Today

- we introduce us
- let's get organized
- simulations are fun!

- let's start:
  Introduction into integers and floating points

We introduce us

- Frauke Gräter, HITS Heidelberg, Interdisciplinary Center for Scientific Computing
- Rüdiger Pakmor, HITS

Exercizes:

- Christopher Zapp, HITS
- Csaba Daday, HITS

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MATHEMATIKON

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Our objective

to reach an active understanding of applicable numerical methods and algorithms

and

to endow you with the capacity

- to identify and classify common numerical problems,
- to solve basic physical problems with adequate numerical techniques, and
- to recognize the range of validity of numerical solutions

Topics

- Basic concepts of numerical simulations, continuous and discrete simulations
- Discretization of ordinary differential equations, integration schemes of different order
- N-body problems, molecular dynamics, collisionless systems
- Discretization of partial differential equations
- Finite element and finite volume methods
- Lattice methods
- Adaptive mesh refinement and multi-grid methods
- Matrix solvers and FFT methods
- Monte Carlo methods, Markov chains, applications in statistical physics

Table 3.4.1: Specialization Computational Physics

Module code	Module	LP/CP	Term
MVComp1	Fundamentals of Simulation Methods	8	WiSe
MVComp2	Computational Statistics and Data Analysis	6	SuSe

Table 3.4.2: Specialization Computational Physics; Specialised lectures and seminars

[The lectures and seminars listed here will be offered on an irregular basis]

Module code	Module	LP/CP	Term
MVSpec	Advanced Monte Carlo Methods	3	WiSe/SuSe
MVSpec	Advanced Parallel Computing	4-6	WiSe/SuSe
MVSpec	Computational Fluid Dynamics	4-6	WiSe/SuSe
MVSpec	Computational Imaging	4-6	WiSe/SuSe
MVSpec	Computational Optics	4-6	WiSe/SuSe
MVSpec	GPU programming	4	WiSe/SuSe
MVSpec	Image Analysis	8	WiSe/SuSe
MVSpec	Introduction to High-Performance Computing	4-6	WiSe/SuSe
MVSpec	Inverse Problems	8	WiSe/SuSe
MVSpec	Machine Learning	8	WiSe/SuSe
MVSpec	Radiative Transfer	4	WiSe/SuSe
MVSpec	Scientific Programming	4-6	WiSe/SuSe
MVSpec	Volume Visualization	8	WiSe/SuSe
MVSem	Computer Vision	6	WiSe/SuSe

Topics

oct			
	18	FG	intro
	20	FG	1.intro
	25	RP	2. ODEs
	27	RP	2. ODEs
nov			
	3	RP	3. collisionless systems
	8	RP	3. collisionless cystems
	10	RP	4. trees
	25	FG	5. Particle-mesh
	17	FG	5. Particle-mesh
	22	FG	6. FT
	24	FG	6. FT
	29	FG	7. iterative solvers
dec			
	1	FG	7. iterative solvers
	6	FG	8. MD
	8	FG	8. MD
	13	RP	8. MD
	15	FG	8. BD
	20	FG	9. MC
	22	FG	9. MC

jan			
	10	RP	10. Gas dynamics
	12	RP	10. Gas dynamics
	17	RP	11. PDEs
	19	RP	11. PDEs
	24	RP	12. SPH
	26	RP	13. FEM
	31	RP	13. FEM
feb			
	2	14	14. Parallelization
	7	14	14. Parallelization
	9	exam	
march			
	9	2nd exam	

Requirements

- you know at least one programming language
- you know at least one plotting software
- you want to learn how to simulate physical problems with the computer

Organizational stuff

Semester	WS 2016/17	**Veranstaltungsnummer**	130000201628001
Veranstaltungskürzel	MVComp1	**Veranstaltungsart**	Vorlesung / Übung
SWS	6	**Leistungspunkte**	8
Erwartete Teilnehmer		**Max. Teilnehmer**	
Sprache	Englisch	**Studienjahr**	
Hyperlink	http://www.h-its.org/teaching-mbm-2016/		

Termine

Tag	Zeit	Rhythmus	Dauer	Dozent	Raum	Status	fällt aus am	Max. Teilnehmer	Bemerkung
Di.	09:15 bis 11:00	wöch		Graeter	INF 227 / HS 2				2. Dozent: R. Pakmor
Do.	09:15 bis 11:00	wöch		Graeter	INF 227 / HS 2				2. Dozent: R. Pakmor
Fr.	11:15 bis 13:00	wöch		Graeter	Philos.-weg 12 / CIP				Exercise; 2. Dozent: R. Pakmor
Fr.	14:15 bis 16:00	wöch		Graeter	INF 227 / CIP-Pool KIP 1.401				Exercise; 2. Dozent: R. Pakmor

Organizational stuff

- lectures 9.30-11.00 – possible?
- please sign up for one of the exercises on Fridays, and be aware of the two different locations!
- Note: active participation in exercises (50% of points) is a requirement for attending the exam!
- teams of 2 are possible
- bring your laptop to the exercises if you want

online material

website:

http://www.h-its.org/teaching-mbm-2016/

script (by Volker Springel, to a minor extent adapted by FG) , exercises etc are provided here:

https://elearning2.uni-heidelberg.de/course/view.php?id=13007

Registration:

`debugging`

exercises

- Exercises will be made available through moodle as well, and they have to be handed in through moodle.
- Group work of 2 (or up to 3) people is allowed/encouraged. You need to reach 50% of the points to be allowed to take the final exam.
- New problem sets are normally made available on Wed evening, to allow first questions to be asked on Friday's exercise class. Due date is normally on the following Thu night.
- Programming can be done in C, C++, Python, IDL, GDL and Fortran if you really feel like it.
- Plotting can be done in Python, IDL/GDL, Gnuplot, Mathematica, xmgrace etc.

Requirements

- you know at least one programming language
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Exercises

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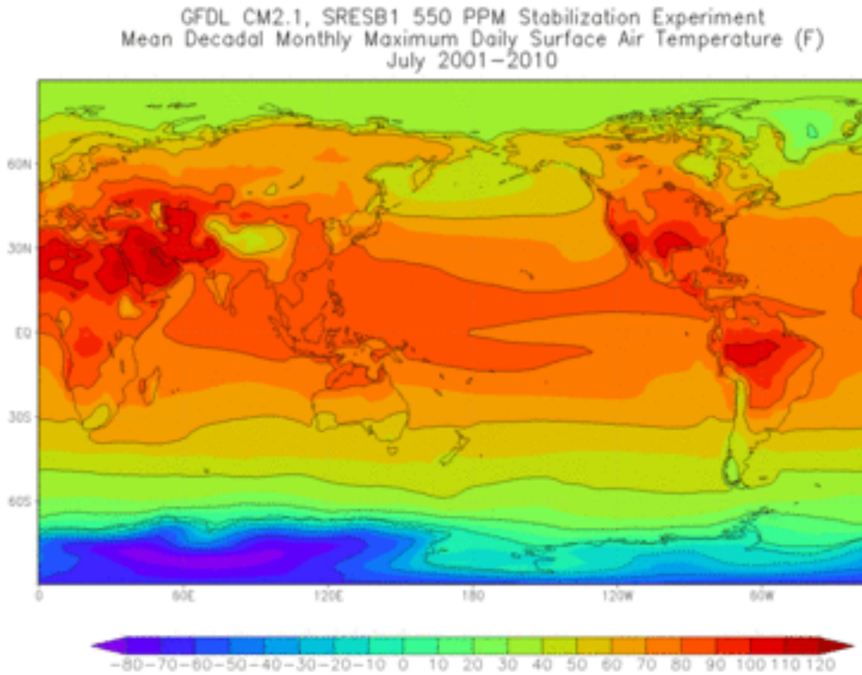
Why simulations?

If we have so many types of fancy experiments?

a) the experiment can not look forward in time
b) the experiment can not look backward in time
c) the experiment has lousy spatial/time resolution

Why simulations?

a) the experiment can not look forward in time

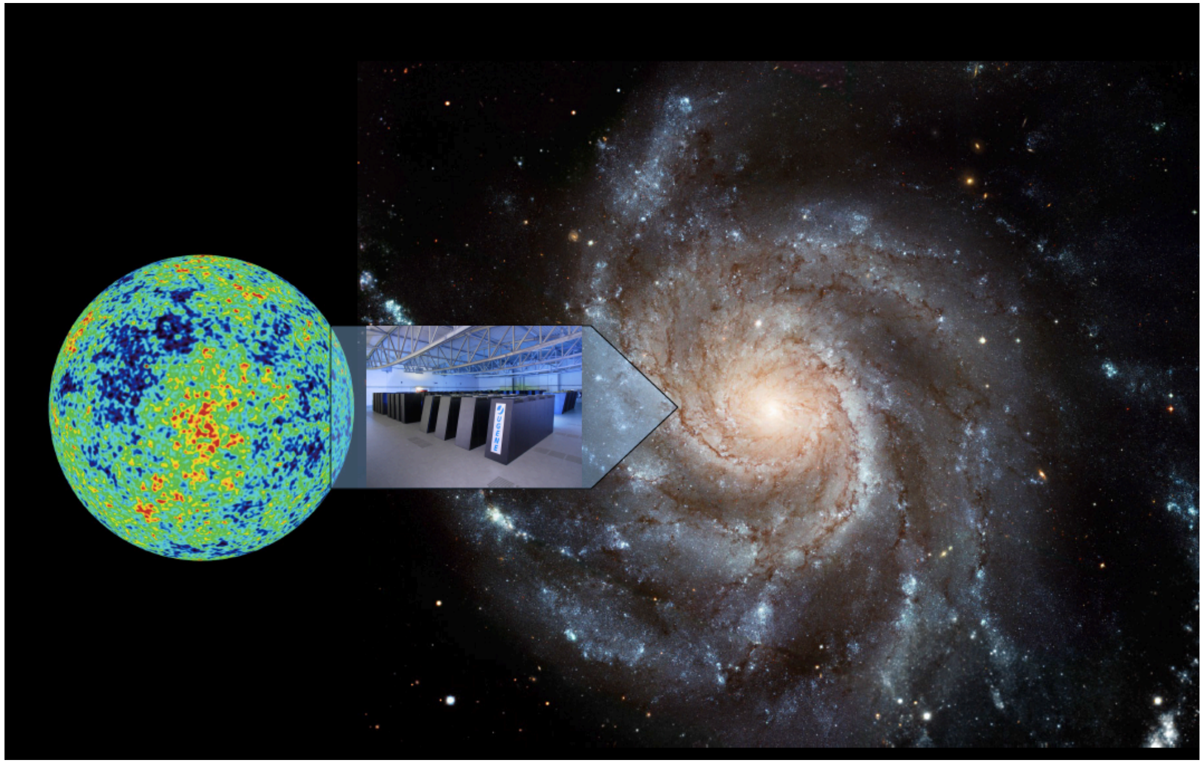


source: NOAA

delta t ~ days, tmax ~ decades
delta x ~ km, xmax ~ the earth
physics: continuous models, fluid dynamics, thermodynamics

Why simulations?

b) the experiment can not look backward in time

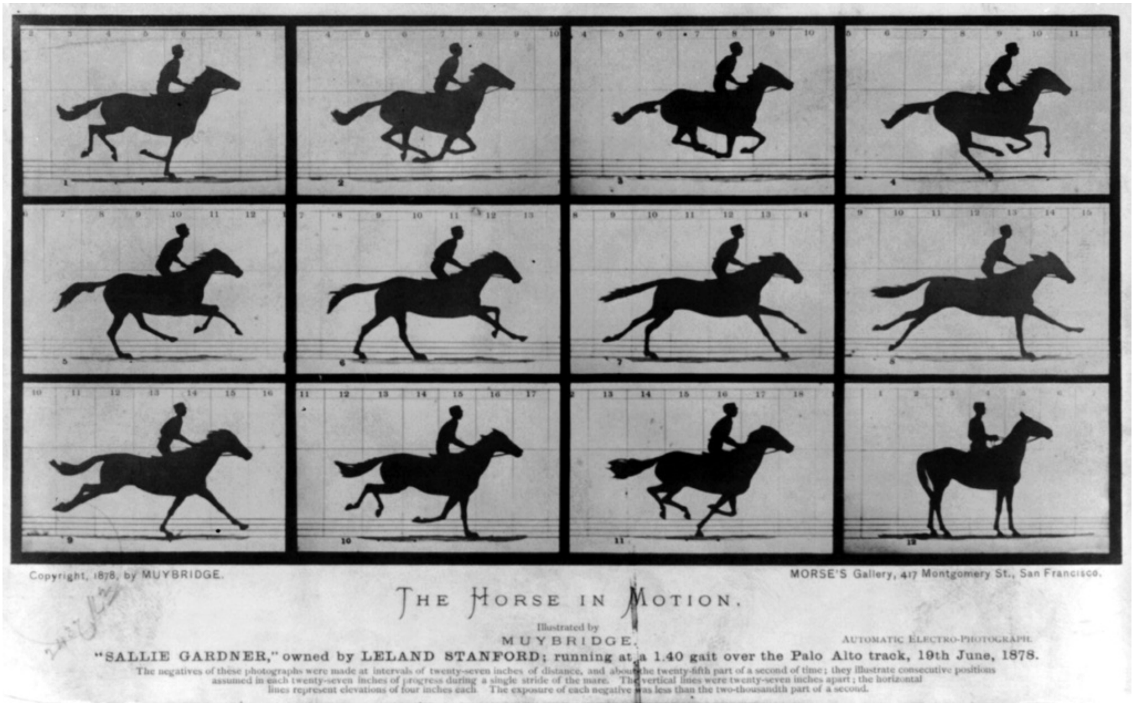


source:
Volker Springel

delta t ~ years, tmax ~ billion of years
delta x ~ lightyears, xmax ~ the universe
physics: particles, hydrodynamics, gravity

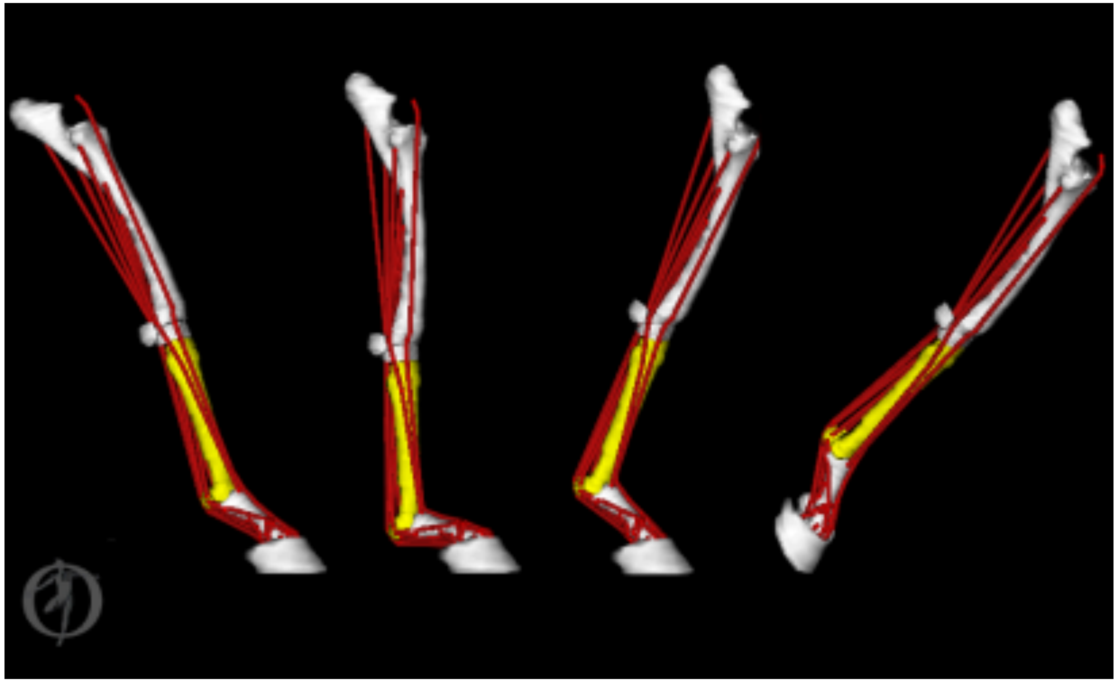
Why simulations?

c) the experiment has lousy spatial/time resolution



Why simulations?

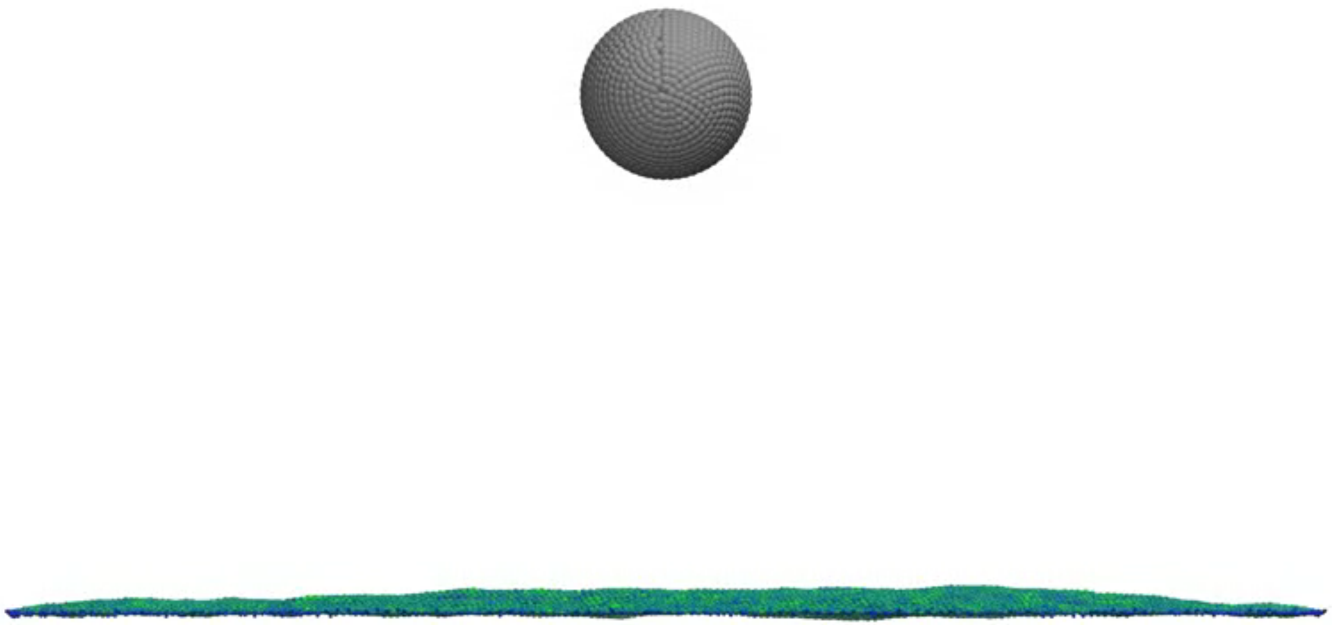
c) the experiment has lousy spatial/time resolution



delta t ~ sub-seconds, tmax ~ minutes
delta x ~ 10^-2m, xmax ~ the horse
physics: continuum mechanics, finite element models

Why simulations?

c) the experiment has lousy spatial/time resolution

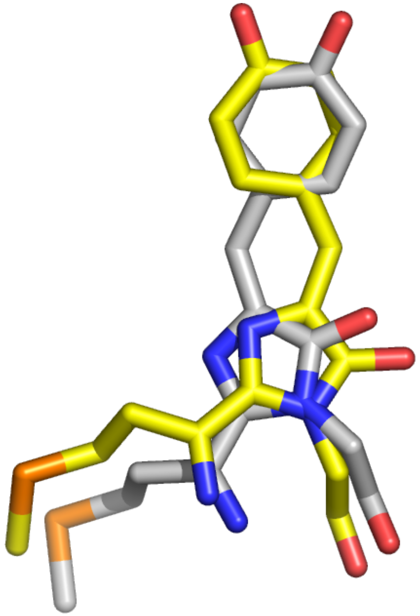


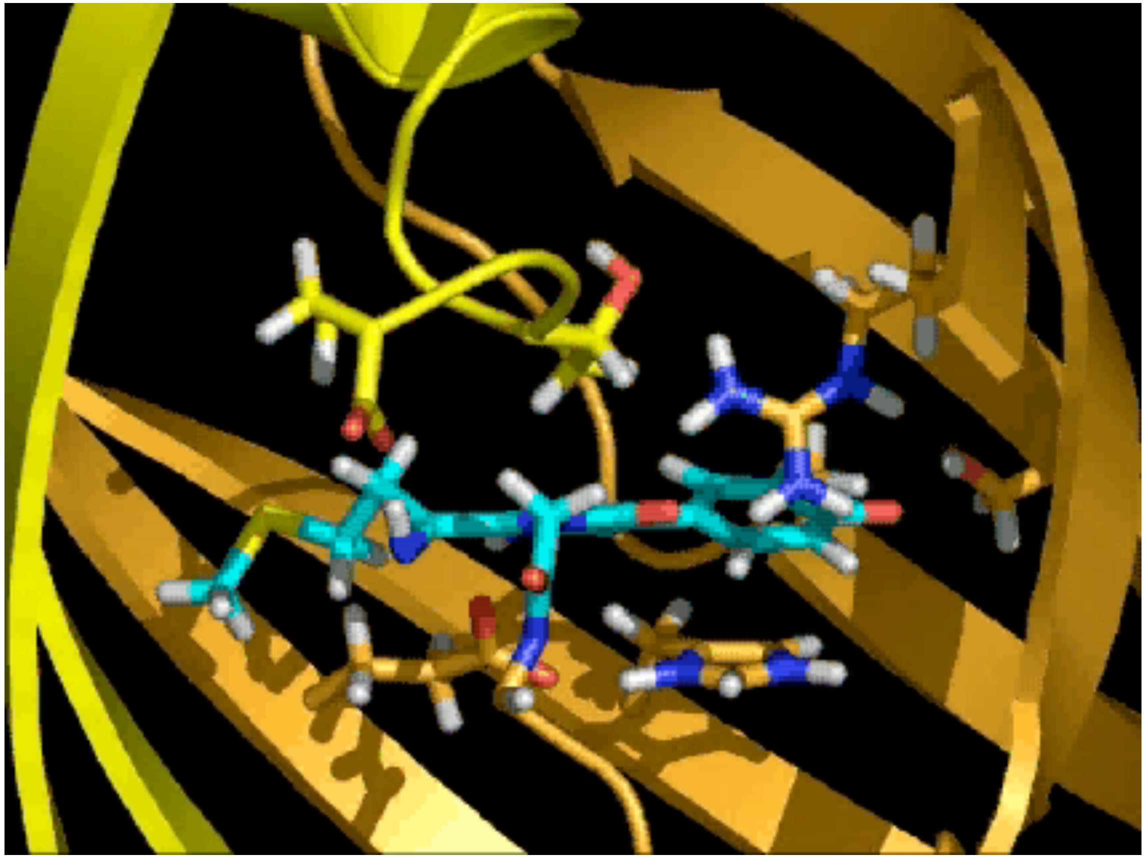
delta t ~ fs, tmax ~ microseconds
delta x ~ 10^-10 m, xmax ~ micrometer
physics: particles, classical mechanics

Examples from our group

(molecular simulations)

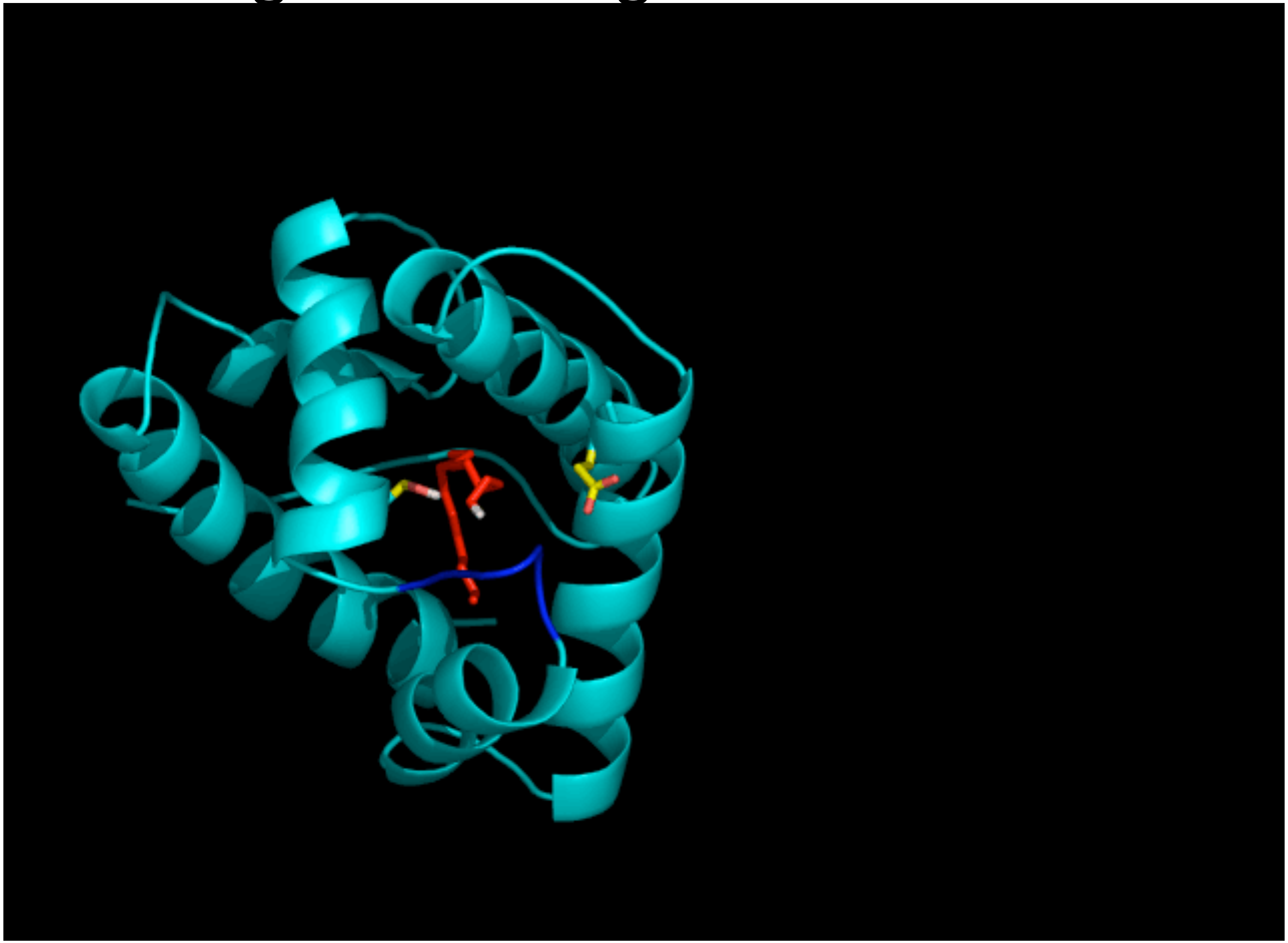
asFP595: trans-cis isomerisation



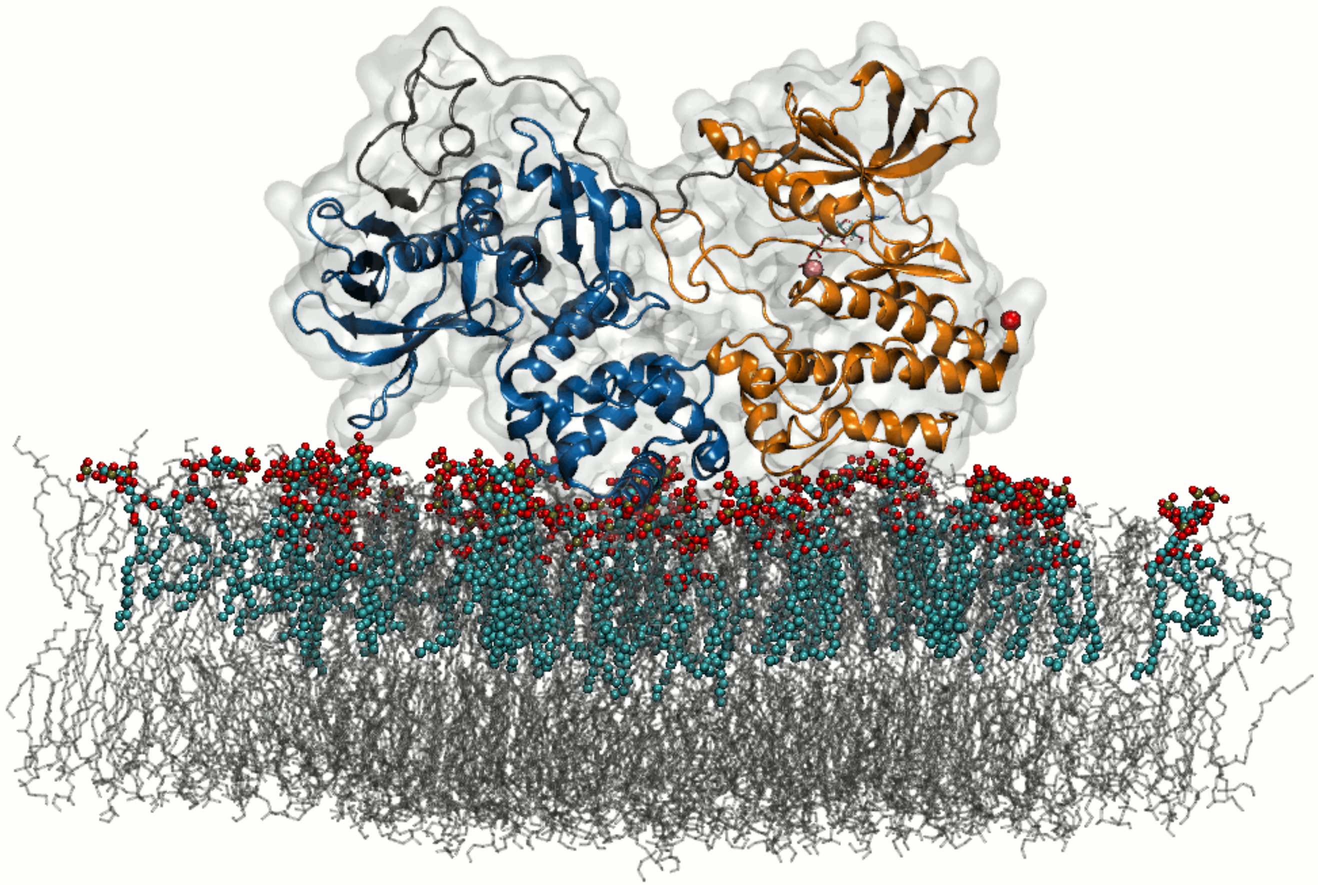


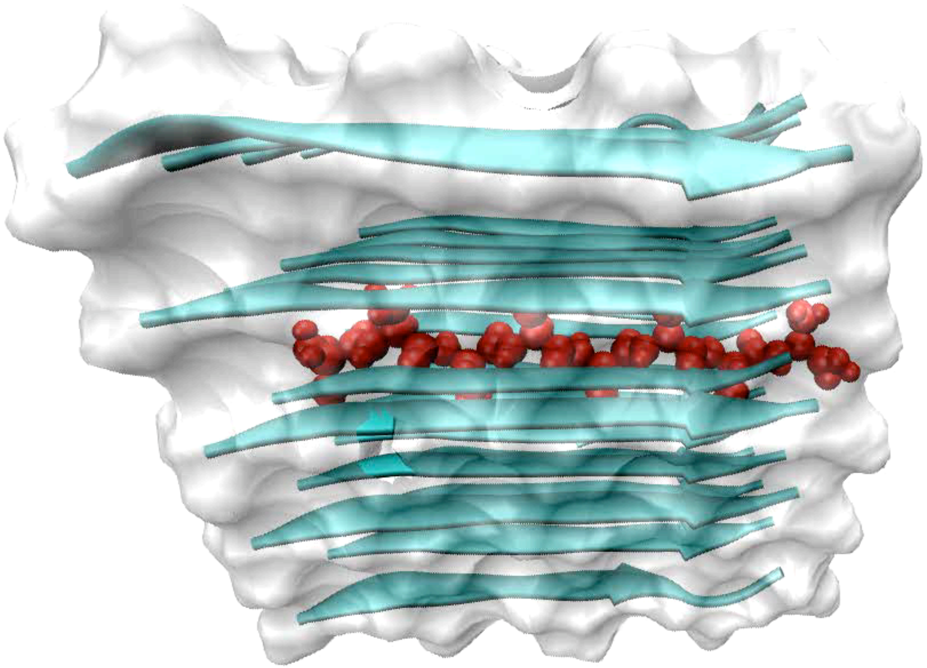
picosecond time scale

protein-ligand binding

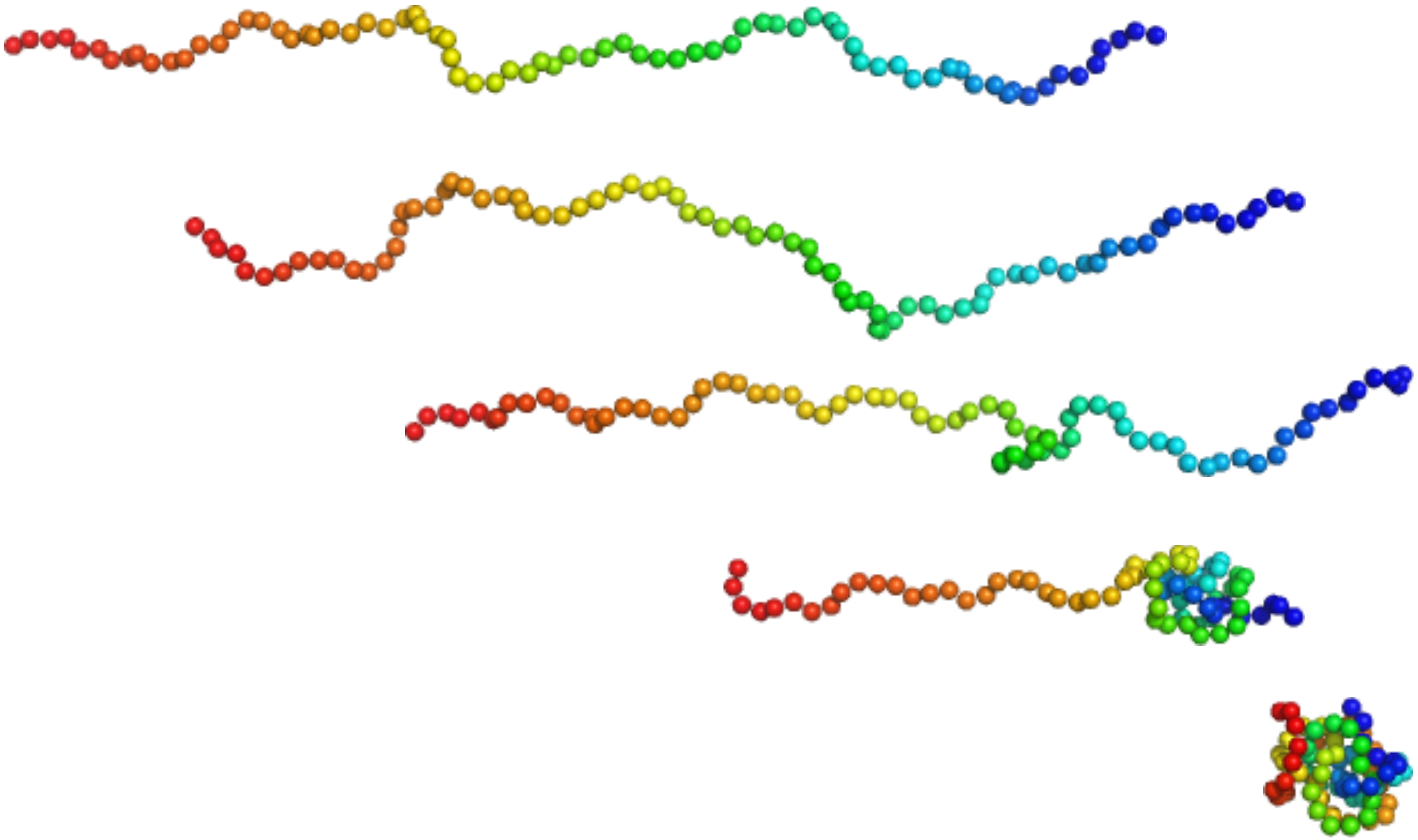


Focal adhesion kinase





Protein collapse and folding



(milli)second time scale

The challenge: big number crunchers

Rank	Site	System	Cores	Rmax (TFlop/s)	Rpeak (TFlop/s)	Power (kW)
1	National Supercomputing Center in Wuxi China	**Sunway TaihuLight** - Sunway MPP, Sunway SW26010 260C 1.45GHz, Sunway NRCPC	10,649,600	93,014.6	125,435.9	15,371
2	National Super Computer Center in Guangzhou China	**Tianhe-2 (MilkyWay-2)** - TH-IVB-FEP Cluster, Intel Xeon E5-2692 12C 2.200GHz, TH Express-2, Intel Xeon Phi 31S1P NUDT	3,120,000	33,862.7	54,902.4	17,808
3	DOE/SC/Oak Ridge National Laboratory United States	**Titan** - Cray XK7 , Opteron 6274 16C 2.200GHz, Cray Gemini interconnect, NVIDIA K20x Cray Inc.	560,640	17,590.0	27,112.5	8,209
4	DOE/NNSA/LLNL United States	**Sequoia** - BlueGene/Q, Power BQC 16C 1.60 GHz, Custom IBM	1,572,864	17,173.2	20,132.7	7,890
5	RIKEN Advanced Institute for Computational Science (AICS) Japan	K computer, SPARC64 VIIIfx 2.0GHz, Tofu interconnect Fujitsu	705,024	10,510.0	11,280.4	12,660
6	DOE/SC/Argonne National Laboratory United States	**Mira** - BlueGene/Q, Power BQC 16C 1.60GHz, Custom IBM	786,432	8,586.6	10,066.3	3,945

The challenge: big number crunchers

Name	Standort	TeraFLOPS (peak)	Konfiguration
Hazel Hen[6]	Höchstleistungsrechenzentrum Stuttgart	7.420,00	Cray Aries Netzwerk; 7712 Nodes mit je 24 Kernen (Intel Xeon E5-2680 v3, 30M Cache, 2,50 GHz)
JUQUEEN[7]	Forschungszentrum Jülich (Deutschland)	5.900,00	IBM BlueGene/Q, 28.672 Power BQC-Prozessoren (16 Kerne, 1,60 GHz)

The challenge: big number crunchers

Why simulations?

increasing impact in science:

simulations

- test existing hypotheses
- generate new hypotheses
- can largely simplify complex phenomena

examples:

~ number papers on simulation increase faster than total number of papers

~ more than half of presentations at biophysical society meeting Germany 2016 included simulations

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Let’s check your background

A you never programmed

B you know some python

C you know some C

D you know C very well

E you know C++ very well

Let’s check your background

A you never plotted

B you can plot with python

C you can plot with gnuplot

D you can plot with IDL

E you can plot with mathematica or matlab

F you can plot with other software

Let’s check your background

A you never plotted (excel does not count!)

B you can plot with pyton

C you can plot with gnuplot

D you can plot with IDL

E you can plot with mathematica or matlab

F you can plot with other software

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Quiz

How is -1 represented in a 16-bit integer?

A 0000000000000000

B 0000000000000001

C 1000000000000000

D 1111111111111110

E 1000000000000001

F 1111111111111111

Quiz

What does this c code print out?

```
int i;
float x=0.0 ;
for (i = 0; i< 100000000; i++)
  x+= 1.0;
printf ("x = %f\n", x);
```

```
A x = 100000000.3200
B x = 99999999.892998
C x = 100000000
D x = 16777216.000000
E x = 100000000.00130
```