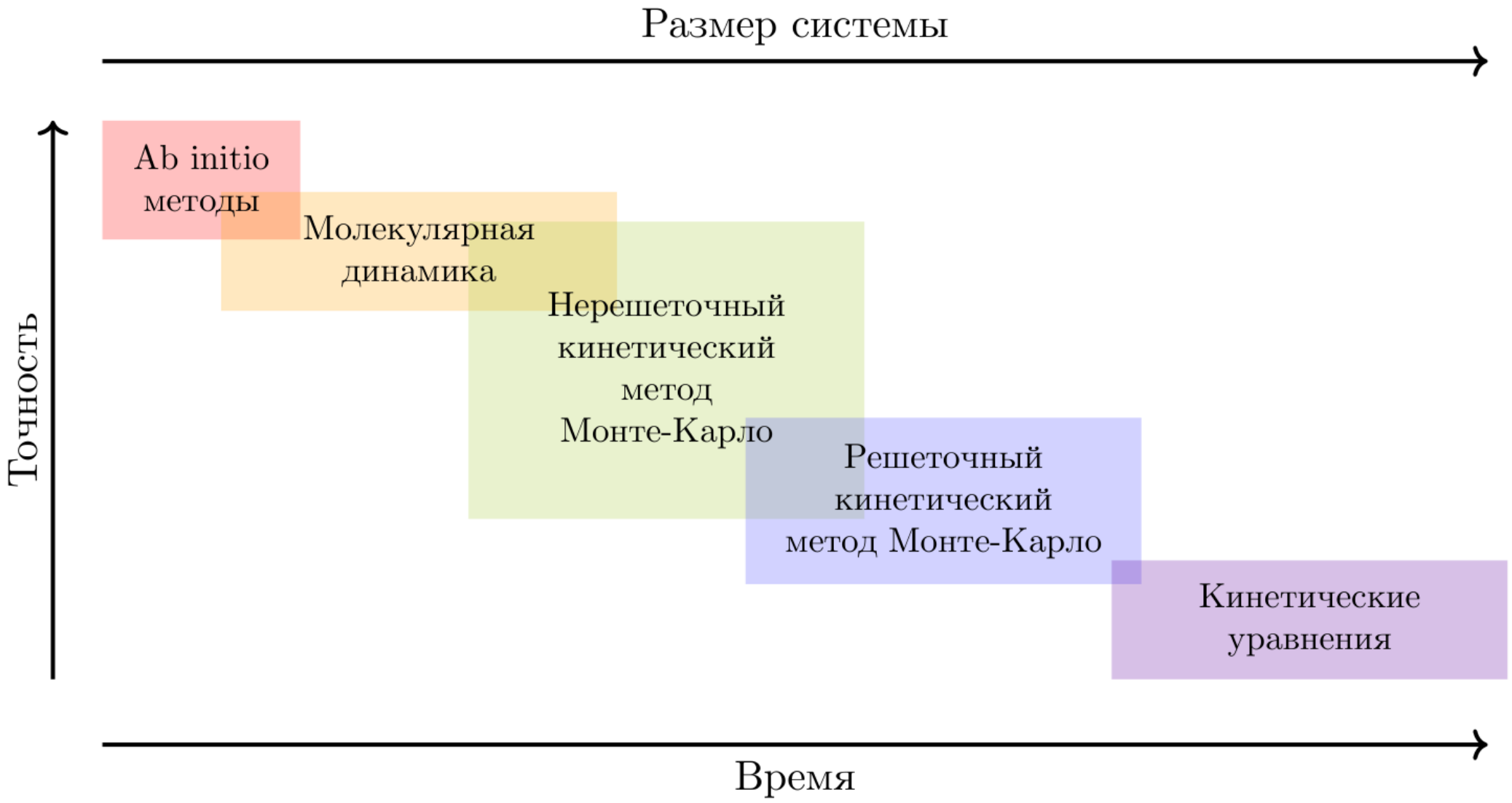
LAMMPS

Часть 1

Что будем делать

- Моделирование реконструкции поверхности Ge(110)
- Визуализация результатов с помощью matplotlib и компании

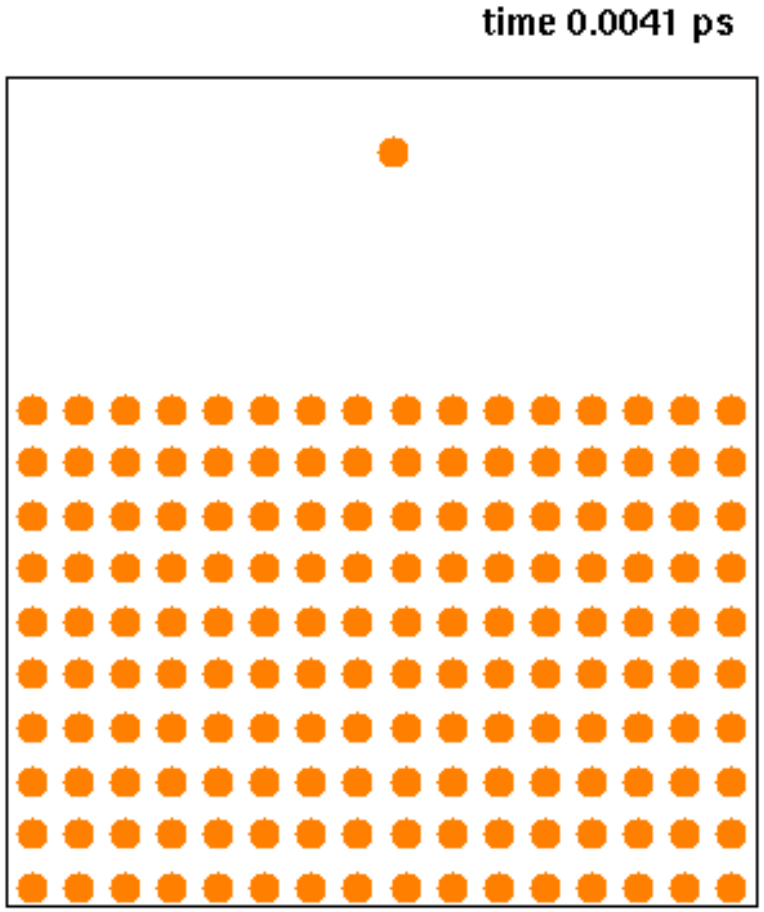
Методы исследования атомных систем



Что такое молекулярная динамика?

Метод молекулярной динамики (метод МД) — метод, в котором временная эволюция системы взаимодействующих атомов или частиц отслеживается интегрированием их уравнений движения

Подробнее – курс С. В. Колесникова, 7 семестр



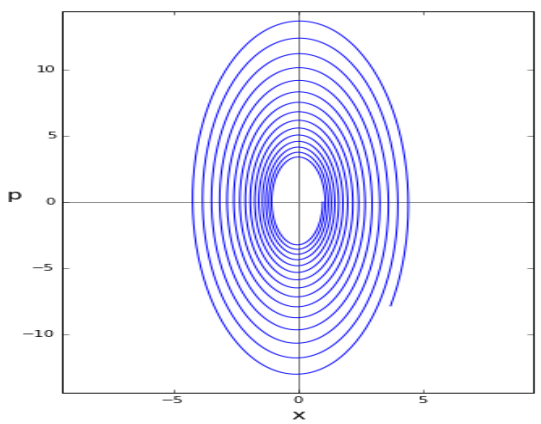
Молекулярная динамика вообще

$$\ddot{\boldsymbol{r}} = \frac{\boldsymbol{F}}{m}$$

Разностные схемы

Схема Эйлера

$$\begin{cases} \boldsymbol{r}^{i+1} = \boldsymbol{r}^i + \boldsymbol{v}^i h \\ \boldsymbol{v}^{i+1} = \boldsymbol{v}^i + \dfrac{\boldsymbol{F}^i}{m} h \end{cases}$$



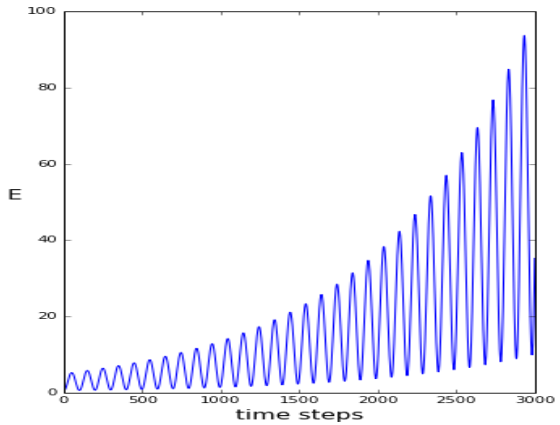
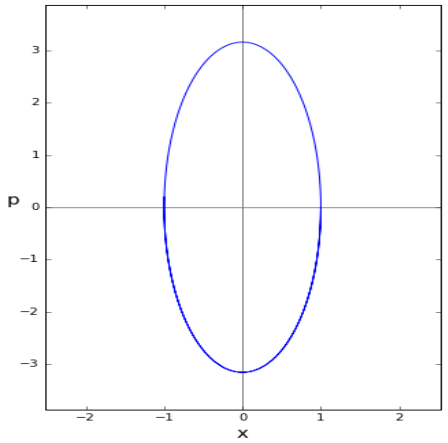
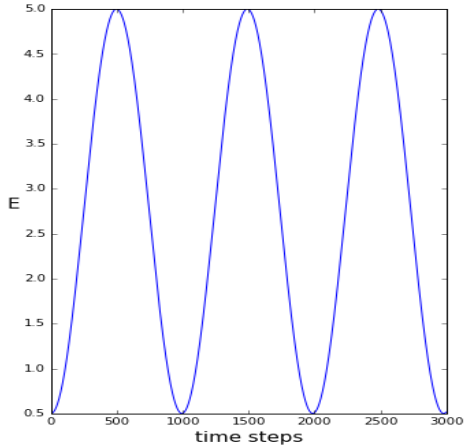


Схема Верле в скоростной форме

$$\begin{cases} \boldsymbol{r}^{i+1} = \boldsymbol{r}^i + \boldsymbol{v}^i h + \dfrac{1}{2}\dfrac{\boldsymbol{F}^i}{m} h^2 \\ \boldsymbol{v}^{i+1} = \boldsymbol{v}^i + \dfrac{1}{2m}(\boldsymbol{F}^i + \boldsymbol{F}^{i+1}) h \end{cases}$$



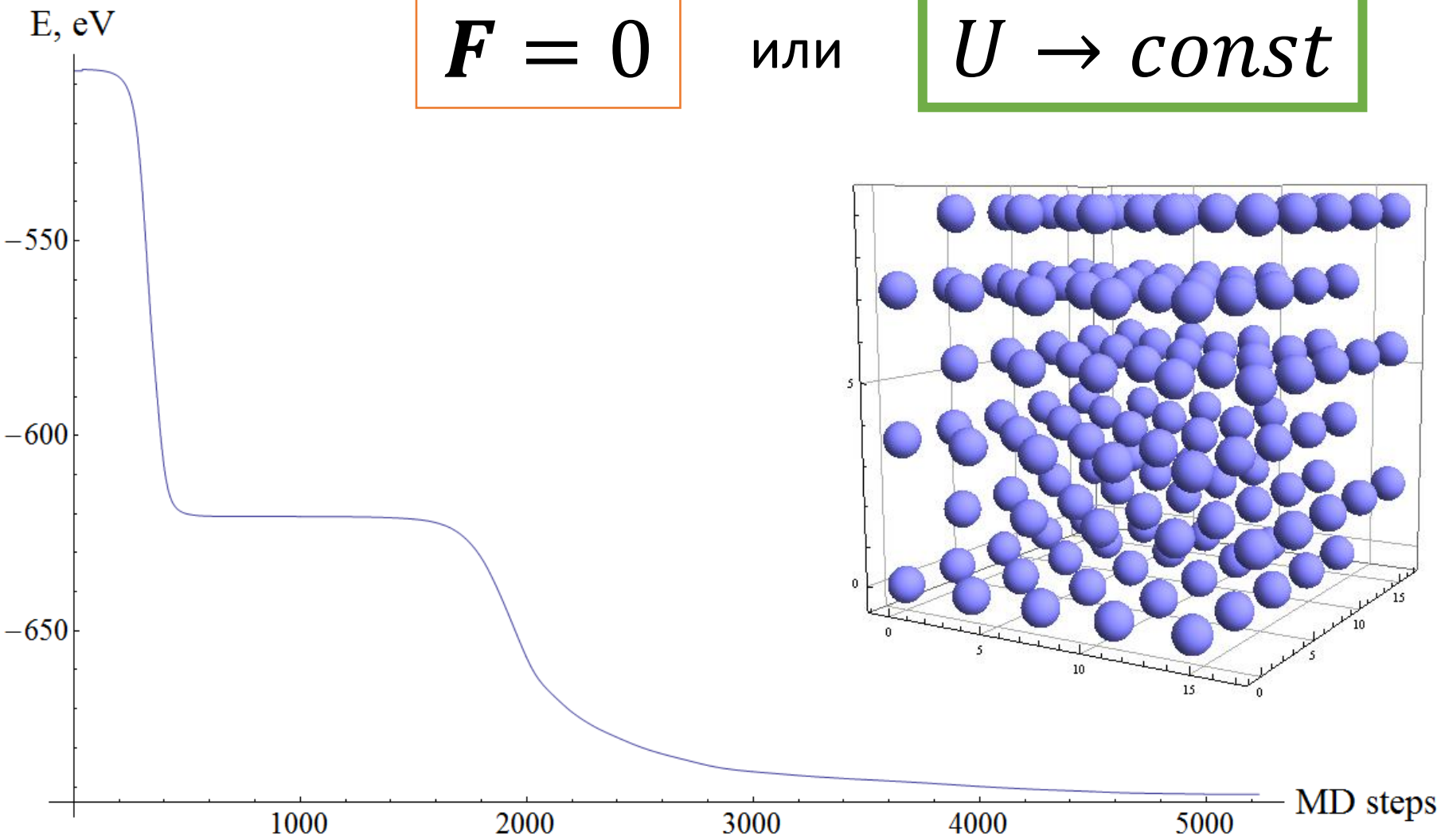


Условие останова

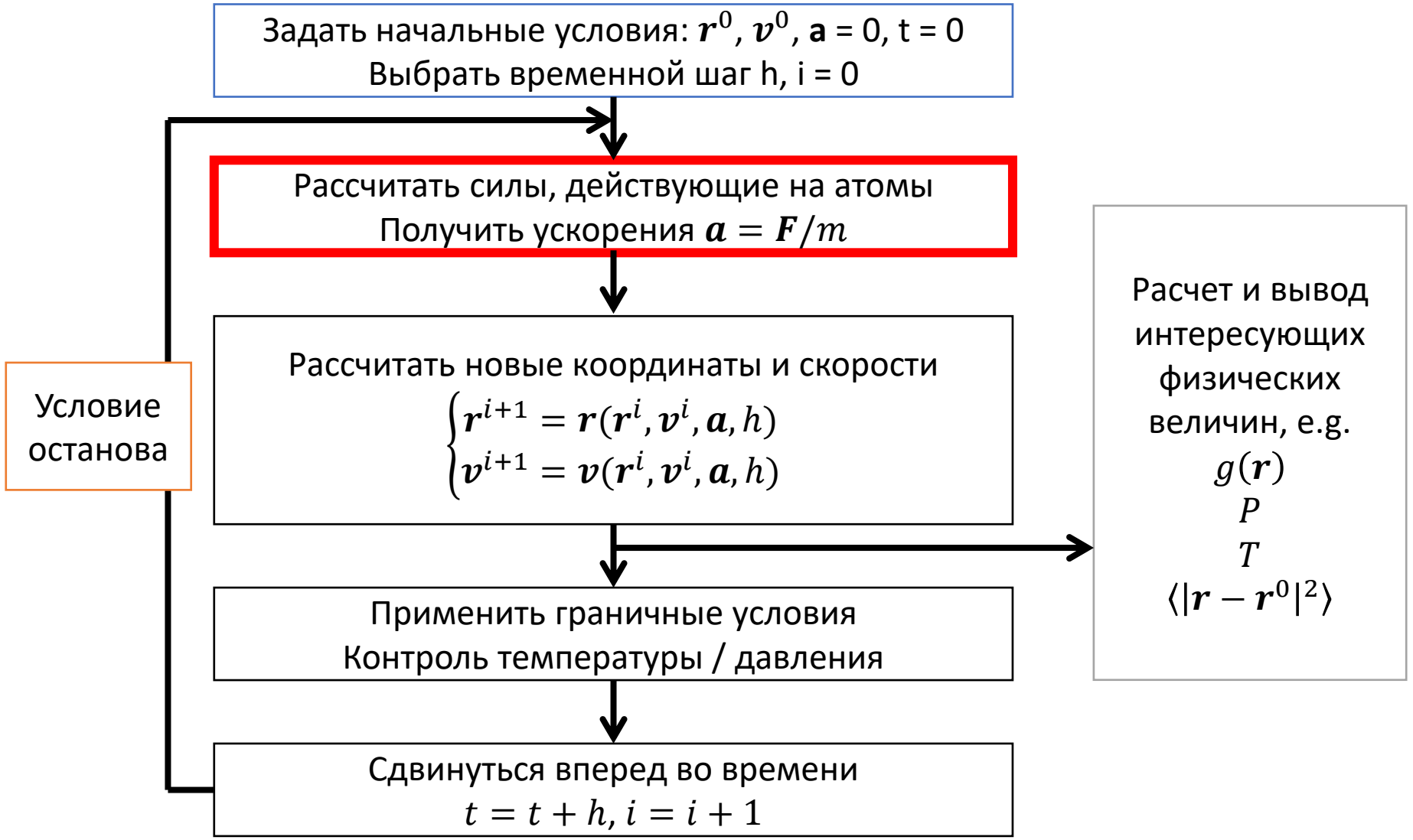
$$\boldsymbol{F} = 0$$

или

$$U \to const$$



Молекулярная динамика вообще



Классическая молекулярная динамика

$$\boldsymbol{F} = -\vec{\nabla} U(\boldsymbol{r}, \underbrace{a_1, a_2, \ldots, a_n}_{\text{параметры}})$$

Движение атомов описывается классической механикой

Межатомные силы = классические потенциальные силы.

Межатомные силы находятся как градиент потенциальной энергии

Молекулярные кристаллы

Потенциал Леннарда-Джонса (6-12)

$$U_{ij}^{LJ}(r) = A\left(\left(\frac{d_0}{r}\right)^{12} - 2\left(\frac{d_0}{r}\right)^{6}\right)$$

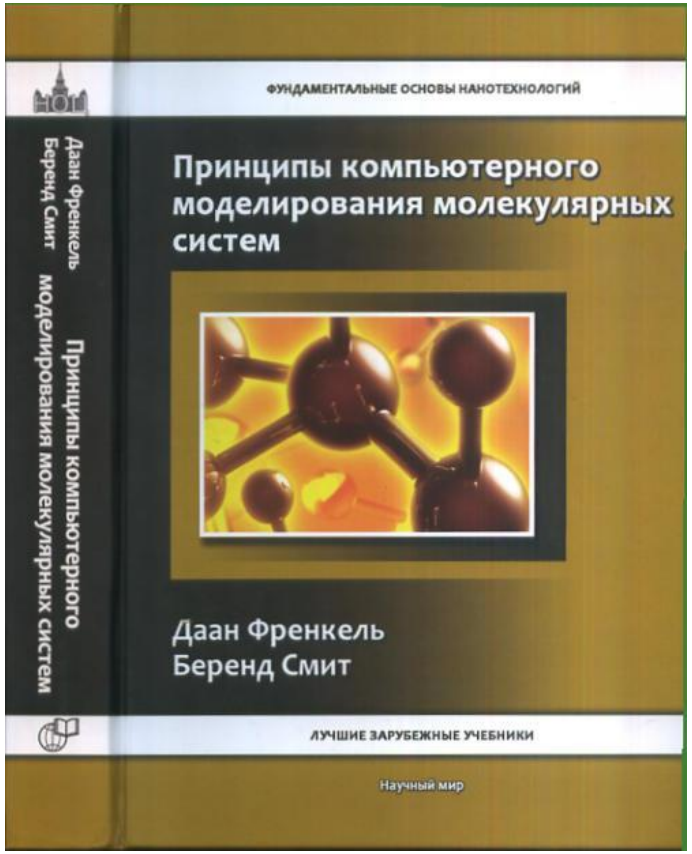
$$F = -\frac{dU_{ij}(r)}{dr} = A\frac{12}{d_0}\left(\left(\frac{d_0}{r}\right)^{13} - \left(\frac{d_0}{r}\right)^{7}\right)$$

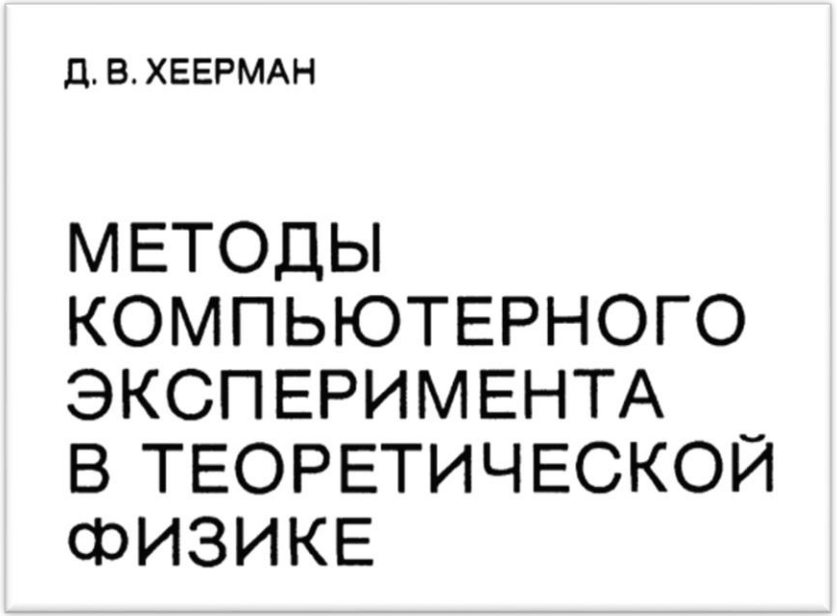
Основные положения

- Для описания движения атомов или частиц применяется классическая механика. Закон движения частиц находят при помощи аналитической механики.
- Силы межатомного взаимодействия можно представить в форме классических потенциальных сил (как градиент потенциальной энергии системы).
- Точное знание траекторий движения частиц системы на больших промежутках времени не является необходимым для получения результатов макроскопического (термодинамического) характера.
- Наборы конфигураций, получаемые в ходе расчетов методом молекулярной динамики, распределены в соответствии с некоторой статистической функцией распределения, например отвечающей микроканоническому распределению.

Литература

спецкурс С. В. Колесникова, 7 семестр

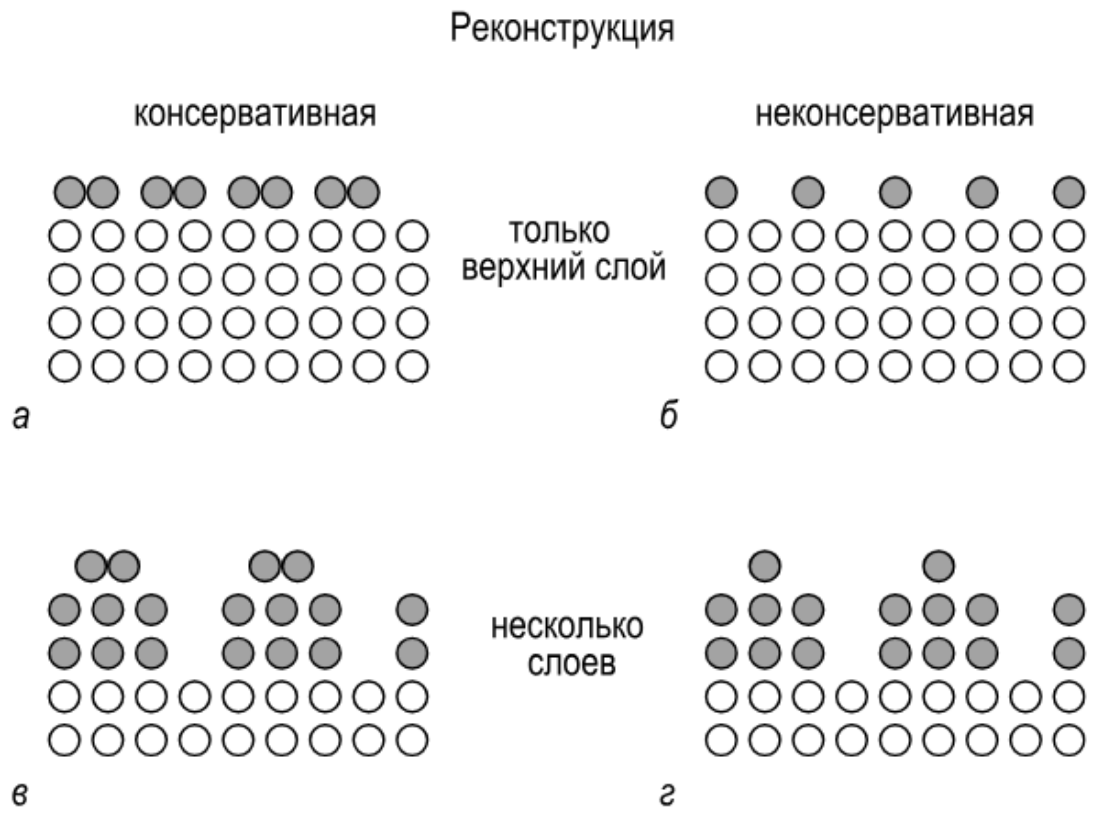




Перестройка поверхности

Выделяют 2 основных типа атомной перестройки поверхности

- Релаксация
- Реконструкция



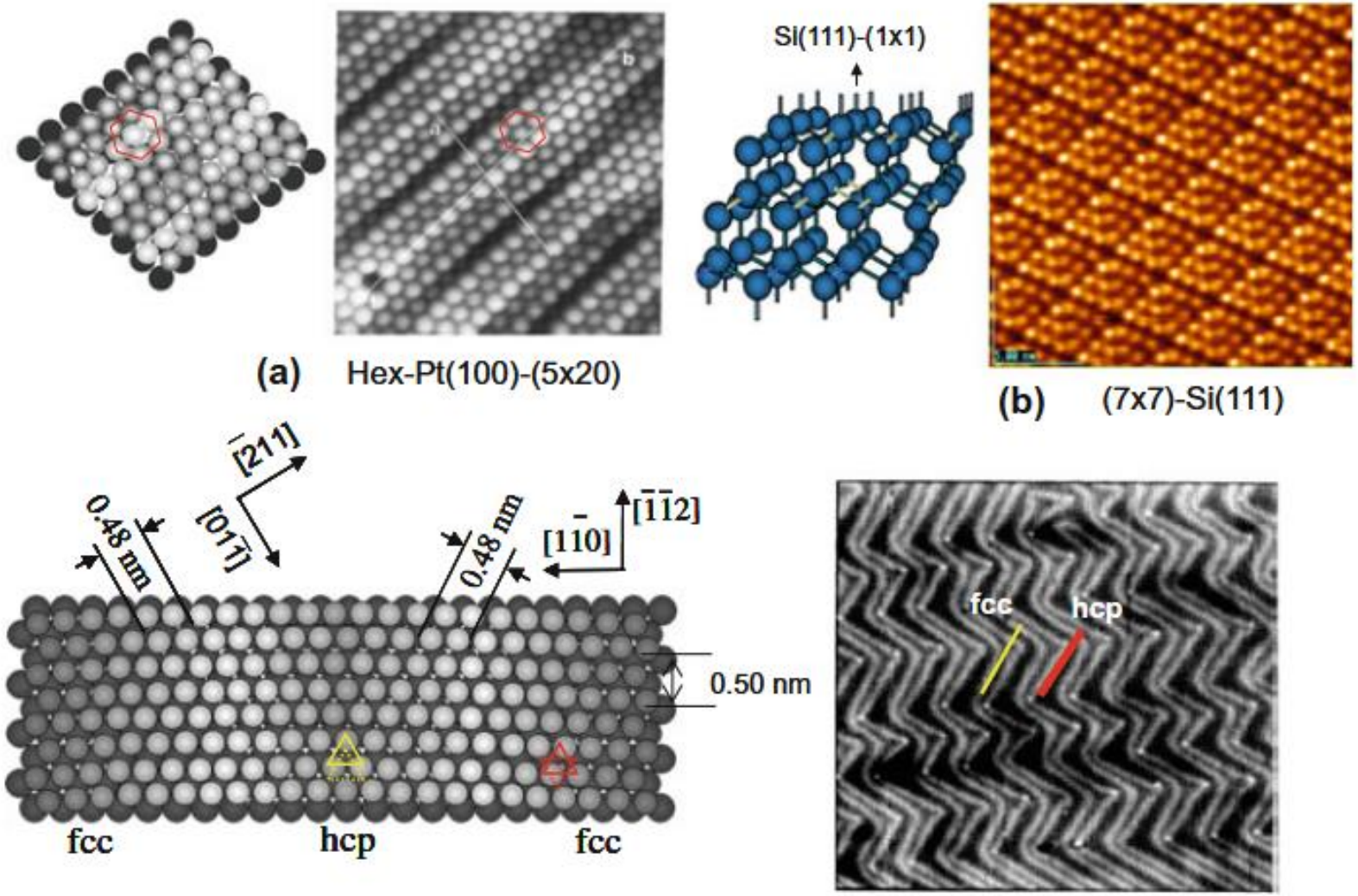


Fig. 2.1 Typical examples of the surface taking a 2-D stabilized conformation: **a** hex-(5 × 20)Pt (100) surface [1], **b** (7 × 7)-Si(111) surface, and **c** (22 × √3)-Au(111) surface, named herringbone structure, formed by alternated stacking of hcp and fcc regions, with bright ridge lines appearing between them, as shown by a model of (22 × √3)-Au(111) [3]

Tanaka, K. *Dynamic Chemical Processes on Solid Surfaces*; Springer: Singapore, 2017. https://doi.org/10.1007/978-981-10-2839-7.

Fe(211)

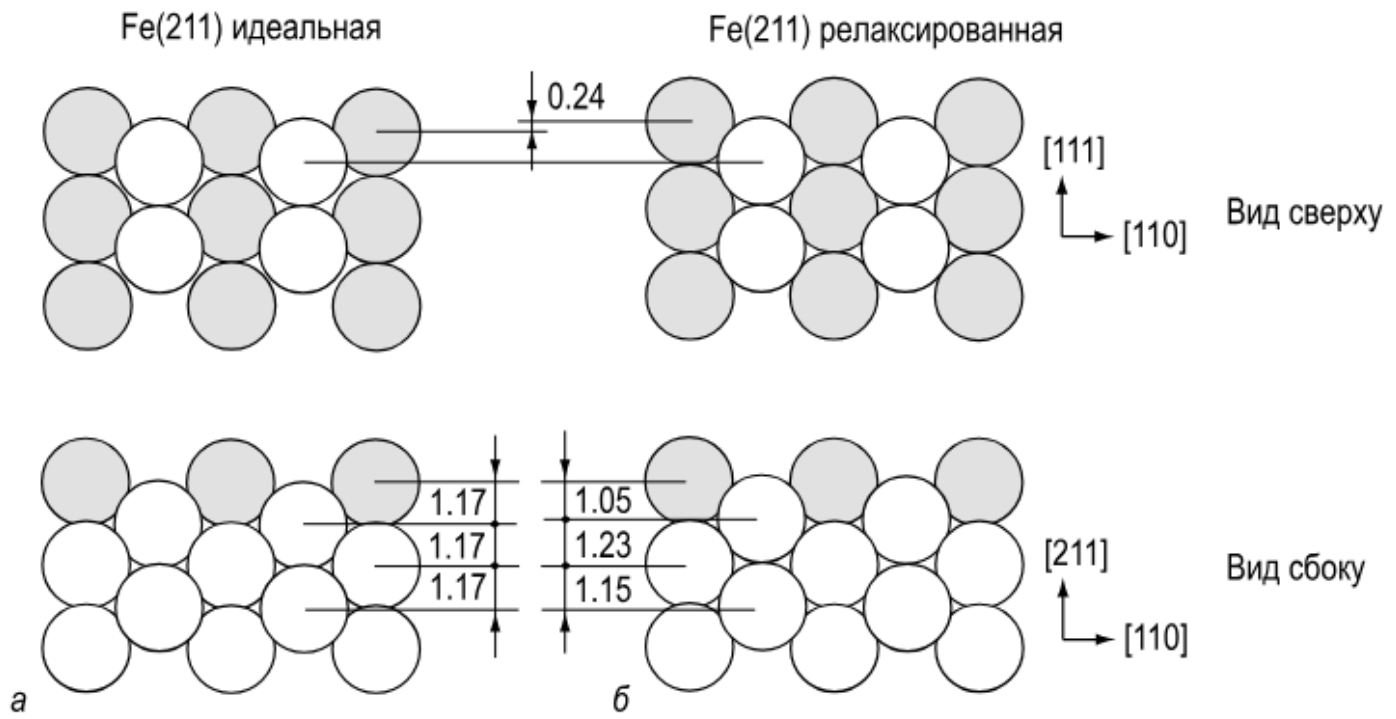


Рис. 7.5. Схематическая диаграмма, показывающая вид сверху и сбоку, *а* – нерелаксированной; *б* – релаксированной поверхности Fe(211). Релаксация включает в себя латеральное смещение верхнего слоя на 14,5 % и осцилляторную нормальную релаксацию межслойных расстояний на $\Delta_{12} = -10,4\,\%$, $\Delta_{23} = +5,4\,\%$ и $\Delta_{34} = -1,3\,\%$ [7.12]

Au(111)

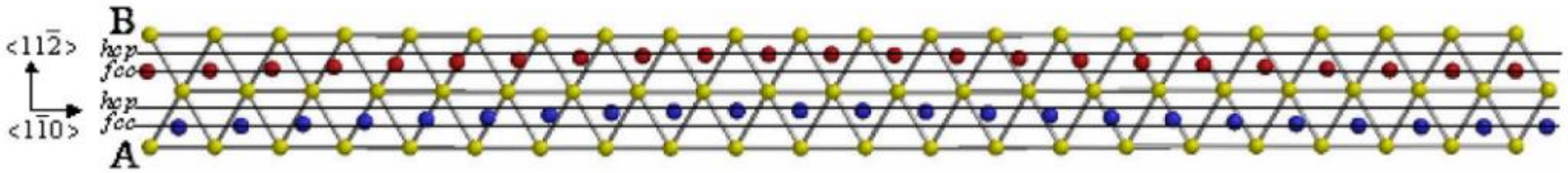


FIG. 1. (Color online) Top view of the reconstructed Au(111) $(22\times\sqrt{3})$ surface unit cell, highlighting the prevalent $\langle 1\bar{1}0\rangle$ and $\langle 11\bar{2}\rangle$ directions as well as the surface atoms in row A (blue) and row B (red) above the subsurface layer (yellow). The locations along the $\langle 11\bar{2}\rangle$ direction of the hcp and fcc sites above the subsurface layer are also indicated; the atoms in the surface layer are located near or between these high-symmetry locations.

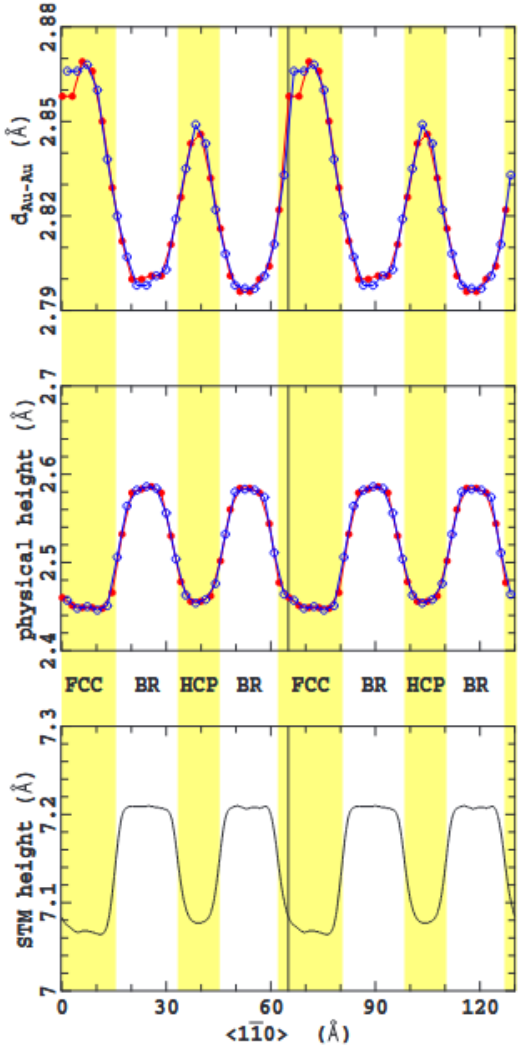


FIG. 2. (Color online) The structure of the topmost surface atoms in the reconstructed Au(111) $(22\times\sqrt{3})$ surface: (a) the shortest nearest-neighbor Au-Au distance $d_{\text{Au-Au}}$, (b) the height with respect to the average location of the second-layer atoms, and (c) the STM tip height obtained using the Tersoff-Hamann approximation at an electron density of 0.000 01 $e/\text{Å}^3$, averaged over the $\langle 11\bar{2}\rangle$ surface coordinate. The blue and red lines and dots correspond to atoms in rows A and B in Fig. 1, respectively, while the vertical shadings depict the fcc, hcp, and bridge ridge surface domains. Results are shown for two copies of the $(22\times\sqrt{3})$ lattice.

Wang, Y.; Hush, N. S.; Reimers, J. R. **Simulation of the Au(111)−(22×√3) surface reconstruction**. *Phys. Rev. B* **2007**, *75* (23), 233416. https://doi.org/10.1103/PhysRevB.75.233416.

Pt(100)

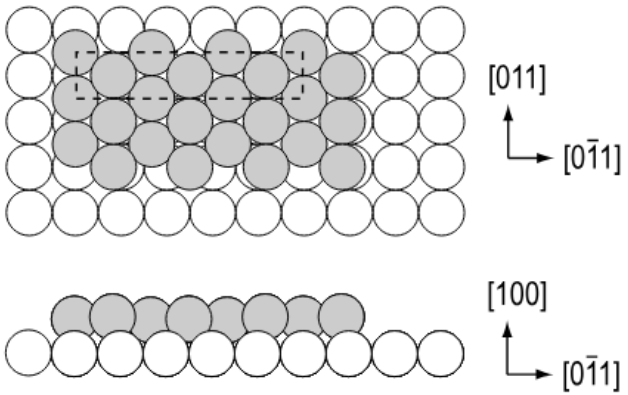


Рис. 7.6. Схематическая диаграмма, иллюстрирующая гексагональную упаковку атомов Pt верхнего слоя (показаны серыми кружками) на атомной плоскости Pt(100) с квадратной решеткой (показаны белыми кружками). В показанной идеальной схеме поверхность имеет периодичность 1×5. В реальности элементарная ячейка суперструктуры гораздо больше или может быть даже несоразмерна по отношению к подложке (см. рис. 7.7)

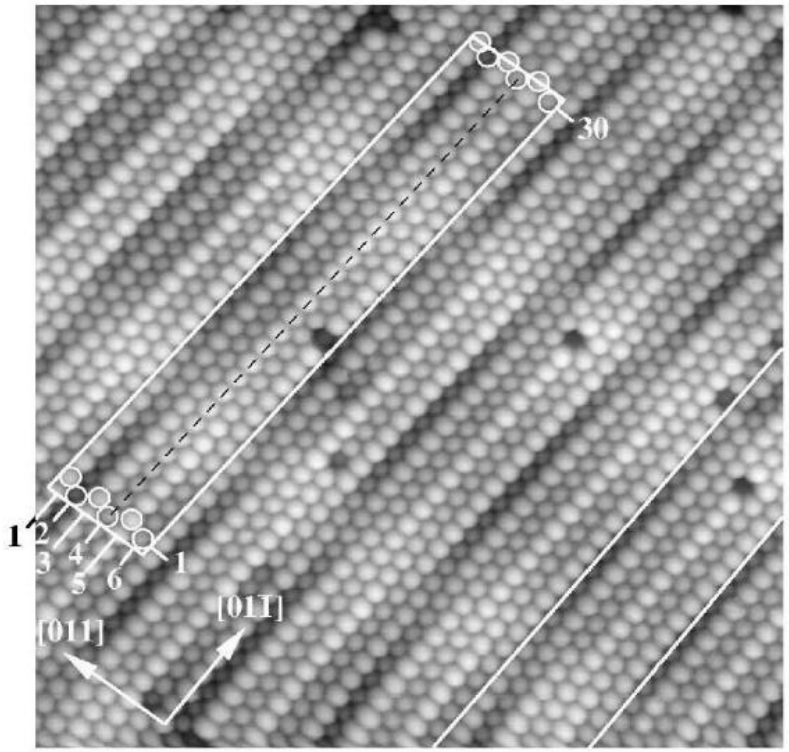


Рис. 7.7. СТМ изображение квазигексагональной реконструированной поверхности Pt(100). Элементарная ячейка суперструктуры содержит более 30 атомов в направлении [01$\bar{1}$] и шесть атомов в направлении [011]. Однако в направлении [011] видны длиннопериодические модуляции, которые указывают на то, что период в этом направлении не равен точно пяти периодом подложки [7.13]

Si(100)

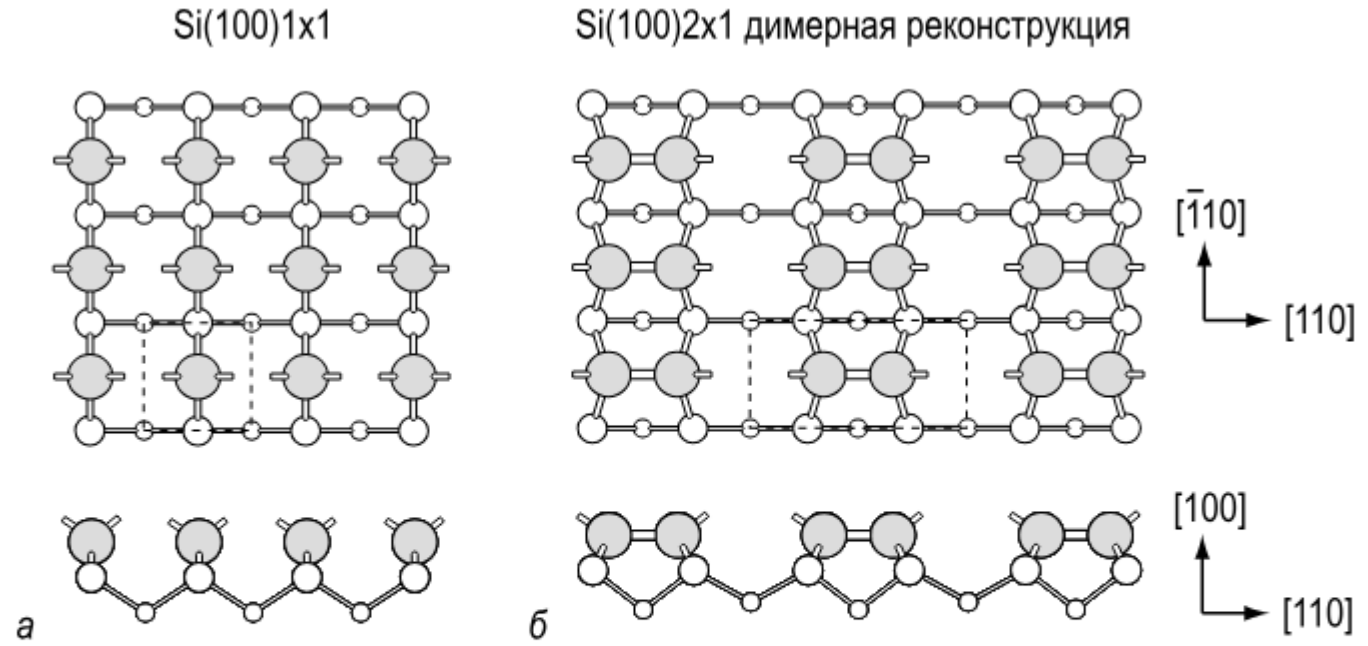


Рис. 7.12. Схематическая диаграмма, иллюстрирующая атомное строение, *а* – идеальной нереконструированной поверхности Si(100)1×1; *б* – реконструированной (димеризованной) поверхности Si(100)2×1. Атомы Si верхнего слоя закрашены, элементарные ячейки обведены штриховой линией

Ge(001)

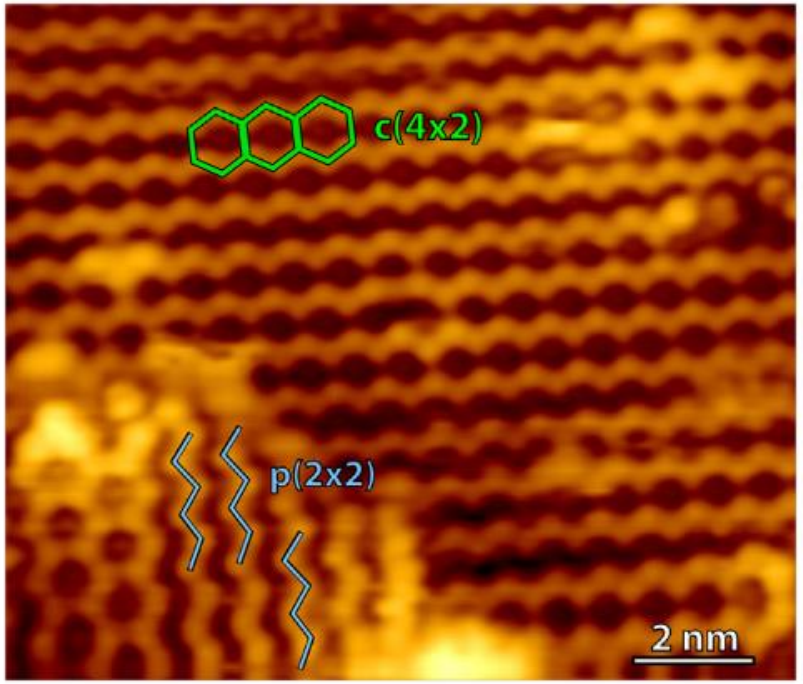
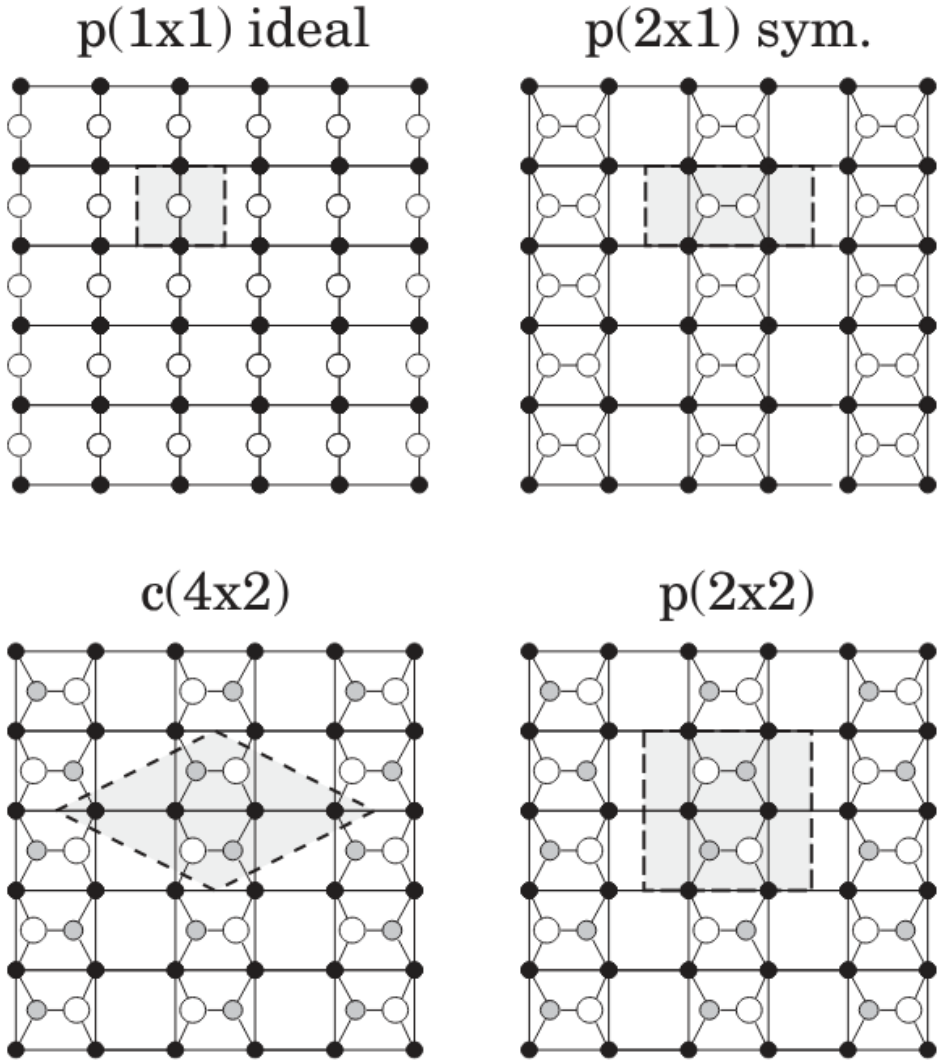


Fig. 1. Scanning tunneling microscopy filled-state image of a clean Ge(001) surface recorded at 77 K. The substrate dimer are buckled leading to local c(4 × 2) regions (adjacent dimer rows are buckled out-of-phase) and p(2 × 2) regions (adjacent dimer rows are buckled in-phase).



Kabanov, N. S., Heimbuch, R., Zandvliet, H. J. W., Saletsky, A. M., & Klavsyuk, A. L. (2017). Atomic structure of self-organizing iridium induced nanowires on Ge(001). *Applied Surface Science*, *404*, 12–17. https://doi.org/10.1016/j.apsusc.2017.01.206

Zandvliet, H. J. W. (2003). The Ge(0 0 1) surface. *Physics Reports*, *388*(1), 1–40. https://doi.org/10.1016/j.physrep.2003.09.001

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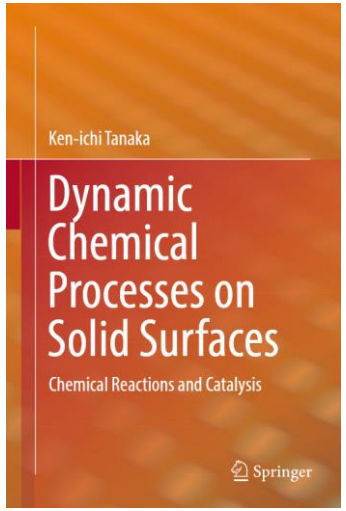
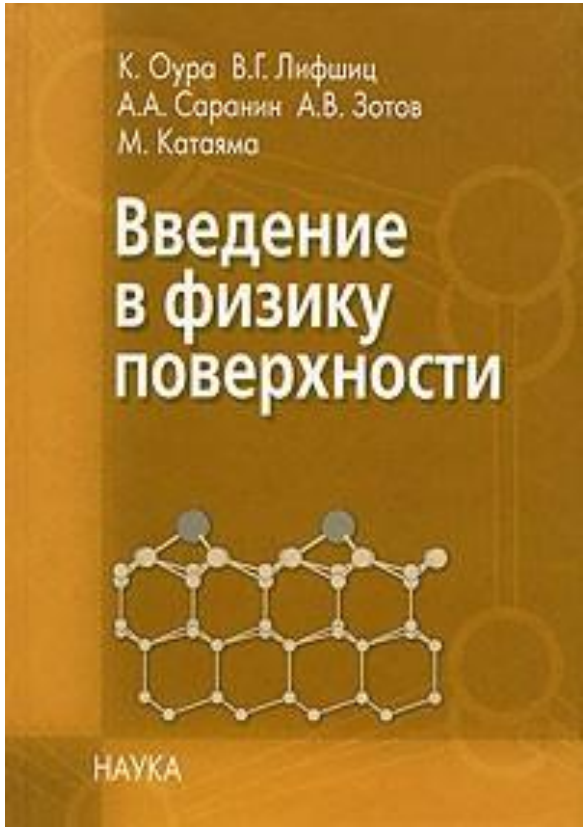
Chan, C. T.; Ho, K. M.; Bohnen, K. P. Chapter 3 - Surface Reconstruction: Metal Surfaces and Metal on Semiconductor Surfaces. In *Handbook of Surface Science*; Unertl, W. N., Ed.; Physical Structure; North-Holland, 1996; Vol. 1, pp 101–136. https://doi.org/10.1016/S1573-4331(96)80008-4.

Tanaka, K. *Dynamic Chemical Processes on Solid Surfaces*; Springer: Singapore, 2017. https://doi.org/10.1007/978-981-10-2839-7.





Потенциал Терсоффа

$$E = \frac{1}{2}\sum_i \sum_{j \neq i} V_{ij}$$

$$V_{ij} = f_C(r_{ij} + \delta)\left[f_R(r_{ij} + \delta) + b_{ij} f_A(r_{ij} + \delta)\right]$$

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

$$f_R(r) = A\exp(-\lambda_1 r)$$

$$f_A(r) = -B\exp(-\lambda_2 r)$$

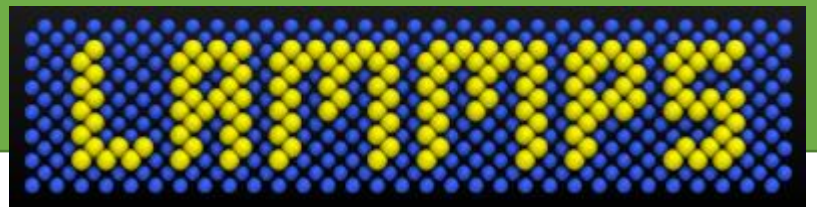
$$b_{ij} = \left(1 + \beta^n {\zeta_{ij}}^n\right)^{-\frac{1}{2n}}$$

$$\zeta_{ij} = \sum_{k \neq i,j} f_C(r_{ik} + \delta) g\left[\theta_{ijk}(r_{ij}, r_{ik})\right] \exp\left[{\lambda_3}^m (r_{ij} - r_{ik})^m\right]$$

$$g(\theta) = \gamma_{ijk}\left(1 + \frac{c^2}{d^2} - \frac{c^2}{\left[d^2 + (\cos\theta - \cos\theta_0)^2\right]}\right)$$

Tersoff, J. Modeling Solid-State Chemistry: Interatomic Potentials for Multicomponent Systems. *Phys. Rev. B* **1989**, *39* (8), 5566–5568. https://doi.org/10.1103/PhysRevB.39.5566.

Что такое LAMMPS?



LAMMPS (англ. ***L**arge-scale **A**tomic/**M**olecular **M**assively **P**arallel **S**imulator*) — свободный пакет для классической молекулярной динамики, написанный группой из Сандийских национальных лабораторий.

Пакет может применяться для крупных расчётов (до десятков миллионов атомов[1]). Для работы на многопроцессорных системах используется интерфейс MPI.

Пакет распространяется по лицензии GPL и доступен в виде исходных кодов, а также скомпилированных пакетов для Linux и Windows.

Дополнительная информация

https://www.lammps.org (через VPN)

http://genphys.phys.msu.ru/rus/sci/nanogroup/sci.html#lammps-stable_22jul2025 (локальная документация +)

На учебном сервере установлен LAMMPS (7 Feb 2024 - Update 1)

SAND2018-7268C

2018

LAMMPS Tutorial

Stan Moore

Modeling Supra-molecular Structures with LAMMPS

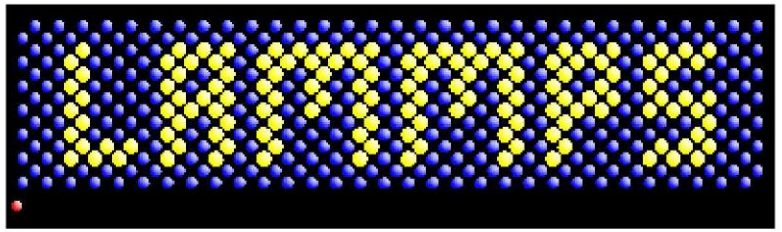
Philadelphia, PA

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA-0003525.. SAND NO. 2011-XXXXP

Tutorial Overview

Sandia National Laboratories

1. LAMMPS theory and methods
2. Download, build, and run LAMMPS
3. Work through two examples: Lennard Jones liquid and rhodopsin (solvated protein)



LAMMPS: Modular and Flexible

Sandia National Laboratories

- LAMMPS is easily extendable (don't need to modify core source code to add a diagnostic)
- Several optional packages can be installed
  - "USER-" packages are maintained by non-core LAMMPS developers
- Many optional diagnostics and commands can be used
  - Computes: only give information about the simulation: e.g. temperature
  - Fixes: modify atom properties such as forces: e.g. thermostat
- LAMMPS is scalable to large number of processors using the MPI domain decomposition method

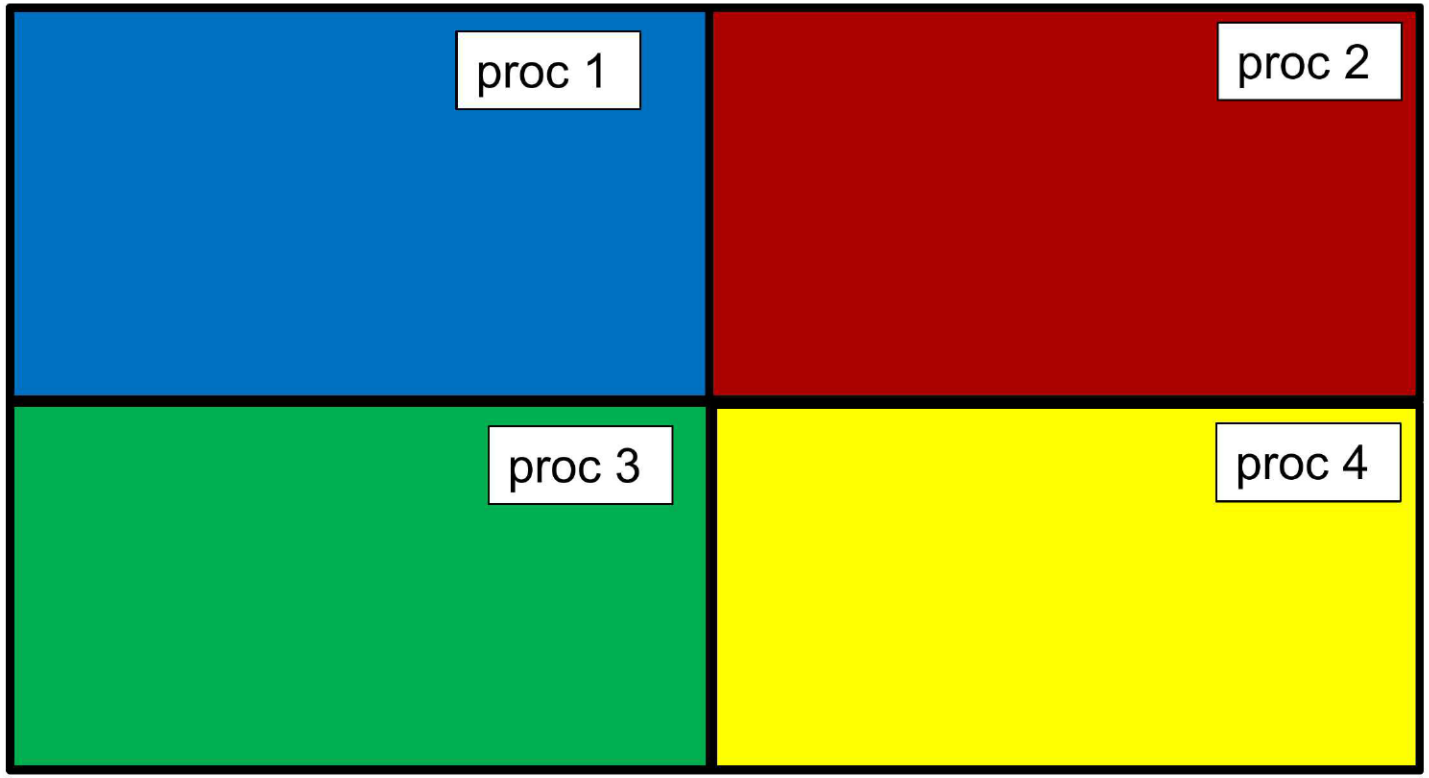
LAMMPS Code Design: C++

Sandia National Laboratories

- Why c++?
  - Allows object-oriented design, encapsulation
  - Allows virtual inheritance, which reduces code duplication
  - Performance still on par with older Fortran version of LAMMPS
- What style of c++?
  - Object-oriented c
  - Use c for low-level operations and c++ for high level (e.g. classes with virtual inheritance)
  - In LAMMPS core, simple data structures, no stl vectors, few templates, etc.
  - Multidimensional arrays are contiguous in memory
  - In USER packages, more freedom (can use stl vectors, templates, etc.)

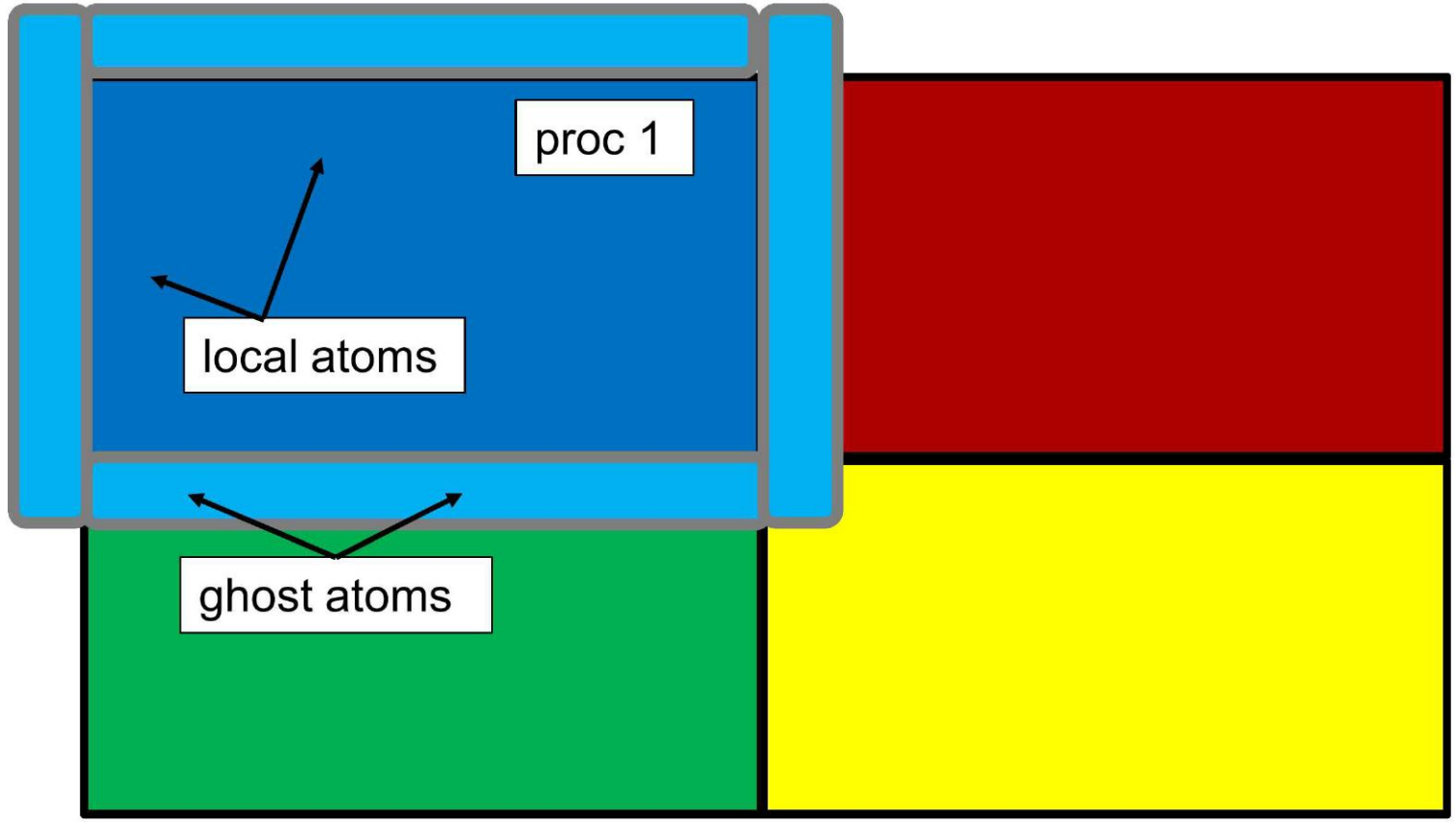
MPI Parallelization Approach

- Domain decomposition: each processor owns a portion of the simulation domain and atoms therein



Ghost Atoms

- The processor domain is also extended include needed ghost atoms (copies of atoms located on other processors)



Communication Patterns

Sandia National Laboratories

- *Forward* communication updates ghost atoms properties (such as positions) from the corresponding real atoms on a different processor
- *Reverse* communication takes properties (such as forces) accumulated on ghost atoms and updates them on the corresponding real atoms on a different processor
- *Exchange* communication migrates real atoms from one processor to another
- *Border* communication creates new ghost atoms
- LAMMPS tries to minimize the number of MPI calls required between subdomains

Strong vs Weak Scaling

Sandia National Laboratories

- Strong scaling: hold system size fixed while increasing processor count (# of atoms/processor decreases)
- Weak scaling: increase system size in proportion to increasing processor count (# of atoms/processor remains constant)
- For perfect strong scaling, doubling the processor count cuts the simulation time in half
- For perfect weak scaling, the simulation time stays exactly the same when doubling the processor count
- Harder to maintain parallel efficiency with strong scaling because the compute time decreases relative to the communication time

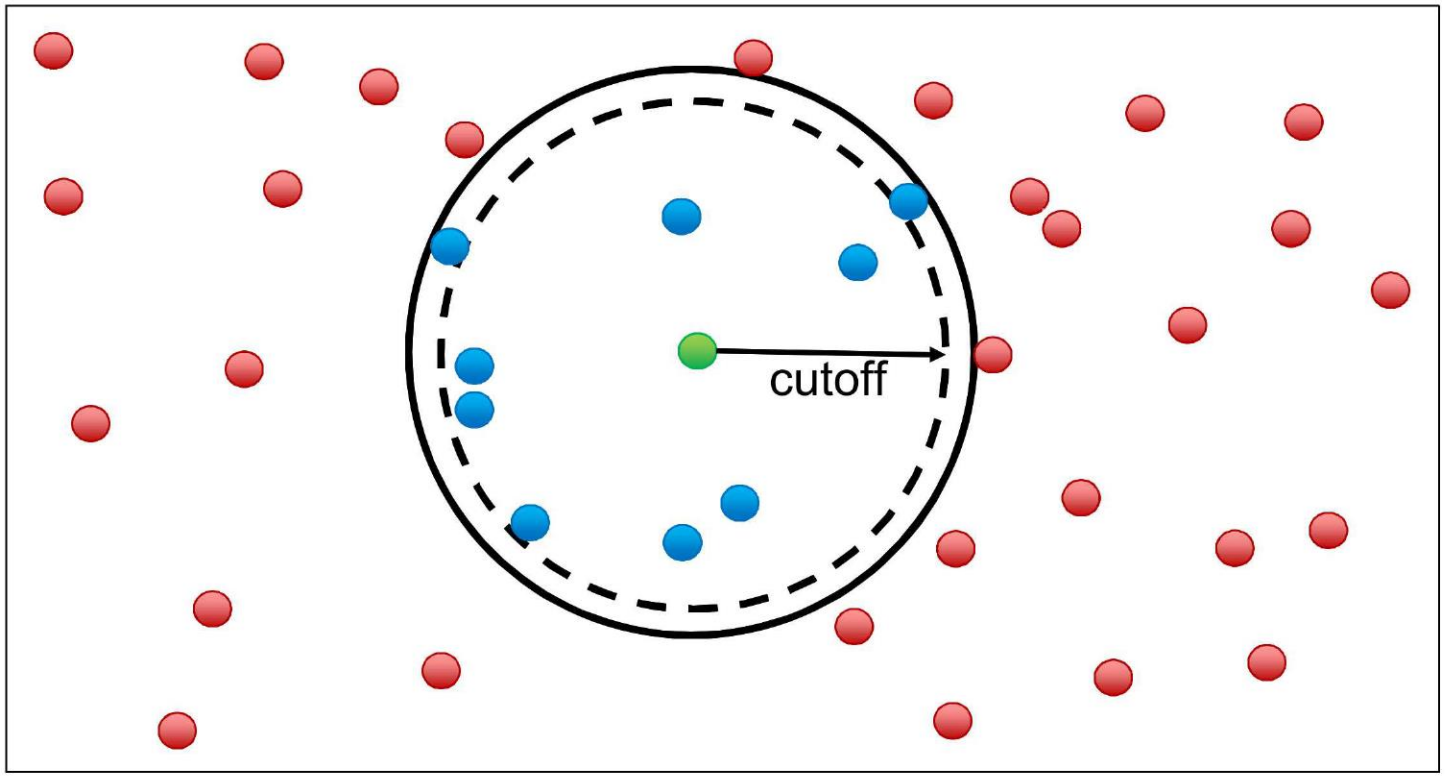
Atom IDs

Sandia National Laboratories

- atom id is a global property stored in atom->tag variable
- *Ntotal* is the total number of atoms in the simulation
- *Nlocal* is the number of atoms owned by each MPI rank
- Local atom IDs run from 0 … *Nlocal* on each processor
- Global atom IDs run from 0 … *Ntotal* across processors
- There can be multiple ghost atoms with the same id for small systems with long cutoffs => no minimum image convention limitation

Neighbor Lists

- Neighbor lists are a list of neighboring atoms within the interaction cutoff + skin for each central atom
- Extra skin allows lists to be built less often



Neighbor Options

Sandia National Laboratories

- *delay* setting means never build new lists until at least N steps after the previous build
- *every* setting means build lists every M steps (after the delay has passed)
- If the *check* setting is *no*, the lists are built on the first step that satisfies the *delay* and *every* settings. If the *check* setting is *yes*, an actual build only occurs if some atom has moved more than half the skin distance (still respects *delay* and *every)*
- *exclude* turns off pairwise interactions between certain pairs of atoms, by not including them in the neighbor list

```
neighbor 0.3 bin
neigh_modify every 2 delay 10 check yes
neigh_modify exclude type 2 3
```

Newton Option

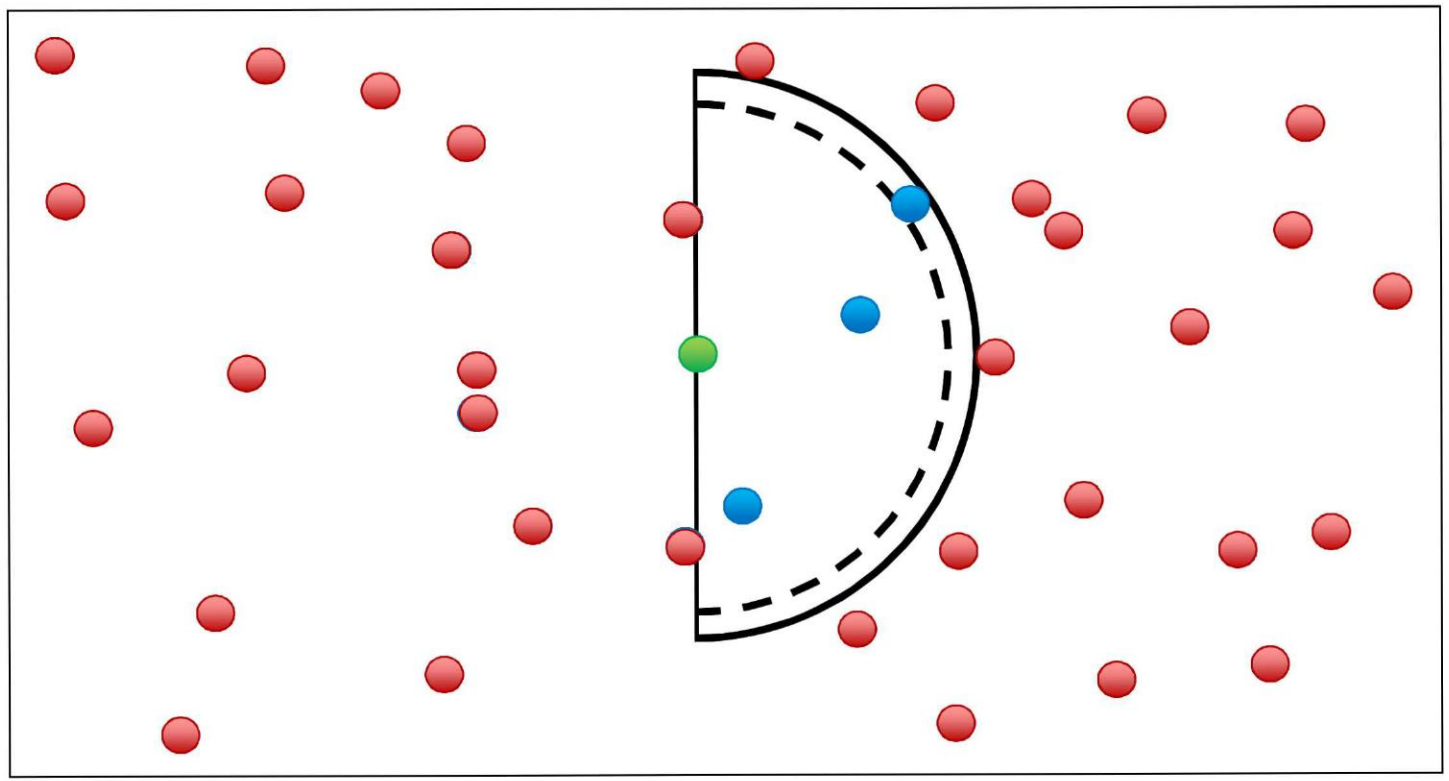
Sandia National Laboratories

- Setting the newton flag to *off* means that if two interacting atoms are on different processors, both processors compute their interaction and the resulting force information is not communicated
- Setting the newton flag to *on* means a modest savings in computation at the cost of two times more communication
- Performance depends on problem size, force cutoff lengths, a machine's compute/communication ratio, and how many processors are being used

```
newton on #default
newton off
```

Half Neighbor List

- With newton flag on, each pair is stored only once (usually better for CPUs)



Full Neighbor List

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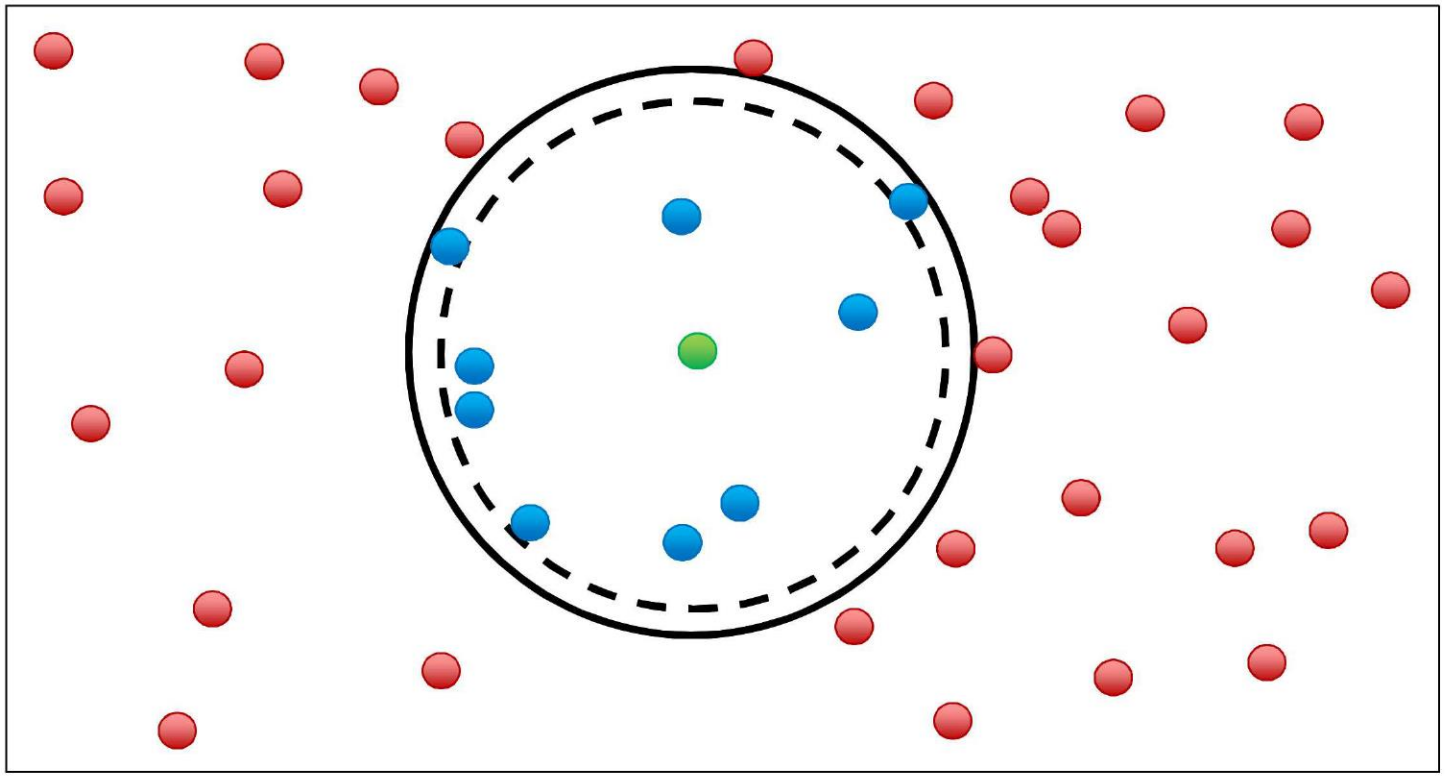
- Each pair stored twice which doubles computation but reduces communication (can be faster on GPUs)



Basic MD Timestep

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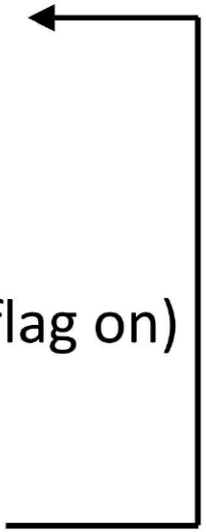
- During each timestep (without neighborlist build):

1. initial integrate
2. MPI forward communication
3. compute forces (pair, bonds, etc.)
4. MPI reverse communication (if newton flag on)
5. final integrate
6. output (if requested on this timestep)



*Computation of diagnostics (fixes or computes) can be scattered throughout the timestep

Pair Styles

Sandia National Laboratories

- In LAMMPS, force fields are called “pair styles”
- Need to specify:
  - style
  - cutoff distance
  - interaction coefficients
  - … and maybe more, depending on the pair style

```
pair_style      lj/cut 2.5
pair_coeff      1 1 1.0 1.0 2.5
```

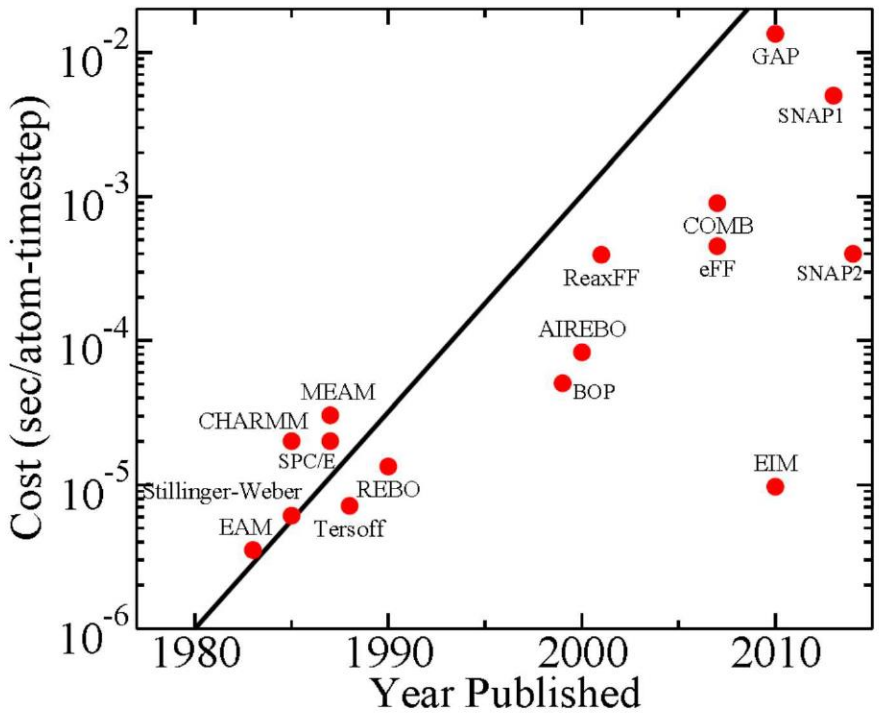
LAMMPS Potentials

Sandia National Laboratories

- See lammps.sandia.gov/bench.html#potentials

Potential	System	Atoms	Timestep	CPU	LJ Ratio
Granular	chute flow	32000	0.0001 tau	5.08e-7	0.34x
FENE bead/spring	polymer melt	32000	0.012 tau	5.32e-7	0.36x
Lennard-Jones	LJ liquid	32000	0.005 tau	1.48e-6	1.0x
DPD	pure solvent	32000	0.04 tau	2.16e-6	1.46x
EAM	bulk Cu	32000	5 fmsec	3.59e-6	2.4x
Tersoff	bulk Si	32000	1 fmsec	6.01e-6	4.1x
Stillinger-Weber	bulk Si	32000	1 fmsec	6.10e-6	4.1x
EIM	crystalline NaCl	32000	0.5 fmsec	9.69e-6	6.5x
SPC/E	liquid water	36000	2 fmsec	1.43e-5	9.7x
CHARMM + PPPM	solvated protein	32000	2 fmsec	2.01e-5	13.6x
MEAM	bulk Ni	32000	5 fmsec	2.31e-5	15.6x
Peridynamics	glass fracture	32000	22.2 nsec	2.42e-5	16.4x
Gay-Berne	ellipsoid mixture	32768	0.002 tau	4.09e-5	28.3x
AIREBO	polyethylene	32640	0.5 fmsec	8.09e-5	54.7x
COMB	crystalline SiO2	32400	0.2 fmsec	4.19e-4	284x
eFF	H plasma	32000	0.001 fmsec	4.52e-4	306x
ReaxFF	PETN crystal	16240	0.1 fmsec	4.99e-4	337x
ReaxFF/C	PETN crystal	32480	0.1 fmsec	2.73e-4	185x
VASP/small	water	192/512	0.3 fmsec	26.2	17.7e6
VASP/medium	CO2	192/1024	0.8 fmsec	252	170e6
VASP/large	Xe	432/3456	2.0 fmsec	1344	908e6

Accuracy = Higher Cost



Moore's Law for Interatomic Potentials

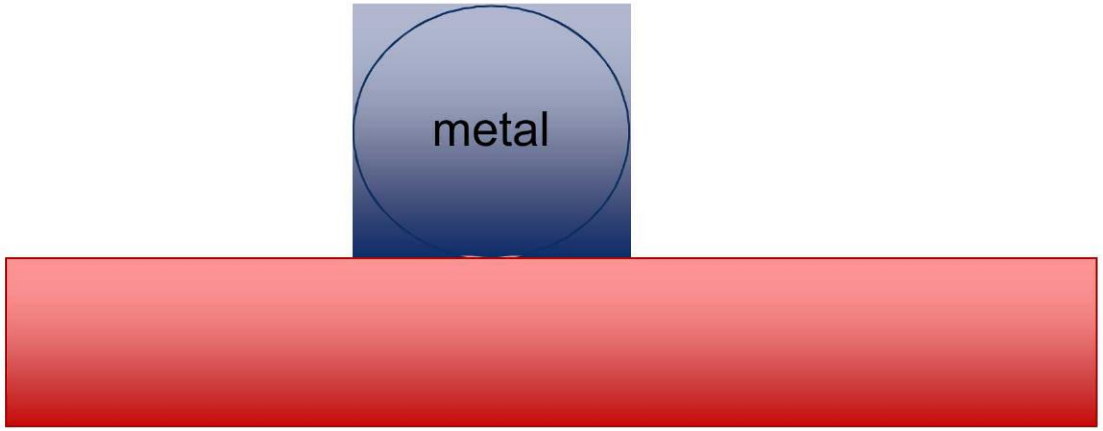
Plimpton and Thompson, MRS Bulletin (2012).

Hybrid force fields

- Pair hybrid: exactly one pair style is assigned to each pair of atom types (can be different pair styles for different atom types)
- Pair hybrid/overlay: one or more pair styles can be assigned to each pair of atom types
- The assignment of pair styles to type pairs is made via the pair_coeff command

Hybrid force fields—Example

- Metal droplet on an LJ surface
  - metal → metal atoms interact with *eam* potential
  - surface → surface atoms interact with *lj/cut* potential
  - metal/surface interaction is also computed via a *lj/cut* potential




```
pair_style hybrid lj/cut/coul/cut 10.0 eam lj/cut 5.0
```

Syntax specifying advanced force field input

Sandia National Laboratories

- Look in the LAMMPS documentation (i.e. http://lammps.sandia.gov/doc/pair_reax.html)
- Shows pair_style name
- Shows syntax with required and optional keywords
- Gives examples of command use
- Gives a description of the keywords
- Also gives restrictions, related commands, and default values of optional keywords

EAM, SW, and Tersoff Syntax

Sandia National Laboratories

```
pair_style eam
pair_coeff * * cuu3
pair_coeff 1*3 1*3 niu3.eam

pair_style sw
pair_coeff * * si.sw Si
pair_coeff * * GaN.sw Ga N Ga

pair_style tersoff
pair_coeff * * Si.tersoff Si
pair_coeff * * SiC.tersoff Si C Si
```

- Can use forcefield files in /potentials folder

Atom-style Formats

Sandia National Laboratories

- Different force fields require different data to be stored with atoms (i.e. positions, charges, bonds, etc.)
- Atomic:
  - Basic style that can be used for simple potentials without bonds or charges
  - E.g. Lennard Jones fluid or metals
- Full:
  - More comprehensive style that includes charges and molecular topology (bonds, angles, dihedrals, and impropers)
  - E.g. water or polymers

```
atom_style    atomic
atom_style    full
```

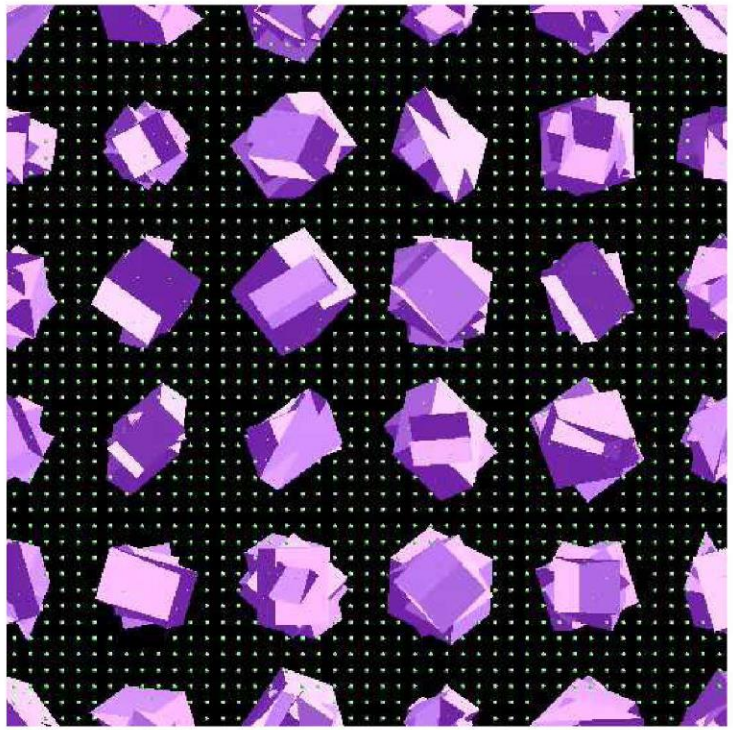
Atom-style Formats

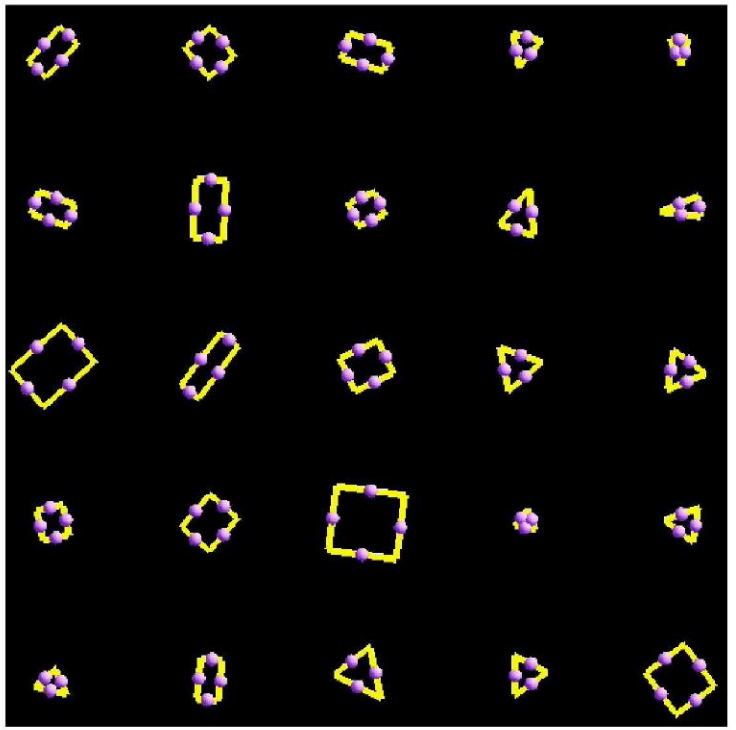
Sandia National Laboratories

angle	atom-ID molecule-ID atom-type x y z
atomic	atom-ID atom-type x y z
body	atom-ID atom-type bodyflag mass x y z
bond	atom-ID molecule-ID atom-type x y z
charge	atom-ID atom-type q x y z
dipole	atom-ID atom-type q x y z mux muy muz
dpd	atom-ID atom-type theta x y z
electron	atom-ID atom-type q spin eradius x y z
ellipsoid	atom-ID atom-type ellipsoidflag density x y z
full	atom-ID molecule-ID atom-type q x y z
line	atom-ID molecule-ID atom-type lineflag density x y z
meso	atom-ID atom-type rho e cv x y z
molecular	atom-ID molecule-ID atom-type x y z
peri	atom-ID atom-type volume density x y z
smd	atom-ID atom-type molecule volume mass kernel-radius contact-radius x y z
sphere	atom-ID atom-type diameter density x y z
template	atom-ID molecule-ID template-index template-atom atom-type x y z
tri	atom-ID molecule-ID atom-type triangleflag density x y z
wavepacket	atom-ID atom-type charge spin eradius etag cs_re cs_im x y z
hybrid	atom-ID atom-type x y z sub-style1 sub-style2 ...

Triangle and line particle examples

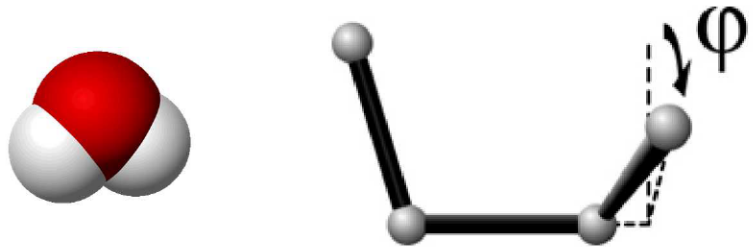
Sandia National Laboratories



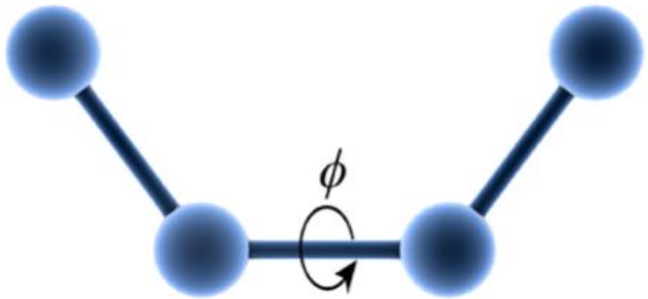


Molecular Topology

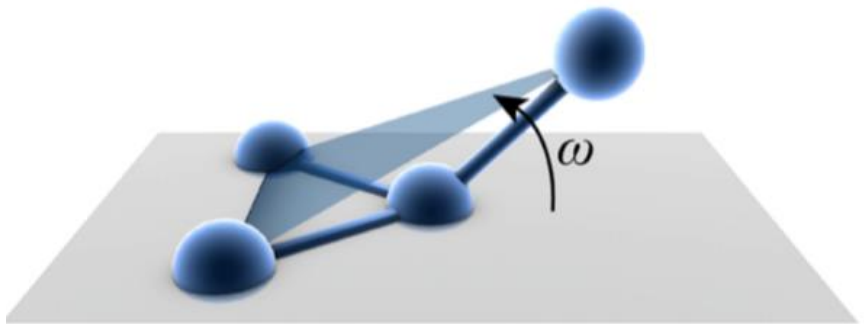
- Bonds: constrained length between two atoms
- Angles: constrained angle between three atoms
- Dihedrals: interactions between quadruplets of atoms
- Impropers: “improper” interactions between quadruplets of atoms




```
bond_style      harmonic
angle_style     charmm
dihedral_style  charmm
improper_style  harmonic
```

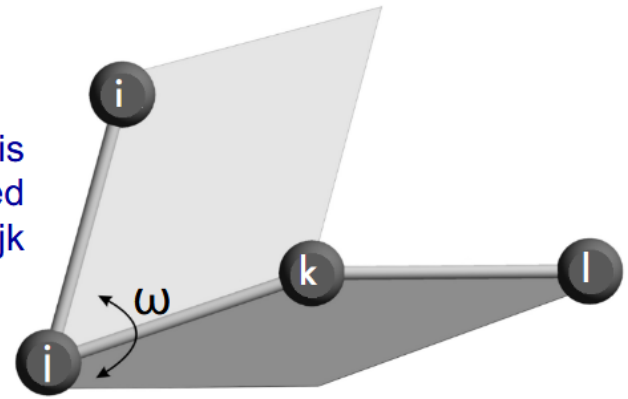


Proper torsion angle



Improper torsion angle

Dihedral angle is defined as signed angle between ijk and jkl planes

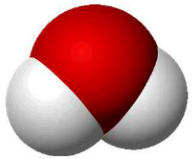


https://storion.ru/cf/lecture_cmd_ak.pdf

Fix Shake and Fix Rattle

Sandia National Laboratories

- Applies bond and angle constraints to specified bonds and angles in the simulation by either the SHAKE or RATTLE algorithms
- Typically enables a longer timestep
- In LAMMPS, only small clusters of atoms can be constrained



```
fix     1 all shake 0.0001 5 0 m 1.0 a 232
```

Special Bonds

Sandia National Laboratories

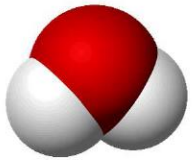
- Allow non-bonded LJ or Coulombic interactions between the pair of atoms to be excluded (or reduced by a weighting factor)
- Weighting factors are a scaling pre-factor on the energy and force between the pair of atoms. 1.0 means include the full interaction; 0.0 means exclude it completely
- Fist coefficient is the weighting factor on 1-2 atom pairs, which are pairs of atoms directly bonded to each other
- Second coefficient is the weighting factor on 1-3 atom pairs which are those separated by 2 bonds
- Third coefficient is the weighting factor on 1-4 atom pairs which are those separated by 3 bonds

```
special_bonds charmm
```

Long-Range Electrostatics

Sandia National Laboratories

- Truncation doesn't work well for charged systems due to long-ranged nature of Coulombic interactions
- Use Kspace style to add long-range electrostatics:
  - PPPM—usually fastest, uses FFTs
  - Ewald—potentially most accurate, but slow for large systems
  - MSM—multigrid method that also works for non-periodic systems
- Usually specify a relative accuracy (1e-4 or 1e-5 typically used)
- Use pair_style *coul/long such as lj/cut/coul/long instead of *coul/cut



```
pair_style      lj/cut/coul/long 10.0
kspace_style    pppm 1e-4
```

2D Slab Geometry with Kspace

Sandia National Laboratories

- The *slab* keyword allows a Kspace solver to be used for a systems that are periodic in x,y but non-periodic in z
- Must use a boundary setting of "`boundary p p f`"
- Actually treats the system as if it were periodic in z, but inserts empty volume between atom slabs and removing dipole inter-slab interactions so that slab-slab interactions are effectively turned off
- May need to use reflecting walls in the z-dimension


```
boundary        p p f
kspace_modify   slab 3.0
```

Run vs Minimize

Sandia National Laboratories

- "run" command updates velocities and positions based on forces. System may blow up and crash LAMMPS if atoms overlap!
- "minimize" command minimizes energy of the system by iteratively adjusting atom coordinates
  - Good to minimize first if you built your system using an external tool
  - Prevents LAMMPS crashing from overlapping atoms
- Can use "run" after "minimize"

```
minimize    1.0e-4 1.0e-6 100 1000
run         100
```

LAMMPS Files

Sandia National Laboratories

- Input file: text file with LAMMPS commands used to run a simulation
- Log file: text file with thermodynamic output from simulation
- Dump file: snapshot of atom properties, i.e. atom forces
- Restart file: binary checkpoint file with data needed to restart simulation
- Data file: text file that can be used to start or restart simulation

LAMMPS Input File

Sandia National Laboratories

- Uses custom powerful scripting language
- Can define variables
- Order of some commands matters
- Can use python
- Many commands take a custom name, and operate “all” atoms

```
compute myKe all ke/atom
fix myHisto all ave/histo 1 1 100 0.0 1.5 10
  c_myKe file temp.histo mode vector
```

Input Script Variables

Sandia National Laboratories

- Can use common math operators such as + and -, as well as common match functions such as sin() and cos()
- Can reference one variable in another variable
- Equal-style variables are scalars
  - `variable beta equal temp/3.0`
  - `variable b1 equal a[234]+0.5*vol`
  - `variable b2 equal sin(a)/2.0`
  - `variable b3 equal c_myTemp`
- Atom-style variables are arrays
  - `variable  atom x*y/vol`
- Other types of variables, see LAMMPS documentation

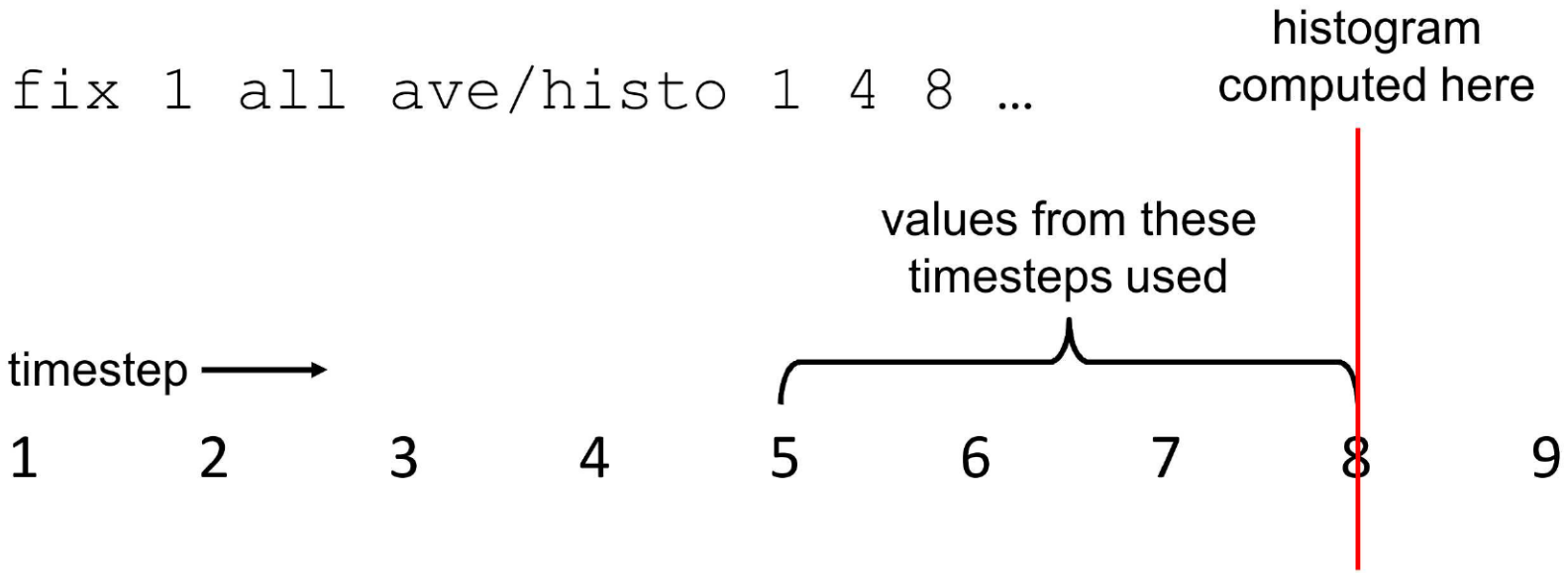
Averaging Frequency

Sandia National Laboratories

```
fix 1 all ave/histo [nevery] [nrepeat] [nfreq]…
```

- Nevery = use input values every this many timesteps
- Nrepeat = # of times to use input values for calculating histogram
- Nfreq = calculate histogram every this many timesteps

```
fix 1 all ave/histo 1 4 8 …
```



LAMMPS Log File

Sandia National Laboratories

- LAMMPS log file contains thermodynamic information about the system (energy, pressure, volume, etc.)
- Can define custom variables and output those to log file
- Per-atom quantities are output in the “dump” file, not log file
- Log file also contains other information such as timing breakdown and estimated memory usage

Data Files

Sandia National Laboratories

- The data file contains basic information such as:
  - size of the problem to be run
  - the initial atomic coordinates
  - molecular topology
  - and (optionally) force-field coefficients
- Data files are text files
- Restart files are binary files which save a system configuration
- Can convert a restart file to a data file using the “-restart” command line option

Data file and molecule file formats

```
LAMMPS Description              (1st line of file)

100 atoms          (this must be the 3rd line, 1st 2 lines are ignored)
95 bonds                (# of bonds to be simulated)
50 angles               (include these lines even if number = 0)
30 dihedrals
20 impropers

5 atom types           (# of nonbond atom types)
10 bond types          (# of bond types = sets of bond coefficients)
18 angle types
20 dihedral types      (do not include a bond,angle,dihedral,improper type
2 improper types            line if number of bonds,angles,etc is 0)

-0.5 0.5 xlo xhi       (for periodic systems this is box size,
-0.5 0.5 ylo yhi        for non-periodic it is min/max extent of atoms)
-0.5 0.5 zlo zhi       (do not include this line for 2-d simulations)
```

Data file and molecule file formats

```
Masses

  1 mass
  ...
  N mass                          (N = # of atom types)

Nonbond Coeffs

  1 coeff1 coeff2 ...
  ...
  N coeff1 coeff2 ...             (N = # of atom types)

Bond Coeffs

  1 coeff1 coeff2 ...
  ...
  N coeff1 coeff2 ...             (N = # of bond types)
(N = # of angle types)
```

Data file and molecule file formats

```
Atoms

  1 molecule-tag atom-type q x y z nx ny nz   (nx,ny,nz are
optional -
  ...                                        see "true flag" input
command)
  ...
  N molecule-tag atom-type q x y z nx ny nz   (N = # of atoms)

Velocities

  1 vx vy vz
  ...
  ...
  N vx vy vz                                 (N = # of atoms)
```

Data file and molecule file formats

Sandia National Laboratories

```
Bonds

  1 bond-type atom-1 atom-2
  ...
  N bond-type atom-1 atom-2          (N = # of bonds)

Angles

  1 angle-type atom-1 atom-2 atom-3  (atom-2 is the center atom in angle)
  ...
  N angle-type atom-1 atom-2 atom-3  (N = # of angles)

Dihedrals

  1 dihedral-type atom-1 atom-2 atom-3 atom-4  (atoms 2-3 form central bond)
  ...
  N dihedral-type atom-1 atom-2 atom-3 atom-4  (N = # of dihedrals)

Impropers

  1 improper-type atom-1 atom-2 atom-3 atom-4  (atom-2 is central atom)
  ...
  N improper-type atom-1 atom-2 atom-3 atom-4  (N = # of impropers)
```

Lattice Command

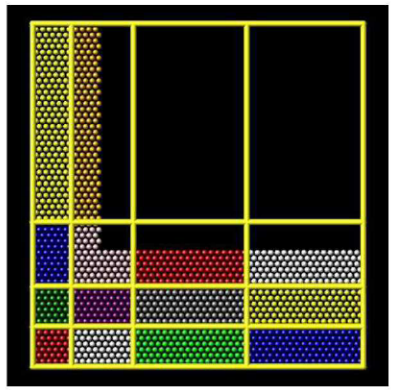
- In LAMMPS, a lattice is simply a set of points in space, determined by a unit cell with basis atoms, that is replicated infinitely in all dimensions
- “Create atoms” command creates atoms on the lattice points inside the simulation box
- For LJ units, the lattice command takes a reduced density, for other units, the lattice command takes the lattice constant

```
lattice       fcc 0.8442
region      box block 0 ${xx} 0 ${yy} 0 ${zz}
create_box    1 box
create_atoms  1 box
```

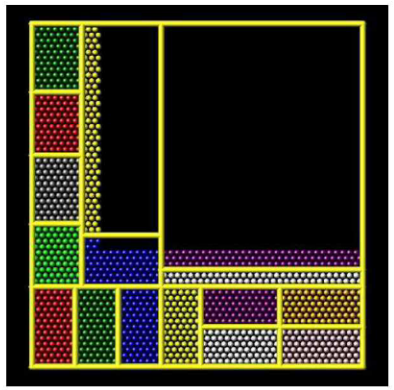
Load Balancing

- Adjusts the size and shape of processor sub-domains within the simulation box
- Attempts to balance the number of atoms or particles and thus indirectly the computational cost (load) more evenly across processors
- Can be static or dynamic

shift



rcb



```
balance 1.0 shift xz 5 1.1
balance 1.1 rcb
```

Accelerator Packages

Sandia National Laboratories

- Some hardware components like GPUs, Xeon Phis, and multithreaded CPUs require special code (i.e. OpenMP, CUDA) to fully take advantage of the hardware
- LAMMPS has 5 accelerator packages:
  - USER-OMP
  - USER-INTEL
  - GPU
  - KOKKOS
  - OPT
- See http://lammps.sandia.gov/doc/Section_accelerate.html (How to build and run with accelerator packages is beyond the scope of this tutorial)

Downloading LAMMPS

Sandia National Laboratories

- LAMMPS Website (http://lammps.sandia.gov)
  - Go to “download” link
  - Download gzipped tar file
- Github (https://github.com/lammps/lammps)
  - https://github.com/lammps/lammps/releases
  - Clone or download button, then download zip file
  - git clone … (beyond this tutorial)
- Stable version: more testing
- Development version: latest features and bug fixes

Running LAMMPS

Sandia National Laboratories

- Syntax: `[executable] -in [input_script]`
- In serial:

```
$ ./lmp_serial -in in.lj
```

- In parallel:

```
$ mpirun -np 2 lmp_mpi -in in.lj
```

- Many other command line options, see http://lammps.sandia.gov/doc/Section_start.html#start-6

Common Errors

Sandia National Laboratories

Lost atoms or out of range atoms - cannot compute PPPM

- Possible causes are
  - bad initial geometry (close contacts), minimize first
  - bad force field parameters or a typo (atoms get too close and then one "shoots" through the system)
  - use of shrinkwrap boundary with lots of extra space (atoms get lost when subdomains move too much (happens only in parallel runs)
  - fixed boundaries without a wall
- To hide the issue, can use `thermo_modify lost ignore`

Common Errors (Continued)

NaN (not a number) in output

- For positions with variable cell: too high potential energy → start with fixed volume, run minimization first
- For positions with fixed volume: close contacts

Unknown XXX style = missing package

Illegal XXX style command = syntax error, often due to version mismatch of online vs. version specific docs

Energy/stress not tallied on current time step

- pe, pressure, pe/atom and stress/atom computes need to be “triggered" by a fix, dump or thermo output either directly or indirectly through a variable

LAMMPS Directories

Sandia National Laboratories

- The "examples" directory has many example inputs, good place to learn commands
- The "potentials" directory has different force field files, such as EAM, Tersoff, etc.
- The "tools" directory has tools, i.e. one can convert inputs from other codes such as CHARMM to LAMMPS
- The "lib" directory has optional libraries bundled with LAMMPS (may require compiling)
- The "bench" directory has canonical benchmarks used to test LAMMPS performance

Example: Lennard Jones

Sandia National Laboratories

1. Run default input script: bench/in.lj
2. Change initial velocity distribution to give higher temperature
3. Change integrator from constant energy (fix nve) to constant temperature (fix nvt)
4. Decrease density of the system
5. Dump atom positions and forces
6. Write out data file and restart file
7. Make a histogram of per-atom kinetic energy

Example: Lennard Jones

Sandia National Laboratories

Run default input script: bench/in.lj

```
$ cd bench
$ ../src/lmp_serial -in in.lj
```

```
Step Temp E_pair E_mol TotEng Press
       0          1.44   -6.7733681             0   -4.6134356   -5.0197073
     100    0.7574531   -5.7585055             0   -4.6223613   0.20726105
Loop time of 3.19363 on 1 procs for 100 steps with 32000 atoms
```

Example: Lennard Jones

Sandia National Laboratories

Change velocity distribution to give higher temperature

```
#velocity all create 1.44 87287 loop geom
velocity  all create 2.0 87287 loop geom
```

```
Step Temp E_pair E_mol TotEng Press
       0            2   -6.7733681             0   -3.7734618     -4.54697
     100    1.0614424   -5.3736027             0   -3.7814889    2.3907499
Loop time of 3.35405 on 1 procs for 100 steps with 32000 atoms
```

now 2.0 instead of 1.44

Example: Lennard Jones

Sandia National Laboratories

Change integrator from constant energy (fix nve) to constant temperature (fix nvt)

```
#fix 1 all nve
fix         1 all nvt 1.0 1.0 0.1
```

```
Step Temp E_pair E_mol TotEng Press
       0          1.44   -6.7733681             0   -4.6134356   -5.0197073
     100   0.92987881   -5.5836548             0   -4.1888802    1.2277583
Loop time of 3.23382 on 1 procs for 100 steps with 32000 atoms
```

close to 1.0

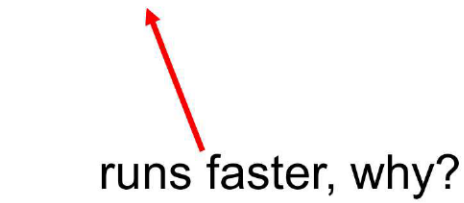
Example: Lennard Jones

Sandia National Laboratories

Decrease density of the system

```
#lattice           fcc 0.8442
lattice           fcc 0.1
```

```
Step Temp E_pair E_mol TotEng Press
       0          1.44      -0.1194            0    2.0405325    0.1202355
     100       1.65803  -0.39464997            0    2.0923173   0.18136994
Loop time of 0.598197 on 1 procs for 100 steps with 32000 atoms
```



runs faster, why?

Example: Lennard Jones

Sandia National Laboratories

Dump atom positions and forces

```
dump myCustom all custom 100 dump.custom id x y
   z fx fy fz
```

```
ITEM: TIMESTEP
100
ITEM: NUMBER OF ATOMS
32000
ITEM: BOX BOUNDS pp pp pp
0.0000000000000000e+00 3.3591923827650149e+01
0.0000000000000000e+00 3.3591923827650149e+01
0.0000000000000000e+00 3.3591923827650149e+01
ITEM: ATOMS id x y z fx fy fz
1 0.227853 0.074729 0.0873785 -20.1615 9.18853 -5.79564
2 0.919519 0.846223 0.101134 0.57499 14.6108 3.75088
3 0.99976 0.0650636 0.951449 -2.22408 8.98378 -9.31871
...
```

Example: Lennard Jones

Sandia National Laboratories

Write out data file and restart file

```
run                 100
write_data          out.data
write_restart       out.rst
```

```
LAMMPS data file via write_data, version 29 Jun 2018, timestep = 100

32000 atoms
1 atom types

0.0000000000000000e+00 3.3591923827650149e+01 xlo xhi
0.0000000000000000e+00 3.3591923827650149e+01 ylo yhi
0.0000000000000000e+00 3.3591923827650149e+01 zlo zhi
...
```

Example: Lennard Jones

Sandia National Laboratories

Make a histogram of per-atom kinetic energy

```
compute myKe all ke/atom
fix myHisto all ave/histo 1 1 100 0.0 1.5 10
  c_myKe file temp.histo mode vector
```