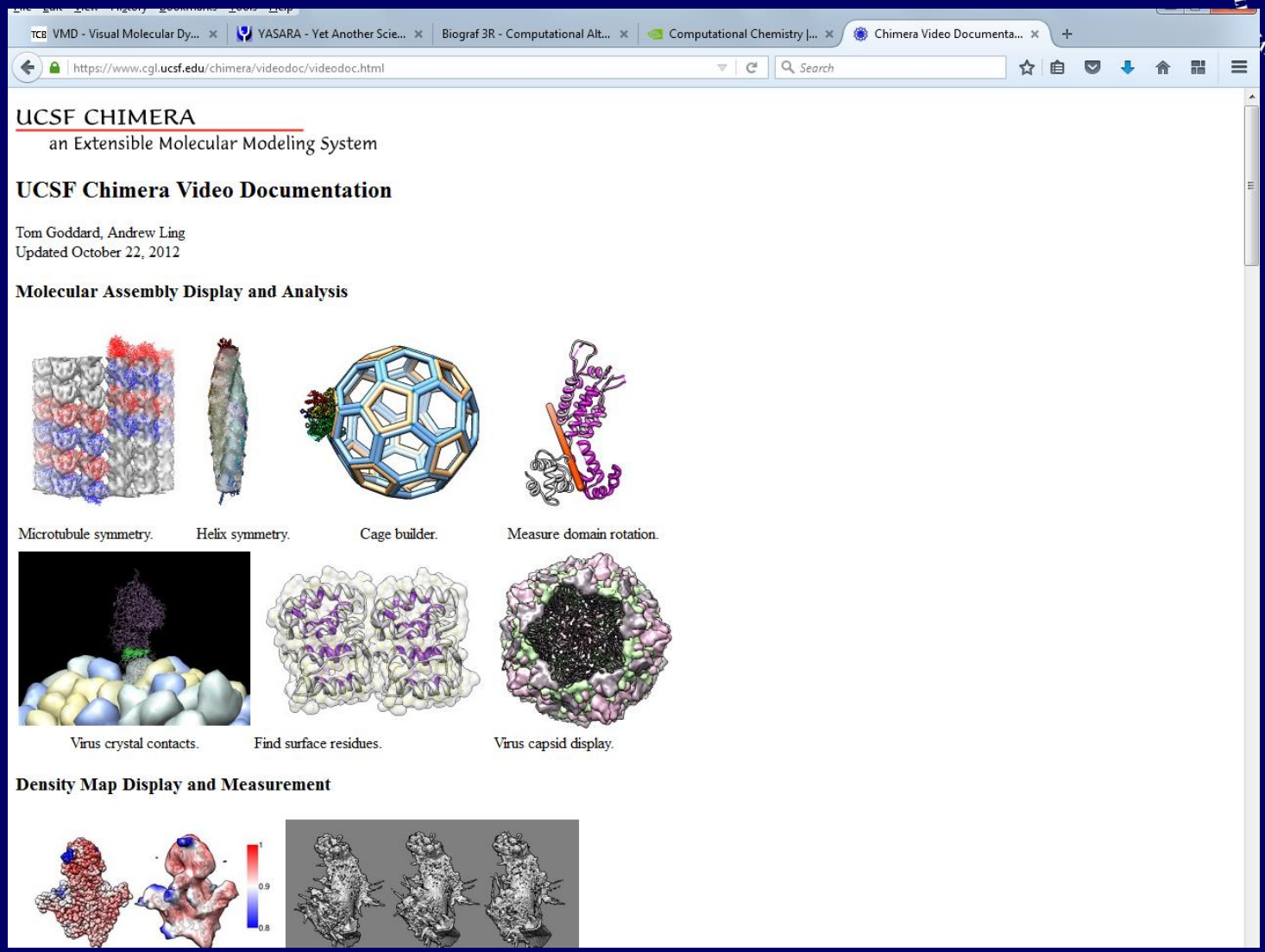
Making animations presented at the NIH Chimera workshop, October 3, 2012. Best viewed in a browser that handles embedded H.264 video (e.g. Chrome or Safari but not Firefox as of Oct 2012).



Making high quality images presented at the National University of Singapore cryoEM workshop, July 12, 2012.



Filtering and segmenting HIV virus electron tomography presented at the NIH Chimera Workshop, October 2-5, 2012, and at the National University of Singapore cryoEM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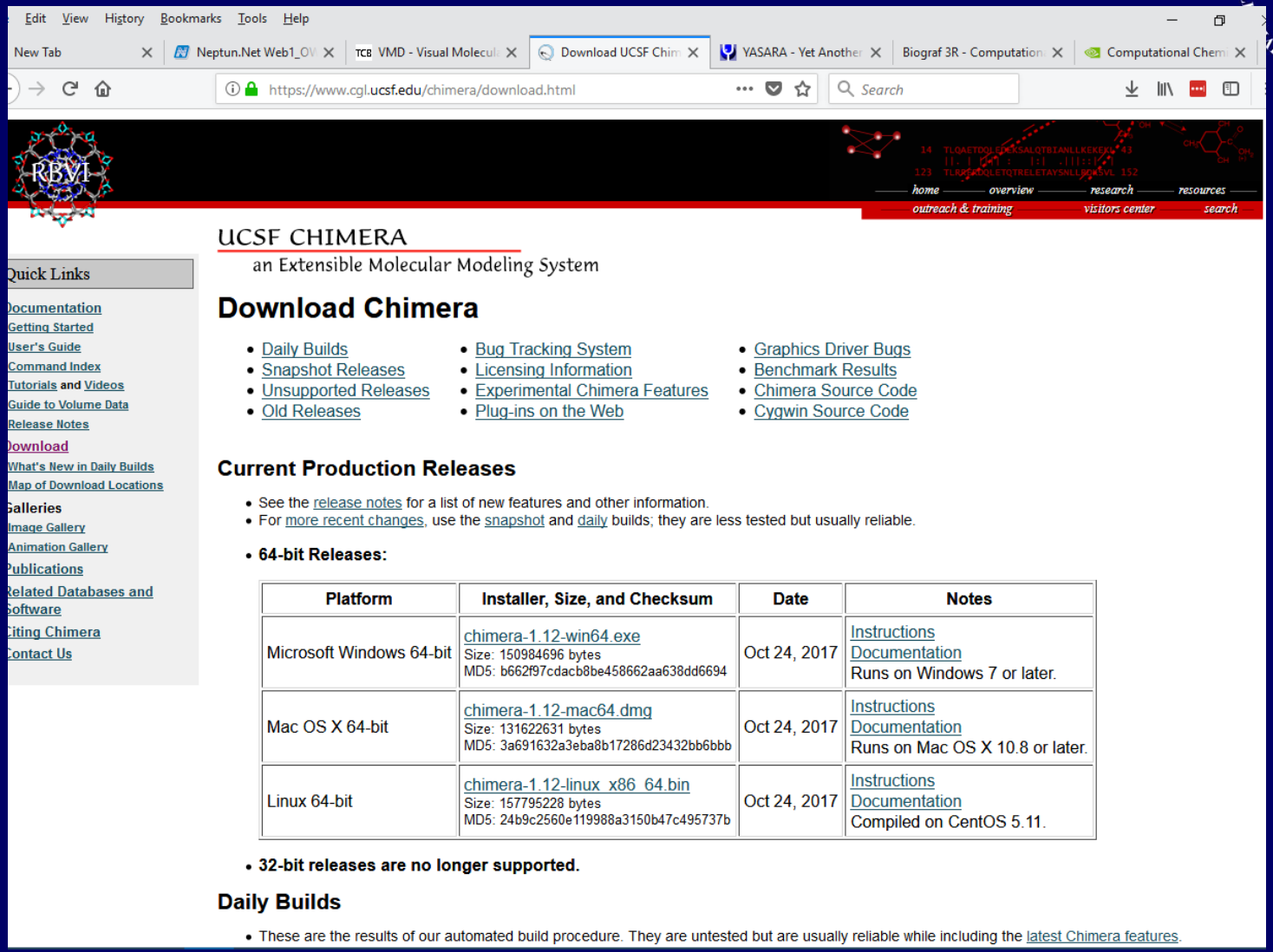
UCSF Chimera Video Documentation
Tom Goddard, Andrew Ling
Updated October 22, 2012
Molecular Assembly Display and Analysis
Microtubule symmetry.
Helix symmetry.
Cage builder.
Measure domain rotation.
Virus crystal contacts.
Find surface residues.
Virus capsid display.
Density Map Display and Measurement



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- Daily Builds
- Snapshot Releases
- Unsupported Releases
- Old Releases
- Bug Tracking System
- Licensing Information
- Experimental Chimera Features
- Plug-ins on the Web
- Graphics Driver Bugs
- Benchmark Results
- Chimera Source Code
- Cygwin Source Code

Current Production Releases

- See the release notes for a list of new features and other information.
- For more recent changes, use the snapshot and daily builds; they are less tested but usually reliable.

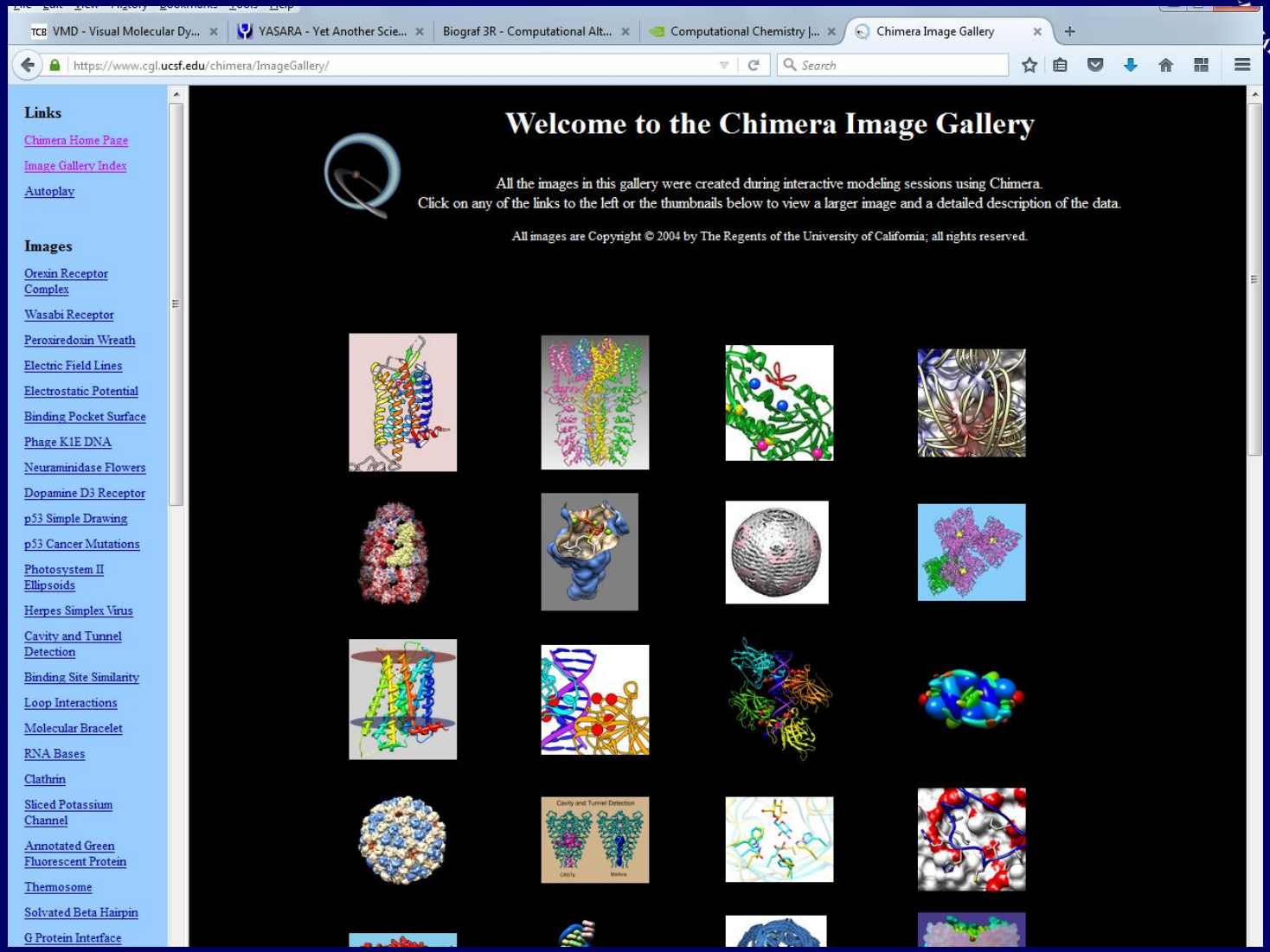
- **64-bit Releases:**

Platform	Installer, Size, and Checksum	Date	Notes
Microsoft Windows 64-bit	chimera-1.12-win64.exe Size: 150984696 bytes MD5: b662f97cdacb8be458662aa638dd6694	Oct 24, 2017	Instructions Documentation Runs on Windows 7 or later.
Mac OS X 64-bit	chimera-1.12-mac64.dmg Size: 131622631 bytes MD5: 3a691632a3eba8b17286d23432bb6bbb	Oct 24, 2017	Instructions Documentation Runs on Mac OS X 10.8 or later.
Linux 64-bit	chimera-1.12-linux_x86_64.bin Size: 157795228 bytes MD5: 24b9c2560e119988a3150b47c495737b	Oct 24, 2017	Instructions Documentation Compiled on CentOS 5.11.

- **32-bit releases are no longer supported.**

Daily Builds

- These are the results of our automated build procedure. They are untested but are usually reliable while including the latest Chimera features.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Computational Chemistry |...
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Wasabi Receptor
Peroxiredoxin Wreath
Electric Field Lines
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Phage K1E DNA
Neuraminidase Flowers
Dopamine D3 Receptor
p53 Simple Drawing
p53 Cancer Mutations
Photosystem II Ellipsoids
Herpes Simplex Virus
Cavity and Tunnel Detection
Binding Site Similarity
Loop Interactions
Molecular Bracelet
RNA Bases
Clathrin
Sliced Potassium Channel
Annotated Green Fluorescent Protein
Thermosome
Solvated Beta Hairpin
G Protein Interface
Welcome to the Chimera Image Gallery
All the images in this gallery were created during interactive modeling sessions using Chimera.
Click on any of the links to the left or the thumbnails below to view a larger image and a detailed description of the data.
All images are Copyright © 2004 by The Regents of the University of California; all rights reserved.

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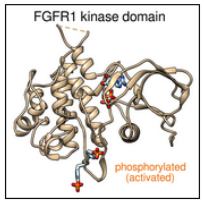
https://www.cgl.ucsf.edu/chimera/animations/animations.html

UCSF CHIMERA

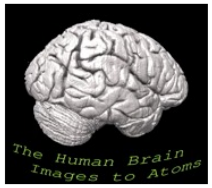
an Extensible Molecular Modeling System

Animations made with UCSF Chimera



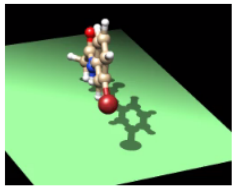
Morphing between the inactive and activated conformations of the FGFR1 kinase domain. June 9, 2014. kinase-morph3.mp4

Morphing between the inactive structure (PDB 3C4F, chain A) and the activated structure (PDB 3GQI, chain A) with phosphorylated tyrosines and bound ATP analog. The protein backbone is shown as a tan ribbon. The tyrosine side chains and ATP analog are shown as sticks, with carbon in light blue, oxygen in red, nitrogen in blue, and phosphorus in orange. Created from Chimera session kinase-morph3.py and command file kinase-morph3.com.



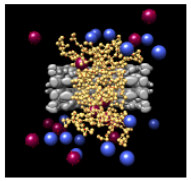
Human Brain: Images to Atoms. January 31, 2014. brain_512x512.mp4 (35 Mb)

Brain imaging and molecular structures. Created for display on a portable planetarium dome for the 2014 Biophysical Society meeting. Video available on YouTube.



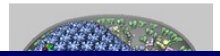
Small molecule rotating and casting shadows on a plane. October 23, 2013.

This simple animation showing interactive shadows was made with the Chimera command script tumble.com. Interactive shadows also work with ribbons and surfaces.



Nuclear pore complex. March 28, 2013. npc.mp4

Brownian dynamics model of transport through the nuclear pore complex. Gray – nuclear pore. Yellow – unstructured FG repeat domains. Red – cargo/transporters. Blue – contaminants.



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https://www.cgl.ucsf.edu/chimera/related/related.html

Chimera-Related Databases and Software

- Databases
- Software
- Mailing Lists

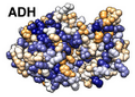
See also: Web services used by UCSF Chimera, sites that provide Chimera Web data, and Chimera plug-ins on the Web

Databases

ASTRAL
Experimentally determined protein structures, divided into domains as defined by SCOP (Structural Classification of Proteins).

Conformational Dynamics Data Bank
Provides conformational dynamics of proteins and protein assemblies from normal mode analysis. CDDB uses Chimera to compute and export surface mesh; data files include density maps that can be viewed in Chimera.

Cube-DB



Database of pre-evaluated conservation and specialization scores for multi-member families of human proteins. Includes downloadable Chimera session files with color-coded structures. Cube-DB is described in Zhang *et al.*, *Nucleic Acids Res* **40**:D490 (2012).

Database for Aligned Ribosomal Complexes (DARC)
Ribosomal structures from the PDB and EMDB aligned into a common frame of reference. Data processed with Chimera, can be viewed with Chimera. DARC is described in Jarasch *et al.*, *Nucleic Acids Res* **40**:D495 (2012).

EM DataBank (EMDB)

This site contains 3D density maps obtained by electron microscopy in CCP4 format that can be shown with Chimera Volume Viewer.

EM Navigator
Presents images, movies, Chimera sessions and details about electron microscopy density maps from the EM DataBank.

Insulin-like Growth Factor Mutation Database
Searchable/browsable repository of IGF mutants and associated receptor-binding data; mutations mapped to structure in Chimera images.

LS-SNP/PDB
A database of human nonsynonymous single-nucleotide polymorphisms (nsSNPs) mapped onto protein structures. Chimera-generated images show SNP locations in the structures and molecular surfaces colored by superfamily sequence conservation and DelPhi-computed electrostatic potential.

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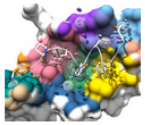
https://www.cgl.ucsf.edu/chimera/related/related.html#software

Software

AlphaSpace



AlphaSpace is a tool for analyzing surface pockets at protein-protein interfaces. AlphaSpace generates a Chimera session file with several "scenes" for viewing the results in different ways. The program is available upon request from the authors for academic use and is described in Rooklin *et al.*, *J Chem Inf Model* **55**:1585 (2015).

Amber

Molecular force field and dynamics simulations. Display trajectories with the Chimera MD Movie extension.

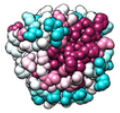
Box Beam Backbone Sculptures

Design protein backbone sculptures made from metal box beams or wood. See also Gurnon, Voss-Andreae, and Stanley, *PLoS Biol* **11**:e1001491 (2013). The new user interface was developed by Evan Zelesnik while the old user interface was made by Tom Goddard.

cellPACK

cellPACK is a tool for assembling large-scale models from molecular building blocks; it integrates structural biology and systems biology data with packing algorithms to assemble comprehensive 3D models of cell-scale structures in molecular detail. Chimera can be used to view and analyze cellPACK models.

ConSurf Server

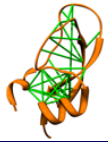


Given a query structure, the server finds related sequences, aligns them, and displays conservation on the structure. Clicking the link to view results in Chimera uses the Chimera web data mechanism to display the structure and sequence alignment colored by conservation, as well as the ConSurf-calculated phylogenetic tree and custom alignment headers (example).

deconSTRUCT Server

The server can compare two structures or search the PDB for structures similar to a query. The resulting pairwise superpositions can be viewed in Jmol and downloaded in various forms, including Chimera sessions.

Direct Coupling Analysis



Direct Coupling Analysis (DCA) is a statistical inference framework for identifying direct co-evolutionary couplings among residue pairs in multiple sequence alignments. A protein multiple sequence alignment can be uploaded to the web service, or the code can be downloaded for local use. The download includes a Matlab implementation and scripts for 3D visualization in Chimera as described in Morcos *et al.*, *Methods Mol Biol* **1137**:55 (2014).

www.nvidia.co.uk/object/molecular_dynamics_uk.html

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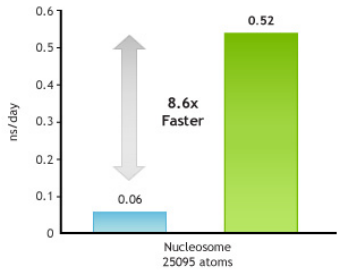
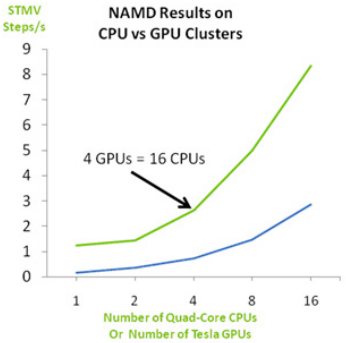
Molecular Dynamics

Molecular dynamics applications are extremely amenable to the massively parallel architecture of NVIDIA's GPUs. In the charts below, we highlight work done on VMD and also molecular dynamics software packages such as NAMD and HOOMD.

With the introduction of NVIDIA Tesla Bio Workbench, it provides bio-physicists and computational chemists the tools to push the boundaries of bio-chemical research, optimizing the scientific workflow and accelerating the pace of research. Learn more.

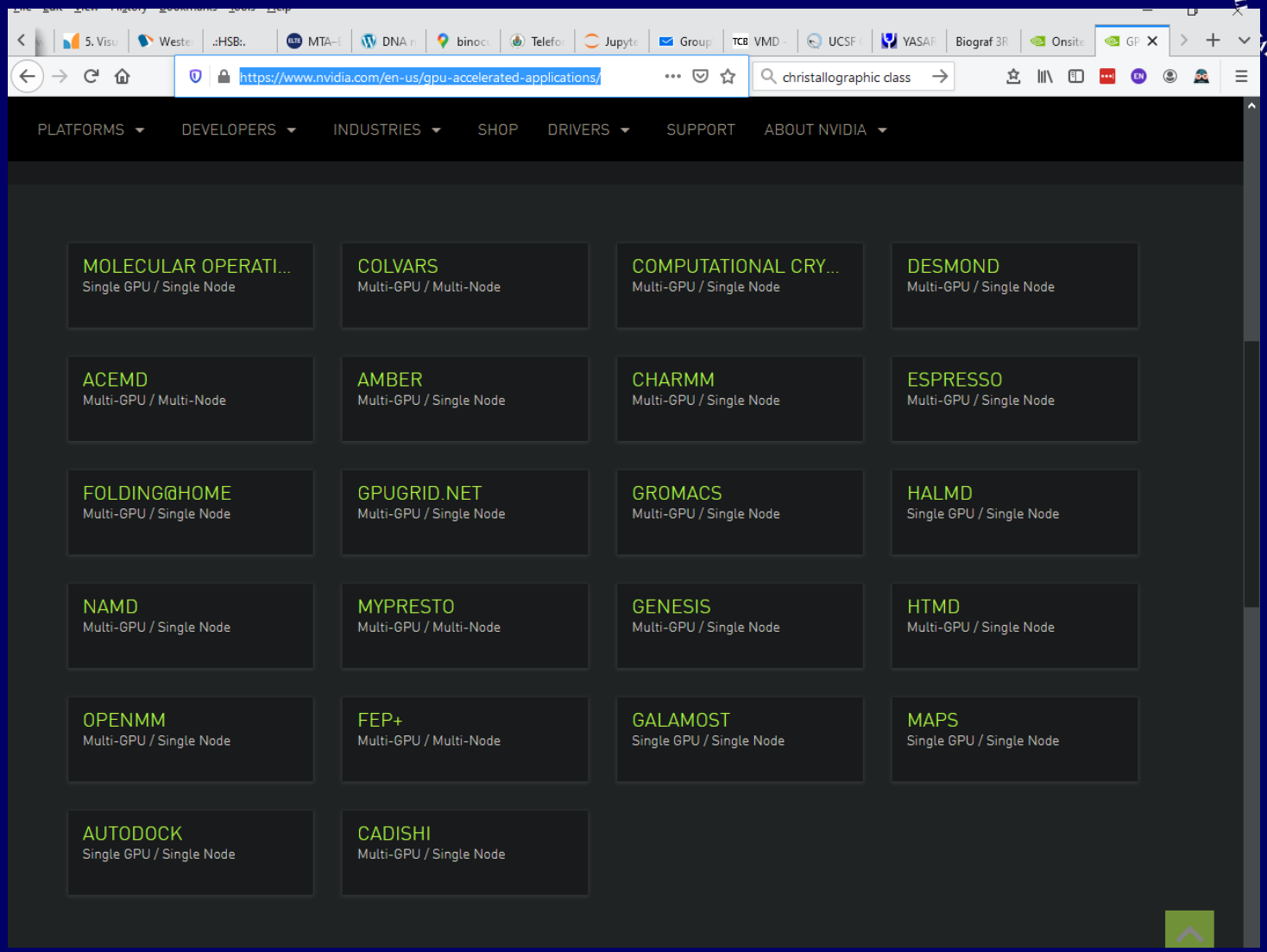


Generalized Born simulation in AMBER
San Diego Supercomputing Center



Scaling of NAMD on a GPU-cluster
Theoretical and Computational Bio-physics Group, UIUC

Learn more about Molecular Dynamic codes by downloading the Life Science Apps Catalog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GROMACS
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NAMD
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GENESIS
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HTMD
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OPENMM
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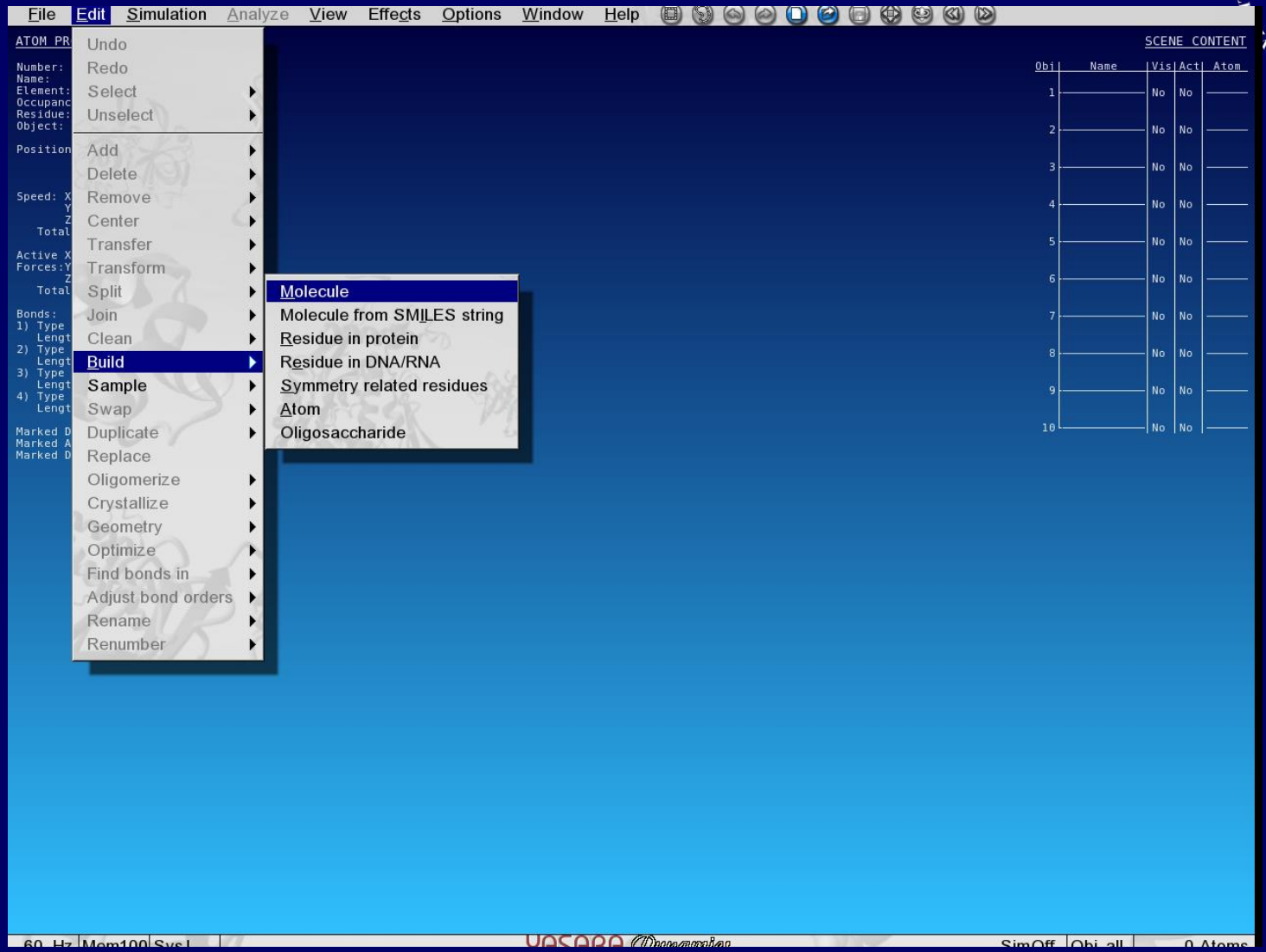
FEP+
Multi-GPU / Multi-Node
GALAMOST
Single GPU / Single Node
MAPS
Single GPU / Single Node
AUTODOCK
Single GPU / Single Node
CADISHI
Multi-GPU / Single Node

Szimuláció indítása előtt

- Vannak hidrogének? (megoldott szerkezetetknél)
- Töltések rendben vannak?
- Erőtér
  - Kiválasztása
  - Hozzárendelése
- Szimulációs lépésköz
- Mehet ……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Swap
Duplicate
Replace
Oligomerize
Crystallize
Geometry
Optimize
Find bonds in
Adjust bond orders
Rename
Renumber
Molecule
Molecule from SMILES string
Residue in protein
Residue in DNA/RNA
Symmetry related residues
Atom
Oligosaccharide
SCENE CONTENT
Obj
Name
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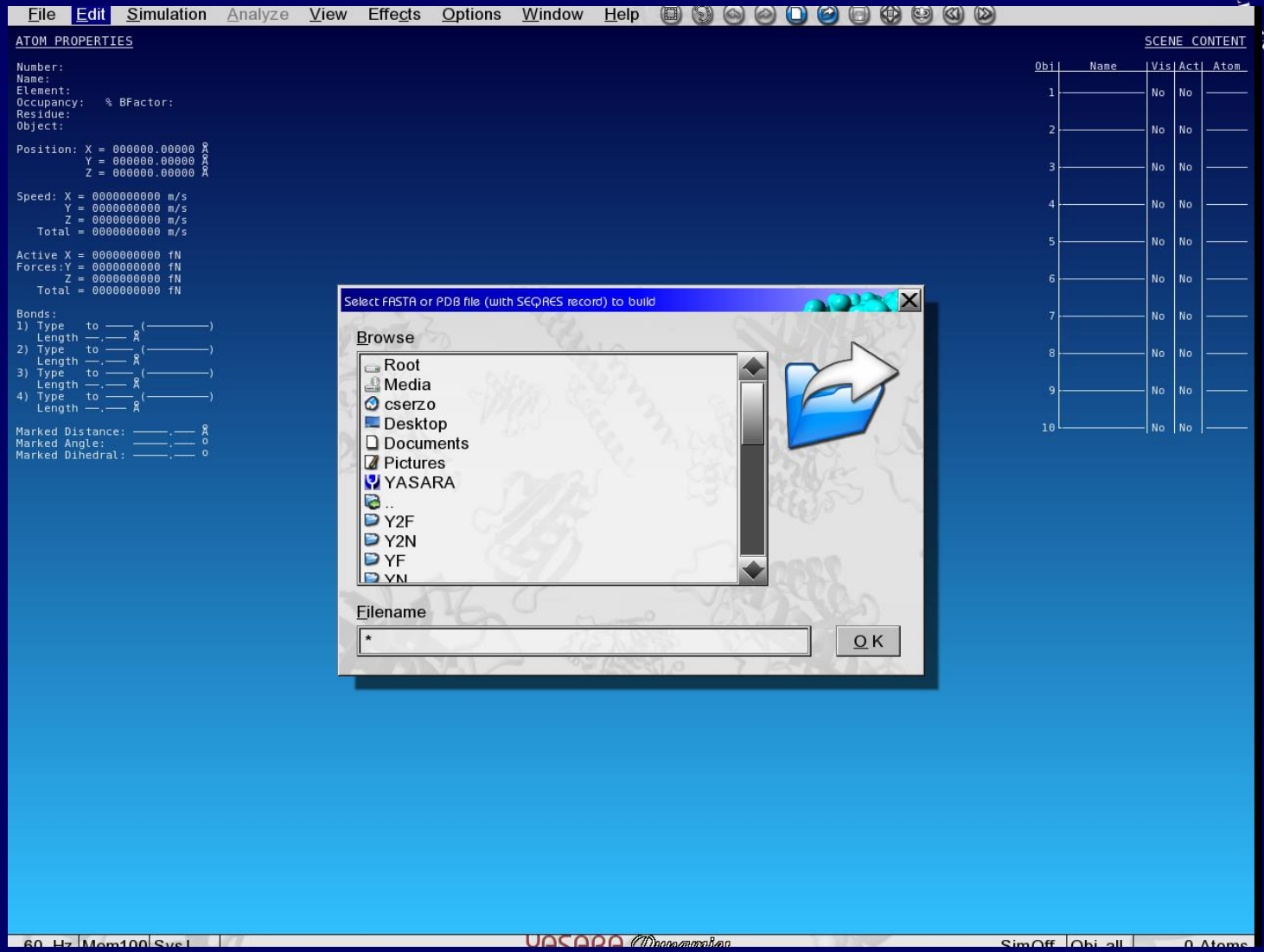
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Y = 0000000000 m/s
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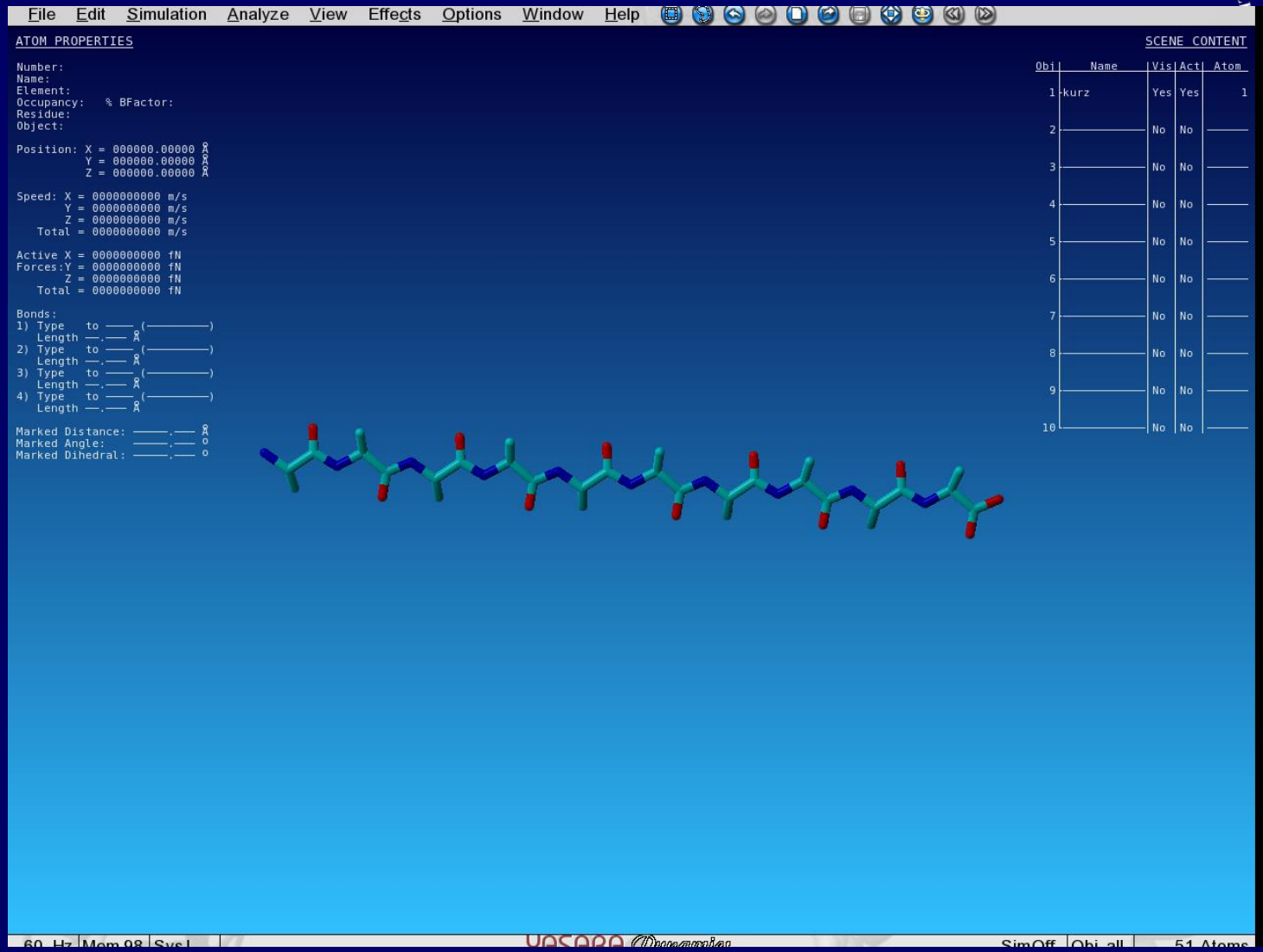
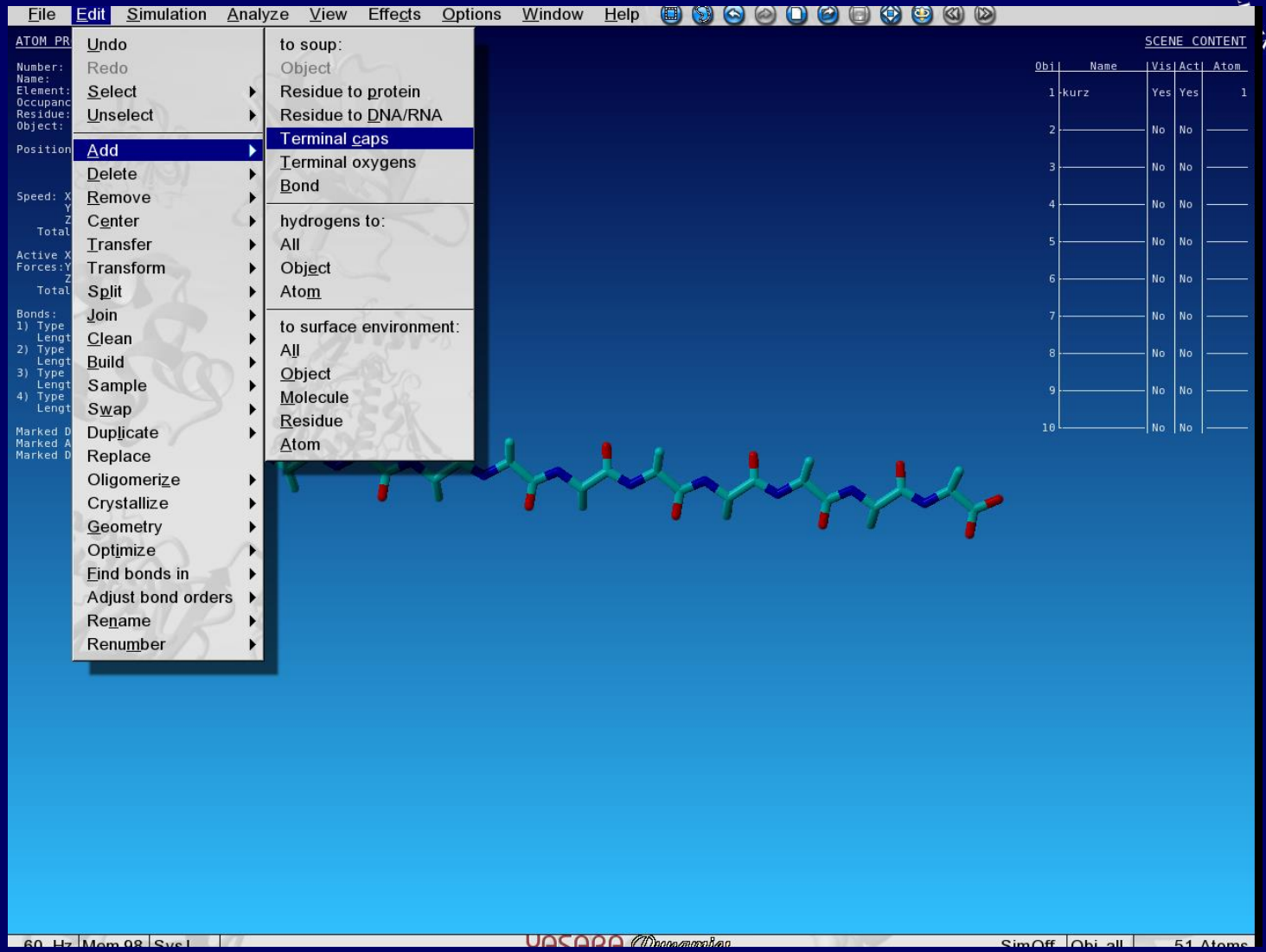
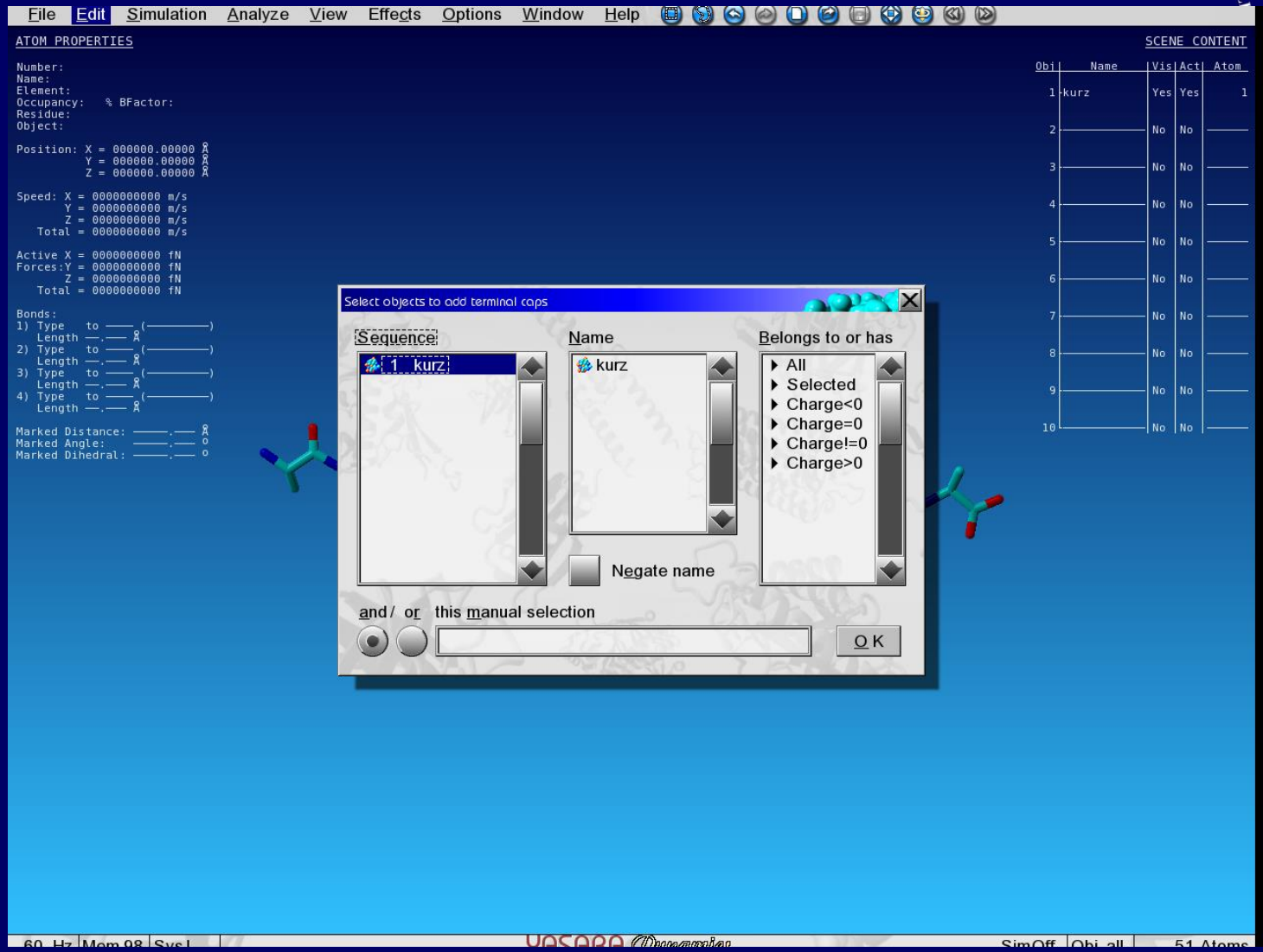
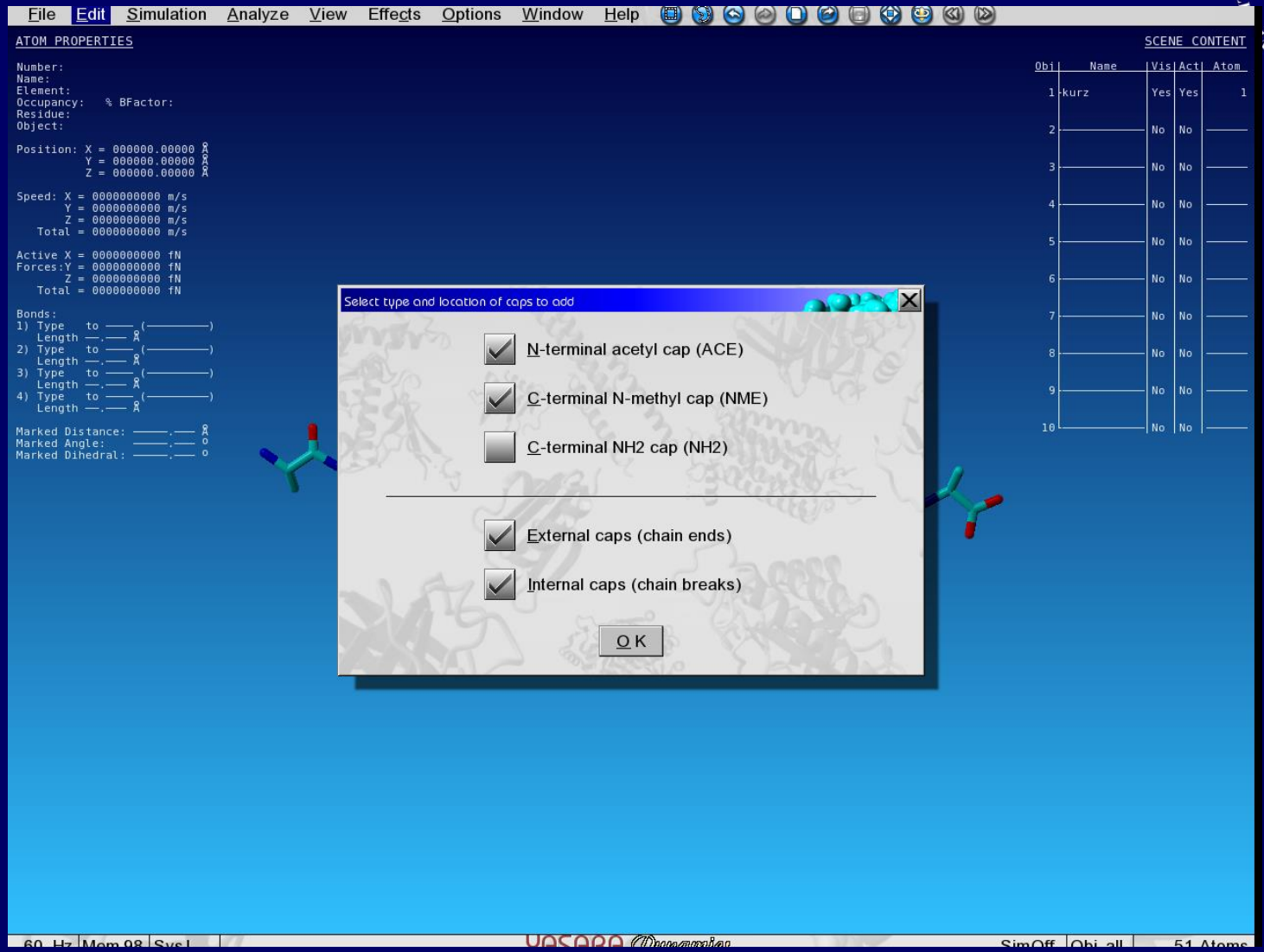
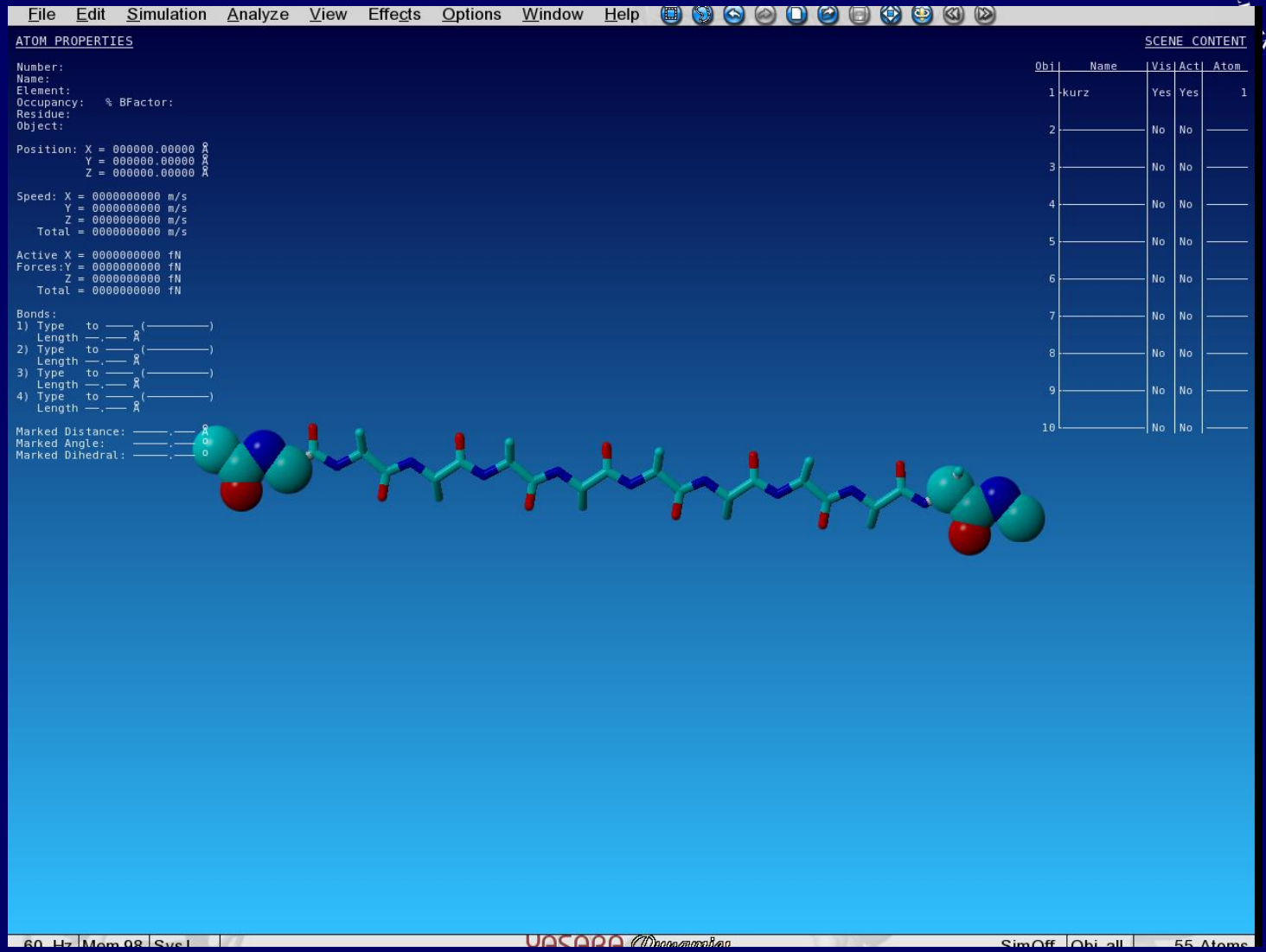
Length ——.—— Å
4) Type to ——— (————————)
Length ——.—— Å
Marked Distance: ———.—— Å
Marked Angle: ———.—— °
Marked Dihedral: ———.—— °
SCENE CONTENT
Obj Name Vis Act Atom
1 No No
2 No No
3 No No
4 No No
5 No No
6 No No
7 No No
8 No No
9 No No
10 No No
Select FASTA or PDB file (with SEQRES record) to build
Browse
Root
Media
cserzo
Desktop
Documents
Pictures
YASARA
..
Y2F
Y2N
YF
YN
Filename
*
OK
60 Hz Mem100 Sys1
SimOff Obj all 0 Atoms

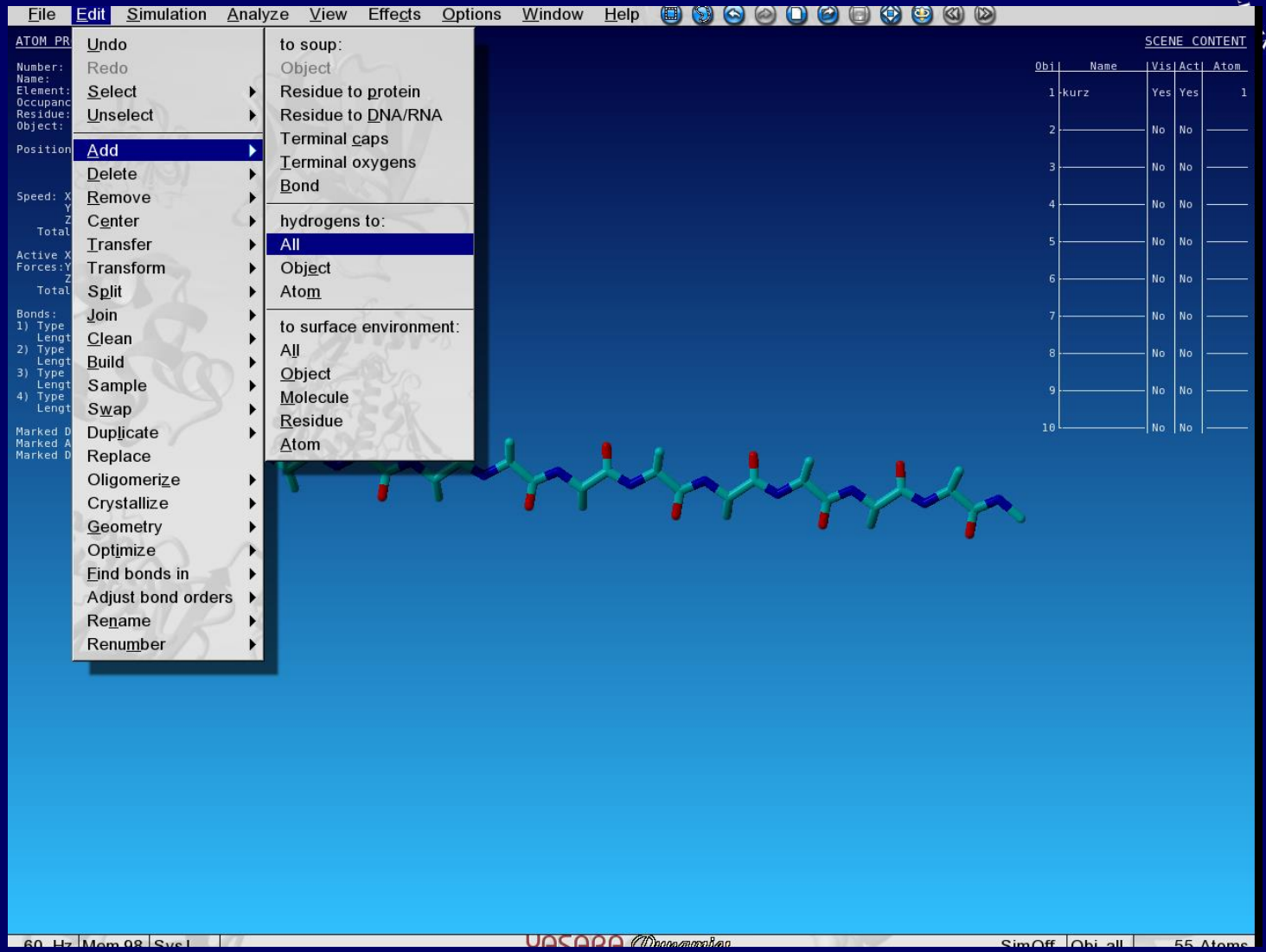

File Edit Simulation Analyze View Effects Options Window Help
ATOM PROPERTIES
Number:
Name:
Element:
Occupancy: % BFactor:
Residue:
Object:
Position: X = 000000.00000 Å
Y = 000000.00000 Å
Z = 000000.00000 Å
Speed: X = 0000000000 m/s
Y = 0000000000 m/s
Z = 0000000000 m/s
Total = 0000000000 m/s
Active X = 0000000000 fN
Forces:Y = 0000000000 fN
Z = 0000000000 fN
Total = 0000000000 fN
Bonds:
1) Type to ——— (————————)
Length ——.—— Å
2) Type to ——— (————————)
Length ——.—— Å
3) Type to ——— (————————)
Length ——.—— Å
4) Type to ——— (————————)
Length ——.—— Å
Marked Distance: ———.—— Å
Marked Angle: ———.—— °
Marked Dihedral: ———.—— °
SCENE CONTENT
Obj Name Vis Act Atom
1 kurz Yes Yes 1
2 No No
3 No No
4 No No
5 No No
6 No No
7 No No
8 No No
9 No No
10 No No
60 Hz Mem 98 Sys I
SimOff Obj all 51 Atoms

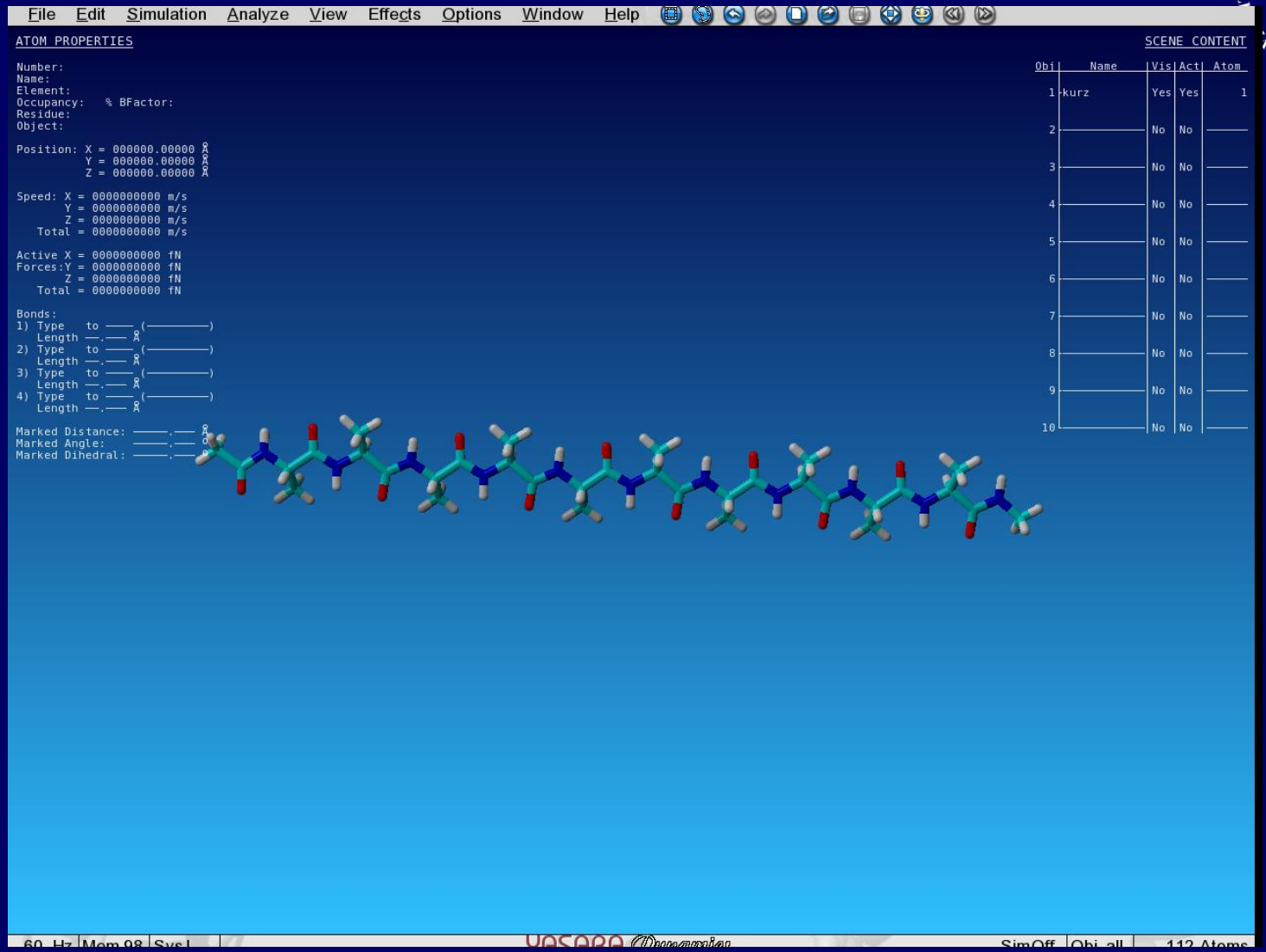

File
Edit
Simulation
Analyze
View
Effects
Options
Window
Help
Undo
Redo
Select
Unselect
Add
Delete
Remove
Center
Transfer
Transform
Split
Join
Clean
Build
Sample
Swap
Duplicate
Replace
Oligomerize
Crystallize
Geometry
Optimize
Find bonds in
Adjust bond orders
Rename
Renumber
to soup:
Object
Residue to protein
Residue to DNA/RNA
Terminal caps
Terminal oxygens
Bond
hydrogens to:
All
Object
Atom
to surface environment:
All
Object
Molecule
Residue
Atom
SCENE CONTENT
Obj
Name
Vis
Act
Atom
1 kurz Yes Yes 1
2 No No
3 No No
4 No No
5 No No
6 No No
7 No No
8 No No
9 No No
10 No No


File Edit Simulation Analyze View Effects Options Window Help
ATOM PROPERTIES
SCENE CONTENT
Select objects to add terminal caps
Sequence
1 kurz
Name
kurz
Belongs to or has
All
Selected
Charge<0
Charge=0
Charge!=0
Charge>0
Negate name
and / or
this manual selection
OK


File Edit Simulation Analyze View Effects Options Window Help
ATOM PROPERTIES
Number:
Name:
Element:
Occupancy: % BFactor:
Residue:
Object:
Position: X = 000000.00000 Å
Y = 000000.00000 Å
Z = 000000.00000 Å
Speed: X = 0000000000 m/s
Y = 0000000000 m/s
Z = 0000000000 m/s
Total = 0000000000 m/s
Active X = 0000000000 fN
Forces:Y = 0000000000 fN
Z = 0000000000 fN
Total = 0000000000 fN
Bonds:
Marked Distance:
Marked Angle:
Marked Dihedral:
SCENE CONTENT
Obj Name Vis Act Atom
1 kurz Yes Yes 1
2 No No
3 No No
4 No No
5 No No
6 No No
7 No No
8 No No
9 No No
10 No No
Select type and location of caps to add
N-terminal acetyl cap (ACE)
C-terminal N-methyl cap (NME)
C-terminal NH2 cap (NH2)
External caps (chain ends)
Internal caps (chain breaks)
O K
60 Hz
SimOff
Obj all
51 Atoms

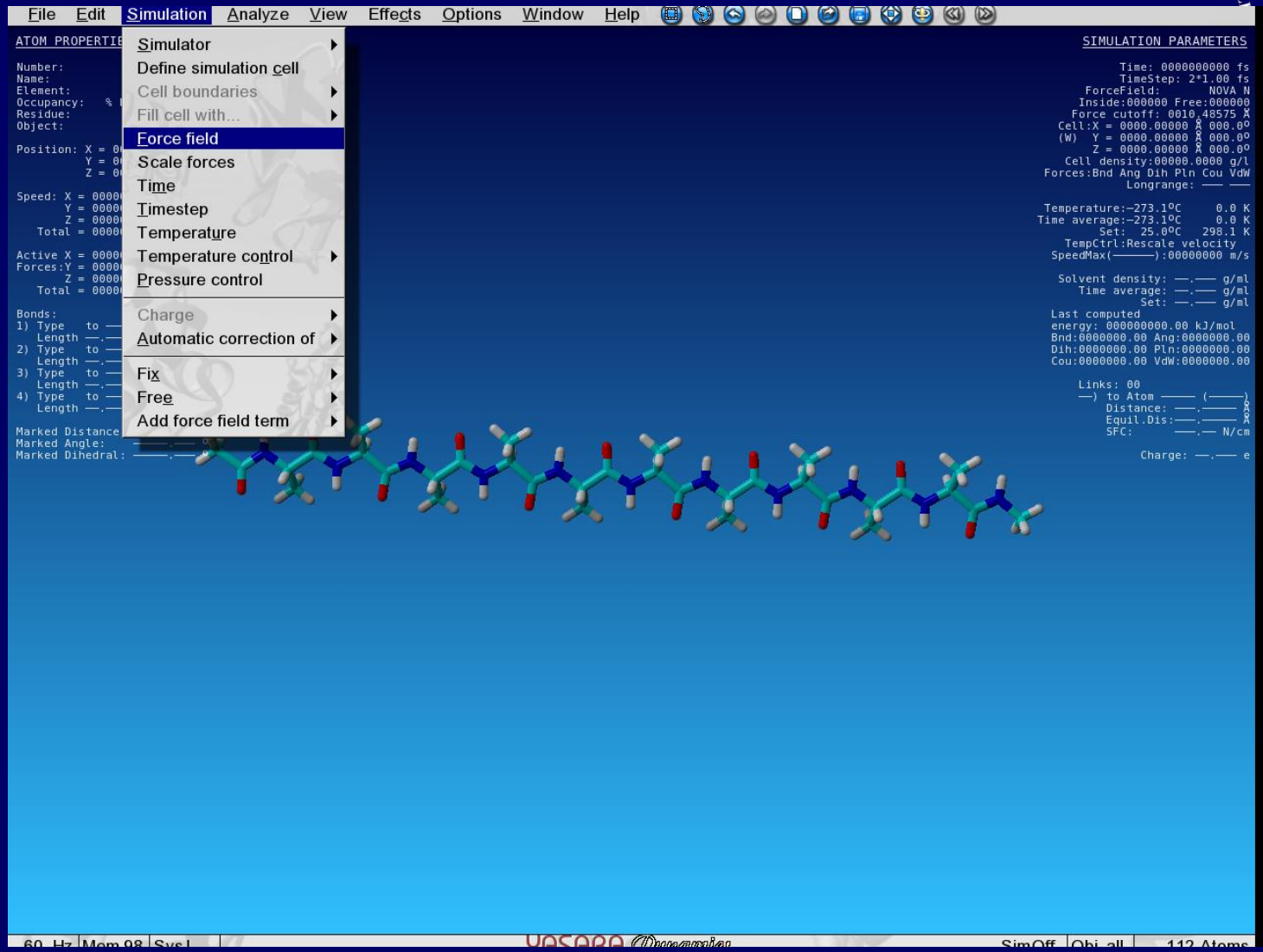

File Edit Simulation Analyze View Effects Options Window Help
ATOM PROPERTIES
Number:
Name:
Element:
Occupancy: % BFactor:
Residue:
Object:
Position: X = 000000.00000 Å
Y = 000000.00000 Å
Z = 000000.00000 Å
Speed: X = 0000000000 m/s
Y = 0000000000 m/s
Z = 0000000000 m/s
Total = 0000000000 m/s
Active X = 0000000000 fN
Forces:Y = 0000000000 fN
Z = 0000000000 fN
Total = 0000000000 fN
Bonds:
1) Type to ——— (————————)
Length ——.—— Å
2) Type to ——— (————————)
Length ——.—— Å
3) Type to ——— (————————)
Length ——.—— Å
4) Type to ——— (————————)
Length ——.—— Å
Marked Distance: ———.—— Å
Marked Angle: ———.——
Marked Dihedral: ———.——
SCENE CONTENT
Obj Name Vis Act Atom
1 kurz Yes Yes 1
2 No No
3 No No
4 No No
5 No No
6 No No
7 No No
8 No No
9 No No
10 No No
60 Hz Mem 98 SysL
SimOff Obj all 55 Atoms

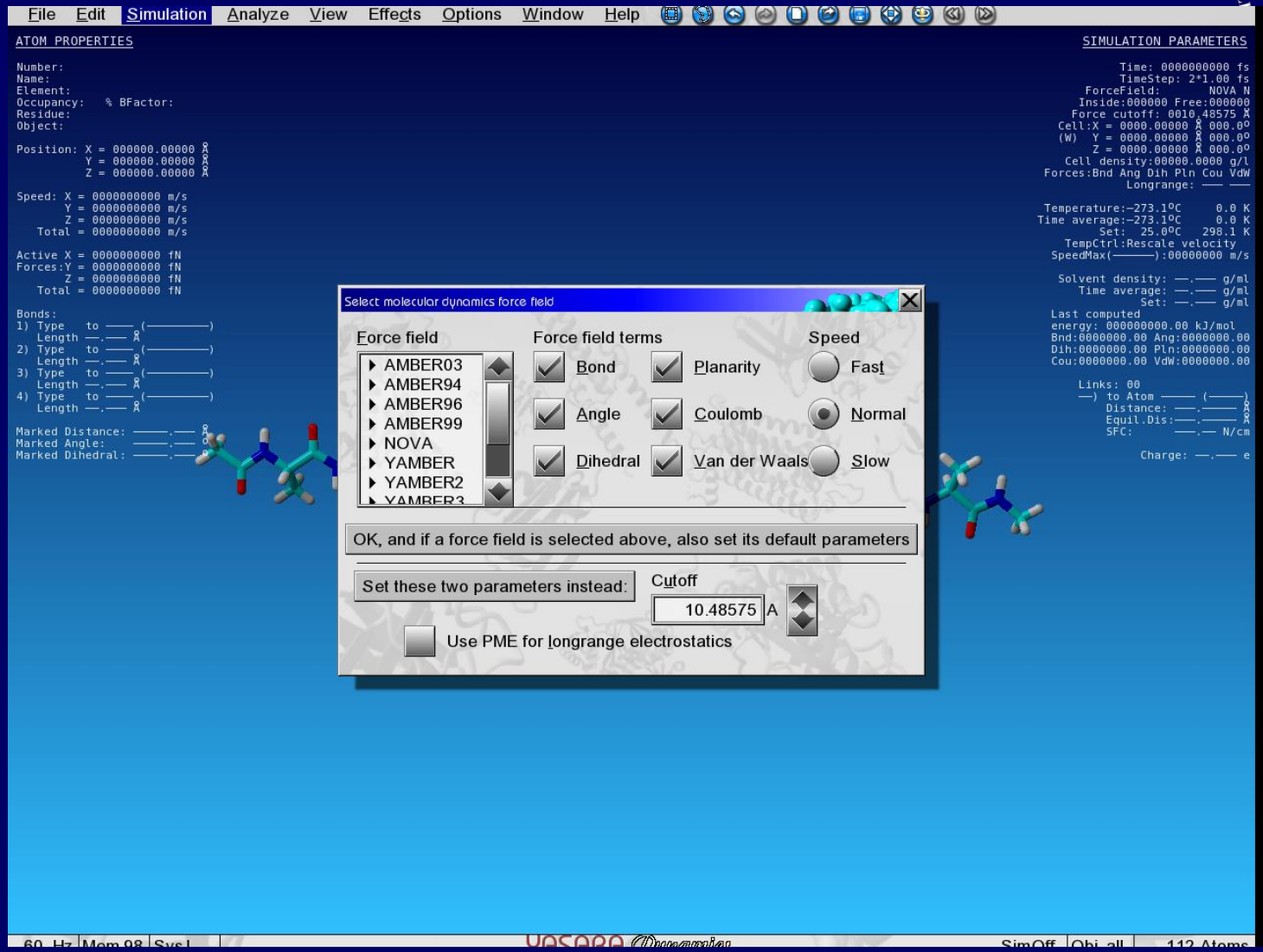

File
Edit
Simulation
Analyze
View
Effects
Options
Window
Help
Undo
Redo
Select
Unselect
Add
Delete
Remove
Center
Transfer
Transform
Split
Join
Clean
Build
Sample
Swap
Duplicate
Replace
Oligomerize
Crystallize
Geometry
Optimize
Find bonds in
Adjust bond orders
Rename
Renumber
to soup:
Object
Residue to protein
Residue to DNA/RNA
Terminal caps
Terminal oxygens
Bond
hydrogens to:
All
Object
Atom
to surface environment:
All
Object
Molecule
Residue
Atom
SCENE CONTENT
Obj
Name
Vis
Act
Atom
1 kurz Yes Yes 1
2 No No
3 No No
4 No No
5 No No
6 No No
7 No No
8 No No
9 No No
10 No No

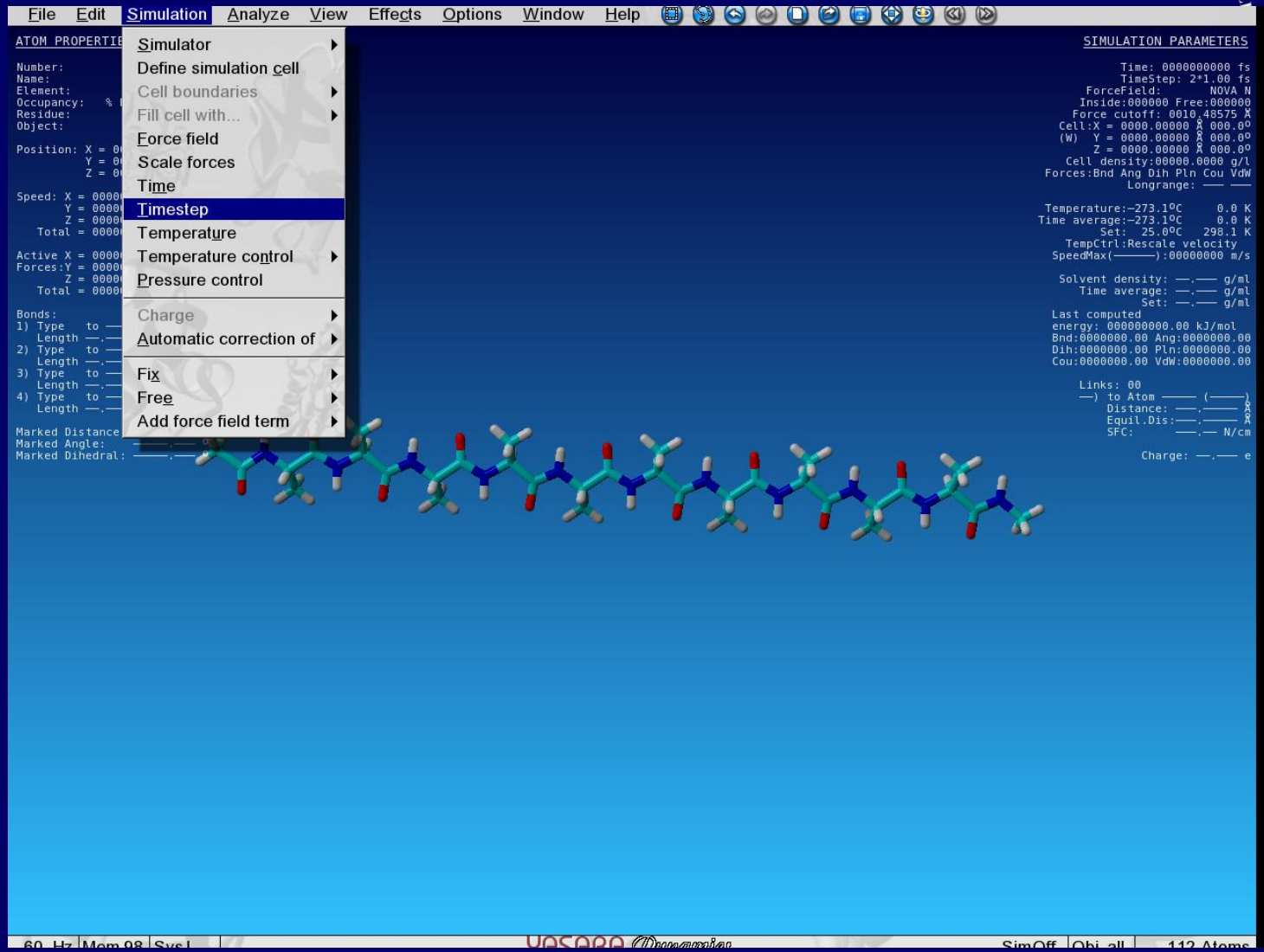

File Edit Simulation Analyze View Effects Options Window Help
ATOM PROPERTIES
Number:
Name:
Element:
Occupancy: % BFactor:
Residue:
Object:
Position: X = 000000.00000 Å
Y = 000000.00000 Å
Z = 000000.00000 Å
Speed: X = 0000000000 m/s
Y = 0000000000 m/s
Z = 0000000000 m/s
Total = 0000000000 m/s
Active X = 0000000000 fN
Forces:Y = 0000000000 fN
Z = 0000000000 fN
Total = 0000000000 fN
Bonds:
1) Type to ——— (————————)
Length ——.—— Å
2) Type to ——— (————————)
Length ——.—— Å
3) Type to ——— (————————)
Length ——.—— Å
4) Type to ——— (————————)
Length ——.—— Å
Marked Distance: ———.—— Å
Marked Angle: ———.—— °
Marked Dihedral: ———.—— °
SCENE CONTENT
Obj Name Vis Act Atom
1 kurz Yes Yes 1
2 No No
3 No No
4 No No
5 No No
6 No No
7 No No
8 No No
9 No No
10 No No
60 Hz Mem 98 Sys I
SimOff Obj all 112 Atoms

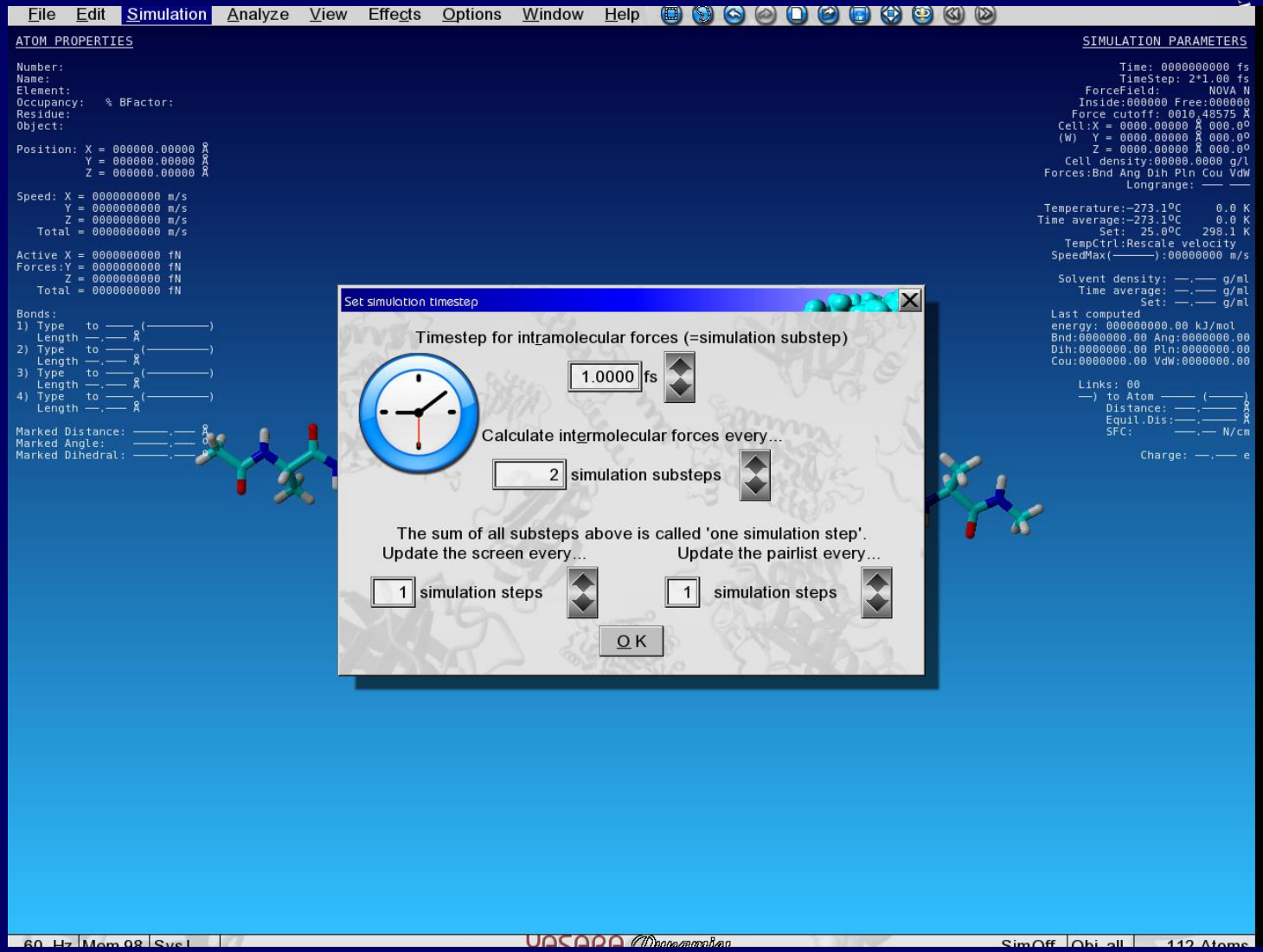
Futtatás

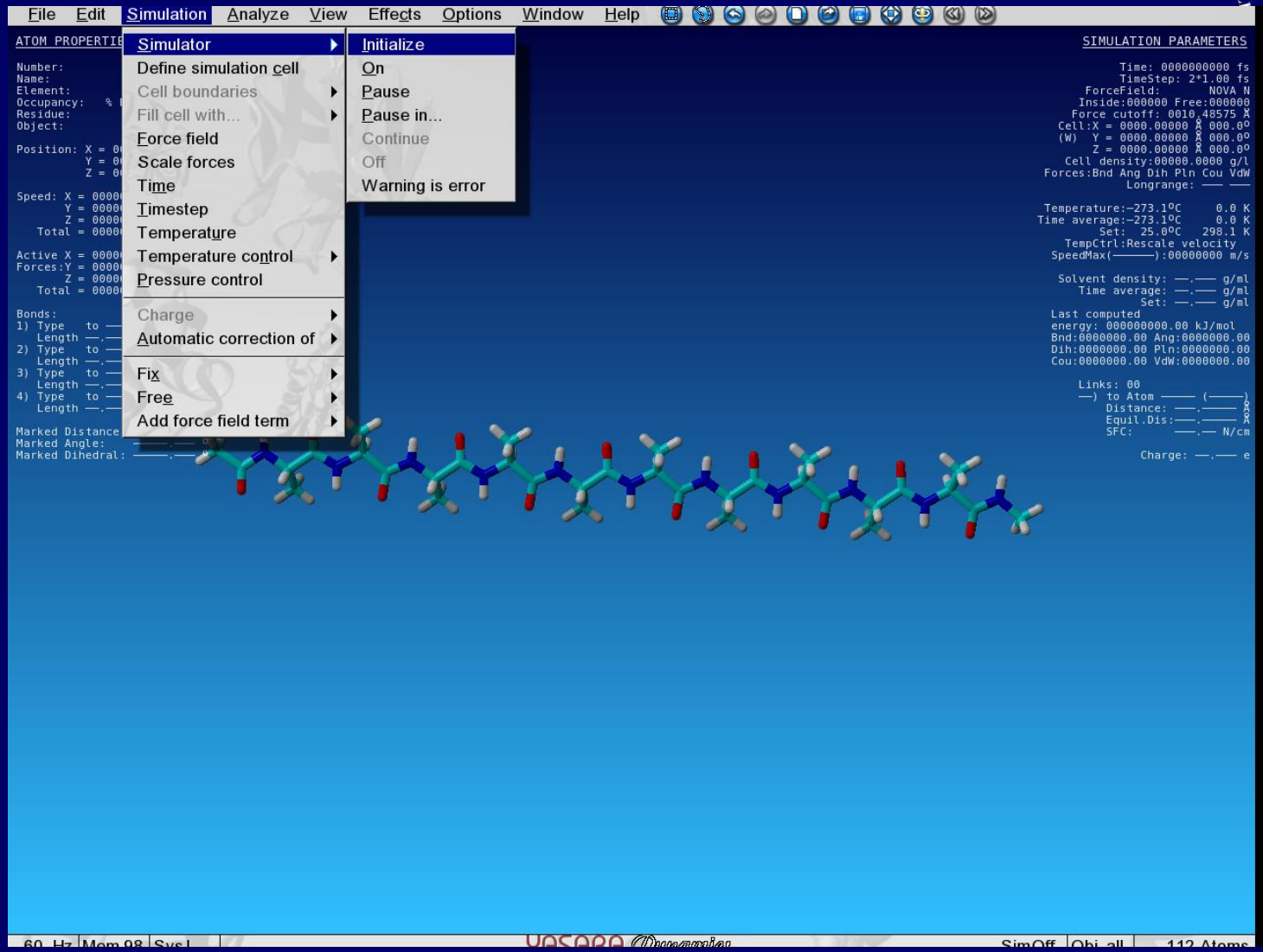
- Kezdeti feszültség oldása: rövid energia minimalizálás
- Dinamika esetén: kezdés alacsony hőmérsékleten – 0 Kº
- Hosszú futás 300 Kº-n – több millió ciklus vagy még több
- Mintavétel pl. 1000 ciklusonként – trajektória

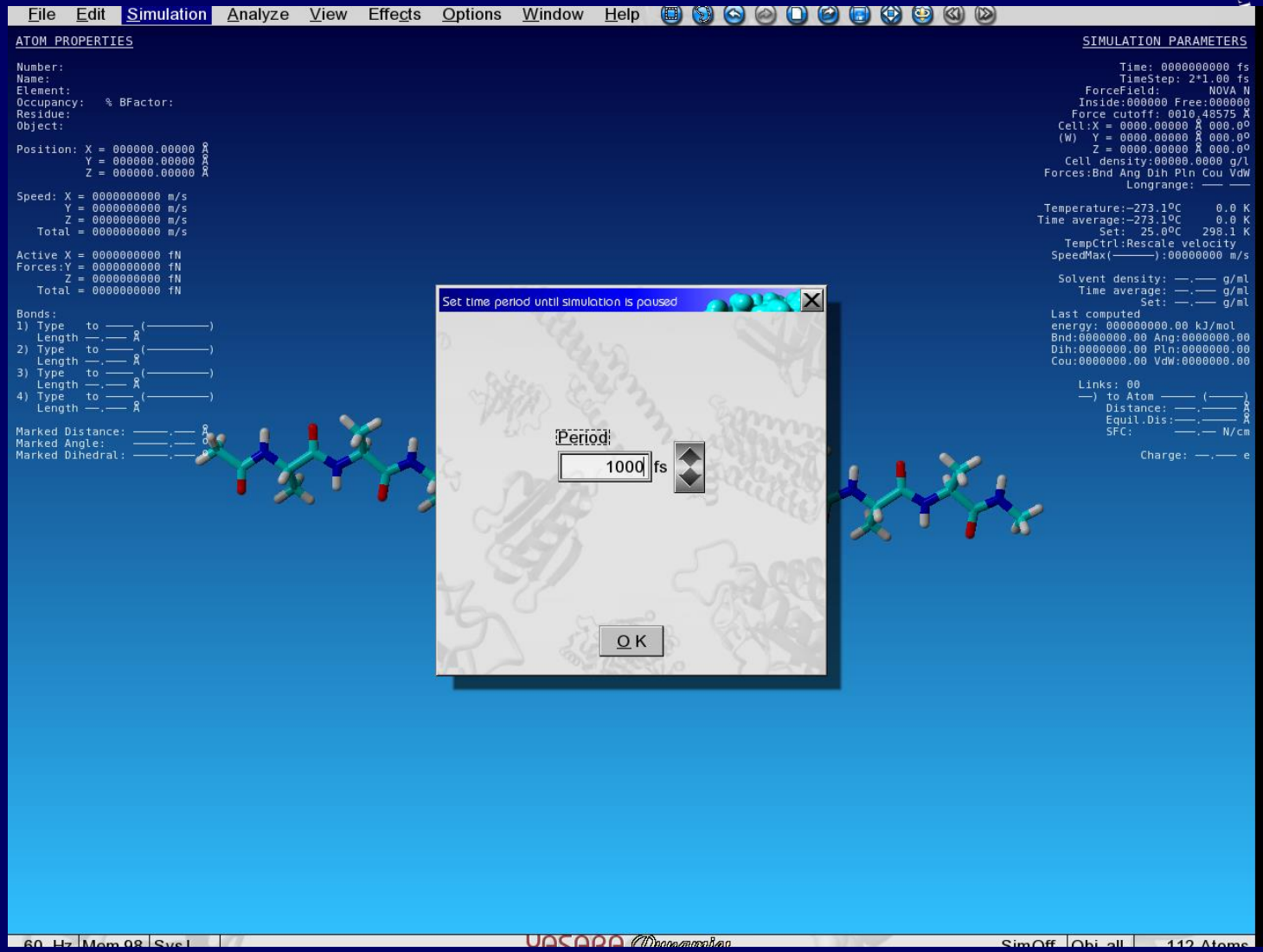

File Edit Simulation Analyze View Effects Options Window Help
Simulator
Define simulation cell
Cell boundaries
Fill cell with...
Force field
Scale forces
Time
Timestep
Temperature
Temperature control
Pressure control
Charge
Automatic correction of
Fix
Free
Add force field term
ATOM PROPERTIE
SIMULATION PARAMETERS
Time: 0000000000 fs
TimeStep: 2*1.00 fs
ForceField: NOVA N
Inside:000000 Free:000000
Force cutoff: 0010.48575 Å
Cell density:00000.0000 g/l
Forces:Bnd Ang Dih Pln Cou VdW
Longrange:
Temperature:-273.1°C 0.0 K
Time average:-273.1°C 0.0 K
Set: 25.0°C 298.1 K
TempCtrl:Rescale velocity
Solvent density:
Time average:
Set:
Last computed
energy: 000000000.00 kJ/mol
Bnd:0000000.00 Ang:0000000.00
Dih:0000000.00 Pln:0000000.00
Cou:0000000.00 VdW:0000000.00
Links: 00
Distance:
Equil.Dis:
SFC:
Charge:
60 Hz
SimOff
112 Atoms

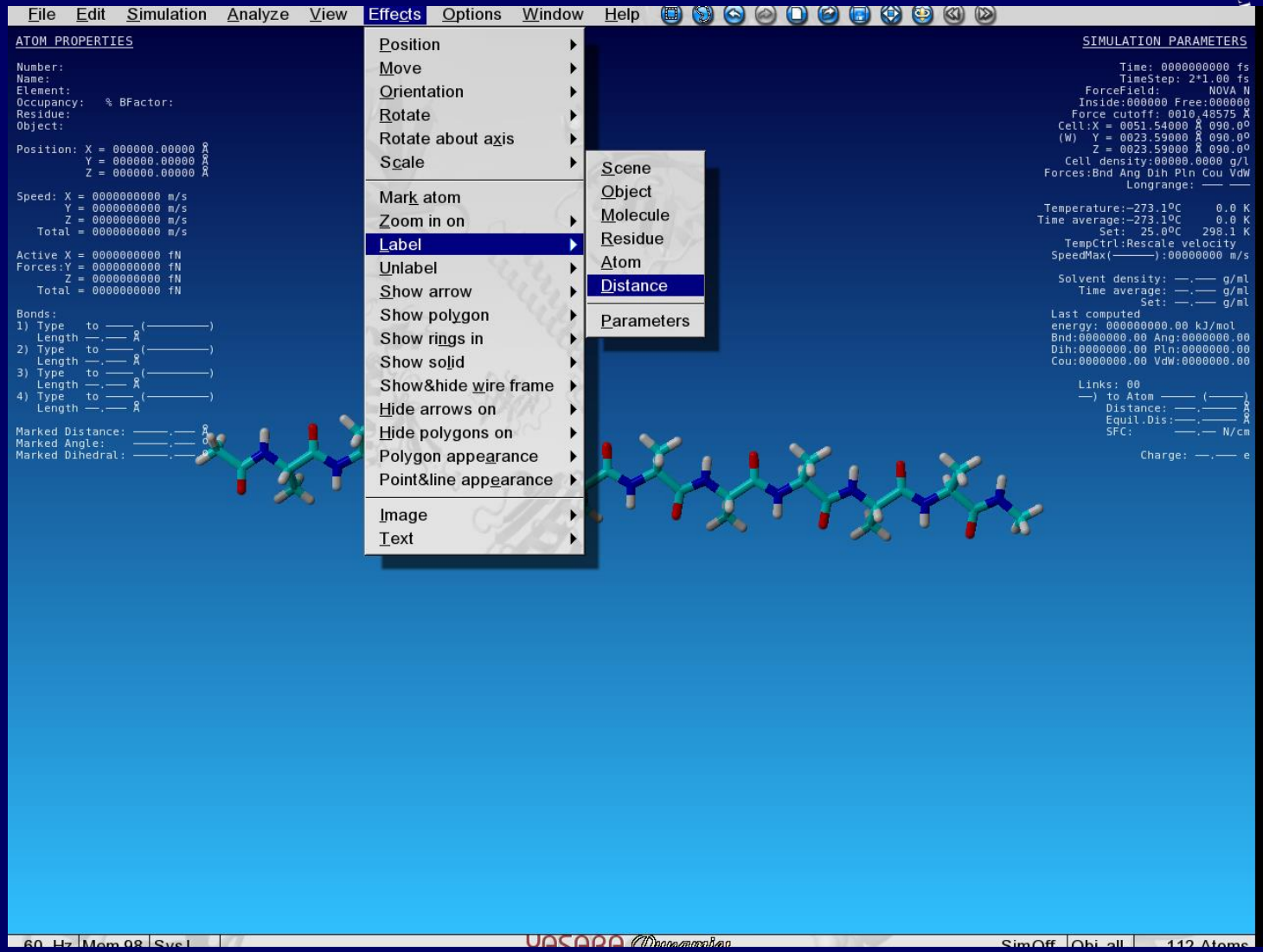

File Edit Simulation Analyze View Effects Options Window Help
ATOM PROPERTIES
SIMULATION PARAMETERS
Select molecular dynamics force field
Force field
AMBER03
AMBER94
AMBER96
AMBER99
NOVA
YAMBER
YAMBER2
Force field terms
Bond
Angle
Dihedral
Planarity
Coulomb
Van der Waals
Speed
Fast
Normal
Slow
OK, and if a force field is selected above, also set its default parameters
Set these two parameters instead:
Cutoff
10.48575 A
Use PME for longrange electrostatics

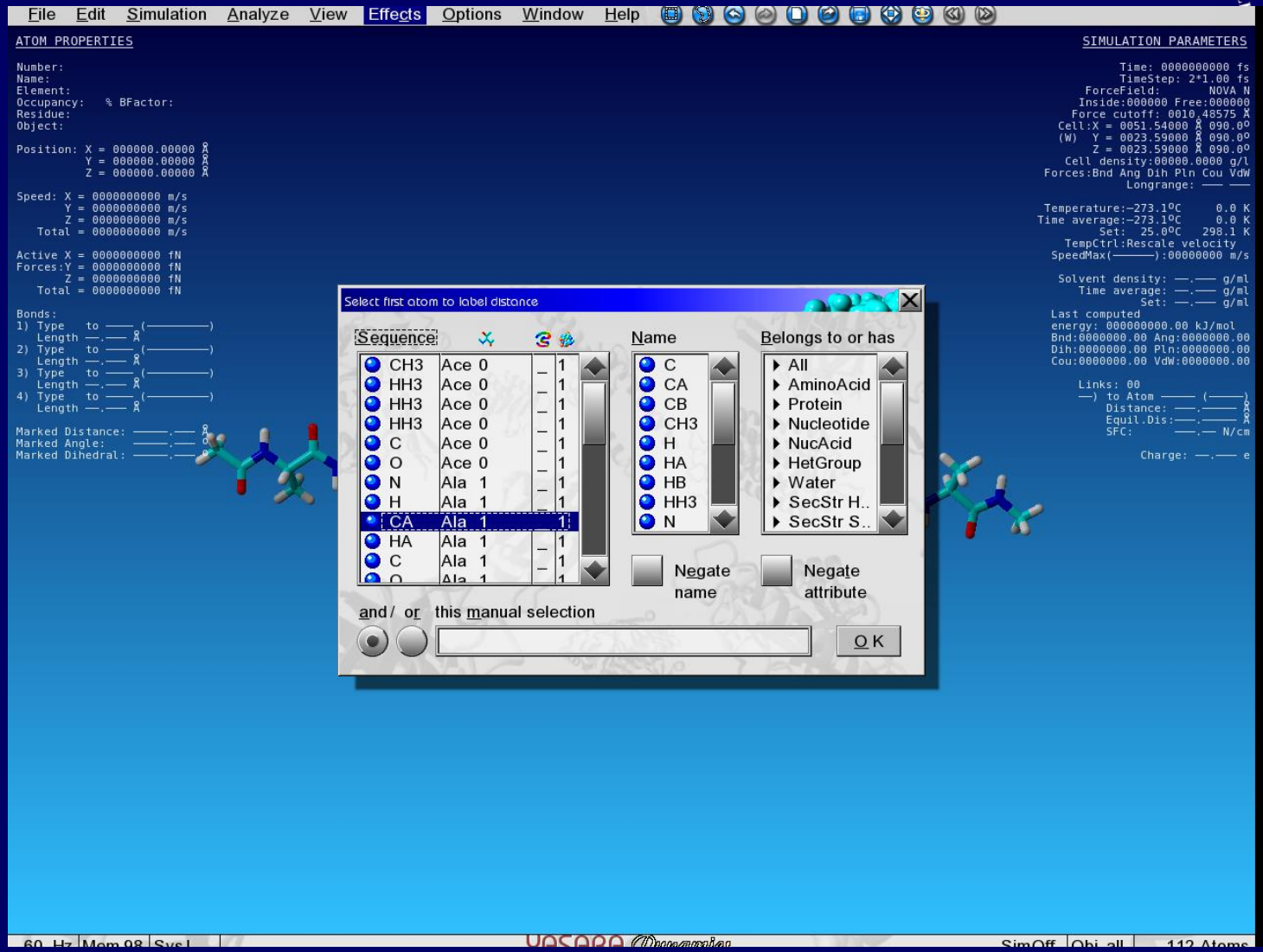

File Edit Simulation Analyze View Effects Options Window Help
Simulator
Define simulation cell
Cell boundaries
Fill cell with...
Force field
Scale forces
Time
Timestep
Temperature
Temperature control
Pressure control
Charge
Automatic correction of
Fix
Free
Add force field term
ATOM PROPERTIES
SIMULATION PARAMETERS
Time: 0000000000 fs
TimeStep: 2*1.00 fs
ForceField: NOVA N
Inside:000000 Free:000000
Force cutoff: 0010.48575 Å
Cell density:00000.0000 g/l
Forces:Bnd Ang Dih Pln Cou VdW
Longrange:
Temperature:-273.1°C 0.0 K
Time average:-273.1°C 0.0 K
Set: 25.0°C 298.1 K
TempCtrl:Rescale velocity
SpeedMax(———):00000000 m/s
Solvent density: —.—— g/ml
Time average: —.—— g/ml
Set: —.—— g/ml
Last computed energy: 000000000.00 kJ/mol
Bnd:0000000.00 Ang:0000000.00
Dih:0000000.00 Pln:0000000.00
Cou:0000000.00 VdW:0000000.00
Links: 00
Charge: —.—— e
60 Hz
SimOff
112 Atoms

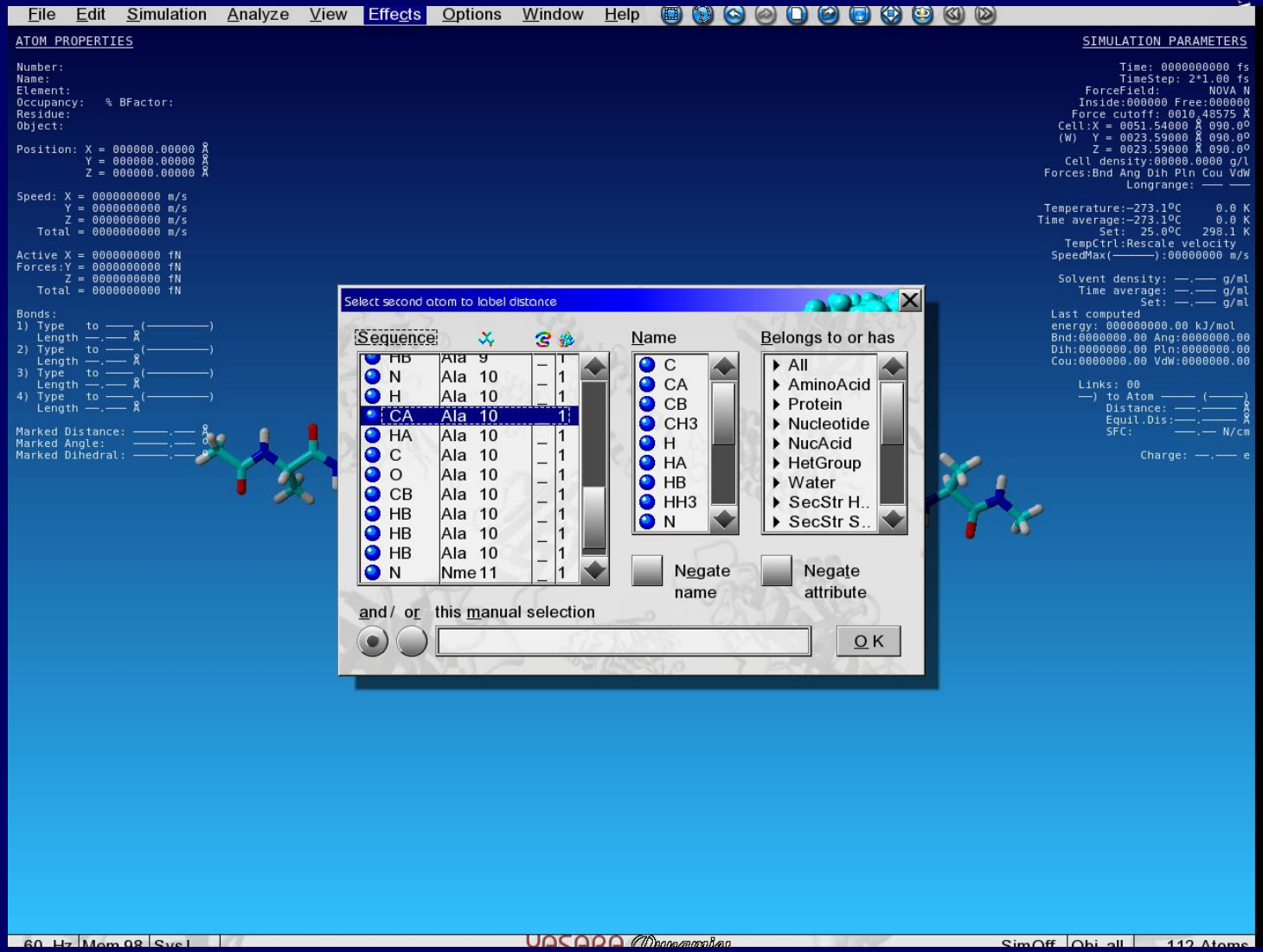

File Edit Simulation Analyze View Effects Options Window Help
ATOM PROPERTIES
SIMULATION PARAMETERS
Set simulation timestep
Timestep for intramolecular forces (=simulation substep)
1.0000 fs
Calculate intermolecular forces every...
2 simulation substeps
The sum of all substeps above is called 'one simulation step'.
Update the screen every...
1 simulation steps
Update the pairlist every...
1 simulation steps
O K

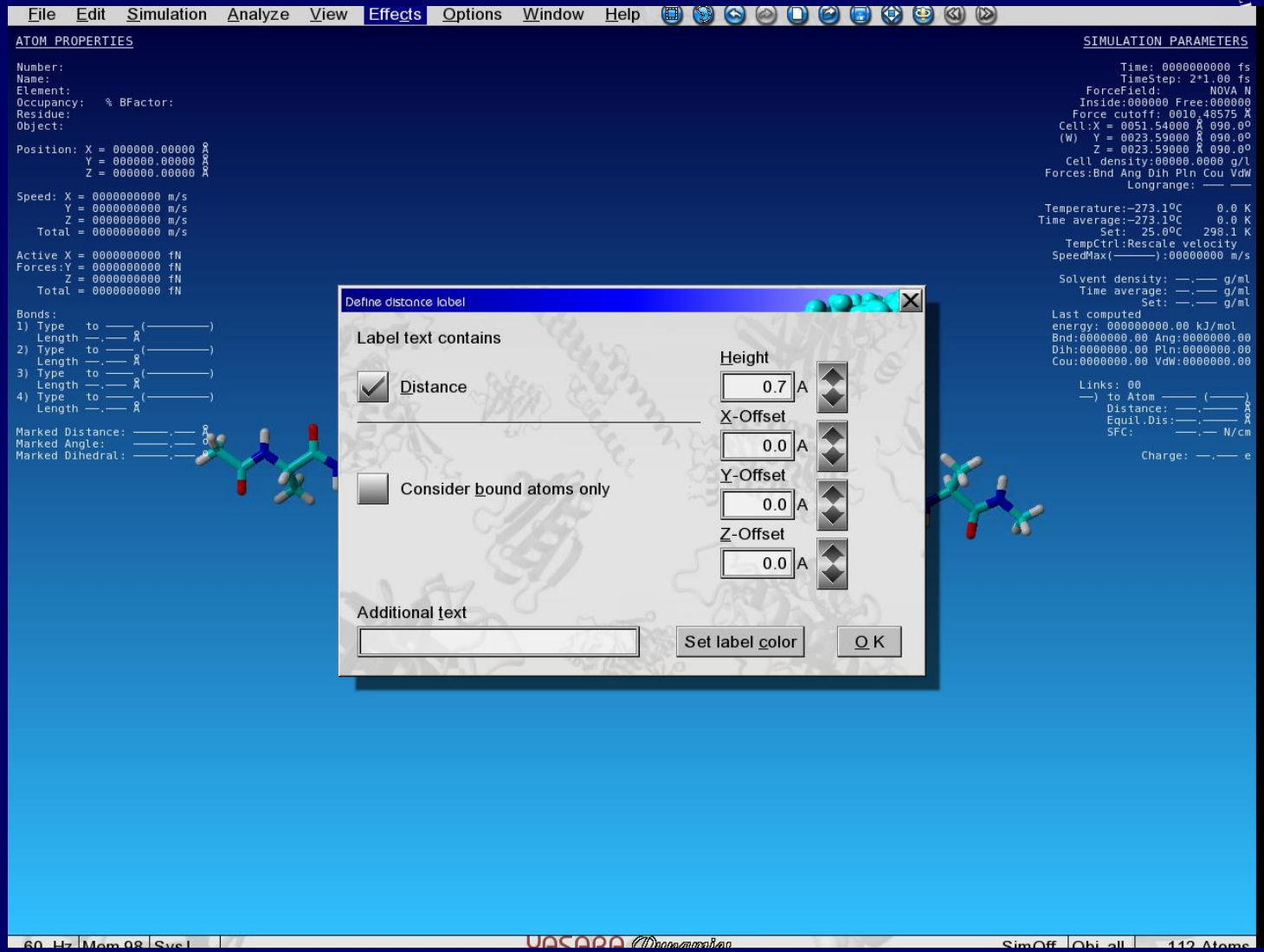

File Edit Simulation Analyze View Effects Options Window Help
Simulator
Define simulation cell
Cell boundaries
Fill cell with...
Force field
Scale forces
Time
Timestep
Temperature
Temperature control
Pressure control
Charge
Automatic correction of
Fix
Free
Add force field term
Initialize
On
Pause
Pause in...
Continue
Off
Warning is error
SIMULATION PARAMETERS

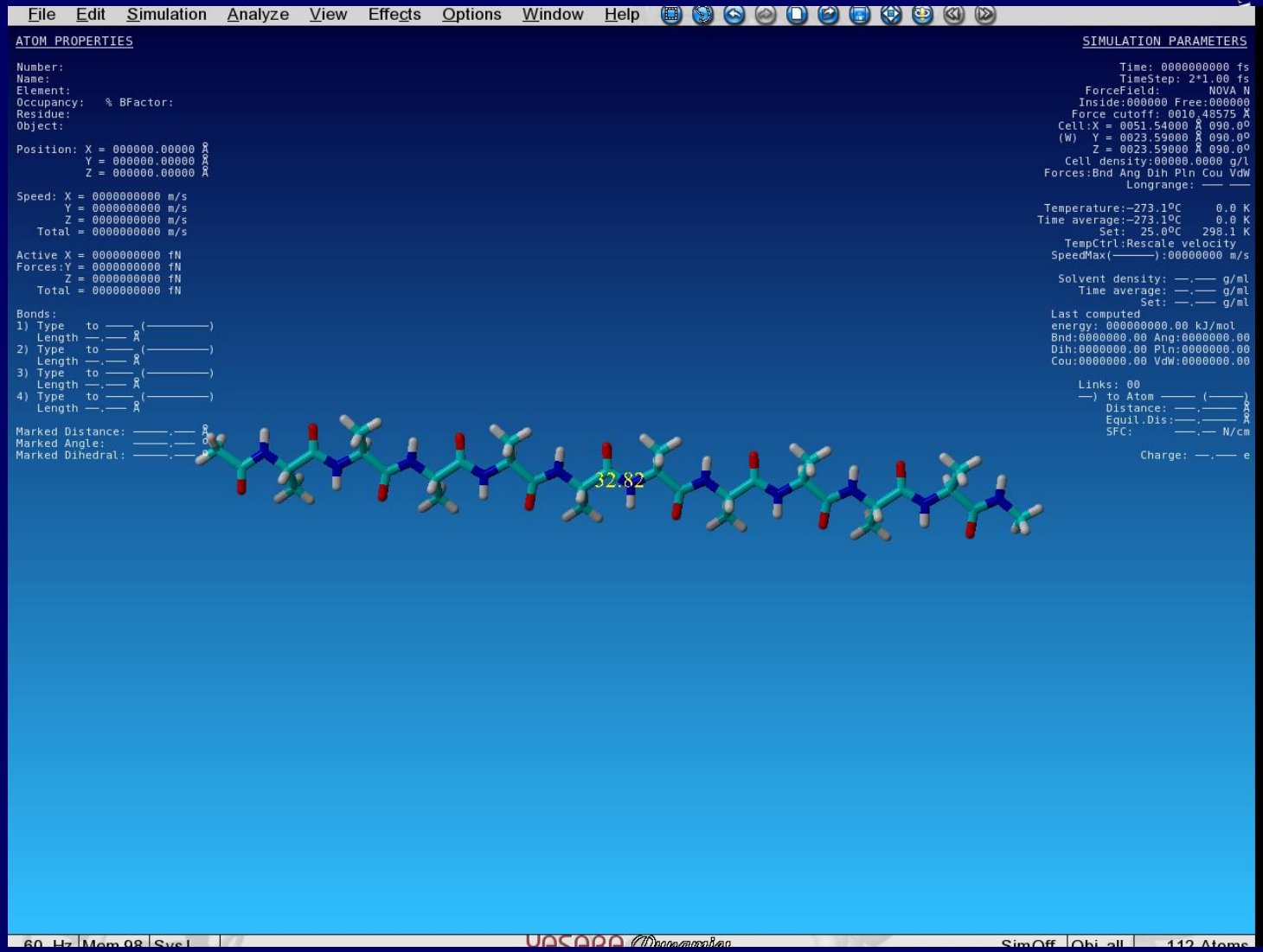

File Edit Simulation Analyze View Effects Options Window Help
ATOM PROPERTIES
SIMULATION PARAMETERS
Set time period until simulation is paused
Period
1000 fs
O K

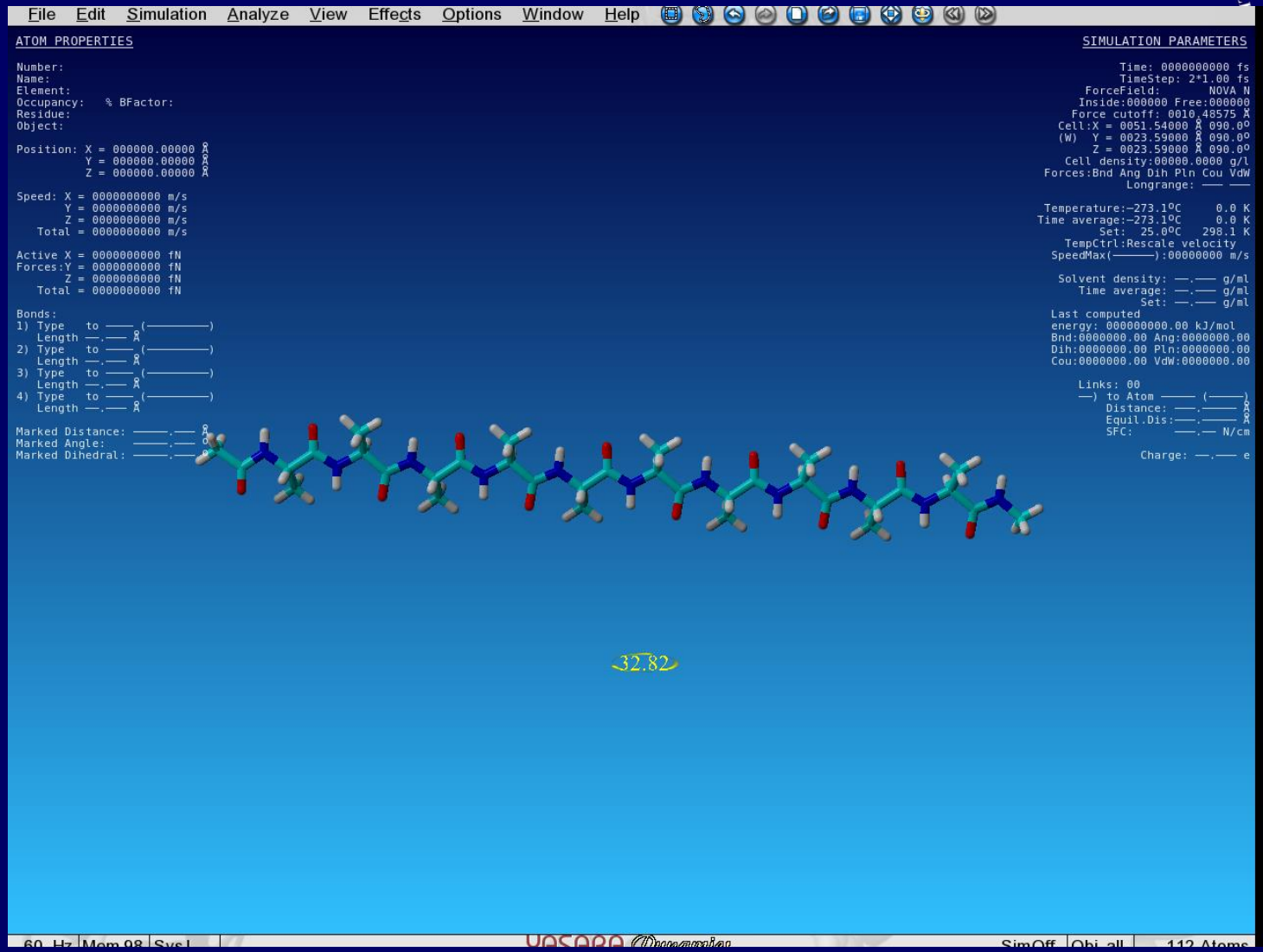

File Edit Simulation Analyze View Effects Options Window Help
ATOM PROPERTIES
Number:
Name:
Element:
Occupancy: % BFactor:
Residue:
Object:
Position: X = 000000.00000 Å
Y = 000000.00000 Å
Z = 000000.00000 Å
Speed: X = 0000000000 m/s
Y = 0000000000 m/s
Z = 0000000000 m/s
Total = 0000000000 m/s
Active X = 0000000000 fN
Forces:Y = 0000000000 fN
Z = 0000000000 fN
Total = 0000000000 fN
Bonds:
1) Type to ——— (———)
Length ——.—— Å
2) Type to ——— (———)
Length ——.—— Å
3) Type to ——— (———)
Length ——.—— Å
4) Type to ——— (———)
Length ——.—— Å
Marked Distance: ———.—— Å
Marked Angle: ———.—— °
Marked Dihedral: ———.—— °
Position
Move
Orientation
Rotate
Rotate about axis
Scale
Mark atom
Zoom in on
Label
Unlabel
Show arrow
Show polygon
Show rings in
Show solid
Show&hide wire frame
Hide arrows on
Hide polygons on
Polygon appearance
Point&line appearance
Image
Text
Scene
Object
Molecule
Residue
Atom
Distance
Parameters
SIMULATION PARAMETERS
Time: 0000000000 fs
TimeStep: 2*1.00 fs
ForceField: NOVA N
Inside:000000 Free:000000
Force cutoff: 0010.48575 Å
Cell:X = 0051.54000 Å 090.0°
(W) Y = 0023.59000 Å 090.0°
Z = 0023.59000 Å 090.0°
Cell density:00000.0000 g/l
Forces:Bnd Ang Dih Pln Cou VdW
Longrange: ——— ———
Temperature:-273.1°C 0.0 K
Time average:-273.1°C 0.0 K
Set: 25.0°C 298.1 K
TempCtrl:Rescale velocity
SpeedMax(———):00000000 m/s
Solvent density: —.—— g/ml
Time average: —.—— g/ml
Set: —.—— g/ml
Last computed
energy: 000000000.00 kJ/mol
Bnd:0000000.00 Ang:0000000.00
Dih:0000000.00 Pln:0000000.00
Cou:0000000.00 VdW:0000000.00
Links: 00
—) to Atom ——— (———)
Distance: ———.——— Å
Equil.Dis:———.——— Å
SFC: ———.— N/cm
Charge: —.—— e
60 Hz
Mem 98
SimOff
Obj all
112 Atoms

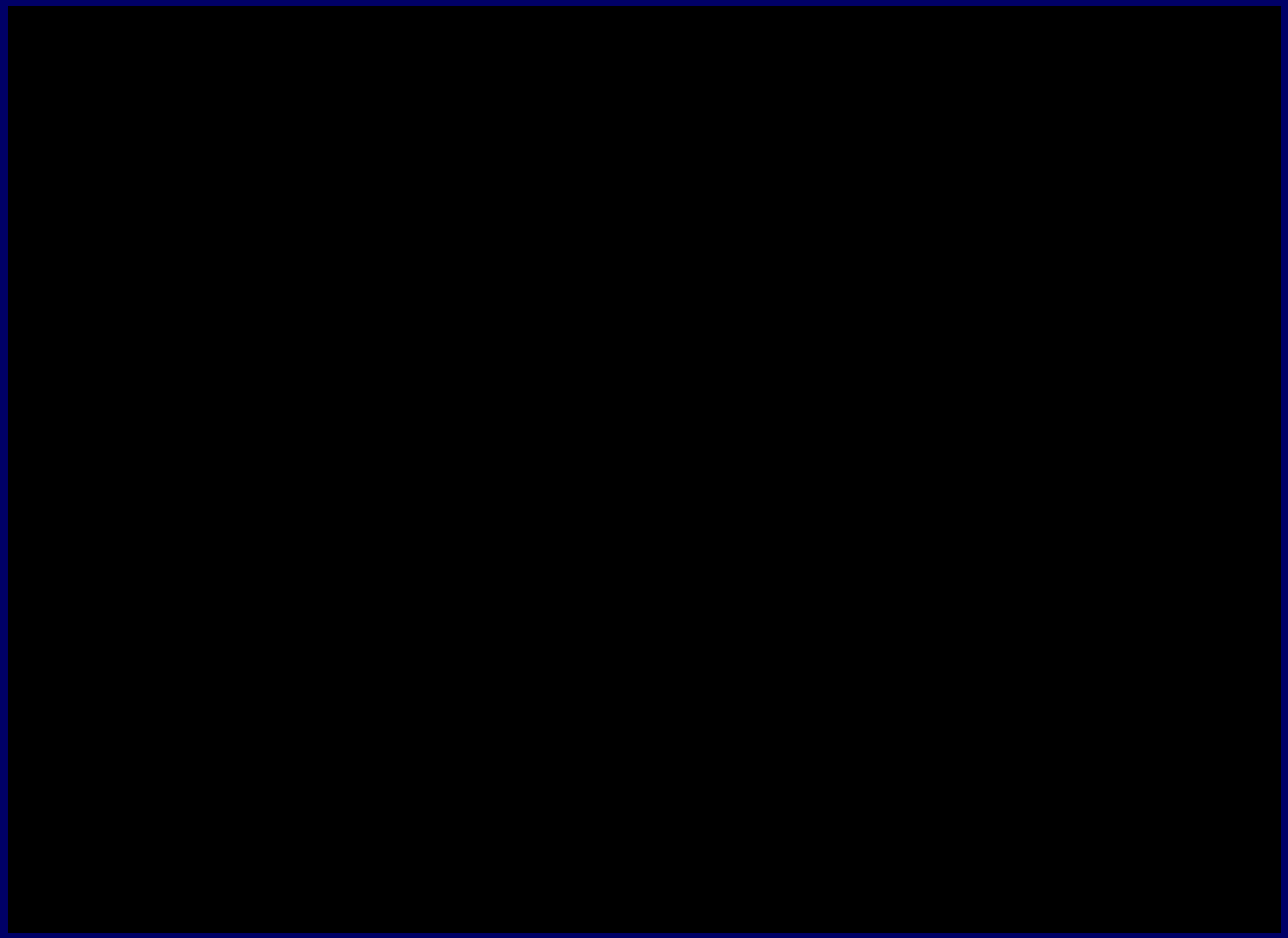

File Edit Simulation Analyze View Effects Options Window Help
ATOM PROPERTIES
SIMULATION PARAMETERS
Select first atom to label distance
Sequence
Name
Belongs to or has
Negate name
Negate attribute
and / or
this manual selection
OK


File Edit Simulation Analyze View Effects Options Window Help
ATOM PROPERTIES
SIMULATION PARAMETERS
Select second atom to label distance
Sequence
Name
Belongs to or has
Negate name
Negate attribute
and / or
this manual selection
OK


File Edit Simulation Analyze View Effects Options Window Help
ATOM PROPERTIES
SIMULATION PARAMETERS
Define distance label
Label text contains
Distance
Consider bound atoms only
Height
0.7 A
X-Offset
0.0 A
Y-Offset
0.0 A
Z-Offset
0.0 A
Additional text
Set label color
O K


File Edit Simulation Analyze View Effects Options Window Help
ATOM PROPERTIES
Number:
Name:
Element:
Occupancy: % BFactor:
Residue:
Object:
Position: X = 000000.00000 Å
Y = 000000.00000 Å
Z = 000000.00000 Å
Speed: X = 0000000000 m/s
Y = 0000000000 m/s
Z = 0000000000 m/s
Total = 0000000000 m/s
Active X = 0000000000 fN
Forces:Y = 0000000000 fN
Z = 0000000000 fN
Total = 0000000000 fN
Bonds:
1) Type to ——— (————————)
Length ——.—— Å
2) Type to ——— (————————)
Length ——.—— Å
3) Type to ——— (————————)
Length ——.—— Å
4) Type to ——— (————————)
Length ——.—— Å
Marked Distance: ———.—— Å
Marked Angle: ———.—— °
Marked Dihedral: ———.—— °
SIMULATION PARAMETERS
Time: 0000000000 fs
TimeStep: 2*1.00 fs
ForceField: NOVA N
Inside:000000 Free:000000
Force cutoff: 0010.48575 Å
Cell:X = 0051.54000 Å 090.0°
(W) Y = 0023.59000 Å 090.0°
Z = 0023.59000 Å 090.0°
Cell density:00000.0000 g/l
Forces:Bnd Ang Dih Pln Cou VdW
Longrange: ——— ———
Temperature:-273.1°C 0.0 K
Time average:-273.1°C 0.0 K
Set: 25.0°C 298.1 K
TempCtrl:Rescale velocity
SpeedMax(————):00000000 m/s
Solvent density: —.——— g/ml
Time average: —.——— g/ml
Set: —.——— g/ml
Last computed
energy: 000000000.00 kJ/mol
Bnd:0000000.00 Ang:0000000.00
Dih:0000000.00 Pln:0000000.00
Cou:0000000.00 VdW:0000000.00
Links: 00
—) to Atom ——— (————)
Distance: ——.——— Å
Equil.Dis:——.——— Å
SFC: ———.— N/cm
Charge: —.——— e
32.82
60 Hz
Mem 98
Sys I
SimOff
Obj all
112 Atoms


File Edit Simulation Analyze View Effects Options Window Help
ATOM PROPERTIES
Number:
Name:
Element:
Occupancy: % BFactor:
Residue:
Object:
Position: X = 000000.00000 Å
Y = 000000.00000 Å
Z = 000000.00000 Å
Speed: X = 0000000000 m/s
Y = 0000000000 m/s
Z = 0000000000 m/s
Total = 0000000000 m/s
Active X = 0000000000 fN
Forces:Y = 0000000000 fN
Z = 0000000000 fN
Total = 0000000000 fN
Bonds:
1) Type to ——— (————————)
Length ——.—— Å
2) Type to ——— (————————)
Length ——.—— Å
3) Type to ——— (————————)
Length ——.—— Å
4) Type to ——— (————————)
Length ——.—— Å
Marked Distance: ———.—— Å
Marked Angle: ———.—— °
Marked Dihedral: ———.—— °
SIMULATION PARAMETERS
Time: 0000000000 fs
TimeStep: 2*1.00 fs
ForceField: NOVA N
Inside:000000 Free:000000
Force cutoff: 0010.48575 Å
Cell:X = 0051.54000 Å 090.0°
(W) Y = 0023.59000 Å 090.0°
Z = 0023.59000 Å 090.0°
Cell density:00000.0000 g/l
Forces:Bnd Ang Dih Pln Cou VdW
Longrange: ——— ———
Temperature:-273.1°C 0.0 K
Time average:-273.1°C 0.0 K
Set: 25.0°C 298.1 K
TempCtrl:Rescale velocity
SpeedMax(———):00000000 m/s
Solvent density: —.——— g/ml
Time average: —.——— g/ml
Set: —.——— g/ml
Last computed
energy: 000000000.00 kJ/mol
Bnd:0000000.00 Ang:0000000.00
Dih:0000000.00 Pln:0000000.00
Cou:0000000.00 VdW:0000000.00
Links: 00
—) to Atom ——— (———)
Distance: ——.——— Å
Equil.Dis:——.——— Å
SFC: ———.— N/cm
Charge: —.——— e
32.82
60 Hz
Mem 98
SimOff
Obj all
112 Atoms



Kiértékelés

- A futás alatt a közbenső állapotokat rendszeresen kiírjuk
- Kiválasztunk néhány paramétert és figyeljük a futás során:
  - Össz-energia
  - Atom-atom távolság
  - Szög …
- Konformaciók összhasonlítása - RMSD

Az eredményekről

- A szimulációt több, független futásban meg kell ismételni
- Csak a többszörösen megerősített eredményt lehet komolyan venni
- A szimuláció mikrosekundumos időskálán dolgozik
- A szimulációk valós ideje több hét
- A rossz konformációk gyorsan szétesnek – a stabil konformáció nem perdöntő

Mit tanultunk ma?

- A molekula modellezés elérhető lehetőség minden laborban
- De nem egyszerű módszer: idő és gépigényes
- Rengeteg közelítést alkalmaz
- Az eredmények értékelése nagy tapasztalatot igényel

Mit tanultunk a félév során?

- A bioinformatika fontos része az orvosbiológiai kutatásnak
- Számos kisérlethez egyenesen nélkülözhetetlen
- Jelentősége tovább fog nőni a jövőben
- Hatékony használatához nem kell programozói tudás
- Az események helyes értékeléséhez sokat segít az algoritmikus háttér ismerete

További lehetőségek

- „Alapfokú számítógép-programozási ismeretek orvosbiológusoknak”, tavaszi félév
- Dr Szalai Csaba: “Genomika” kurzusa a második félévben
  - Searls DB (2012): **An online bioinformatics curriculum.** PLoS Comput Biol. 8(9)
  - Searls DB (2014) **A New Online Computational Biology Curriculum.** PLoS Comput Biol 10(6)