

EURO

Moleküler Dinamik Simülasyon Çalışmalarının ABC'si

29 Eylül 2022

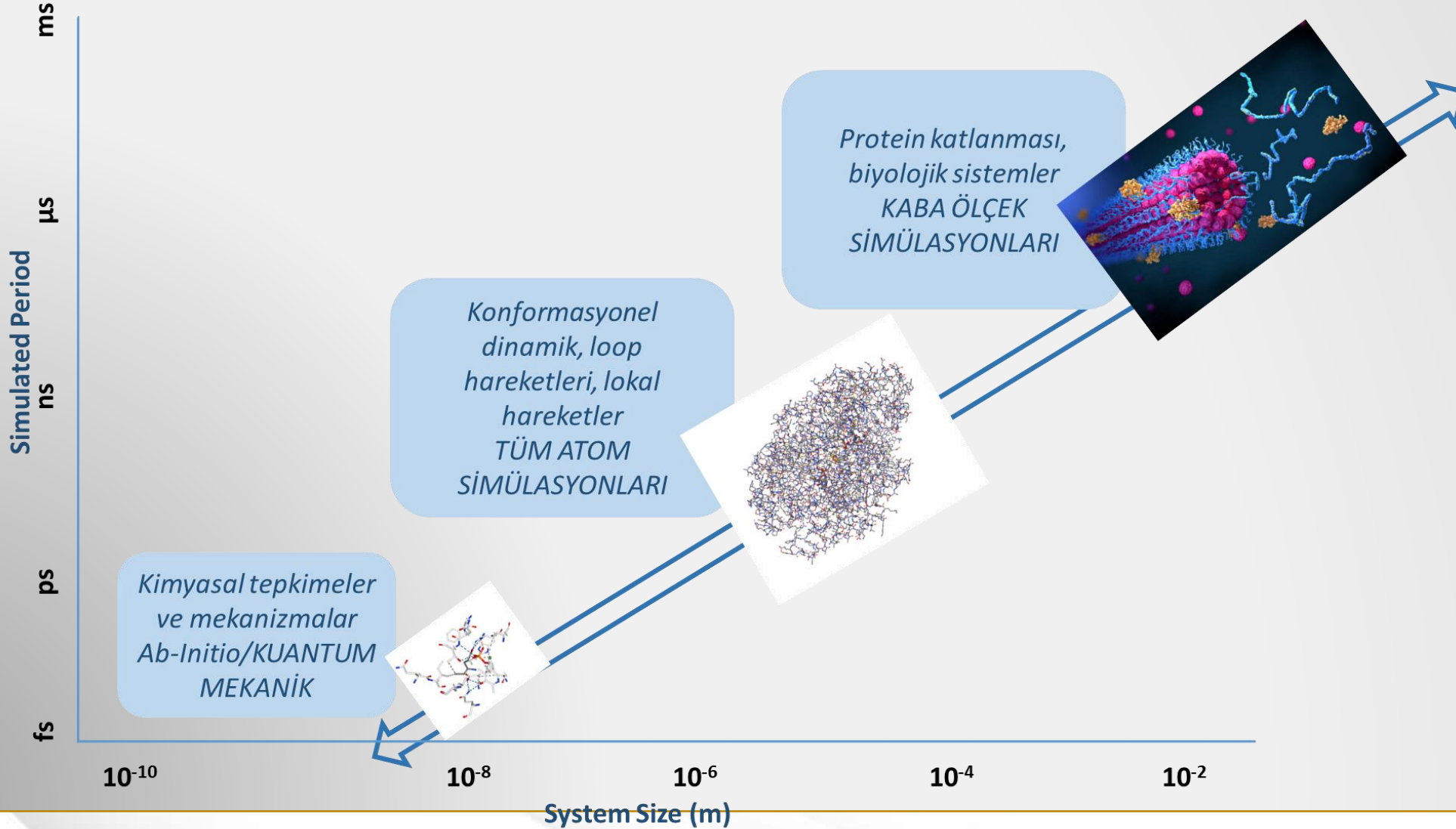
F. Aylin Sungur

Başlangıç olarak...

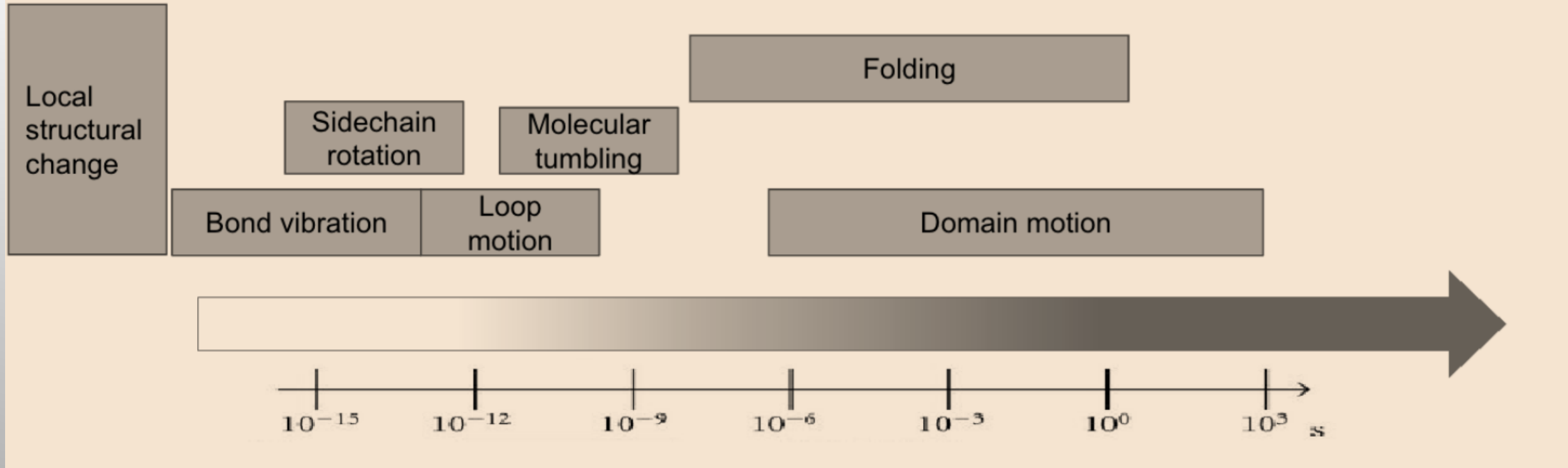
“Every sentence I utter must be understood not as an affirmation but as a question. “

Niels Bohr (1885–1962).

Moleküler Modelleme



Protein Yapısal Değişiklik Süreleri



Moleküler Dinamik Simülasyon ??????

- Deneysel olarak yapısı belirlenmiş bir protein bağlı ligandı çıkarın ve ardından ligandın çıkarılmasının protein konformasyonuna etkisini
- Bağlı bir ligandı farklı bir ligandla değiştirin veya deneysel yapıda bulunmayan bir ligand ekleyin
- Proteindeki bir veya daha fazla amino asit rezidüsünü mutasyona uğratarak mutasyonun işlevsel etkisini açıklamak veya tahmin etmek
- Transmembran voltajının veya mekanik gerilmenin etkisini yakalamak için atomlara dış kuvvetler uygulamak

Hangi bilgisayar?

- Dizüstü ?
- Masaüstü?
- İş istasyonu
- Sunucu (CPU)
- GPU

Tarihsel Gelişim

- 1971 Protein Data Bankası kuruldu
- 1975 Databankta 50 adet çözümlenmiş yapı bulunuyordu
- 1985 NSF 5 tane Ulusal HPC merkezini kurdu
- 1998 İyon kanalı protein kristal yapısı çözüldü
- 2003 İnsan genom sekansı tanımlandı



- **Kuvvet alanı (Force Fields)**

- 20. yy ilk yarısı vibrational spectroscopy
- İlk formülasyon “Urey, HC; Bradley, CA., Jr. Phys. Rev. **1931** 38 pp 1969. “
 - Hooke’s Law – Morse Potential

- **1946**

- Molekül yapılarının hesaplanması/modellenmesi için

Sterik etkileşimler ve bağ germe(bond stretching) , açı bükme (angle bending) ve burulma (torsional) titreşim modlarının Newton mekaniği ile kombinasyonu üzerinden MOLEKÜLER MEKANİK (AMPİRİK KUVVET ALANI) çalışmaları

Tarihsel Gelişimi

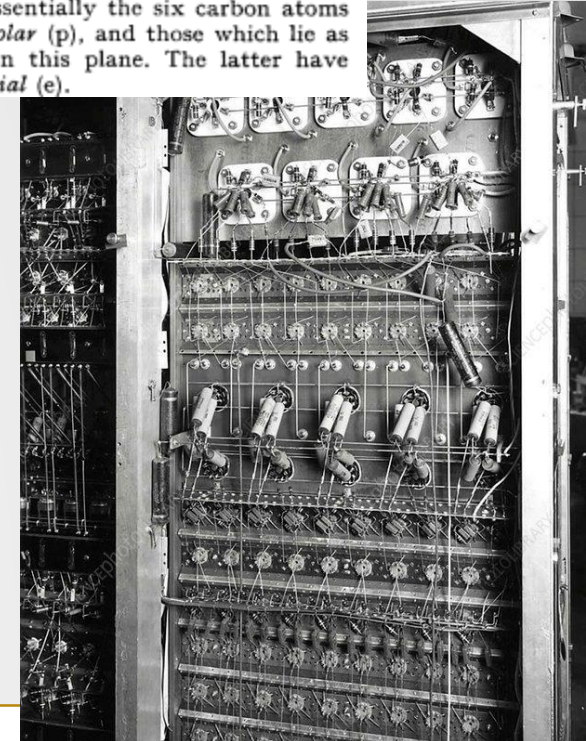
- **1950**
 - Barton'un steroidlerin konformasyonlarının kimyalarını nasıl etkilediğine dair kısa notunun yayınlanmasıyla
 - 3D yapılar ve konformasyonel analiz -> Yapı kararlılığı ve reaktivite
- **1953**
 - Los Alamos'dan bir grup
 - "Equation of State Calculations by Fast Computing Machines."
 - Bilgisayar : MANIAC
 - Simulated annealing -Metropolis algoritması-Monte Carlo yöntemi
 - Moleküler Dinamik Hesapları için ilk adımlar

STUDIORUM PROGRESSUS

The Conformation¹ of the Steroid Nucleus

By D. H. R. BARTON², Cambridge, Mass.

In recent years it has become generally accepted that the chair conformation of cyclohexane is appreciably more stable than the boat. In the chair conformation it is possible^{3,4} to distinguish two types of carbon-hydrogen bonds; those which lie as in (Ia) perpendicular to a plane containing essentially the six carbon atoms and which are called³ *polar* (p), and those which lie as in (Ib) approximately in this plane. The latter have been designated³ *equatorial* (e).



- **1957** Alder ve Wainwright
 - atomların yalnızca mükemmel çarpışmalar yoluyla etkileştiği “hard sphere” modelini kullanarak en eski MD simülasyonu

Phase Transition for a Hard Sphere System

B. J. ALDER AND T. E. WAINWRIGHT

University of California Radiation Laboratory, Livermore, California

• (Received August 12, 1957)

A CALCULATION of molecular dynamic motion has been designed principally to study the relaxations accompanying various nonequilibrium phenomena. The method consists of solving exactly (to the number of significant figures carried) the simultaneous classical equations of motion of several hundred particles by means of fast electronic computers. Some of the details as they relate to hard spheres and to particles having square well potentials of attraction have been described.^{1,2} The method has been used also to calculate equilibrium properties, particularly the equation of state of hard spheres where differences with previous Monte Carlo³ results appeared.

We gratefully acknowledge Mrs. Shirley Campbell's and Mary Shephard's help with the coding problems.

Tarihsel Gelişimi

- **1961**

- Kuvvet alanlarını hesapları için bilgisayar kullanımı -
Hendrickson
- Moleküler yapının ampirik kuvvet alanı hesaplamaları -> orta büyüklükteki halkaların konformasyonları inceleniyor



Tarihsel Gelişimi

- **1965- WIBERG**
- Konformasyonel analizi için bilgisayarda kuvvet alanı hesaplamaları
- “steepest descent” algoritması
- Wiberg Kartezyen koordinatlarını iç koordinatlara dönüştürmek, bu koordinatlardan bağ uzunluklarını, bağ açılarını ve burulma açılarını hesaplamak için algoritmalar
- Hidrojenlerin metilen karbonu üzerindeki yerini tahmin etmek için geometri algoritması yazıyor.



Tarihsel Gelişimi

- **1968 BOYD**
- Siklofanların kuvvet alanı hesaplamaları -> strain energy minimization”
- “modifiye Newton-Raphson yöntemi

- **1969 SNOW**
- Boyd’s yöntemi kullanarak kobalt pentaamin şelatlarında geometri optimizasyonunun sonuçları

Boyd, RH. J. Chem. Phys. 1968 49 2574.

Snow, MR.; Buckingham, DA.; Marzili, PA.; Sargeson, AM. J. Chem. Soc. Chem. Commun. ~~1969~~ 891

CHEMICAL COMMUNICATIONS, 1969

891

The Absolute Configurations and Conformations of Chlorocobalt(III) Tetraethylenepenta-amine Complexes

By M. R. SNOW*

(Department of Physical and Inorganic Chemistry, University of Adelaide, Adelaide, South Australia)

and D. A. BUCKINGHAM, P. A. MARZILLI, and A. M. SARGESON

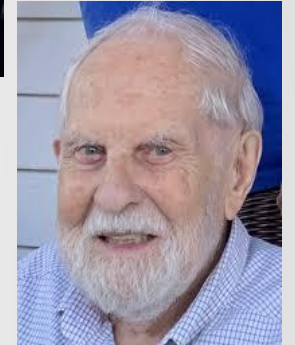
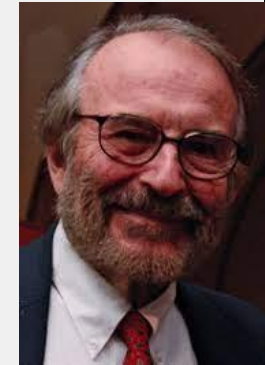
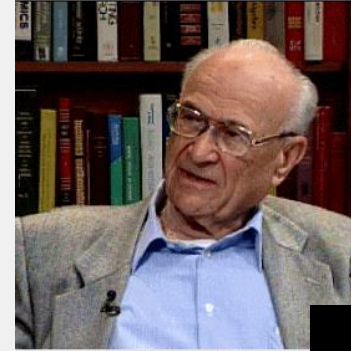
(Research School of Chemistry, Australian National University, Canberra, Australia)

Summary The absolute configurations, circular dichroism spectra, crystal structure, equilibria, and the results of energy minimization calculations are presented for a pair of diastereoisomeric chlorocobalt(III) tetraethylenepenta-amine complexes. $b = 12.44(1)$, $c = 8.43(1)$ Å; $(\alpha\beta R)a = 17.26(2)$, $b = 12.03(1)$, $c = 8.72(3)$ Å. The absolute configurations were determined by anomalous scattering of Cu- K_{α} X-rays by cobalt. The IUPAC symbol⁵ is given for each chelate ring

Both isomers were submitted to the strain energy minimization procedure of Boyd⁶ using force constants^{7,8} and nonbonded potentials^{9,10} from the literature. With

Tarihsel Gelişimi

- İlk ağ bağlantısı (**Internet**) **Ekim 1969'da** devletin desteğiyle UCLA'daki bir bilgisayar ve Stanford Research Institute Menlo Park'taki bir bilgisayar arasında kuruldu.
- 70'lerin ilk başında
 - **UNICEPP** -> Scheraga et al.,
 - Consistent Force Field (**CFF**) -> Lifson and Warshel
 - **MMI** force field -> Allinger et al.,
 - **EAS** force field -> Schleyer et al.



Tarihsel Gelişimi

- **1972 Wiberg ve Boyd,**
 - sistematik olarak torsiyon açısına dayalı konformasyonel dönüşümler için algoritma oluşturarak yayınladılar
- **1974 Lemieux ve grubu ,**
 - Oligosakkaritlerin bilgisayar destekli moleküler modellemesi

Tetrahedron. Vol. 30, pp. 1933 to 1944. Pergamon Press 1974. Printed in Great Britain

THE CONFORMATIONAL PROPERTIES OF GLYCOSIDIC LINKAGES

R. U. LEMIEUX and S. KOTO*

Department of Chemistry, The University of Alberta, Edmonton, Alberta, Canada

(Received in the UK 14 February 1974)

Wiberg, KB; Boyd, RH. J. Am. Chem. Soc. **1972** 94 8426.
Lemieux, RU; Koto, S. Tetrahedron **1974** 30 1933;

Tarihsel Gelişimi

- **1977 McCammon, Gelin & Karplus**
- ampirik bir enerji fonksiyonunu kullanarak gerçekleştirilen ilk protein MD simülasyonu.
- Bovine pancreatic trypsin inhibitörünün (BPTI-500 atom) simülasyon süresi 9.2 ps.

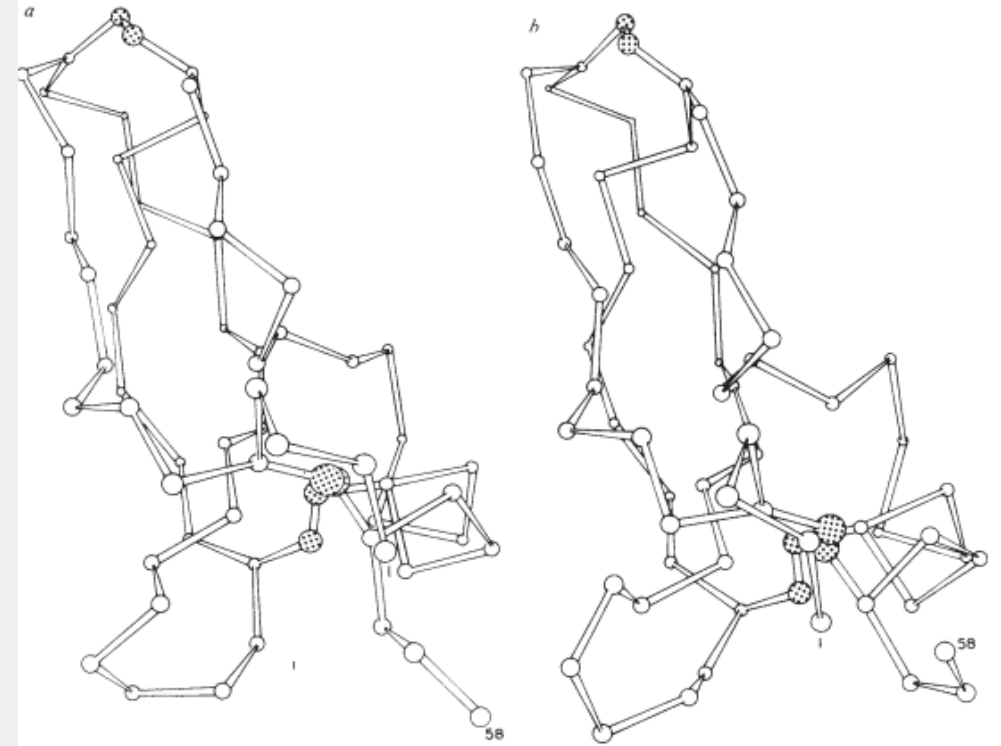


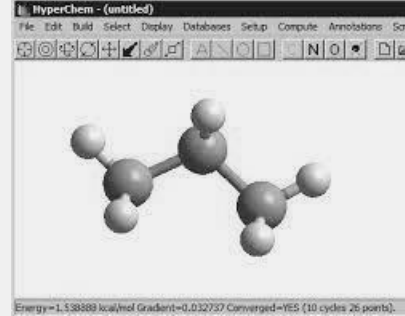
Fig. 1 The peptide backbone (α carbons) and disulphide bonds of PTI. *a*, X-ray structure²¹. *b*, Time evolved structure after 3.2 ps of dynamical simulation.

McCammon, J., Gelin, B. & Karplus, M.
Dynamics of folded proteins. *Nature* **267**,
585–590 (1977).

<https://doi.org/10.1038/267585a0>

Tarihsel Gelişimi

- **1980'ler,**
 - ✓ Kişisel bilgisayar
 - ✓ Bilgisayarların erişilebilirliği
 - ✓ Grafiksel kullanıcı arabiriminin (GUI) kullanımındaki artış
- **1980** : H. C. Andersen - MD method for NPH, NVT, NPT ensembles
- **1986** : R. Car and M. Parrinello Ab initio MD (includes electronic degrees of freedom)



Understanding Molecular Simulation

From Algorithms to Applications

Daan Frenkel

FOM Institute for Atomic and Molecular Physics,
Amsterdam, The Netherlands

Department of Chemical Engineering,
Faculty of Sciences
University of Amsterdam
Amsterdam, The Netherlands

Berend Smit

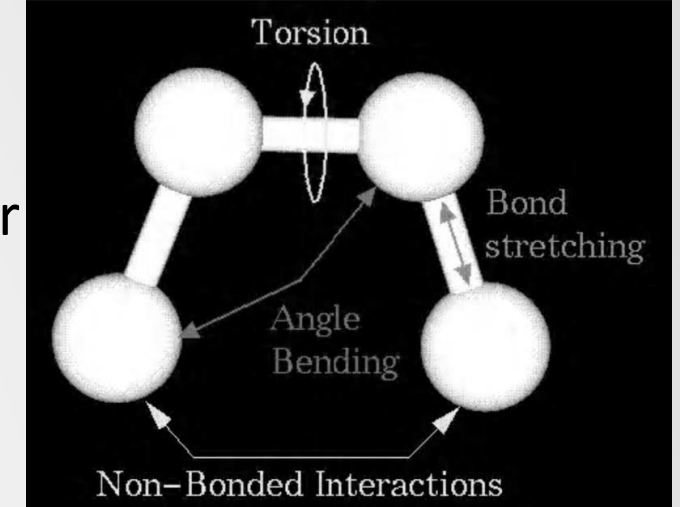
Department of Chemical Engineering
Faculty of Sciences
University of Amsterdam
Amsterdam, The Netherlands

- **Klasik Fizik – Hooke Kanunu**

- Moleküllerde birbirine bağlı atomlar arasında farklı kuvvetler
- İtme ve çekmelere sebep olabilecek yükler

- ✓ **Kuvvet Alanları**

- ✓ **Sınıf I**
- ✓ CHARMM, CHARMM (Biovia) AMBER, OPLS, GROMOS, SYBYL(Tripos)
- ✓ **Sınıf II**
- ✓ MMFF94, UFF, ...
- ✓ **Sınıf III**
- ✓ DRUDE, AMOEBA (Tinker)



MM Enerjisi

$$E_{\text{total}} = E_{\text{stretch}} + E_{\text{bend}} +$$

Bağ içeren enerji terimleri

$$E_{\text{torsion}} + E_{\text{vdW}} + E_{\text{electrostatic}}$$

Bağ içermeyen enerji terimleri

$$+ E_{\text{cross}}$$

Yüksek dereceli (coupling) $E_{\text{stretch-bend}}$

$$+ E_{\text{other}}$$

Özel olarak eklenene $E_{\text{H-bonding}}$

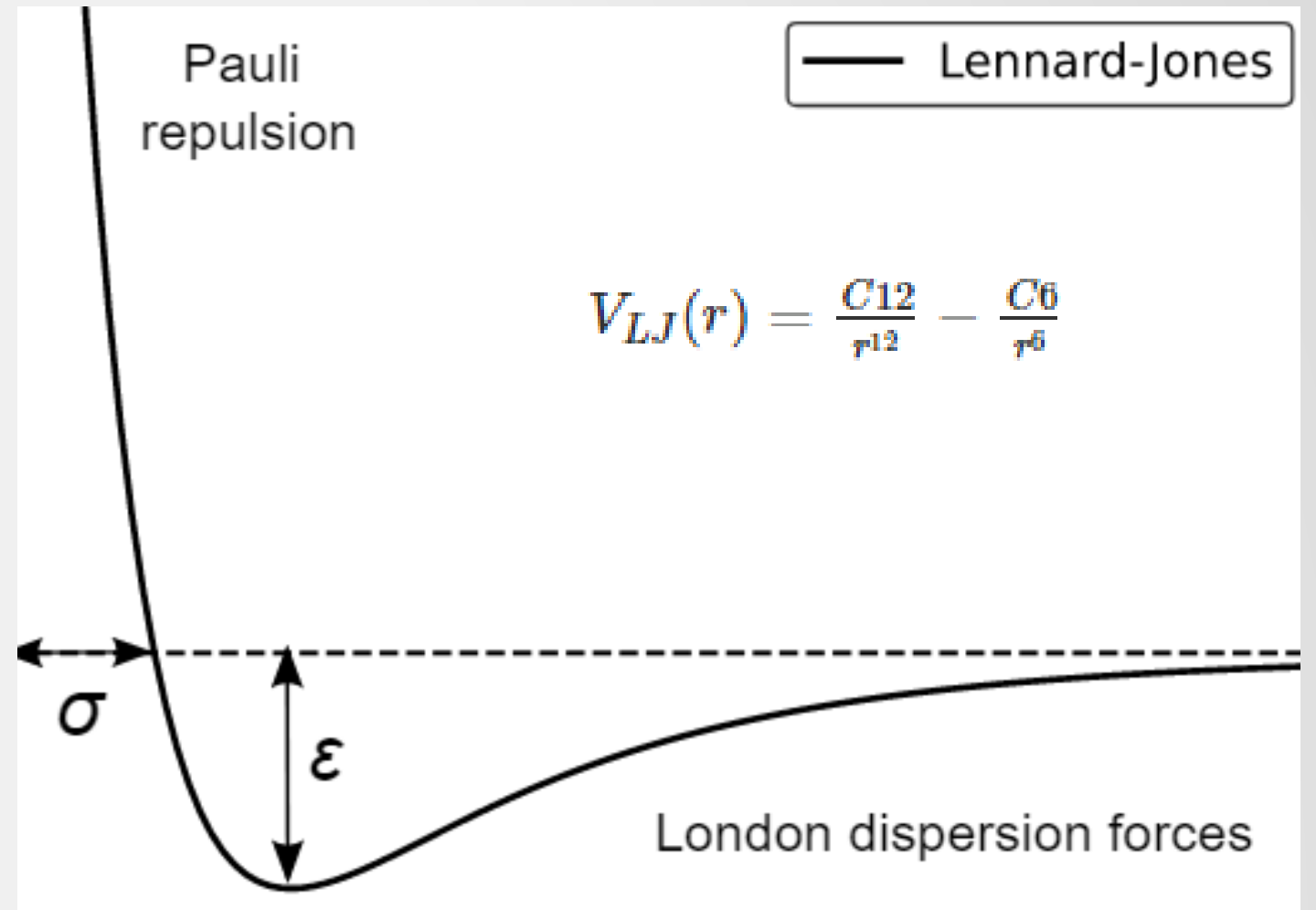
Bağ içermeyen terimler

VDW – Lennard Jones Potansiyeli

- 6-12 Terimi

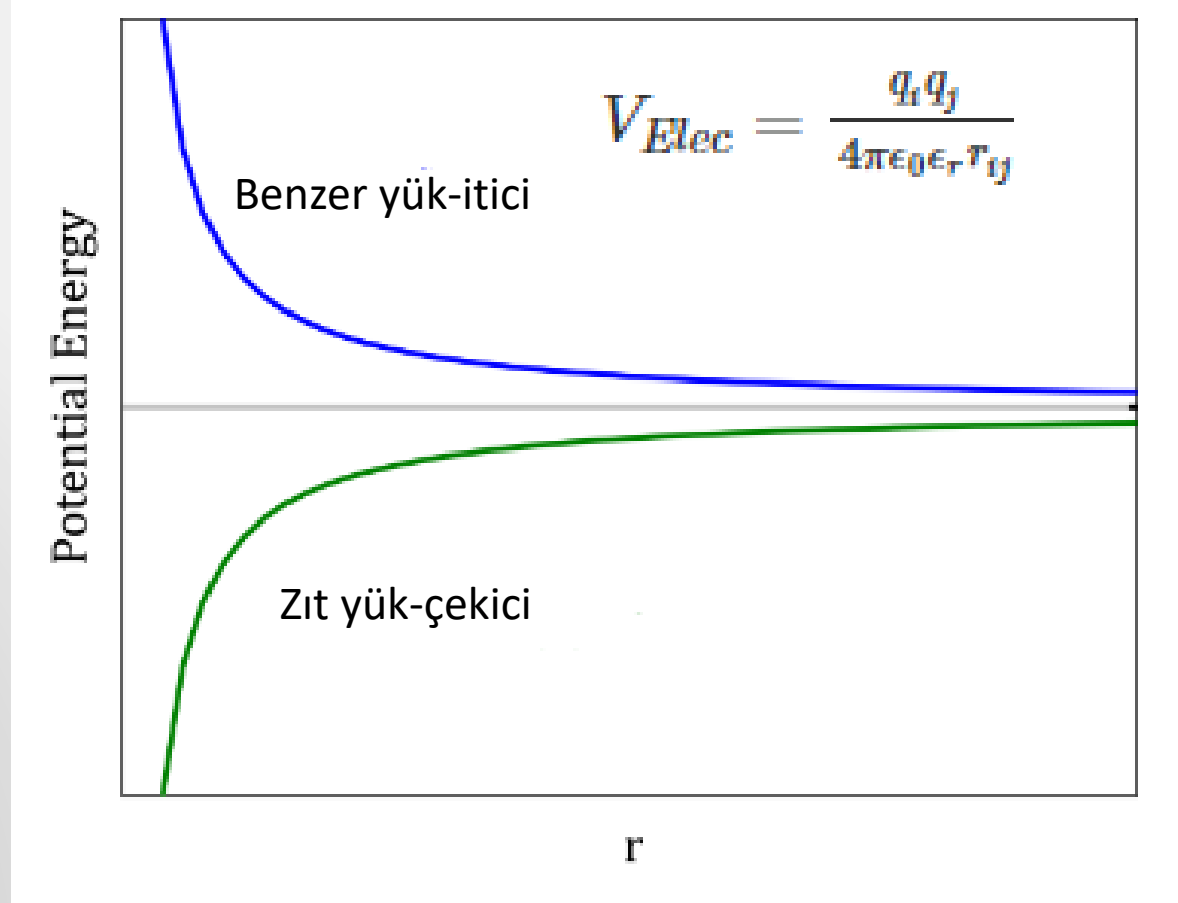
$$V_{LJ}(r) = \frac{C_{12}}{r^{12}} - \frac{C_6}{r^6}$$

- The Buckingham Potential hesapsal açıdan pahalı



Bağ içermeyen terimler

Elektrostatik Potansiyel



Bağ içeren terimler

- Bağ potansiyeli-harmonic

$$V_{Bond} = k_b(r_{ij} - r_0)^2$$

- Açı Potansiyeli-harmonic

$$V_{Angle} = k_\theta(\theta_{ijk} - \theta_0)^2$$

- Dihedral Potansiyeli-Trigonometrik

$$V_{Dihed} = k_\phi(1 + \cos(n\phi - \delta)) + \dots$$

- Uyumsuz (Improper) torsiyon potansiyeli-harmonik

$$V_{Improper} = k_\phi(\phi - \phi_0)^2$$

KUVVET ALANLARI

- Additive Kuvvet Alanlari
 - AMBER: Assisted Model Building with Energy Refinement.
 - CHARMM: Chemistry at Harvard Macromolecular Mechanics.
- Polarizable Kuvvet alanlari
 - Drude
 - AMOEBA

MD Simülasyonları

- Moleküler simulasyon nedir?

Moleküler Dinamik

Deterministik

Hareket Denklemlerinin Integrasyonu
(Integration of equations of motions)

Zaman elemanı içerir

MD Simülasyonları

MD: “N body” sistem için hareket denklemlerinin sayısal integrali

- Kuvvet -> İvme -> Hız -> Pozisyon

- Newtonian

$$F_i = m_i a_i = m_i \frac{d^2 x_i(t)}{dt^2}$$

Gradient of the potential -> Force

$$F_i = - \frac{\partial V(r^N)}{\partial r_i}$$

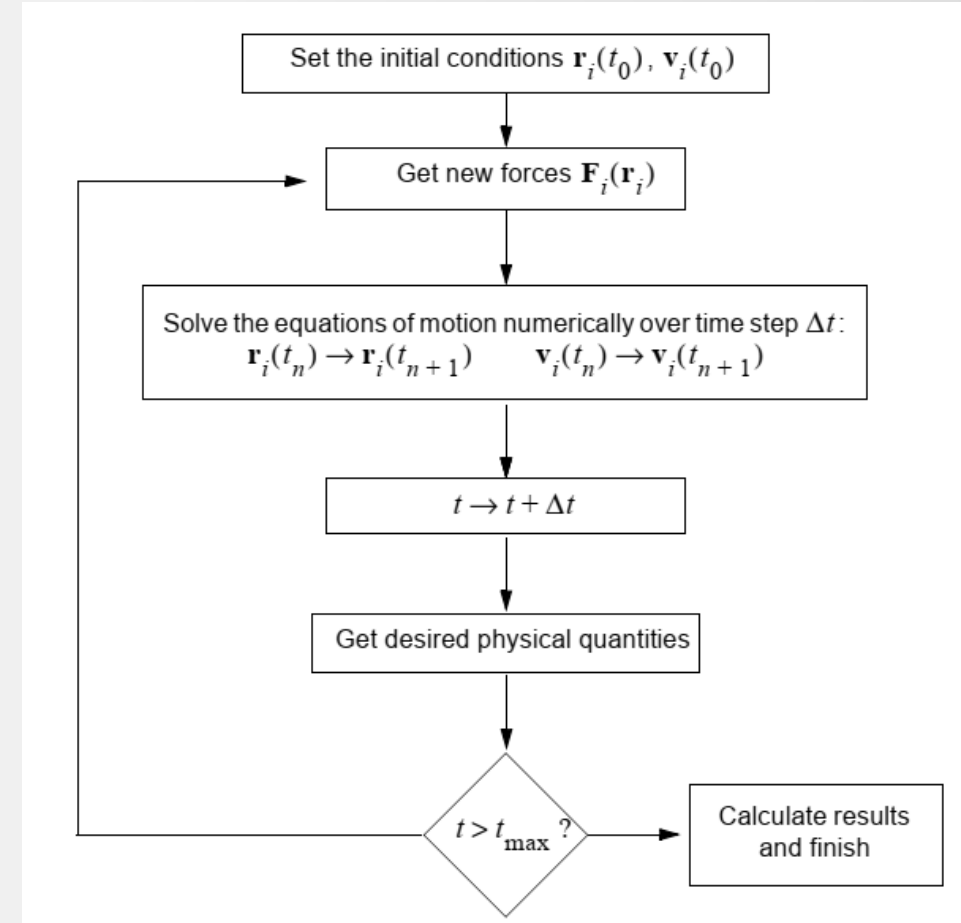
$$\Delta v = a \cdot \Delta t$$

$$v = v_0 + \Delta v$$

$$\Delta r = v \cdot \Delta t$$

MD Programı

1. Temel parametreleri oku (sıcaklık, atomlar, zaman adımı, vb.)
2. Sistemi başlat - pozisyonlar ve hızlar
3. Kuvvetleri hesapla
4. Hareket denklemlerini integralini bul
5. Hesaplamalar için tanımlanan yeterli süre sonunda dur



MD Simülasyonları

Hareket Denklemlerinin Integrasyonu: N-body problem –numerik çözüm

- Verlet algoritması
- Leap-frog algoritması
- Beeman's algoritması

Tercih edilen:

Velocity Verlet:

$$r(t+\Delta t) = r(t) + v(t)\Delta t + (1/2) a(t)\Delta t^2$$

Update of positions

$$v(t+\Delta t) = v(t) + (1/2) [a(t) + a(t + \Delta t)]\Delta t$$

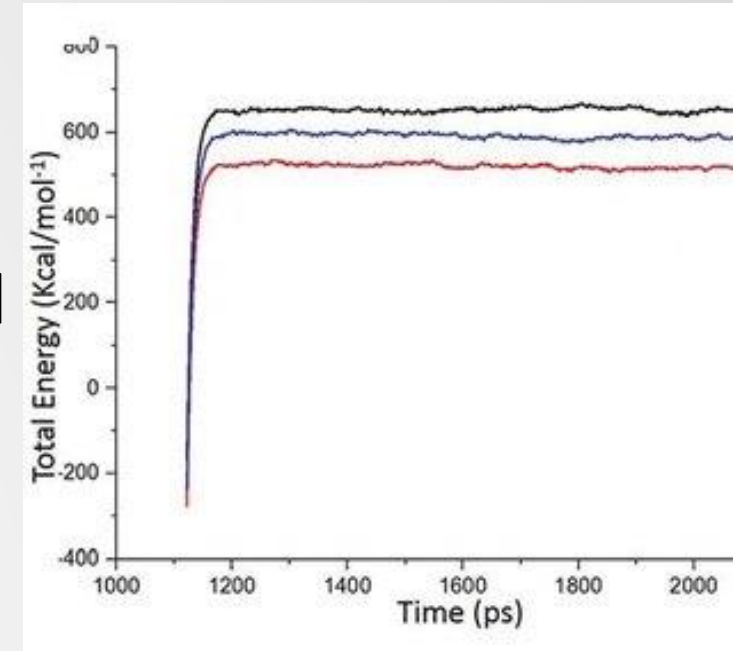
Update of velocities

Başlangıç hızları rassal belirlenir.

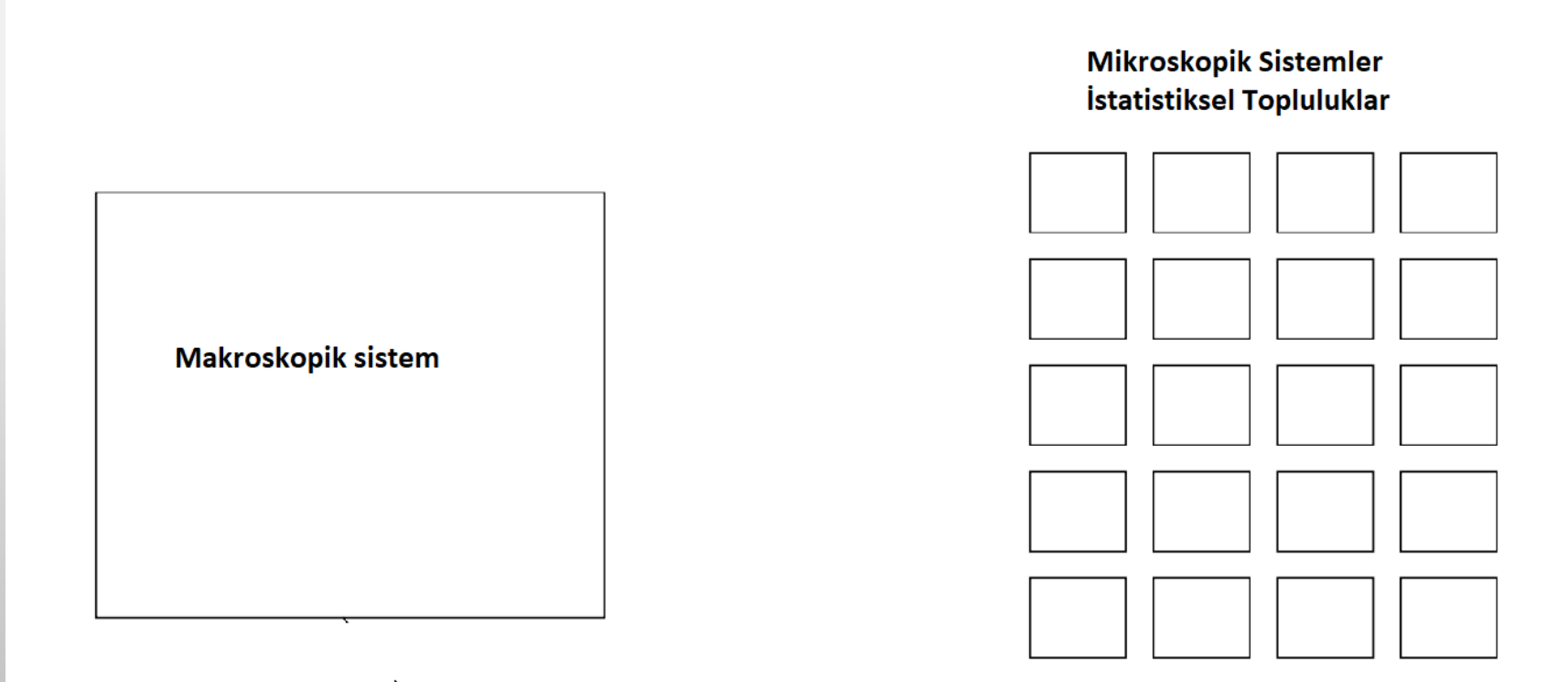
MD Programı- Time step seçimi

- Newton denklemleri toplam enerjisini (E) korur.
- Sayısal çözümlerin doğruluğu, enerjinin ne kadar sabit kaldığı ile kontrol edilebilir.
- **Time step seçilmesi:** Enerjinin korunmasında sayısal kararlılık ve doğruluk için,
- Çok küçük zaman adımları XXXX
- Çok büyük zaman adımları, XXXX

Zaman adımı (Δt) en hızlı hareketin periyodunun 1/10 ila 1/100'ü arasında seçilir.



Istatistiksel Toplulukları



Sistemin Özelliđi = Tüm sistemlerdeki ortalama özellik
(Topluluk/Küme Ortalaması)

NVE, NVT, NPT Toplulukları

Topluluklar termodinamik deęişkenlerin sabit deęerleri ile karakterize edilir:

Enerji

Sıcaklık

Basınç

Hacim

Parçacık sayısı

Kimyasal Potansiyel

NVE, NVT, NPT Simülasyonları

NVE: Sabit parçacık sayısı, sabit hacim, sabit toplam enerji (Micro canonical)
Sıcaklık ve Basınç

NVT: Sabit parçacık sayısı, sabit hacim, sabit sıcaklık (canonical)
Toplam Enerji ve Basınç
-thermostat : sıcaklığı sabit tutmak için enerji ekleyen ve çıkaran algoritma
Berendsen thermostat, Anderson thermostat

NPT: sabit parçacık sayısı, sabit basınç, sabit sıcaklık (isothermal-isobaric)
Toplam Enerji ve Hacim
-thermostat ve barostat : basıncı sabit tutmak için hacmi değiştiren
algoritma

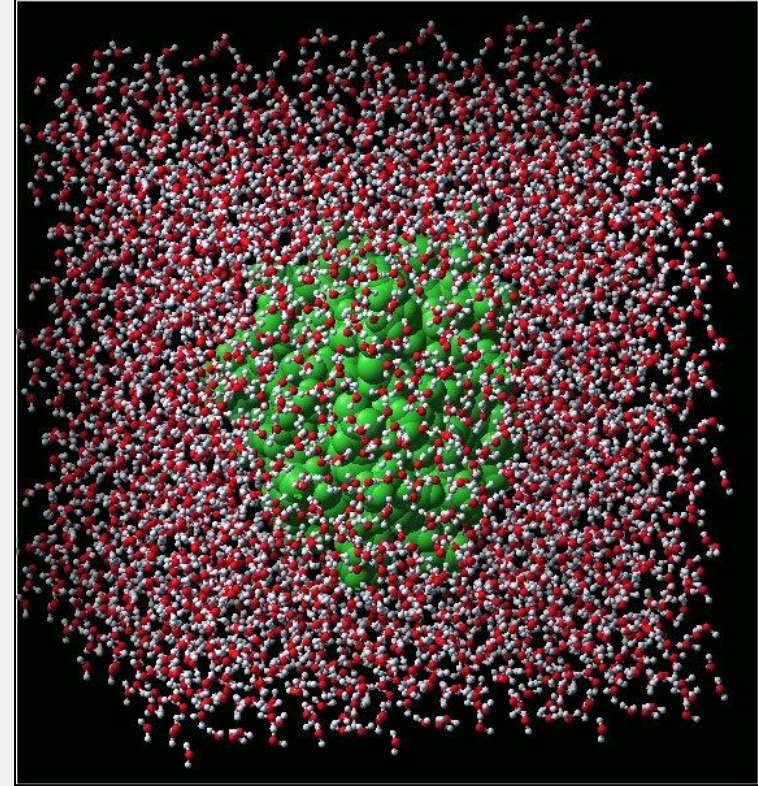
Termostatlar



- Berendsen
- Andersen
- Nose-Hoover
- Langevin

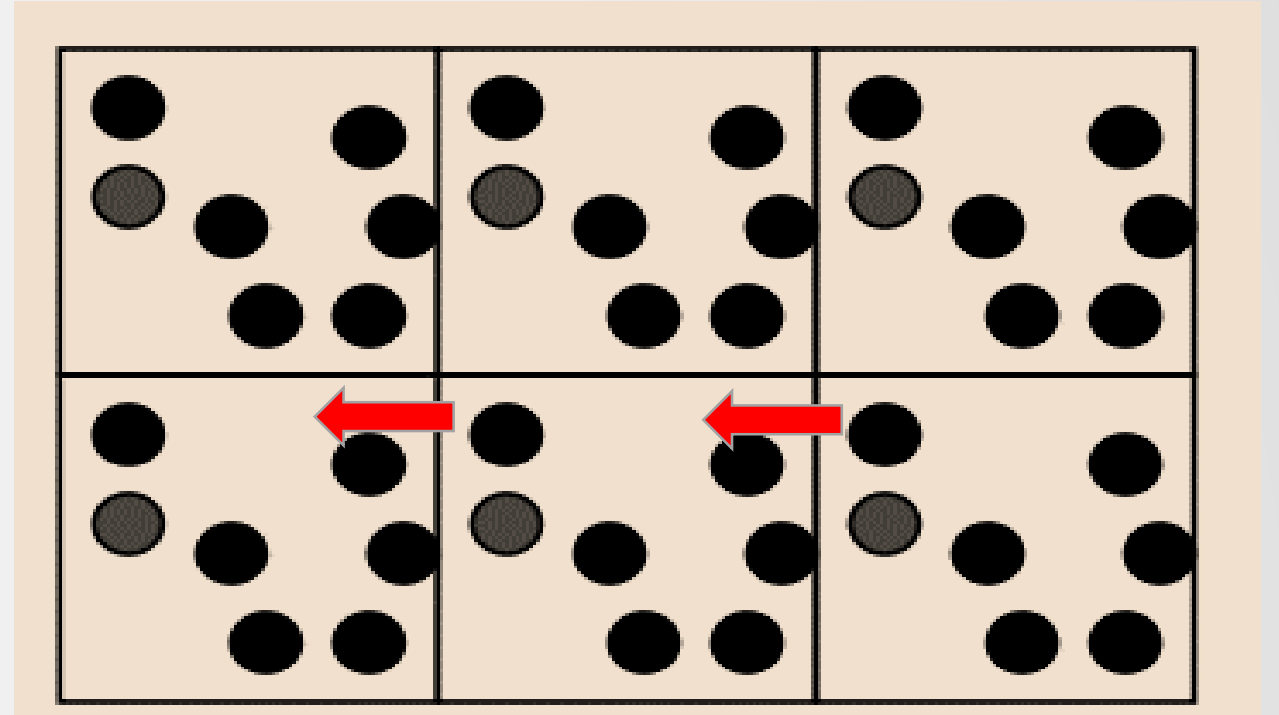
Çözücü içinde Simülasyon

- Biomoleküller –Su
- EXPLICIT (AÇIK) YA DA IMPLICIT (ÖRTÜK)
- Su modelleri
- TIP3P , SPC, TIP4P



Periodik Sınır Koşulları

- SİSTEME GÖRE KARAR VERİLECEKLER
- Kutu Büyüklüğü
- Kutu Tipleri
 - Kübik
 - Truncated Octahedron



Ewald Sum-- Particle Mesh Ewald

- Coulomb etkileşimleri $\rightarrow 1/r$
- Particle Mesh Yöntemleri
- Kısa (Hızlı azalan) ve uzun (yavaş azalan) menzil olarak ayırır .
- Kısa menzil 😊 Parçacıklararası direkt ikili etkileşim (Particle)-Real Space
- Uzun Menzilli Yavaş Azalan Elektrostatik Etkileşimler (Mesh)- Fourier Space
- Yük nötr olmalı
- AMBER programında :
- Particle Mesh Ewald (PME) yöntemi, $ntb = 0$ olmadığı sürece her zaman "açık"tır.

Kullanılan Yazılımlar

- 3 Boyutlu Görselleştirme
- MD Simülasyon
- Homoloji Modellemesi
- Yardımcı Yazılımlar

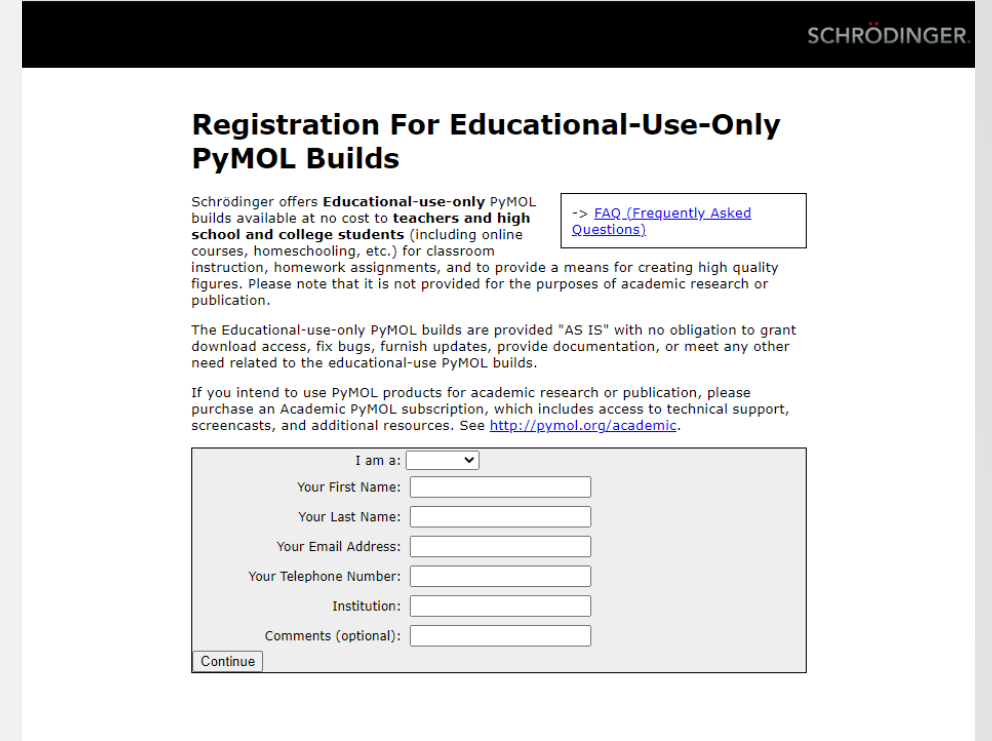
Kullanılan Yazılımlar-3 B Görselleştirme

- Pymol
- UCSF Chimera
- VMD
- DS Visualizer

Kullanılan Yazılımlar Pymol

- Python ile yazılmış, açık kaynak kodlu, kullanıcı destekli, moleküler görselleştirme sistemi.
- built-in betik yazabilme
- Windows, Mac ve Linux için.
- Öğrenci Eğitimci ücretsiz
- Schrödinger grubu tarafından ücretli olarak dağıtılan bir versiyonda var

<https://pymol.org/edu/>



SCHRÖDINGER

Registration For Educational-Use-Only PyMOL Builds

Schrödinger offers **Educational-use-only** PyMOL builds available at no cost to **teachers and high school and college students** (including online courses, homeschooling, etc.) for classroom instruction, homework assignments, and to provide a means for creating high quality figures. Please note that it is not provided for the purposes of academic research or publication.

[-> FAQ \(Frequently Asked Questions\)](#)

The Educational-use-only PyMOL builds are provided "AS IS" with no obligation to grant download access, fix bugs, furnish updates, provide documentation, or meet any other need related to the educational-use PyMOL builds.

If you intend to use PyMOL products for academic research or publication, please purchase an Academic PyMOL subscription, which includes access to technical support, screencasts, and additional resources. See <http://pymol.org/academic>.

I am a:

Your First Name:

Your Last Name:

Your Email Address:

Your Telephone Number:

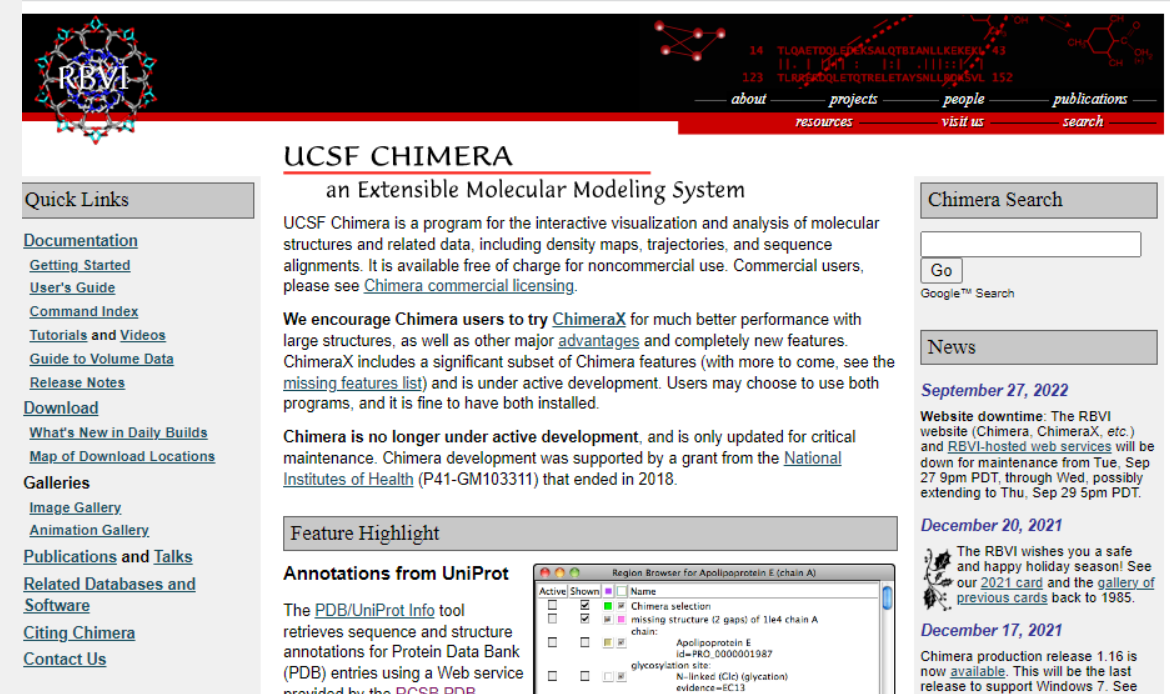
Institution:

Comments (optional):

Kullanılan Yazılımlar UCSF Chimera

- Moleküler yapıların ve ilgili verilerin etkileşimli görselleştirilmesi ve analizi için açık kaynak program.
- Akademik, devlet, kar amacı gütmeyen ve kişisel kullanım için ücretsiz.
- Windows, Mac ve Linux için.


<https://www.cgl.ucsf.edu/chimera/index.html>



The screenshot shows the UCSF Chimera website. At the top, there is a navigation bar with links for 'about', 'projects', 'people', 'publications', 'resources', 'visit us', and 'search'. Below this, the main heading reads 'UCSF CHIMERA an Extensible Molecular Modeling System'. The main text describes Chimera as a program for the interactive visualization and analysis of molecular structures and related data. It mentions ChimeraX as a newer version with more features. A 'Feature Highlight' section titled 'Annotations from UniProt' shows a screenshot of the UniProt interface for Apolipoprotein E. On the right side, there is a 'Chimera Search' box and a 'News' section with dates like 'September 27, 2022' and 'December 20, 2021'.

Kullanılan Yazılımlar- VMD

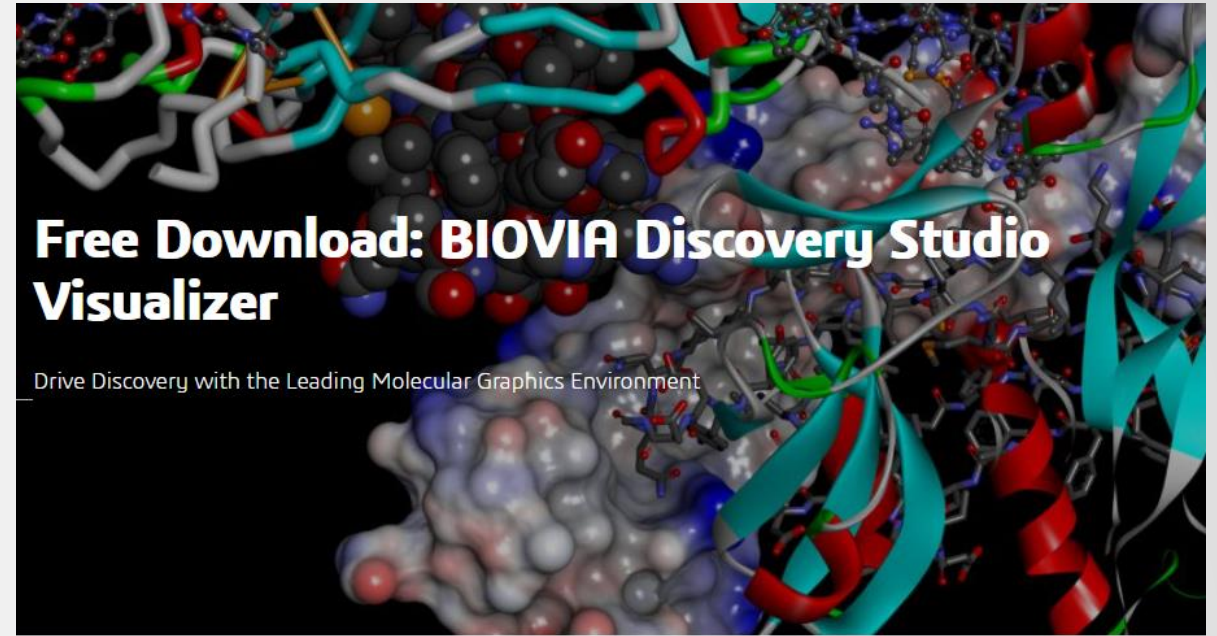
- 3 boyutlu grafikler ve built-in betik yazabilme
- büyük biyomoleküler sistemleri görüntülemek, animasyonu ve analiz etmek için ücretsiz açık kaynaklı moleküler görselleştirme programı.
- MacOS X, Unix veya Windows için.
- <http://www.ks.uiuc.edu/Research/vmd/>



The screenshot shows the homepage of the Visual Molecular Dynamics (VMD) website. The header includes the NIH Center for Macromolecular Modeling & Bioinformatics and the University of Illinois at Urbana-Champaign. The main navigation bar lists Home, Research, Publications, Software, Instruction, News, Galleries, Facilities, and About Us. The left sidebar contains a navigation menu with links to Home, Overview, Publications, Research, Software, Outreach, and various mailing lists and manuals. The main content area features the VMD logo and a description of the software as a molecular visualization program for displaying, animating, and analyzing large biomolecular systems. A 'Spotlight' section highlights the software's capability to work with very large structures, mentioning a 1,000,000+ atom Mosaic Virus simulation. Below this, there are sections for 'Overview' and 'News and Announcements', which lists several recent publications and news items, many marked as 'NEW'.

Kullanılan Yazılımlar- DS Visualizer

- Discovery Studio'nun ücretsiz 3D görselleştiricisi
- 2D ligand-reseptör etkileşim diyagramları oluşturur..
- Linux veya Windows için.
- <https://discover.3ds.com/discovery-studio-visualizer-download>



Free Download: BIOVIA Discovery Studio Visualizer

Drive Discovery with the Leading Molecular Graphics Environment

Molecular visualization is a key aspect of the **analysis and communication** of modeling studies. If you need a commercial-grade graphics visualization tool for **viewing, sharing, and analyzing protein and modeling data**, complete the form below to receive the free Discovery Studio Visualizer for interactive 3D visualization.

Kullanılan Yazılımlar- MD Simülasyonu

- **AMBER-AmberTools**
- NAMD
- Desmond
- Tinker <https://dasher.wustl.edu/tinker/>
- CHARMM <https://www.charmm.org/>
- GROMACS <https://www.gromacs.org/>
- LAMMPS <https://www.lammps.org/#gsc.tab=0>
-

Kullanılan Yazılımlar-AMBER

ambermd.org



The Amber Home Page

Tools for Molecular Simulations

AmberTools22 Amber22 Manuals Tutorials Force Fields Contacts History

Useful links:

- Download Amber
- Installation
- Amber Citations
- GPU Support
- Updates
- Mailing Lists
- For Educators
- File Formats

The Amber Mail Reflectors

Amber The Mail Reflector exists to provide a forum for discussions on the use of the Amber software and for release of bugfixes. Before posting please read the manual, consult the FAQ, and search the previous items discussed on the Amber Reflector using the Google search box provided on the [archive site](#).

Mail reflectors distribute mail sent to the reflector address to all subscribers.

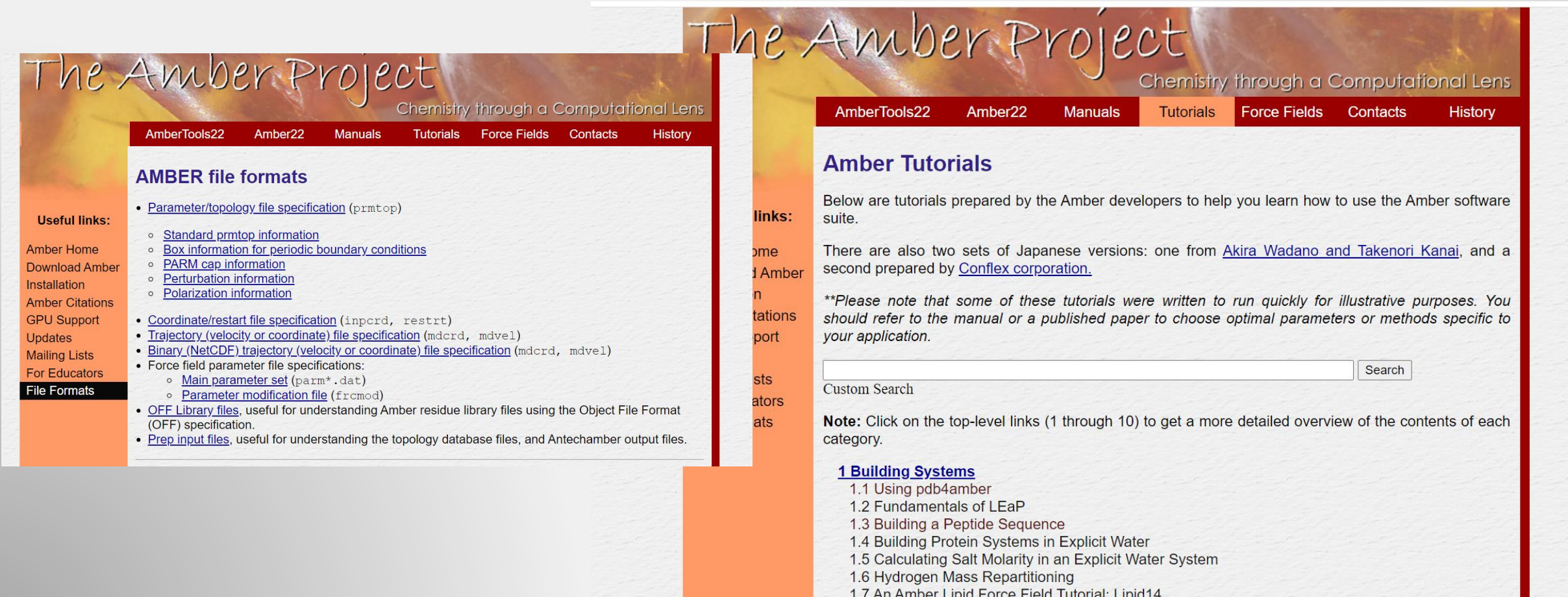
- [Archive of Users' Mail Reflector](#)
- [Archive of Developers' Mail Reflector](#)

Only subscribers to the reflector can post. To join or leave the reflector, please see: <http://lists.ambermd.org/mailman/listinfo/amber>. To post or mail to the list (subscribers only), e-mail (in plain text) to: amber@ambermd.org.

Search 

Welcome to Amber!

Amber is a suite of biomolecular simulation programs. It began in the late 1970's, and is maintained by an active development community; see our [history page](#) and our [contributors page](#) for more information.



The Amber Project

Chemistry through a Computational Lens

AmberTools22 Amber22 Manuals Tutorials Force Fields Contacts History

AMBER file formats

- [Parameter/topology file specification](#) (prmtop)
 - [Standard prmtop information](#)
 - [Box information for periodic boundary conditions](#)
 - [PARM cap information](#)
 - [Perturbation information](#)
 - [Polarization information](#)
- [Coordinate/restart file specification](#) (inpcrd, restrt)
- [Trajectory \(velocity or coordinate\) file specification](#) (mdcrd, mdvel)
- [Binary \(NetCDF\) trajectory \(velocity or coordinate\) file specification](#) (mdcrd, mdvel)
- Force field parameter file specifications:
 - [Main parameter set](#) (parm*.dat)
 - [Parameter modification file](#) (frcmod)
- [OFF Library files](#), useful for understanding Amber residue library files using the Object File Format (OFF) specification.
- [Prep input files](#), useful for understanding the topology database files, and Antechamber output files.

Amber Tutorials

Below are tutorials prepared by the Amber developers to help you learn how to use the Amber software suite.

There are also two sets of Japanese versions: one from [Akira Wadano and Takenori Kanai](#), and a second prepared by [Conflex corporation](#).

***Please note that some of these tutorials were written to run quickly for illustrative purposes. You should refer to the manual or a published paper to choose optimal parameters or methods specific to your application.*

Custom Search

Note: Click on the top-level links (1 through 10) to get a more detailed overview of the contents of each category.

1 Building Systems

- 1.1 Using pdb4amber
- 1.2 Fundamentals of LEaP
- 1.3 Building a Peptide Sequence
- 1.4 Building Protein Systems in Explicit Water
- 1.5 Calculating Salt Molarity in an Explicit Water System
- 1.6 Hydrogen Mass Repartitioning
- 1.7 An Amber Lipid Force Field Tutorial: Lipid14

Kullanılan Yazılımlar- NAMD

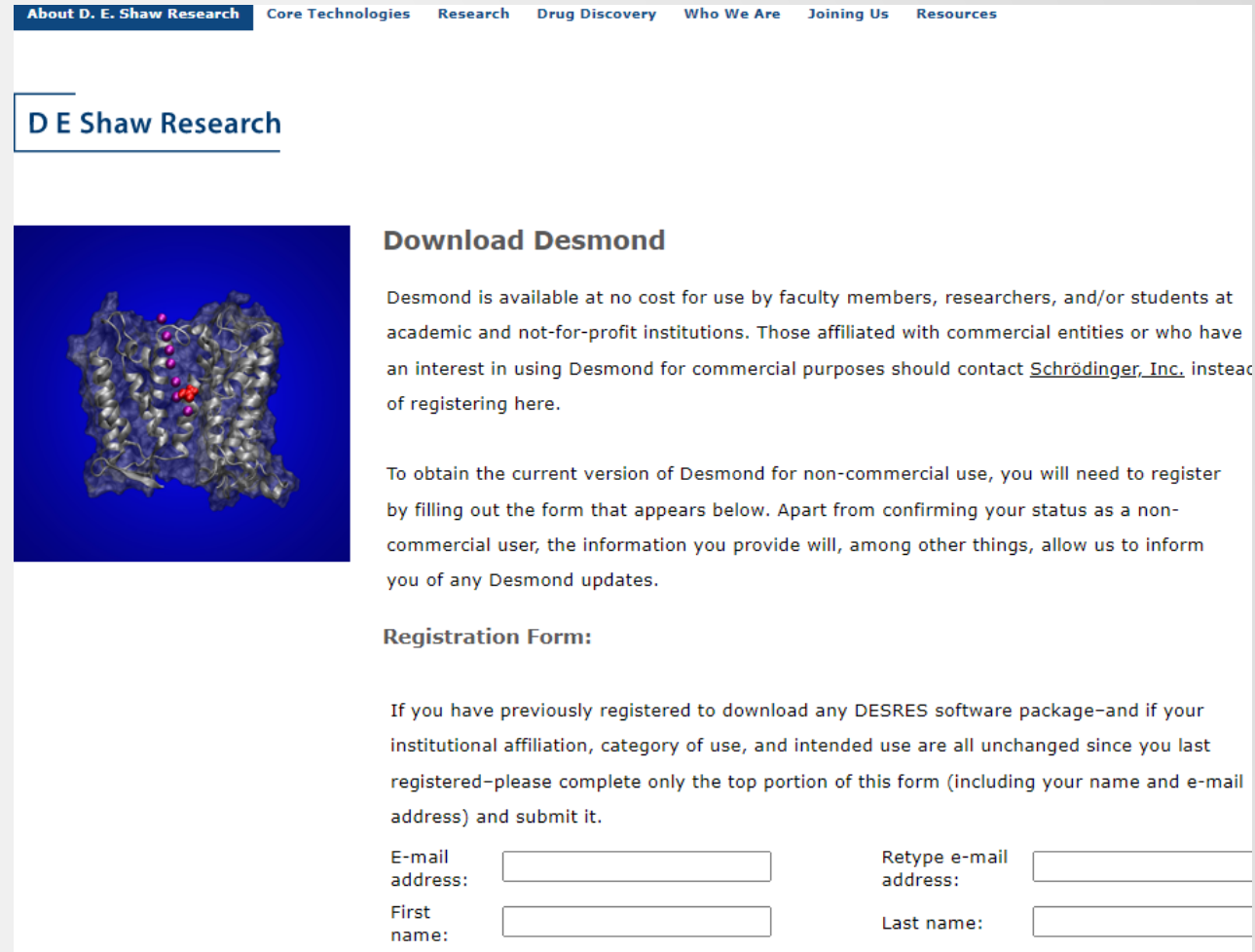
- <http://www.ks.uiuc.edu/Research/namd/>
- Kaynak koduyla birlikte ücretsiz olarak dağıtılır.



The screenshot shows the NAMD website homepage. At the top, it identifies the NIH Center for Macromolecular Modeling & Bioinformatics at the University of Illinois at Urbana-Champaign. The main header reads "THEORETICAL and COMPUTATIONAL BIOPHYSICS GROUP". A navigation menu includes Home, Research, Publications, Software, Instruction, News, Galleries, Facilities, and About Us. A sidebar on the left lists various resources under categories like Home, Overview, Publications, Research, Software (with sub-items for NAMD, VMD, GPU Computing, Lattice Microbes, Atomic Resolution Brownian Dynamics, MDFF, QwikMD, and Other), Outreach, Download NAMD, Download VMD, and Parallel Programming Laboratory. The main content area features the NAMD logo and a description of the software as a parallel molecular dynamics code. It highlights awards such as the 2002 Gordon Bell Award, 2012 Sidney Fernbach Award, and 2020 Gordon Bell Prize. A search bar is provided for finding resources. Below this, a "Breaking News" section features a banner for the 2020 ACM Gordon Bell Special Prize in HPC-based COVID-19 Research, awarded to a team for their work on AI-driven multiscale simulations of SARS-CoV-2 spike dynamics. The banner lists participating institutions like UC San Diego, Argonne National Laboratory, and the University of Illinois. At the bottom, a text block states that the University of Illinois has established a oneAPI academic Center of Excellence to address exascale computing challenges. A footer note mentions that NAMD version 3.0alpha achieves 9x throughput on NVIDIA A100 GPUs.

Kullanılan Yazılımlar- Desmond

- https://www.deshawresearch.com/downloads/download_desmond.cgi/
- Belirli GPU'larda çalışan bir MD simülasyon yazılım paketi.
- Akademik ve kar amacı gütmeyen kurumlardaki öğretim üyeleri, araştırmacılar ve/veya öğrencilere ücretsiz.



About D. E. Shaw Research Core Technologies Research Drug Discovery Who We Are Joining Us Resources

D E Shaw Research

Download Desmond

Desmond is available at no cost for use by faculty members, researchers, and/or students at academic and not-for-profit institutions. Those affiliated with commercial entities or who have an interest in using Desmond for commercial purposes should contact [Schrodinger, Inc.](#) instead of registering here.

To obtain the current version of Desmond for non-commercial use, you will need to register by filling out the form that appears below. Apart from confirming your status as a non-commercial user, the information you provide will, among other things, allow us to inform you of any Desmond updates.

Registration Form:

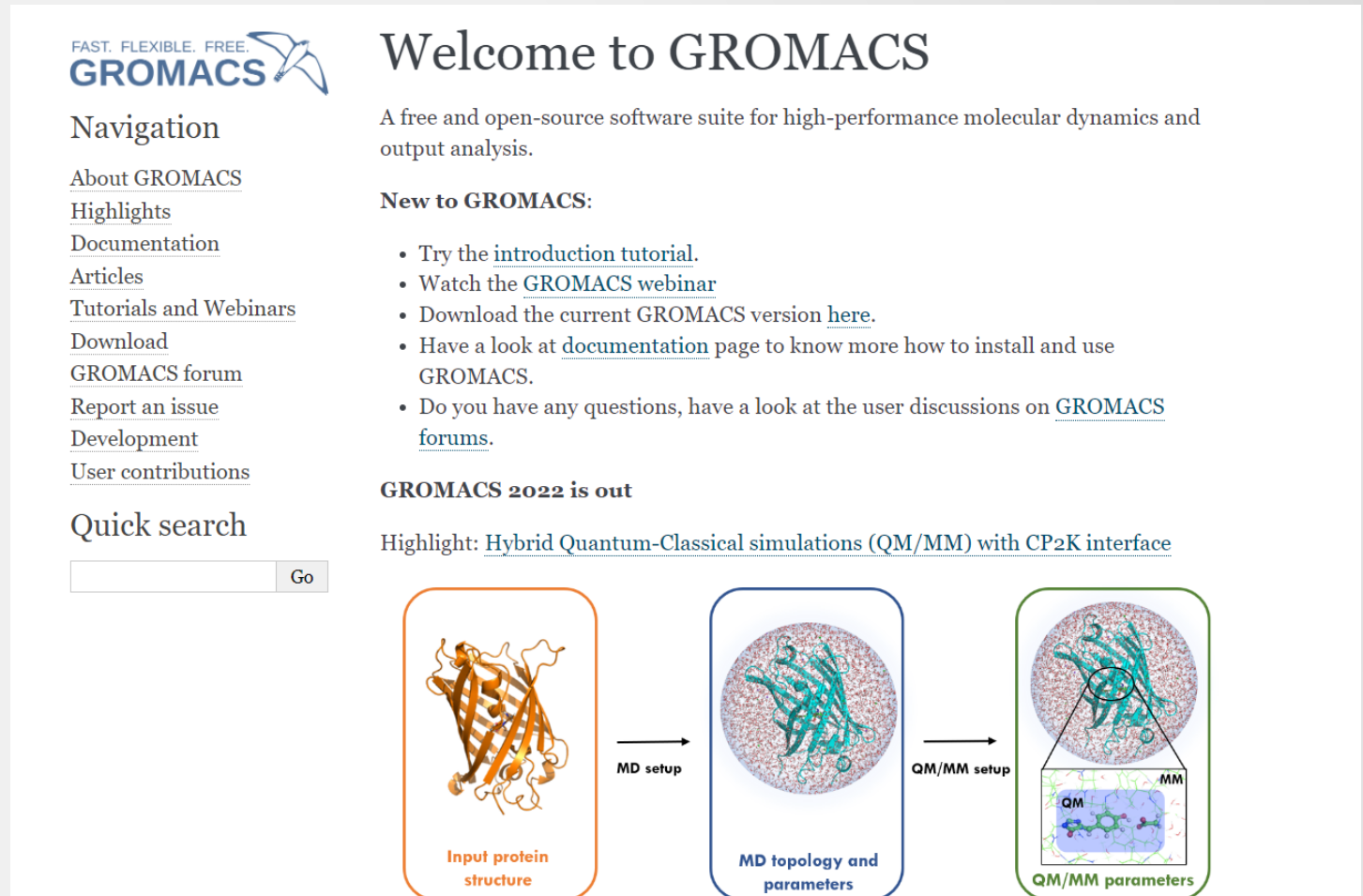
If you have previously registered to download any DESRES software package—and if your institutional affiliation, category of use, and intended use are all unchanged since you last registered—please complete only the top portion of this form (including your name and e-mail address) and submit it.

E-mail address: Retype e-mail address:

First name: Last name:

Kullanılan Yazılımlar- GROMACS

- Açık kaynak



FAST. FLEXIBLE. FREE.
GROMACS

Welcome to GROMACS

A free and open-source software suite for high-performance molecular dynamics and output analysis.

New to GROMACS:

- Try the [introduction tutorial](#).
- Watch the [GROMACS webinar](#)
- Download the current GROMACS version [here](#).
- Have a look at [documentation](#) page to know more how to install and use GROMACS.
- Do you have any questions, have a look at the user discussions on [GROMACS forums](#).

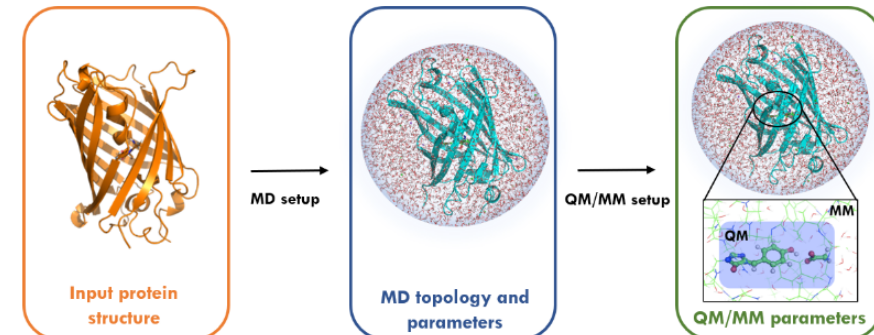
GROMACS 2022 is out

Highlight: [Hybrid Quantum-Classical simulations \(QM/MM\) with CP2K interface](#)

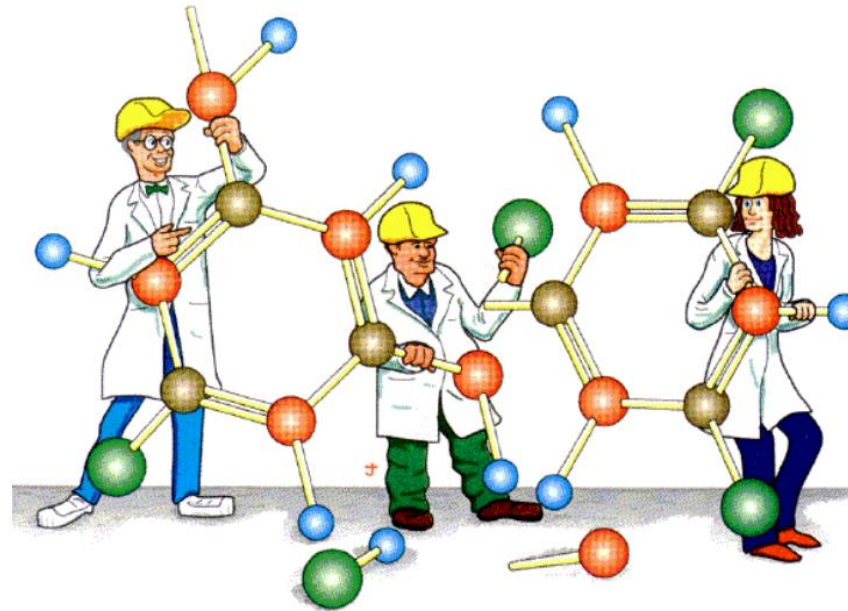
Navigation

- [About GROMACS](#)
- [Highlights](#)
- [Documentation](#)
- [Articles](#)
- [Tutorials and Webinars](#)
- [Download](#)
- [GROMACS forum](#)
- [Report an issue](#)
- [Development](#)
- [User contributions](#)

Quick search



Tinker Molecular Modeling



Tinker - Software Tools for Molecular Design

Current Major Version: Tinker 8.10

Kullanılan Yazılımlar-Homoloji Modellemesi



- Modeller- Akademik Kullanım Bedava
- Web Servisleri
 - Robetta
 - Swiss-Model
 - I-TASSER
 - Alphafold

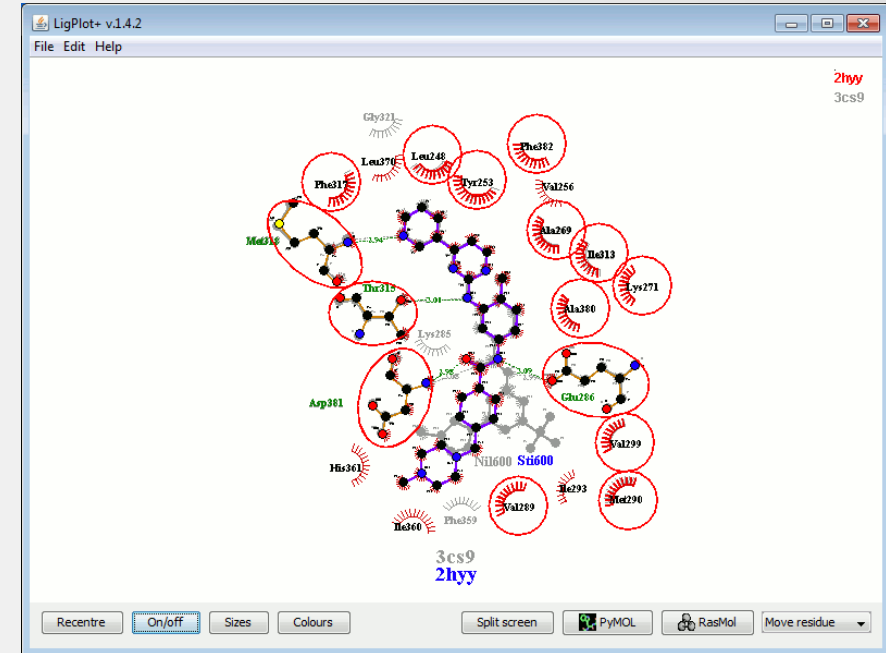
Kullanılan Yazılımlar- pKa tahmini

- PDB2PQR Server. Web sunucusu. Protein pKa are calculated using PROPKA.
- PROPKA. GitHub 'dan indirilebilir.
- H++. Web sunucusu

Yardımcı Yazılımlar

- OpenBabel- dosya formatları çevirici
- PDB Binder Bağlanma bölgesi tahmini
- Autodock/Vina- Kenetleme
- Dock- Kenetleme

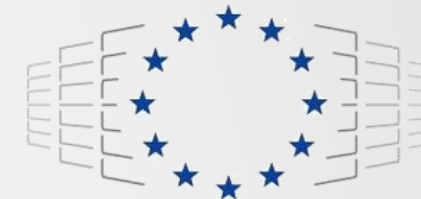
Ligplot



MD Protokolü

- Minimizasyon (Minimization) –PE fonksiyonundaki minimum yapı
- Dengeleme (Equilibration)- Toplam E –ortalama bir deęer etrafında dalgalanır (KE \leftrightarrow PE)
- Üretim (Production Runs)
- Analiz ve Görselleştirme

Teşekkürler!



EuroHPC
Joint Undertaking

This project has received funding from the European High-Performance Computing Joint Undertaking (JU) under grant agreement No 951732. The JU receives support from the European Union's Horizon 2020 research and innovation programme and Germany, Bulgaria, Austria, Croatia, Cyprus, Czech Republic, Denmark, Estonia, Finland, Greece, Hungary, Ireland, Italy, Lithuania, Latvia, Poland, Portugal, Romania, Slovenia, Spain, Sweden, United Kingdom, France, Netherlands, Belgium, Luxembourg, Slovakia, Norway, Switzerland, Turkey, Republic of North Macedonia, Iceland, Montenegro