Parallelization of Molecular Dynamics (with focus on Gromacs)

Outline

- A few words on MD applications and the GROMACS package
- The main work in an MD simulation
- Parallelization
- Stream computing

Supercomputers

Beskow (PDC)
Cray XC40
53623 Intel Haswell cores
1.4 - 2 PetaFLOPS

Piz Daint (CSCS Switzerland)
Cray XC50 computer
nodes with a 12-core Haswell
(0.5 TeraFLOPS) + 1 NVIDIA
P100 GPU (5 TeraFlops)

Challenges for exascale computing

Issues:

- Power usage (K computer: 10 MW, cooling doubles this)
- Reliability, chance of components failing increases
- Interconnect speed needs to keep up with millions of cores
- Data handling
- Software does not scale!

Question:

- Do we really need an exaflop computer?
- Does that get us better science?

Two general computing trends

Over the past decades:

- Moore's law transistor count doubles every two years
- Processor speed doubles every 18 months
- Memory speed does not increase this fast
- Result: memory access relatively expensive!

Second important development:

- Past two decades: slow increase of parallel computing
- This decade: no MHz increase, instead core count increase
- Arrival of GPGPUs: even mores cores!
- Result: parallel algorithms very important

MD versus “typical” HPC applications

Other “typical” HPC applications, e.g. turbulence:

- Weak scaling: scale problem size with computer size
- Calculation times stay the same

Molecular dynamics:

- Little increase in problem size
- Time per step decrease (sub millisecond)
- Need lots of computing power, but use of supercomputers is challenging
- Algorithms need to be re-designed

How to write efficient code for MD?

Hardware and software:

- Multi-core CPUs: C (SIMD intrinsics?) or Fortran + MPI + OpenMP
- GPUs: CUDA or OpenCL
- Intel Xeon 5 (Larabee, MIC, ...): C or something else?
- FPGAs ?
- OpenACC for everything: much less work

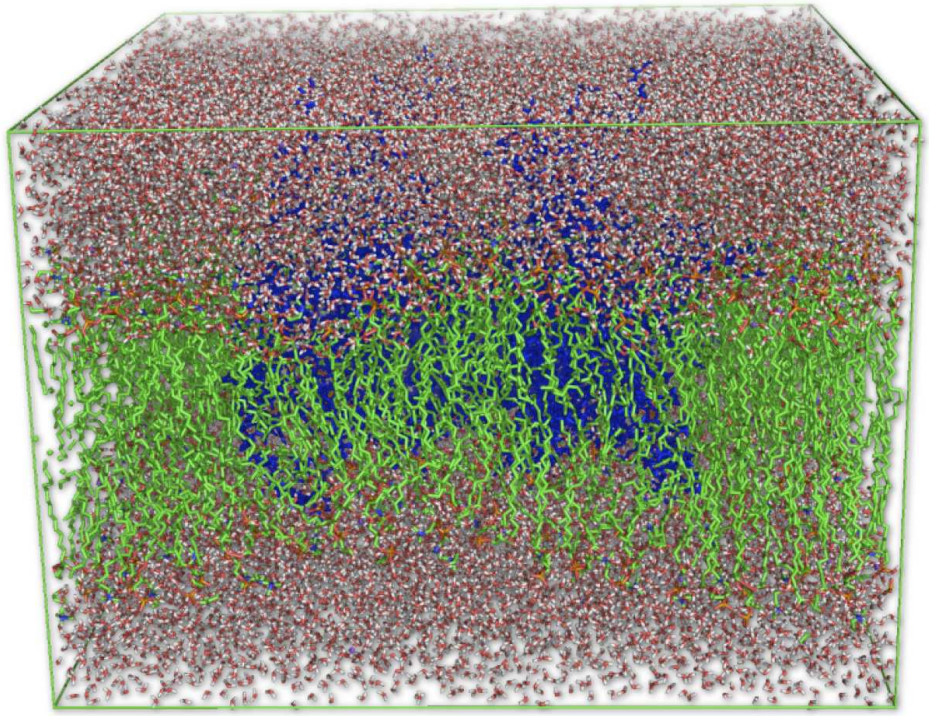
Molecular dynamics need sub-millisecond iterations times:
we need low-level optimization: C + SIMD intrinsics + CUDA

A lot of work, but it might be worth it

Classical molecular simulation

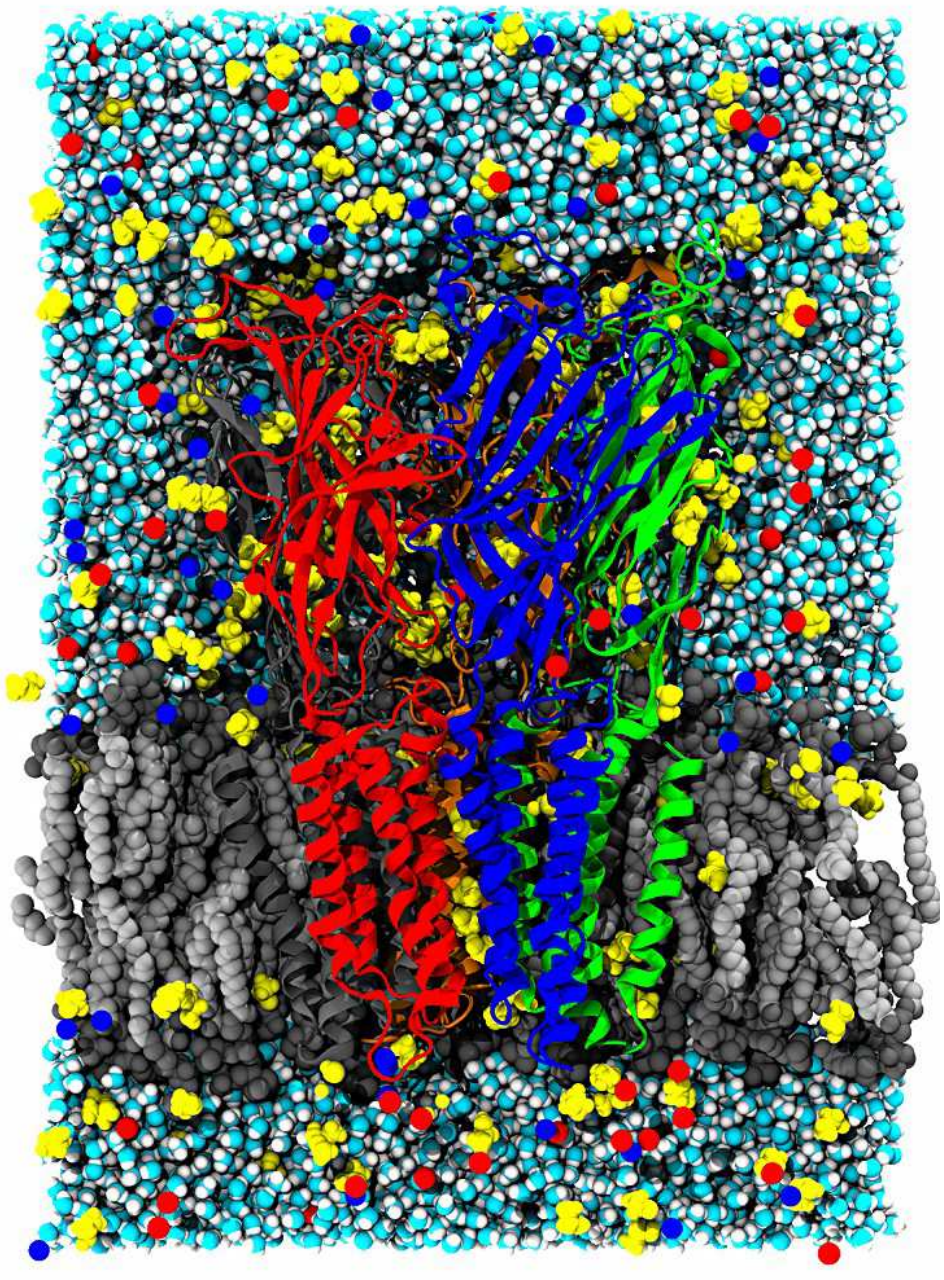
Common applications:

"simple" liquids	10^3 - 10^4 atoms	ns - μs
peptide/protein folding	10^4 - 10^5 atoms	μs - s
protein functional motions	10^5 - 10^6 atoms	μs - s
polymers	10^4 - 10^6 atoms	μs - ?
materials science	10^4 - 10^8 atoms	ns - ?



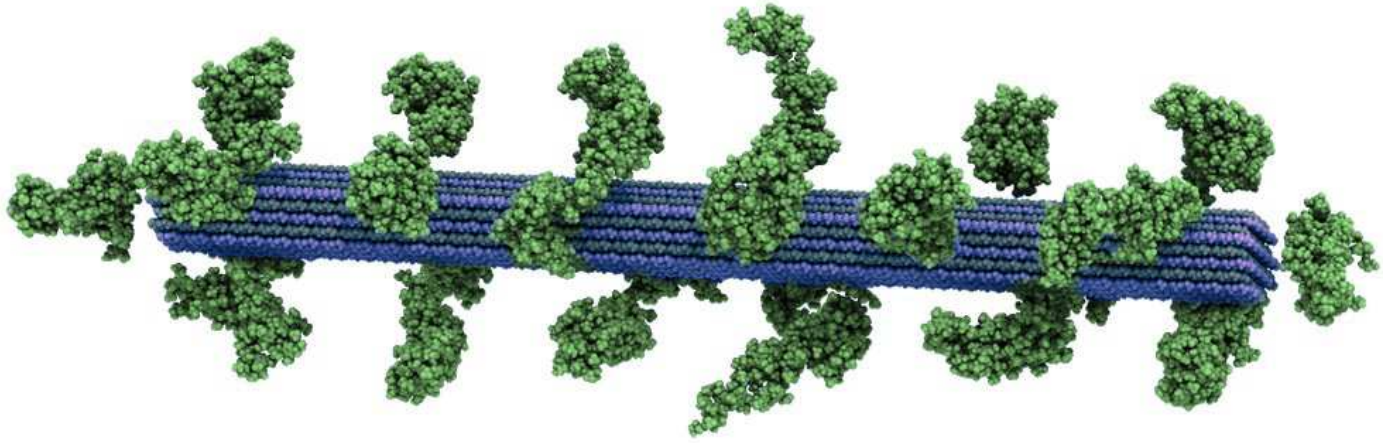
Simulations of bio-molecules

- Proteins, DNA, RNA
- Fixed system sizes
- Functional motions
- Overdamped dynamics
- Stochastic kinetics
- Need to sample many events
- The time scales often increase exponentially with system size

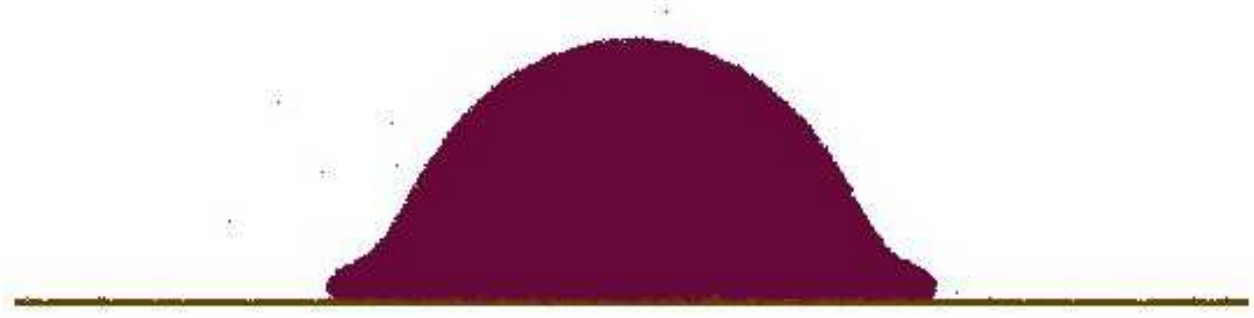


Simulations in (Chemical) Physics

Simulations of biomass for bio-ethanol
(millions of atoms)



Understanding and controlling interactions of droplets on surfaces
(100 million particles)



Molecular Dynamics

Basically solving Newton's equation of motion:

$$m_i \frac{d^2 \mathbf{x}_i}{d\,t^2} = -\nabla_i V(\mathbf{x}) = \mathbf{F}_i(\mathbf{x}) \qquad i = 1, \ldots, N_{\text{atoms}}$$

Symplectic leap-frog integrator:

$$\mathbf{v}_i(n + \frac{1}{2}) = \mathbf{v}_i(n - \frac{1}{2}) + \frac{\Delta t}{m_i} \mathbf{F}_i(\mathbf{x}(n))$$

$$\mathbf{x}_i(n + 1) = \mathbf{x}_i(n) + \Delta t\, \mathbf{v}_i(n + \frac{1}{2})$$

$$V(\mathbf{x}) = \sum_{\text{bondeds}} V_{\text{b}}(\mathbf{x}) + \sum_{i<j} A_{ij} \mathbf{r}_{ij}^{-12} - B_{ij} \mathbf{r}_{ij}^{-6} + \frac{q_i q_j}{r_{ij}}$$

Computational cost:

integration:	$c\,N$
force calculation:	$C\,N^2$

Molecular Dynamics in practice

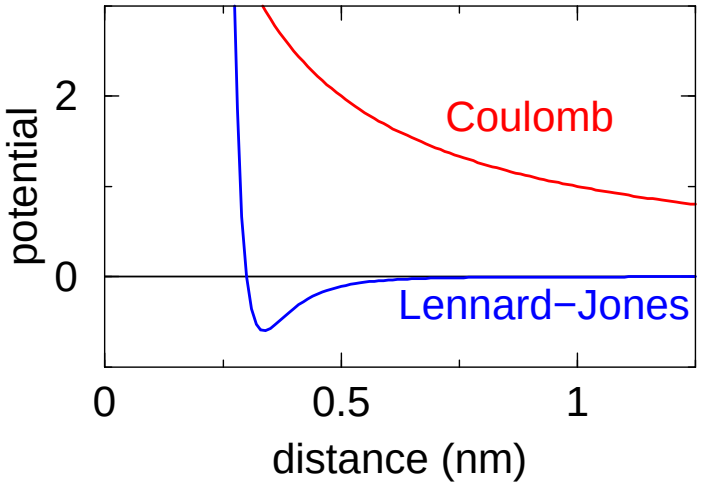
Setting up simulations requires a lot of physical/chemical/biological knowledge

The force field (parameters) is critical:
the results are as good/bad as the force field

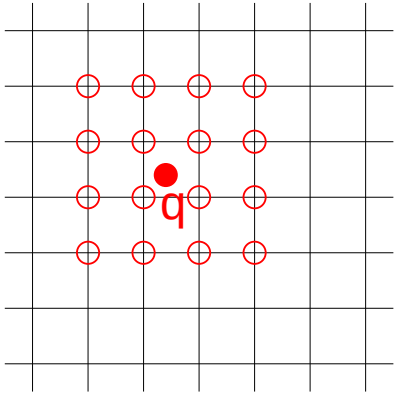
Developing algorithms for simulations is a completely different business, but you need to know the application needs

Computational cost: force calculation

All forces are short ranged,
except for the Coulomb forces



Thus use a (smooth) cut-off for the particle-particle interactions
and do the remaining part of the Coulomb interaction on a grid



Particle Mesh Ewald electrostatics:

Solve the Poisson equation
in reciprocal space using a 3D FFT

Computational breakdown

computation	cost	communication	
bonded forces	$c\,O(N)$	along with nbf	
non-bonded forces	$c\,M \times N$	local	M = 10^2 - 10^3
spread charge	$C\,N$	local	
3D FFT	$c\,N \log N$	global	
gather forces	$C\,N$	local	
integration	$c\,N$		
constraints	$c\,N$	local	Δt: $\times$ 4
virtual sites	$c\,N$	local	Δt: $\times$ 2

Time step: 2 - 5 fs, simulation length 10^7 to 10^9 steps.

A step takes 1 - 100 milliseconds.

CPU vs GPU

How many pair interactions per second?

Intel Core i7, 2.67 GHz
4 cores + Hyperthreading

NVidia GTX580, 1.5 GHz
512 CUDA Cores

CPU vs GPU

How many pair interactions per second?

Intel Core i7, 2.67 GHz
4 cores + Hyperthreading

192 million per core
960 million total

NVidia GTX580, 1.5 GHz
512 CUDA Cores

3200 million total

Speeding up simulations

For many applications we would like orders of magnitude more sampling

Speed up simulations through:

- Increasing the time step (constraints, virtual interaction sites)
- Use less particles (triclinic, more spherical periodic cells)
- Use more processors: parallelize
- Use stream computing

Parallelization nowadays is MPI + threads

Scaling limits

Strong scaling limited by:

all communication latencies/bandwith and load imbalance

Weak scaling limited by:

electrostatics global communication

Electrostatics solvers:

- PME/PPPM: $O(N \log N)$, small pre-factor
- Multi level methods: $O(N)$, large pre-factor
- Fast multipole: $O(N)$, discontinuous gradient

Note:
(nearly) embarrassing parallelizm, run 1 - 1000 simulations in parallel

GROMACS simulation package

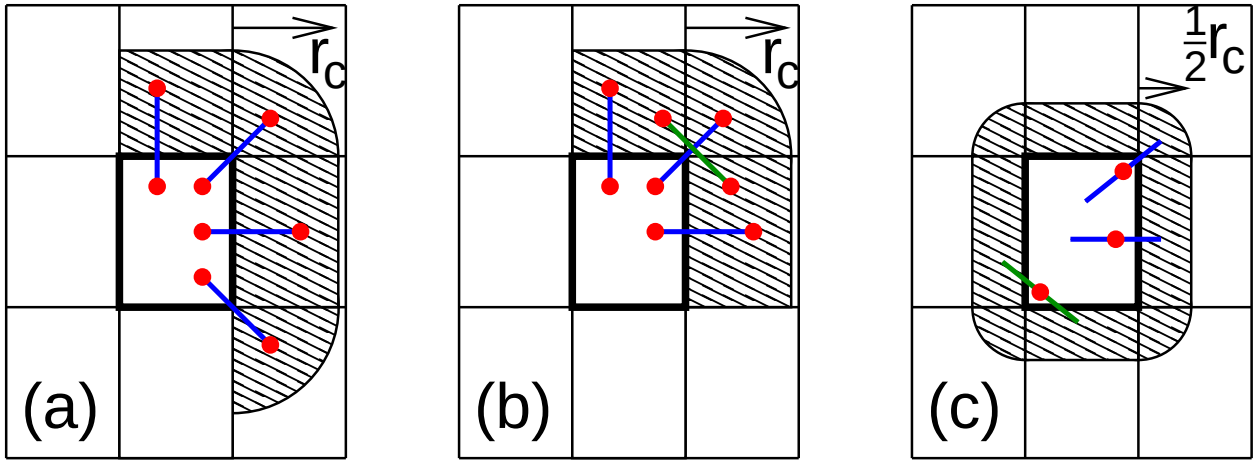
Started at the University of Groningen in the early 1990s.
Now all main developers are in Sweden (Stockholm/Uppsala)

Thousands of users world wide
A million users through Folding@home

- Open source (GPL), `www.gromacs.org`
- Support for all major biomolecular force fields
- Highly optimized algorithms and code
- Advanced algorithms for increasing the time step
- Language: C and essential parts in assembly: SSE2/Altivec/CUDA/...
- Efficient single processor performance
- Since three years efficient parallelization

Hess, Kutzner, Van der Spoel, Lindahl; J. Chem. Theory Comput. 4, 435 (2008)

Domain decomposition methods



comm.	cut-off	Half Shell	Eighth Shell	Midpoint
#cells	$r_c < L_d$	13	7	26
	$r_c < 2L_d$	62	26	26
volume	$r_c = \frac{1}{2}L_d$	2.94 L_d^3	2.15 L_d^3	
	$r_c = L_d$	9.81 L_d^3	5.88 L_d^3	
	$r_c \to \infty$	$\frac{1}{2}$ sphere	$\frac{1}{8}$ sphere	

Eighth shell: Liem, Brown Clarke; Comput. Phys. Commun. 67(2), 261 (1991)

Midpoint: Bowers, Dror, Shaw; JCP 124, 184109 (2006)

Full, dynamic load balancing

Load imbalance can occur due to three reasons:

- imhomogeneous particle distribution
- inhomogeneous interaction cost distribution (charged/uncharged, water/non-water due to GROMACS water innerloops)
- statistical fluctuation (only with small particle numbers)

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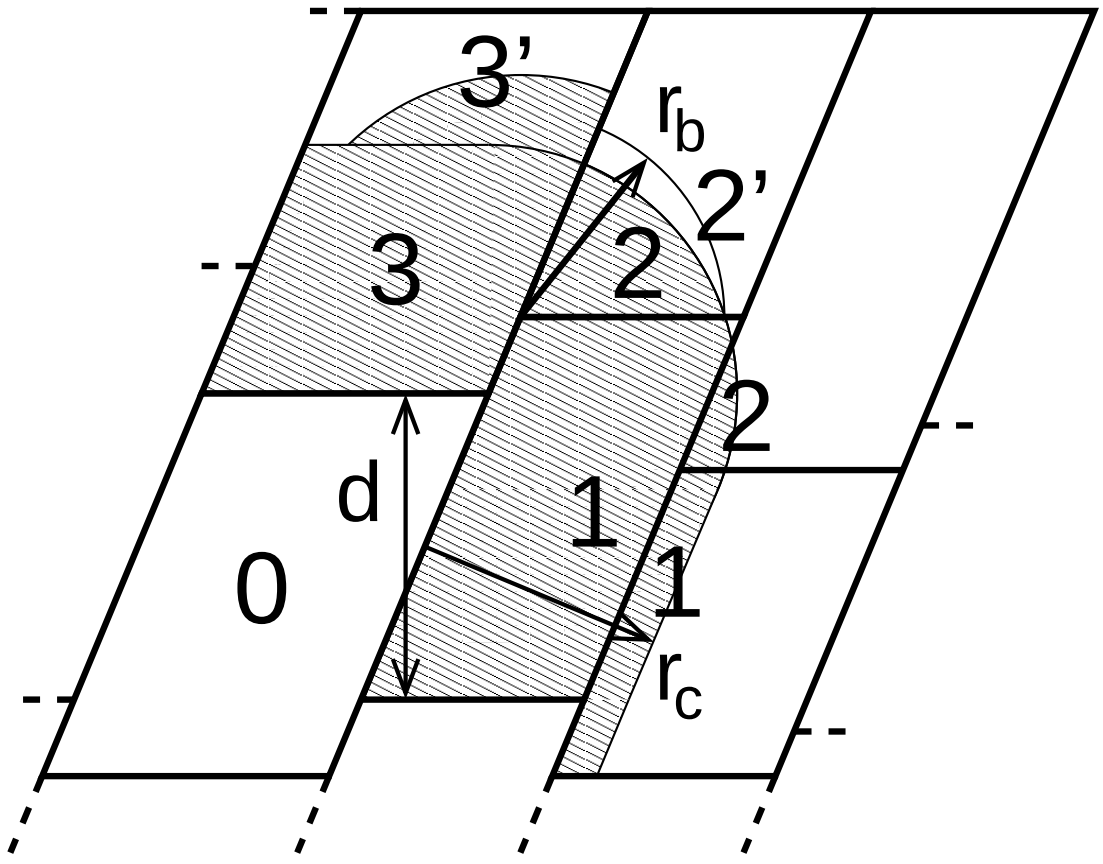
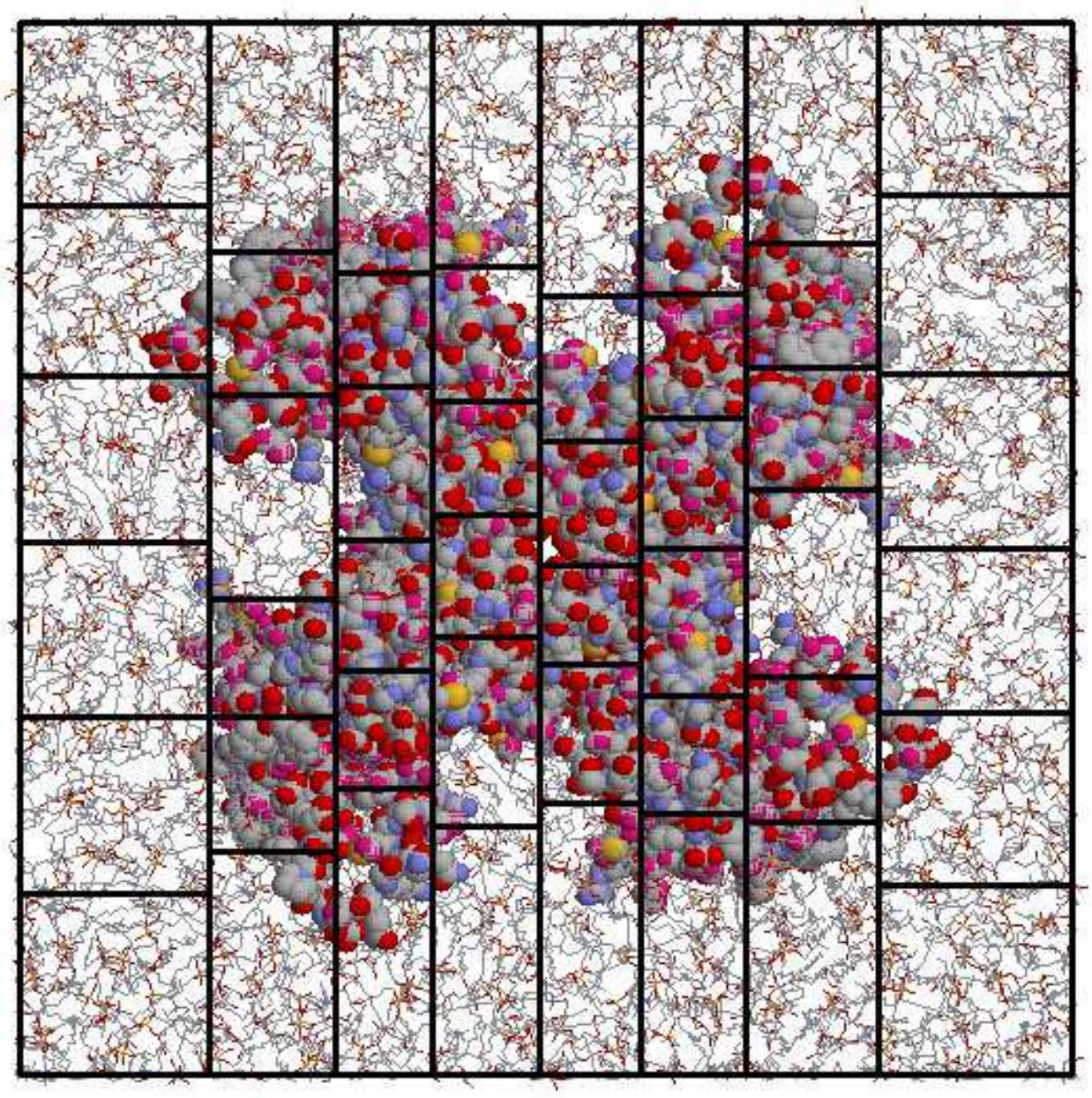
So we need a dynamic load balancing algorithm
where the volume of each domain decomposition cell
can be adjusted **independently**

Triclinic unit cells with load balancing



Dynamic load balancing in action

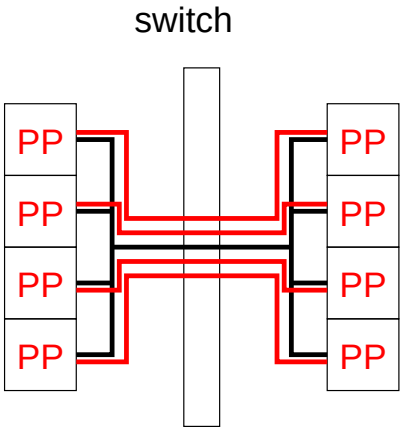


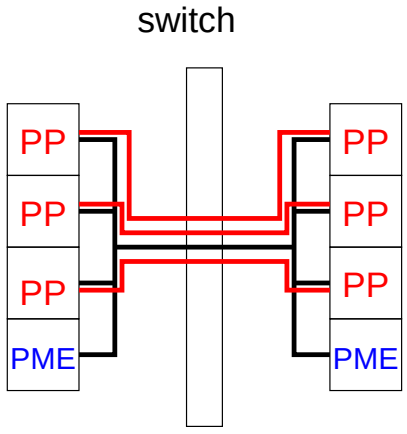
Multiple-program, multiple data PME

SP−MD

MP−MD

PP

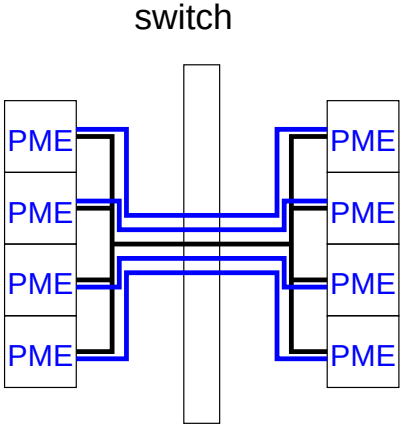


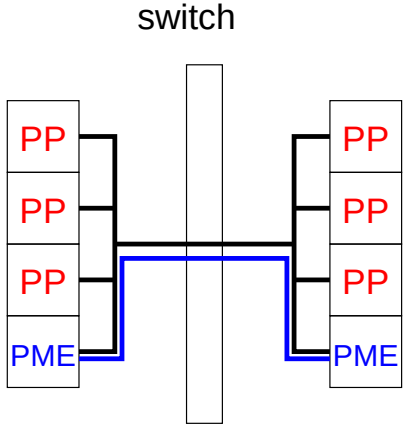


latency 4/3 lower

bandwith 4/3 higher

PME



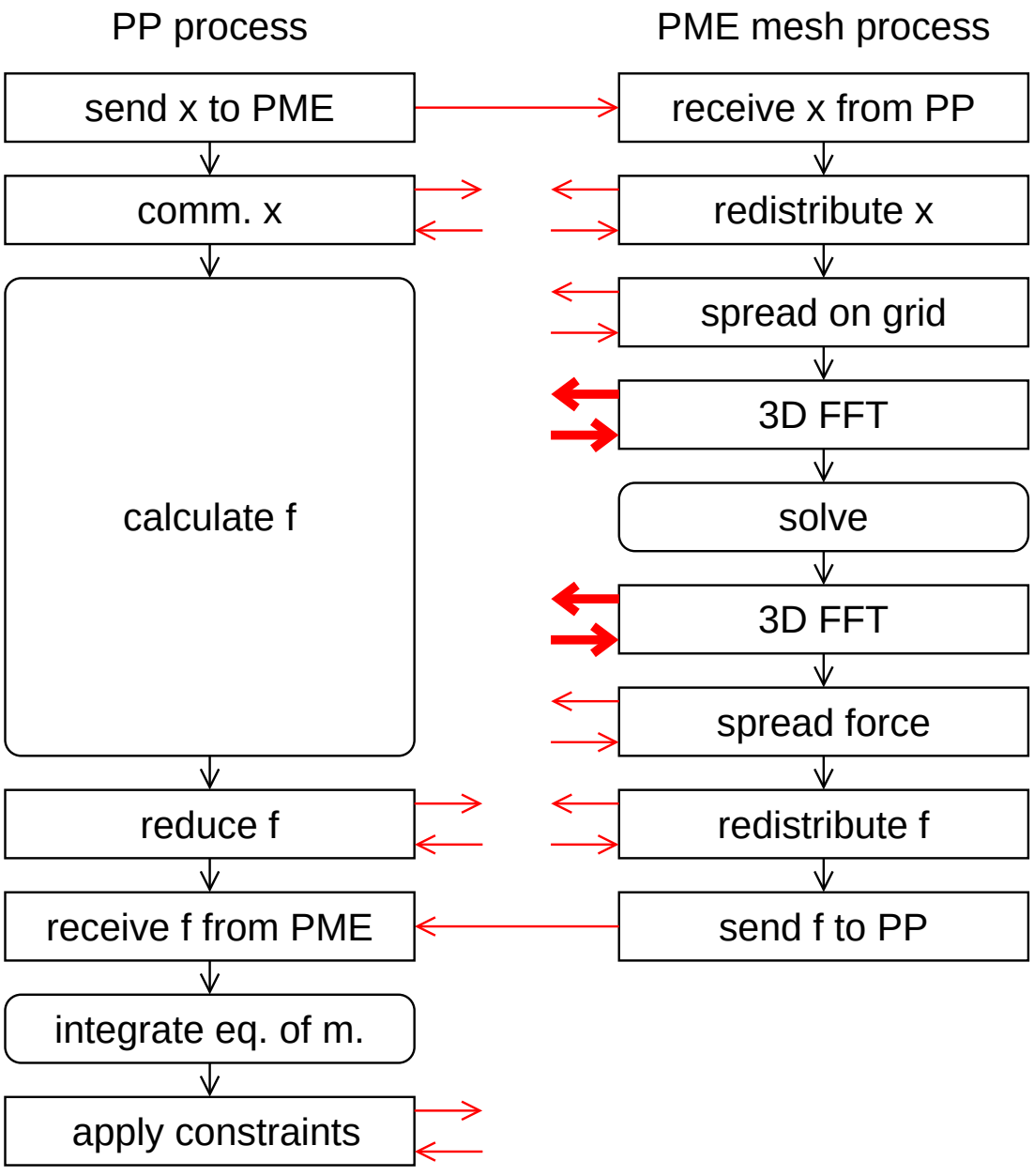


latency 4 x lower

Futher advantage: 4 to 16 times less MPI messages

Enables 4x further scaling!

Flow chart, CPU only

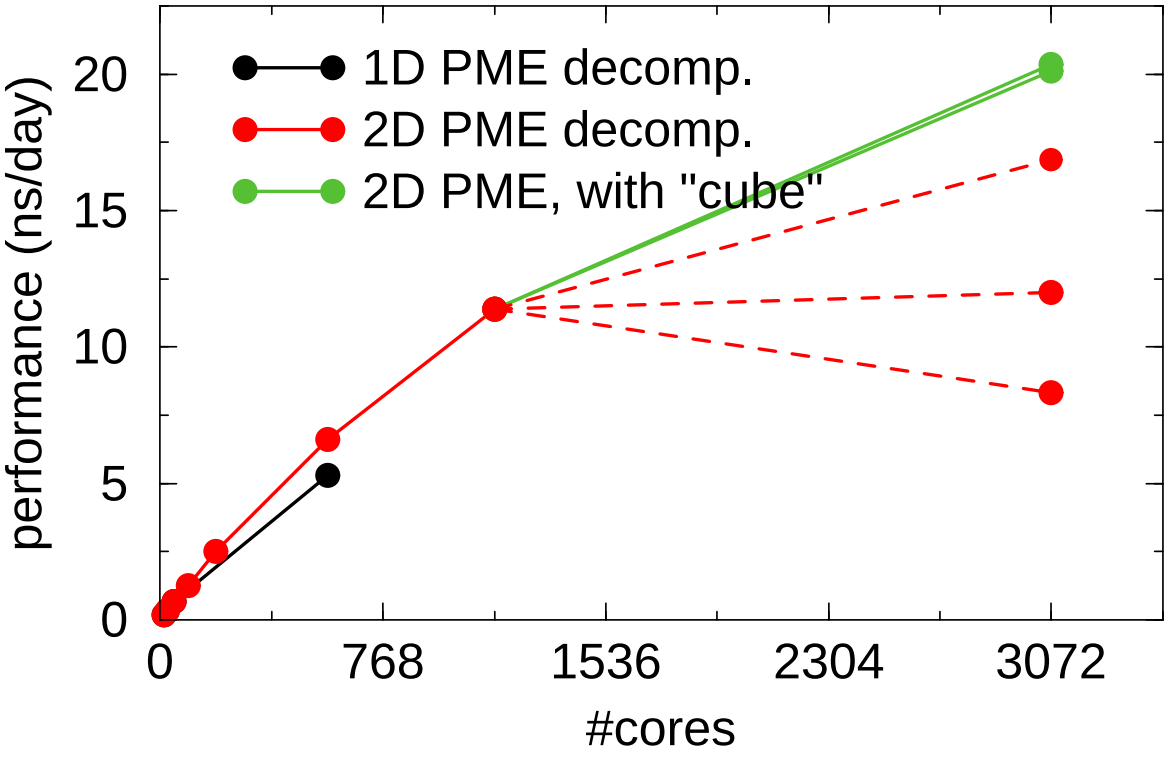


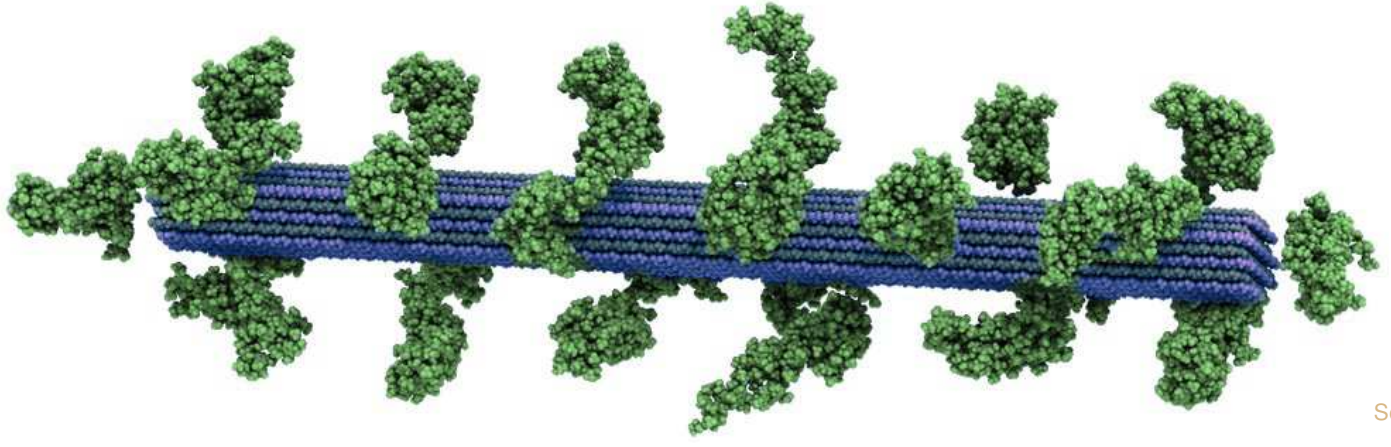
2D PME (pencil) decomposition

cellulose +
lignocellulose +
water

2.2 million atoms

Cray XT5

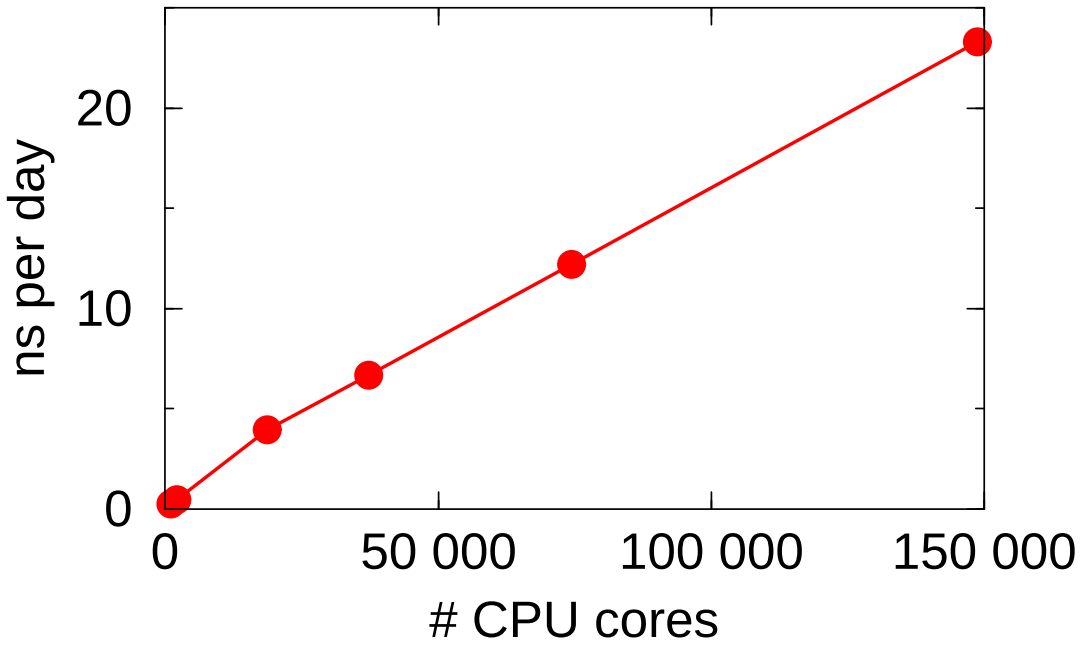




How far can we scale?

100 million atoms
half protein half water
no PME (!)

Jaguar Cray XT5
at Oak Ridge



Issues:

- a μs is far too short for a 100 million atom system
- no full electrostatics

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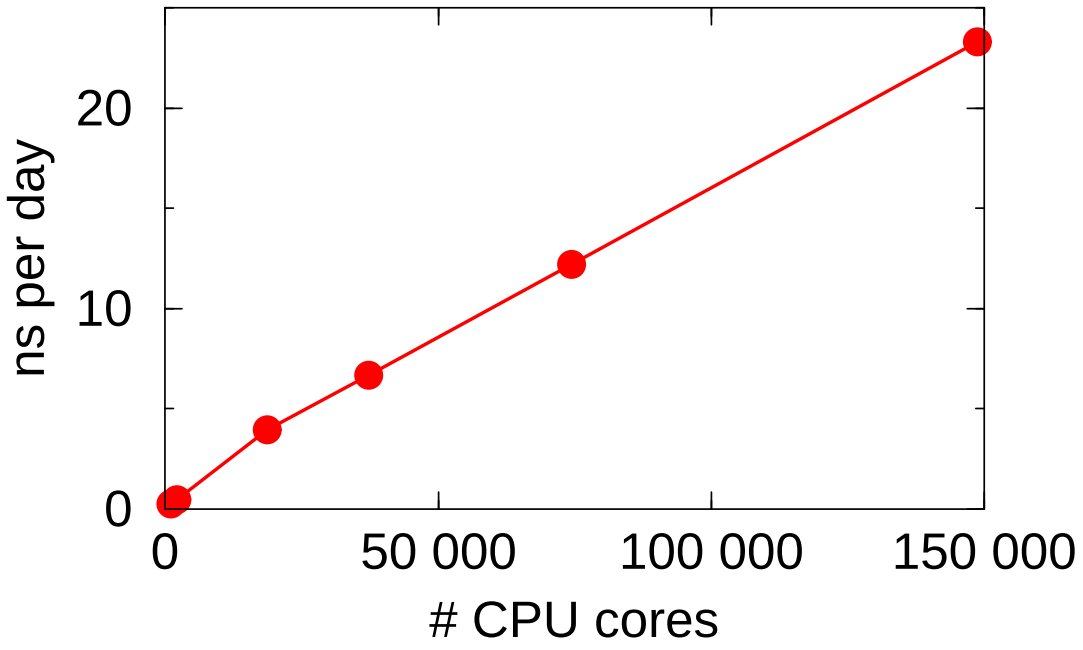

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Solutions:

- combine thread and MPI parallelization (a lot of work)
- develop electrostatics methods with less communication

Stream calculations

Single CPU-code: focus on functions

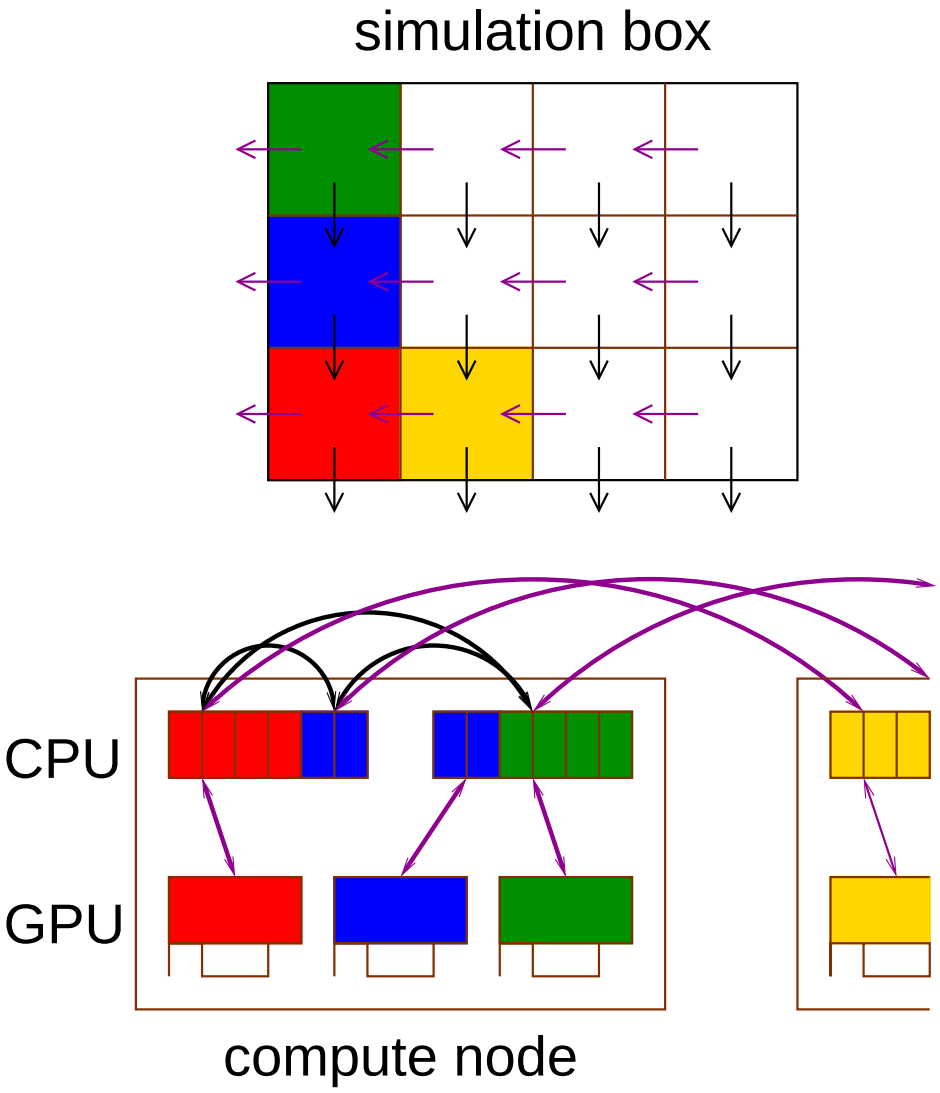
Stream calculations: focus on data streams, operations done in parallel

Common stream type archtectures:

- SSE: operations on 4 floats at once (or 2 doubles)
- AVX: operations on 8 floats at once (Intel Sandy Bridge, AMD Bulldozer)
- CUDA (NVidia GPUs): operations of 32 floats/doubles at once

So 4 to 32 times speedup, assuming the same #cores and frequency

Hybrid acceleration



GPU only does non-bonded

Re-use most of the CPU code

Use the GPU for what it's good at

Cut-off schemes in Gromacs

Gromacs $\leq$ 4.5 "group" cut-off scheme, based on (ancient) charge-groups

Gromacs 4.6 "Verlet" buffered cut-off scheme optional

Gromacs 5.0 "Verlet" cut-off scheme default

Group cut-off scheme:

- Fast, since we process groups of atoms at once; water is a group $\Rightarrow$ very fast
- No Verlet list buffer by default, but optional: energy drift

Verlet cut-off scheme:

- Fast on wide SIMD and GPUs
- Verlet list buffer by default
- Supports OpenMP parallelization (+MPI)

Later today

- What is stream computing (SIMD, GPUs, CUDA)
- How to use it efficiently in MD