

**Prof. Dr. rer. nat. habil. Martin O. Steinhauser**

**Frankfurt University of Applied Sciences, Germany**

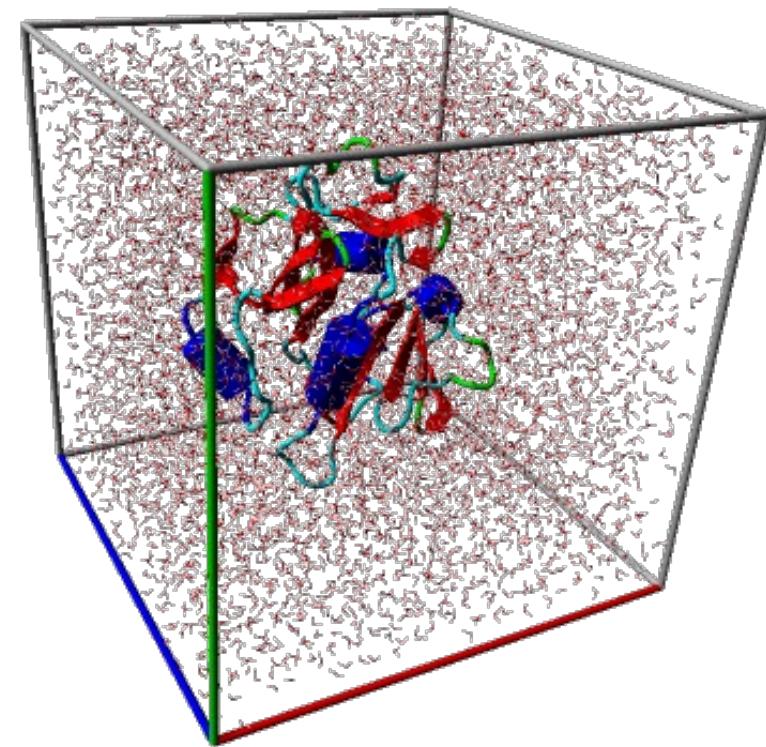
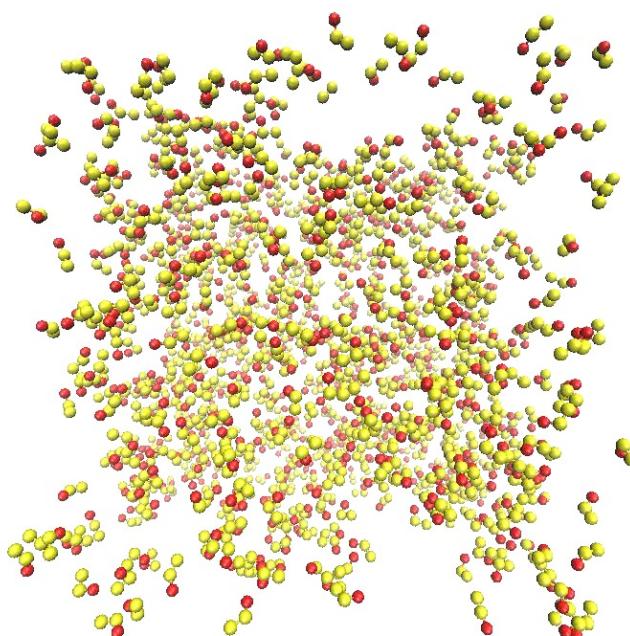
Faculty of Computer Science and Engineering



**Short Lecture Course:**

**Introduction to Computational Science with Applications in Molecular Dynamics**

**Session 1: Introduction**



# Overview of this short course

## ■ **Topics Covered** (subject to change)

- 1st Session: Lec. 1-2                          Introduction & Bits and Bytes
- 2nd Session: Lec 3                          (2x)                  Bits and Bytes continued
- 3rd Session: Lec 4-6                          Molecular Dynamics
- 4th Session: Lec 7-8                          MD continued / Algorithms
- 5th Session: Lec 9                          (2x)                  Algorithms/ Problem of Sorting
- 6th Session: Lec 10-11                          Asymptotic Analysis of Algorithms
- 7th Session: Lec 12-13                          Monte Carlo/Random Numbers

# Overview of this short course

## ■ **Objectives:**

The course is aimed at advanced undergraduate or beginning graduate students who want to learn some **basics of the Molecular Dynamics Method** and obtain an **introduction in to Computational Science**

## ■ **Instructor:**

Prof. Dr. habil. Martin Steinhauser

## ■ **Prerequisites:**

Some basic familiarity with computers (writing programs, scripts,...), classical mechanics or thermodynamics is helpful, but not required.

## ■ **Class Meetings:**

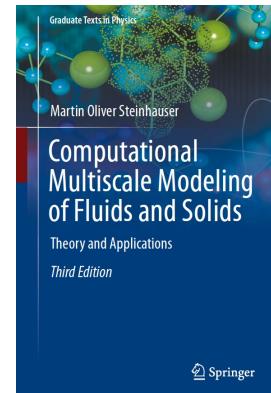
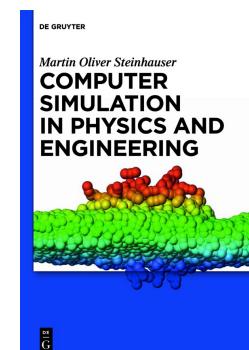
A total of 8 sessions of varying length and intensity

## ■ **Textbooks:**

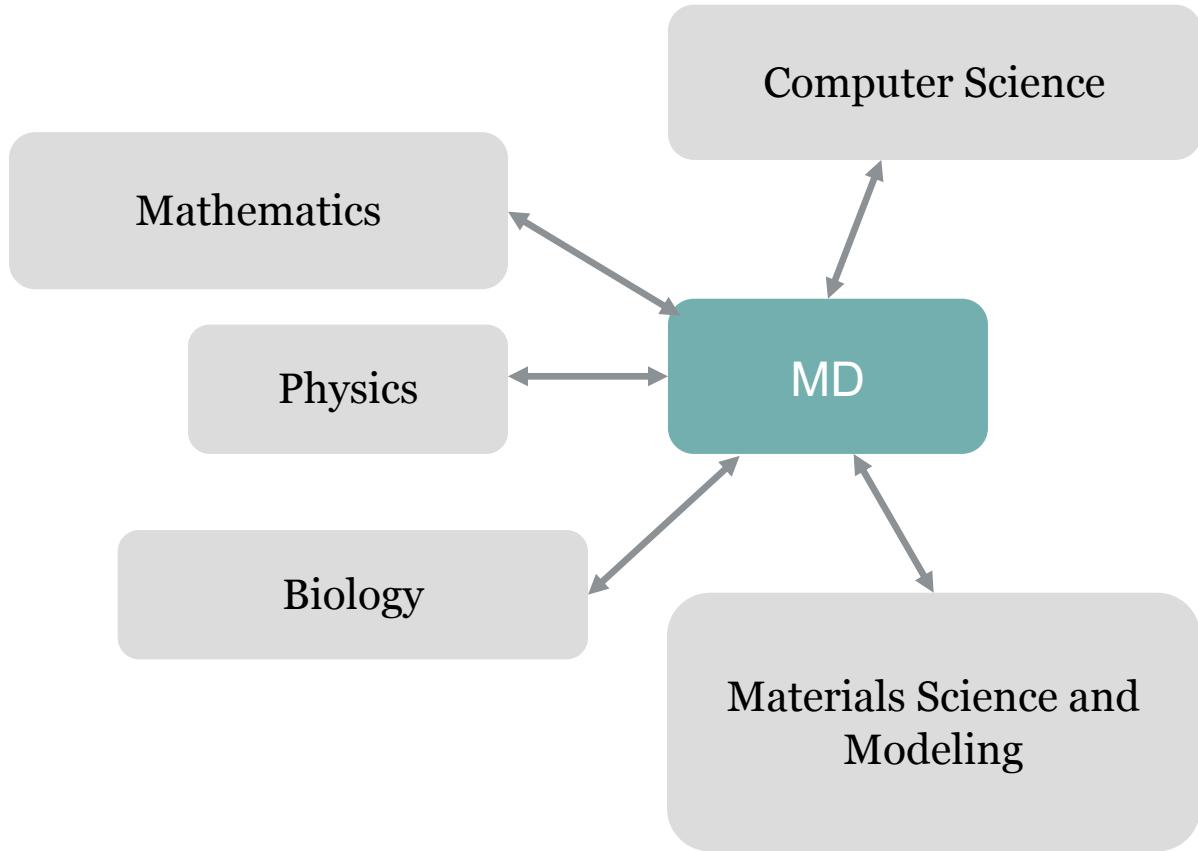
No specific textbooks are needed or used for this course

# General Course Literature / Textbooks

- **M.P. Allen and Tildesley:** „Computer Simulation of Liquids“, Oxford Science Publishers 1998.
- **D. Frenkel and B. Smit:** „Understanding Molecular Simulation“, Academic Press 2002.
- **D. C. Rappaport:** „The Art of Molecular Dynamics Simulation“, Cambridge University Press 2004.
- **K. Binder and D. W. Heermann:** “Monte Carlo Simulation in Statistical Physics”, Springer 2010.
- **J. M. Haile:** „Molecular Dynamics Simulation: Elementary Methods“, Wiley & Sons 1997.
- **M. O. Steinhauser:** „Computational Multiscale Modeling of Fluids and Solids – Theory and Applications“, 2nd edition, Berlin, Heidelberg, Springer 2017.
- Book, covering parts of this course:  
**M. O. Steinhauser:** „Computer Simulation in Physics and Engineering“, de Gruyter, 2012.



# Importance of the Molecular Dynamics Method



# Session 1: Introduction to Scientific Computing (Overview)

## ■ OUTLINE OF LECTURE

- Introduction to Scientific Computing / Bits and Bytes
- ◆ Handout 1: A Survival Guide to the Language C

To download lecture material, please go to Github:

<https://github.com/Kosmokrat/JapanLecture2024>

# Session 1: Lecture 1/2

## 1 A short Introduction to Scientific Computing

# Introduction to Scientific Computing

“I think there is a world market for maybe five computers.”

*Statement attributed to Thomas Watson, IBM chairman, 1943*

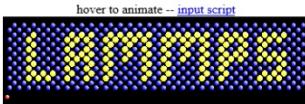


[http://800ceoread.com/book/blog/9780385042352-My\\_Years\\_with\\_General\\_Motors](http://800ceoread.com/book/blog/9780385042352-My_Years_with_General_Motors)

# MD Resources on the WWW: Large-scale Atomic/Molecular Massively Parallel Simulator

## LAMMPS Molecular Dynamics Simulator

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



physical analog (start at 3:25) & [explanation](#)

Big Picture	Code	Documentation	Results	Related Tools	Context	User Support
<a href="#">Features</a>	<a href="#">Download</a>	<a href="#">Manual</a>	<a href="#">Publications</a>	<a href="#">Offsite LAMMPS packages</a>	<a href="#">Authors</a>	<a href="#">Mail list</a>
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			<a href="#">Citina LAMMPS</a>			<a href="#">Contribute to LAMMPS</a>



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

LAMMPS has potentials for soft materials (biomolecules, polymers) and solid-state materials (metals, semiconductors) 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. 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](#).

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## Recent LAMMPS News

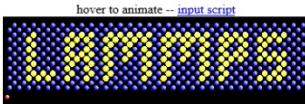
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- [NEW](#) (8/11) Release of the USER-CUDA package which provides accelerated versions for NVIDIA GPUs of 28 pair styles, 14 fixes, and 4 computes, with the ability to run an input script entirely on the GPU(s) until a timestep on which CPU calculations are required. See [this section](#) of the manual for details.
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<http://lammps.sandia.gov/>

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<http://lammps.sandia.gov/>

# Smooth Particle Hydrodynamics (SPH)

## Our Implementation became part of the LAMMPS Package

The implementation of Smooth Particle Hydrodynamics in  
LAMMPS.

A guide to the SPH-USER package.

Martin O. Steinhauser\* and Georg C. Ganzenmüller  
Fraunhofer Ernst-Mach Institut für Hochgeschwindigkeitsdynamik  
Freiburg, Germany

Paul Van Liedekerke  
Faculty of Bio-Engineering, MEBIOS Division  
Katholieke Universiteit Leuven  
Leuven, Belgium

\*martin.steinhauser@emi.fraunhofer.de

<http://lammps.sandia.gov>

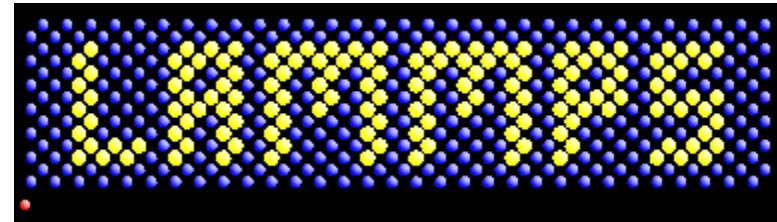
*SPH-USER Documentation*

*Contents*

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  - 3.3. SPH approximation of the Navier-Stokes continuity equation
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  - 5.4. Shear cavity flow



# MD Resources on the WWW: GROningen MAchine for Chemical Simulations

The screenshot shows a Mozilla Firefox browser window with multiple tabs open. The active tab displays the Gromacs homepage (<http://www.gromacs.org/>). The browser interface includes a toolbar with various icons like Print, Tab Groups, and AiOS-Toolbar. A sidebar on the left contains links for Bookmarks, History, Downloads, Add-ons, MultiPanel, and Page Info. The main content area features the Gromacs logo and navigation links for Log in, Register, Search, Main pages, and Gromacs documentation. It also includes links for getting source code, searching the mailing list, viewing the online manual, and accessing the git repository. A news section at the bottom provides updates from April 8, 2011, through January 6, 2012.

Gromacs - Gromacs - Mozilla Firefox

File Edit View History Bookmarks Tile Tools Help

Help - Eclipse SDK dict.leo.org – Ergebnisse f... Fortran – Wikipedia Gromacs - Gromacs

Back Forward http://www.gromacs.org/ Reload Stop Google Home

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The development of Gromacs would not have been possible without generous funding support from the European Research Council, the Swedish Research Council, the Swedish Foundation for Strategic Research, the Swedish National Infrastructure for Computing, and the Swedish Foundation for International Cooperation in Research and Higher Education. Several other grant agencies also provide funding to researchers involved in Gromacs development, in particular NIH and NSF in the US, and the DFG in Germany. For more information, see [funding](#).

Gromacs is one of the applications that are part of the ScalaLife Competence Center (<http://scalalife.eu>). The Competence Center is being developed as a one-stop-shop for users and developers of Life Science software. Various training events on high-performance computing and optimization techniques for improving scalability and performance will be organized by the center.

ScalaLife

**News**

April 8, 2011

Updated version 1.1.1 of xdrfile is available for download: <ftp://ftp.gromacs.org/pub/contrib/xd...e-1.1.1.tar.gz>. It contains compilation fixes and sample Python code for reading xtc files etc. from Python scripts.

March 22, 2011

Updated version 4.5.4 of the Gromacs manual is available at <ftp://ftp.gromacs.org/pub/manual/manual-4.5.4.pdf>.

March 21, 2011

New maintenance release: [gromacs-4.5.4.tar.gz](#). Here are the [release notes](#).

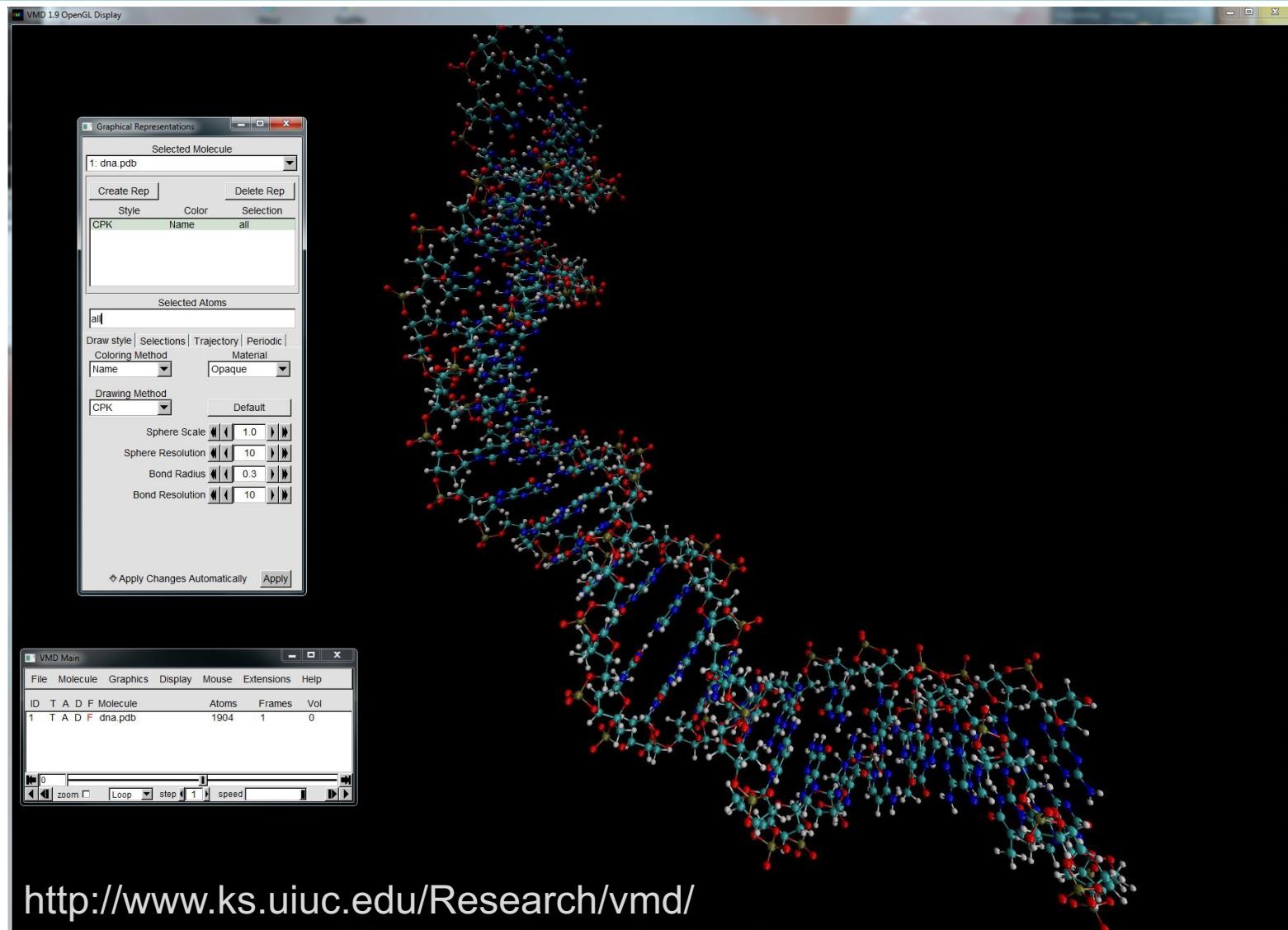
January 6, 2011

Happy New Year!

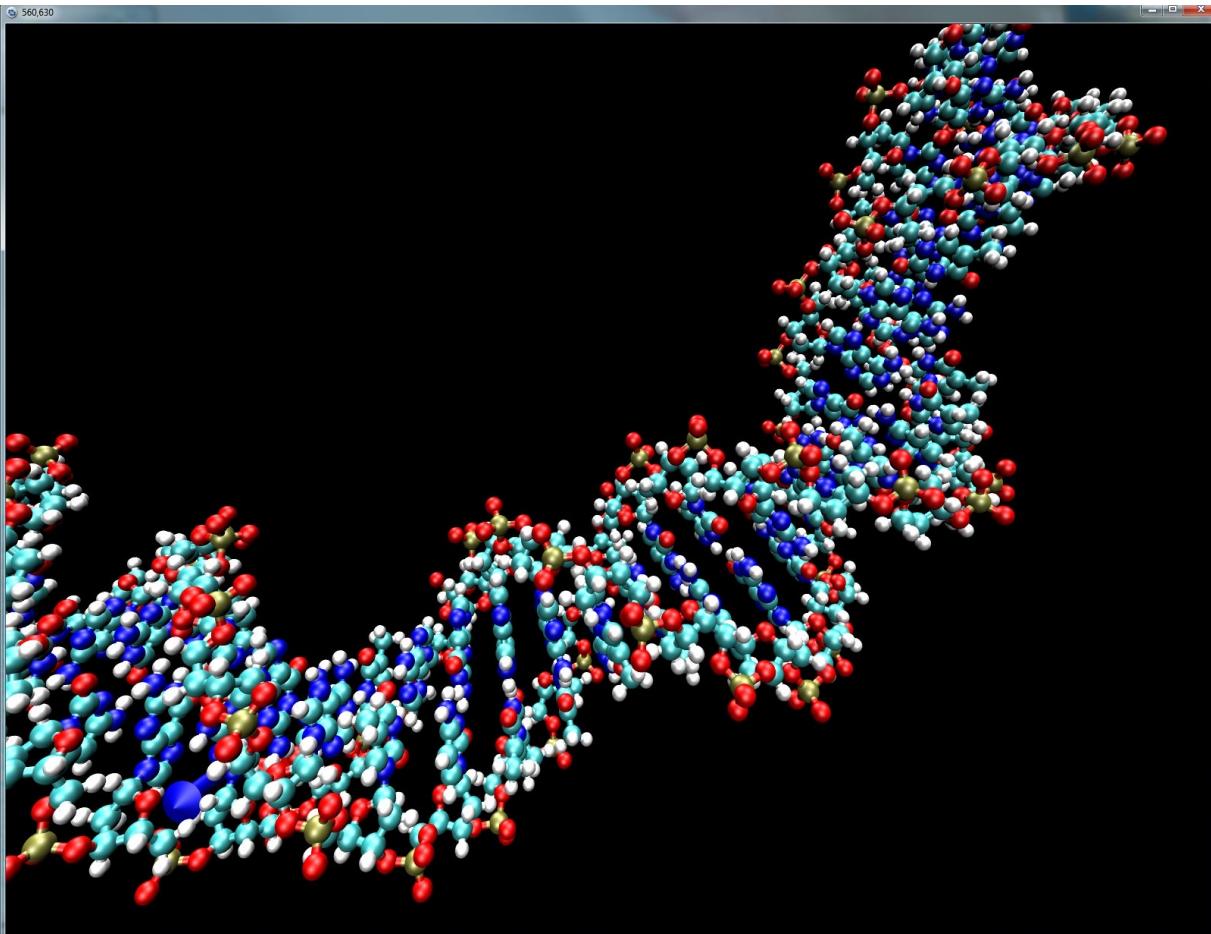
We've been discussing for a while moving away from Bugzilla and start using Redmine for bugtracking and project management. The latter offers a richer platform that we hope will be more helpful for our collaborative efforts. It is now available at <http://redmine.gromacs.org>, and the old bugzilla

[www.gromacs.org](http://www.gromacs.org)

# Visualization of MD Results



# Visualization of MD Results

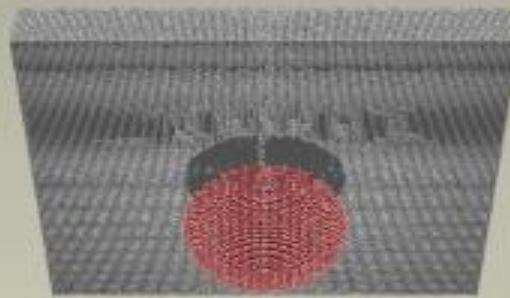


<http://www.povray.org/>

# Povray (raytracer)

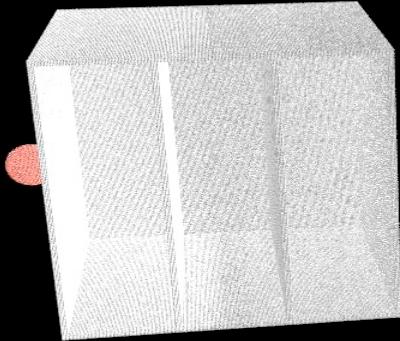
## Example from my own research:

Impact Simulation of a Solid at  $v = 6.5 \text{ km/s}$



## Example from my own research:

Simple CubeSat Numerical Model impacted in Space



$$\emptyset = 15 \text{ mm}$$

$$V = 10 \text{ km/s}$$

10 x 10 x 10 cm CubeSat

$1.22 \times 10^6$  Simulation Particles

# Simple CubeSat Numerical Model impacted in Space

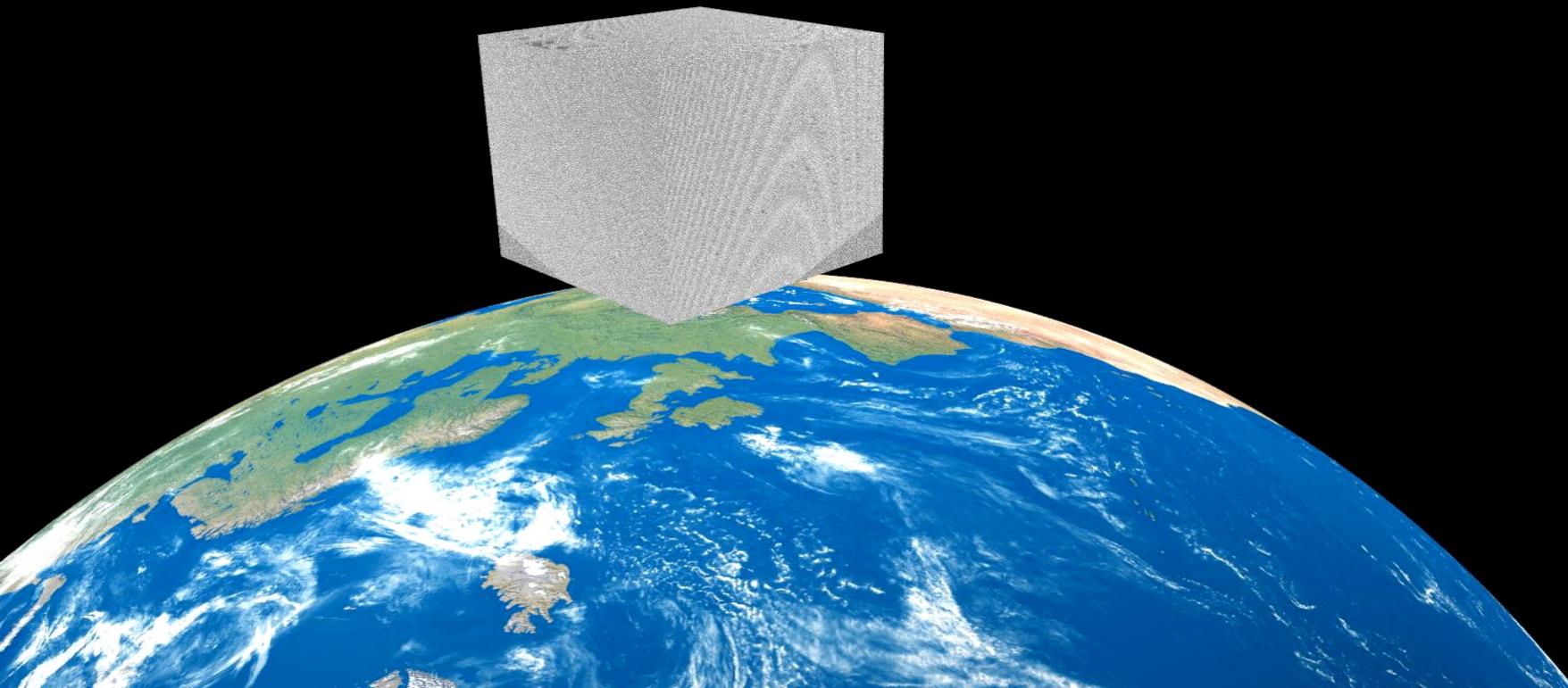
Simple CubeSat Numerical Model impacted in Space

$\emptyset = 15 \text{ mm}$

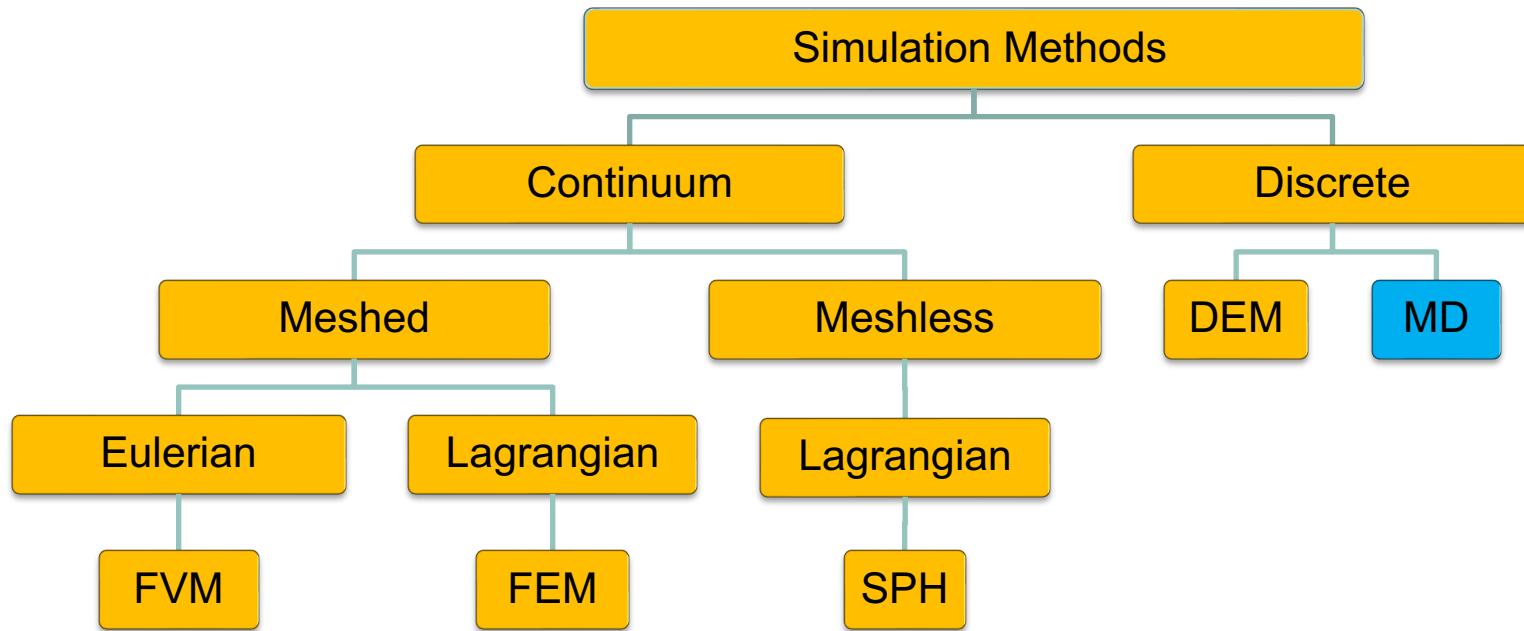
$V = 10 \text{ km/s}$

$10 \times 10 \times 10 \text{ cm CubeSat}$

$1.22 \times 10^6 \text{ Simulation Particles}$

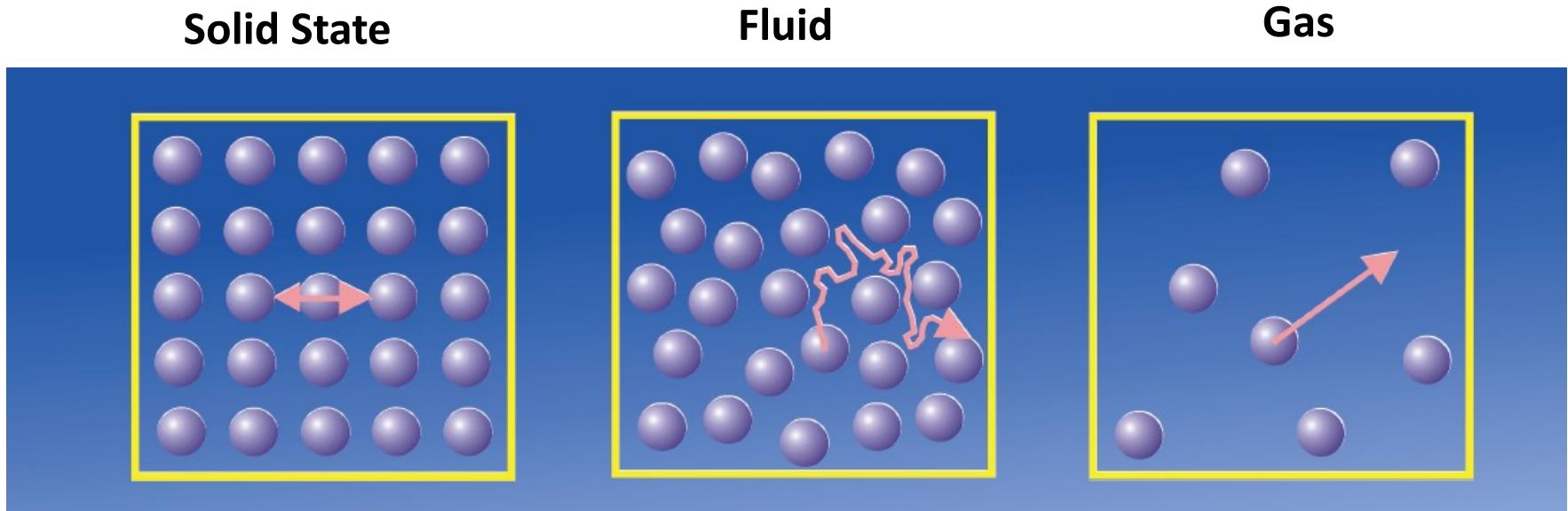


# A very simplified Overview of Simulation Methods



# Why Computer Simulation?

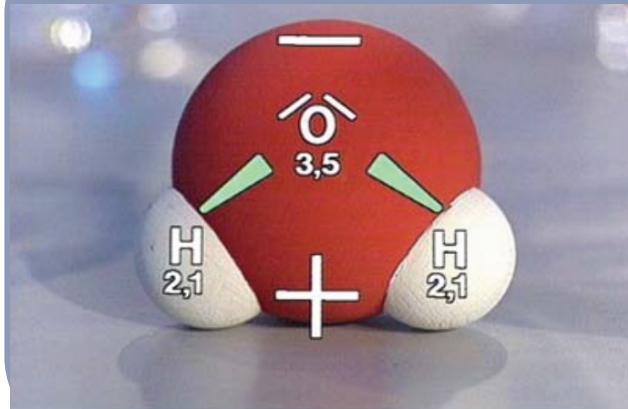
- All processes of life happen in the fluid state (in aqueous solutions)
- Many chemical syntheses and technical processes are done in the fluid phase



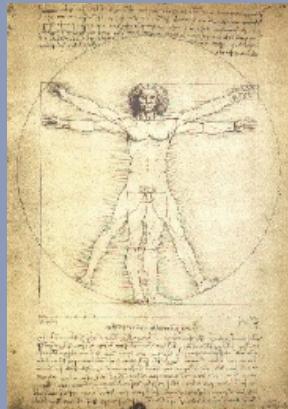
- But: There is no real „Theory of the Fluid State“

# Length and Time Scales in Nature

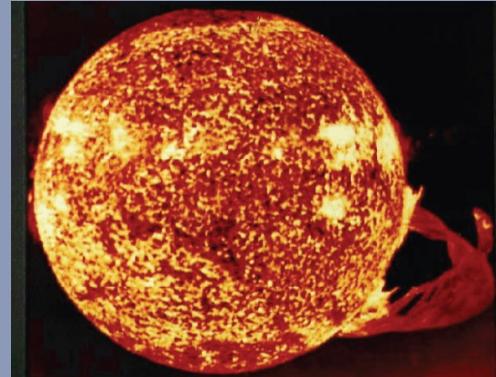
$3 \times 10^{-10} \text{ m}$



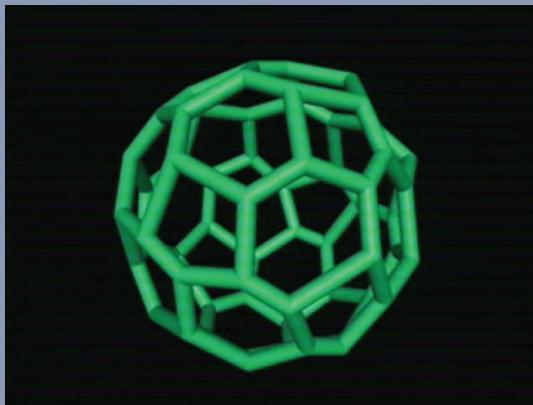
1.8m



$15 \times 10^{15} \text{ m}$



$2 \times 10^{-15} \text{ s}$



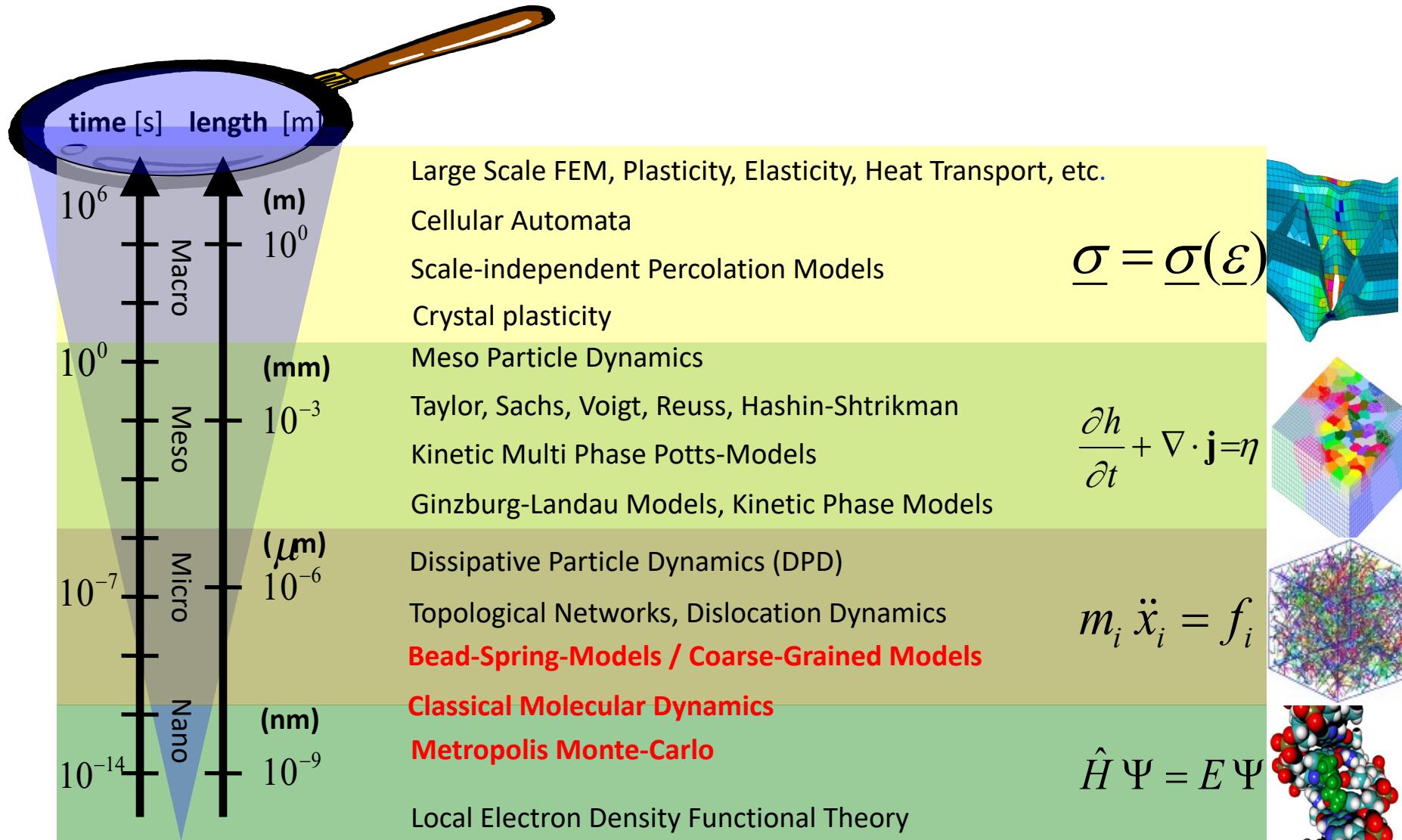
60s



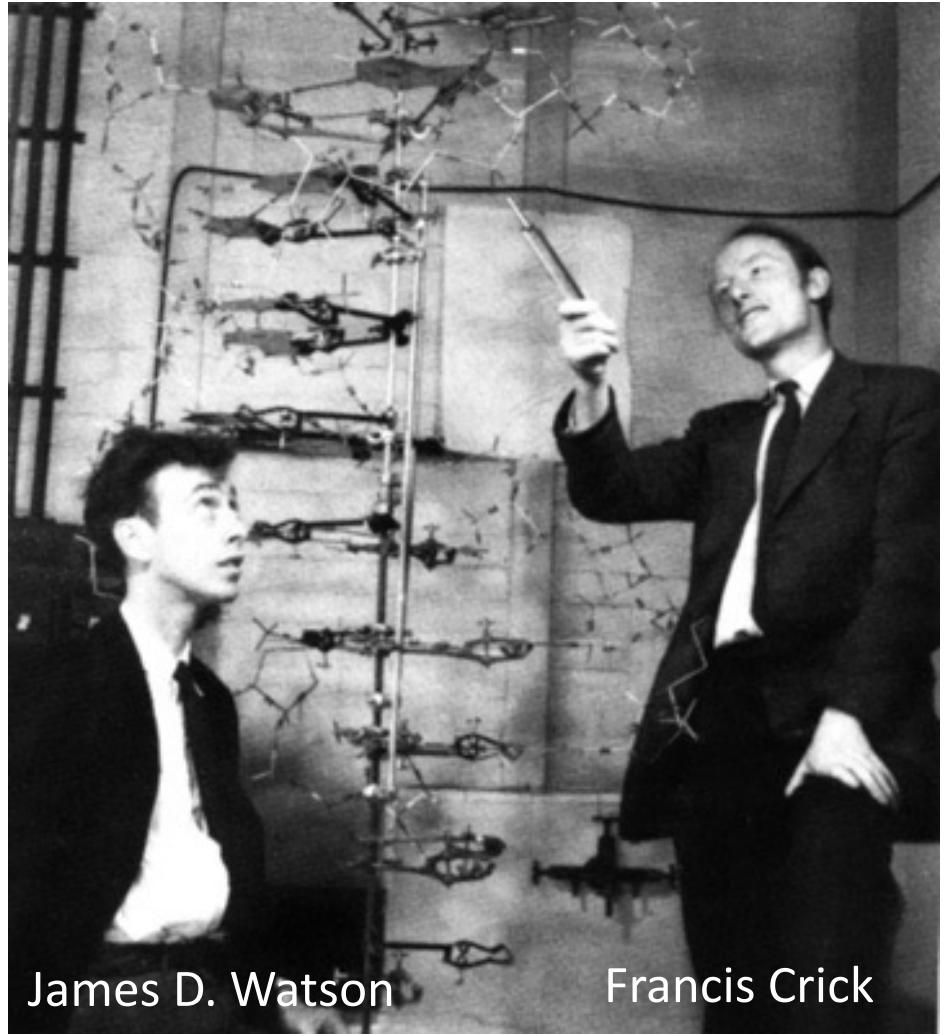
$1.5 \times 10^{15} \text{ s}$



# Length and Time Scales and Associated Numerical Schemes



# Static Models can be quite useful...



James D. Watson

Francis Crick

From: James D. Watson, "The Double Helix: A Personal Account of the Discovery of the Structure of DNA", Touchstone 2001

NO. 4356 April 25, 1953

NATURE

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equipment, and to Dr. G. E. R. Deacon and the captain and officers of R.R.S. *Discovery II* for their part in making the observations.

<sup>1</sup> Young, F. B., Gerard, H., and Jeavons, W., *Phil. Mag.*, **40**, 149 (1920).

<sup>2</sup> Longuet-Higgins, M. S., *Mon. Not. Roy. Astro. Soc., Geophys. Suppl.*, **8**, 285 (1949).

<sup>3</sup> Von Hippel, W. S., Woods Hole Papers in Phys. Oceanogr. Meteor., **11** (3) (1956).

<sup>4</sup> Ekman, V. W., *Arkiv. Mat. Astron. Fysik. (Stockholm)*, **2** (11) (1905).

## MOLECULAR STRUCTURE OF NUCLEIC ACIDS

### A Structure for Deoxyribose Nucleic Acid

WE wish to suggest a structure for the salt of deoxyribose nucleic acid (D.N.A.). This structure has novel features which are of considerable biological interest.

A structure for nucleic acid has already been proposed by Pauling and Corey<sup>1</sup>. They kindly made their manuscript available to us in advance of publication. Their model consists of three intertwined chains, with the phosphates near the fibre axis, and the bases on the outside. In our opinion, this structure is unsatisfactory for two reasons: (1) We believe that the material which gives the X-ray diagrams is the salt, not the free acid. Without the acidic hydrogen atoms it is not clear what forces would hold the structure together, especially as the negatively charged phosphates near the axis will repel each other. (2) Some of the van der Waals distances appear to be too small.

Another three-chain structure has also been suggested by Fraser (in the press). In his model the phosphates are on the outside and the bases on the inside, linked together by hydrogen bonds. This structure as described is rather ill-defined, and for this reason we shall not comment on it.

We wish to put forward a radically different structure for the salt of deoxyribose nucleic acid. This structure has two helical chains each coiled round the same axis (see diagram). We have made the usual chemical assumptions, namely, that each chain consists of phosphate ester groups joining  $\beta$ -D-deoxy-ribofuranose residues with  $3',5'$  linkages. The two chains (but not their bases) are related by a dyad perpendicular to the fibre axis. Both chains follow right-handed helices, but owing to the dyad the sequences of the atoms in the two chains run in opposite directions. Each chain loosely resembles Furberg's<sup>2</sup> model No. 1; that is, the bases are on the inside of the helix and the phosphates on the outside. The configuration of the sugar and the atoms near it is close to Furberg's 'standard configuration'; the sugar being roughly perpendicular to the attached base. There

The figure is a diagrammatic representation. It shows two parallel helical ribbons symbolizing the two phosphate-sugar chains, and the horizontal rod is the pair of bases holding the chains together. The vertical line marks the fibre axis.

is a residue on each chain every 3.4 Å. in the z-direction. We have assumed an angle of  $36^\circ$  between adjacent residues in the same chain, so that the structure repeats after 10 residues on each chain, that is, after 34 Å. The distance of a phosphorus atom from the fibre axis is 10 Å. As the phosphates are on the outside, cations have easy access to them.

The structure is an open one, and its water content is rather high. At lower water contents we would expect the bases to tilt so that the structure could become more compact.

The novel feature of the structure is the manner in which the two chains are held together by the purine and pyrimidine bases. The planes of the bases are perpendicular to the fibre axis. They are joined together in pairs, a single base from one chain being hydrogen-bonded to a single base from the other chain, so that the two lie side by side with identical z-coordinates. One of the pair must be a purine and the other a pyrimidine for bonding to occur. The hydrogen bonds are made as follows: purine position 1 to pyrimidine position 1; purine position 6 to pyrimidine position 6.

If it is assumed that the bases only occur in the structure in the most plausible tautomeric forms (that is, with the keto rather than the enol configurations) it is found that only specific pairs of bases can bond together. These pairs are: adenine (purine) with thymine (pyrimidine), and guanine (purine) with cytosine (pyrimidine).

In other words, if an adenine forms one member of a pair, on either chain, then on these assumptions the other member must be thymine; similarly for guanine and cytosine. The sequence of bases on a single chain does not appear to be restricted in any way. However, if only specific pairs of bases can be formed, it follows that if the sequence of bases on one chain is given, then the sequence on the other chain is automatically determined.

It has been found experimentally<sup>3,4</sup> that the ratio of the amounts of adenine to thymine, and the ratio of guanine to cytosine, are always very close to unity for deoxyribose nucleic acid.

It is probably impossible to build this structure with a ribose sugar in place of the deoxyribose, as the extra oxygen atom would make too close a van der Waals contact.

The previously published X-ray data<sup>5,6</sup> on deoxyribose nucleic acid are insufficient for a rigorous test of our structure. So far as we can tell, it is roughly compatible with the experimental data, but it must be regarded as unproved until it has been checked against more exact results. Some of these are given in the following communications. We were not aware of the details of the results presented there when we devised our structure, which rests mainly though not entirely on published experimental data and stereochemical arguments.

It has not escaped our notice that the specific pairing we have postulated immediately suggests a possible copying mechanism for the genetic material.

Full details of the structure, including the conditions assumed in building it, together with a set of co-ordinates for the atoms, will be published elsewhere.

We are much indebted to Dr. Jerry Donohue for constant advice and criticism, especially on interatomic distances. We have also been stimulated by a knowledge of the general nature of the unpublished experimental results and ideas of Dr. M. H. F. Wilkins, Dr. R. E. Franklin and their co-workers at

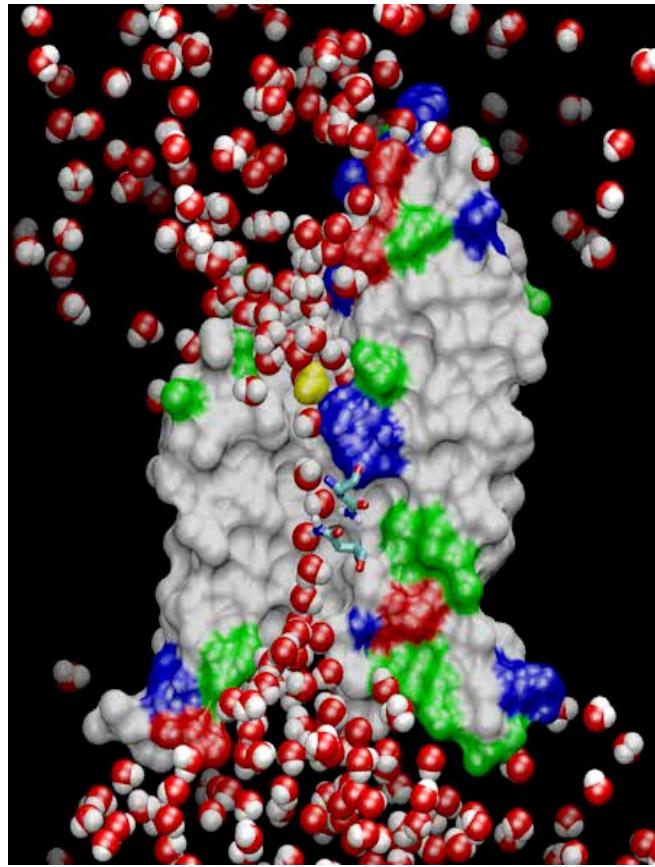
## But...

- Molecules are *flexible* structures, able to change their conformations
- Molecules do *not* naturally *occur isolated* in almost all cases
- Molecules usually *build aggregates* (macromolecular complexes)
- Many physiological processes occur *at interfaces*
- Some experiments are *too dangerous or impossible* to be performed
- Simulations can *realize thought experiments!*

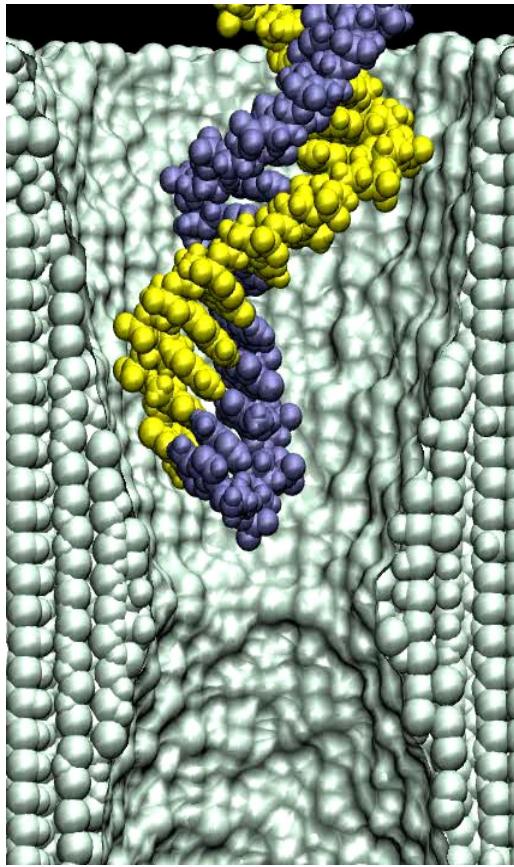
**GOOD REASONS FOR SCIENTIFIC COMPUTING!**

# Examples from Soft Matter Physics

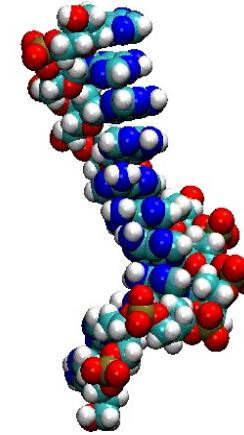
Motion of water through a membrane  
Water channel, aquaporin



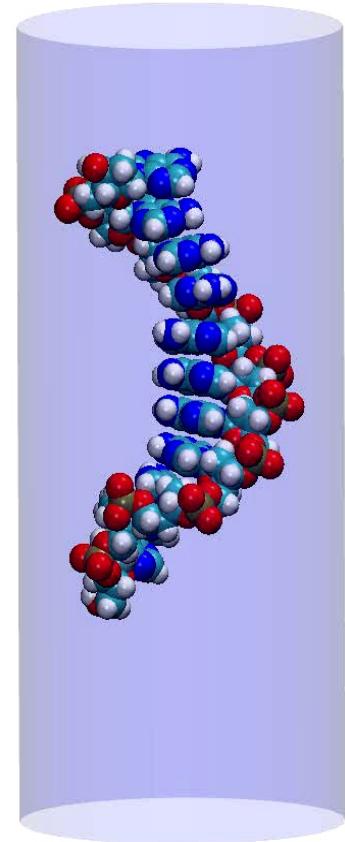
DNA, forced through small nanopore



Stretching DNA



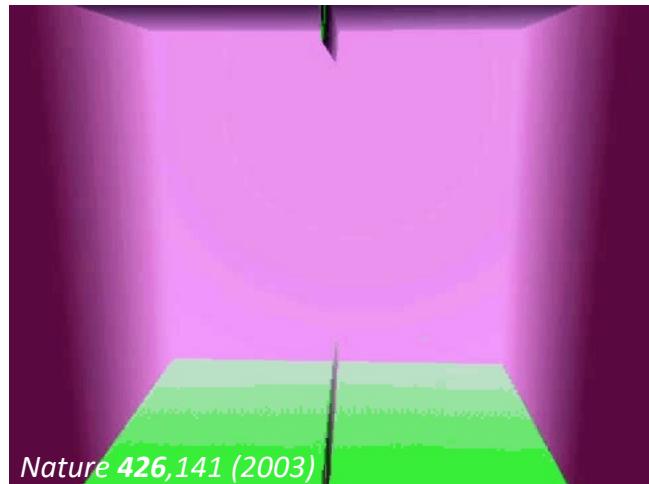
Confining DNA



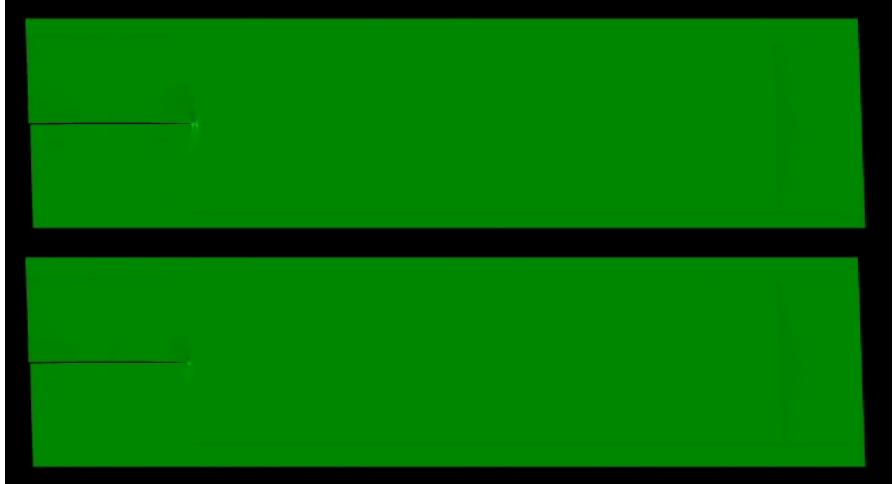
[www.ks.uiuc.edu/Gallery/Movies/](http://www.ks.uiuc.edu/Gallery/Movies/)

# Examples from Hard Matter Physics

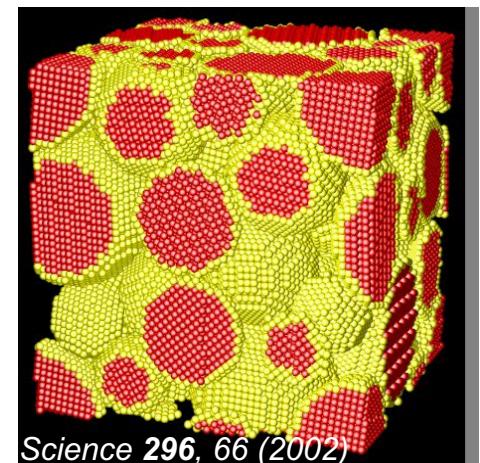
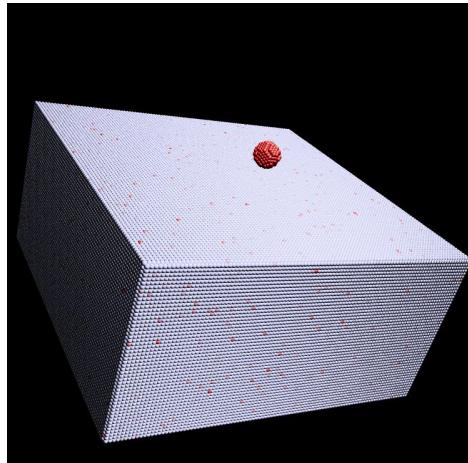
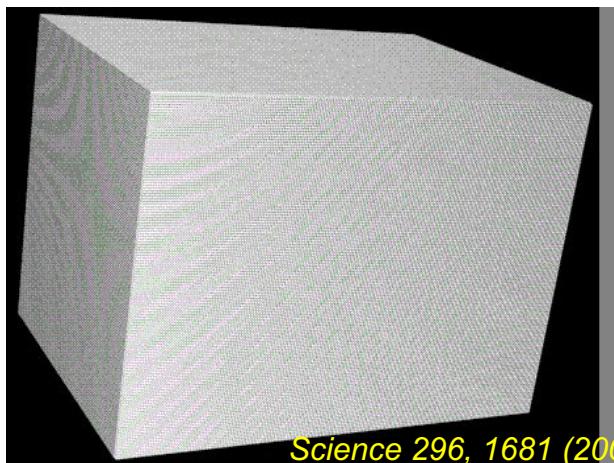
Dislocations in a crystal



Supersonic crack propagation

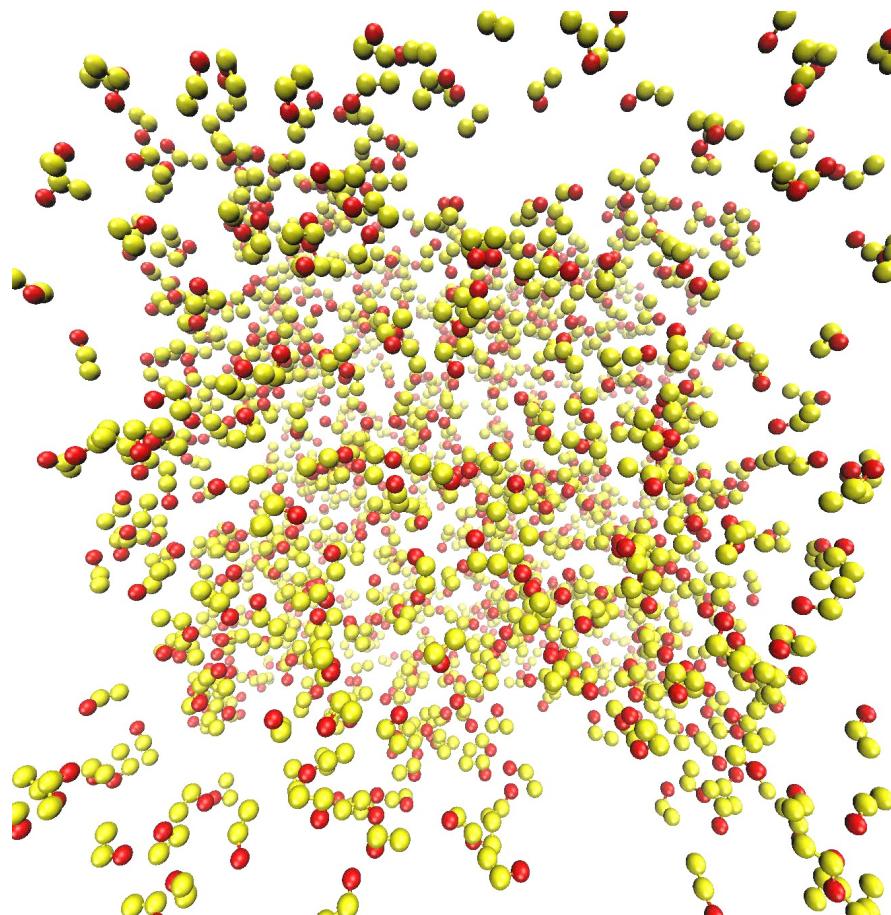


Shocked, impacted and loaded crystals



# Example from Current Research in Computational Biology

## How do Complex Structures of Biomolecules arise ?



# Prerequisite: Fast Computers



**ENIAC 1953**  
(30000 vacuum tubes)



**HP Frontier at Oak Ridge NL 2024**  
(24.3 Mio cores)

$1.0 \times 10^3$  FLOPS     $\leftarrow 10^{13} \rightarrow > 4 \times 10^{16}$  FLOPS

[www.top500.org/](http://www.top500.org/)

**Hardware is not Everything!**

Hardware without Software is  
Noware

# Whiteboard Notes...

# Summary

- Today, computer simulation is predominant in science and research
- In Scientific computing, visualizations of data are important, too!
- In order to use computers, **one must learn (scientific) programming**
- There are certain best practices for programming style: (See Handout)
- The first **computers for everyone** appeared only roughly 40 years ago
- Keep in Mind: Scientific Programming REALLY is a lot of fun !



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