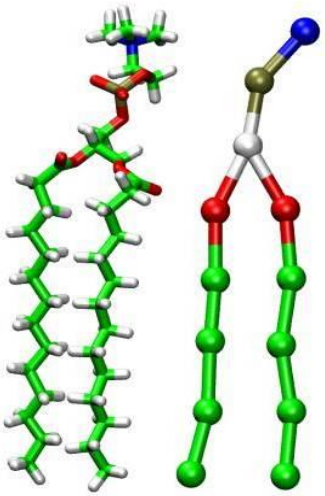
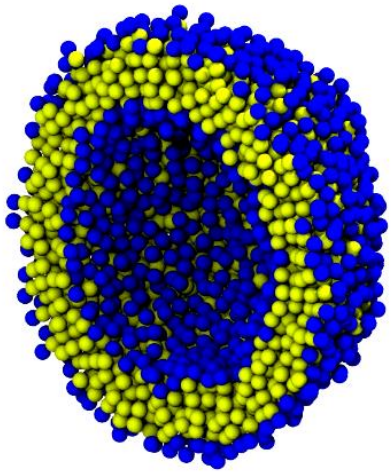
Сучасні комп’ютерні методи дослідження нанорозмірних та біологічних систем

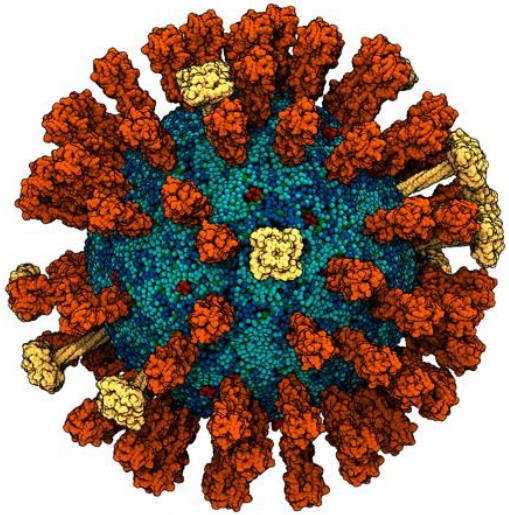
ХІМІЧНИЙ ФАКУЛЬТЕТ
ХАРКІВСЬКИЙ НАЦІОНАЛЬНИЙ УНІВЕРСИТЕТ імені В. Н. КАРАЗІНА

Лекція № 9

Крупно-зерниста модель ліпіду та ліпідної мембрани. Порівняльна характеристика та області застосування різних МД моделей







професор кафедри неорганічної хімії Кириченко О.В. 2020

План Лекції № 9

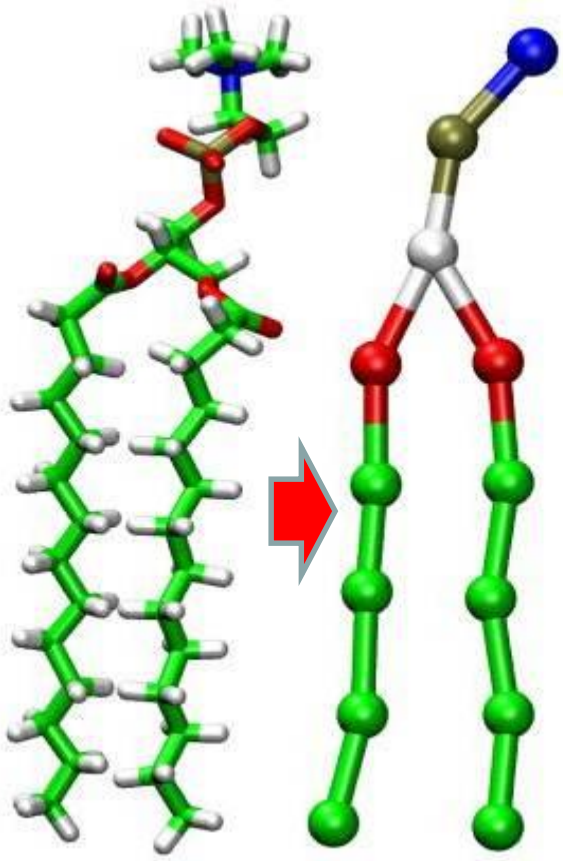
- **Фрагментовані та “зернисті” моделі ліпіду та ліпідної мембрани**

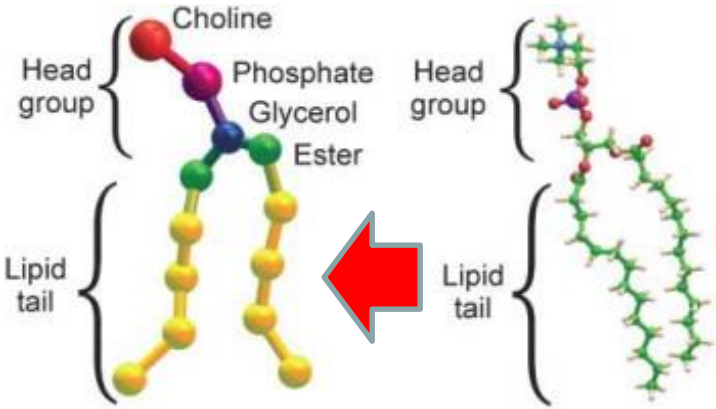
- **Поширені силові поля та програми для МД моделювання ліпідних систем**

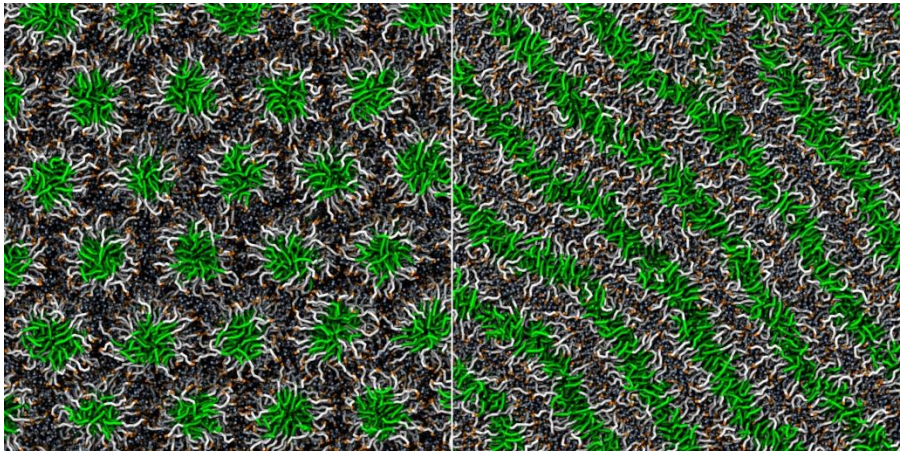
- **Порівняльна характеристика та області застосування різних МД моделей**

- **Наявні програмні пакети для МД моделювання біологічних мембран**

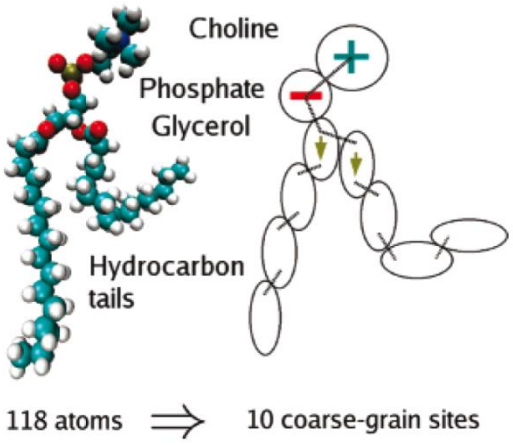
“Фрагментарная”, “крупно-зернистая” или “грубо-зернистая” (coarse-grained) МД модель липида

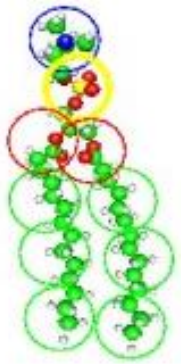




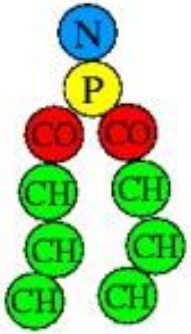


“Фрагментарная” или “крупно-зернистая” МД модель липида

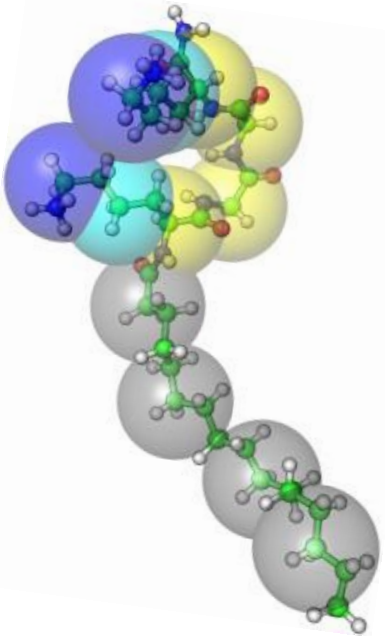




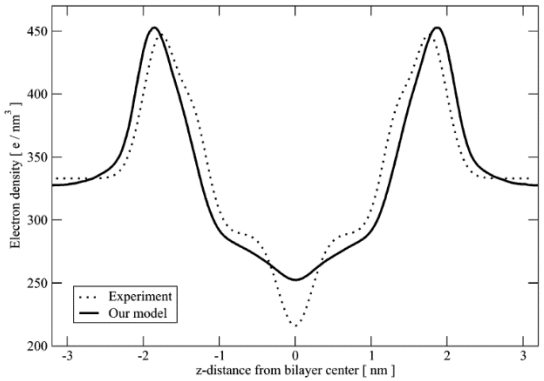
полноатомная модель (118 атомов)

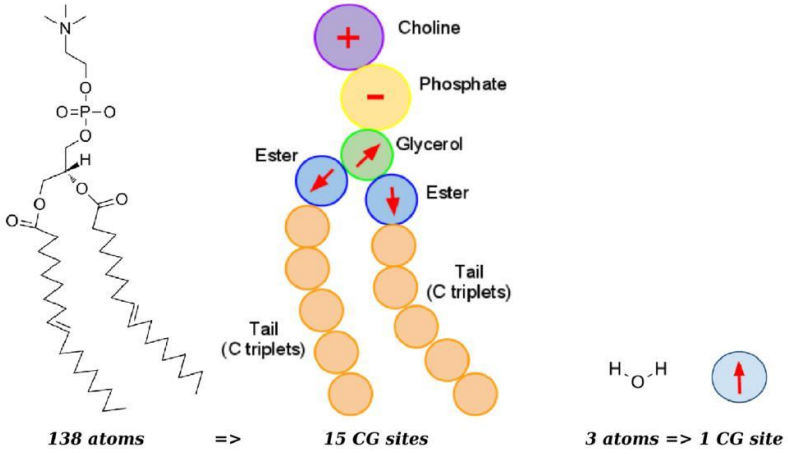


фрагментарная модель (10 центров взаимодействия)

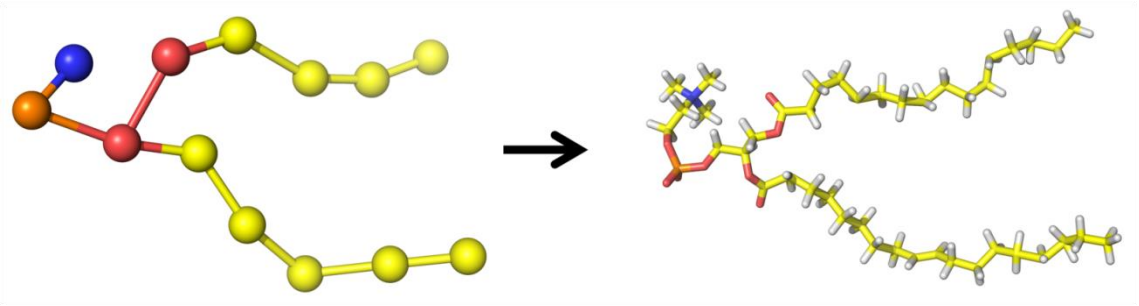


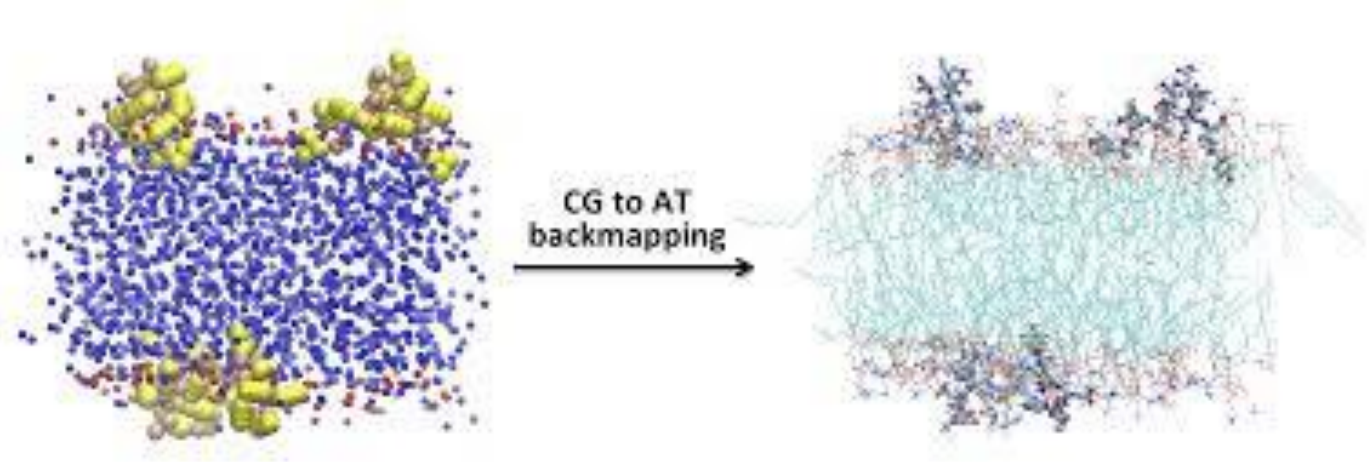
критерий успешности модели



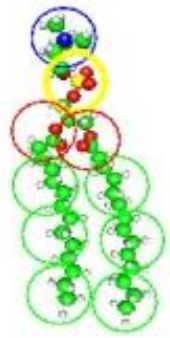


Обратная трансформация “крупнозернистой” модели в полноатомную модель

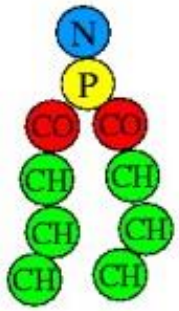




“Фрагментарная” МД модель липида



полноатомная модель (118 атомов)



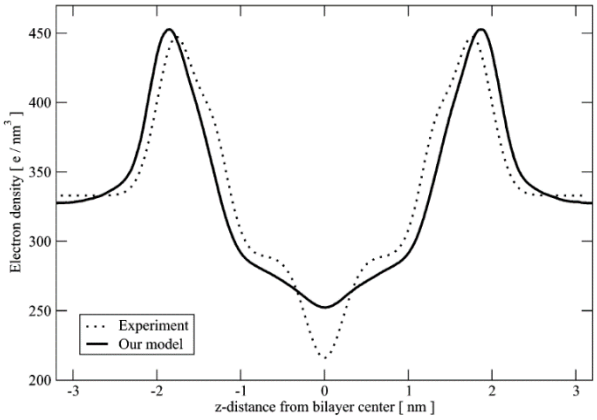
фрагментарная модель (10 центров взаимодействия)

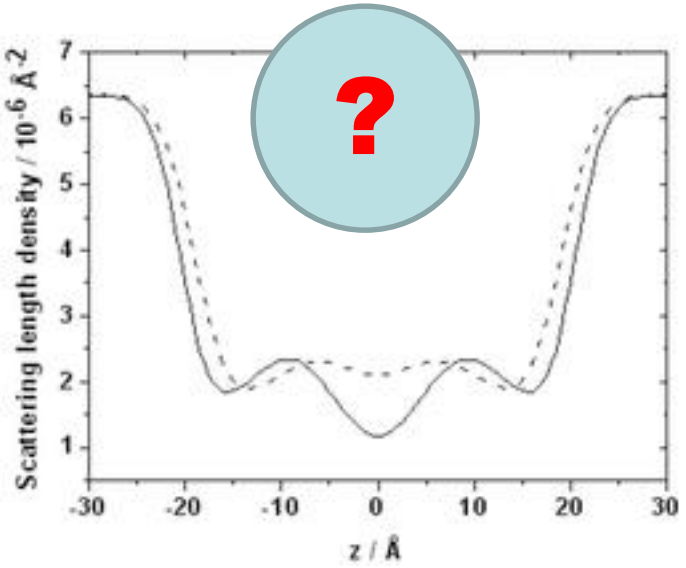
Уже предложено 8 различных моделей, с разной степенью фрагментации одной молекулы липида.

однако

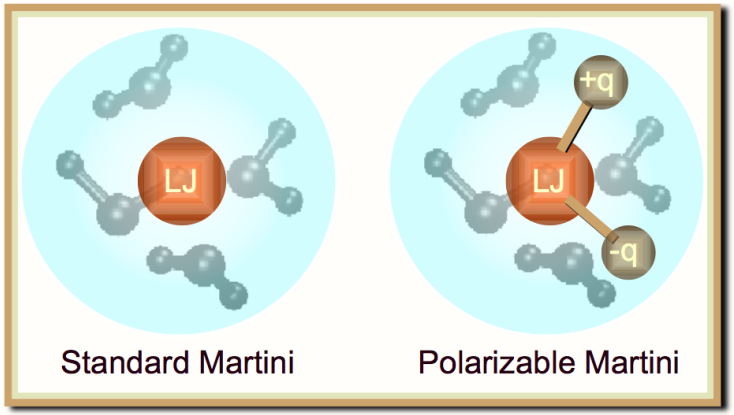
на определенном этапе происходит потеря разрешающей способности фрагментированной модели …

критерий успешности модели = воспроизведение эксперимента





“Фрагментарные” МД модели воды



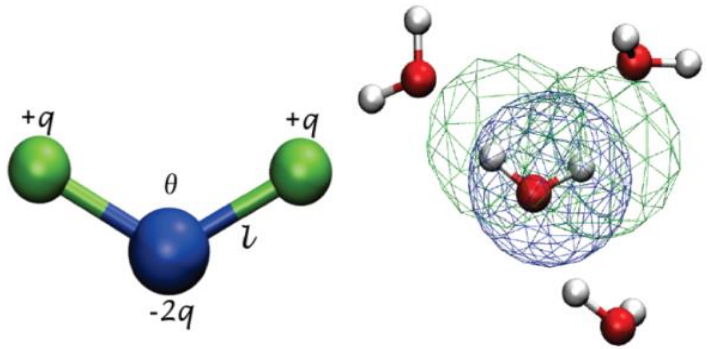
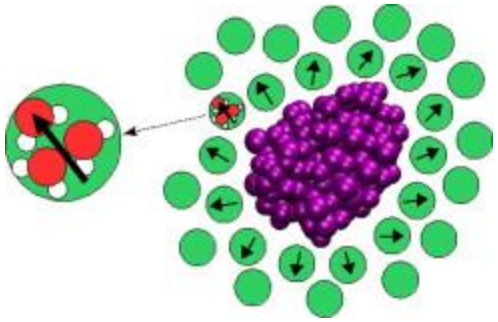
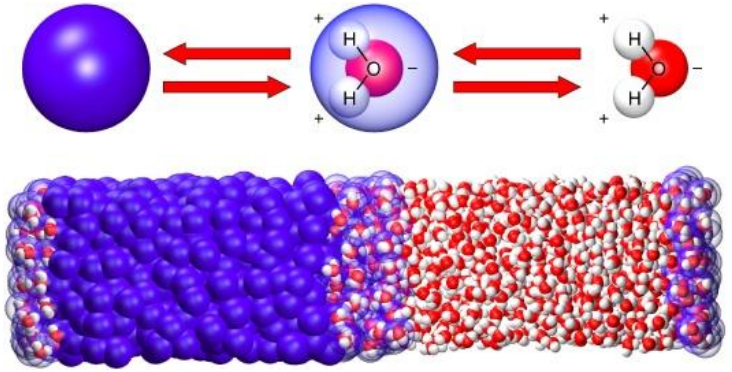
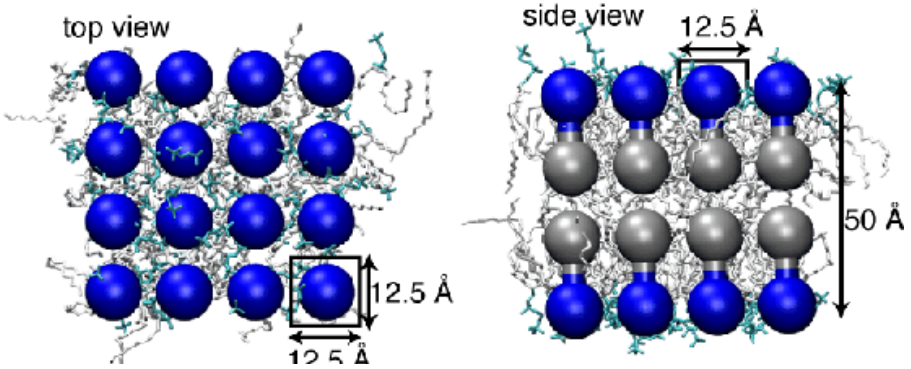


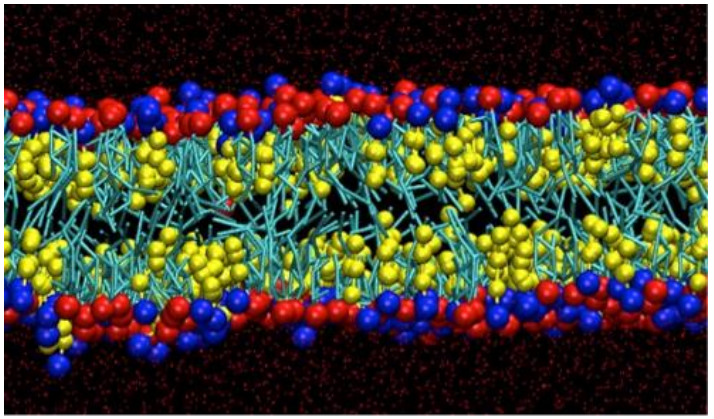
Figure 2. A 4-water cluster is coarse grained into a three-site model with $\theta = 120°$, $l = 1.2$ Å, $q = 1e^{-}$.

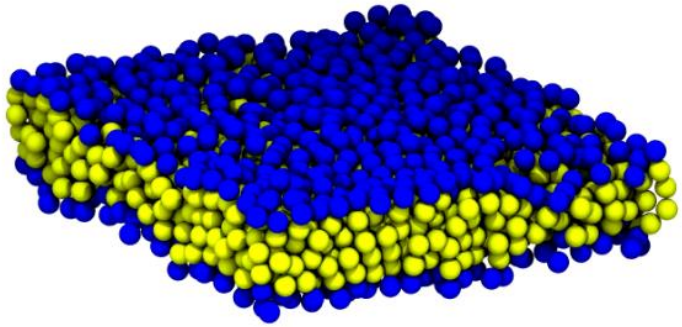


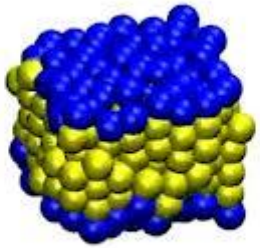


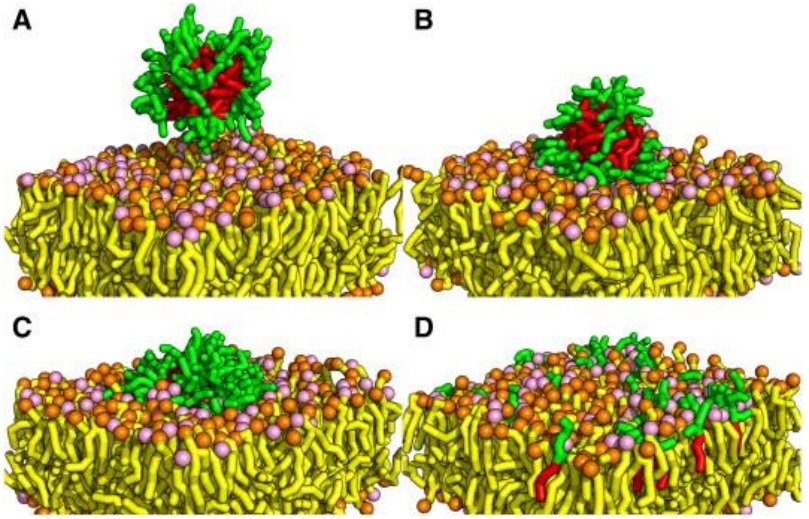
“Фрагментарная” МД модель мембраны







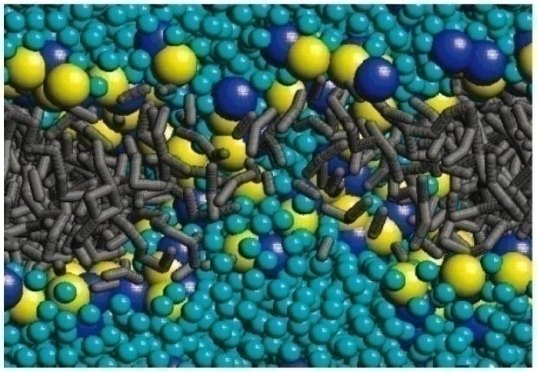




“Фрагментарная” МД модель мембраны

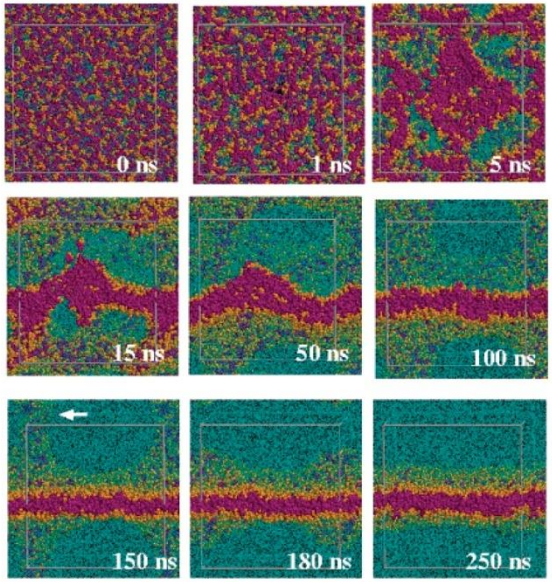
Преимущества:

Адекватное описание макроскопических параметров мембран и везикул. Позволяет изучать процессы образования и слияния индивидуальных везикул. Позволяет проводить МД расчет в микросекундной шкале!

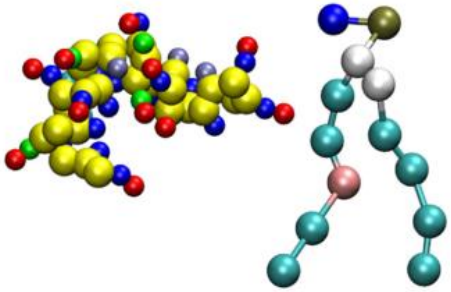


Недостатки:

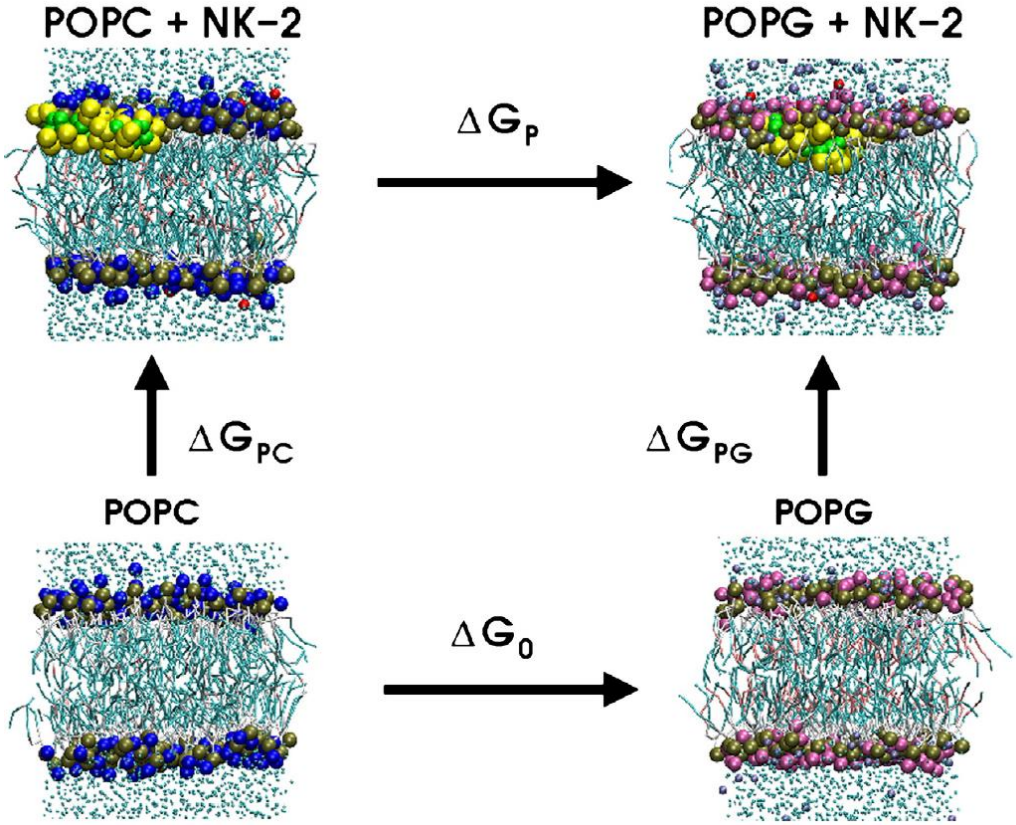
Утрачивается атомное разрешение в строение изучаемой системы. Невозможно различить детали межмолекулярного взаимодействия. Отсутствие адекватных моделей для водной фазы



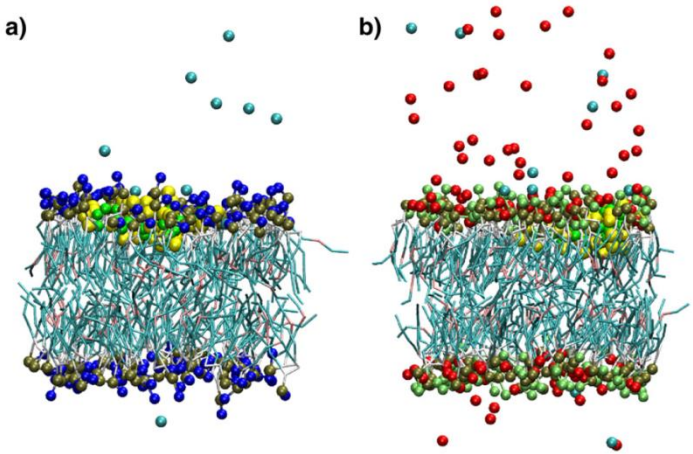
Пример “крупнозернистой” МД модели



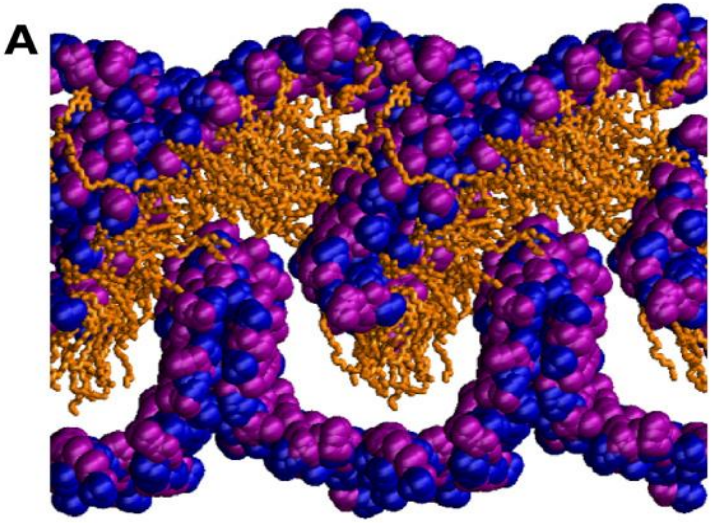
Пептид POPC липид

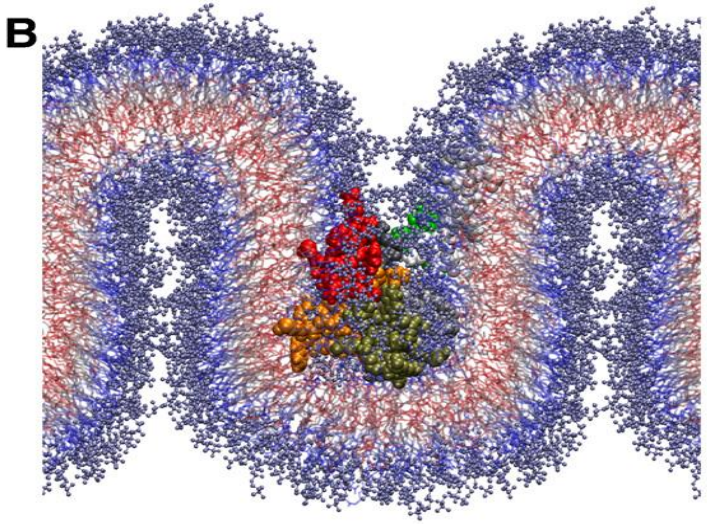


C.I.E. von Deuster, V. Knecht / Biochimica et Biophysica Acta 1808 (2011) 2867–2876



Примеры “крупнозернистой” МД модели





Biochimica et Biophysica Acta 1788 (2009) 149–168

Contents lists available at ScienceDirect

Biochimica et Biophysica Acta

journal homepage: www.elsevier.com/locate/bbamem

Review

Lipids on the move: Simulations of membrane pores, domains, stalks and curves

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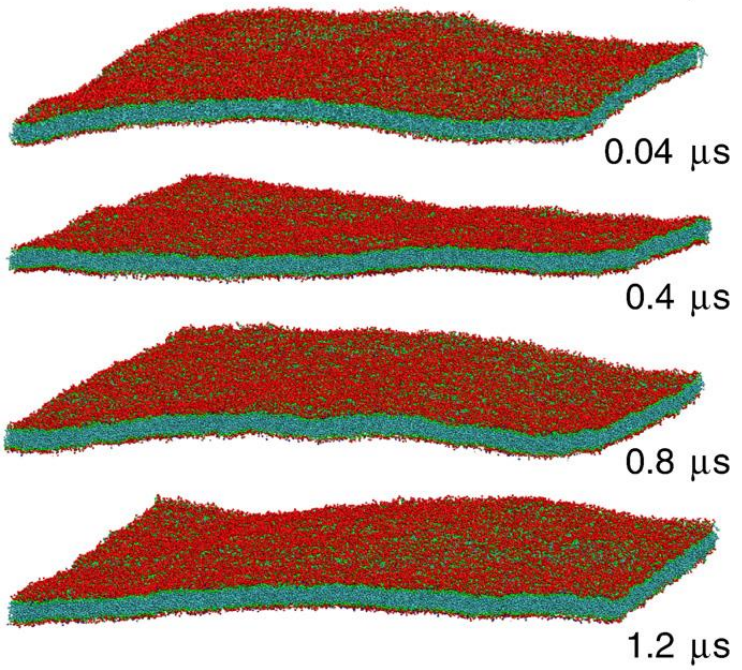
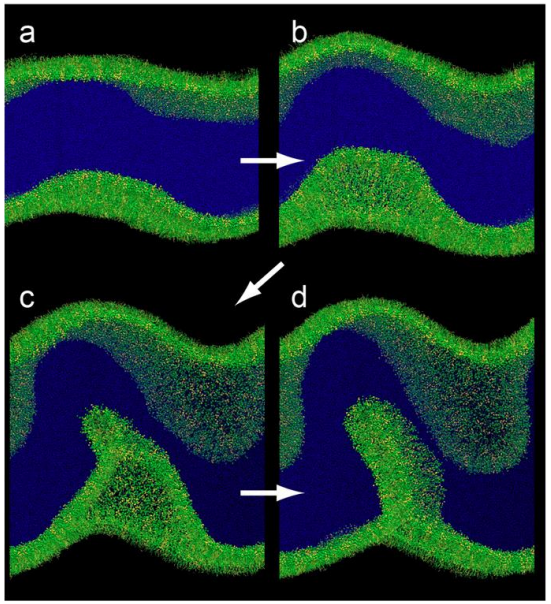
ABSTRACT

In this review we describe the state-of-the-art of computer simulation studies of lipid membranes. We focus on collective lipid–lipid and lipid–protein interactions that trigger deformations of the natural lamellar membrane state, showing that many important biological processes including self-aggregation of membrane components into domains, the formation of non-lamellar phases, and membrane poration and curving, are now amenable to detailed simulation studies.



Примеры “крупнозернистой” МД модели



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Computer simulations of lung surfactant☆

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Lipid monolayer
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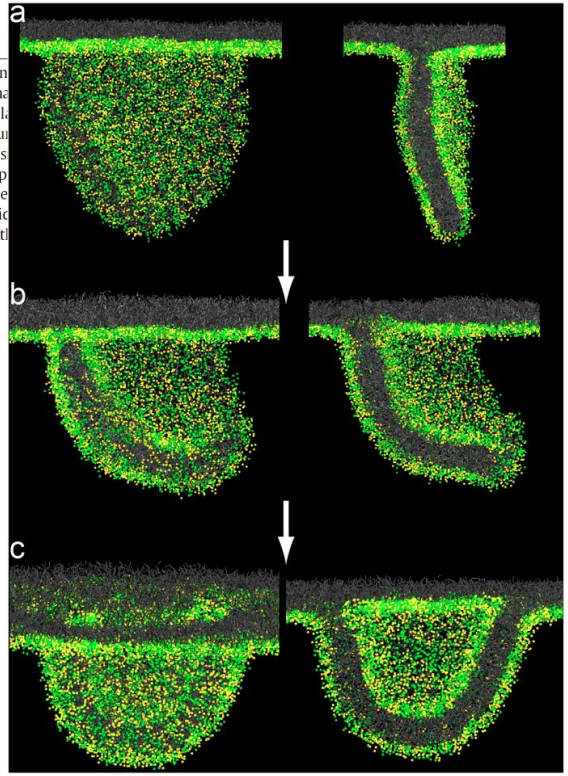
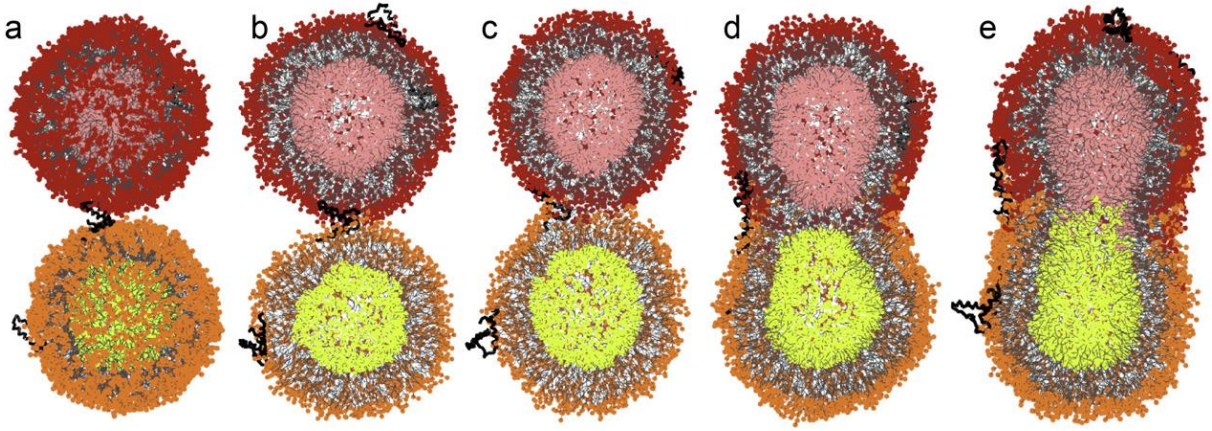
ABSTRACT

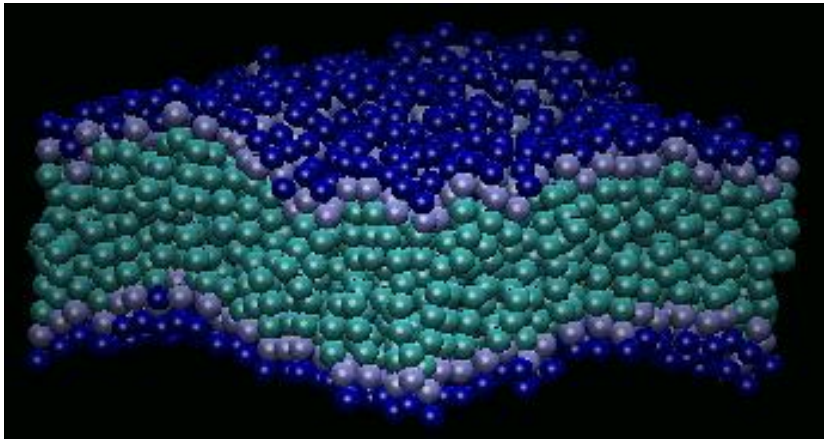
Lung surfactant lines the gas-exchange in
for breathing. Lung surfactant consists ma
the air–water interface connected to bila
between the monolayer and bilayers du
the monolayer; selected species are poss
lung surfactant and the exact roles of lip
review recent simulation studies on the
monolayer–bilayer transformations, lipi
This article is part of a Special Issue entitl



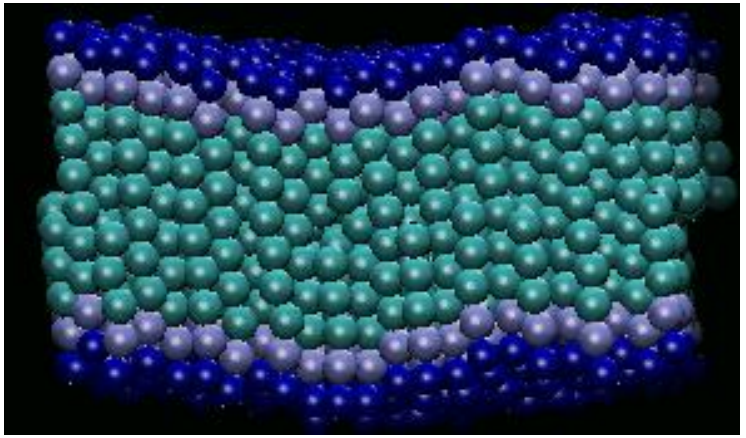


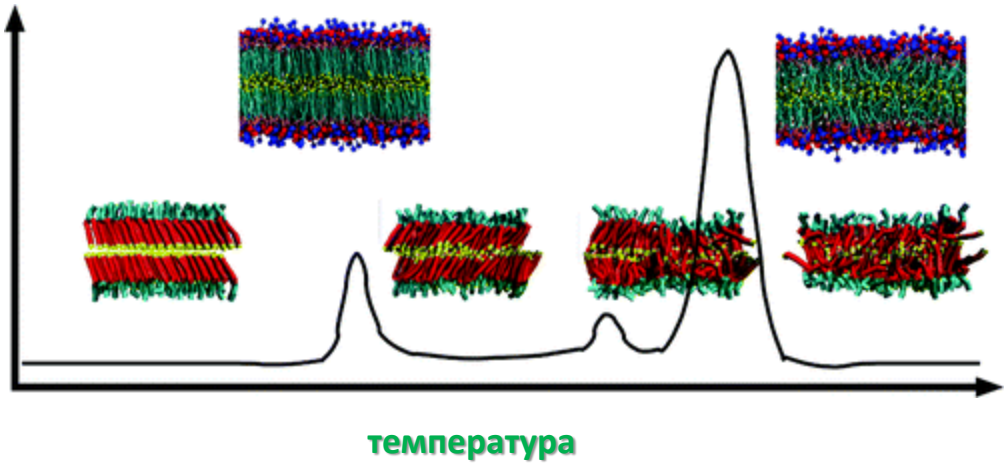
МД моделирование фазового перехода с использованием крупнозернистой модели липида

“Жидкокристаллическое”

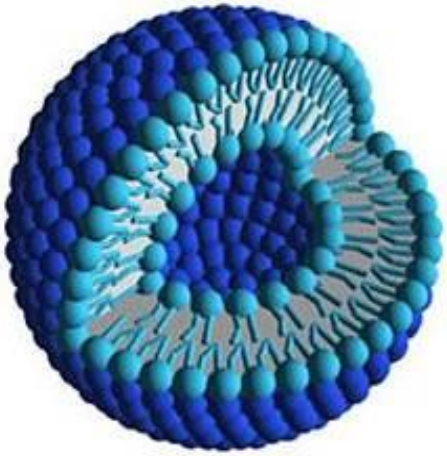


“Гелеобразное”

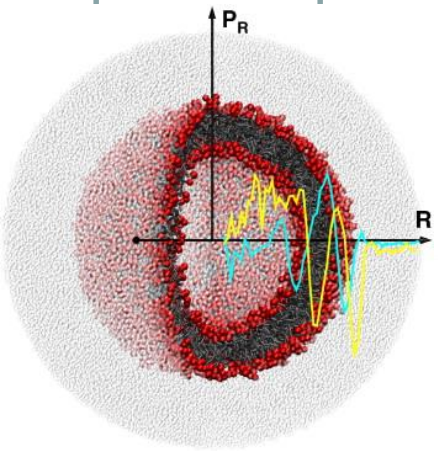


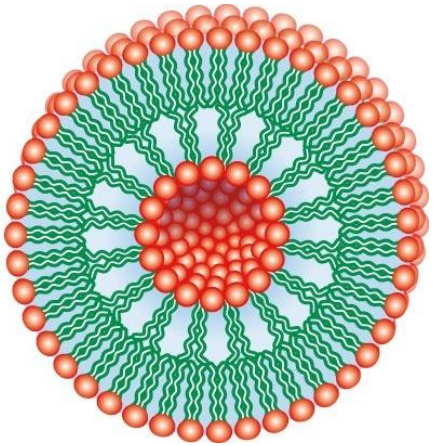


МД моделирование липидных везикул

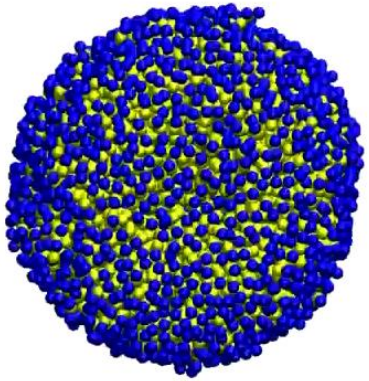


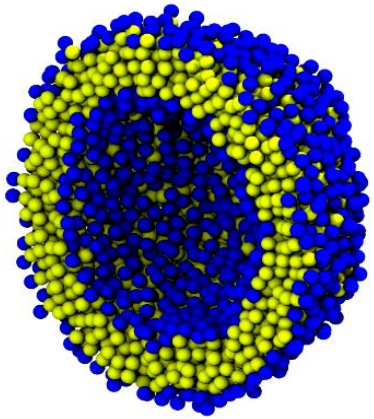
Липосома (липидная везикула) (от греч. липос – жир и сома – тельце или частица) – это замкнутая, сферическая система, которая образуется самопроизвольно в смесях фосфолипидов с водой.





фосфолипидная молекула





биохимический микрореактор

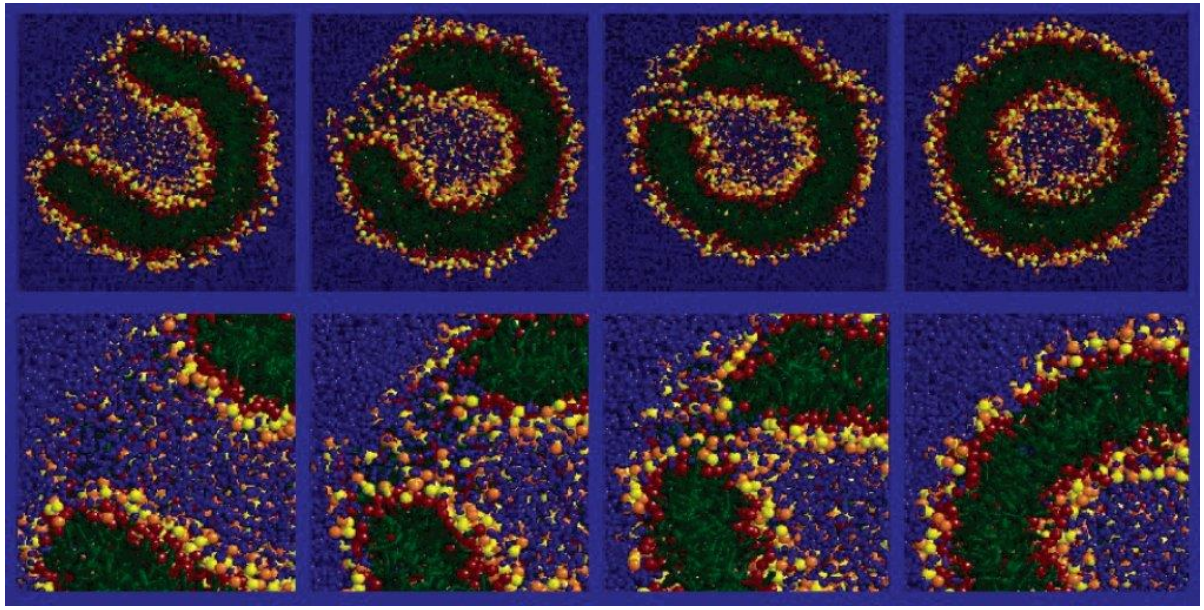
Силовое поле “MARTINI”

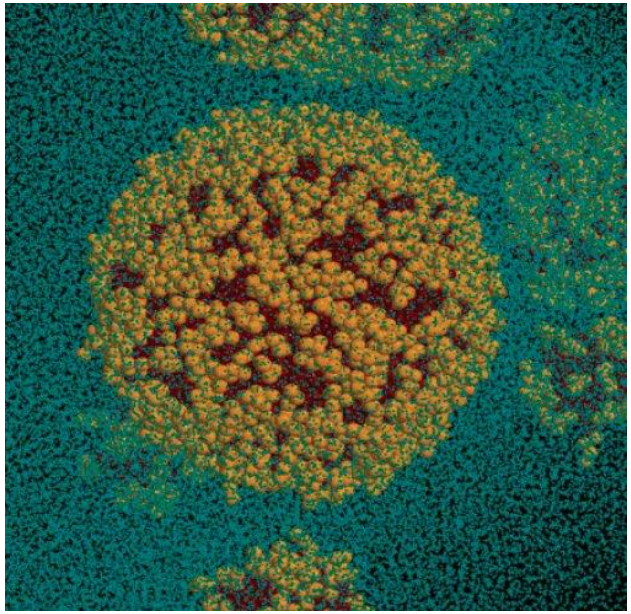
7812 *J. Phys. Chem. B* **2007,** *111,* 7812−7824

The MARTINI Force Field: Coarse Grained Model for Biomolecular Simulations

Siewert J. Marrink,*,† H. Jelger Risselada,† Serge Yefimov,‡ D. Peter Tieleman,§ and Alex H. de Vries†

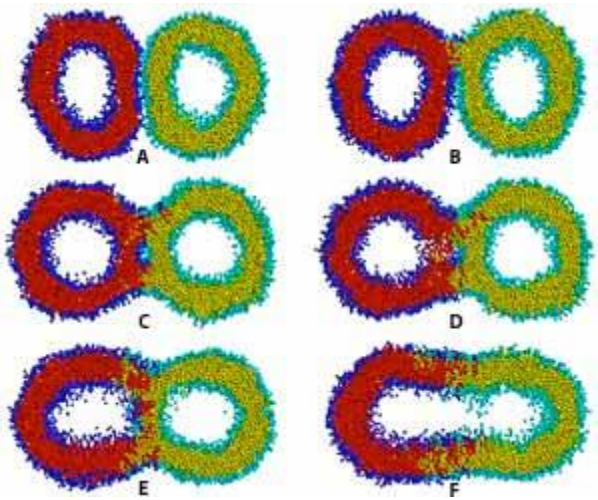
Groningen Biomolecular Sciences and Biotechnology Institute & Zernike Institute for Advanced Materials, Department of Biophysical Chemistry, University of Groningen, Nijenborgh 4, 9747 AG Groningen, The Netherlands, Zernike Institute for Advanced Materials, Department of Applied Physics, University of Groningen, Nijenborgh 4, 9747 AG Groningen, The Netherlands, and Department of Biological Sciences, University of Calgary, 2500 University Drive NW, Calgary AB T2N 1N4, Canada





S.J. Marrink and A.E. Mark *JACS* **125** (2003) 15233-15242

МД моделирование липидных везикул



J. Phys. Chem. B **2009,** *113,* 4443–4455

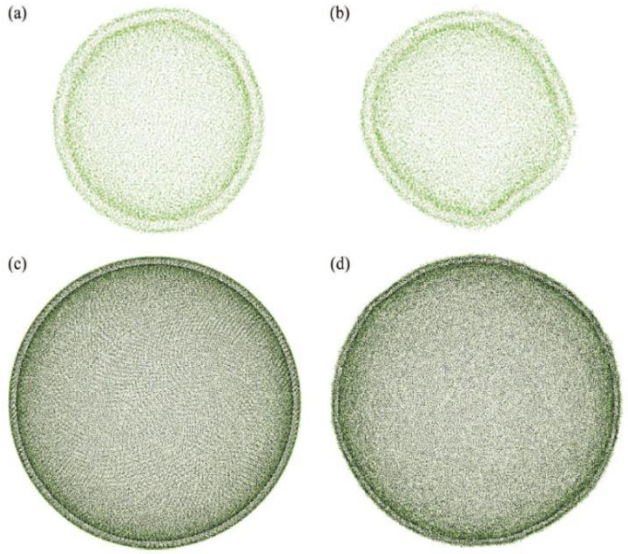
Solvent-Free Lipid Bilayer Model Using Multiscale Coarse-Graining

Sergei Izvekov and Gregory A. Voth*

Department of Chemistry and Center for Biophysical Modeling and Simulation, University of Utah, 315 S. 1400 E. Rm. 2020, Salt Lake City, Utah 84112-0850

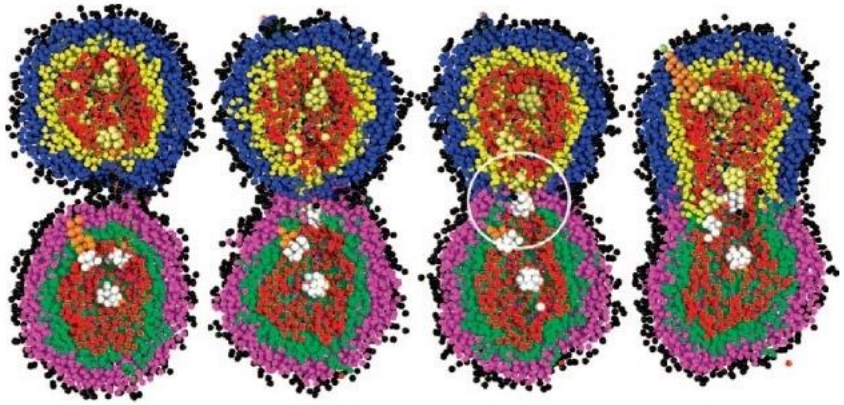
Received: November 27, 2008; Revised Manuscript Received: January 17, 2009

12000 липидов



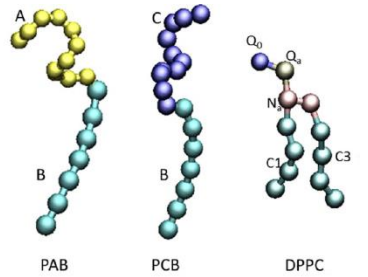
79300 липидов

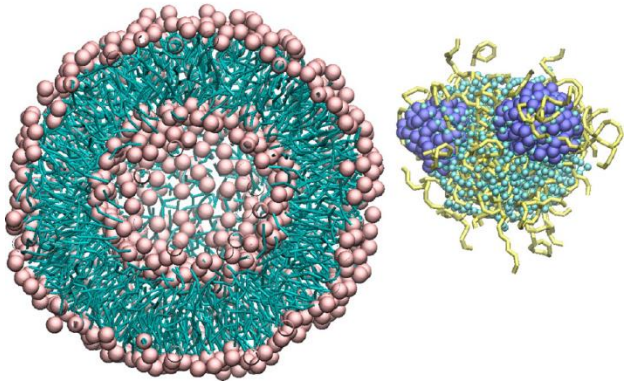
слияние липидных везикул

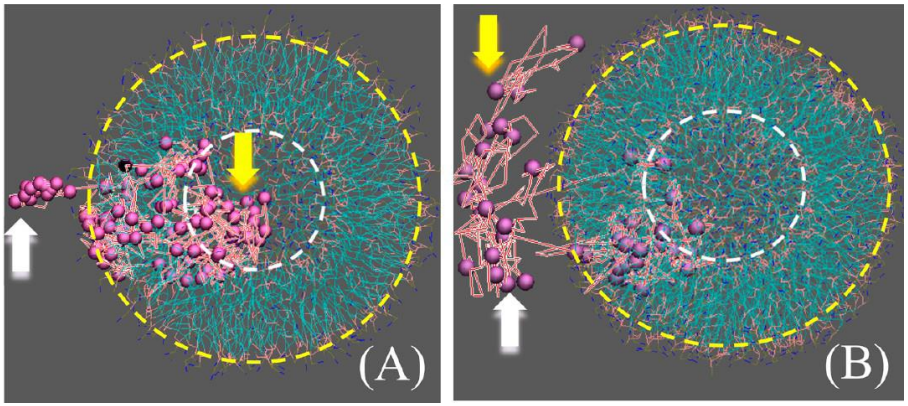


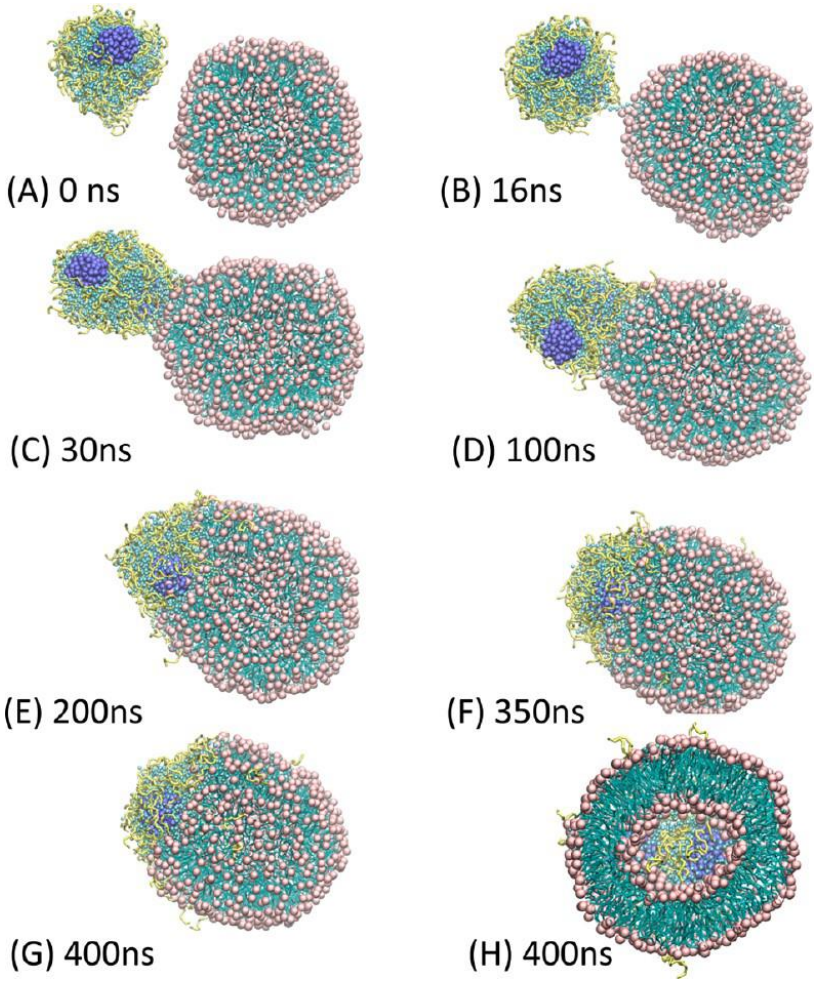
256000 “фрагментов” (beads)

Крупнозернистое МД моделирование липидных везикул и мицелл



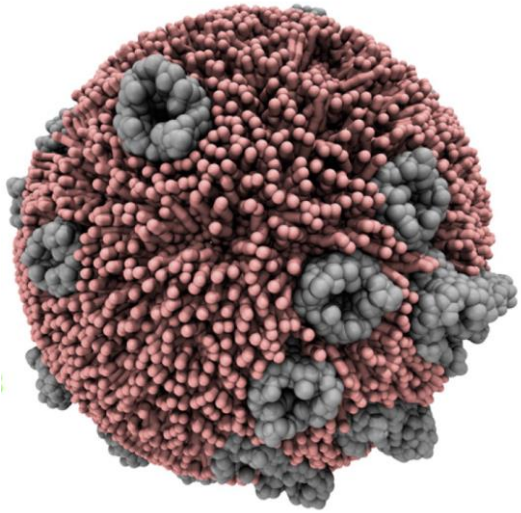


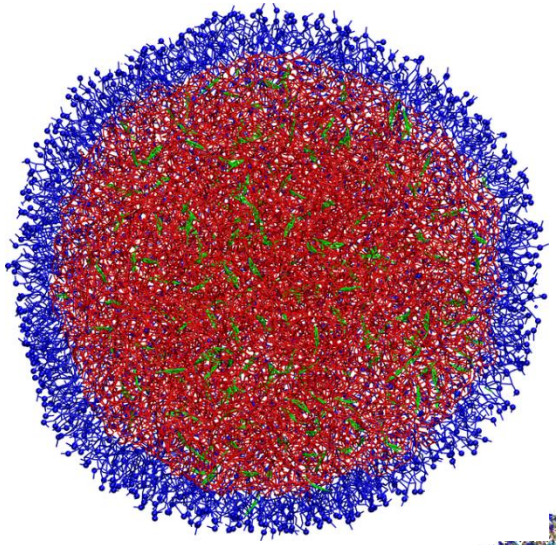


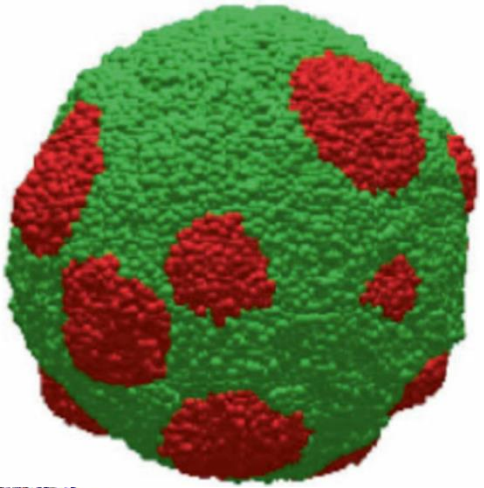


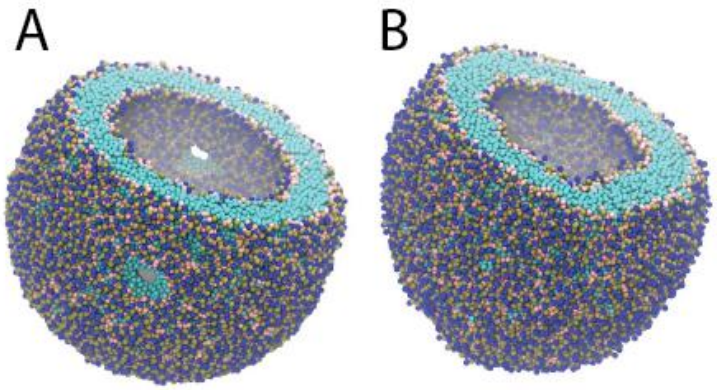
J. Phys. Chem. B 2013, 117, 12095−12104

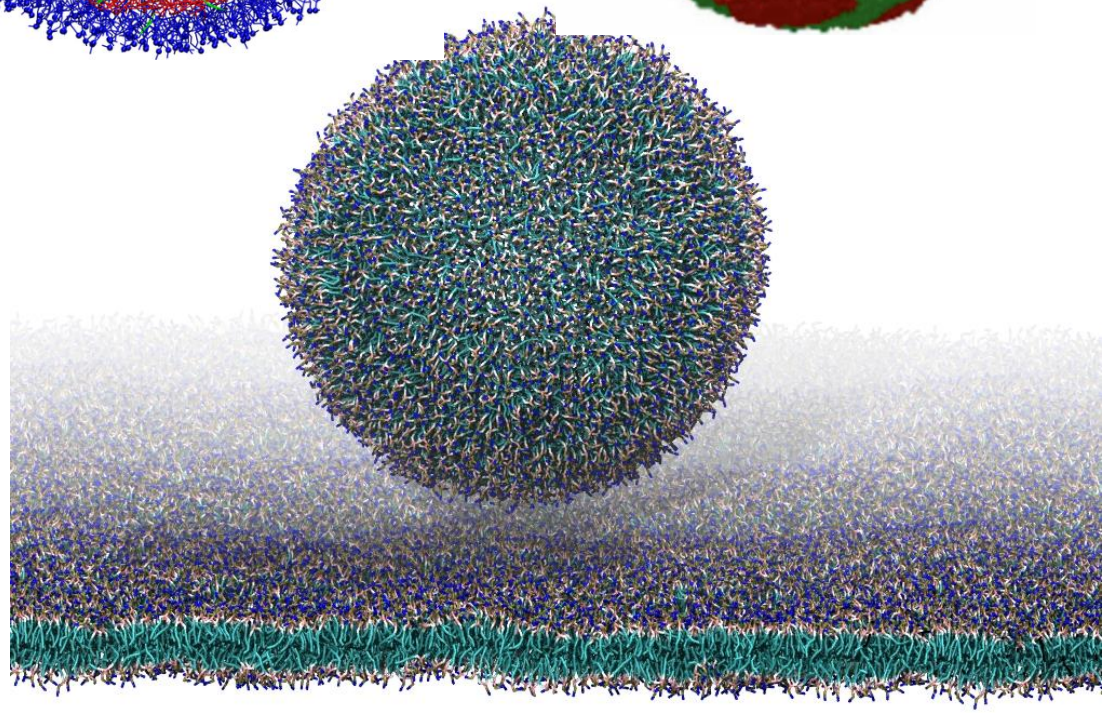
Крупнозернистое МД моделирование липидных везикул и мембранных белков



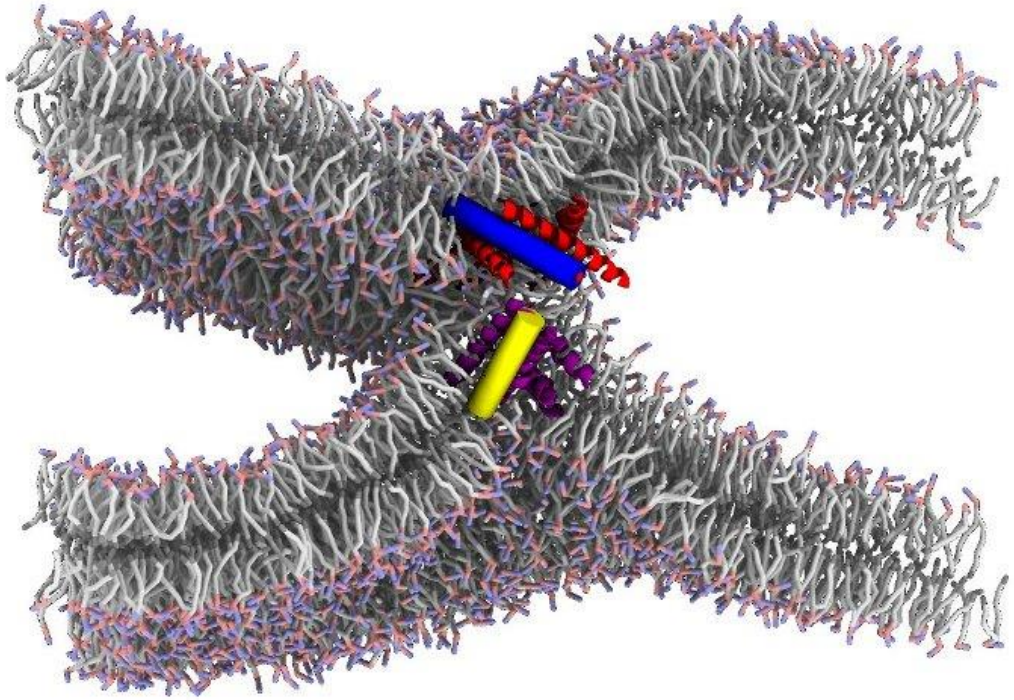








Примеры “крупнозернистого” МД моделирования биомембран



Изучение процессов слияния двух везикул, индуцированное определенными биомакромолекулами

Нобелевская премия по физиологии и медицине в 2013

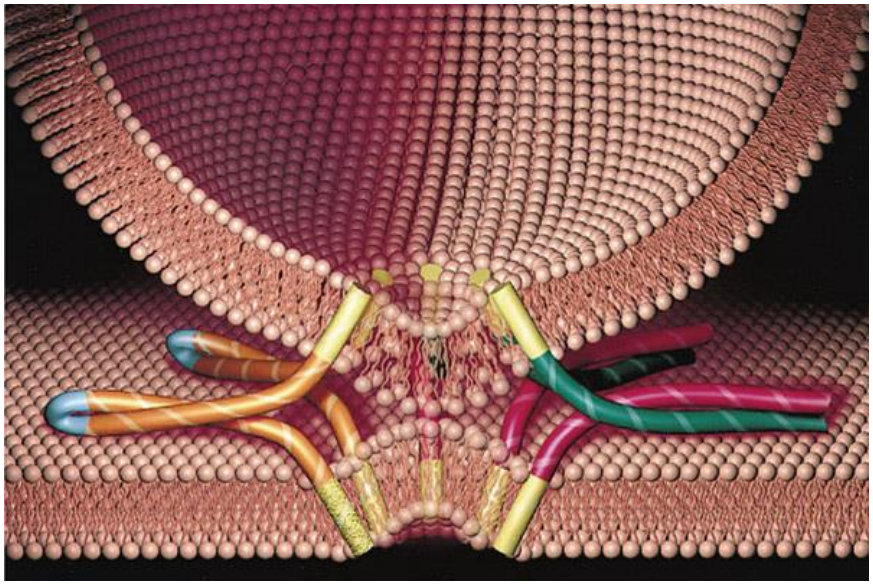
Нобелевскую премию по физиологии и медицине в 2013 году получили три американских ученых

Ренди Шекман, Джеймс Ротман и Томас Зюдоф

за

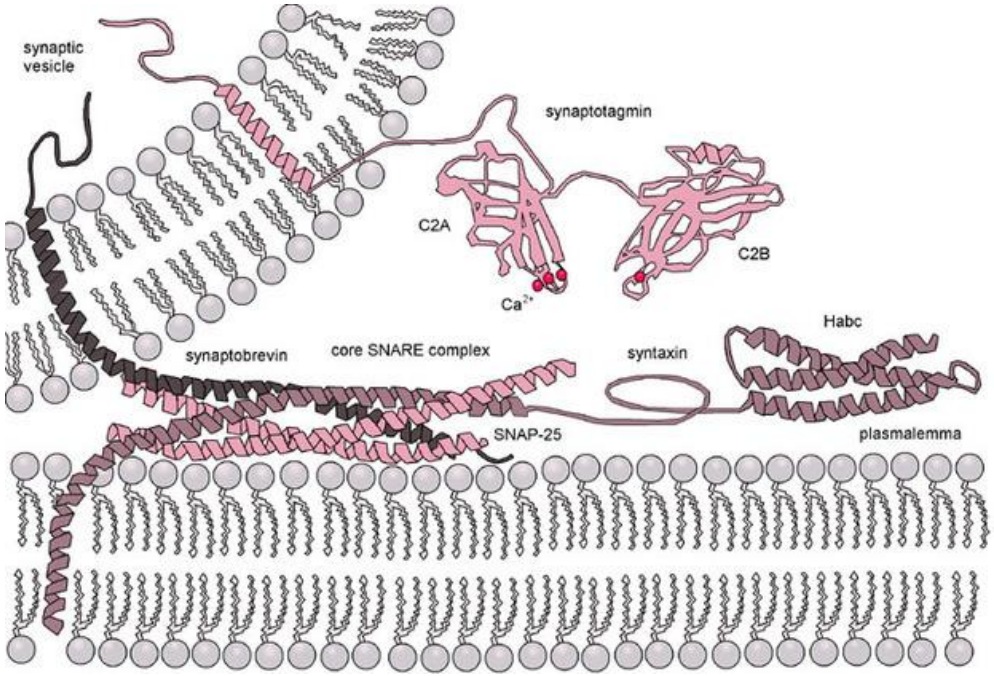
«Исследование механизмов, регулирующих везикулярный транспорт»

Нобелевская премия по физиологии и медицине в 2013



Слияние везикулы с клеточной мембраной: цилиндрами показаны белки-рецепторы SNARE (справа) и вирусные белки, имитирующие их работу (слева).

Нобелевская премия по физиологии и медицине в 2013



SNARE комплекс формируется в результате сплетения четырех альфа-спиралей белков синаптобревина (v-SNARE), синтаксина (t-SNARE) и SNAP-25. Синаптотагмин служит кальциевым сенсором.

Нобелевская премия по химии в 2013

Nobelpriset 2013 The Nobel

The Nobel Prize in Chemistry 2013

Martin Karplus
Université de Strasbourg, France and Harvard University, Cambridge, MA, USA

Michael Levitt
Stanford University School of Medicine, CA, USA

Arieh Warshel
University of Southern California, Los Angeles, CA, USA

”För utvecklandet av flerskalemodeller för komplexa kemiska system.”

“For the development of multiscale models for complex chemical systems.”

Нобелевская премия по химии в 2013

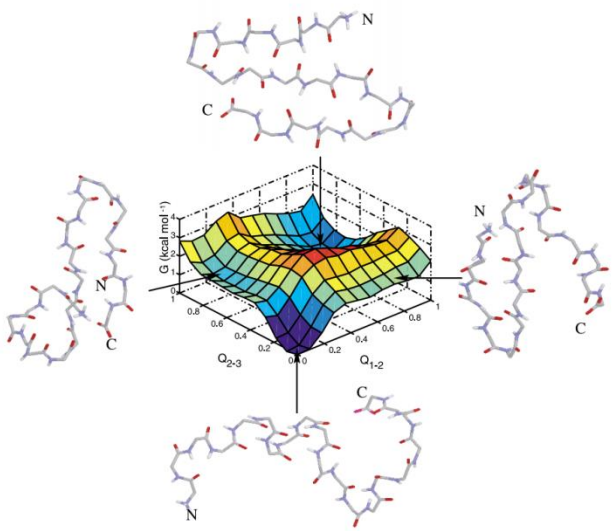
Мартин Карплус

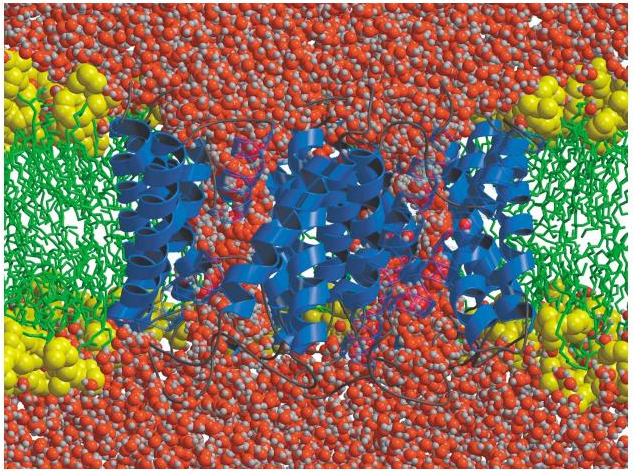
review

Molecular dynamics simulations of biomolecules

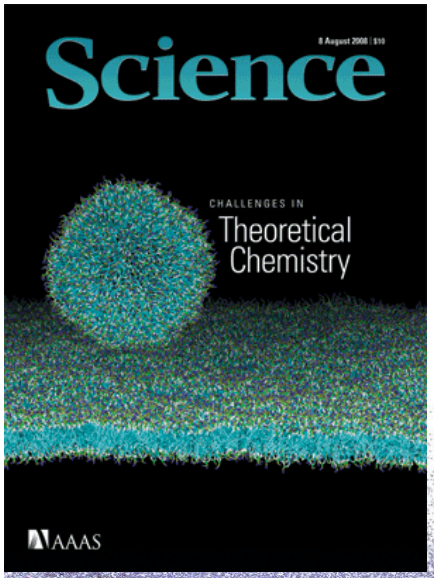
Martin Karplus[1,2] and J. Andrew McCammon[3]

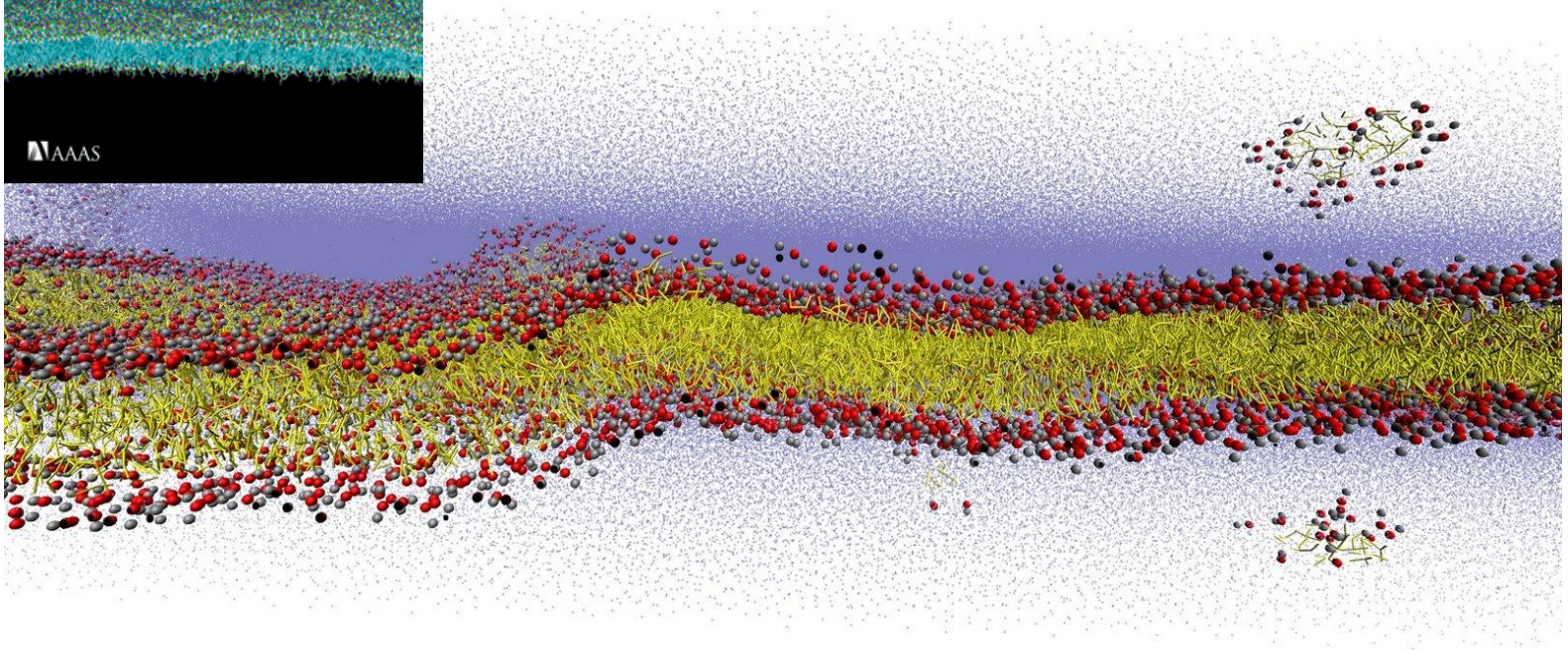
Molecular dynamics simulations are important tools for understanding the physical basis of the structure and function of biological macromolecules. The early view of proteins as relatively rigid structures has been replaced by a dynamic model in which the internal motions and resulting conformational changes play an essential role in their function. This review presents a brief description of the origin and early uses of biomolecular simulations. It then outlines some recent studies that illustrate the utility of such simulations and closes with a discussion of their ever-increasing potential for contributing to biology.





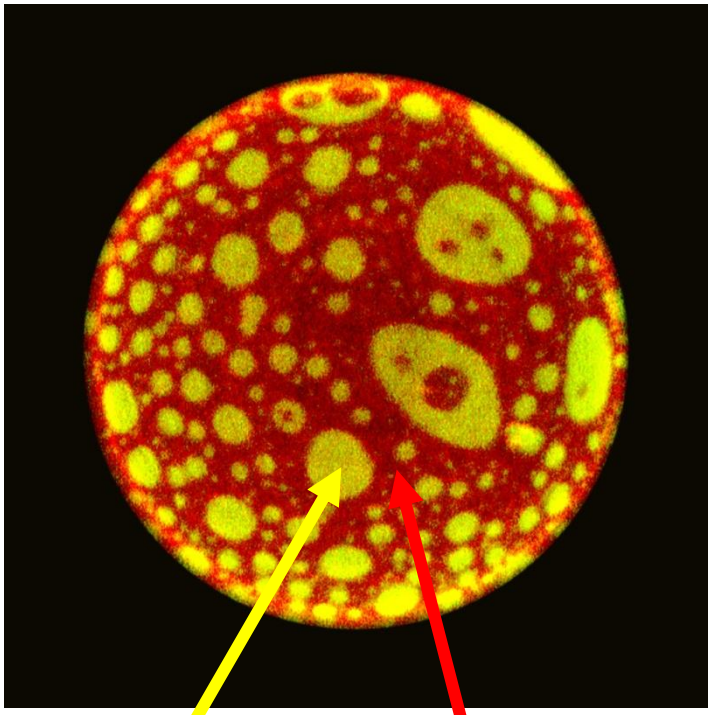
Примеры “крупнозернистого” МД моделирования биомембран





“крупнозернистая” модель биомебраны состоящая из 2 000 000 частиц …

Образование труднорастворимых холестериновых доменов в мембране

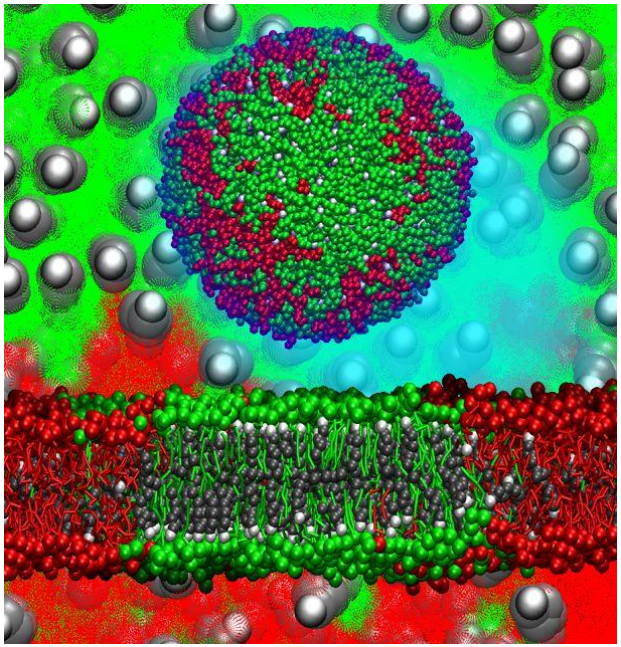


эксперимент

Холестерин

POPC липид

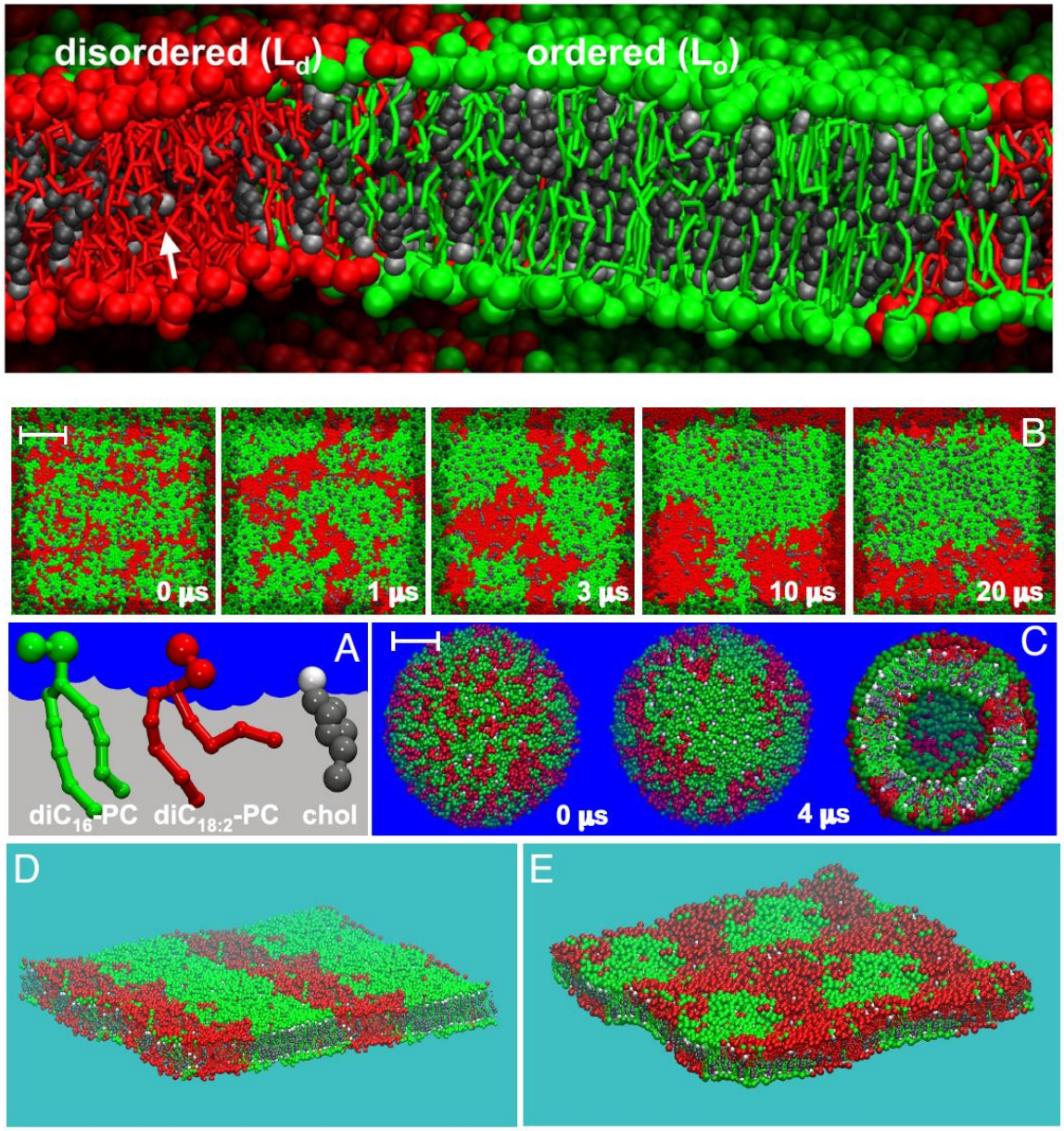
http://www.memphys.sdu.dk



http://md.chem.rug.nl/cgmartini/index.php/about/martini-projects/rafts

МД модель

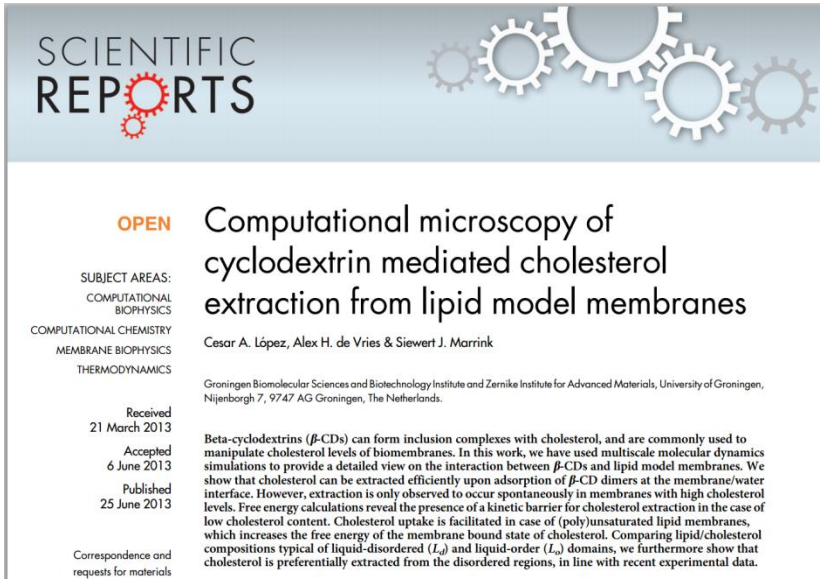
Формирование фосфолипидных доменов в мембране



Силовое Поле MARTINI
Вычисления выполнены в GROMACS 3.3

The Molecular Face of Lipid Rafts in Model Membranes.
H. J. Risselada and S. J. Marrink, Proceedings of the National Academy of Science of USA, 2008, v104, 17367–17372

Моделирование процессов экстракции холестерина молекулами циклодекстрина из липидных доменов в мембране



SCIENTIFIC REPORTS

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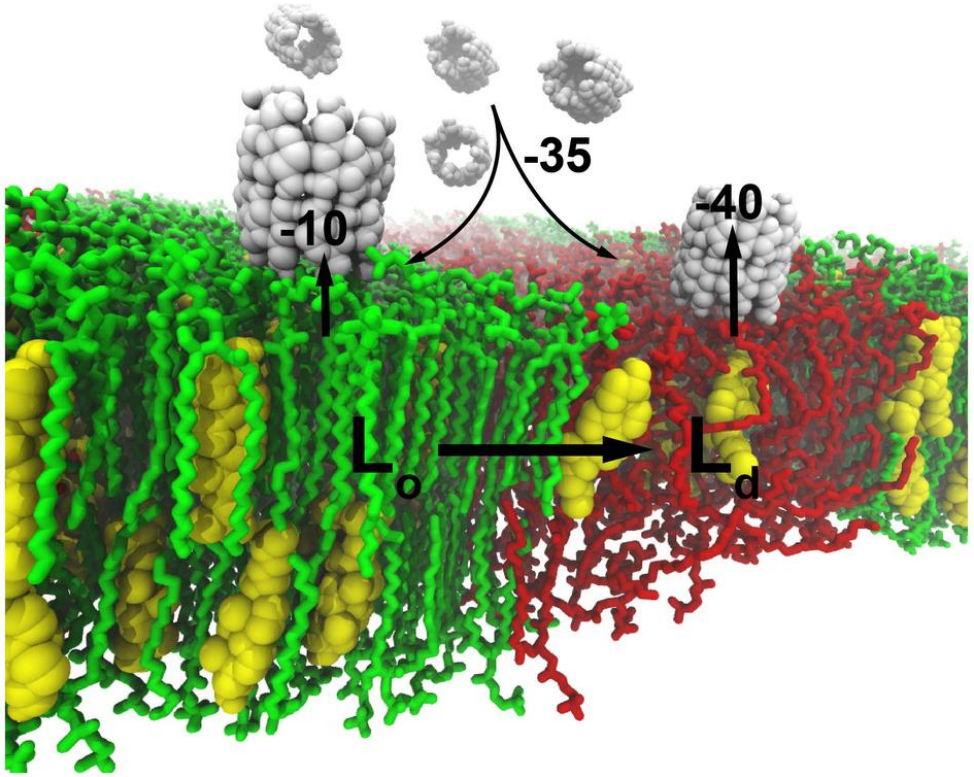
Computational microscopy of cyclodextrin mediated cholesterol extraction from lipid model membranes

Cesar A. López, Alex H. de Vries & Siewert J. Marrink

Groningen Biomolecular Sciences and Biotechnology Institute and Zernike Institute for Advanced Materials, University of Groningen, Nijenborgh 7, 9747 AG Groningen, The Netherlands.

Beta-cyclodextrins (β-CDs) can form inclusion complexes with cholesterol, and are commonly used to manipulate cholesterol levels of biomembranes. In this work, we have used multiscale molecular dynamics simulations to provide a detailed view on the interaction between β-CDs and lipid model membranes. We show that cholesterol can be extracted efficiently upon adsorption of β-CD dimers at the membrane/water interface. However, extraction is only observed to occur spontaneously in membranes with high cholesterol levels. Free energy calculations reveal the presence of a kinetic barrier for cholesterol extraction in the case of low cholesterol content. Cholesterol uptake is facilitated in case of (poly)unsaturated lipid membranes, which increases the free energy of the membrane bound state of cholesterol. Comparing lipid/cholesterol compositions typical of liquid-disordered (L_d) and liquid-order (L_o) domains, we furthermore show that cholesterol is preferentially extracted from the disordered regions, in line with recent experimental data.



www.nature.com

“Очень крупнозернистая” МД модель мембраны и везикулы

JCTC Journal of Chemical Theory and Computation — Article
pubs.acs.org/JCTC
J. Chem. Theory Comput. 2014, 10, 4730−4744

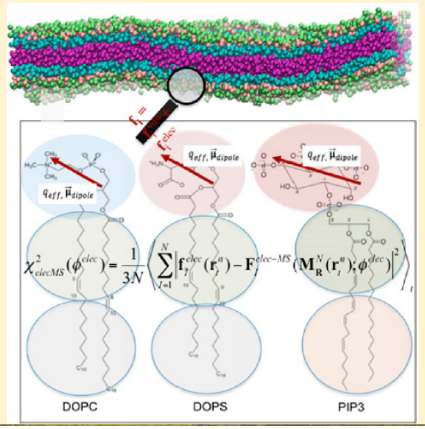
Solvent-Free, Highly Coarse-Grained Models for Charged Lipid Systems

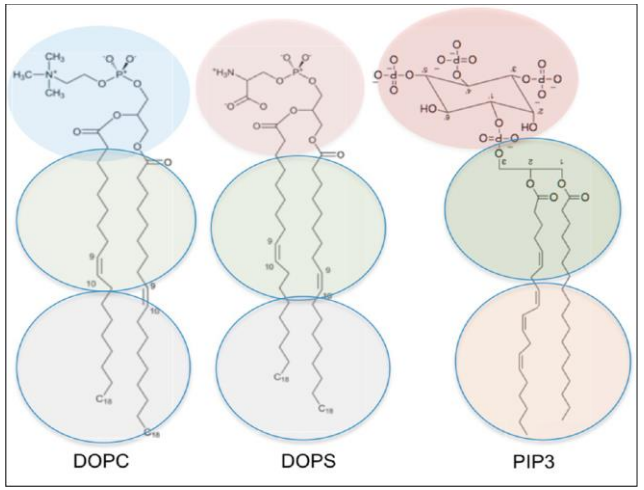
Anand Srivastava and Gregory A. Voth*

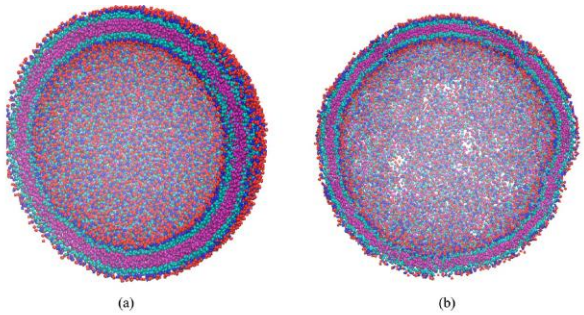
Department of Chemistry, Institute for Biophysical Dynamics, James Franck Institute, and Computation Institute, The University of Chicago, 5735 S. Ellis Ave., Chicago, Illinois 60637, United States

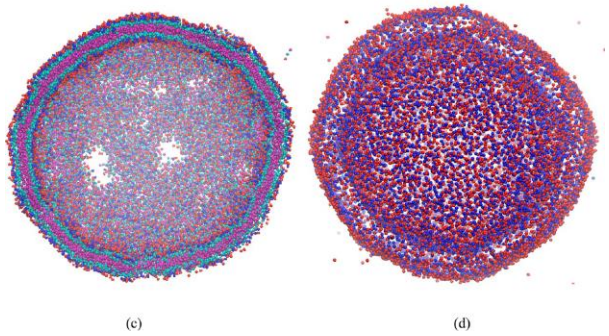
Supporting Information

ABSTRACT: We present a methodology to develop coarse-grained lipid models such that electrostatic interactions between the coarse-grained sites can be derived accurately from an all-atom molecular dynamics trajectory and expressed as an effective pairwise electrostatic potential with appropriate screening functions. The reference non-bonded forces from the all-atom trajectory are decomposed into separate electrostatic and van der Waals (vdW) forces, based on the multiscale coarse-graining method. The coarse-grained electrostatic potential is assumed to be a general function of unknown variables and the final site−site interactions are obtained variationally, where the residual of the electrostatic forces from the assumed field is minimized. The resulting electrostatic interactions are fitted to screened electrostatics functions, with a special treatment for distance-dependent dielectrics and screened dipole−dipole interactions. The vdW interactions are derived separately. The resulting charged hybrid coarse-graining method is applied to various solvent-free three-site models of anionic lipid systems.









$$U_{SR}(R_{IJ}) = 4\varepsilon\left[\left(\frac{\sigma}{R_{IJ}}\right)^{m} - \left(\frac{\sigma}{R_{IJ}}\right)^{n}\right] \qquad R_{IJ} \le R_{SR}$$

Современные тенденции и перспективы в “крупнозернистом” МД моделировании мембран и везикул

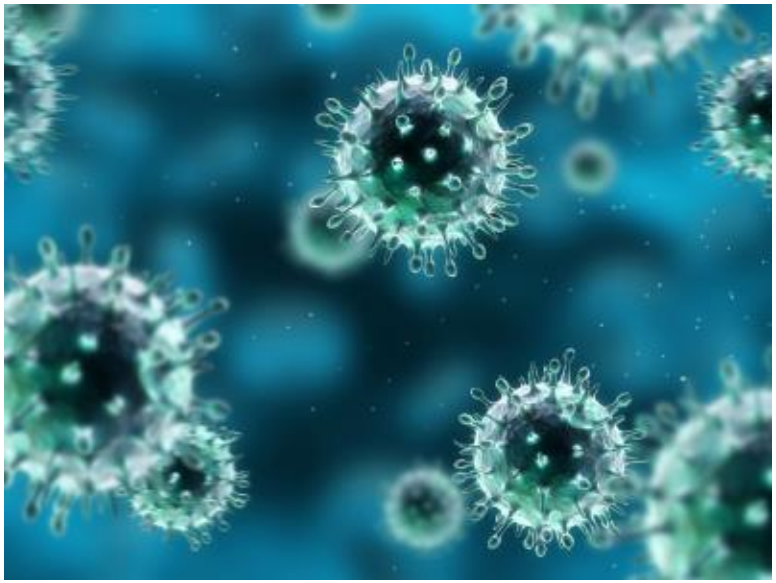
- Разработка новых “супер-крупнозернистых” (ultra coarse graining) МД моделей

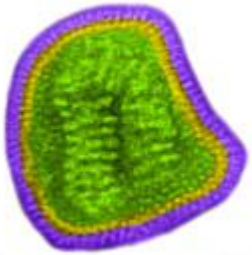
- Разработка МД моделей в неявных (implicit) растворителях

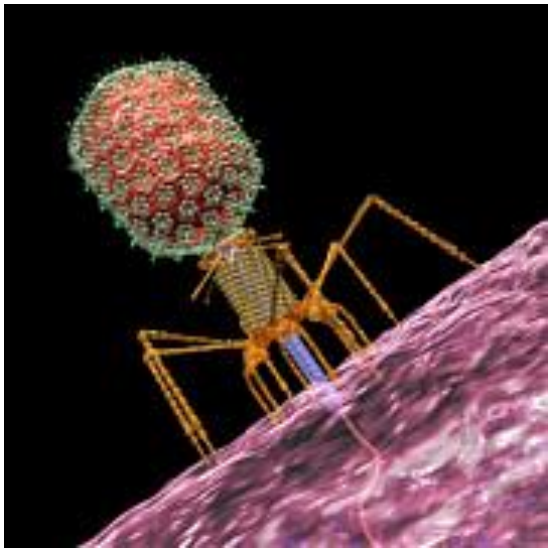
- Обязательная проверка МД модели на воспроизведение “самосборки”

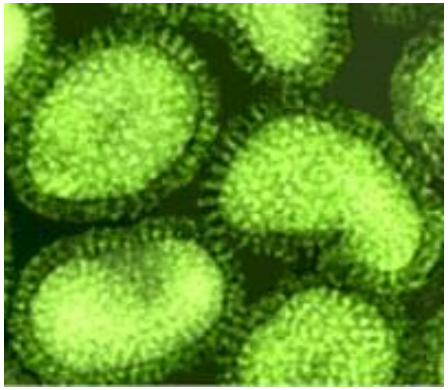
- Обязательная возможность обратной трансформации к полноатомной модели

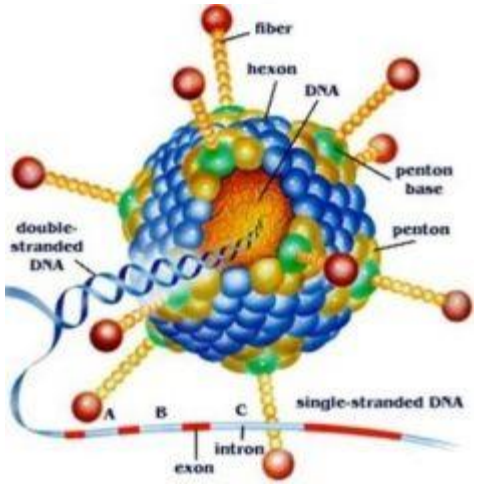
Есть ли возможность МД моделирование вирусов?



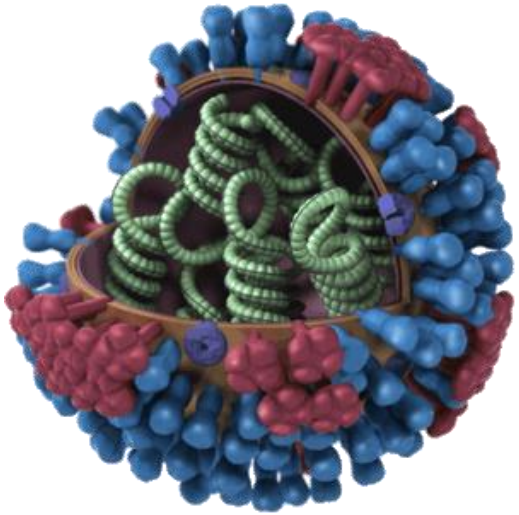


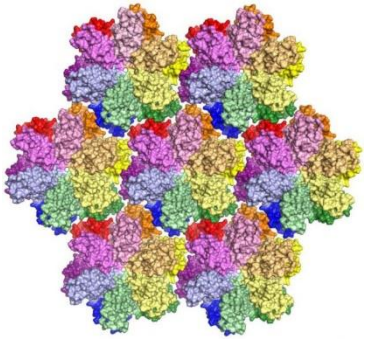


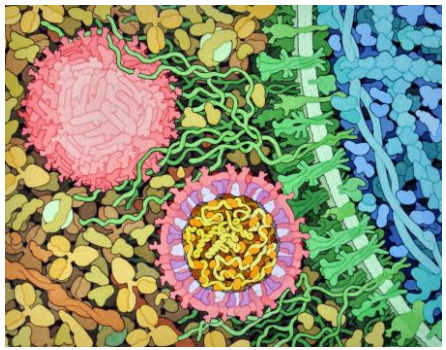


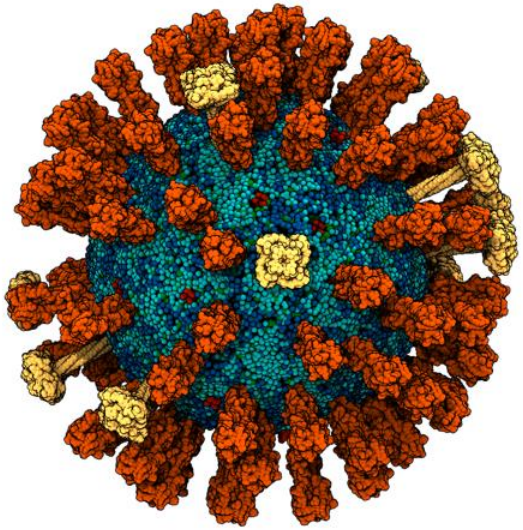


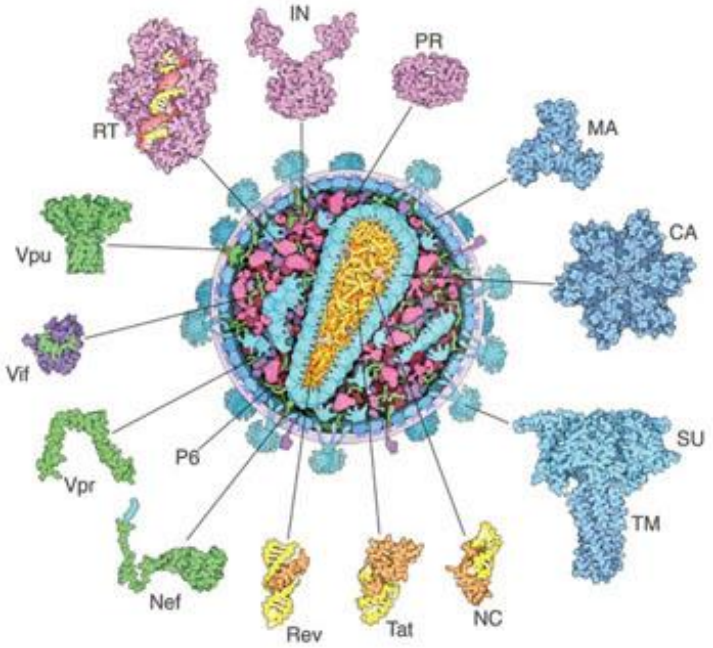
“Крупнозернистое” МД моделирование вирусов



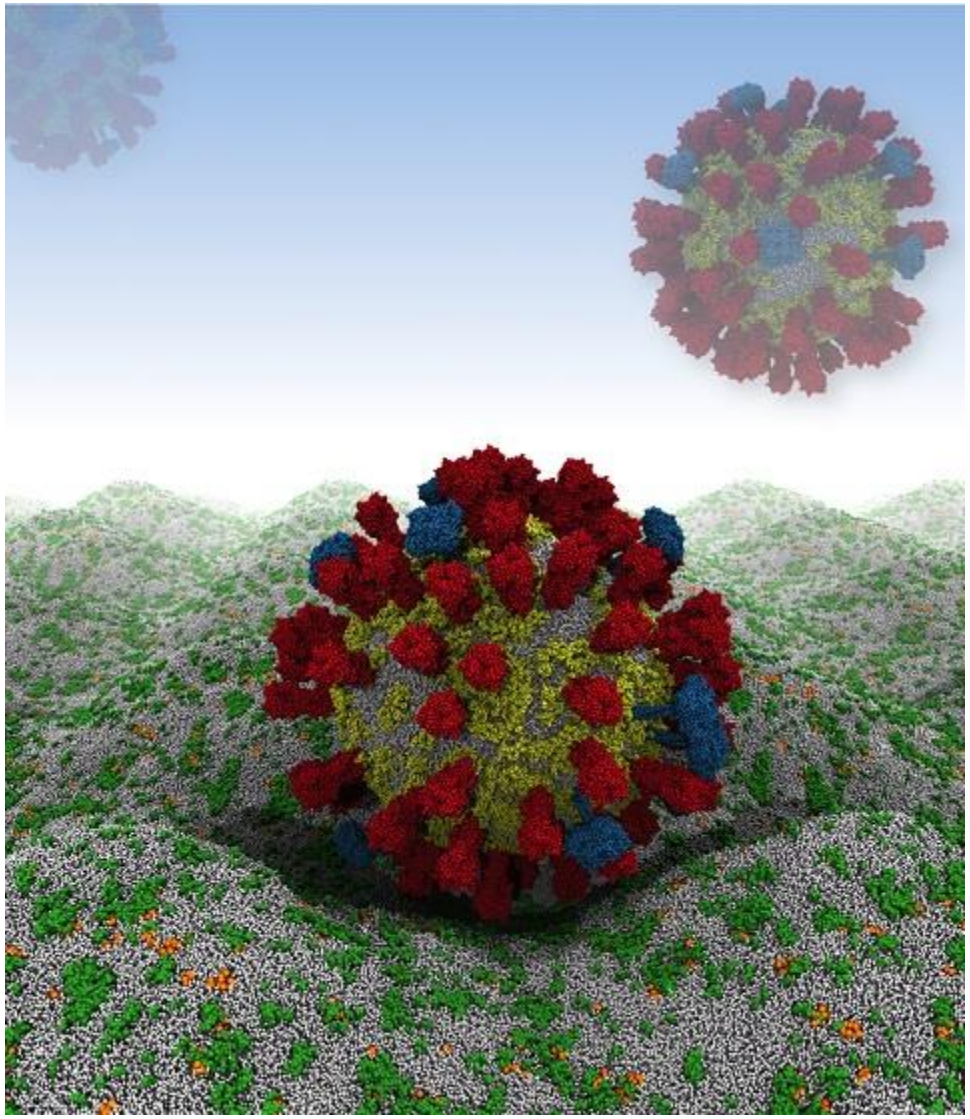




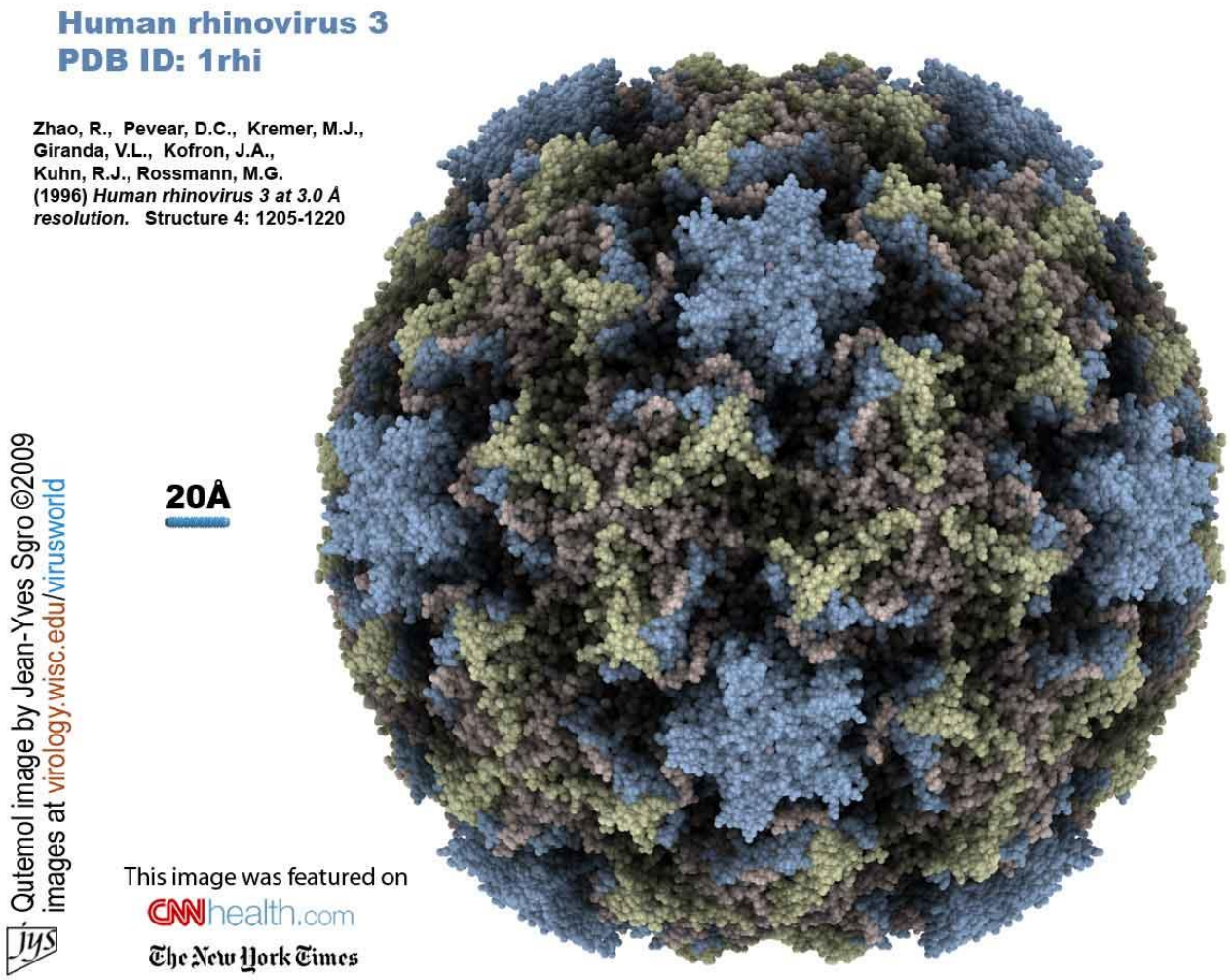




“Крупнозернистое” МД моделирование инфлуенза вируса

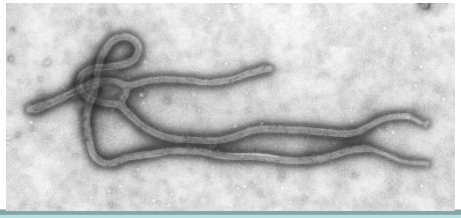


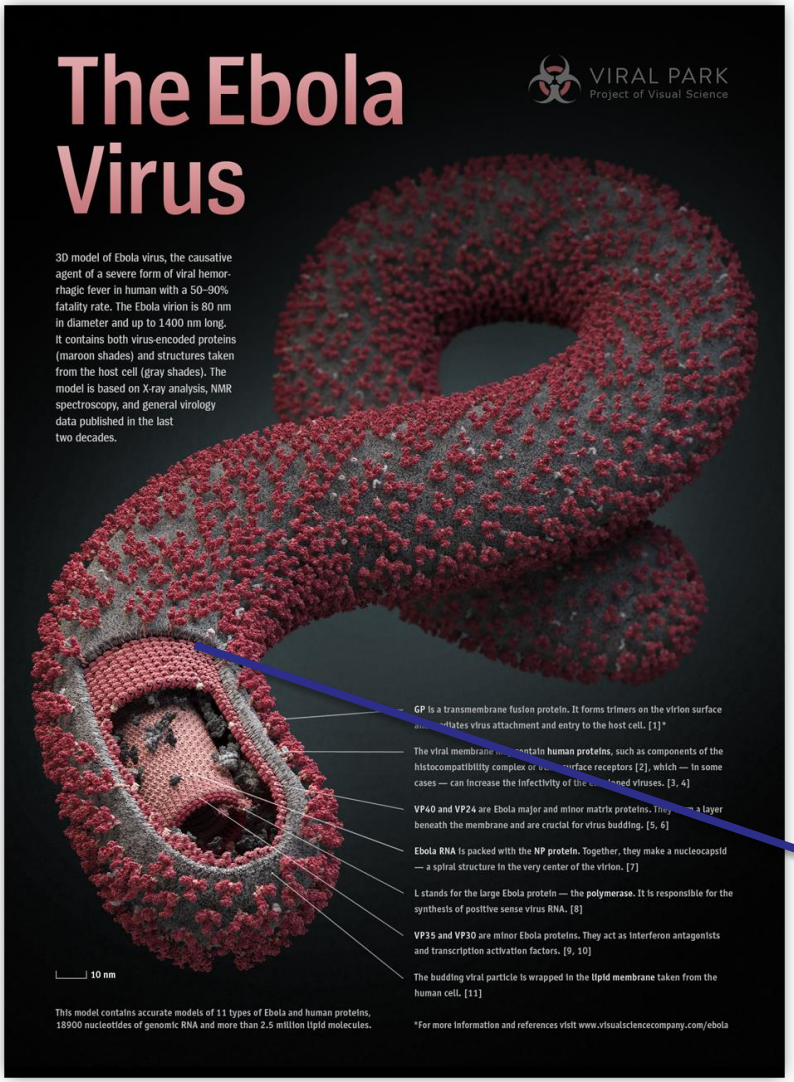
“Крупнозернистое” МД моделирование риновируса человека



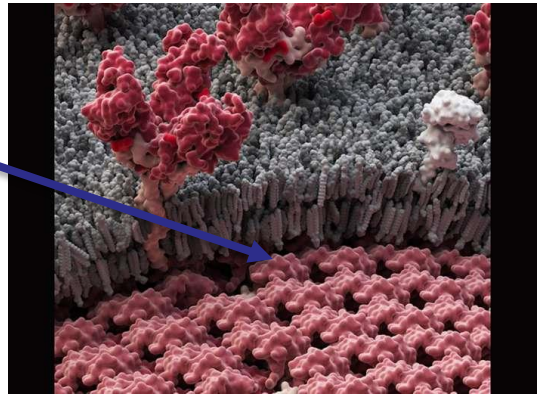
Риновирусы (лат. *Rhinovirus*, от др.-греч. ῥίς / ῥινός — нос) — группа мелких РНК-содержащих видов вирусов рода энтеровирусов, вирионы которых не имеют наружной оболочки, а геном представлен одноцепочечной линейной нефрагментированной молекулой РНК, связанной с белком VPg; включает возбудителей острых респираторных заболеваний (ОРЗ).

“Крупнозернистое” МД моделирование вируса Эбола

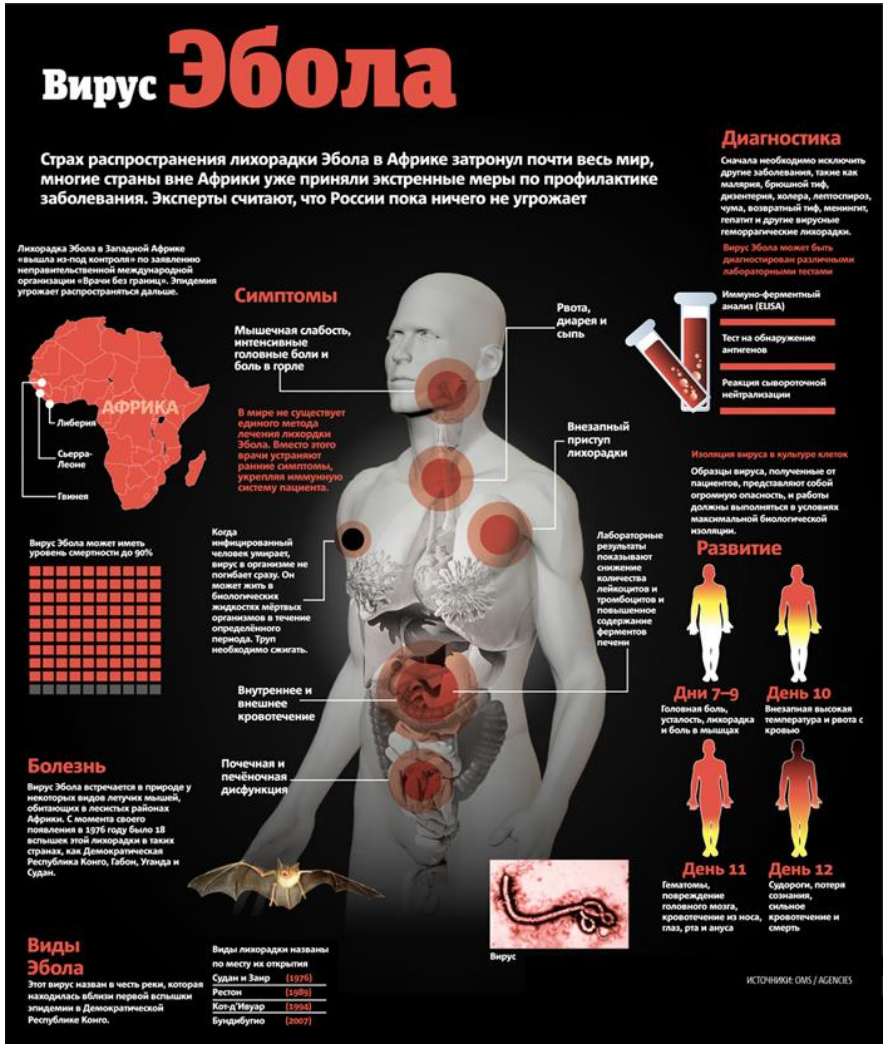


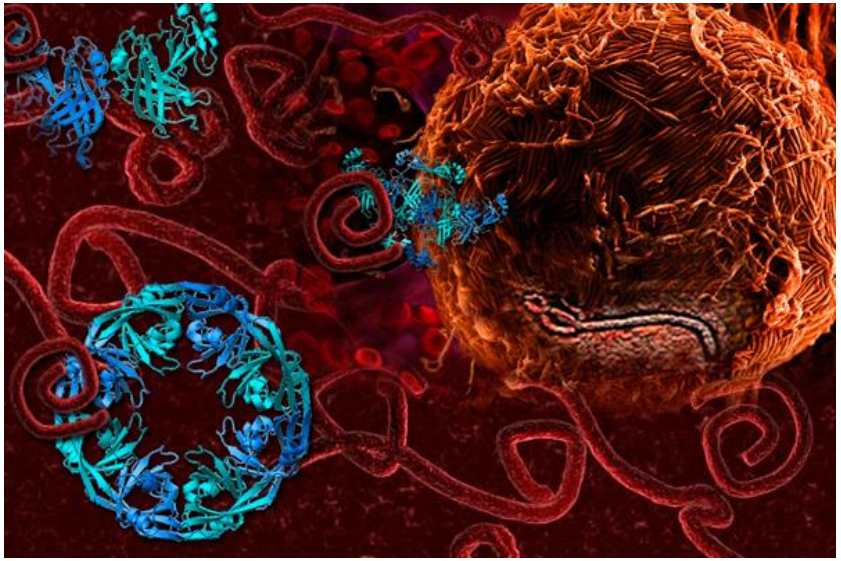


Ebolavirus (**эбóлавирус**, **вирус Эбóла** или **вирус Э́бола**) — род вирусов из семейства филовирусов (*Filoviridae*), вызывающих геморрагическую лихорадку Эбола у высших приматов. Морфологические признаки эболавирусов схожи с вирусом Марбург, также принадлежащим семейству филовирусов и вызывающим подобное заболевание. Кроме рода, вирусом Эбола могут называть конкретного представителя рода — чаще всего *Zaire ebolavirus*, который был выделен первым из рода в 1976 году в бассейне реки Эбóла в Заире, от чего и образовалось название. Эболавирусы, особенно вид *Zaire ebolavirus*, стали причиной нескольких широко освещённых серьёзных эпидемий



Моделирование биологической активности вируса Эбола





Перспективные направления в области МД моделирования мембранных систем

- **Гибридные МД модели**, в которых различные компоненты системы, такие как мембрана, сольватная среда и изучаемое соединение могут рассматриваться на разном уровне молекулярной детализации, включая полноатомные, упрощенные и фрагментированные модели.

- **Смешаные молекулярно-динамические\квантово-химические** модели (MM/QM), в которых изучаемое соединение рассматривается на уровне ab-initio, в то время мембрана и водная фаза описываются силовым полем МД.

- ***Ab-initio*** **молекулярная динамика** всей системы мембрана\вода.

Программные пакеты для МД моделирования

Практически все популярные МД программы имеют готовые полноатомные и упрощенные силовые поля и геометрии липидных мембран для простых однокомпонентных липидных систем!

Программы:

GROMOS
http://www.gromos.net/

GROMACS
http://www.gromacs.org/

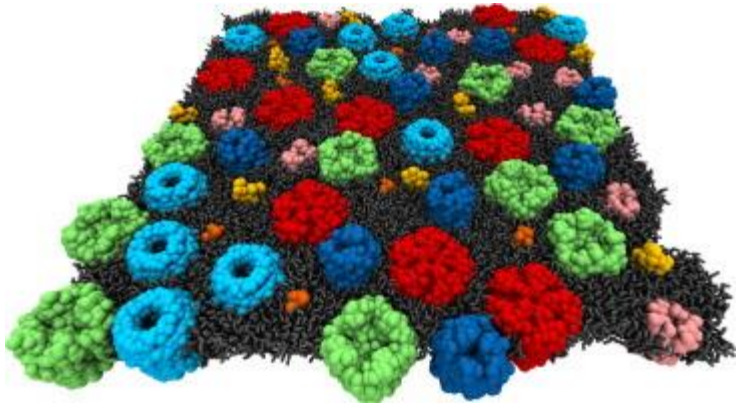
NAMD
http://www.ks.uiuc.edu/Research/namd/

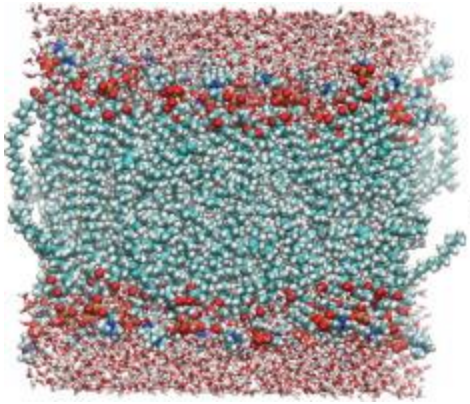
CHARMM
http://www.charmm.org/

AMBER
http://ambermd.org/

LAMMPS
http://lammps.sandia.gov/

DL_POLY
http://www.stfc.ac.uk





$$m\vec{a} = \vec{F} = \begin{cases} \text{CHARMM ?} \\ \text{AMBER ?} \\ \text{GROMOS ?} \\ \text{Slipids ?} \\ \ldots ? \end{cases}$$

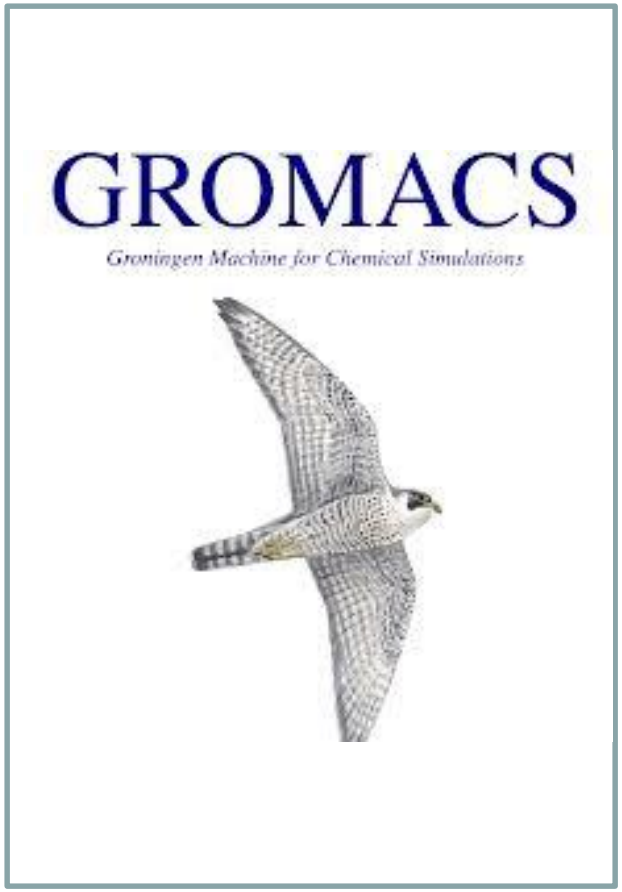
Ваша собственная программа …

Популярные программные пакеты для МД моделирования

GROMACS

http://www.gromacs.org/

GROMACS FAST. FLEXIBLE. FREE.



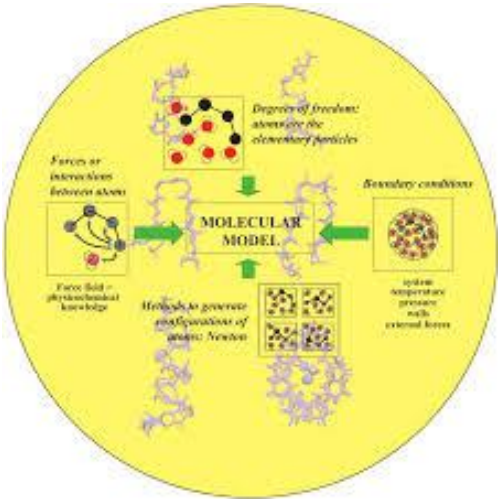
Linux

UNIX®

Популярные программные пакеты

GROMOS

http://www.gromos.net/



Linux

UNIX®

GROMOS

LOGIN

- About GROMOS
- How to get GROMOS
- Downloads
- GROMOS updates
- BIOMOS
- FAQ
- Contact

About the GROMOS software for biomolecular simulation

1. **What is GROMOS**

GROMOS™ is an acronym of the GROningen MOlecular Simulation computer program package, which has been developed since 1978 for the dynamic modelling of (bio)molecules, until 1990 at the University of Groningen, The Netherlands, and since then at the ETH, the Swiss Federal Institute of Technology, in Zürich, Switzerland. Its development is driven by the research group of Wilfred van Gunsteren.

Since the last official release of the GROMOS software and manual in 1996, called GROMOS96, no comprehensive release occurred. Yet the GROMOS software has seen a steady development since 1996, see e.g. Christen *et al.* J. Comput. Chem. **26** (2005) 1719. The programming language has been changed from FORTRAN to C++, the documentation has been put into electronic form, and many new features have been included in the software.

To the development of the new code and manuals many current and former members of the research group for Informatikgestützte Chemie (igc) have contributed : Jane Allison, Dirk Bakowies, Ulf Börjesson, Roland Bürgi, Alexandra Choutko, Clara Christ, Markus Christen, Jozica Dolenc, Andreas Eichenberger, Daan Geerke, Alice Glättli, Halvor Hansen, Bruno Horta, Philippe Hünenberger, Mika Kastenholz, Anna-Pitschna Kunz, Katharina Meier, Chris Oostenbrink, Christine Peter, Maria Reif, Sereina Riniker, Heiko Schäfer, Nathan Schmid, Denise Steiner, Dongqi Wang, Haibo Yu, to mention a few.

The GROMOS *software* is to be distinguished from the GROMOS *force fields* for biomolecular systems, of which the latest versions are coded as:

45A3/4	J. Comput. Chem. **22** (2001) 1205-1218
	Eur. Biophys. J. **32** (2003) 67-77
	J. Comput. Chem. **26** (2005) 725-737
	J. Comput. Chem. **26** (2005) 1400-1412
53A5/6	J. Comput. Chem. **25** (2004) 1656-1676
54A7	J. Comput. Chem. **31** (2010) 1117-1125
	Eur. Biophys. J. **40** (2011) 843-856

2. **GROMOS documentation**

The GROMOS software manuals that accompanied the major releases of 1987 and 1996 are:

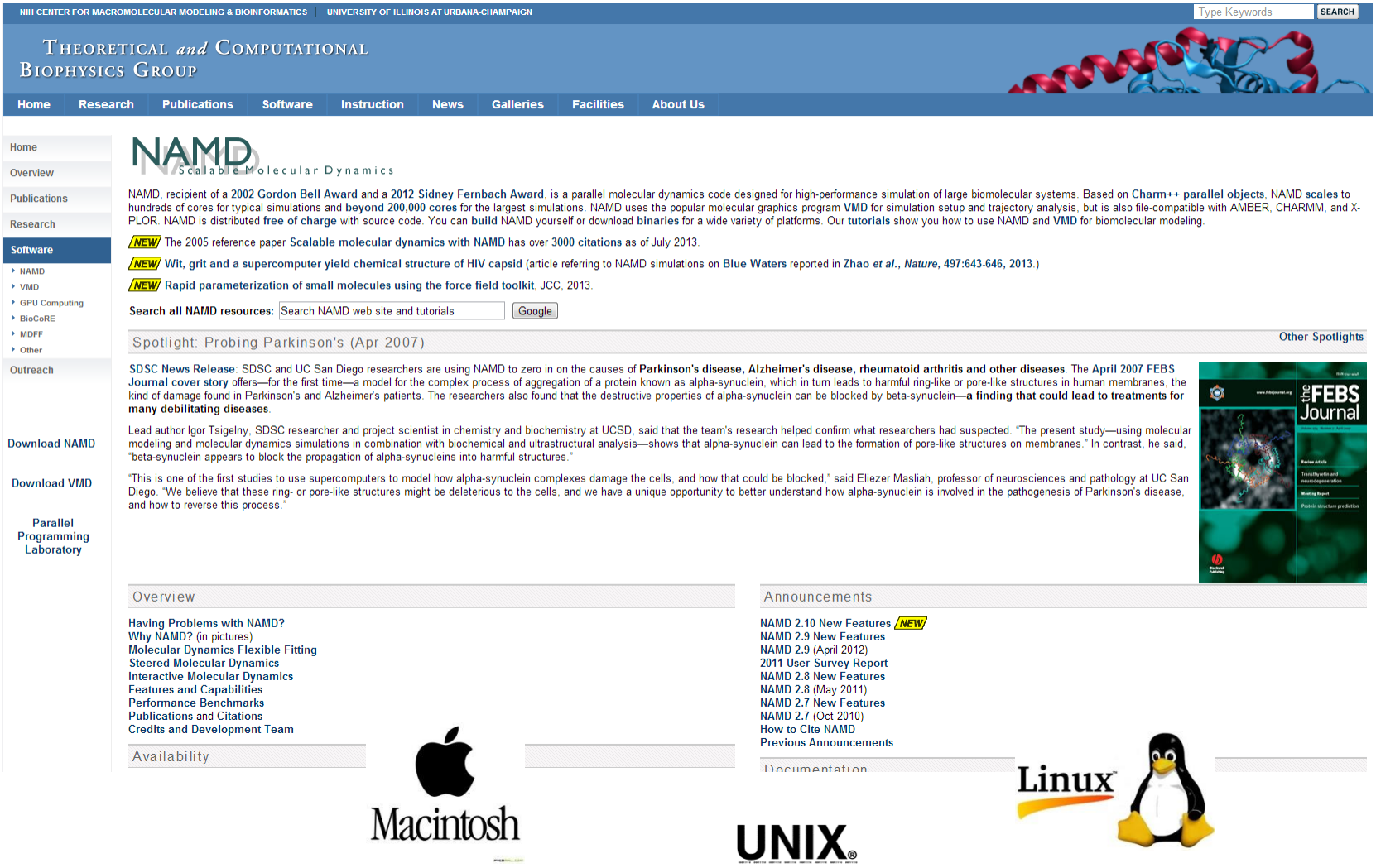
W. F. van Gunsteren and H. J. C. Berendsen, *Groningen Molecular Simulation (GROMOS) Library Manual,* Biomos, Groningen, The Netherlands, 1987, pp. 1-221.

Популярные программные пакеты

NAMD

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

NAMD Scalable Molecular Dynamics



Популярные программные пакеты

CHARMM

http://www.charmm.org/

- ▶ CHARMM
- ▶ Package
- ▶ Development
- ▶ Documentation

CHARMM

CHARMM News (Oct. 22, 2012):

The most recent release of CHARMM makes available to users significant performance enhancements for conventional molecular dynamics calculations, e.g., MD with explicit solvent and periodic boundary conditions using PME. This enhanced performance comes from the development and introduction of the DOMDEC module, by Antti-Pekka Hynninen and Michael Crowley, for simulations on parallel architectures, and for GPU accelerated molecular dynamics from the CHARMM/OpenMM interface, developed by Michael Garrahan and Charles Brooks, which leverages the relatively mature OpenMM API developed by Vijay Pande and coworkers at Stanford. For more information, please see this page.

CHARMM News (Apr. 30, 2012):

An advanced CHARMM tutorial will be held from May 7-10, 2012, at the National Institutes of Health main campus in Bethesda, MD. A full schedule may be found on the CHARMM forums.

CHARMM (Chemistry at HARvard Macromolecular Mechanics):

- is a versatile and widely used molecular simulation program with broad application to many-particle systems
- has been developed with a primary focus on the study of molecules of biological interest, including peptides, proteins, prosthetic groups, small molecule ligands, nucleic acids, lipids, and carbohydrates, as they occur in solution, crystals, and membrane environments
- provides a large suite of computational tools that encompass numerous conformational and path sampling methods, free energy estimates, molecular minimization, dynamics, and analysis techniques, and model-building capabilities
- is useful for a much broader class of many-particle systems
- can be utilized with various energy functions and models, from mixed quantum mechanical-molecular mechanical force fields, to all-atom classical potentials with explicit solvent and various boundary conditions, to implicit solvent and membrane

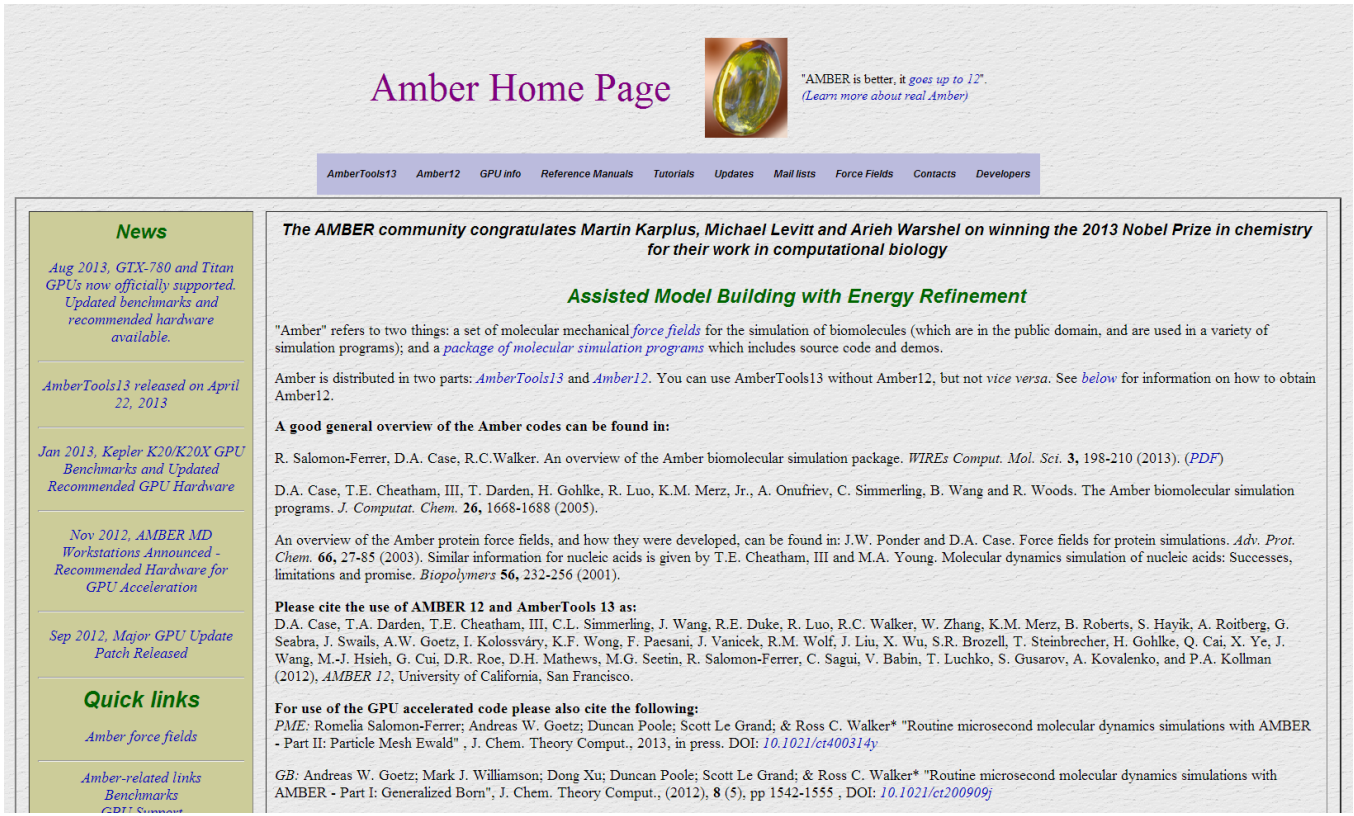
Linux

Macintosh

Популярные программные пакеты

AMBER

http://ambermd.org/



Amber Home Page

"AMBER is better, it goes up to 12".
(Learn more about real Amber)

AmberTools13 | Amber12 | GPU info | Reference Manuals | Tutorials | Updates | Mail lists | Force Fields | Contacts | Developers

News

Aug 2013, GTX-780 and Titan GPUs now officially supported. Updated benchmarks and recommended hardware available.

AmberTools13 released on April 22, 2013

Jan 2013, Kepler K20/K20X GPU Benchmarks and Updated Recommended GPU Hardware

Nov 2012, AMBER MD Workstations Announced - Recommended Hardware for GPU Acceleration

Sep 2012, Major GPU Update Patch Released

Quick links

Amber force fields

Amber-related links
Benchmarks
GPU Support

The AMBER community congratulates Martin Karplus, Michael Levitt and Arieh Warshel on winning the 2013 Nobel Prize in chemistry for their work in computational biology

Assisted Model Building with Energy Refinement

"Amber" refers to two things: a set of molecular mechanical *force fields* for the simulation of biomolecules (which are in the public domain, and are used in a variety of simulation programs); and a *package of molecular simulation programs* which includes source code and demos.

Amber is distributed in two parts: *AmberTools13* and *Amber12*. You can use AmberTools13 without Amber12, but not *vice versa*. See *below* for information on how to obtain Amber12.

A good general overview of the Amber codes can be found in:

R. Salomon-Ferrer, D.A. Case, R.C.Walker. An overview of the Amber biomolecular simulation package. *WIREs Comput. Mol. Sci.* **3,** 198-210 (2013). (*PDF*)

D.A. Case, T.E. Cheatham, III, T. Darden, H. Gohlke, R. Luo, K.M. Merz, Jr., A. Onufriev, C. Simmerling, B. Wang and R. Woods. The Amber biomolecular simulation programs. *J. Computat. Chem.* **26,** 1668-1688 (2005).

An overview of the Amber protein force fields, and how they were developed, can be found in: J.W. Ponder and D.A. Case. Force fields for protein simulations. *Adv. Prot. Chem.* **66,** 27-85 (2003). Similar information for nucleic acids is given by T.E. Cheatham, III and M.A. Young. Molecular dynamics simulation of nucleic acids: Successes, limitations and promise. *Biopolymers* **56,** 232-256 (2001).

Please cite the use of AMBER 12 and AmberTools 13 as:
D.A. Case, T.A. Darden, T.E. Cheatham, III, C.L. Simmerling, J. Wang, R.E. Duke, R. Luo, R.C. Walker, W. Zhang, K.M. Merz, B. Roberts, S. Hayik, A. Roitberg, G. Seabra, J. Swails, A.W. Goetz, I. Kolossváry, K.F. Wong, F. Paesani, J. Vanicek, R.M. Wolf, J. Liu, X. Wu, S.R. Brozell, T. Steinbrecher, H. Gohlke, Q. Cai, X. Ye, J. Wang, M.-J. Hsieh, G. Cui, D.R. Roe, D.H. Mathews, M.G. Seetin, R. Salomon-Ferrer, C. Sagui, V. Babin, T. Luchko, S. Gusarov, A. Kovalenko, and P.A. Kollman (2012), *AMBER 12*, University of California, San Francisco.

For use of the GPU accelerated code please also cite the following:
PME: Romelia Salomon-Ferrer; Andreas W. Goetz; Duncan Poole; Scott Le Grand; & Ross C. Walker* "Routine microsecond molecular dynamics simulations with AMBER - Part II: Particle Mesh Ewald" , J. Chem. Theory Comput., 2013, in press. DOI: *10.1021/ct400314y*

GB: Andreas W. Goetz; Mark J. Williamson; Dong Xu; Duncan Poole; Scott Le Grand; & Ross C. Walker* "Routine microsecond molecular dynamics simulations with AMBER - Part I: Generalized Born", J. Chem. Theory Comput., (2012), **8** (5), pp 1542-1555 , DOI: *10.1021/ct200909j*

Популярные программные пакеты

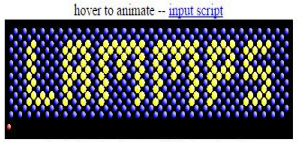
LAMMPS

http://lammps.sandia.gov/

LAMMPS Molecular Dynamics Simulator

lamp: *a device that generates light, heat, or therapeutic radiation; something that illumines the mind or soul* -- www.dictionary.com

hover to animate -- input script



physical analog (start at 3:25) & explanation

Big Picture	Code	Documentation	Results	Related Tools	Context	User Support
Features	Download	Manual	Publications	Pre/Post processing	Authors	Mail list
Non-features	SourceForge	Developer guide	Pictures	Pizza.py Toolkit	History	Workshops
FAQ	Latest features & bug fixes	Tutorials	Movies	Offsite LAMMPS packages & tools	Funding	User scripts and HowTos
Wish list	Unfixed bugs	MD to LAMMPS glossary	Benchmarks	Visualization	Open source	Contribute to LAMMPS
.	Pull requests	Commands	Citing LAMMPS	Related modeling codes	.	.

LAMMPS is a classical molecular dynamics code, and an acronym for Large-scale Atomic/Molecular Massively Parallel Simulator.

LAMMPS has potentials for solid-state materials (metals, semiconductors) and soft matter (biomolecules, polymers) and coarse-grained or mesoscopic systems. It can be used to model atoms or, more generically, as a parallel particle simulator at the atomic, meso, or continuum scale.

LAMMPS runs on single processors or in parallel using message-passing techniques and a spatial-decomposition of the simulation domain. Many of its models have versions that provide accelerated performance on CPUs, GPUs, and Intel Xeon Phis. The code is designed to be easy to modify or extend with new functionality.

LAMMPS is distributed as an open source code under the terms of the GPL. The current version can be downloaded here. Links are also included to older F90/F77 versions. Periodic releases are also available on SourceForge.

LAMMPS is distributed by Sandia National Laboratories, a US Department of Energy laboratory. The main authors of LAMMPS are listed on this page along with contact info and other contributors. Funding for LAMMPS development has come primarily from DOE (OASCR, OBER, ASCI, LDRD, Genomes-to-Life) and is acknowledged here.

The LAMMPS web site is hosted by Sandia, which has this Privacy and Security statement.

Search the LAMMPS web pages

Популярные программные пакеты

DL_POLY

http://www.stfc.ac.uk

Выводы

В зависимости от поставленной задачи необходимо выбрать адекватную по молекулярной детализации и сложности МД модель мембраны и программный пакет

Рекомендуемая литература

[1]. A computer perspective of membranes: Molecular dynamics studies of lipid bilayer systems / Tieleman D. P., Marrink S. J. and Berendsen H. J. C. // Biochim Biophys Acta Rev Biomembr. — 1997. — V. 1331, № 3. — P. 235-270.

[2] Martinez-Seara H. and Róg T., Molecular dynamics simulations of lipid bilayers: Simple recipe of how to do it, *in Biomolecular simulations,* L. Monticelli and E. Salonen, Editors. 2013, Humana Press. p. 407-429.

[3]. Computer simulations of transport through membranes: Passive diffusion, pores, channels and transporters / Tieleman D. Peter // Proc. Australian Physiol. Soc. — 2006. — V. 37, — P. 15-27.

[4]. The importance of membrane defects—lessons from simulations / Bennett W. F. D. and Tieleman D. P. // Acc. Chem. Res. — 2014. — V. 47, № 8. — P. 2244-2251.