MSU Nanotechnology Education and Research Center
International School “Computer simulation of advanced materials”, 16–21 July 2012

ATOMISTIC SIMULATIONS ON SUPERCOMPUTERS USING OPEN SOURCE CODES

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Joint Institute for High Temperatures
of Russian Academy of Sciences

July 19, 2012

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   - **Molecular Dynamics (MD)**
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   - **Interaction models**
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First papers on MD simulations

Phase Transition for a Hard Sphere System

B. J. Alder and T. E. Wainwright
University of California Radiation Laboratory, Livermore, California
(Received August 12, 1957)

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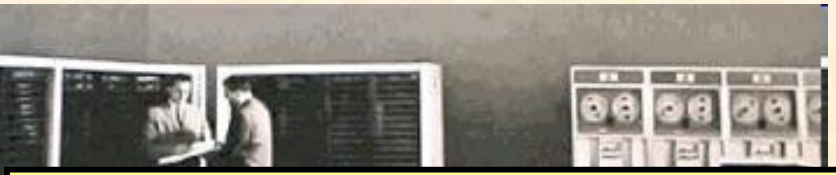
The record numbers of particles taken for MD simulations in different years



1964	1.000	Rahman
1984	200.000	Abraham
1990	1.000.000	Swope, Anderson
1994	100.000.000	Beazley, Lomdahl
1997	1.213.857.792	Stadler
1997	1.399.440.000	Müller
1999	5.180.116.000	Roth
2000	8.500.000.000	Vashishta
2003	19.000.416.964	Kadau, Germann, Lomdahl
2005	160.000.000.000	Kadau, Germann, Lomdahl
2006	320.000.000.000	Kadau, Germann, Lomdahl
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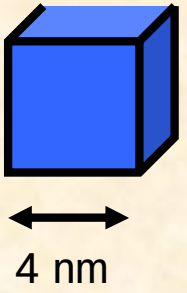
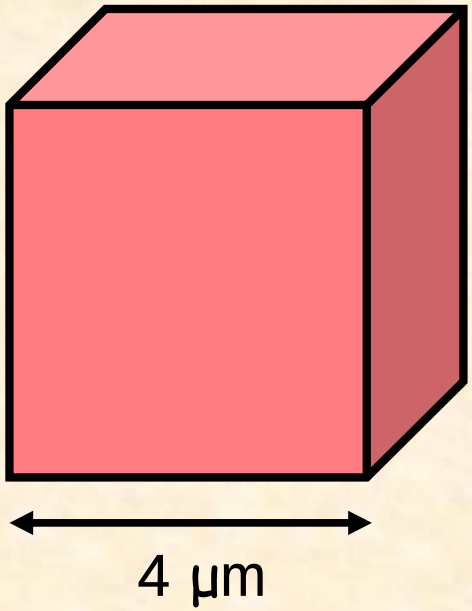
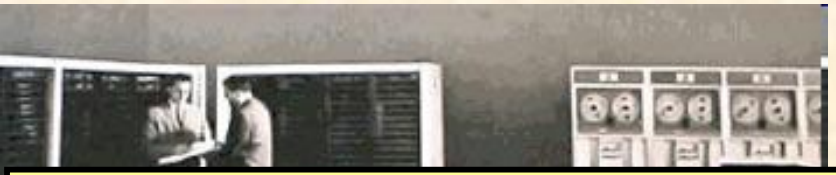




Years, Flop/s and the numbers of cores

Mflops	1964 г.	CDC 6600	10 MHz	1 CPUs
Gflops	1985 г.	Cray 2	125 MHz	8 CPUs
Tflops	1997 г.	ASCI Red	200 MHz	9152 CPUs
Pflops	2008 г.	Roadrunner	3,2 GHz	122400 Cores
Eflops	≈ 2018 г.			10^8 – 10^9

The record numbers of particles taken for MD simulations in different years



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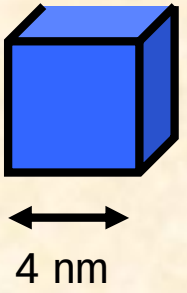
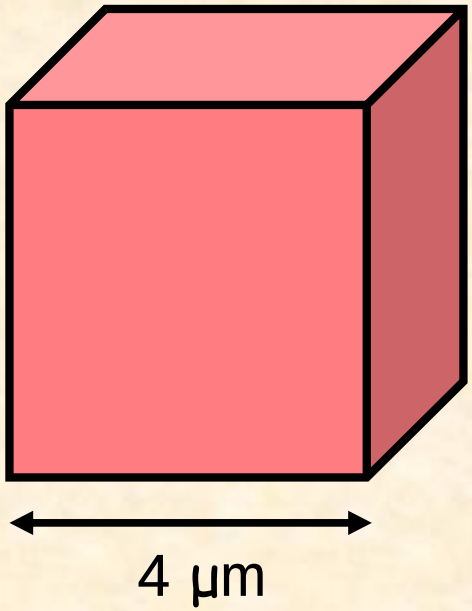
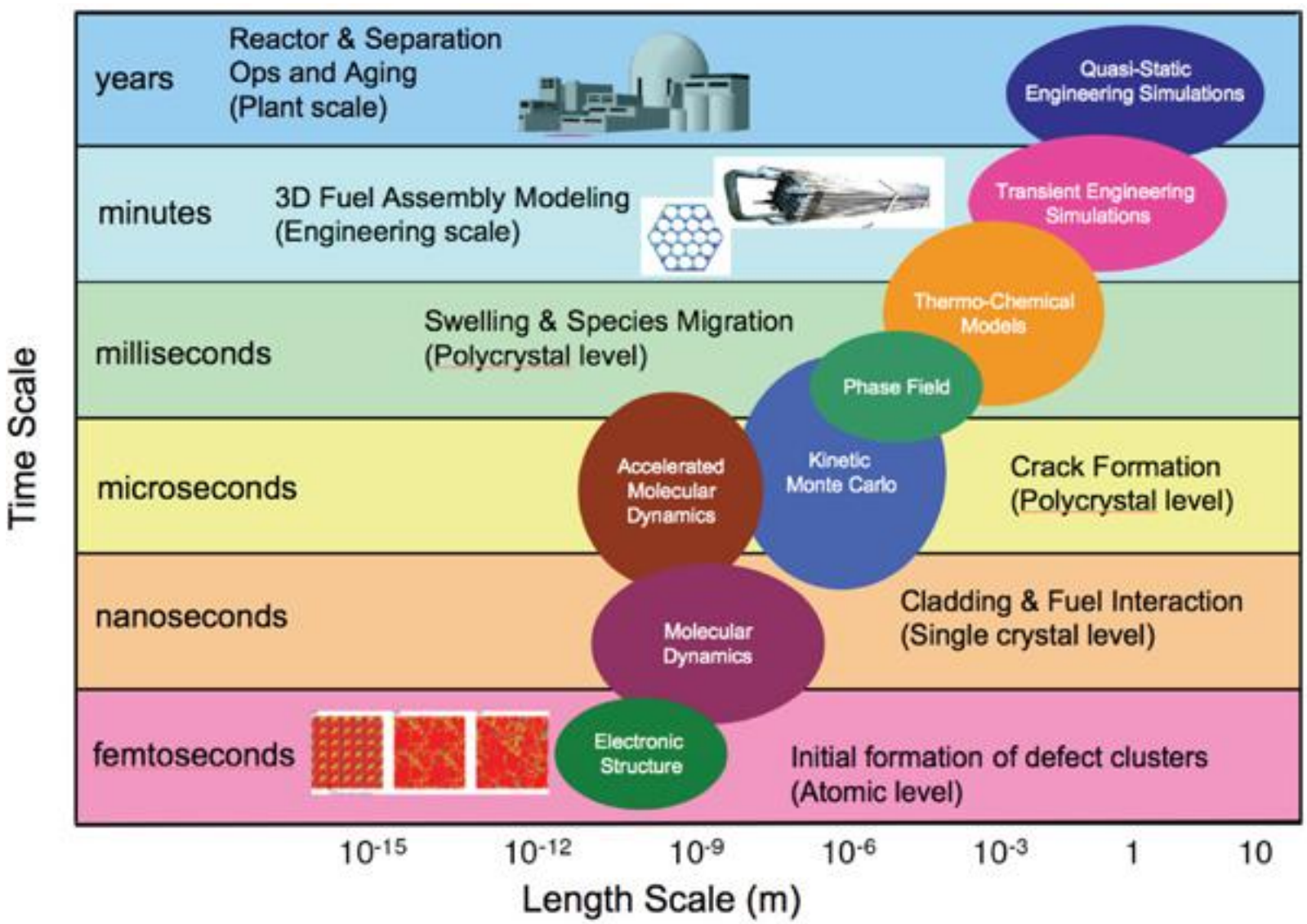




Multiscale approach in material sciences



Original at Berkeley Lab We site: **http://www.lbl.gov/CS/html/exascale4energy/nuclear.html**

Choice of the simulation code

Open source

- Free of charge ☺
- Allows modifications
- Implements cutting edge technologies
- Tested by many users over the internet
- Supported by a community of developers

Proprietary

- Reliable
- Easier to install and configure
- Professional support
- Usually has better support for different platforms

Creating new code on the basis of an open source project

Key features of atomistic simulation codes

- ***Basic simulation algorithms***
  MD, MC, energy minimization, thermostats, boundary conditions, neighbor lists, optimized electrostatics
- ***Particle interaction models***
  Force fields for pair and many-body potentials, customization
- ***Trajectory analysis tools***
  Binary trajectory output, plausible modules for calculation of thermodynamics, correlation functions, etc. including averaging
- ***Parameter input and variation***
  Parameter input languages, batch runs, workflows
- ***Parallel execution***
  Parallel efficiency on modern supercomputing clusters
- ***Optimization for a special hardware, GPU***
- ***Visualization***

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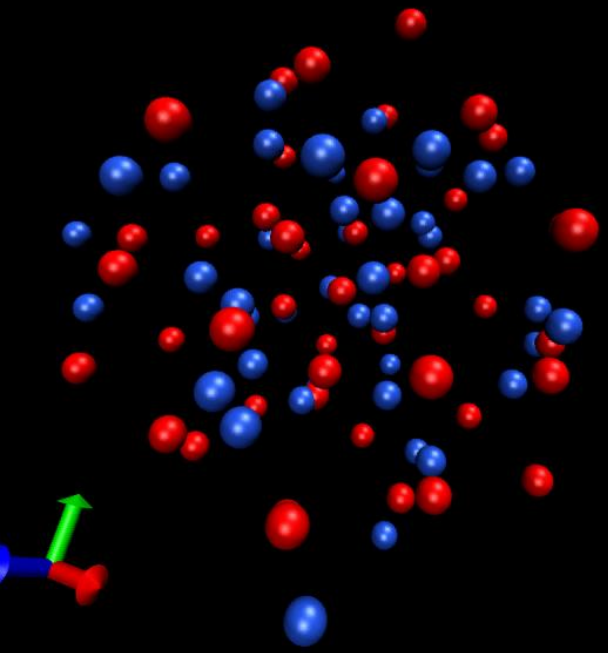
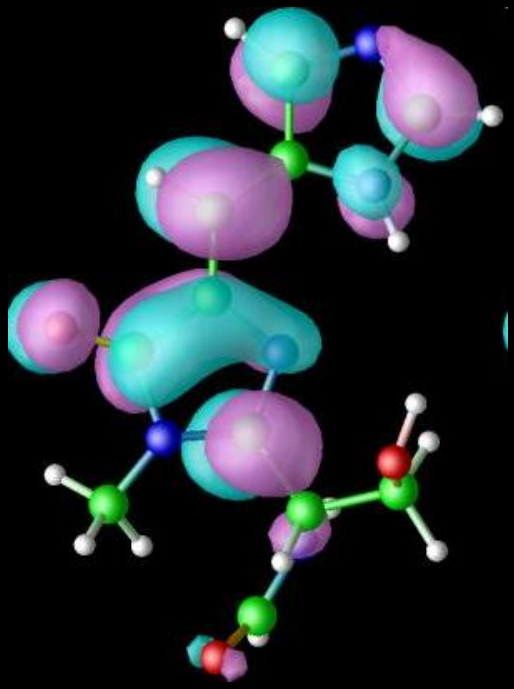
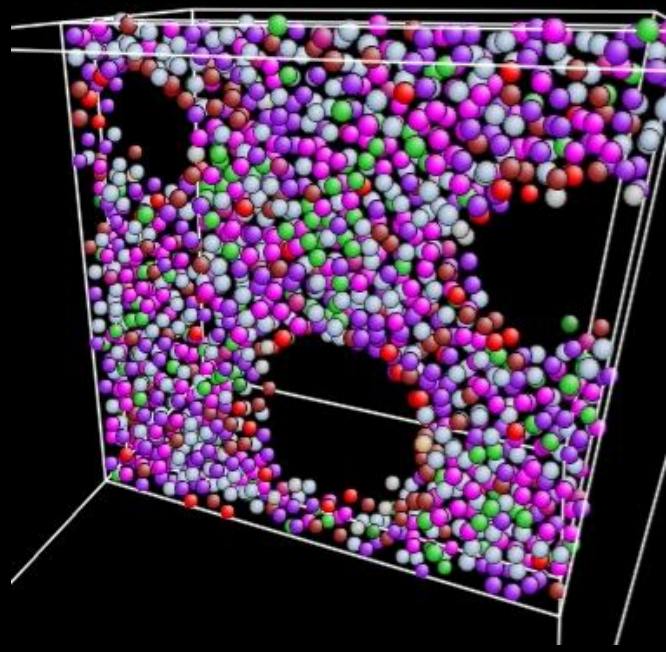
Open source packages for atomistic simulations

Package name	Language	GPU	Parallel	Min	MD	MC	Comment
Adun	C			+	+		User specified force field (FFML), QM/MM calculations with Empirical Valence Bond (EVB)
DL_POLY*	Fortran, C++, Java				+		General purpose MD, HDF5 output, Java GUI
GROMACS	C	+	MPI		+		High performance MD, designed for biological systems and polymers
HALMD	C++	++			+		High-precision MD for the large-scale simulation of simple and complex liquids, HDF5 output
HOOMD-blue	C++, Python	++		+	+		General-purpose MD highly optimized for GPUs
LAMMPS	C++	+	MPI	+	+	+	High parallel scalability, wide range of potentials and analysis tools
MDynaMix	Fortran		MPI		+		Parallel MD for AMBER force field
MOIL	Fortran, Tcl		MPI	+	+		Basic algorithms and force fields, Replica exchange, coarse-grained models, Tcl GUI
NAMD/VMD	C++	+	MPI				High parallel scalability, designed for biomolecular, visualization (VMD)
RedMD	C/C++	-		+	+	+	Coarse-grained models of proteins and nucleic acids
TINKER	Fortran		OpenMP	+	+	+	Simple MD, QM/MM, molecular design
XMD	C		pthreads	+	+	+	MD for metals and ceramics

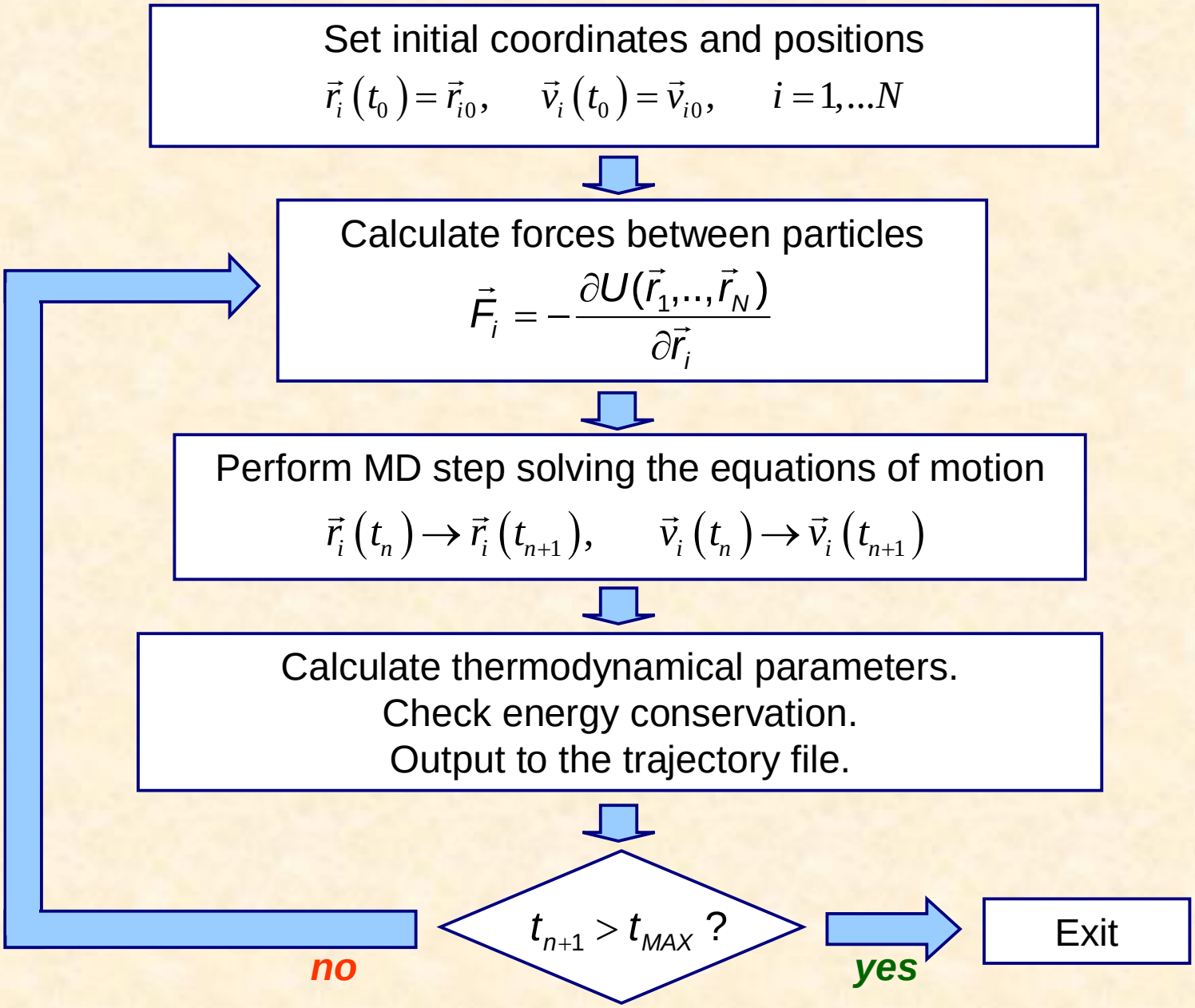
SIMULATION ALGORITHMS



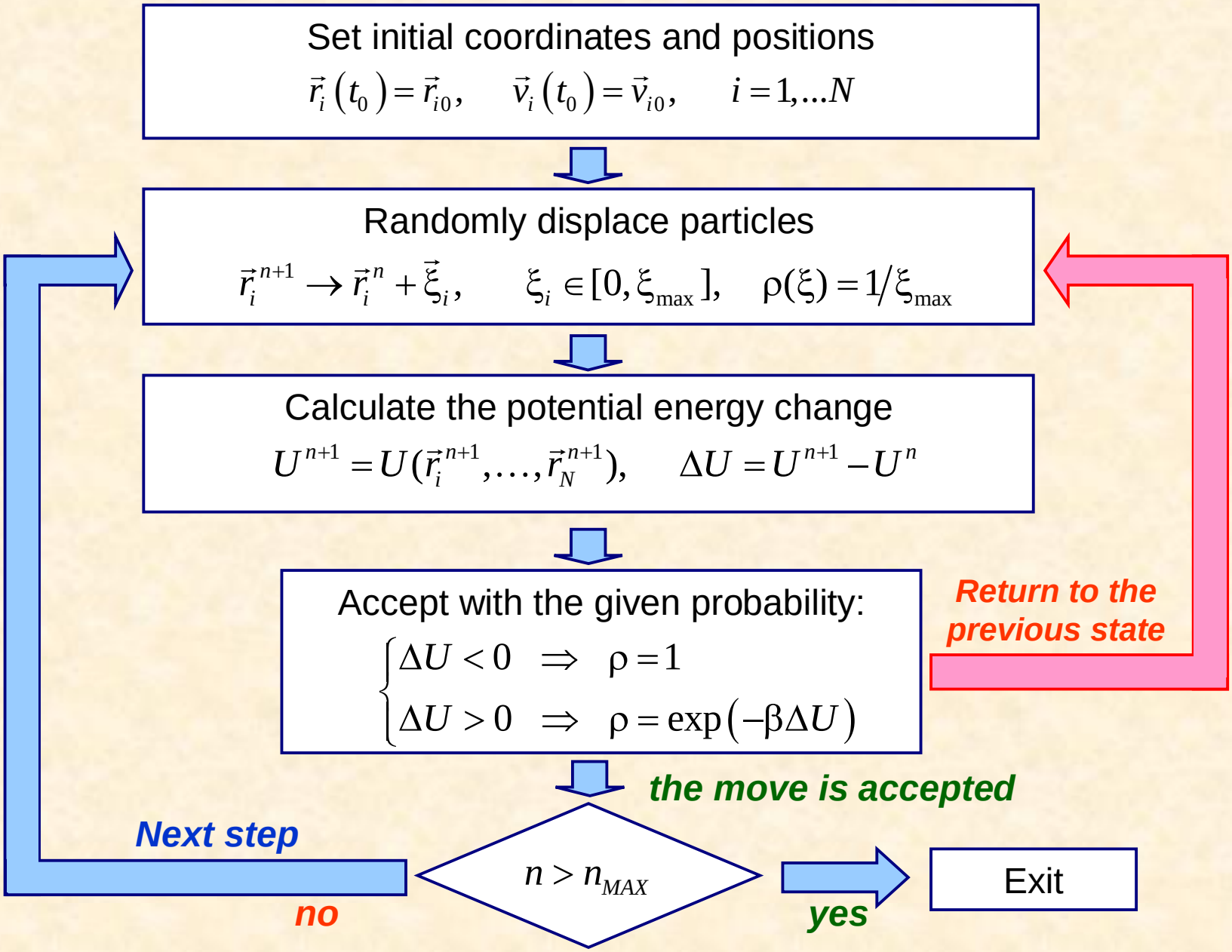




Molecular Dynamics: Trajectory Calculation

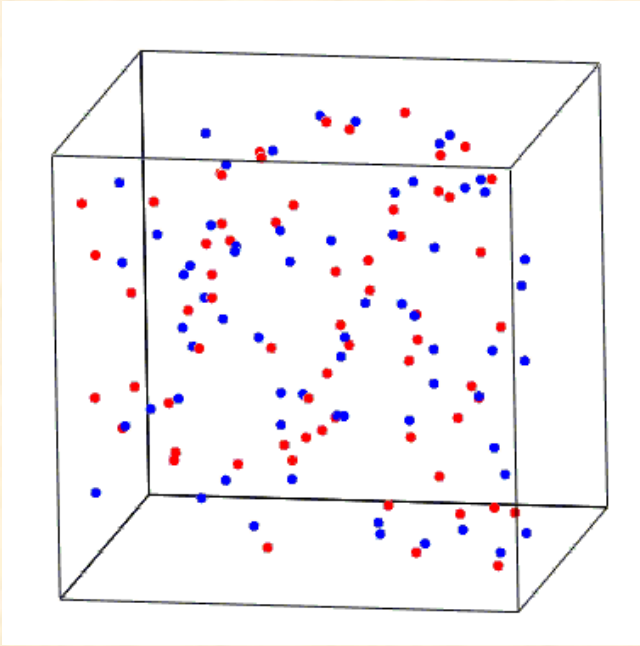


Monte-Carlo: Metropolis algorithm



Equations of motion in Classical MD

Consider a system of N particles with positions $\vec{R} = \{\vec{r}_1, ..., \vec{r}_N\}$ and velocities $\vec{V} = \{\vec{v}_1, ..., \vec{v}_N\}$.



The Newton's equations of motion:

$$\begin{cases} \vec{r}_k\,''(t) = \dfrac{1}{m_k}\vec{F}_k(t, \vec{r}_1, ..., \vec{r}_N), \qquad k = \overline{1, N}, \\ \vec{R}(0) = \vec{R}_0, \qquad \vec{V}(0) = \vec{V}_0. \end{cases}$$

Force acting of k-th particle: $\vec{F}_k(\vec{R}) = -\dfrac{\partial U(\vec{R})}{\partial \vec{r}_k}$

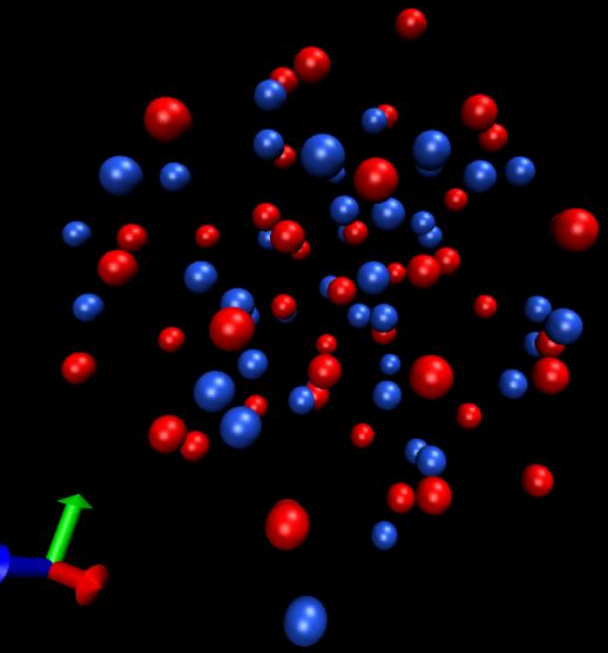
General form of the interaction potential:

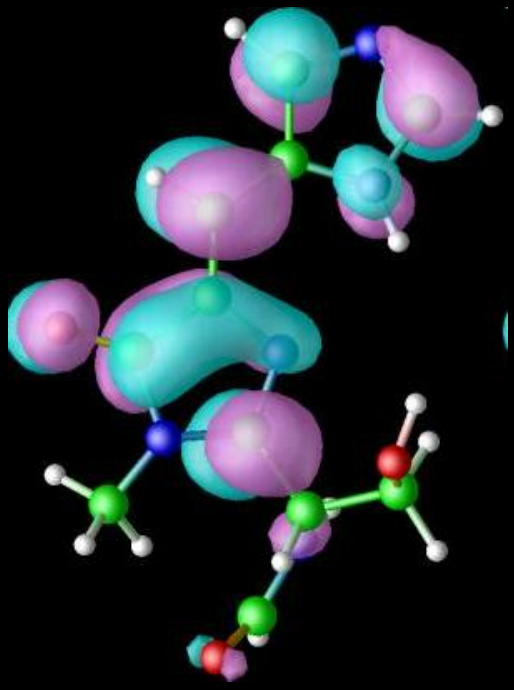
$$U(\vec{R}) = \sum_k U^{ext}(t, \vec{v}_k, \vec{r}_k) + \sum_{i<j} U(\vec{r}_i, \vec{r}_j) + \sum_{i<j<k} \Phi(\vec{r}_i, \vec{r}_j, \vec{r}_k) + ...$$

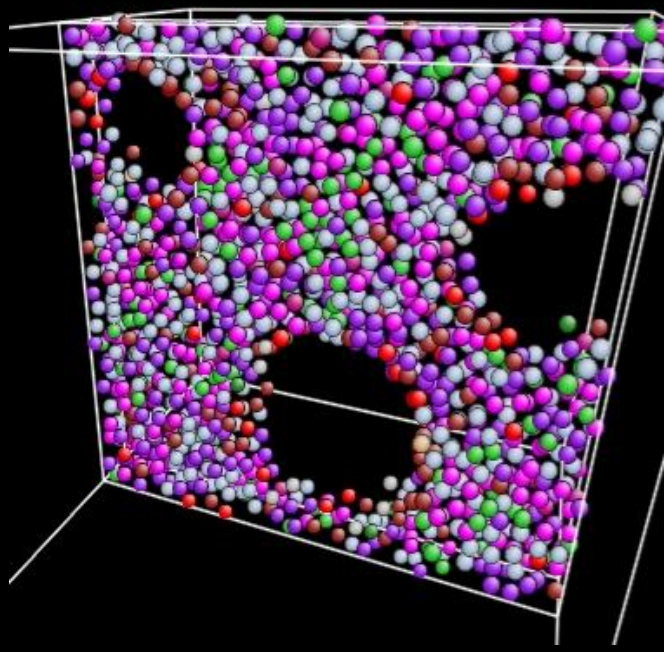
Particular case of the pairwise potential:

$$U(\vec{r}_i, \vec{r}_j) = U(|\vec{r}_i - \vec{r}_j|) = U(r_{ij}) \qquad \vec{F}_k^{\,pair} = -\sum_j \frac{\vec{r}_{kj}}{r_{kj}} \frac{\partial U(r_{kj})}{\partial r_{kj}} = \sum_j \frac{\vec{r}_{kj}}{r_{kj}} f(r_{kj})$$

INTERACTION MODELS







Interaction models and simulation techniques

- Particle-in-cell, hydrodynamic codes
- Coarse-grained, discontinuous molecular dynamics

Atomistic simulations

- Simple pairwise potentials for atoms or molecules with fixed atomic bonds
- Complicated many-body potentials for atoms (EAM, MEAM, ReaxFF, Tersoff, etc.)
- Classical MD for electrons and ions
- Wave Packet MD, Electron Force Field

- QM/MM hybrid models
- Quantum MD (Car-Parinello, DFT, TD-DFT)
- Numerical solution of the Schrödinger equation

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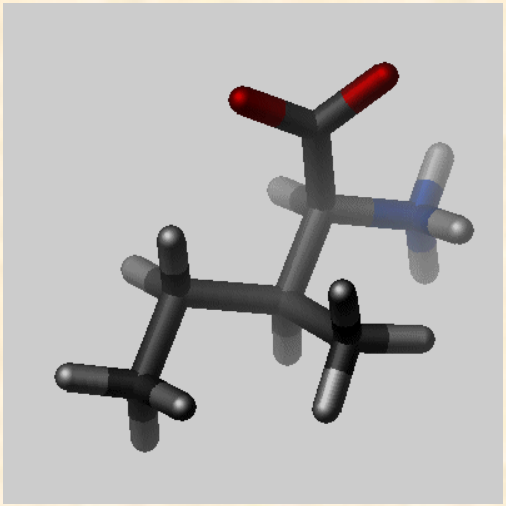
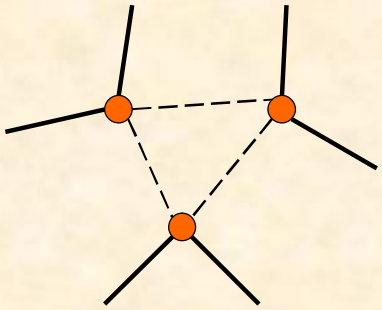
Atomistic simulations

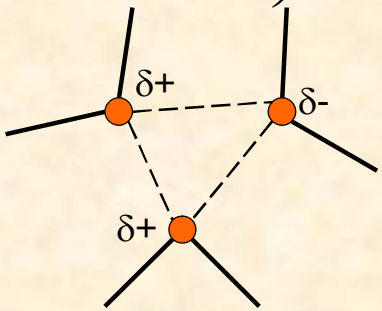
Force field for interaction of atoms in a molecule

$$U(\vec{r}_1,\ldots,\vec{r}_N) = \sum_{i=1}^{N}\sum_{j=i+1}^{N}\left(4\varepsilon_{ij}\left[\left(\frac{\sigma_{ij}}{r_{ij}}\right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}}\right)^{6}\right] + \frac{q_i q_j}{4\pi\varepsilon_0 r_{ij}}\right) +$$





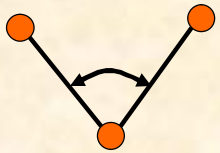
Non-bonded interactions
(van der Waals)



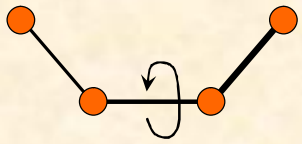
Non-bonded interactions
(electrostatic)

$$+ \sum_{bonds}\frac{k_i}{2}(l_i - l_{i,0})^2 + \sum_{angles}\frac{\tilde{k}_i}{2}(\theta_i - \theta_{i,0})^2 + \sum_{torsions}\frac{V_n}{2}(1+\cos(n\omega-\gamma))$$

Bond stretching



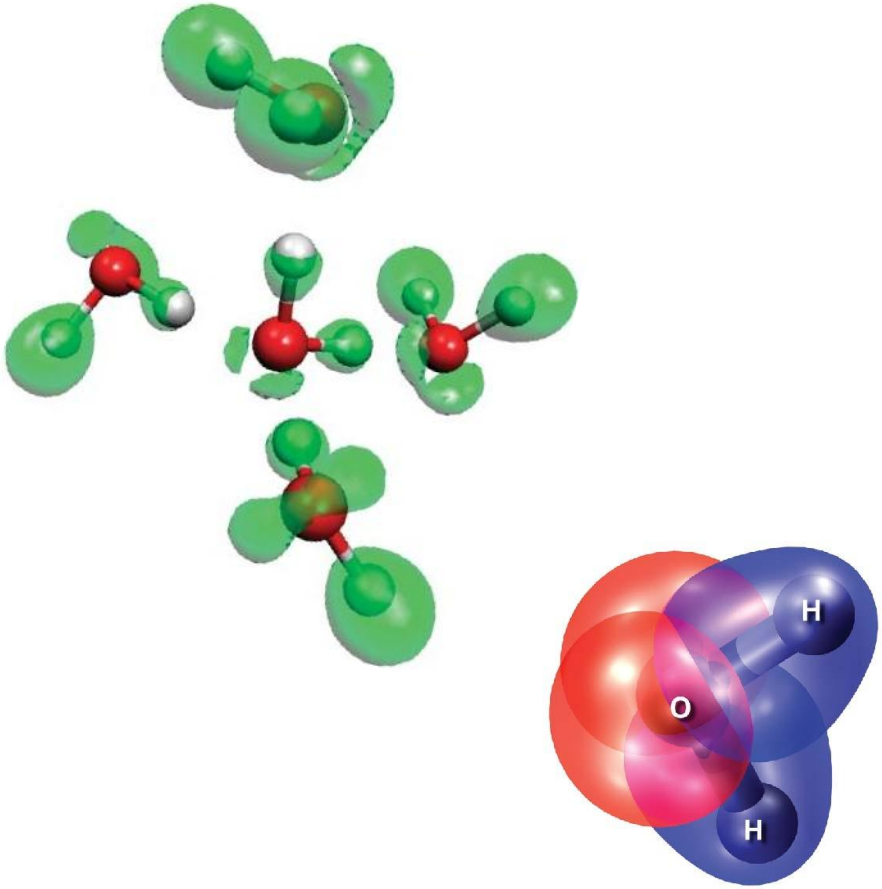
Angle bending



Bond rotation
(torsion)

Source: Pingwen Zhang, Molecular Dynamics Simulations (http://math.xtu.edu.cn/myphp/math/image/MD.ppt)

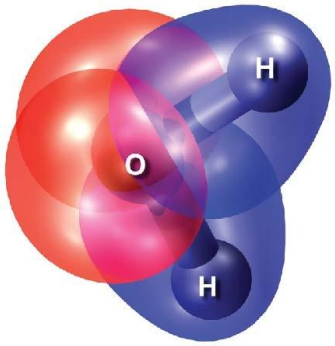
Classical Molecular Models of Water

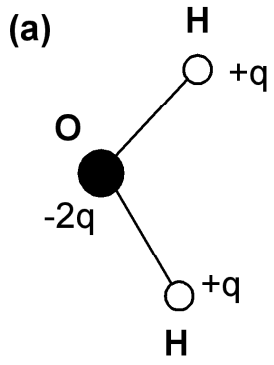


Acronym (date)	Reference	Status	Type	Sites	$\mu_g(D)$	$\mu_l(D)$
BF (1933)	7	empirical	R	4	2.0	2.0
R (1951)	21	empirical	R	5	1.84	1.84
BNS (1971)	22	empirical	R	5	2.17	2.17
ST2 (1973,1993)	23	empirical	R	5	2.35	2.35
CF (1975,1978,1995)	24	empirical	F	3	1.86	1.98
MCY (1976)	25	ab initio	R	4	2.19	2.19
DCF (1978,1980,1993)	26	empirical	F,D,P	3	1.855	-
PE (1979)	27	empirical	P	1	1.855	2.50
SPC (1981)	14	empirical	R	3	2.27	2.27
TIP3P (1981,1983)	15	empirical	R	3	2.35	2.35
RWK (1982)	28	empirical	F	4	1.85	1.89
TIP4P (1983)	15	empirical	R	4	2.18	2.18
BJH (1983)	29	empirical	F	3	1.87	1.99
SPC/F (1985)	30	empirical	F	3	2.27	2.42
MCYL (1986)	31	ab initio	F	4	2.19	2.26
SPC/E (1987)	32	empirical	R	3	2.35	2.35
WK (1989)	33	empirical	R	4	2.60	2.60
SPCP (1989)	34	empirical	P	3	1.85	2.90
CKL (1990)	35	empirical	F,P	4	1.88	2.20
MCHO (1990)	36	ab initio	P	6	2.12	≈3.0
NCC (1990)	37	ab initio	P	6	1.85	2.80
NEMO (1990,1995)	38	ab initio	P	5	2.04	2.89
PTIP4P (1991)	39	empirical	P	4	1.85	2.80
SPC/FP (1991)	40	empirical	F,P	3	1.85	2.44
PSRWK (1991)	41	empirical	P	4	1.88	2.63
KJ (1992)	42	empirical	P	4	1.85	-
NCCvib (1992)	37b	ab initio	F,P	6	1.85	3.11
ASP-W (1992,1998)	43	ab initio	P	3	1.85	2.90
RPOL (1992)	44	empirical	P	3	2.02	2.62
CPMD (1993,1999)	45	DFT+CP	F,D,P	nucl.+el.	1.87	2.95
PPC (1994)	46	ab initio	P	4	2.14	2.51
SPC/FQ (1994)	47	empirical	P	3	1.85	2.83
TIP4P/FQ (1994)	47	empirical	P	4	1.85	2.62
KKY (1994)	48	empirical	F,D	3	2.38	2.21
SQPM (1995)	49	valence bond	P	4	1.85	2.62
SCPDP (1996)	50	empirical	P	4	1.85	2.87
TAB/10D (1998)	51	SCF+MD	P	5	1.85	2.65
NSPCE (1998)	52	empirical	R	3	2.18	2.18
NCF (1998)	53	empirical	F	3	1.85	1.90
MCDHO (2000)	54	ab initio	F, P	4	1.85	3.01
TIP5P (2000)	55	empirical	R	5	2.29	2.29
SPC/HW (2001)	56	empirical	R	3	2.41	2.41
DEC (2001)	57	empirical	R	3	1.85	1.85
SWFLEX (2001)	58	empirical	P	4	1.85	2.59
POLARFLEX (2001)	59	valence bond	F,P	3	1.85	2.55
POL5 (2001)	60	ab initio	P	5	1.85	2.71

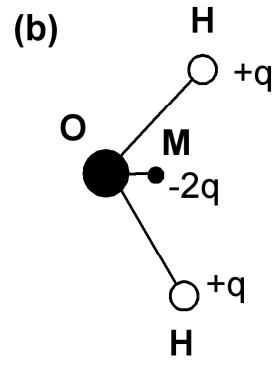
- Guillot B (2002) What we have learnt during three decades of computer simulations on water. *Journal of Molecular Liquids* **101**, 219-260.
- Finney JL (2004) Water? What's so special about it? *Phil. Trans. R. Soc. Lond.* **B 359**, 1145-1165.

The Structure of H_2O Molecule and Classical Intermolecular Potentials

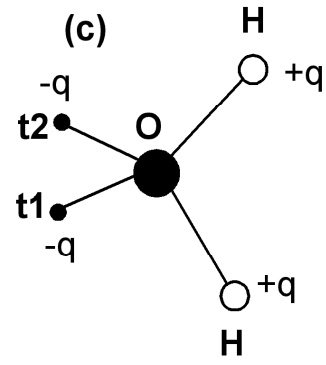




SPC
SPC/E
TIP3P



MCY
TIPS2
TIP4P



BNS
ST2
TIP5P

$$U = \Sigma\Sigma(A_{ij}/r_{ij}^{12} - B_{ij}/r_{ij}^{6} + q_i q_j /\varepsilon_0 r_{ij}) +$$

Short-range repulsion Van der Waals Coulombic

$$+ \Sigma\, ½\, k_b(r_{ij} - r_0)^2 + \Sigma\, ½\, k_\theta(\theta_{ij} - \theta_0)^2$$

bond stretching bond bending

- *Ab-initio* quantum mechanical
- Empirical and semi-empirical
- Rigid vs flexible
- Point polarizability
- “Charges on springs” models
- Core-shell models

Interaction models and simulation techniques

- Particle-in-cell, hydrodynamic codes
- Coarse-grained, discontinuous molecular dynamics

Atomistic simulations

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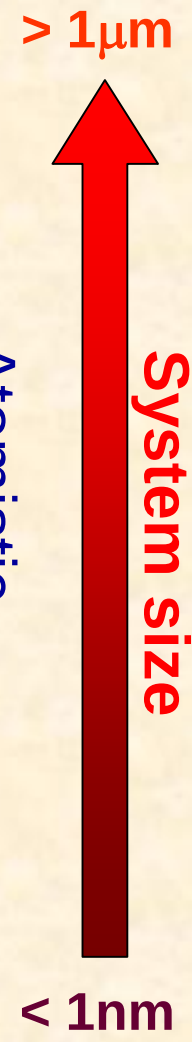


Many-body Tersoff potential

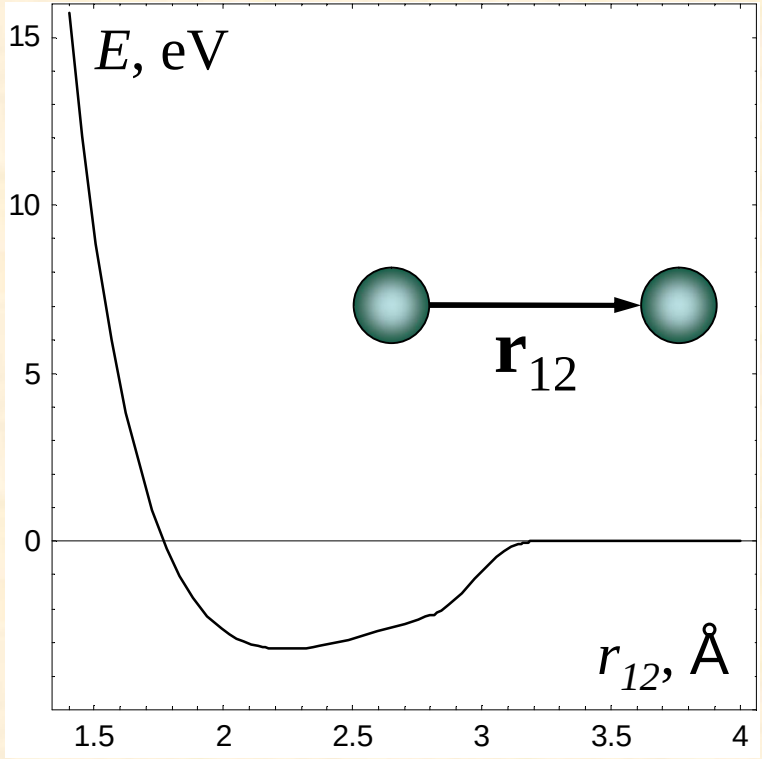
$$E = \sum_{i<j} U_{ij}$$

$$U_{ij} = \left[A e^{-\lambda_1 r_{ij}} - B_{ij}\, e^{-\lambda_2 r_{ij}} \right] f_c(r_{ij})$$

$$B_{ij} = B_0 e^{-z_{ij}/b},$$

$$z_{ij} = \sum_{k \neq i,j} \left[\frac{w(r_{ik})}{w(r_{ij})} \right]^n \left(c + e^{-d \cos\theta_{ijk}} \right),$$

$$w(r) = f_c(r) e^{-\lambda_2 r}.$$



$A = 2280$ eV, $B_0 = 171$ eV, $\lambda_1 = 2\lambda_2$, $\lambda_2 = 1.465$ Å^{-1},

$b = 1.324$, $c = 6.5$, $d = 6.02$, $n = 4$,

$$f_c = \begin{cases} 1, & r < R - D, \\ \frac{1}{2} - \frac{1}{2}\sin\left[\frac{1}{2}\pi (r - R)/D\right], & R - D < r < R + D, \\ 0, & r > R + D, \end{cases}$$

$R = 3.0$ Å, $D = 0.2$ Å

Parameters for Si:

(J. Tersoff, Phys. Rev. B, **37** (1988) 6991)

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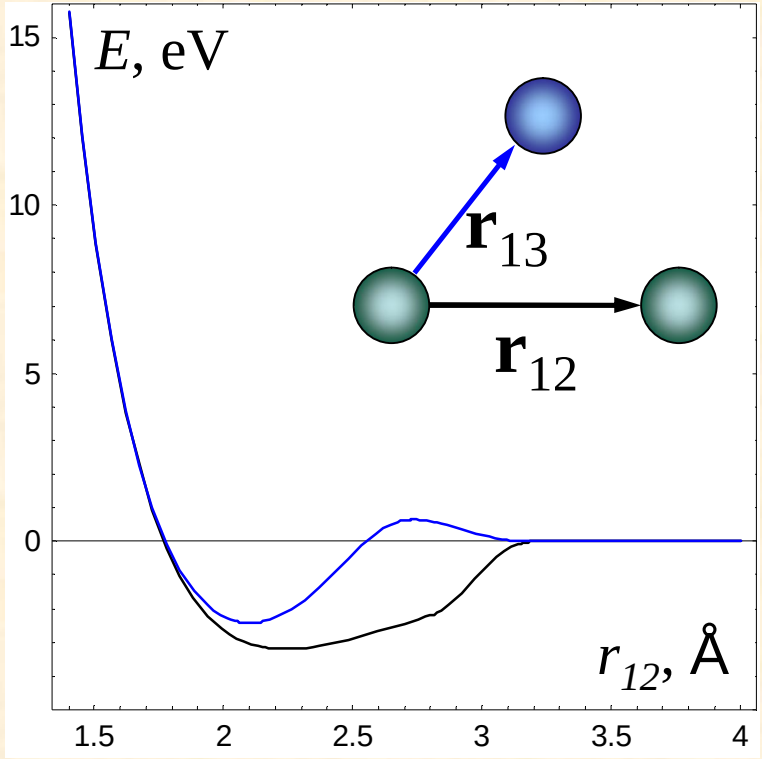

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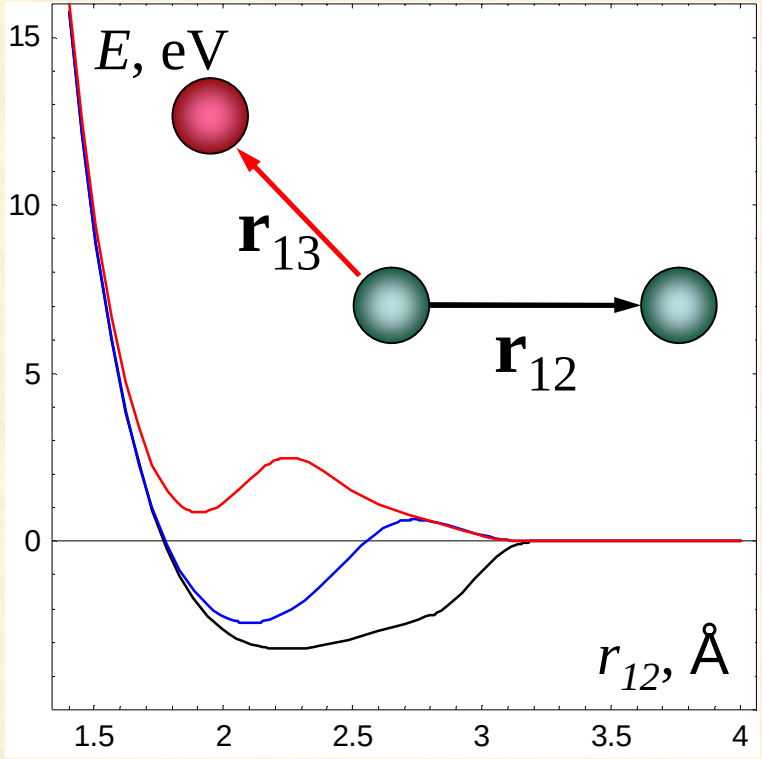

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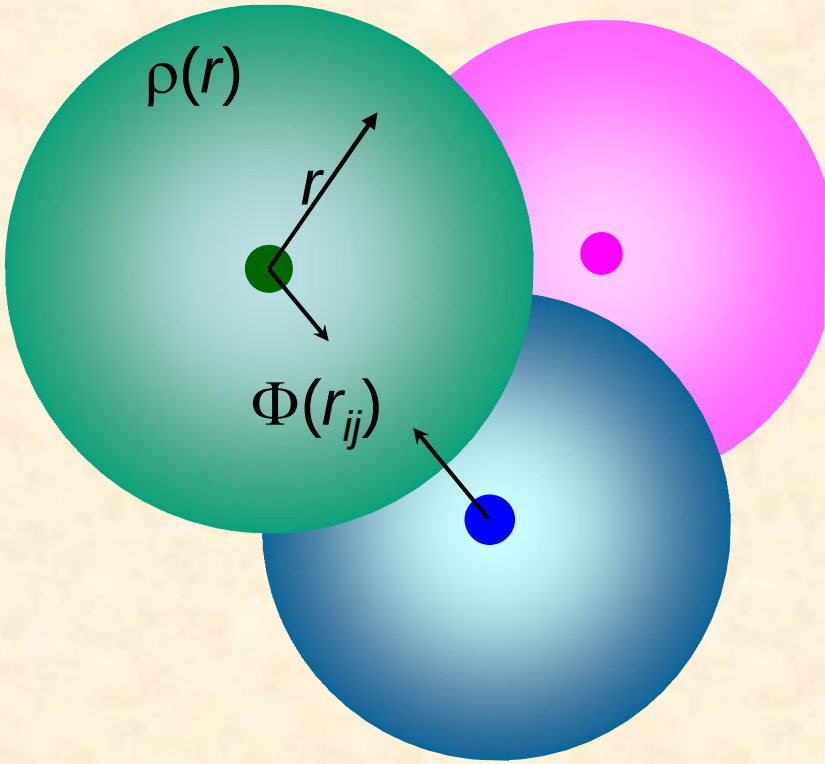
Embedded Atom Method - EAM

Electron density
(transfer function)

$$U = \sum_i F_i\left(\sum_{j\neq i}\rho_j\left(r_{ij}\right)\right) + \sum_{i<j}\Phi_{ij}\left(r_{ij}\right) \overset{?}{\neq} \sum_i\sum_{j\neq i} U(\vec{r}_{ij})$$

Embedding function

Pair potential



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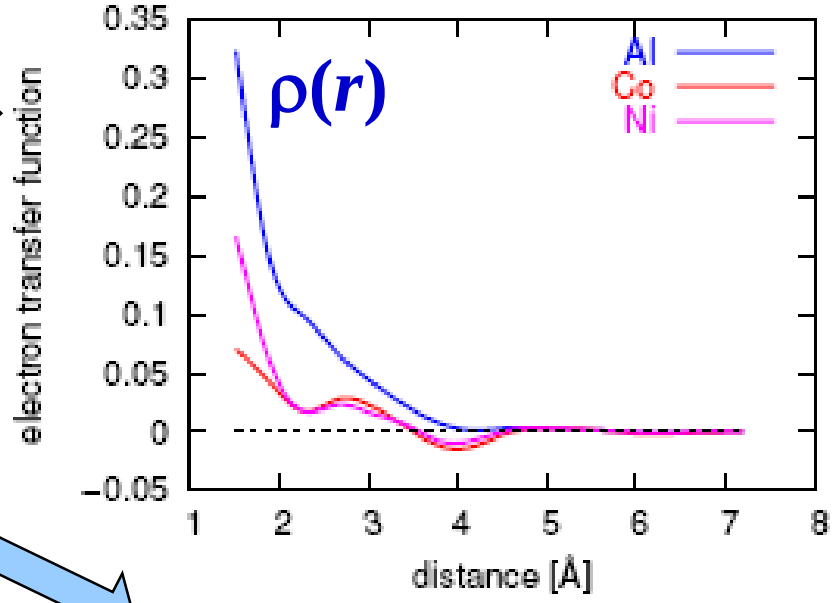
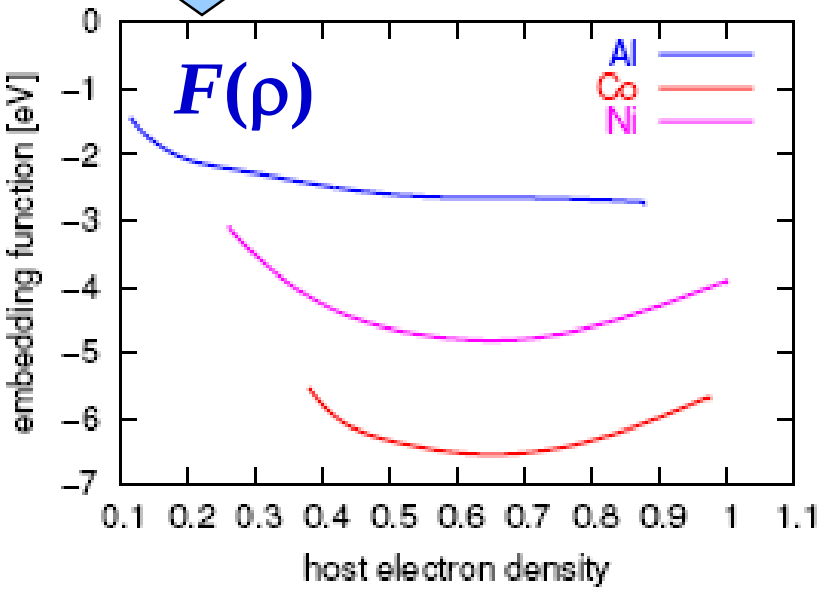
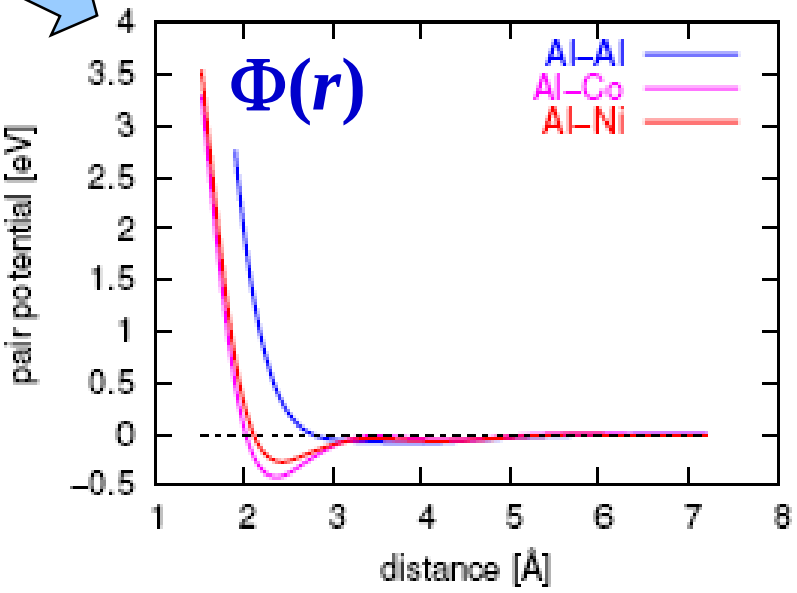
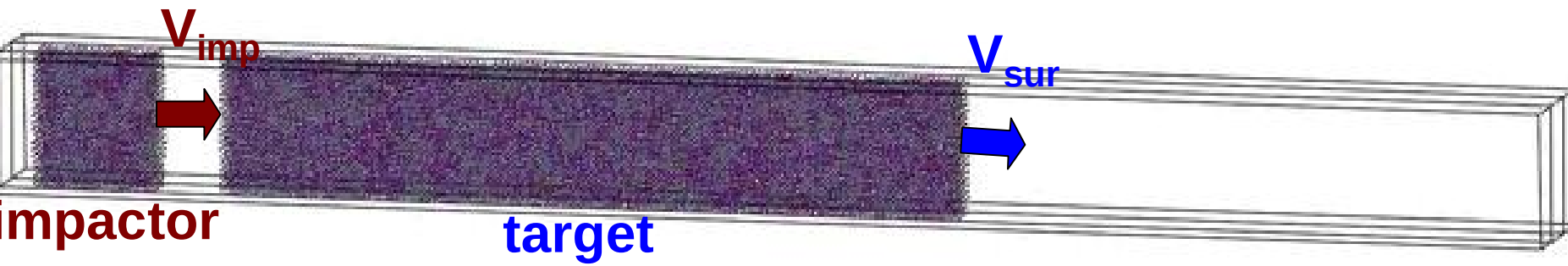
Embedding function **Pair potential**







Atomistic model of spallation process at high rate shock*

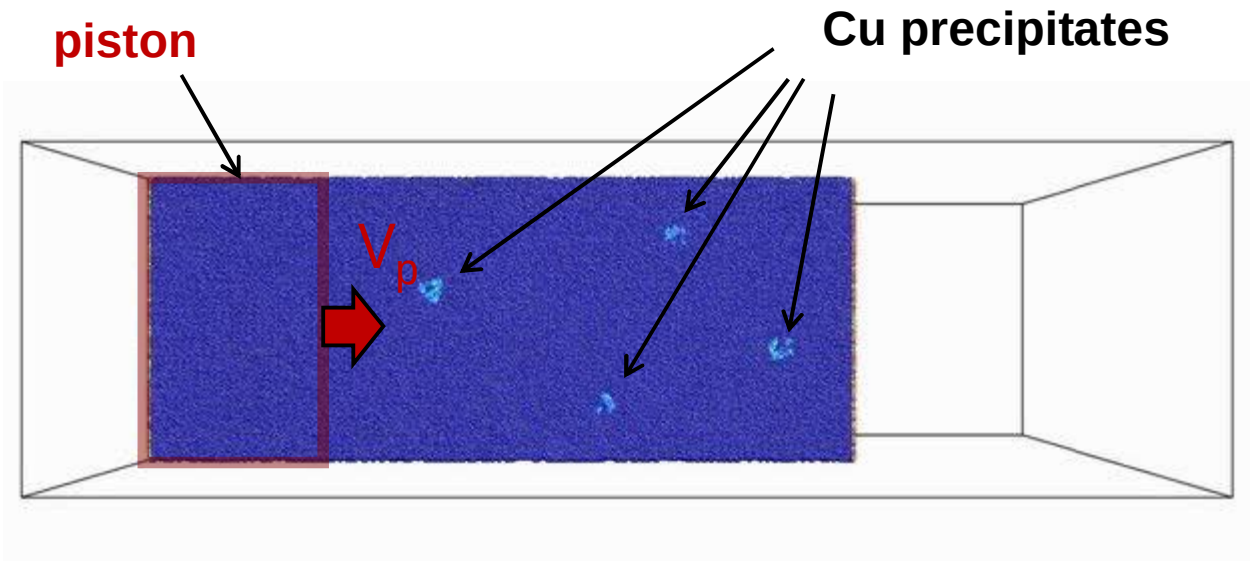


Model parameters:

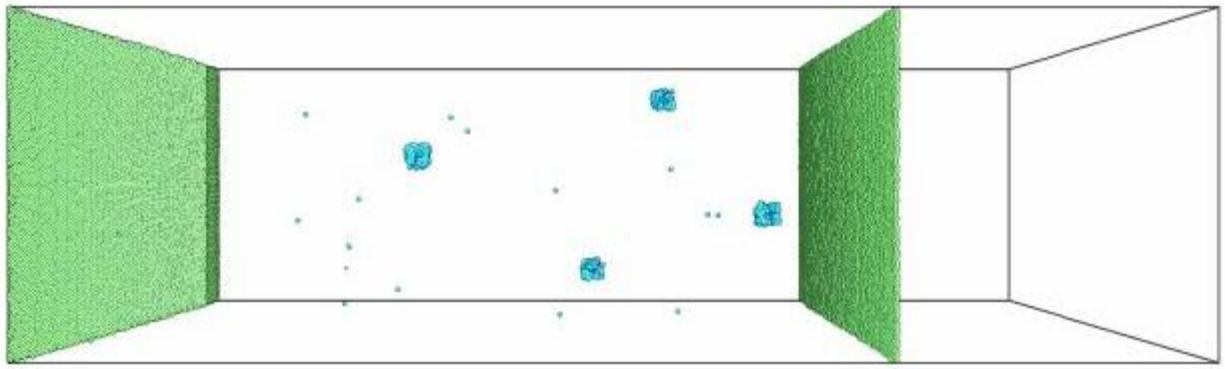
1. **T = 300 K**
2. **Number of Cu atoms 112 000**
3. **Impactor / target mass ratio 1/6**
4. **Initial defect number density 0.05**

* A. Yu. Kuksin, G.E.Norman, V. V. Stegailov, and A. V. Yanilkin
Thermophysics, 2009, Vol. 18, No. 3, pp. 197–226.

Shock wave in Al crystal with Cu precipitates



thin slice



atoms
of defects

200x80x80 N = 5 million atoms V_p = 1800 m/s T=300K

* A. Yu. Kuksin, G.E.Norman, V. V. Stegailov, and A. V. Yanilkin // Journal of Engineering Thermophysics, 2009, Vol. 18, No. 3, pp. 197–226.

The ReaxFF Interatomic Potential

Developed by Adri van Duin:

van Duin ACT, Dasgupta S, Lorant F, Goddard WA, *J. Phys. Chem A.* 105 9396 (2001) (183 citations up to Feb 2010)

Describes bond formation and charge transfer in condensed phases, especially organics

Bonded interactions generated on-the-fly, based on distance-dependent bond-order functions.

Bond-orders adjusted to compensate for atomic over/under-coordination

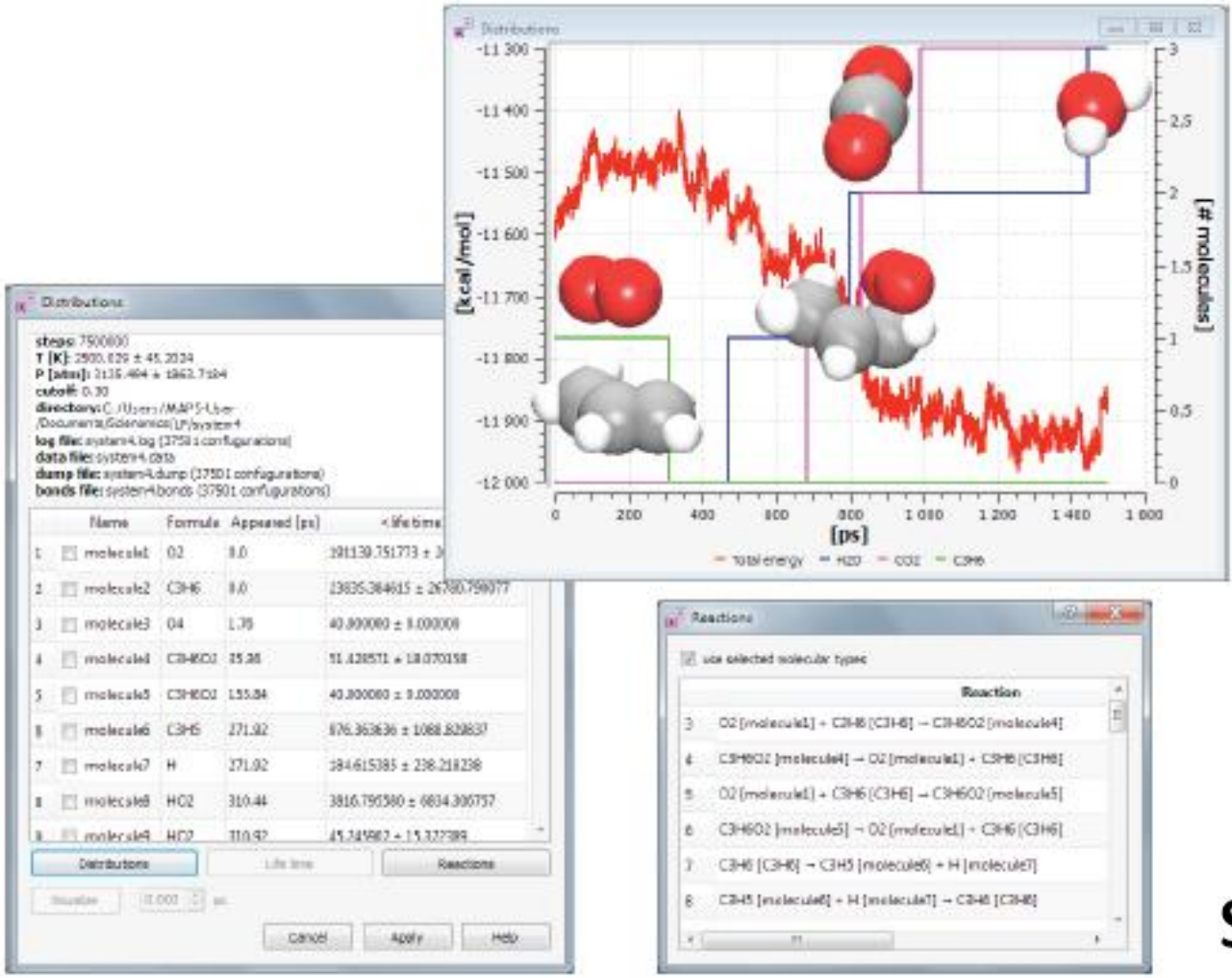
Atom charges computed using electro-negativity equalization i.e. minimizing quadratic function in *N* charges (Coulombic plus ionization energies)

$$E_{System} = E_{bond} + E_{over/under} + E_{lp} + E_{pen} + E_{coa} + E_{hb} + E_{tors} + E_{conj} + E_{val} + E_{vdW} + E_{Coul}$$
$$= E(\text{bond-order}) + E(\text{non-bond}) + E(\text{charge equilibration})$$

Sandia National Laboratories

Source: http://lammps.sandia.gov/workshops/Feb10/Aidan_Thompson/ReaxFF_LAMMPS_2010.pdf

The ReaxFF Interatomic Potential



Butene oxidation, characteristic configuration obtained after 1.5 ns

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Interaction models and simulation techniques

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- Coarse-grained, discontinuous molecular dynamics

- Simple pairwise potentials for atoms or molecules with fixed atomic bonds
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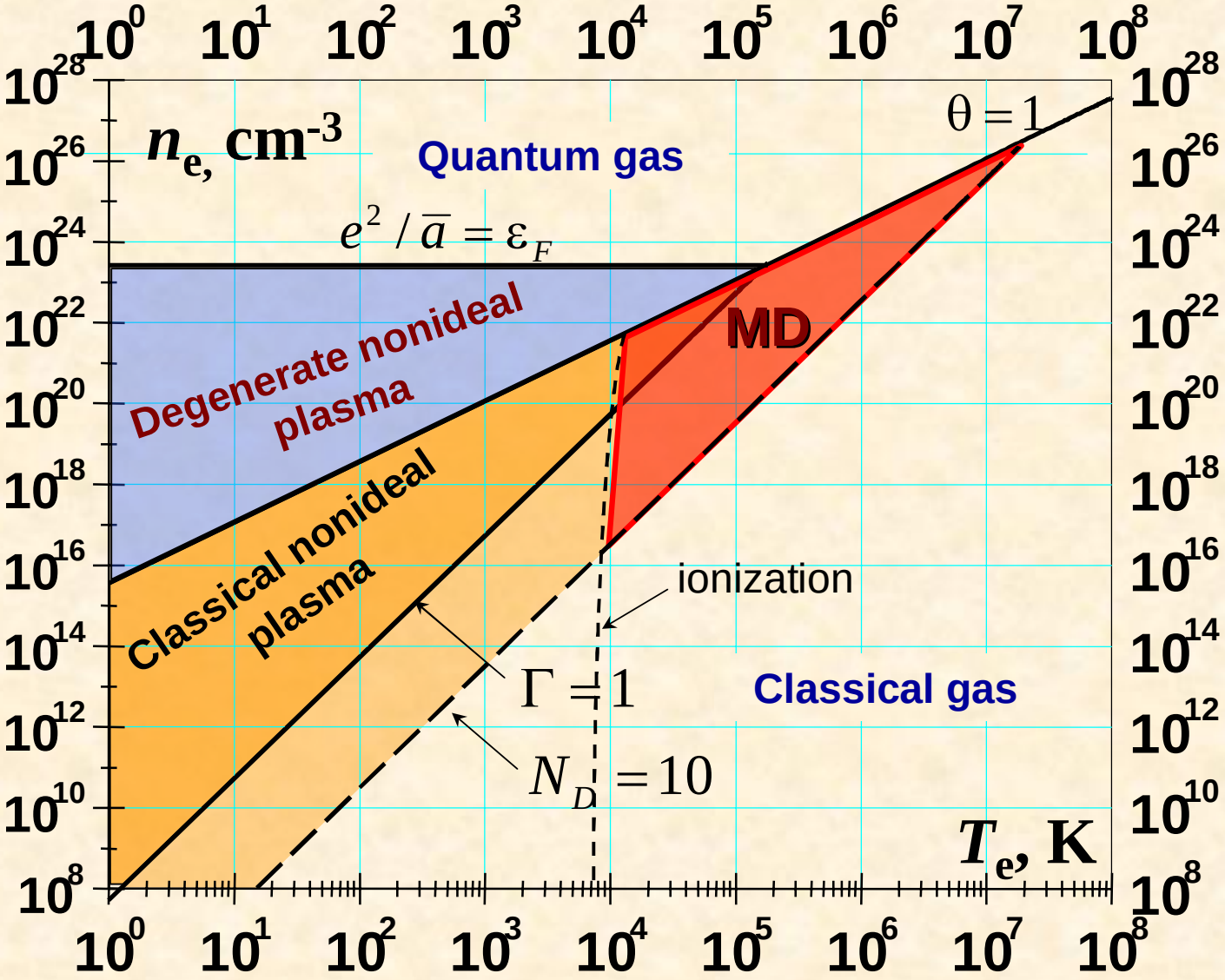
Atomistic simulations

Density-Temperature Diagram



Nonideality parameter for electrons

$$\Gamma = \left(\frac{4\pi n_e}{3}\right)^{1/3} \frac{e^2}{kT}$$

Number of electrons in the Debye sphere

$$N_D = \frac{4\pi r_D^3}{3} n_e$$

Degeneracy parameter

$$\theta = \varepsilon_F / kT$$

Breaking into the atom

Approximations, restrictions and gains

1. BO approx. (adiabatic approx.)
   No nonadiabatic processes (charge-transfer reactions, photochemistry)
2. Ground state
   No electronic excitations, no electron-phonon coupling, etc
3. Classical approx. for nuclei movement
   No proton transfer, atom tunneling, etc

On the good side – big systems, long evolution times, nice parallelization and scaling

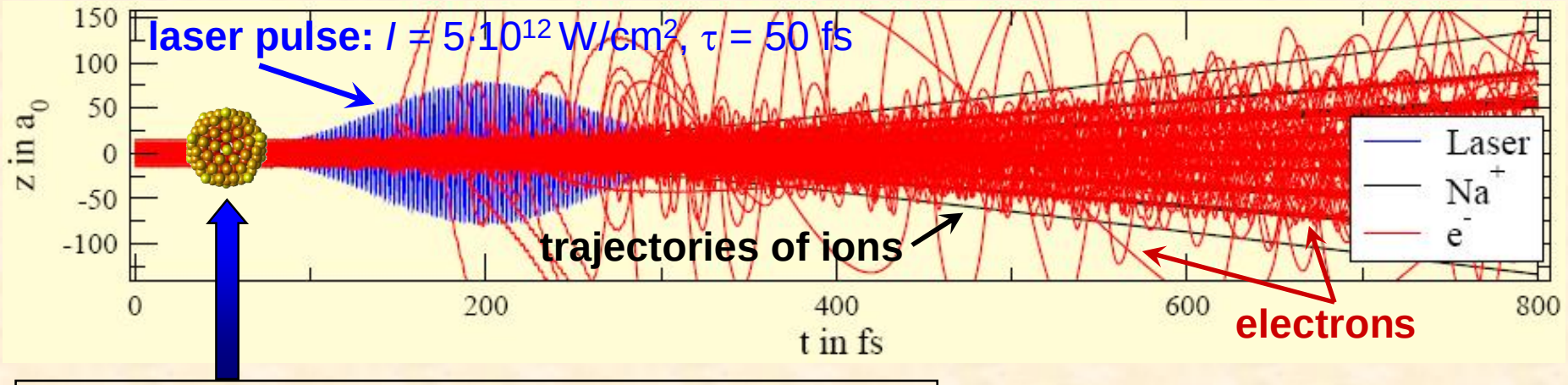
TD Schrödinger eq. – 3 atoms

MD – 10^9 atoms, up to milliseconds

Source: Alexey Shaitan, International School "Computer simulation of advanced materials", Moscow, Russia, July 16–21, 2012

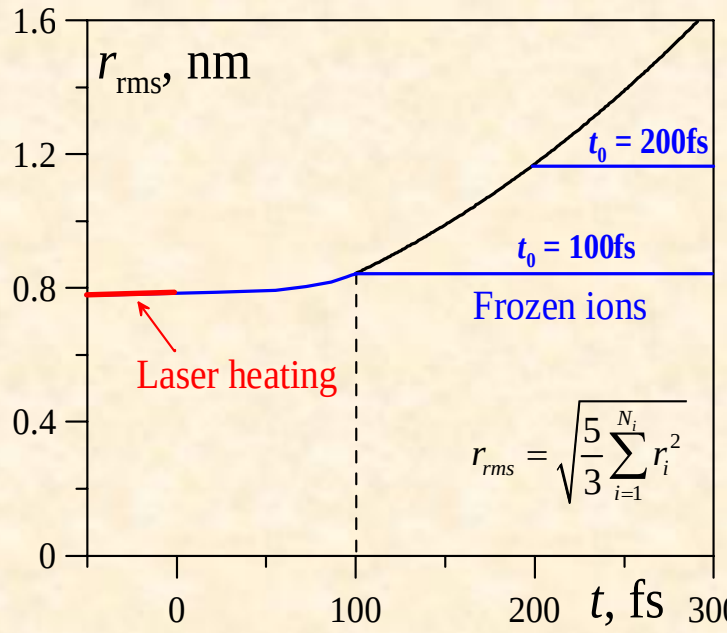
MD simulations of ionized sodium clusters

Ionization and cluster expansion «Coulomb explosion»



- In the initial state the ions are located in the nodes of Na55 icosahedral crystal. Electrons are on top of ions.
- Ion-electron mass ratio is 41910
- Erf-like electron ion potential is used with U_{min} = - 5.1eV
- Typical times of:
  cluster expansion > 100fs
  electron oscillations < 1fs

Cluster expansion



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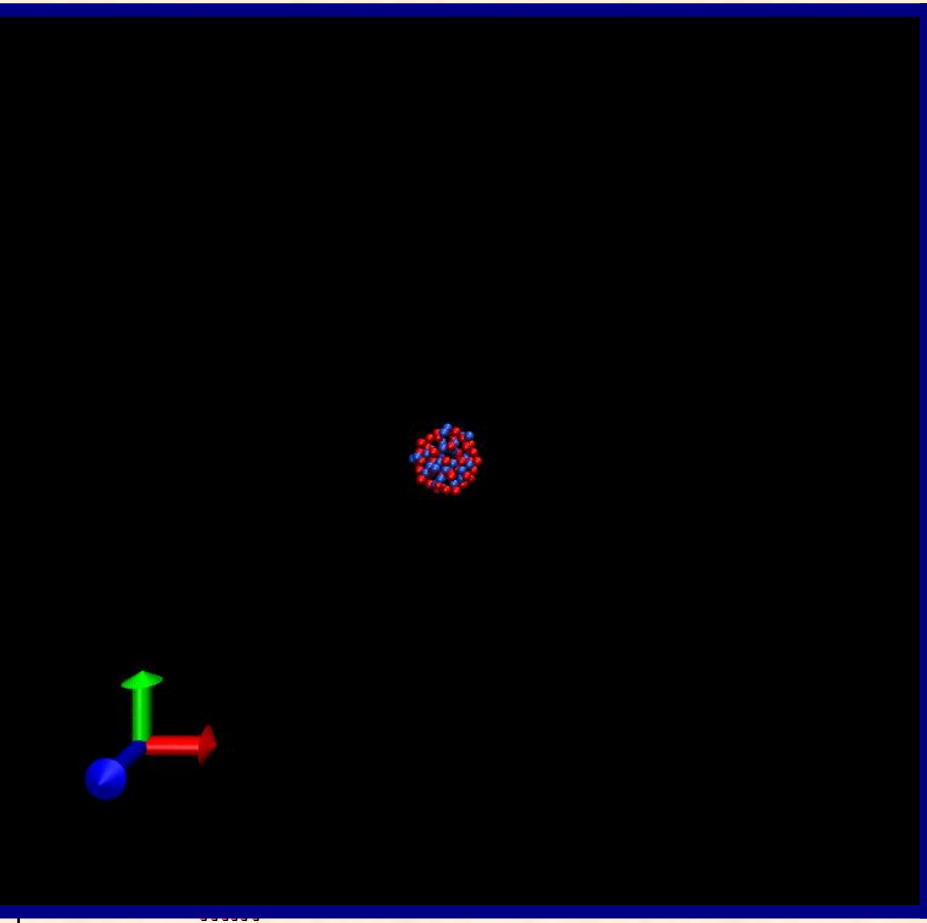

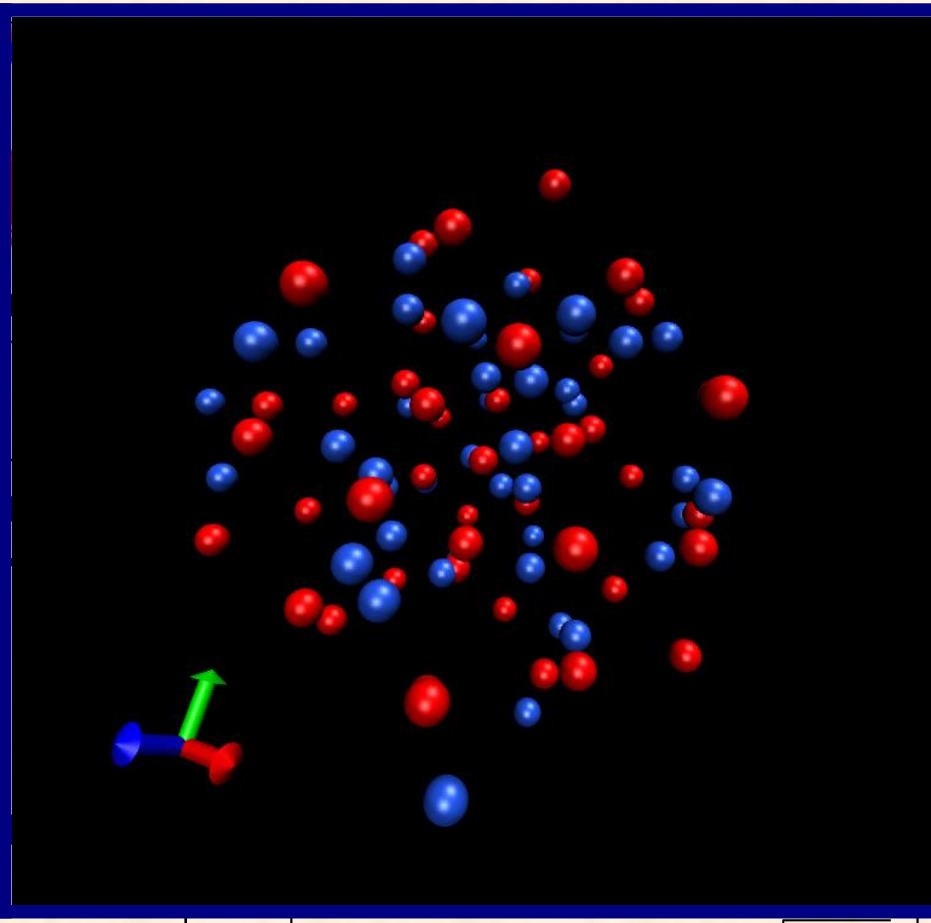

- **Typical times of:**
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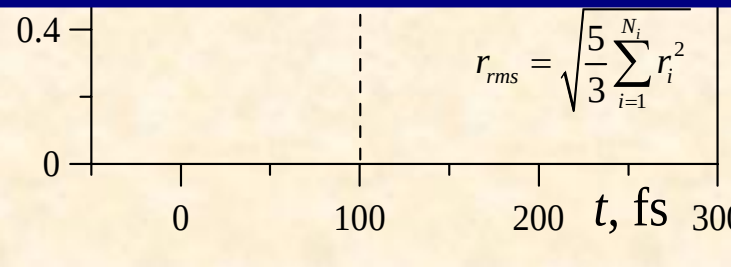
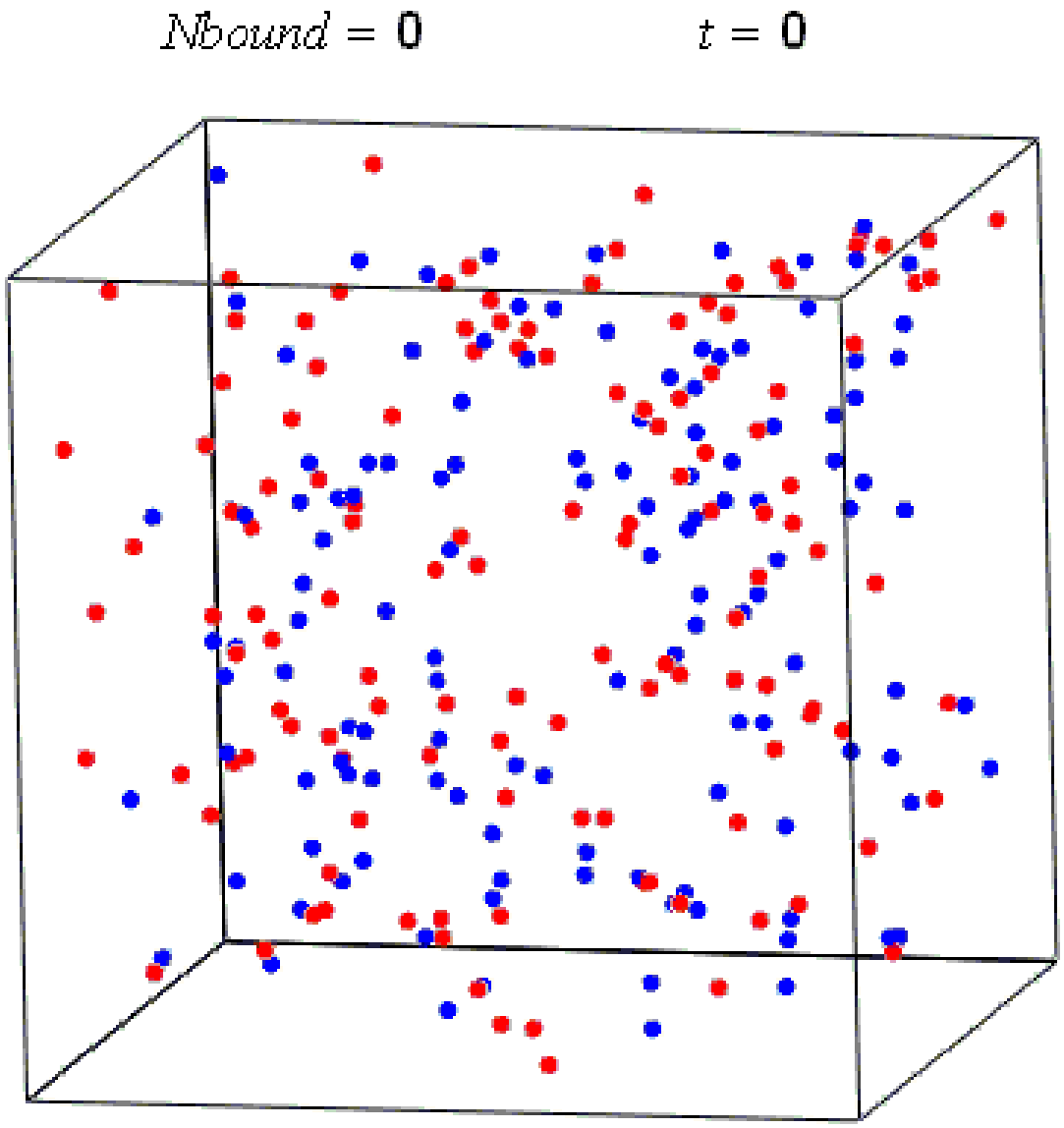


Visualization of particle motion in MD cell



- – electron
- – ion
- – bound electron
- – bound ion

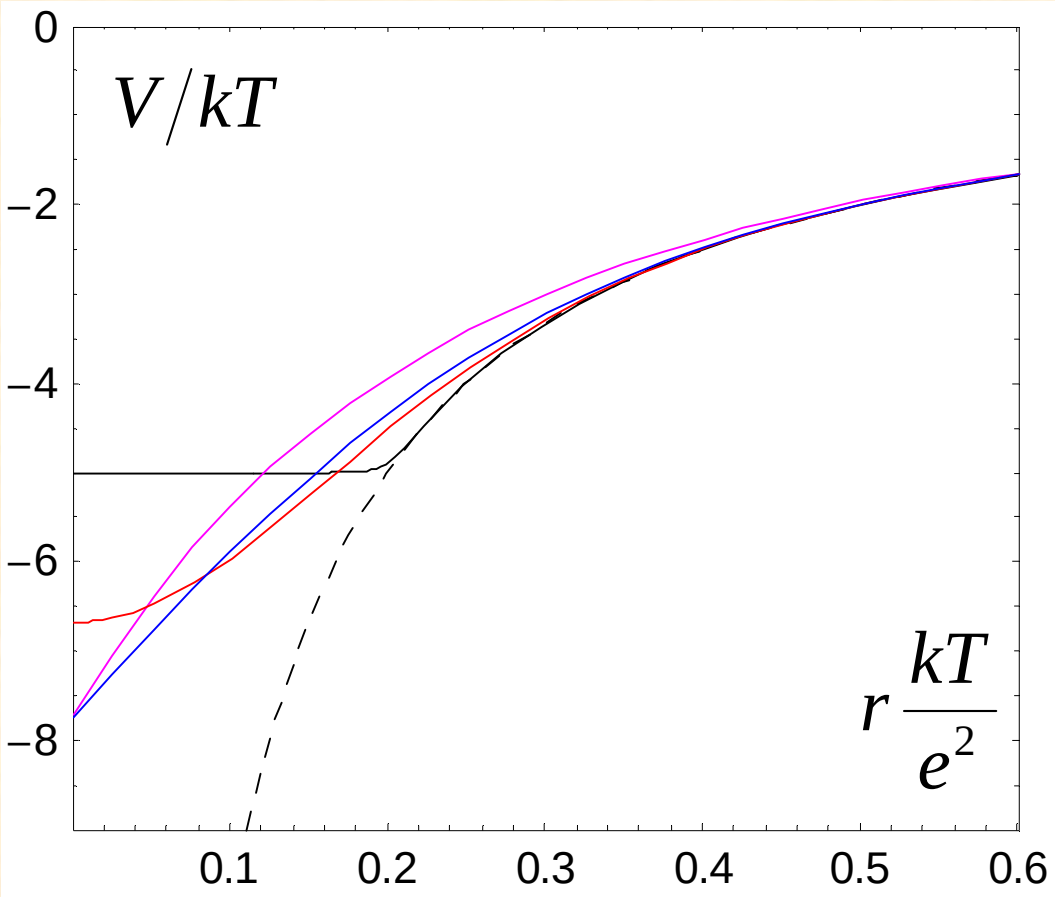
An electron is marked as bound if it makes at least one complete revolution around an ion.

$N = 128$

$\Gamma = 1.28$

$M/m = 10$

Models for electron-ion interaction potentials



Coulomb $\frac{1}{r}$

Cut-off $\frac{1}{r},\ r > \frac{1}{\varepsilon};\qquad -\varepsilon,\ r \le \frac{1}{\varepsilon}$

Deutsch $\frac{1}{r}\left[1-\exp\left(-\frac{r}{\lambda_{ei}}\right)\right]$

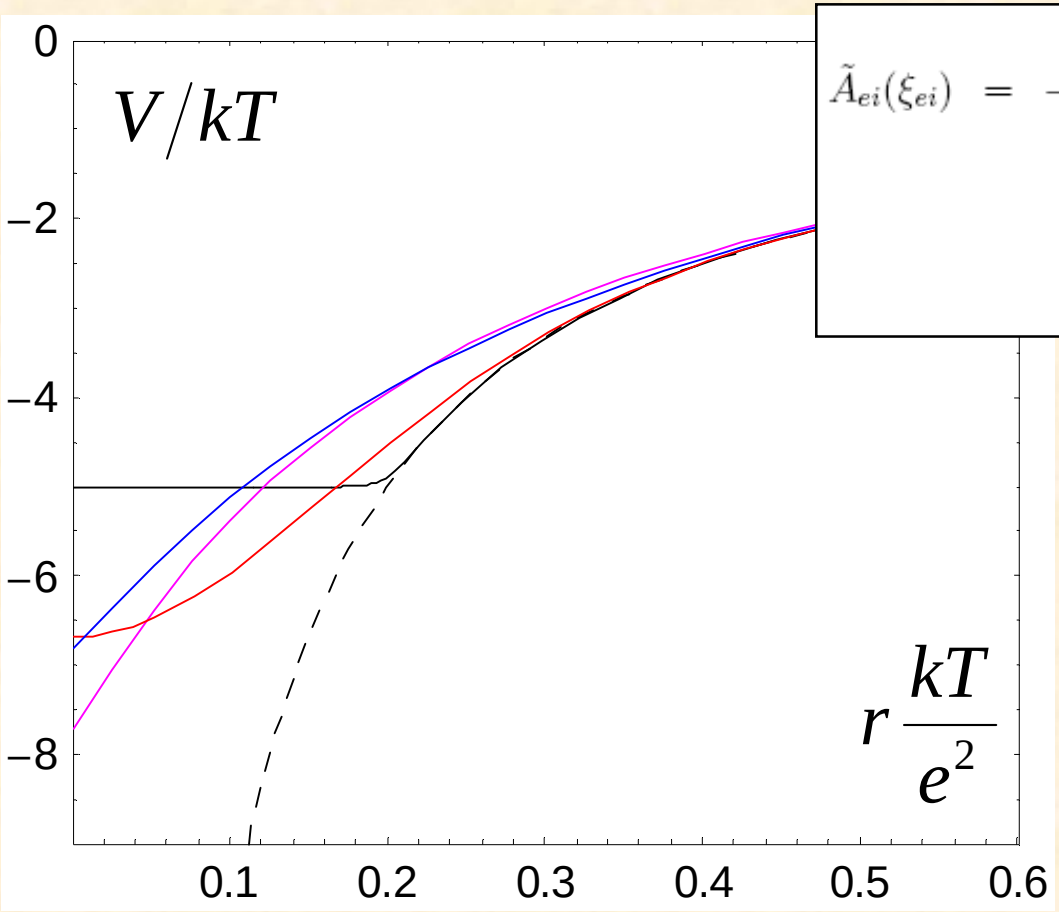
$$\lambda_{ie} = \lambda_{th} = \hbar/\sqrt{mkT}$$

Error function $\frac{1}{r}\operatorname{erf}\left(-\frac{r}{\lambda_{ei}}\right)$

Kelbg $\frac{1}{r}F\left(\frac{r}{\Lambda_{ei}}\right)$

$$F(x) = 1-\exp(-x^2)+\sqrt{\pi}x(1-\operatorname{erf}(x)) \qquad \Lambda_{ie} = \hbar/\sqrt{2mkT}$$

Models for electron-ion interaction potentials



$$\tilde{A}_{ei}(\xi_{ei}) = -\sqrt{\pi}\xi_{ei} + \ln\left[\sqrt{\pi}\xi_{ie}^3\left(\zeta(3) + \frac{1}{4}\zeta(5)\xi_{ie}^2\right) + 4\sqrt{\pi}\xi_{ei}\int_0^\infty \frac{y\exp(-y^2)\,dy}{1-\exp(-\pi\xi_{ei}/y)}\right]$$

Deutsch $\dfrac{1}{r}\left[1-\exp\left(-\dfrac{r}{\lambda_{ei}}\right)\right]$

$$\lambda_{ie} = \lambda_{th} = \hbar/\sqrt{mkT}$$

Error function $\dfrac{1}{r}\operatorname{erf}\left(-\dfrac{r}{\lambda_{ei}}\right)$

Corrected Kelbg $\dfrac{1}{r}\left[F\left(\dfrac{r}{\Lambda_{ei}}\right) + r\dfrac{kT}{e^2}\tilde{A}_{ei}\left(\dfrac{e^2}{kT\Lambda_{ei}}\right)\exp\left(-\left(\dfrac{r}{\lambda_{ei}}\right)^2\right)\right]$

$$F(x) = 1-\exp(-x^2) + \sqrt{\pi}x(1-\operatorname{erf}(x)) \qquad \Lambda_{ie} = \hbar/\sqrt{2mkT}$$

Interaction models and simulation techniques

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- Coarse-grained, discontinuous molecular dynamics

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Atomistic simulations

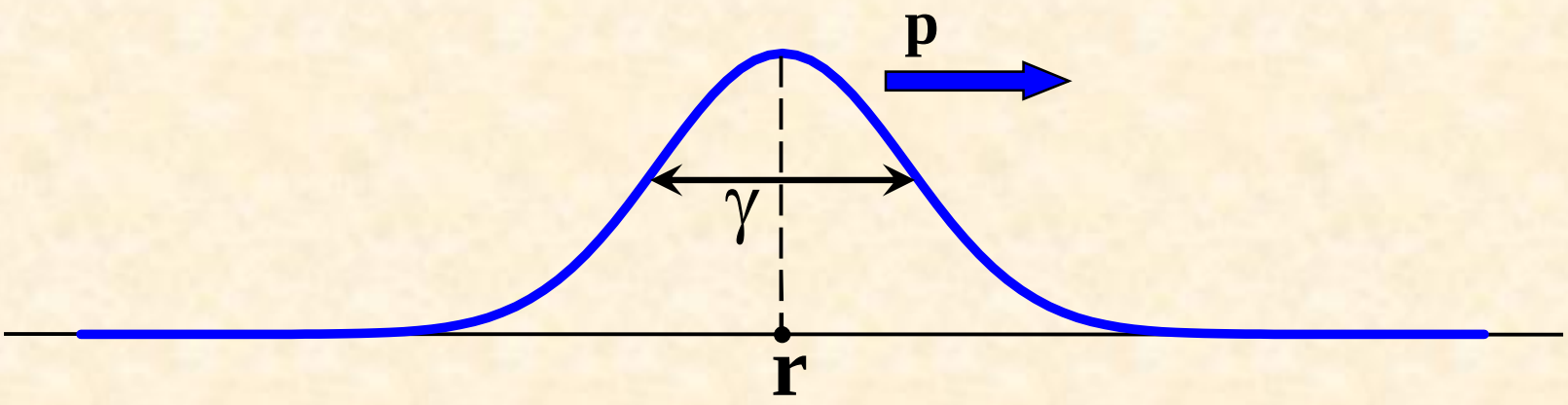
Wave Packet Molecular Dynamics

Gaussian wave packet (WP) for a single particle:

$$\varphi(\mathbf{x},t)=\left(\frac{3}{2\pi\gamma^2}\right)^{3/4}\exp\left\{-\left(\frac{3}{4\gamma^2}-\frac{ip_\gamma}{2\hbar\gamma}\right)(\mathbf{x}-\mathbf{r})^2+\frac{i}{\hbar}\mathbf{p}\cdot(\mathbf{x}-\mathbf{r})\right\}$$

"Physical" parameters (8 real numbers per particle):

$(\mathbf{r}, \mathbf{p})$	particle coordinate and momentum (3D vectors)
γ	width of the packet ($\gamma > 0$)
p_γ	"momentum" of the width



Wave Packet Molecular Dynamics

Hamiltonian

$$\hat{H} = \hat{K}_e + \hat{V}_{ei} + \hat{V}_{ee} + \hat{H}_{ext} = -\sum_k \frac{\hbar^2}{2m}\Delta_k - \sum_{k,i} \frac{eq_i}{\left|\hat{\mathbf{x}}_k - \mathbf{R}_i\right|} + \sum_{k<m} \frac{e^2}{\left|\hat{\mathbf{x}}_k - \hat{\mathbf{x}}_m\right|} + \hat{H}_{ext}$$

Many-electron wave function

$$\Psi(\{\mathbf{x}_k\}, t) = \prod_k \varphi(\mathbf{x}_k, t)$$ (Hartree approximation)

Total energy

$$H = \left\langle \Psi \middle| \hat{H} \middle| \Psi \right\rangle = \sum_k \left(\frac{\mathbf{p}_k^2}{2m} + \frac{\mathbf{p}_{\gamma_k}^2}{2m} \right) + \sum_k \frac{9\hbar^2}{8m\gamma_k^2} + \sum_{k<l} \frac{e_k e_l}{r_{kl}} \operatorname{erf}\left(\frac{r_{kl}}{\sqrt{2(\gamma_k^2 + \gamma_l^2)/3}} \right) + H_{ex}$$

Norm-matrix

$$N_{\alpha\beta} = \frac{\partial}{\partial q_\alpha^* \partial q_\beta} \ln \left\langle \Psi(\mathbf{q}^*) \middle| \Psi(\mathbf{q}) \right\rangle$$

$$\mathbf{N} = \begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

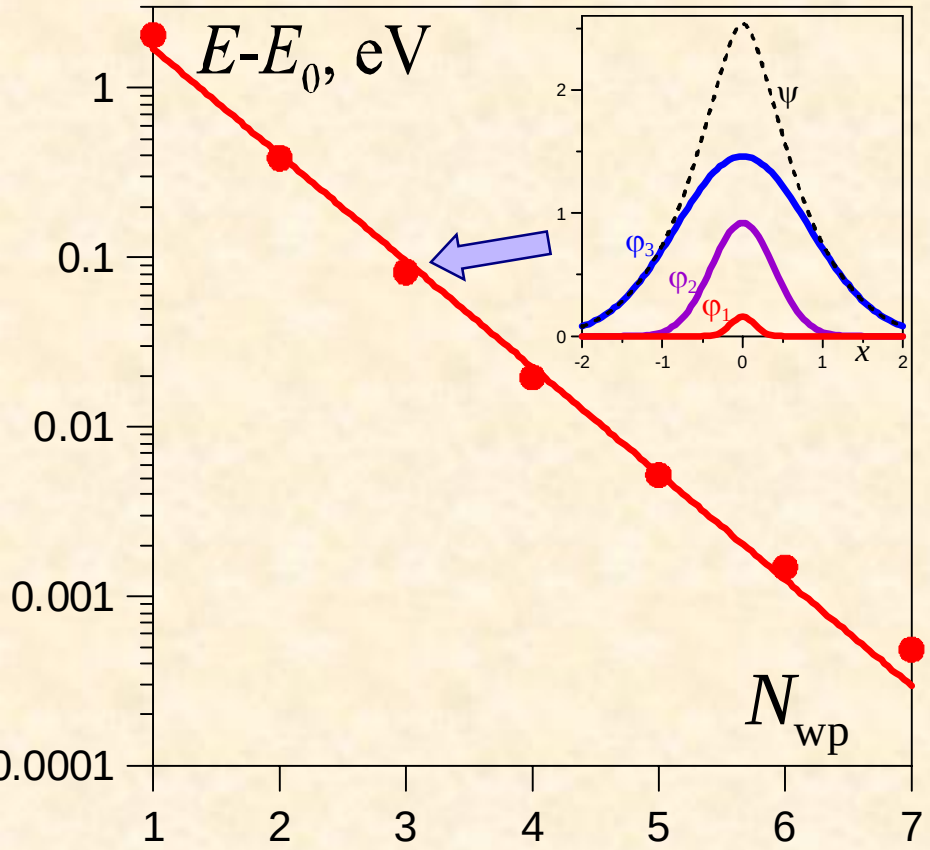
Equations of motion

$$\sum_\alpha N_{\alpha\beta} \frac{dq_\alpha}{dt} = \frac{\partial H}{\partial q_\beta},$$

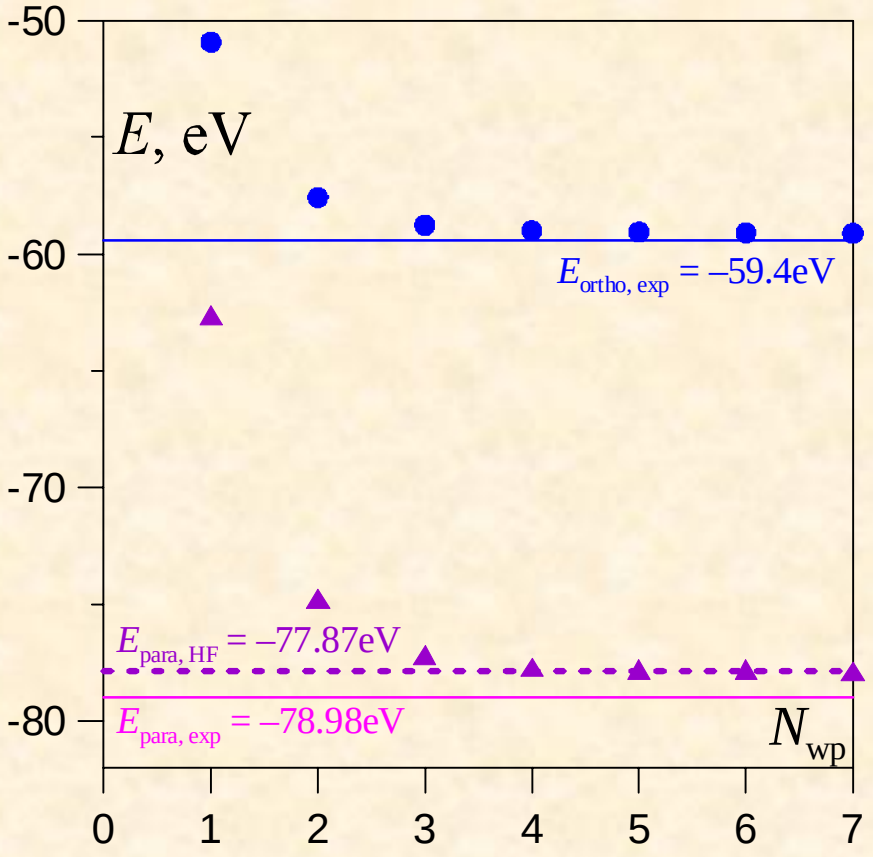
$$\dot{\mathbf{r}}_k(t) = \frac{\partial H}{\partial \mathbf{p}_k}, \quad \dot{\mathbf{p}}_k(t) = -\frac{\partial H}{\partial \mathbf{r}_k}, \quad \dot{\gamma}_k(t) = \frac{\partial H}{\partial p_{\gamma_k}}, \quad \dot{p}_{\gamma_k}(t) = -\frac{\partial H}{\partial \gamma_k}$$

Ground state of simple atoms represented by multiple Gaussian wave packets

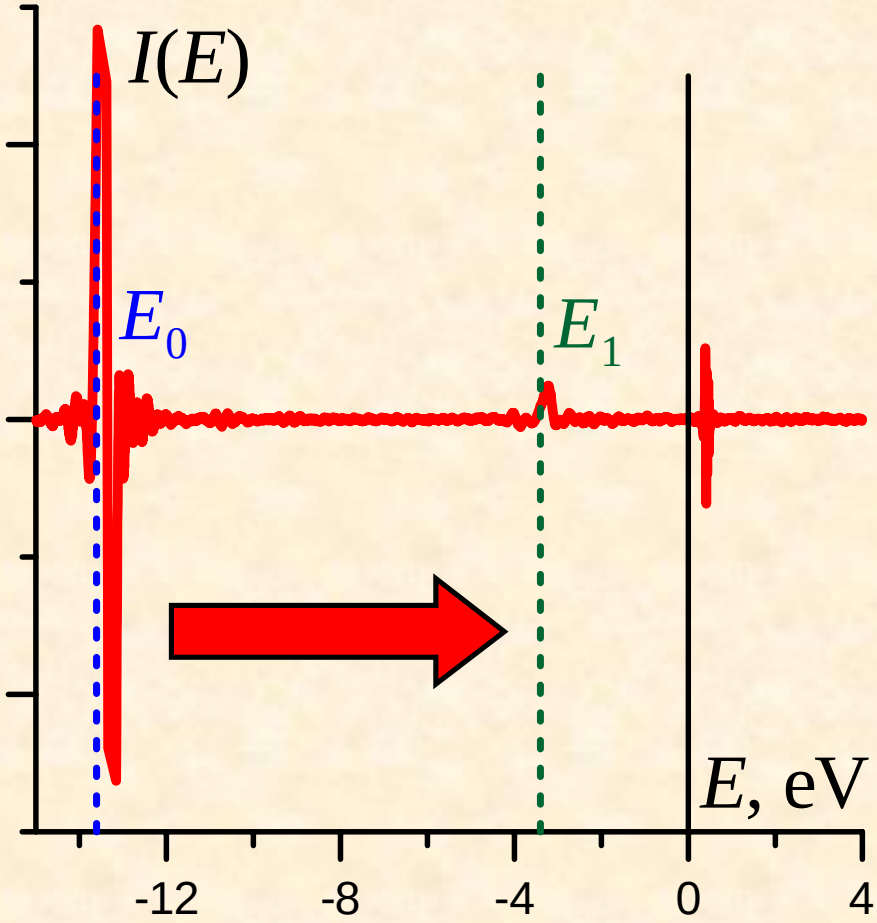
Hydrogen



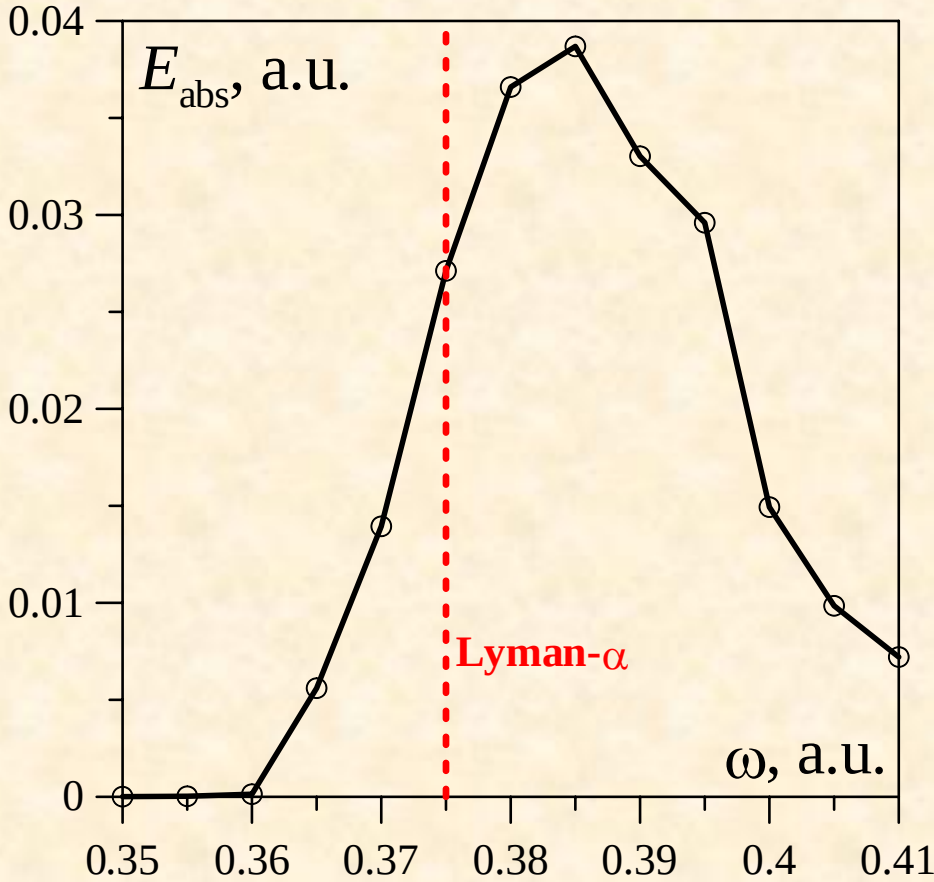
Helium



Excited states of Hydrogen represented by multiple Gaussian wave packets



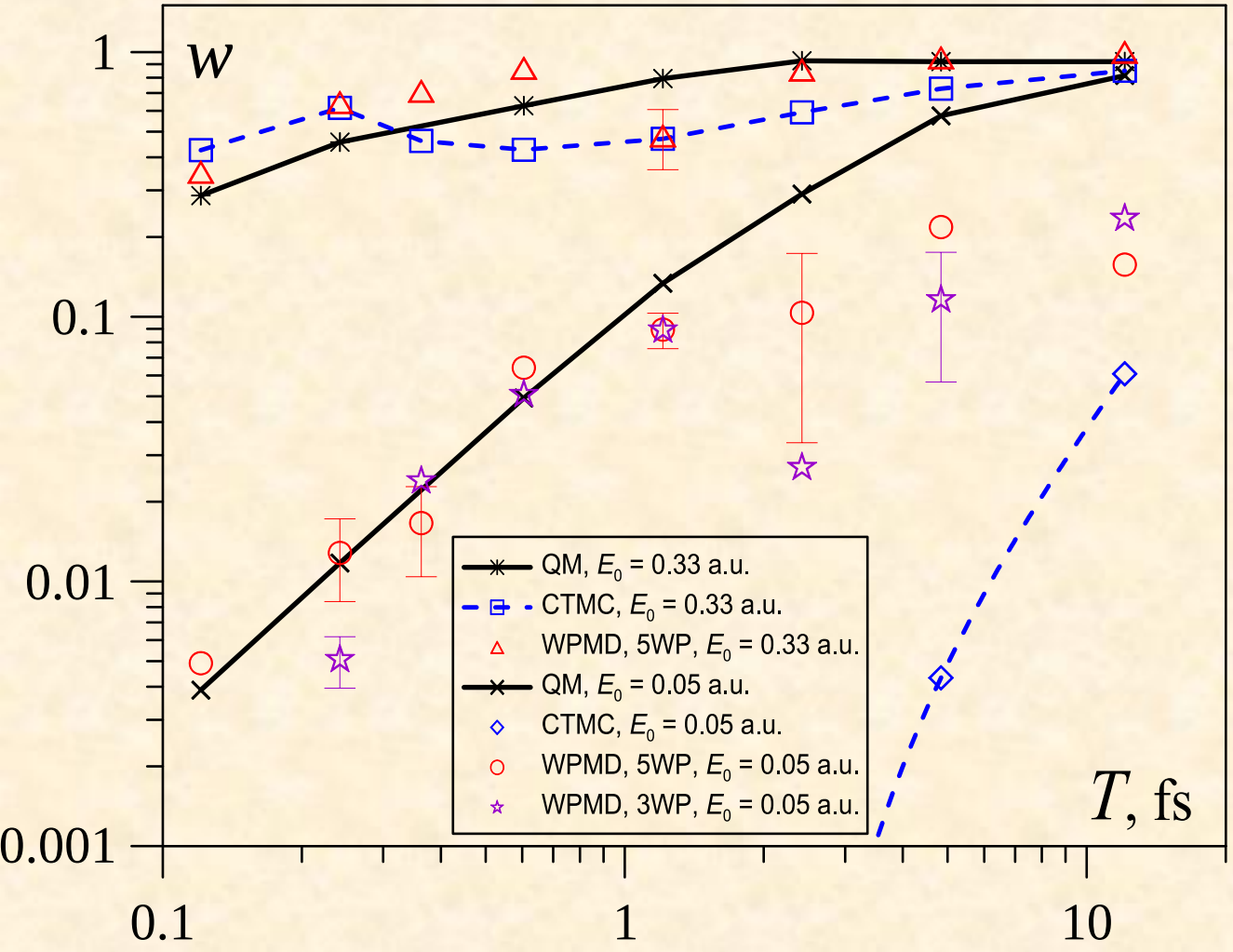
Spectrum of the time correlation function after excitation



Absorbed energy depending on the laser frequency in the area of 1s → 2s transition

N_{wp} = 5, T = 200a.u., E_0 = 0.005a.u.

Ionization of H(1s) atom by a laser pulse*



Classical Trajectory Motne-Carlo (CTMC):

$$P = \frac{N_{E_{part}>0}}{N_{tot}}$$

WPMD (1 electron, 3 WPs):

$$\psi = \psi_{\text{bound}} + \psi_{\text{free}}$$

$$P = \frac{\langle \psi_{\text{free}} | \psi_{\text{free}} \rangle}{\langle \psi | \psi \rangle}$$

* Comparison with *J.P. Hansen, J. Lu, L.B. Madsen, H.M. Nilsen* // Phys. Rev. A, 2001, V. 64, P. 033418.

Electron force field approach*

$$E_{\text{elec-elec}} = \frac{1}{4\pi\varepsilon_0}\sum_{i<j}\frac{1}{r_{ij}}Erf\left(\frac{\sqrt{2}r_{ij}}{\sqrt{s_i^2+s_j^2}}\right),$$

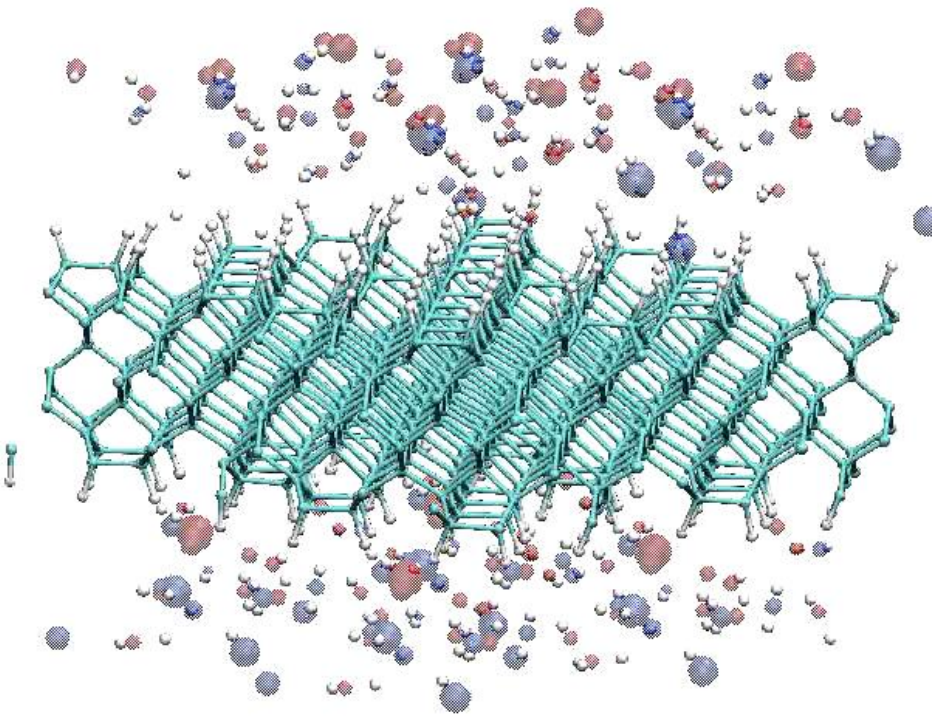
$$E_{\text{Pauli}} = \sum_{\sigma_i=\sigma_j} E(\uparrow\uparrow)_{ij} + \sum_{\sigma_i\neq\sigma_j} E(\uparrow\downarrow)_{ij},$$

$$E(\uparrow\uparrow)_{ij} = \left(\frac{S_{ij}^2}{1-S_{ij}^2} + (1-\rho)\frac{S_{ij}^2}{1+S_{ij}^2}\right)\Delta T_{ij}$$

$$E(\uparrow\downarrow)_{ij} = \frac{\rho S_{ij}^2}{1+S_{ij}^2}\Delta T_{ij},$$

$$\Delta T_{ij} = \frac{\hbar^2}{m_e}\left[\frac{3}{6}\left(\frac{1}{\bar{s}_i^2}+\frac{1}{\bar{s}_j^2}\right) - \frac{6\left(\bar{s}_i^2+\bar{s}_j^2\right)-4\bar{r}_{ij}^2}{\left(\bar{s}_i^2+\bar{s}_j^2\right)^2}\right], \quad S_{ij} = \left(\frac{2}{\bar{s}_i/\bar{s}_j+\bar{s}_j/\bar{s}_i}\right)^{3/2} e^{-\bar{r}_{ij}^2/(\bar{s}_i^2+\bar{s}_j^2)},$$

$$\rho = -0.2,\ \bar{x}_{ij} = x_{ij}\times 1.125,\ \text{and}\ \bar{s}_i = s_i \times 0.9.$$



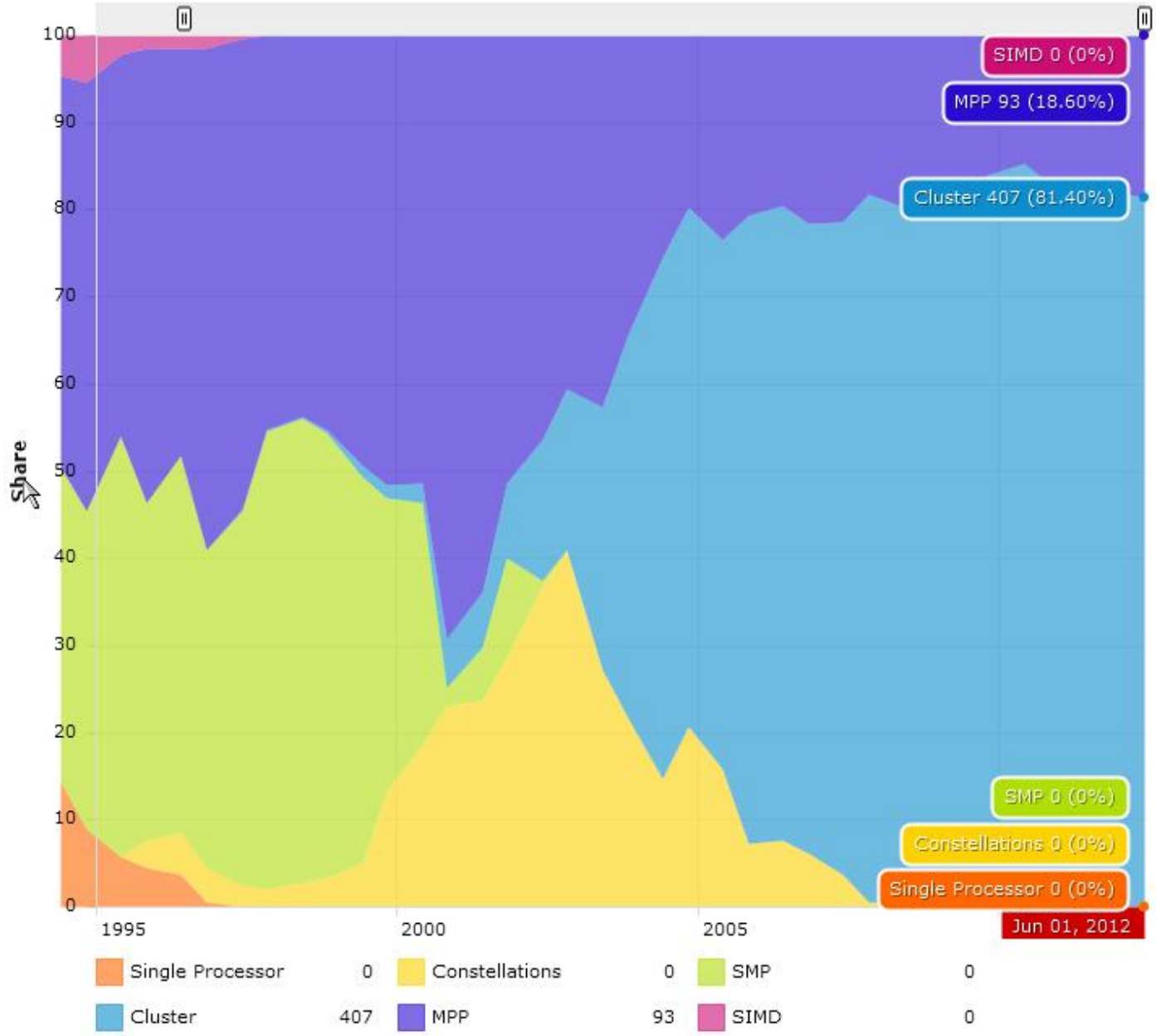
*** J.T. Su, W.A. Goddard III**, *Excited Electron Dynamics Modeling ofWarm Dense Matter*, Phys. Rev. Lett., 2007, v. 99, p. 185003.

PARALLEL EXECUTION

LLNL Sequoia Supercomputer

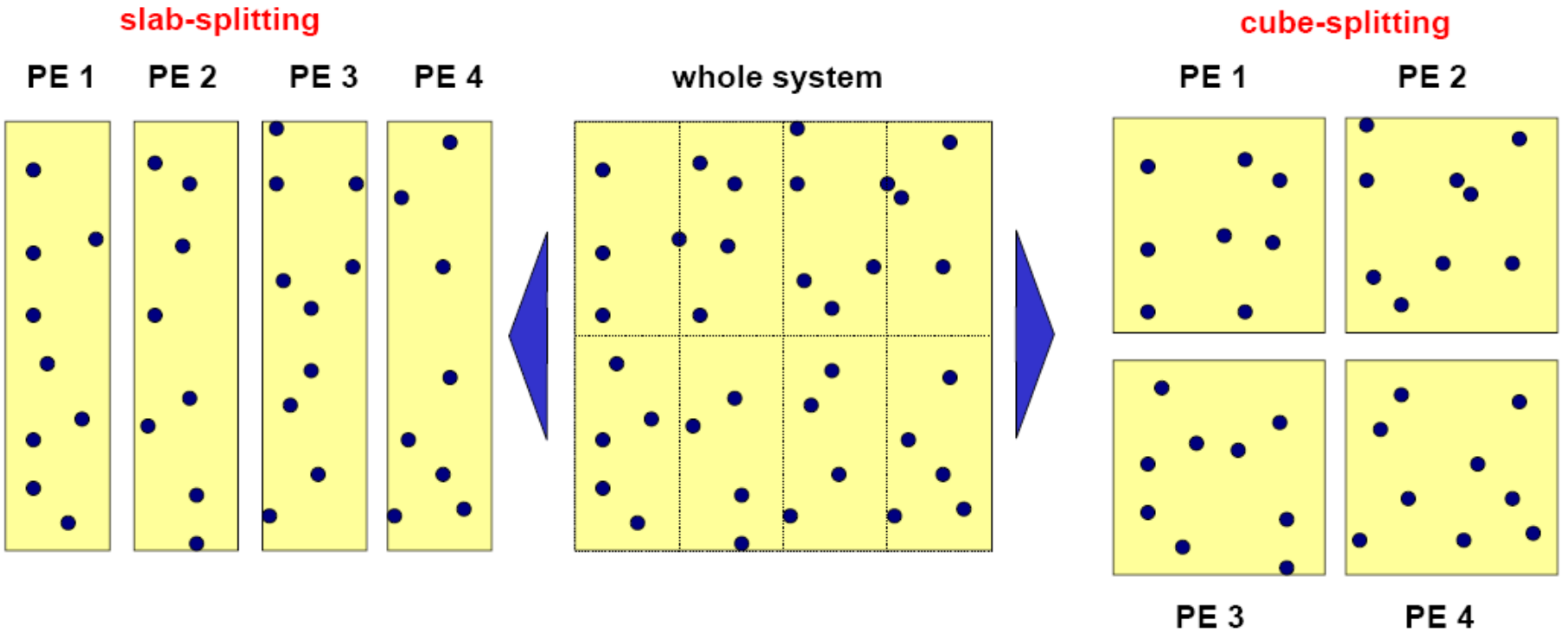
National Nuclear Security Administration

Top-500: System Architecture



Domain Decomposition

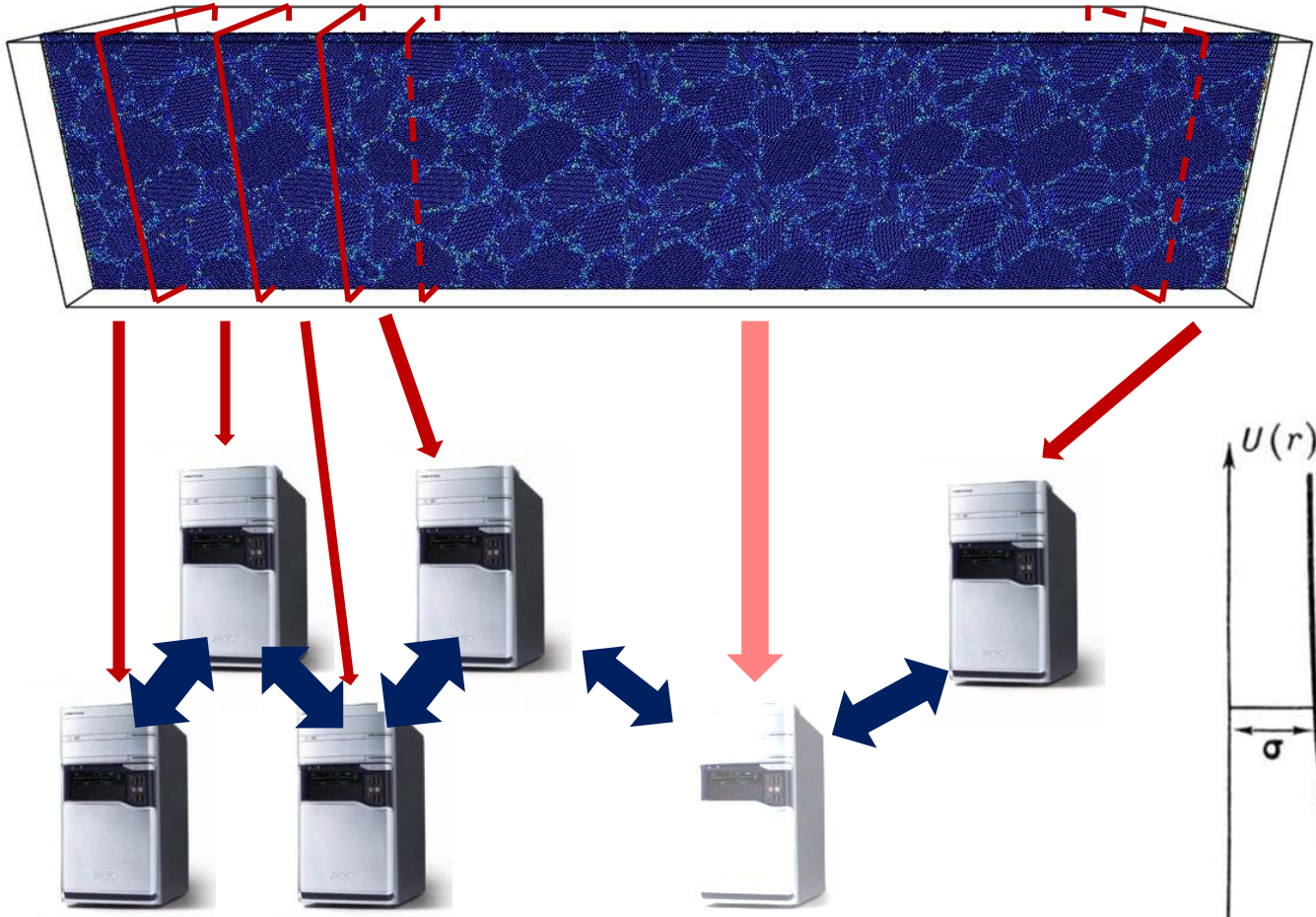
Principle:
- Distribute the spatial domain most uniform among processors
- Particles can move across different processors
- Only local communications required (interacting particles are on the local and neighbored processors)

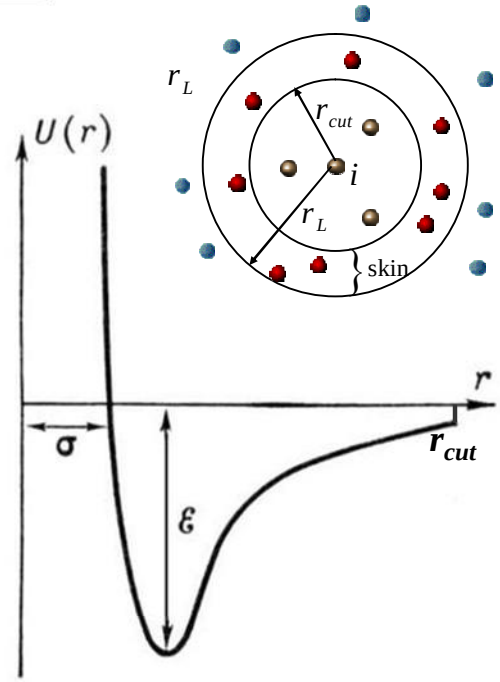


small number of neighbor cells:
2 neighbors

small surface area:
8 / 26 neighbors (2-/3-dim)

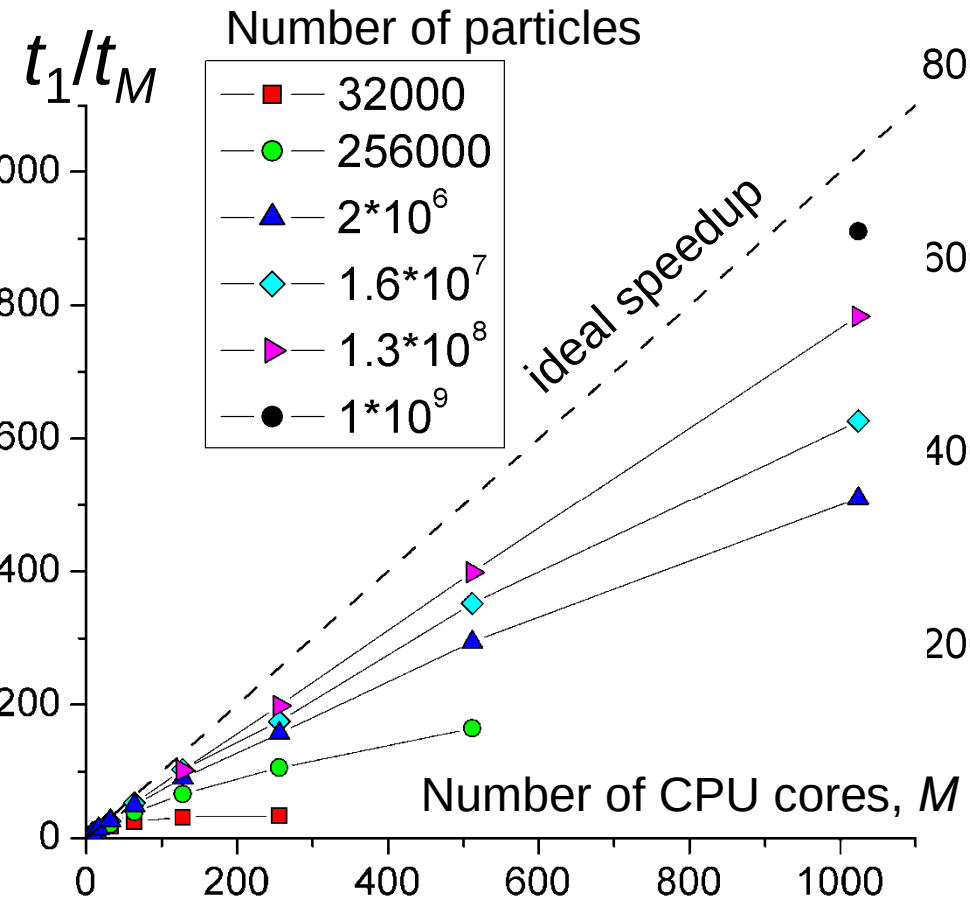
Domain decomposition



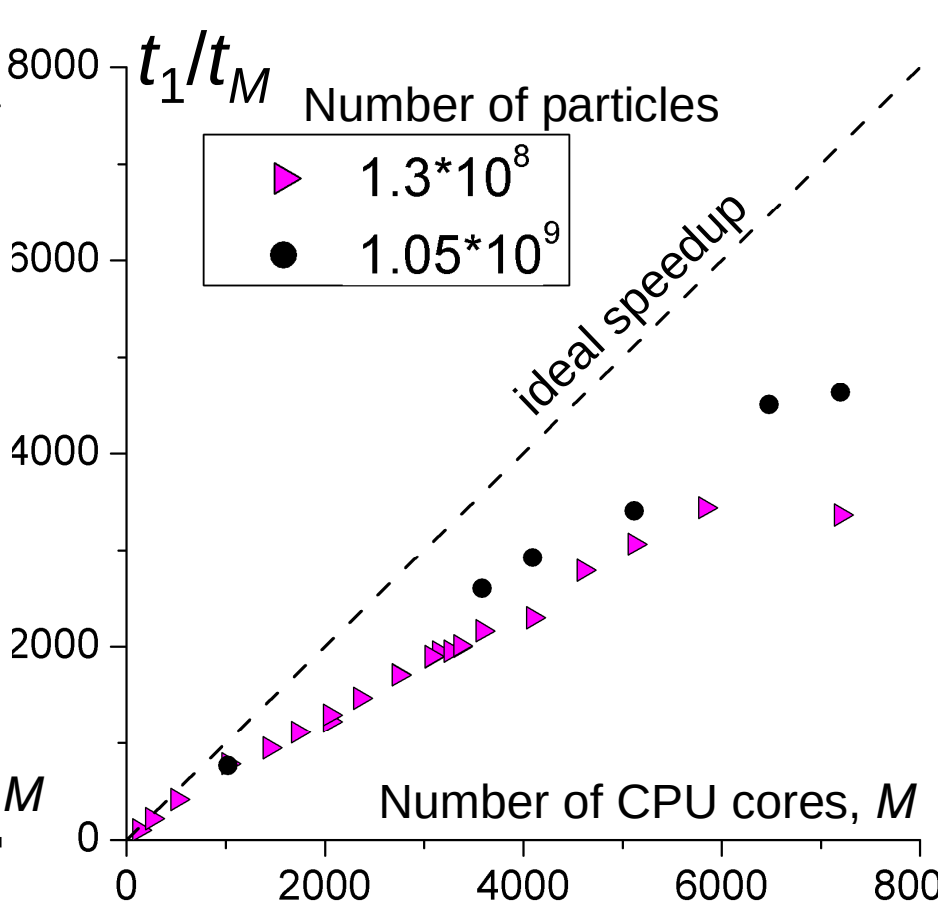


Speedup depending on the number of CPU cores*

Simulations were performed at the MVS-100K cluster of JSCC RAS using LAMMPS



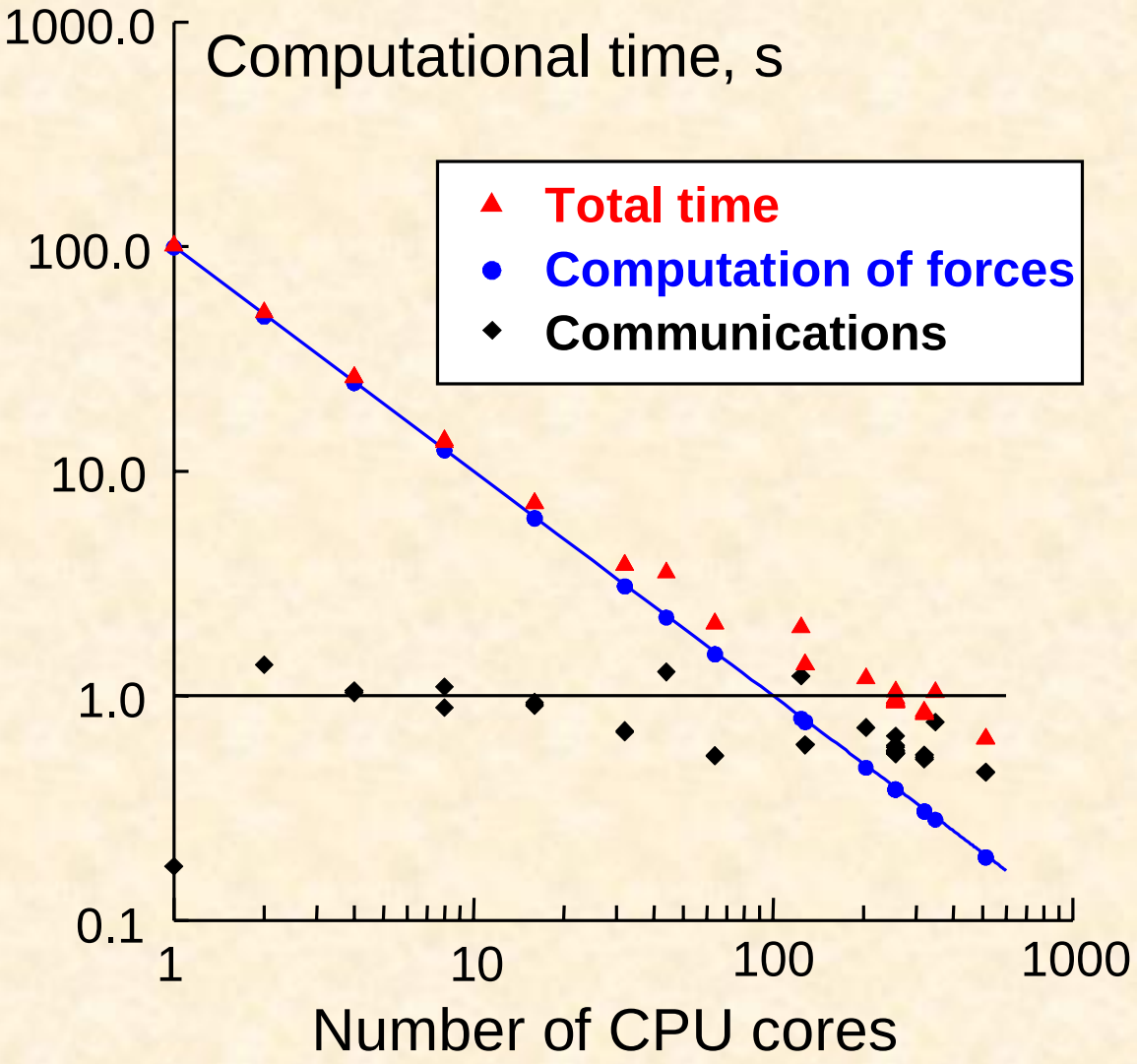
Lennard-Jones



EAM, Al

* **A. Yu. Kuksin, G.E.Norman, V. V. Stegailov, and A. V. Yanilkin // Journal of Engineering Thermophysics, 2009, Vol. 18, No. 3, pp. 197–226.**

CPU number limit due to interprocess communications



The number of particles is fixed to
N = 32 000

Lennard-Jones interaction potential with large cut-off length
R_{cut} = 7.0

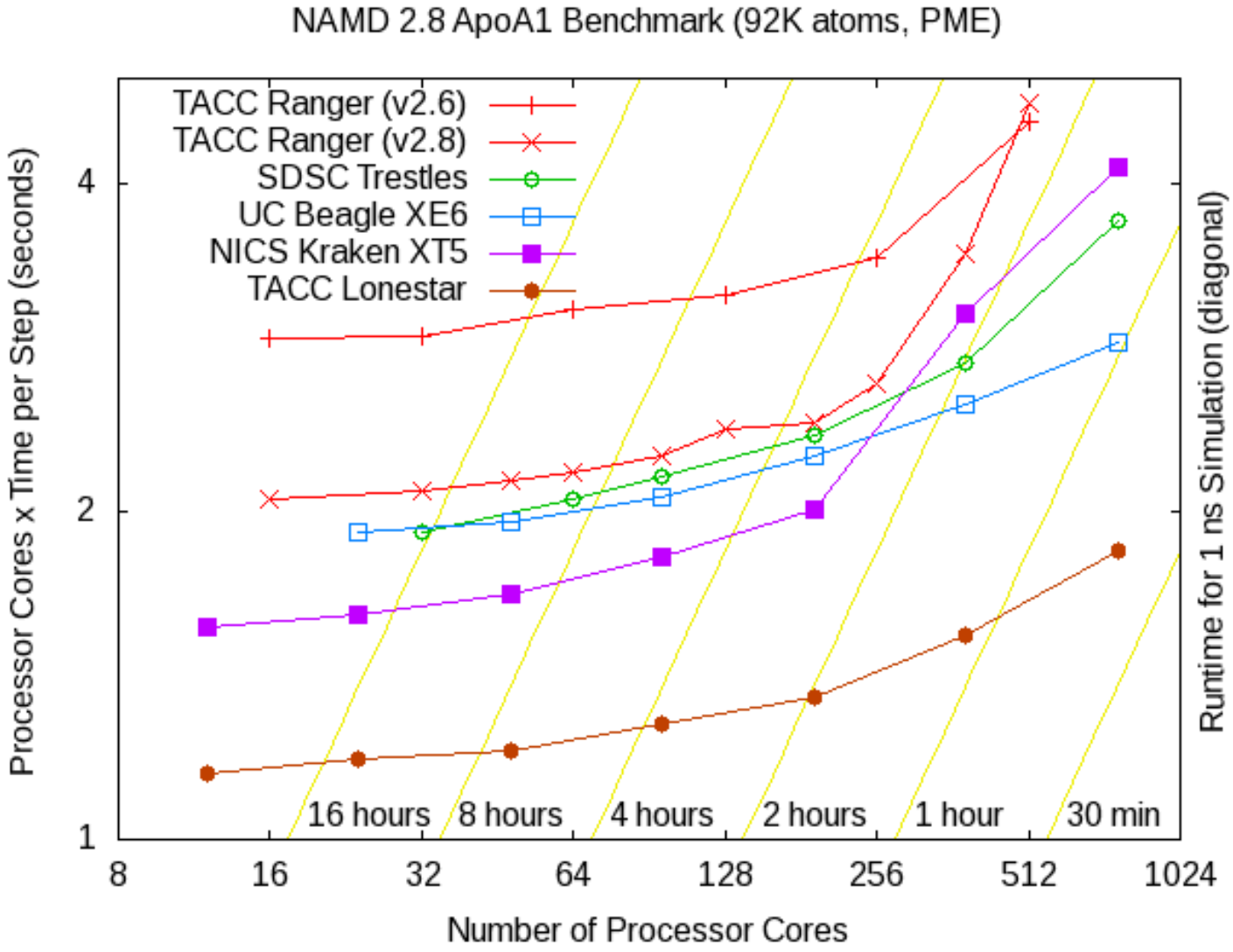
Computing cluster
MIPT–60

Application
LAMMPS

* A. Yu. Kuksin, G.E.Norman, V. V. Stegailov, and A. V. Yanilkin // Journal of Engineering Thermophysics, 2009, Vol. 18, No. 3, pp. 197–226.

NAMD: weak scaling for different clusters

92,224 atoms, 12A cutoff + PME every 4 steps, periodic



Source: http://www.ks.uiuc.edu/Research/namd/performance.html

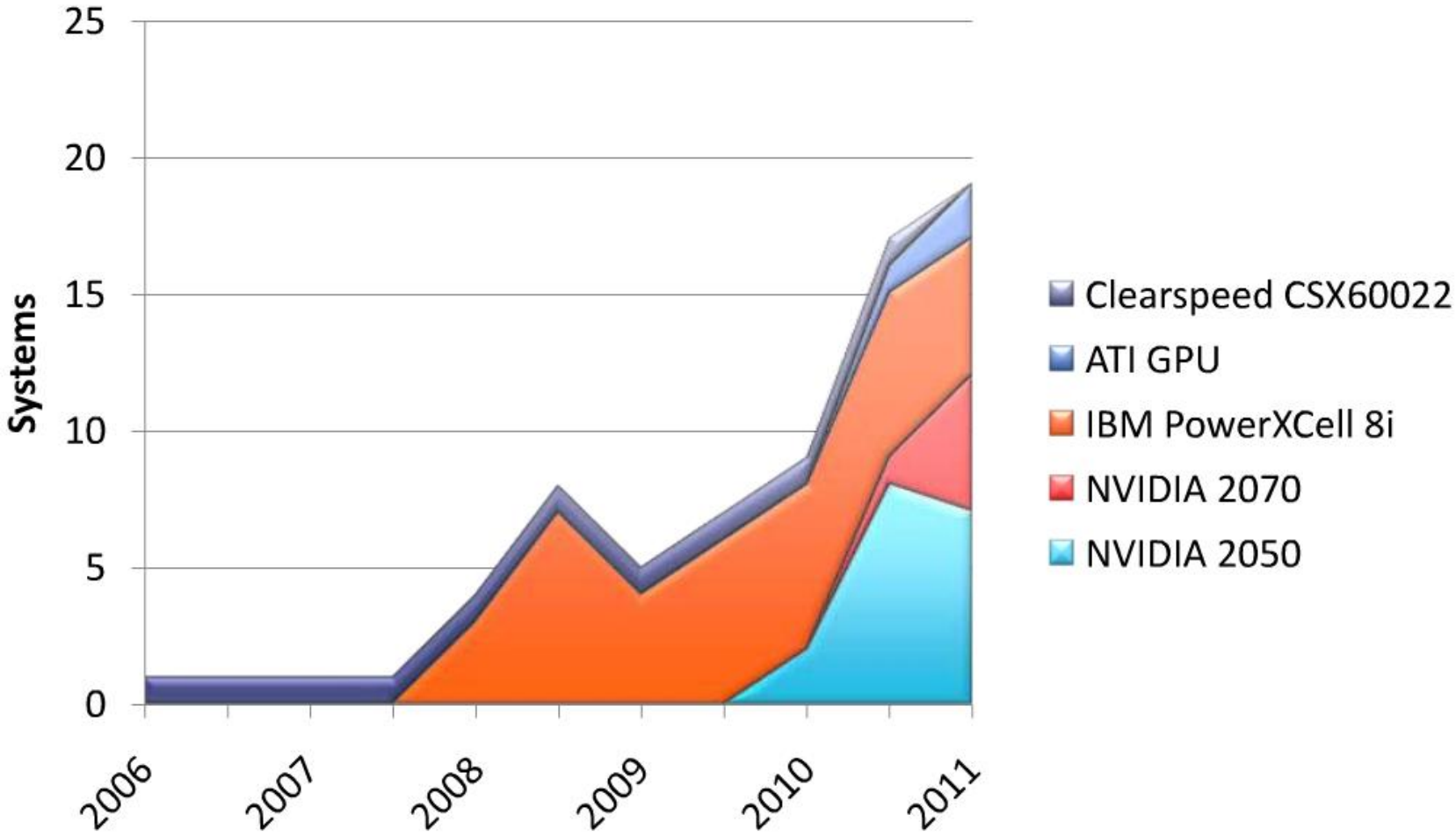

ACCELERATION USING GPUs

Top 500 Supercomputers (June 2012)*

Rank	Site	Computer/Year Vendor	Cores	R_{max}	R_{peak}	Power
1	DOE/NNSA/LLNL United States	**Sequoia** - BlueGene/Q, Power BQC 16C 1.60 GHz, Custom / 2011 IBM	1572864	16324.75	20132.66	7890.0
2	RIKEN Advanced Institute for Computational Science (AICS) Japan	K computer, SPARC64 VIIIfx 2.0GHz, Tofu interconnect / 2011 Fujitsu	705024	10510.00	11280.38	12659.9
3	DOE/SC/Argonne National Laboratory United States	**Mira** - BlueGene/Q, Power BQC 16C 1.60GHz, Custom / 2012 IBM	786432	8162.38	10066.33	3945.0
4	Leibniz Rechenzentrum Germany	**SuperMUC** - iDataPlex DX360M4, Xeon E5-2680 8C 2.70GHz, Infiniband FDR / 2012 IBM	147456	2897.00	3185.05	3422.7
5	National Supercomputing Center in Tianjin China	**Tianhe-1A** - NUDT YH MPP, Xeon X5670 6C 2.93 GHz, NVIDIA 2050 / 2010 NUDT	186368	2566.00	4701.00	4040.0
6	DOE/SC/Oak Ridge National Laboratory United States	**Jaguar** - Cray XK6, Opteron 6274 16C 2.200GHz, Cray Gemini interconnect, NVIDIA 2090 / 2009 Cray Inc.	298592	1941.00	2627.61	5142.0
7	CINECA Italy	**Fermi** - BlueGene/Q, Power BQC 16C 1.60GHz, Custom / 2012 IBM	163840	1725.49	2097.15	821.9
8	Forschungszentrum Juelich (FZJ) Germany	**JuQUEEN** - BlueGene/Q, Power BQC 16C 1.60GHz, Custom / 2012 IBM	131072	1380.39	1677.72	657.5
9	CEA/TGCC-GENCI France	**Curie thin nodes** - Bullx B510, Xeon E5-2680 8C 2.700GHz, Infiniband QDR / 2012 Bull	77184	1359.00	1667.17	2251.0
10	National Supercomputing Centre in Shenzhen (NSCS) China	**Nebulae** - Dawning TC3600 Blade System, Xeon X5650 6C 2.66GHz, Infiniband QDR, NVIDIA 2050 / 2010 Dawning	120640	1271.00	2984.30	2580.0

http://www.top500.org

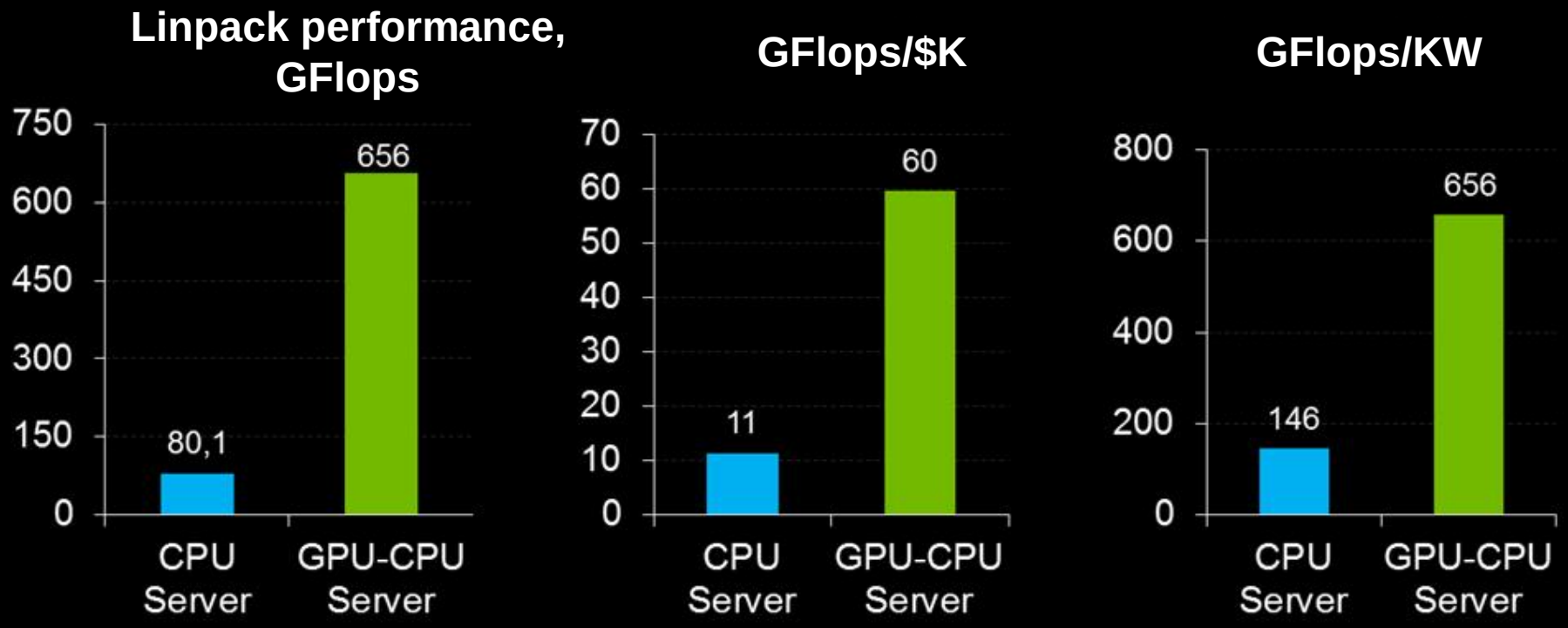
Accelerators in supercomputers



Источник: Top500.org

Горбас С.А., XIII Международная суперкомпьютерная конференция «Научный сервис в сети интернет: экзафлопсное будущее», 14-24 сентября 2011г.

GPU vs CPU: Performance, Cost, Energy Saving*

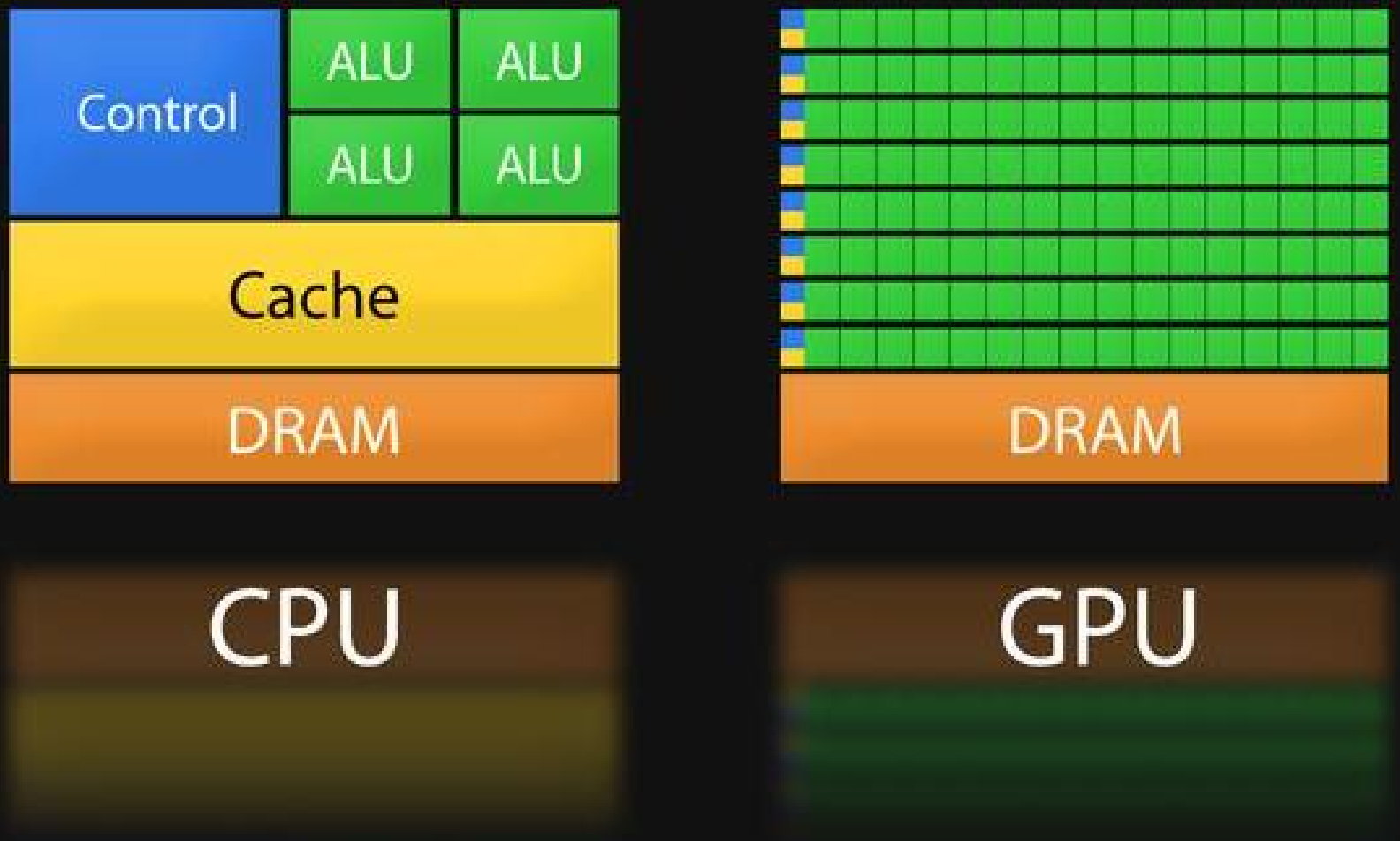


CPU 1U Server: 2x Intel Xeon X5550 (Nehalem) 2.66 GHz, 48 GB memory, $7K, 0.55 kw

GPU-CPU 1U Server: 2x Tesla C2050 + 2x Intel Xeon X5550, 48 GB memory, $11K, 1.0 kw

Anton Dzhoraev, The 1st Research and Practice Conference “High Performance Computing on GPUs”, Perm, Russia, May 21-25, 2012

Comparison of CPU and GPU architectures*



*Original location: http://www.chepr.ru/index.php?rasd=info&id=75

GPU-enabled MD simulation packages

LAMMPS

Large-scale Atomic/Molecular Massively Parallel Simulator
Sandia National Lab, USA
http://lammps.sandia.gov, Free.

HOOMD-blue

Highly Optimized Object Oriented Molecular Dynamics
Developers: J.A. Anderson, A. Travesset
Iowa State University, Ames, IA 50011, USA
http://codeblue.umich.edu/hoomd-blue/, Free.

NAMD Scalable Molecular Dynamics
VMD Visual Molecular Dynamics

NAMD/VMD
University of Illinois at Urbana-Champaign (UIUC), USA
http://www.ks.uiuc.edu/Research/namd, Free.

GROMACS + OpenMM

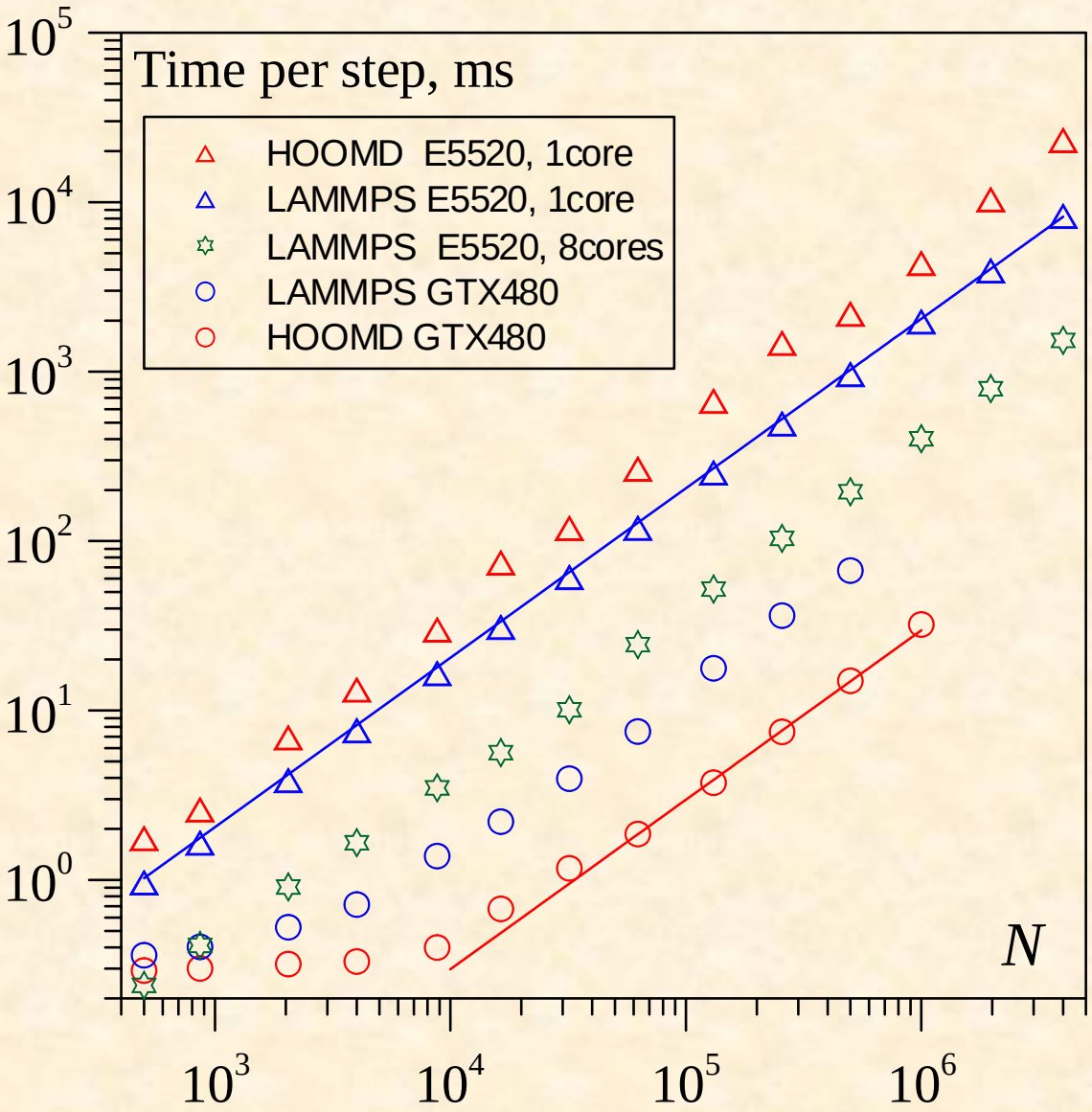
MDGPU

AMBER

ACE-MD

HALMD

Time of a single step execution (the lower the better) for different number of particles



Benchmarks for Lennard-Jones liquid:

$\rho = 0.84$, $T=0.64$,

$r_{cut} = 3$, $r_{skin} = 0.8$

MD simulation packages:

LAMMPS (18 Feb 2011)

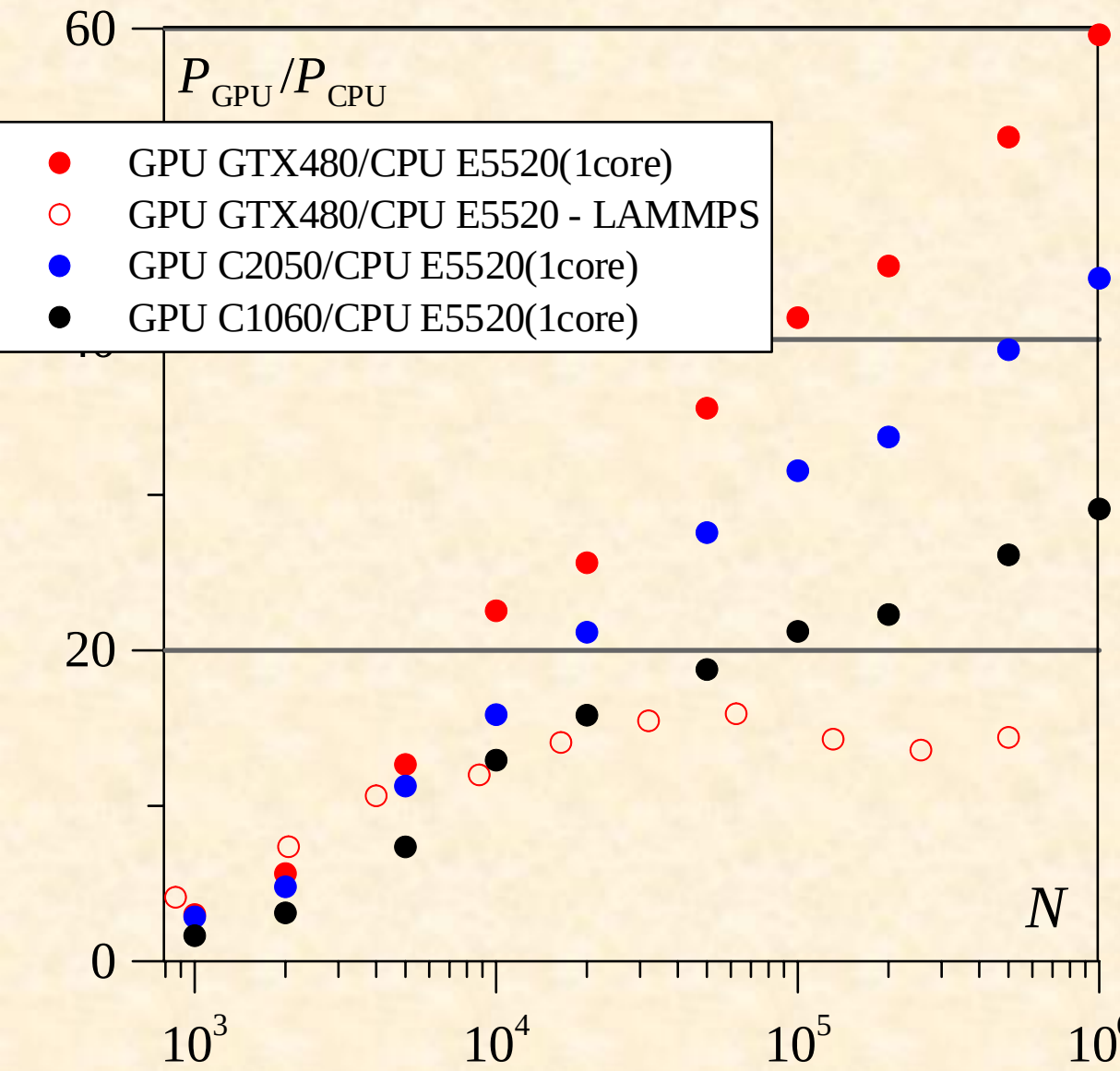
HOOMD ver. 0.9.1

Compilers:

icc 11.0 20090318

CUDA 3.2, V0.2.1221

Ratio between GPU and CPU performances depending on the number of particles



60 X

Benchmarks for Lennard-Jones liquid:

$\rho = 0.19$, $T=1.0$,

$r_{cut} = 3$, $r_{skin} = 0.8$

MD simulation packages:

LAMMPS (20 May 2010)

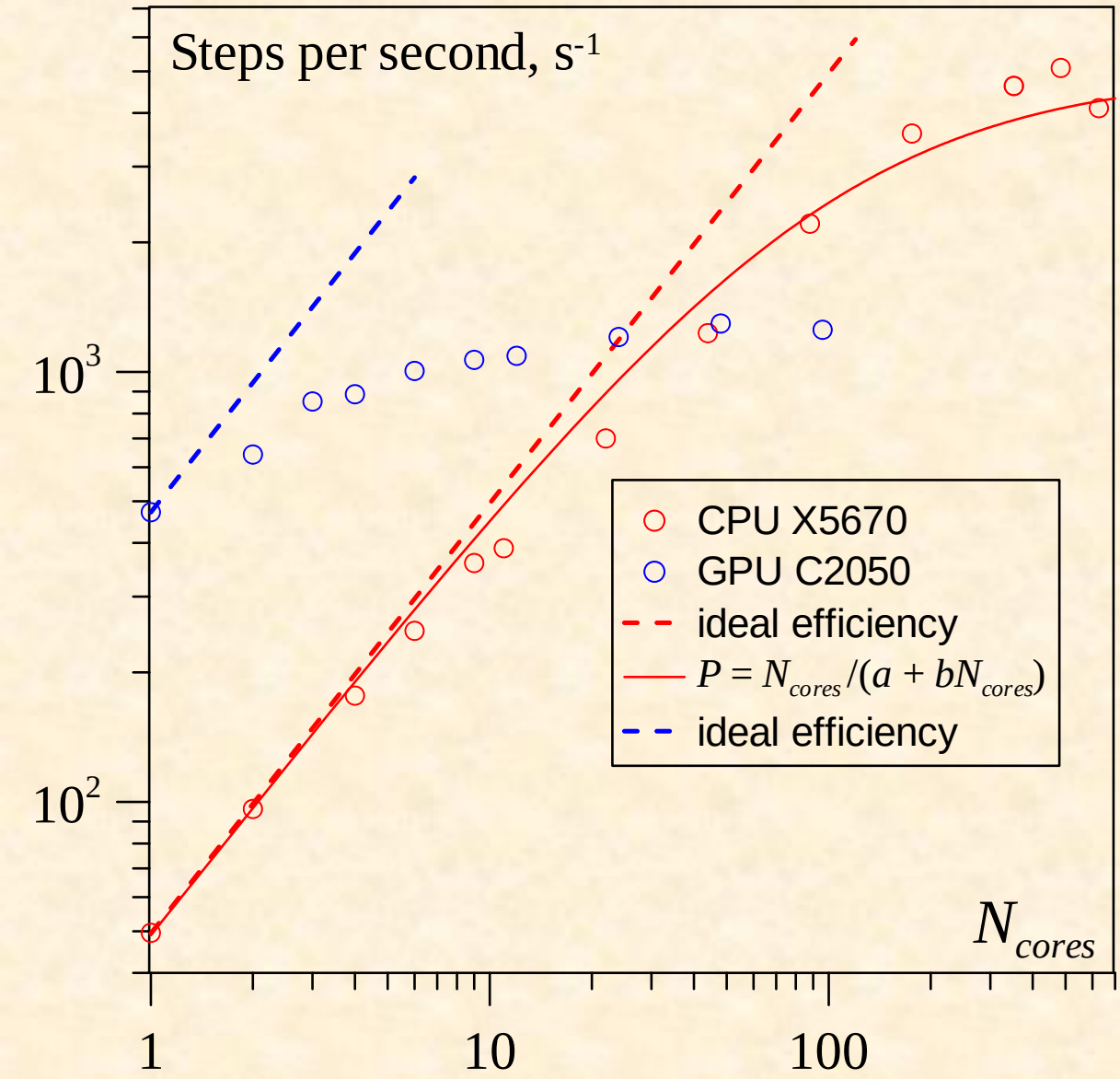
HOOMD ver. 0.9.0

Compilers:

icc 11.0 20090318

CUDA 3.2, V0.2.1221

Time of a single step execution for different number of CPU/GPU cores of the hybrid cluster



$N_{part} = 16 \cdot 10^3$

Benchmarks for LJ liquid:

$\rho = 0.19$, $T=1.0$,

$r_{cut} = 3$, $r_{skin} = 0.8$

MD simulation packages:

LAMMPS (5 Apr 2011)

Compilers:

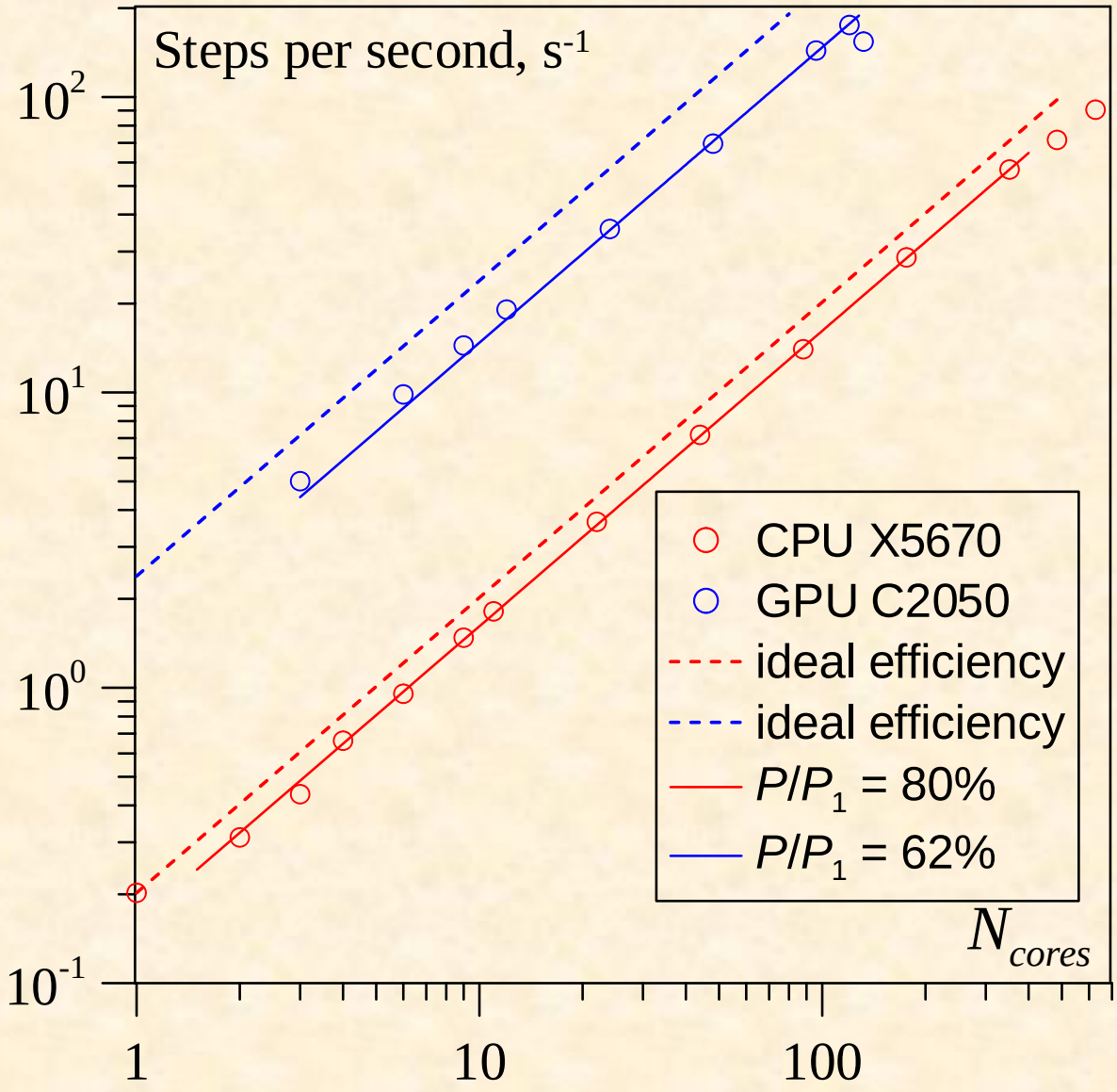
icc 11.1 20100414

CUDA 3.2, V0.2.1221

Cluster:

K100 (KIAM RAS)

Time of a single step execution for different number of CPU/GPU cores of the hybrid cluster



$N_{part} = 4 \cdot 10^6$

Benchmarks for LJ liquid:

$\rho = 0.19$, $T = 1.0$,

$r_{cut} = 3$, $r_{skin} = 0.8$

MD simulation packages:

LAMMPS (5 Apr 2011)

Compilers:

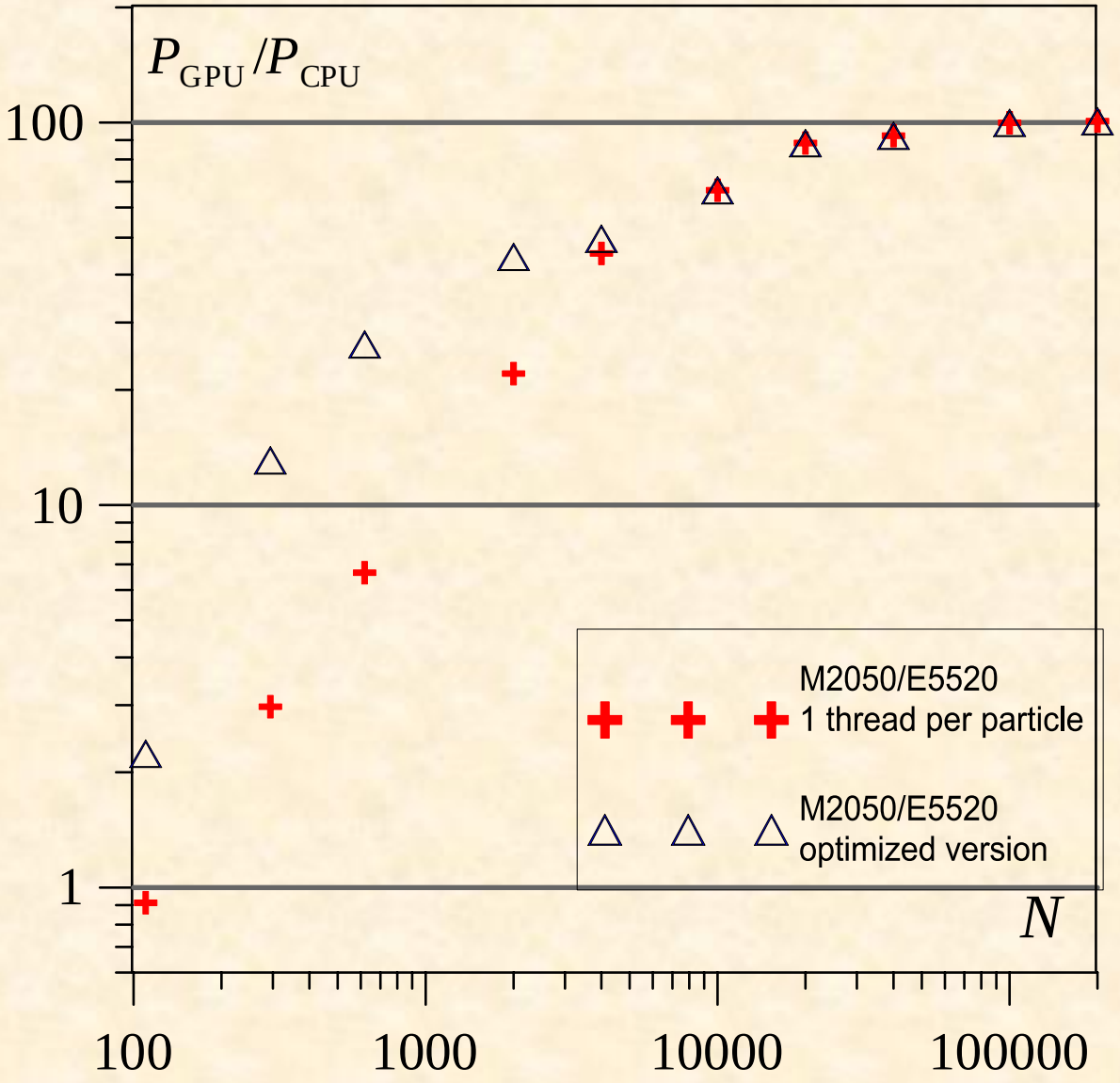
icc 11.1 20100414

CUDA 3.2, V0.2.1221

Cluster:

K100 (KIAM RAS)

Ratio between GPU and CPU performances depending on the number of particles



100 X

GPU:
NVIDIA Tesla M2050
CUDA 4.0, V0.2.1221

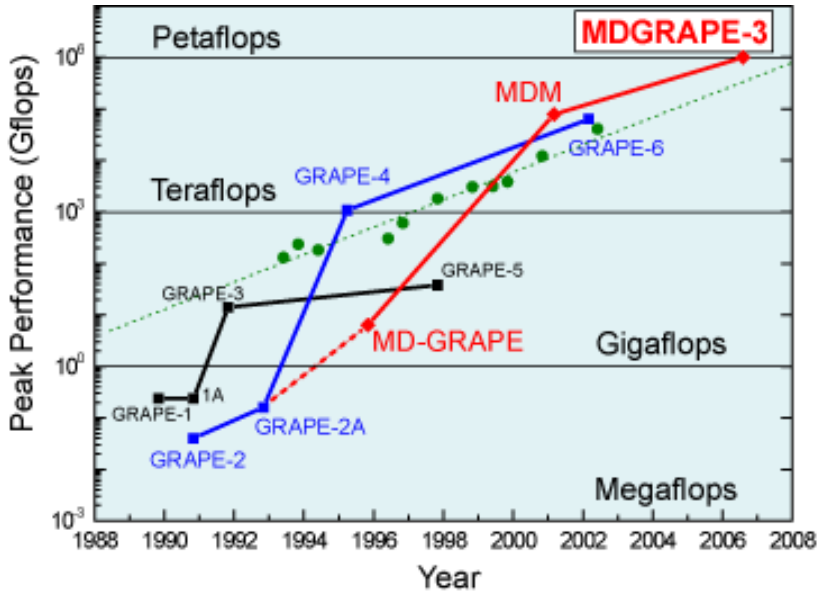
CPU:
Xeon E5520
(Nehalem),
2.27GHz, 8Mb L3
Intel compiler
ver. 11.0.083

Interactions:
Coulomb
(long-range)

RIKEN "Protein Explorer": special purpose system for molecular dynamics

1 unit = Dual-core Intel Xeon CPU
+
24 MD-GRAPE chips

201 units achieve 1 PFlops for MD



ATOMISTIC SIMULATIONS ON THE GRID

Requirements to Grid middleware

MD (or MC) numerical experiment usually goes through a number of stages:

Low level:

- prepare system in the initial state
- propagate it through the chain of other states
- obtain system properties from the MD trajectory

need for workflow

High level:

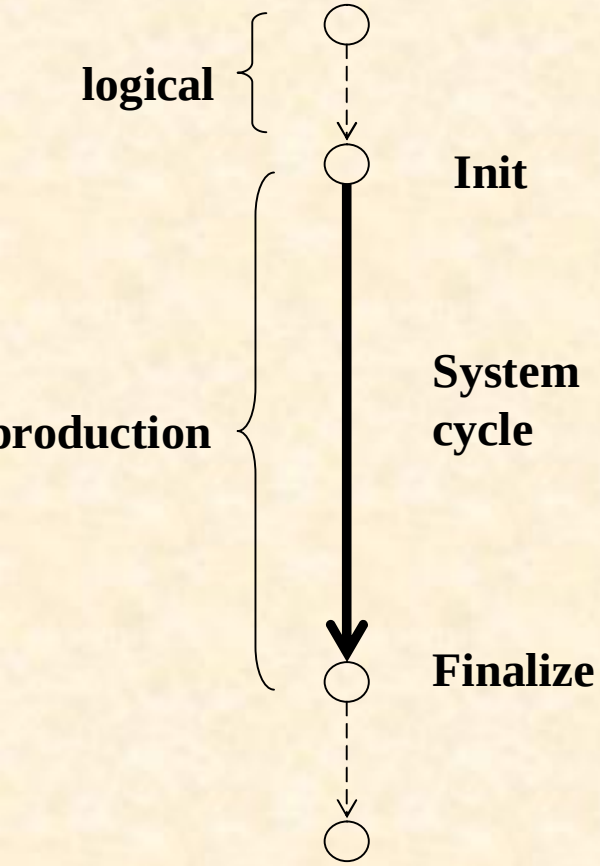
- average over a set of initial states
- perform parameter sweep
- perform optimal parameter search

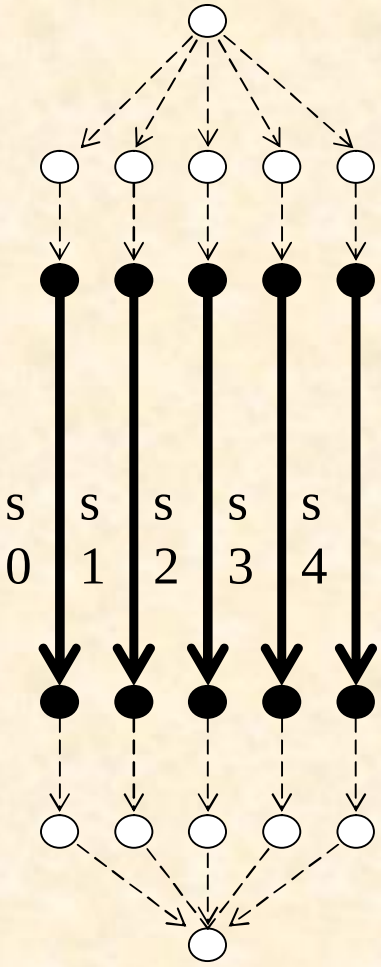
etc

need for predefined workflow scenarios

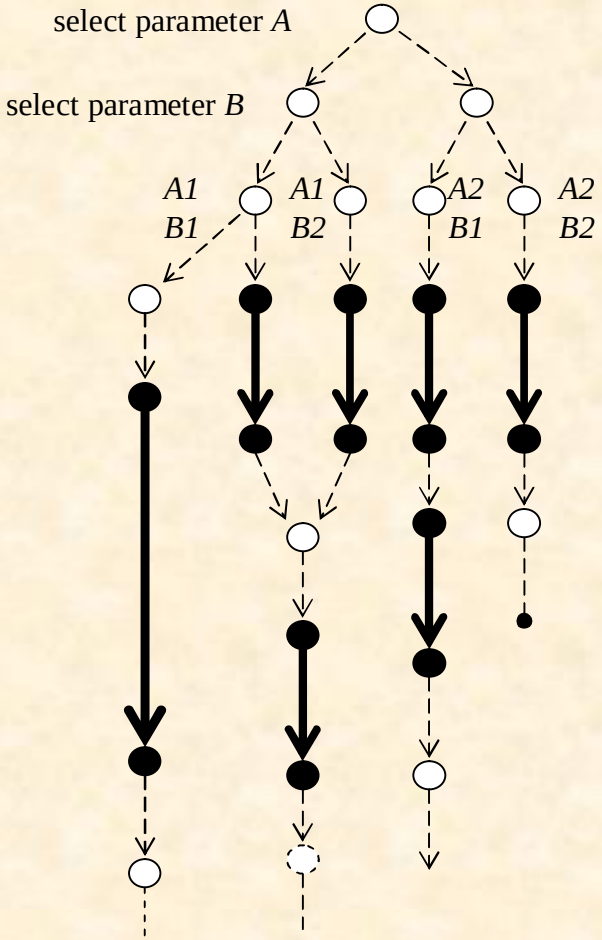
Scenarios and workflow graphs

Graph elements

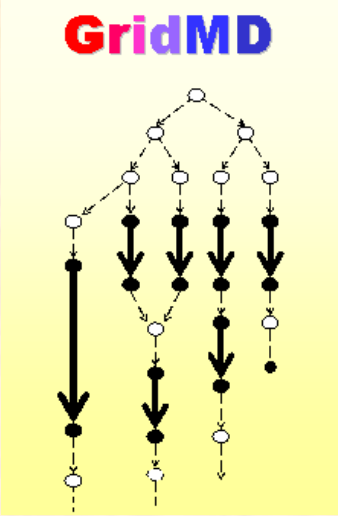




Scenario examples



Open source GridMD library



GridMD is a C++ class library intended for constructing simulation applications and running them in distributed environments

- Single application for serial (debug) and distributed execution
- Automatic workflow generation from GridMD function calls inside the main application
- Component architecture, easy interfacing to other MD packages.
- All required components for MD experiment: boundary conditions, thermodynamic ensembles, etc.)
- Support for various job managers
- Cross-platform design, compiled for Linux and Windows
- Open source code (available at http://gridmd.sourceforge.net)

Submission of the tasks to parallel and distributed systems

User code

MPI

Simulation program

local shell, ssh, Globus, *etc*

Batch system (PBS, ...)

Cluster

Working node

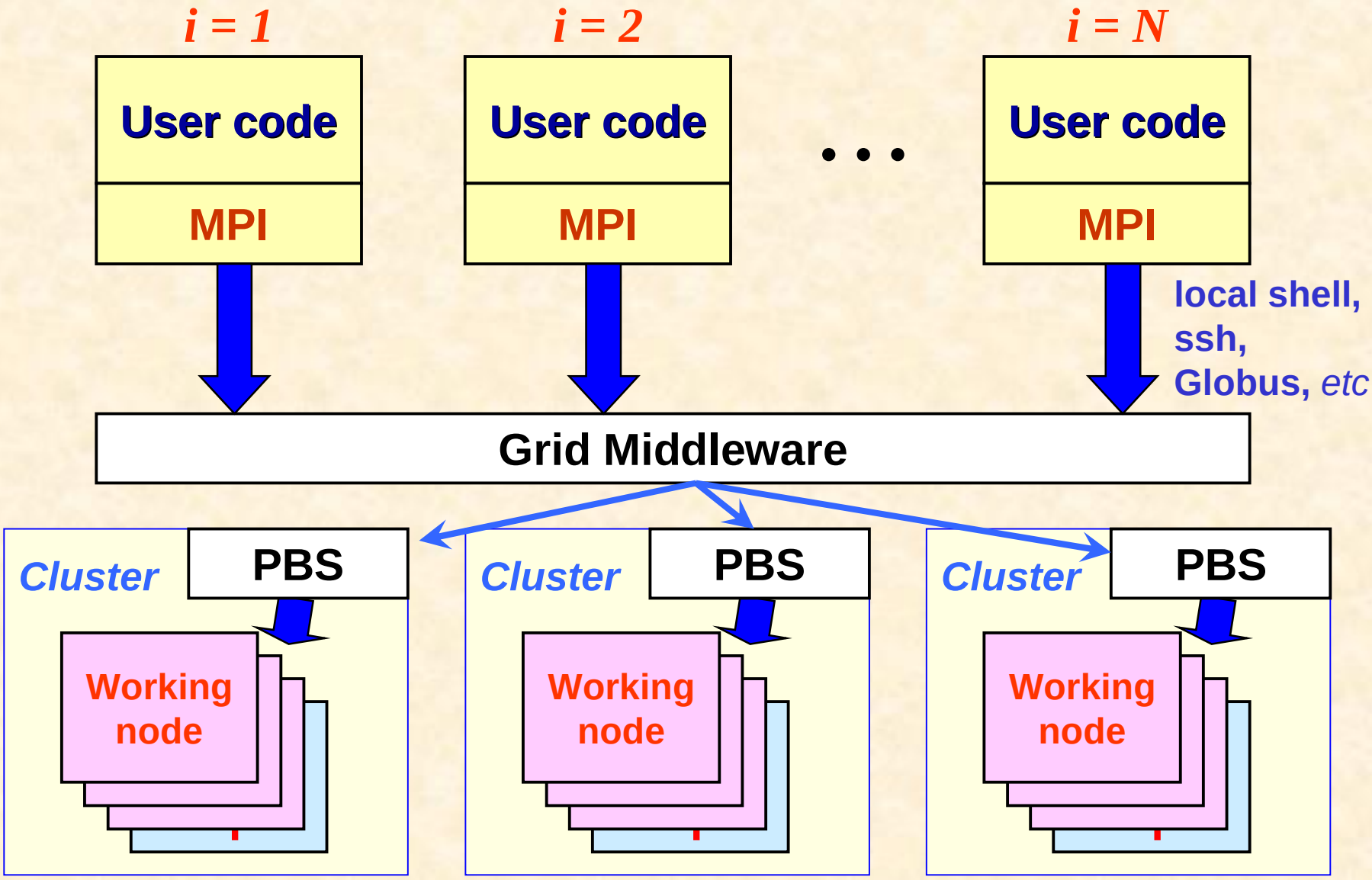
Working node

Working node

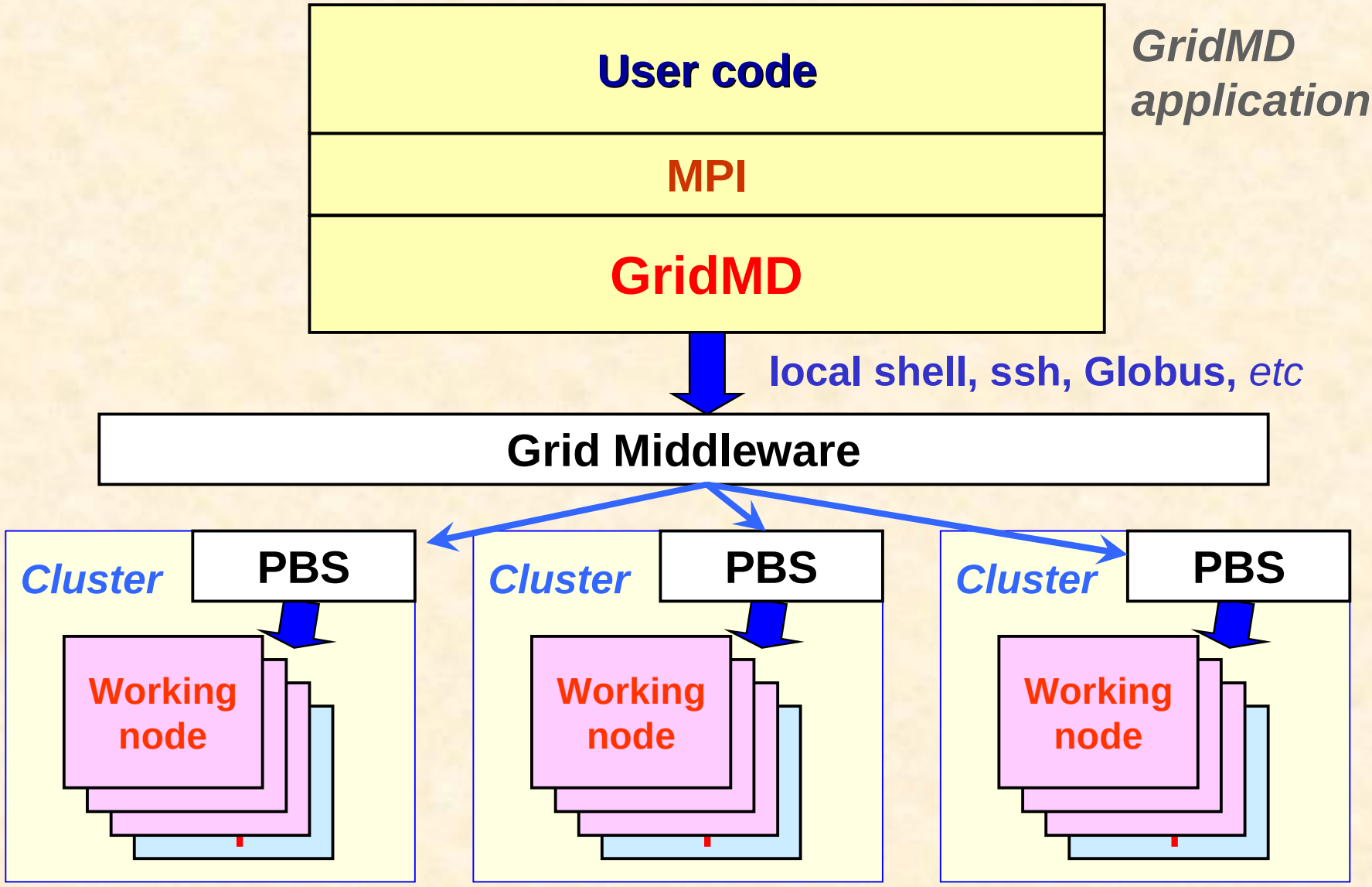
• • •

Working node

Submission of the tasks to parallel and distributed systems



Submission of the tasks to parallel and distributed systems



Submission of the tasks to parallel and distributed systems

User code
parameter sweep, optimization, workflows

MPI

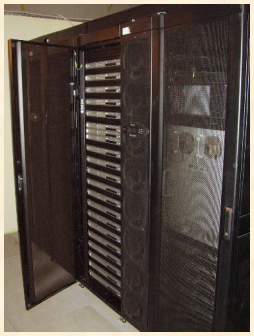
GridMD
workflow scenarios, internal job manager

GridMD application

Nimrod workflows

local shell,
ssh,
Globus, *etc*

PBS



JSCC RAS

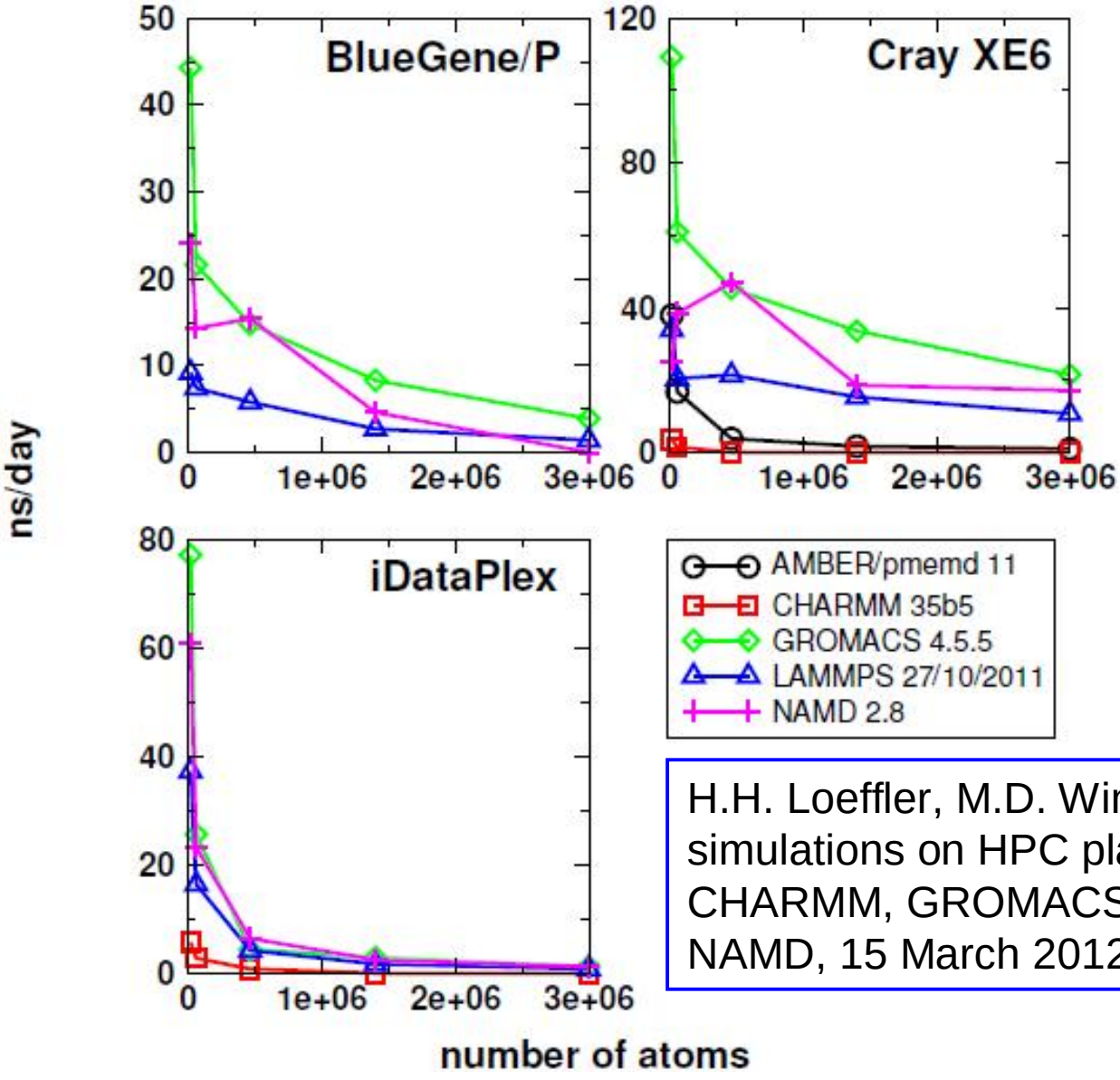
DEISA Shell

Distributed
European
Infrastructure for
Supercomputing
Applications

Open source packages for atomistic simulations

Package name	Language	GPU	Parallel	Min	MD	MC	Comment
Adun	C			+	+		User specified force field (FFML), QM/MM calculations with Empirical Valence Bond (EVB)
DL_POLY*	Fortran, C++, Java				+		General purpose MD, HDF5 output, Java GUI
GROMACS	C	+	MPI		+		High performance MD, designed for biological systems and polymers
HALMD	C++	++			+		High-precision MD for the large-scale simulation of simple and complex liquids, HDF5 output
HOOMD-blue	C++, Python	++		+	+		General-purpose MD highly optimized for GPUs
LAMMPS	C++	+	MPI	+	+	+	High parallel scalability, wide range of potentials and analysis tools
MDynaMix	Fortran		MPI		+		Parallel MD for AMBER force field
MOIL	Fortran, Tcl		MPI	+	+		Basic algorithms and force fields, Replica exchange, coarse-grained models, Tcl GUI
NAMD/VMD	C++	+	MPI				High parallel scalability, designed for biomolecular, visualization (VMD)
RedMD	C/C++	-		+	+	+	Coarse-grained models of proteins and nucleic acids
TINKER	Fortran		OpenMP	+	+	+	Simple MD, QM/MM, molecular design
XMD	C		pthreads	+	+	+	MD for metals and ceramics

Benchmarks for bimolecular simulations



H.H. Loeffler, M.D. Winn, Large biomolecular simulations on HPC platforms: III. AMBER, CHARMM, GROMACS, LAMMPS and NAMD, 15 March 2012

Source: http://www.stfc.ac.uk/cse/resources/pdf/biomolbenchiii.pdf

CONCLUSIONS

- Open source projects are particularly suitable for scientific research because they are customizable, extensible, implement a variety of ionization models and optimization techniques.
- Quasiclassical atomistic simulations of chemical reactions, ionization/recombination processes and electron-ion relaxation are still a challenge.
- GPUs can highly accelerate MD simulations in particular for long-ranged interactions.
- Averaging and parameter sweep lead allow to run simulations on Grid and Cloud environments.

Our web site: http://www.ihed.ras.ru/norman