機器學習於材料資訊的應用
Machine Learning on Material Informatics

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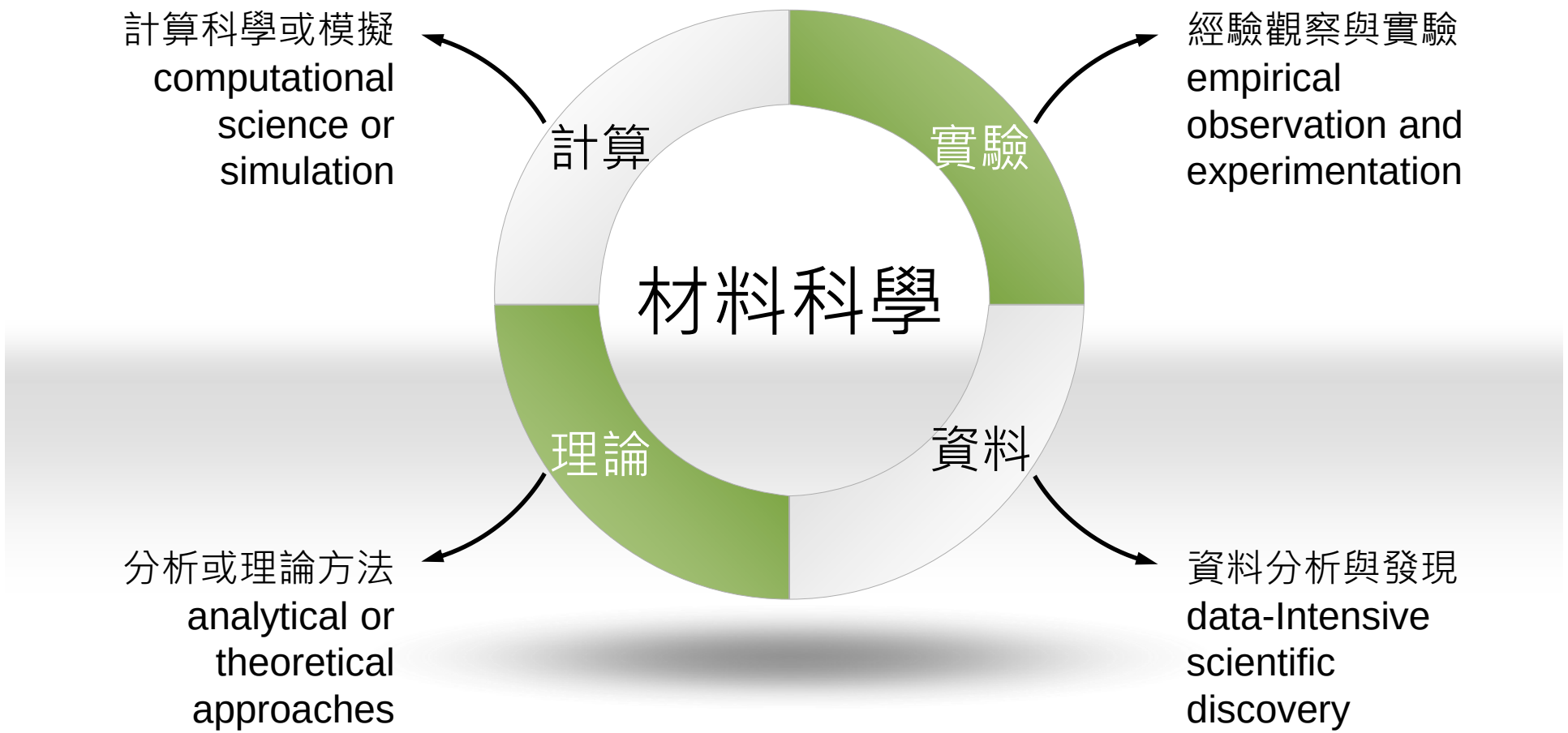
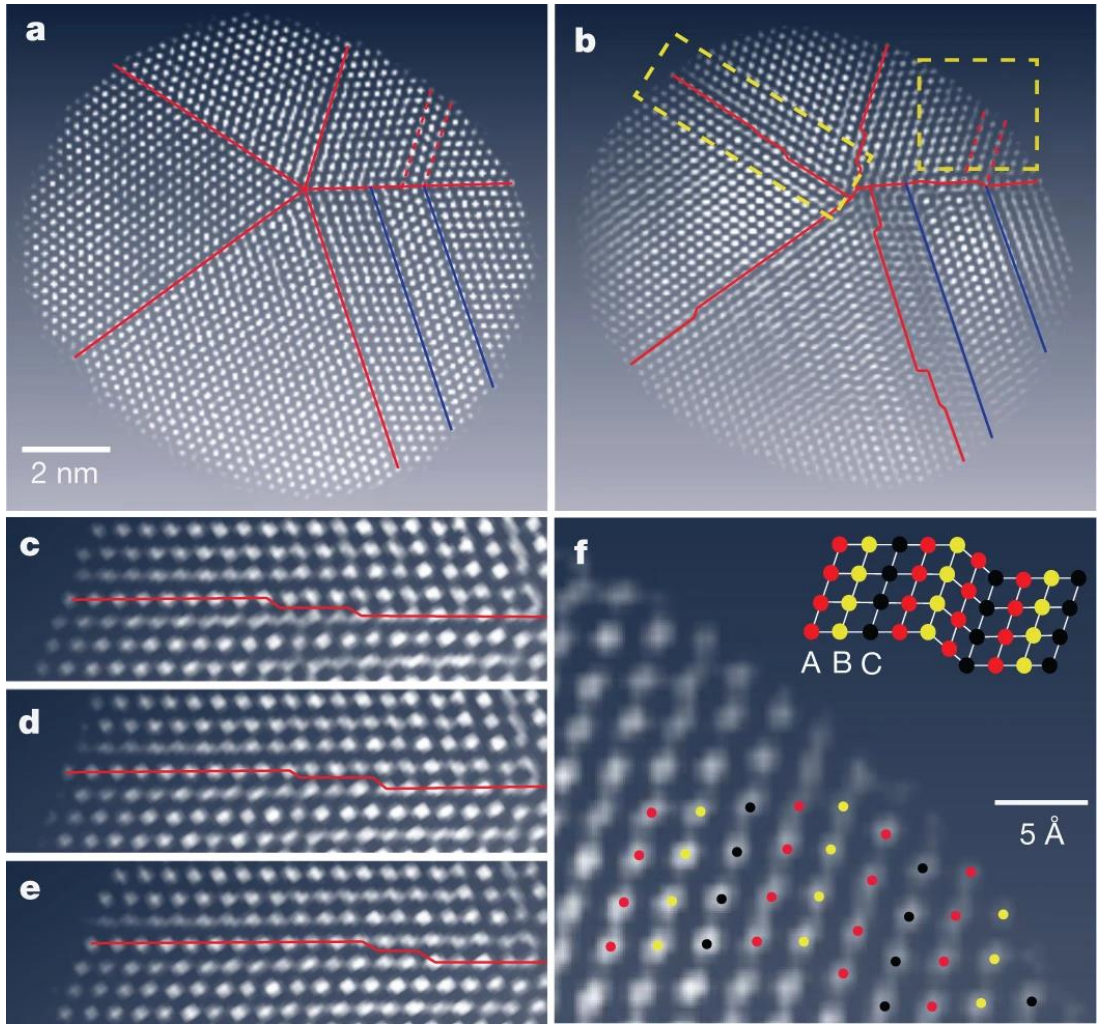
材料科學的分支

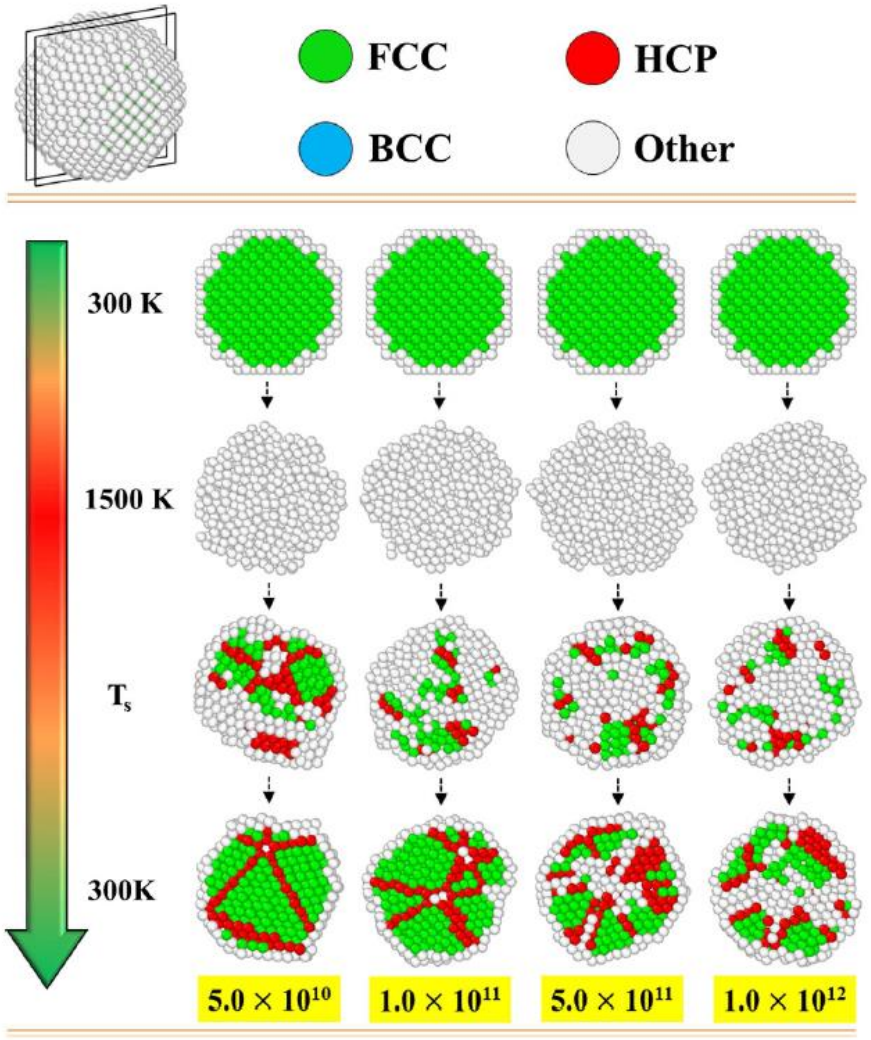

計算科學或模擬
computational science or simulation
經驗觀察與實驗
empirical observation and experimentation
計算
實驗
材料科學
理論
資料
分析或理論方法
analytical or theoretical approaches
資料分析與發現
data-Intensive scientific discovery

實驗與測量



Chen, C., Zhu, C., White, E. et al. Three-dimensional imaging of dislocations in a nanoparticle at atomic resolution. Nature 496, 74–77 (2013).

計算或模擬

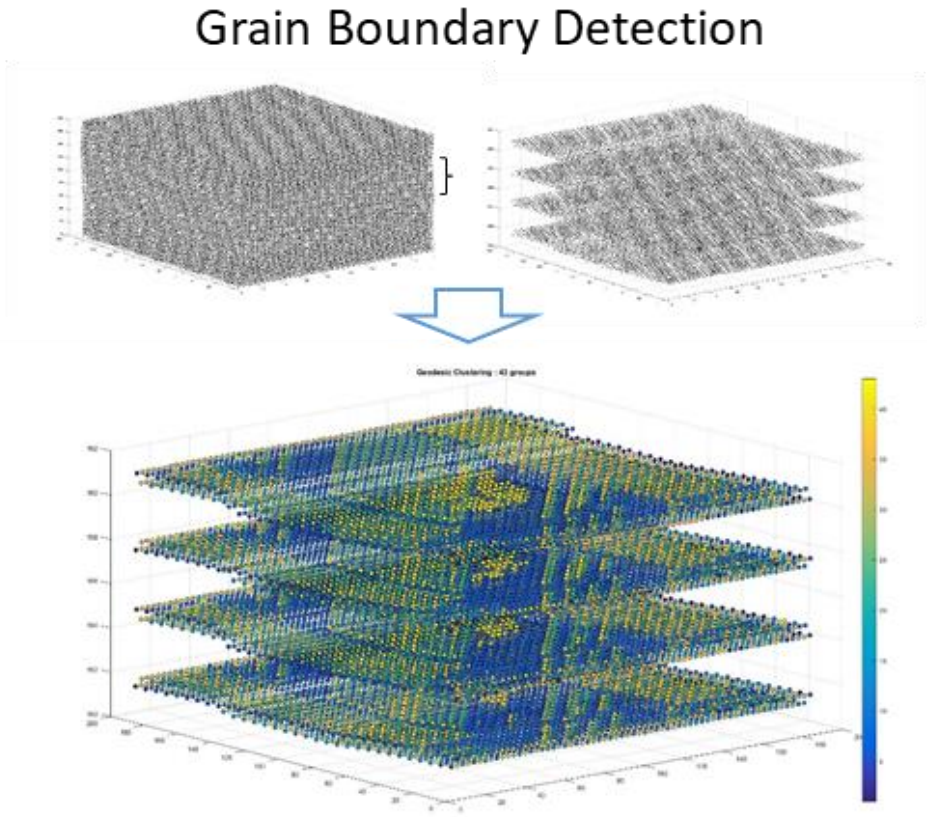


Vo, T.Q., Kim, B. A molecular dynamics study on cooling rate effect on atomic structure of solidified silver nanoparticles. Eur. Phys. J. D 73, 183 (2019).

Case1-晶粒邊界辨識

晶粒邊界分群機器

合作計畫	無
合作團隊	交大材料鄒年棣實驗室

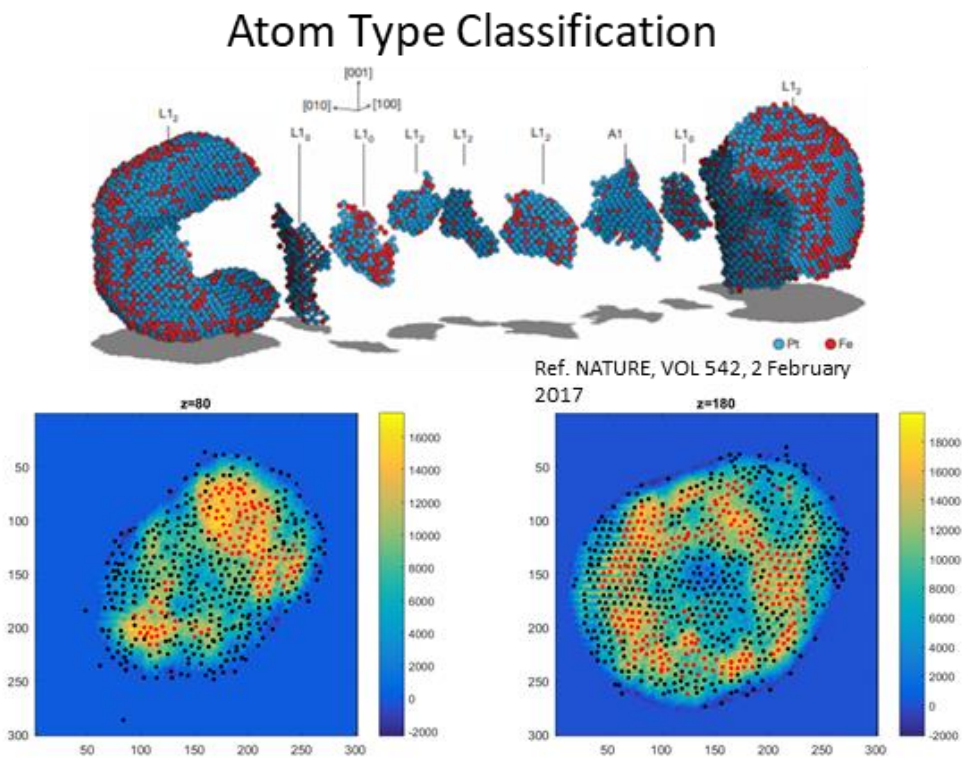


案例	透過非監督式學習，完成晶粒邊界辨識、結構分群
客戶目標	晶粒邊界辨識，達成結構分群，以進行區塊結構相似度分析，並與人為經驗公式相互驗證
問題困難描述	人工觀察大量模擬結果資料耗工費時，傳統分群方法需要先前知識才能協助分群。
訓練資料來源	分子動力學模擬結果
機器學習引擎	Modularity
結果	針對晶粒邊界辨識與其結構達成自動分群，與人工經驗法則結果一致。
Status	會議論文已發表 論文撰寫中

Case2-奈米粒子影像重建

種類與缺陷型態深度辨識機器

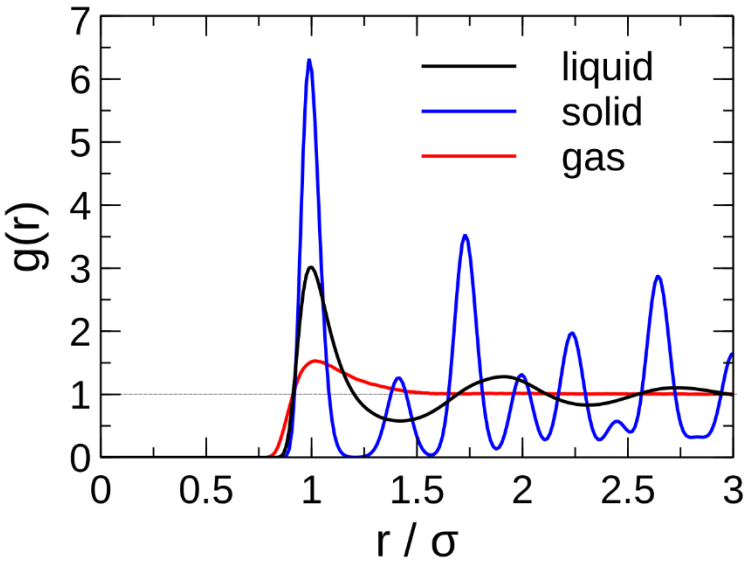
合作計畫	國研院創新計畫
合作團隊	清大工科陳健群實驗室

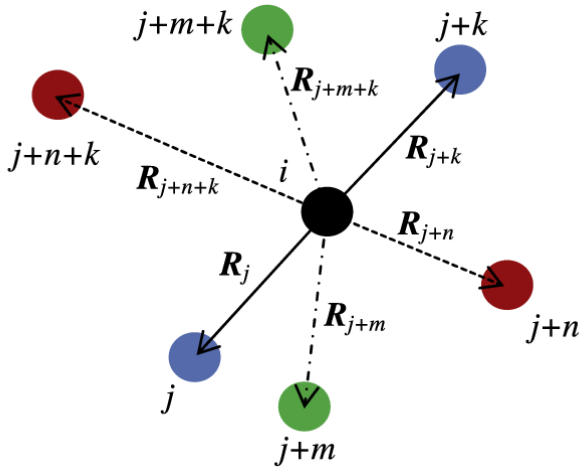


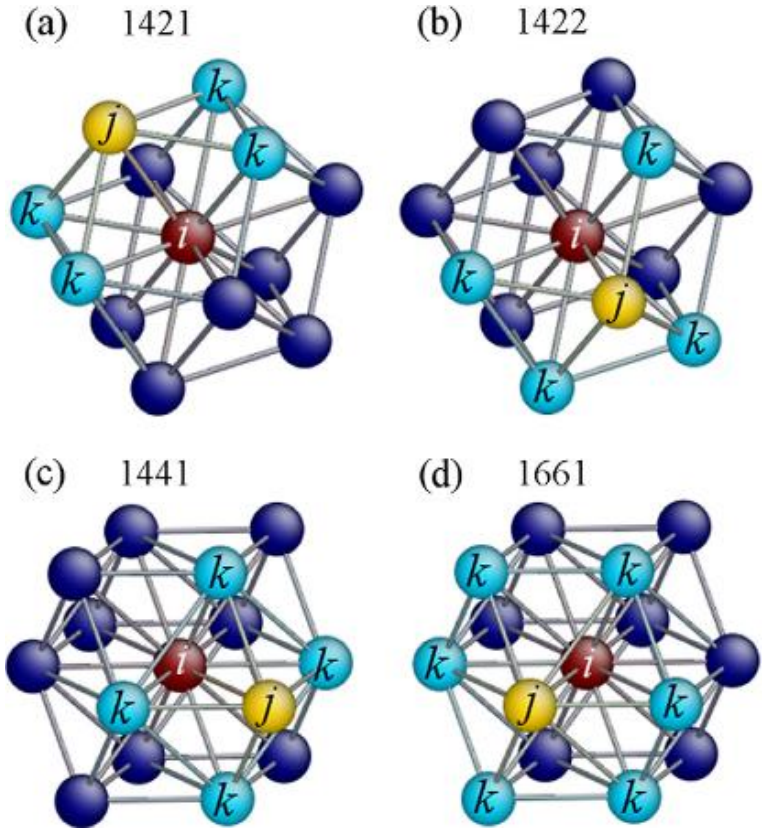
案例	三維斷層造影之原子種類與缺陷型態辨識
客戶目標	透過深度學習技術，定位原子座標、辨識原子種類、分析缺陷型態
問題困難描述	需要人工判斷原子種類與缺陷邊界，會因人為偏見造成不一致性的誤判。
訓練資料來源	原子級三維斷層造影顯微技術之實驗資料
機器學習引擎	Convolutional Neural Network, Ensemble Learning, Active Learning
結果	成功完成原子座標定位、種類辨識、缺陷邊界型態與相似度分析。降低人為誤判機會。
Status	通過實驗組驗證 論文撰寫中(Nature Materials)

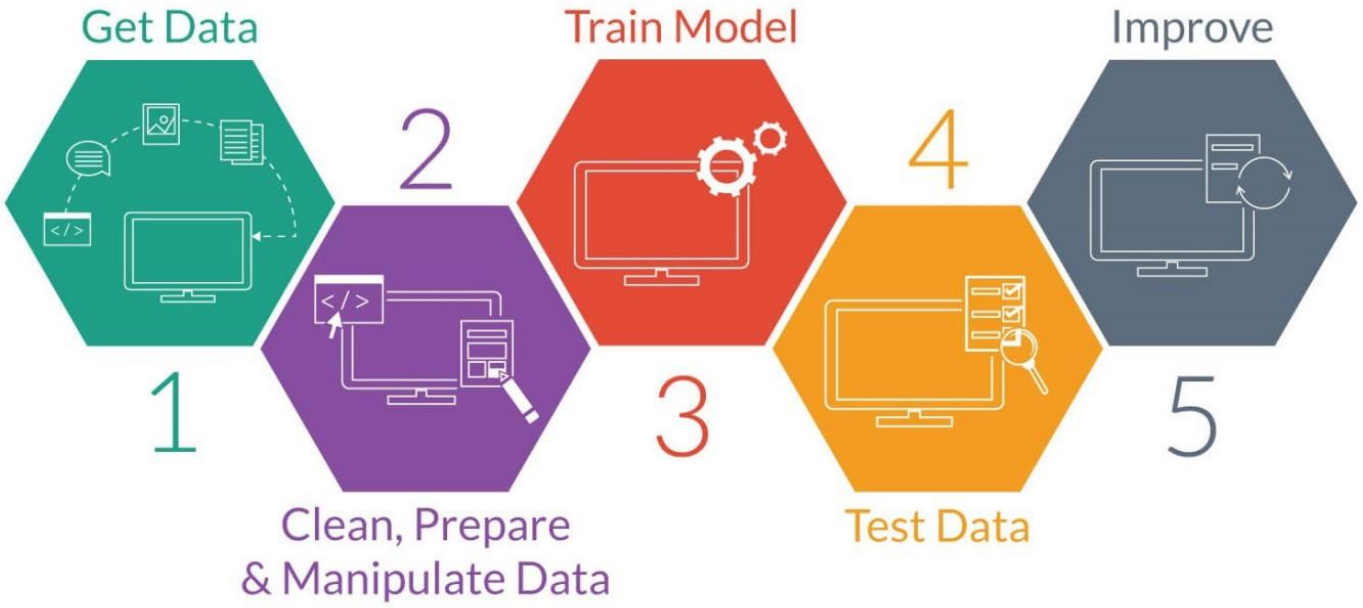
Classification of Crystallographic Groups by Machine Learning

A new powerful approach helping us to Identify the microstructure.









使用軟體產生資料

檔案處理

特徵萃取

建立網路

分群演算法

用測試資料檢驗演算法

調整萃取特徵方法

LAMMPS

NumPy

SciPy

MD ANALYSIS

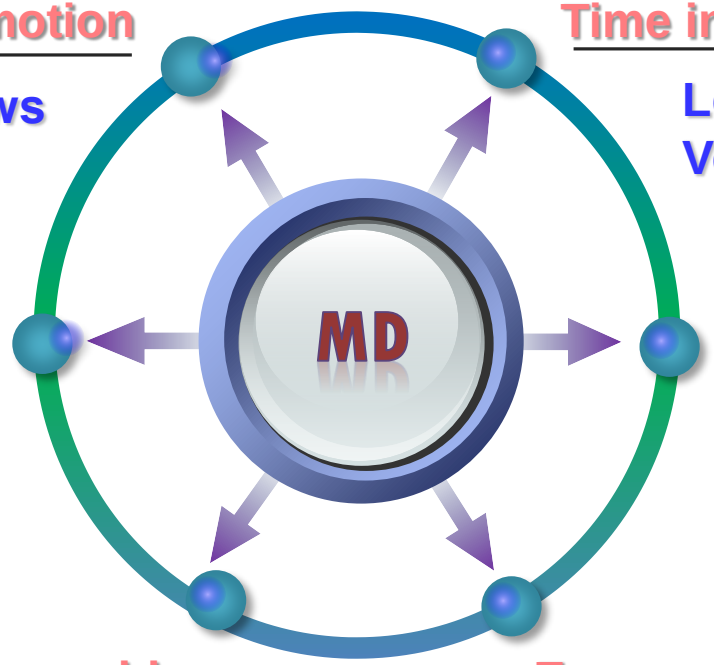
ASE

scikit learn

Molecular Dynamics (MD)

- **A computer simulation technique that allows one to predict the time evolution of a system of interacting particles (atoms, molecules,.. etc.)**
- **N-body simulation**
- 利用一個描述原子間作用關係來描述一個系統。
- 系統內的所有原子遵循著牛頓運動定律。

Quantum Molecular Dynamics; Classical Molecular Dynamics



Equation of motion

Newton's 2nd Laws

Time integral

Leap-frog Verlet
Velocity Verlet algorithm

Numerical algorithm

Force truncation
neighbor List
PBC

Force Field/ Potential

CHARMm
ENCAD
AMBER
TB
EAM
SW

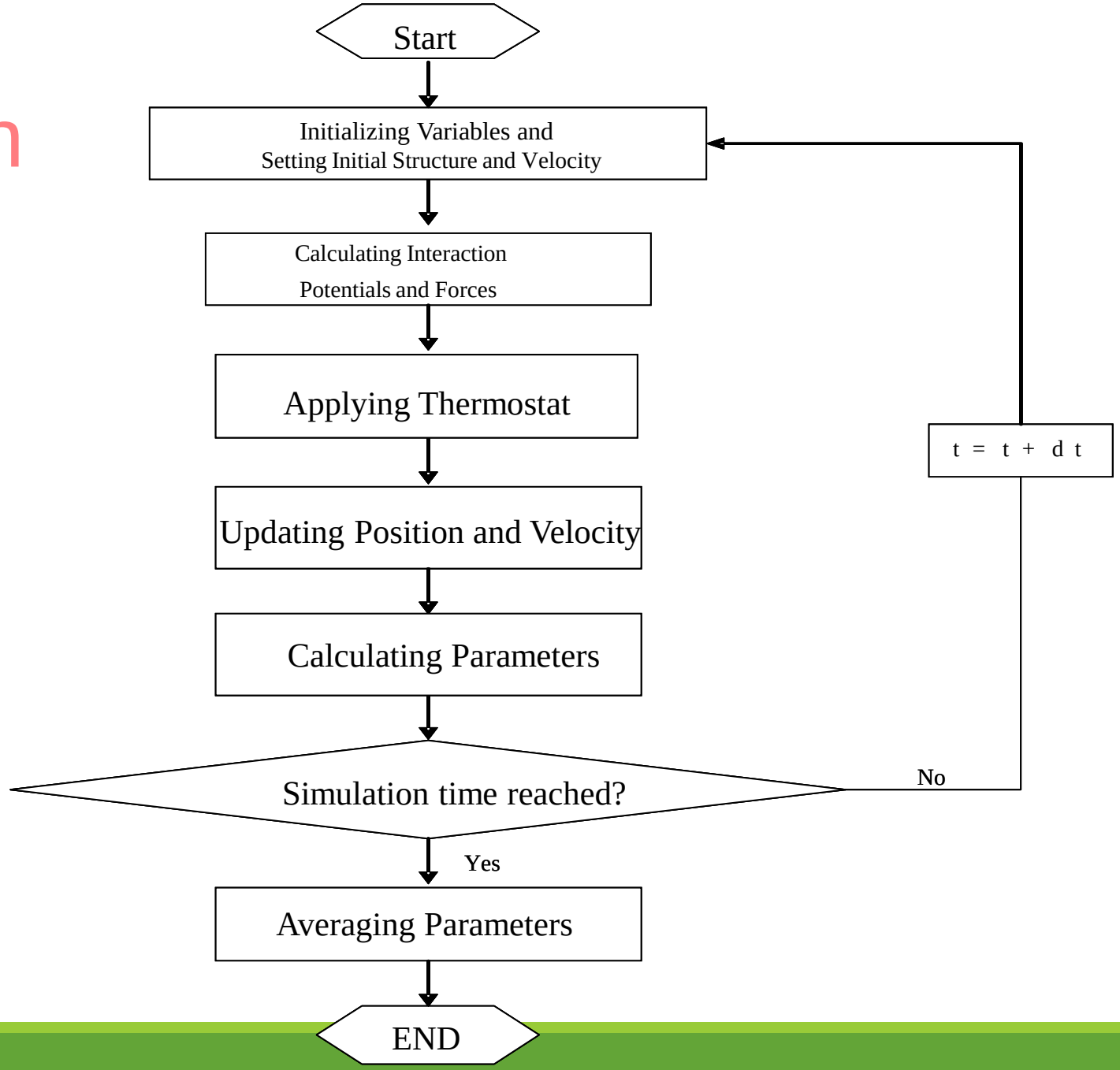
Ensemble

NPT
Isobaric-Isothermal Ensemble
NVT
Canonical Ensemble
NVE
Microcanonicalensemble

Energy minimization

Conjugate gradient
Steepest Descent
Fire algorithm

Flow Chart of MD simulation



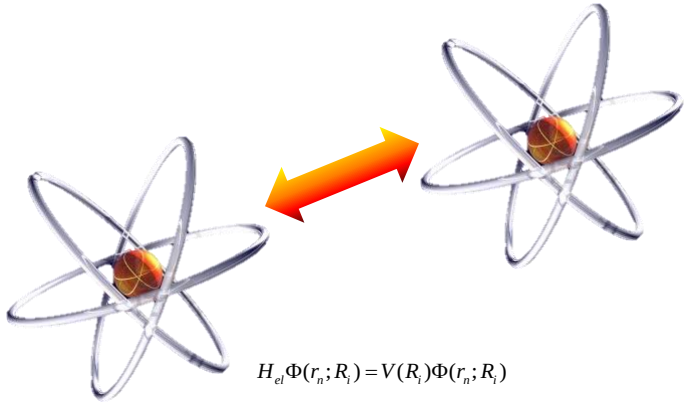
Initial velocity and energy conservation

- Velocities are randomly assigned to the atoms. To achieve faster equilibration atoms can be assigned velocities with the expected equilibrium velocity, i.e. Maxwell distribution.
- Momentum and energy are to be conserved throughout the simulation period.
- Energy conservation is sensitive to the choice of integration method and size of the time step.
- Angular momentum conservation.

Equation of motion

How Does Molecular Dynamics Work?

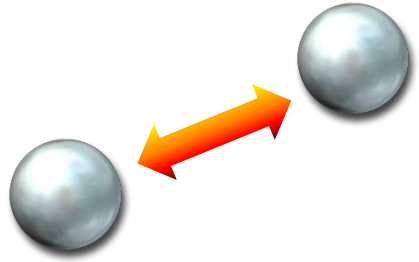
In the molecular dynamics method, each atom is treated as a point mass in space



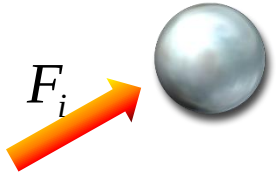
$H_{el}\Phi(r_n;R_i) = V(R_i)\Phi(r_n;R_i)$

Born and Oppenheimer $\sqrt{\frac{M}{m}} \approx 100$

Simplify



Once the force on each atom is computed, atomic motion is determined through application of Newton's Laws



$$F_i(t) = m_i \frac{d^2 r_i(t)}{dt^2} = -\frac{\partial \Phi(r_i)}{\partial r_i}$$

Second-order ordinary differential equation which can be numerically integrated to find new atomic positions!

Time integration

First-order

Euler method

Backward Euler method

Exponential Euler

…

Second-order

Leap-frog Verlet algorithm

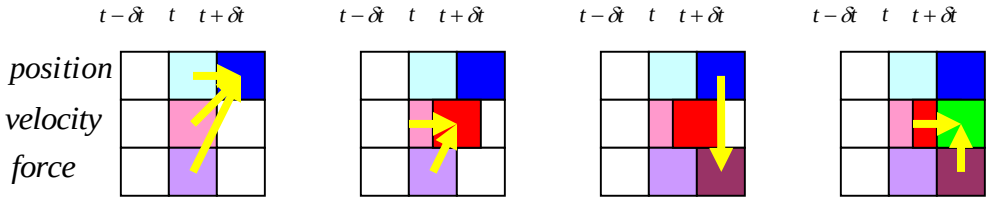
$$r(t+\delta t) = r(t) + v(t+\frac{1}{2}\delta t)\delta t$$

$$v(t+\frac{1}{2}\delta t) = v(t-\frac{1}{2}\delta t) + a(t)\delta t$$

Velocity Verlet algorithm

$$r(t+\delta t) = r(t) + v(t)\delta t + \frac{1}{2}a(t)\delta t^2$$

$$v(t+\delta t) = v(t) + \frac{1}{2}(a(t) + a(t+\delta t))\delta t$$



High-order

Runge–Kutta methods

SSPRK3

…

Ensembles

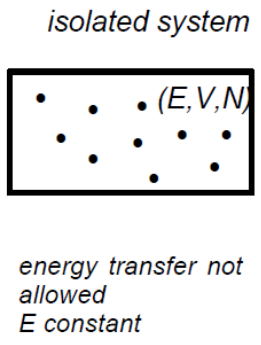
An ensemble is a collection of all possible systems which have different microscopic states but have an identical macroscopic or thermodynamic states. There exist different ensembles with different characteristics.

- **Microcanonical ensemble** (NVE) : The thermodynamic state characterized by a fixed number of atoms, N, a fixed volume, V, and a fixed energy, E. (isolated system)

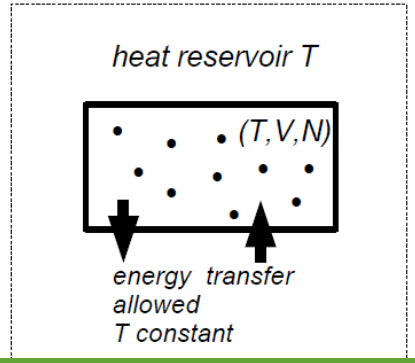
- **Canonical Ensemble** (NVT): This is a collection of all systems whose thermodynamic state is characterized by a fixed number of atoms, N, a fixed volume, V, and a fixed temperature, T. (system in thermostat)

- **Isobaric-Isothermal Ensemble** (NPT): This ensemble is characterized by a fixed number of atoms, N, a fixed pressure, P, and a fixed temperature, T. (system in barostat)

• *Microcanonical ensemble*



• C*anonical ensemble*



Temperature Control

- Velocity Rescaling

  This method is appropriate and efficient for a **homogeneous** system or an inhomogeneous system with **slight difference of mass among atoms**. In the latter case, this method is only appropriate in initial stages of equilibrating the system to relax the random noise of initial velocity.

- Weak coupling method :Berendsen Thermostat / Brownian motion

  This method does generate a fluctuation at about the desired temperature, but has disadvantages similar to the rescaling method.

- Stochastic collision method : Andersen thermostat

  The drawback of this method is that it cannot generate a smooth trajectory and has **less realistic dynamics**. Therefore, it has been rarely used for molecular dynamics simulations.

- Extended system coupling (Extended Lagrangian) method :

  Although the addition of the extended Lagrangian has definitely carried out a correct canonical distribution in property and produced a fluctuation of energy, this assumption of an extended system still cannot make a connection to statistical mechanics.

Temperature Control

- Velocity Rescaling $V_i^{new} = V_i^{old}\lambda$ $\lambda = \sqrt{T_d / T_\alpha}$
- Weak coupling method :Berendsen Thermostat / Brownian motion

$$m\dot{v} = F_i - m_i\gamma_i v_i + R(t)$$ (Langevin' s equation)

- Stochastic collision method : Andersen thermostat
- Extended system coupling (Extended Lagrangian) method :
  - The Nose-Hoover extended system method

$$\dot{\mathbf{r}}_i = \frac{\mathbf{p}_i}{m_i}$$

$$\dot{\mathbf{p}}_i = -\nabla_i V - \zeta \mathbf{p}_i$$

$$\zeta = \frac{\left(\sum_i \frac{\mathbf{p}_i^2}{m_i} - g\,k_B T\right)}{Q} = \nu_T\left[\frac{\sum_i \frac{\mathbf{p}_i^2}{m_i}}{g\,k_B T} - 1\right] = \nu_T\left[\frac{T^*}{T} - 1\right]$$

Notice that: (1) for $T^* > T$ (system too hot), ζ will increase (if it is positive the system cools down)
(2) for $T^* < T$ (system too cold), ζ will decrease (if it is negative the system heat up)

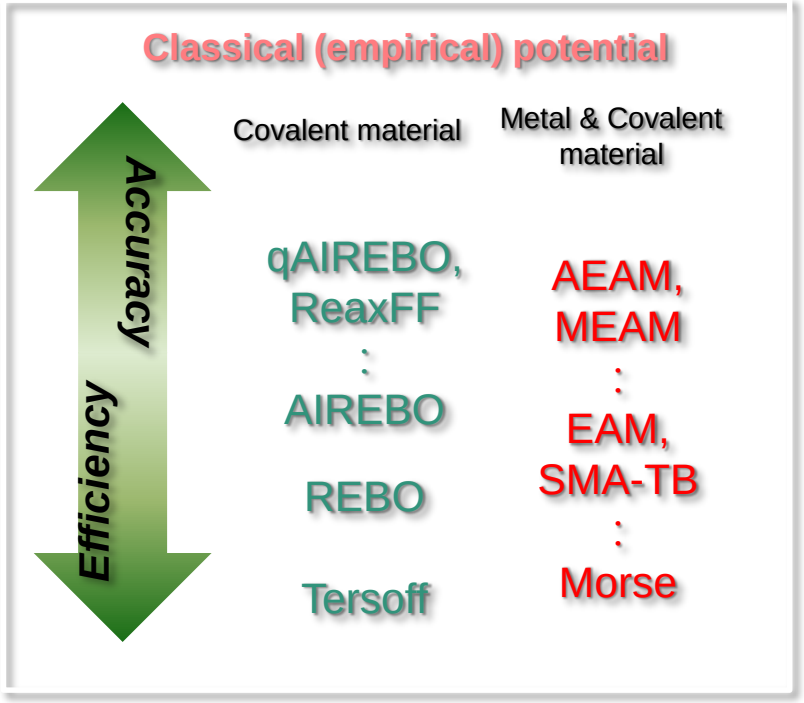
Force Field

In the context of molecular modeling, a force field refers to the form and parameters of mathematical functions used to describe the potential energy of a system of particles (typically molecules and atoms). Force field functions and parameter sets are derived from both experimental work and high-level quantum mechanical calculations. "All-atom" force fields provide parameters for every type of atom in a system.

The usage of the term "force field" in chemistry and computational biology differs from the standard usage in physics. In chemistry it is a system of potential energy functions rather than the gradient of a scalar potential.

To be effective, an analytic Force Field (potential) must possess the following critical properties:

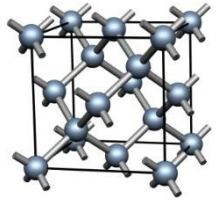
- Accuracy (reproduce properties of interest as closely as possible)
- Computational speed (calculations are fast with simple potentials)
- Transferability (can be used to study a variety of properties for which it was not fit)
- Flexibility (accommodate a wide range of structures in a fitting database)



The potential parameters in the force field are derived from

- ab-initio quantum mechanics
- Crystallography.
- Spectroscopy
- ….

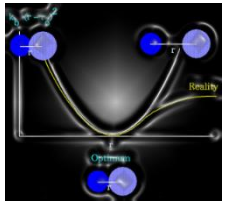
$$\nu = \frac{1}{2\pi}\sqrt{\frac{K}{\mu}}$$



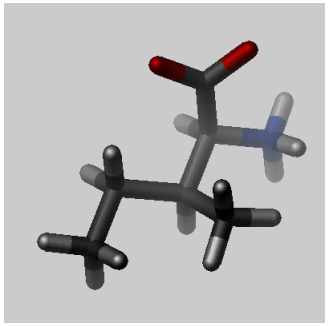
Nonreactive force field (AMBER,CHARMM…)

$$U_{total} = U_{bond} + U_{bending} + U_{dihedral} + U_{vdw} + U_{col}$$

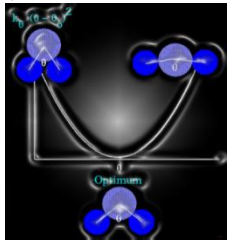
(a) Bond strength



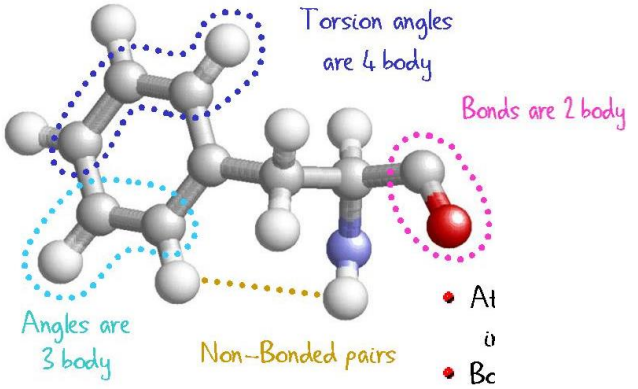
$$U_{bond\ length} = \sum_{N=1}^{N_0} \frac{1}{2} K_b^i (b_i - b_0^i)^2$$



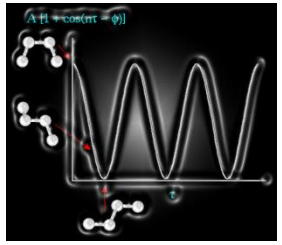
(b) Bond bending



$$U_{bending} = \sum_{N=1}^{N_0} \frac{1}{2} K_\theta^i (\theta_i - \theta_0^i)^2$$

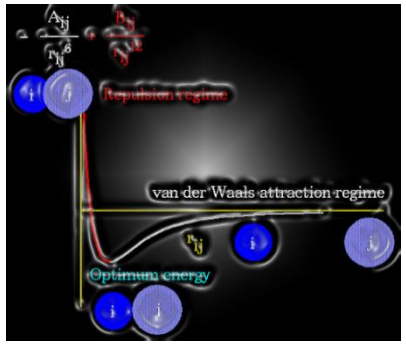


(c) Dihedral Angle



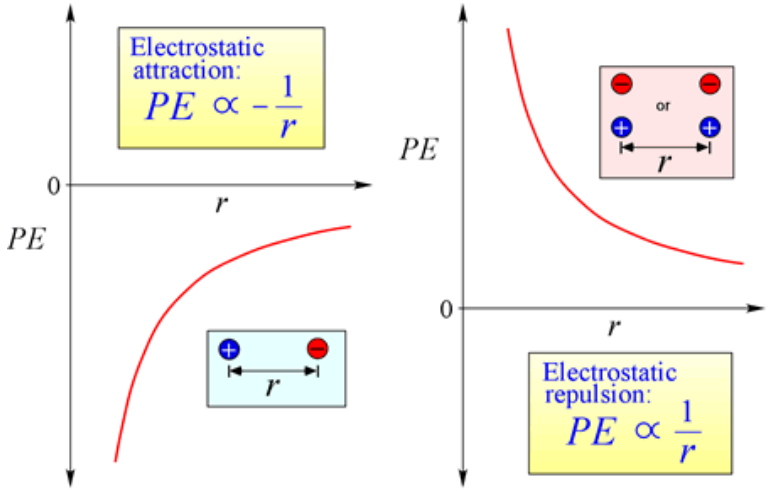
$$U_{dihedral} = \sum_{N=1}^{N_\varphi} K_\varphi^i \left\{1 - \cos\left[N^i\left(\varphi_i - \varphi_0^i\right)\right]\right\}$$

(d) Van der Wail



$$U_{vdw} = \left[\varepsilon^{ij} \left(r_0^{ij} / r_{ij} \right)^{12} - 2\varepsilon^{ij} \left(r_0^{ij} / r_{ij} \right)^{6} \right]$$

(e) Coulomb force



$$U_{col} = \sum_{partialcharges} q^i q^j / r_{ij}\varepsilon$$

Treating Long-Range Electrostatic Interactions

particle-mesh Ewald (PME); Ewald sum

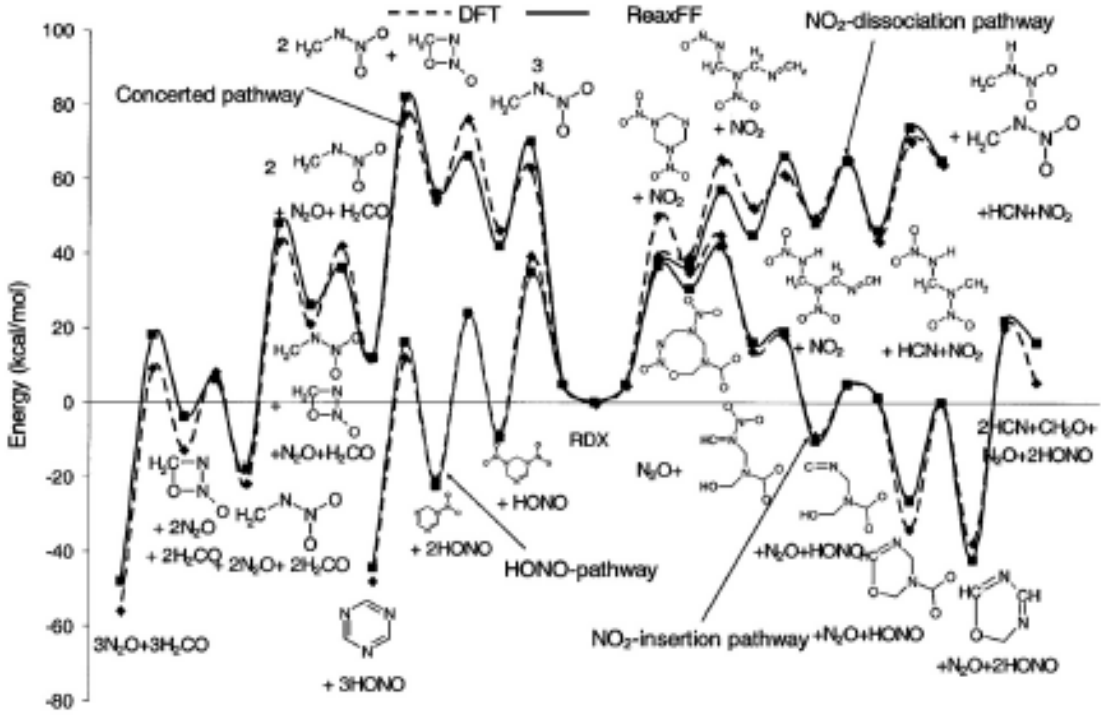
ReaxFF Potential Energy Function

$$E_{system} = E_{bond} + E_{lp} + E_{over} + E_{under} + E_{val} + E_{pen} + E_{coa} + E_{C2} + E_{triple} + E_{tors} + E_{conj} + E_{H\text{-}bond} + E_{vdWaals} + E_{Coulomb}$$

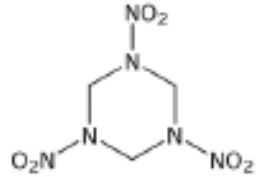
- E_{bond}: bond energy; attractive term, directly derived from bond orders
- E_{lp}: Lone pair energy; penalty for breaking up lone pairs in O, N
- E_{over} : Overcoordination energy: penalty for overcoordinating atoms
- E_{under} : Undercoordination energy: stabilizes undercoordinated atoms
- E_{val} : Angle strain; equilibrium angle depends on bond order central atom
- E_{pen} : Penalty for 'allene'-type molecules (H2C=C=CH2)
- E_{coa} : Angle conjugation; stabilizes –NO2 groups
- E_{C2} : C2 correction: destabilizes C=C
- E_{triple} : triple bond related, first mentioned in publications from 2008
- E_{tors} : Torsion energy: bond-order dependent V2-term
- E_{conj} : Torsion conjugation: general conjugation stability
- $E_{H\text{-}bond}$: Hydrogen bond
- $E_{vdWaals}$: van der Waals: calculated between every atom
- $E_{Coulomb}$: Coulomb interaction: calculated between every atom; polarizable charges get updated every iteration

ReaxFF/*Ab Initio* Comparison

ReaxFF can decribe a wide variety of chemical reactions.



e.g., unimolecular decomposition of RDX



Strachan, et al, *JCP*, 122, 054502 ('05).

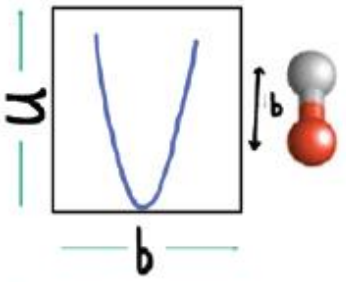
(Original slide from Quenneville presentation)

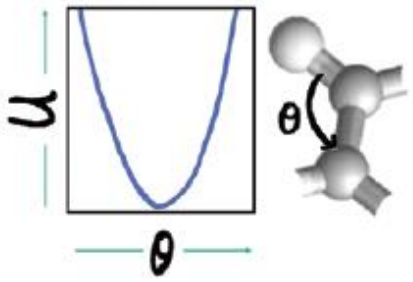
MOLECULAR POTENTIAL ENERGY

$$U = \sum \tfrac{1}{2} K_b (b - b_0)^2 + \sum \tfrac{1}{2} K_\theta (\theta - \theta_0)^2$$

All — All

Hooke 1635

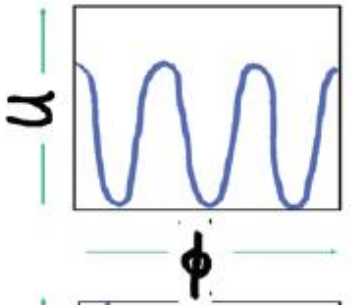


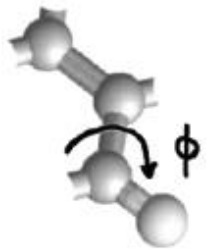


$$+ \sum K_\phi [1 - \cos(n\phi + \delta)]$$

All Torsion

Fourier 1768

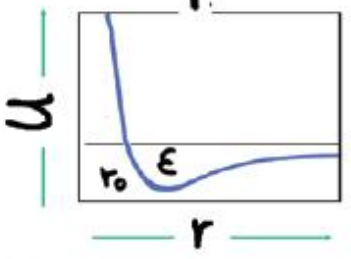


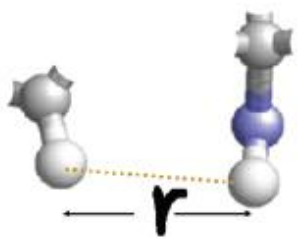


$$+ \sum \varepsilon \left[\left(r_0 / r \right)^{12} - 2 \left(r_0 / r \right)^{6} \right]$$

All Nonbonded

Van der Waals 1837



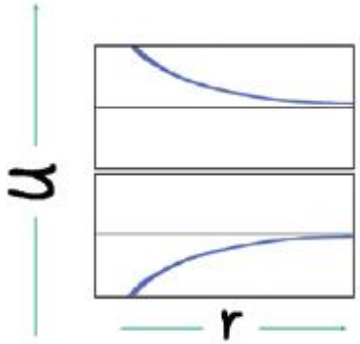


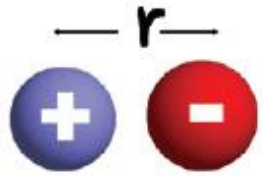
$$+ \sum 332 q_i q_j / r$$

All partial

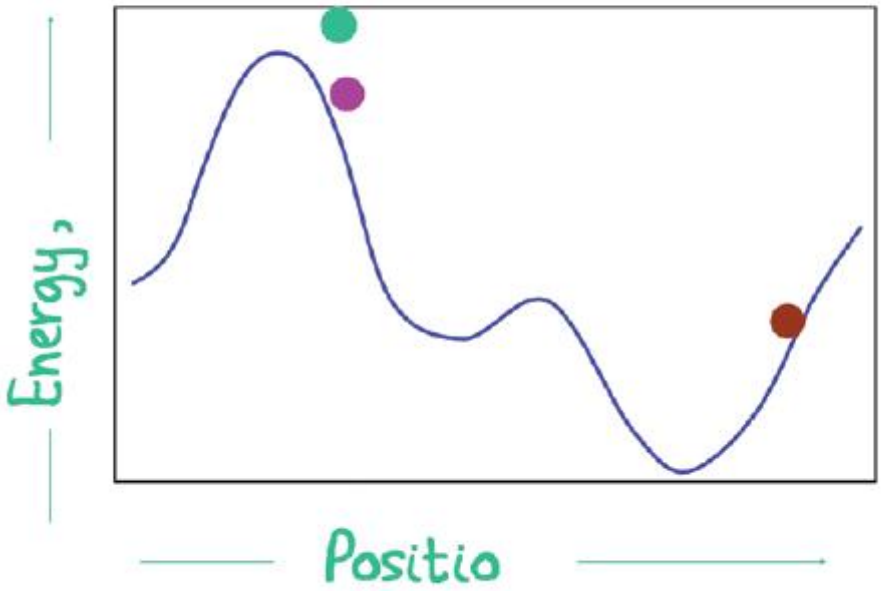
Coulomb 1736

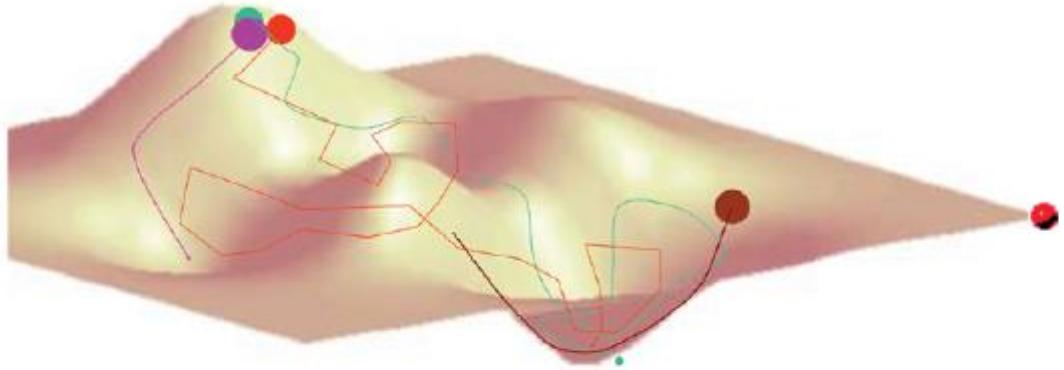
Simple sum over many terms





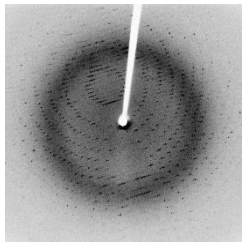
MOVING OVER ENERGY SURFACE

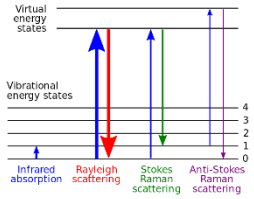


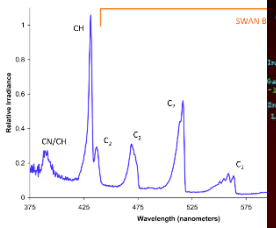


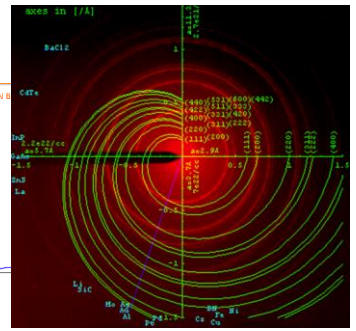
- EM: Energy Minimization drops into local minimum.
  Euclid 325 BC
- NMD: Normal Mode Dynamics vibrates about minimum.
  Galileo 1564
- MD: Molecular Dynamics uses thermal energy to move smoothlu over surface.
  Newton 1643
- MC: Monte Carlo Moves are random. Accept with probability $\exp(-\Delta U/kT)$.
  Metropolis 1915

Fitting energy surface in high dimensional data space with Machine Learning



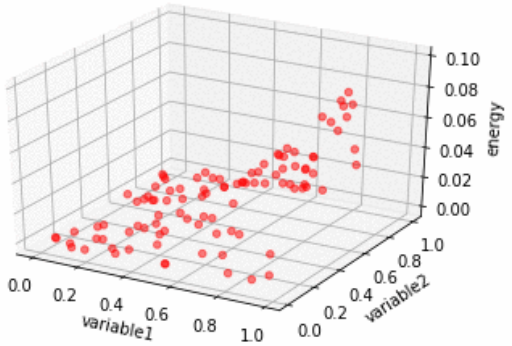






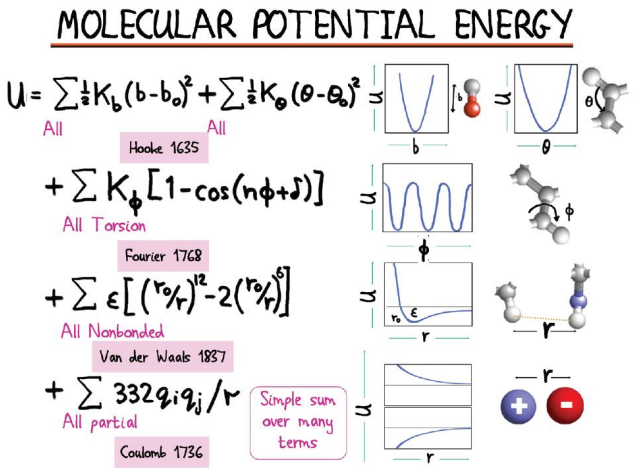
Experimental measurement

Real P.E.S.

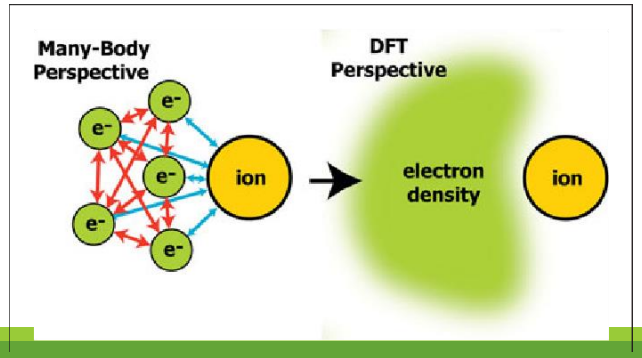


Human fitting

Ordinary approach



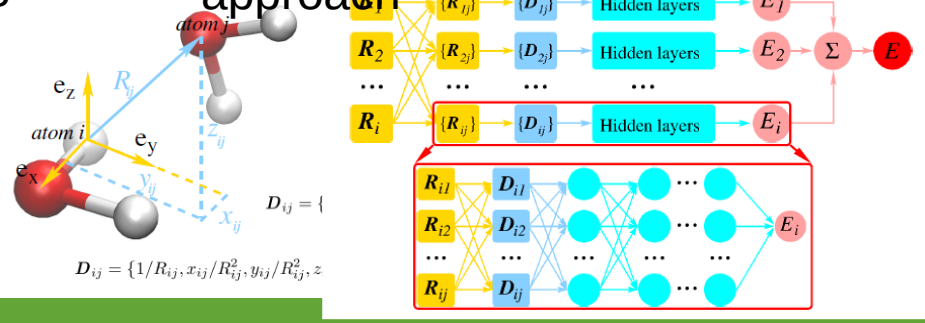
Ab initio calculation

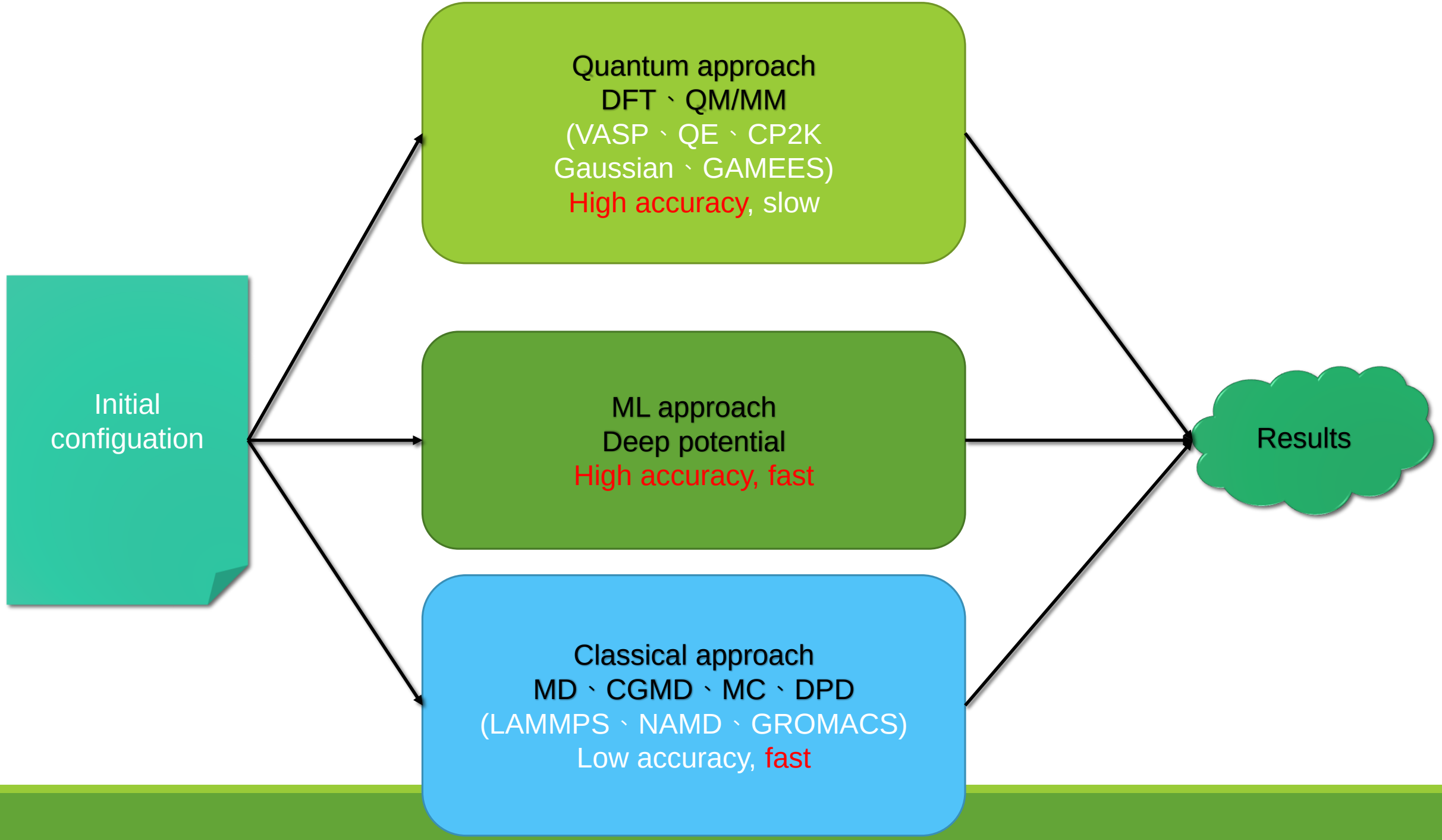


$H\Psi = E\Psi$

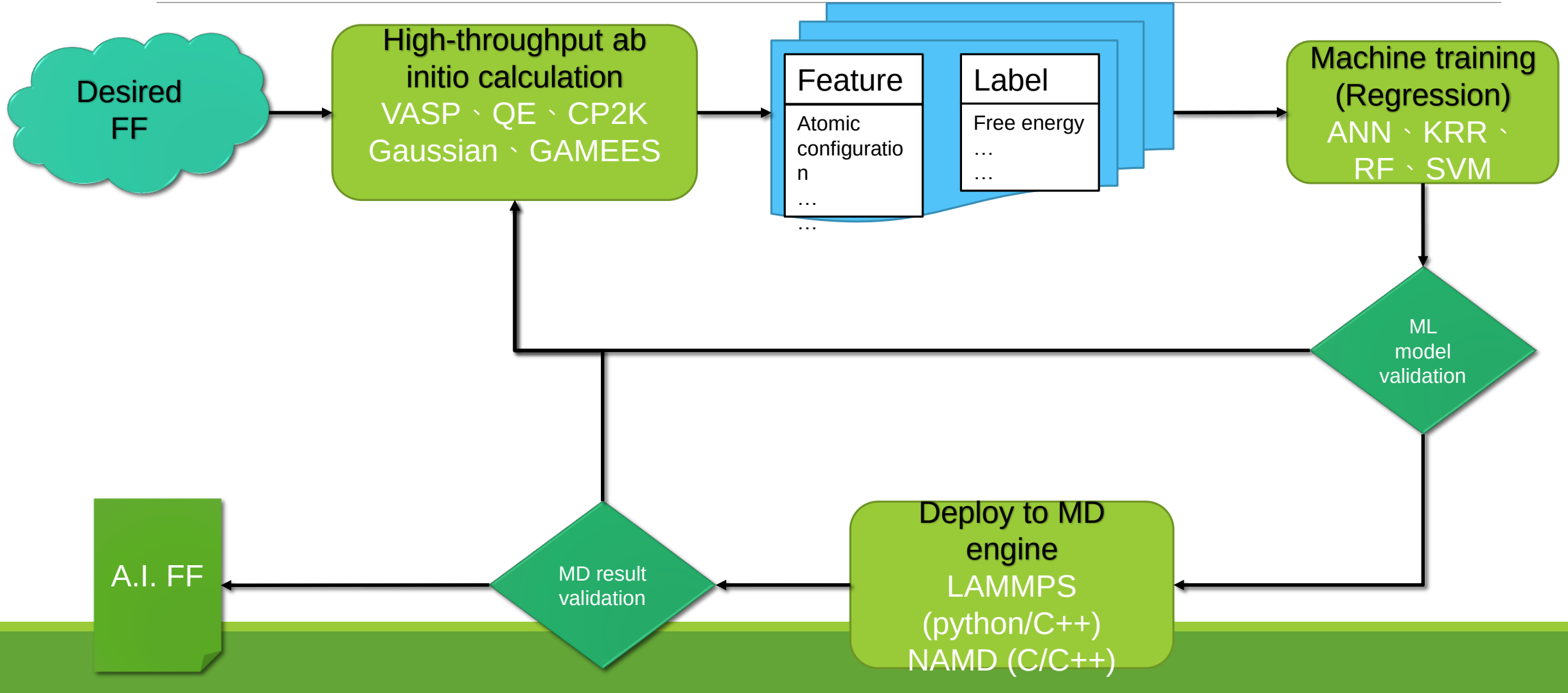
NN fitting

Neuron Network approach




Quantum approach
DFT、QM/MM
(VASP、QE、CP2K
Gaussian、GAMEES)
High accuracy, slow
Initial configuation
ML approach
Deep potential
High accuracy, fast
Results
Classical approach
MD、CGMD、MC、DPD
(LAMMPS、NAMD、GROMACS)
Low accuracy, fast

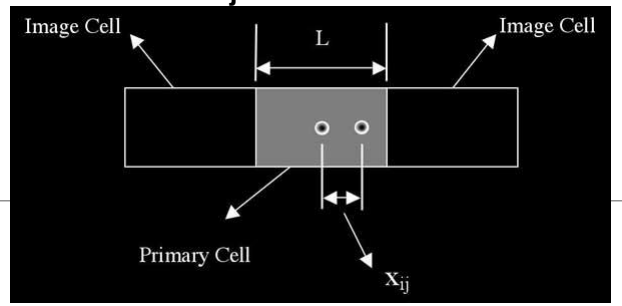
Flow chart for Deep Potential



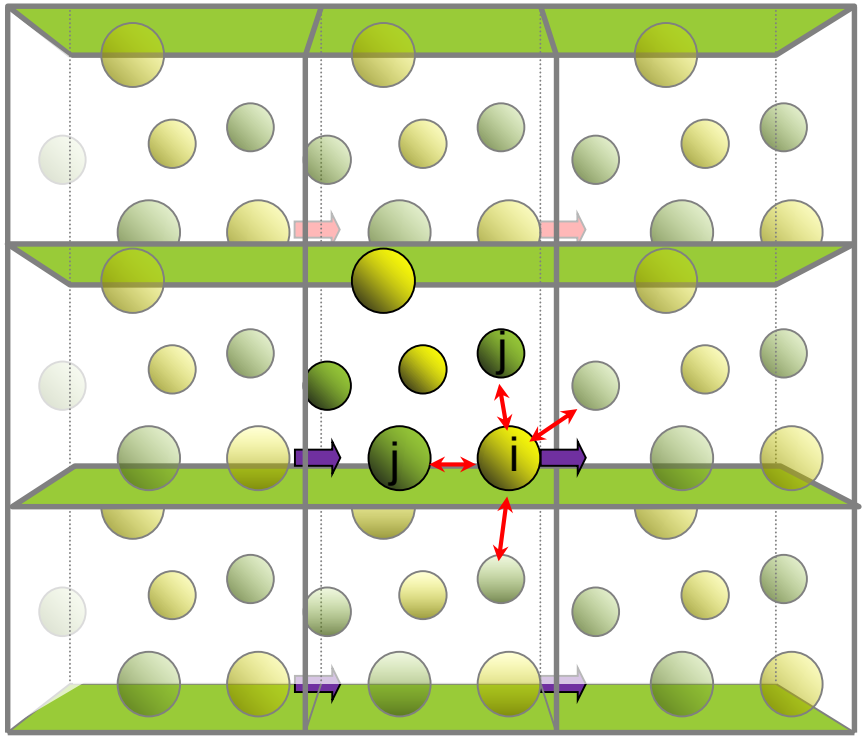
Numerical algorithm

- Periodic Boundary Condition
- Minimum Image Criterion

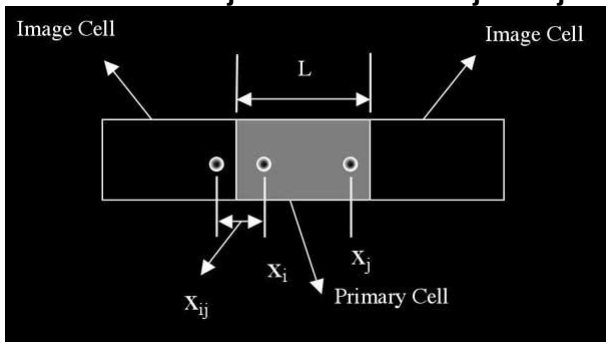
Case A: x_{ij} is less than 0.5L



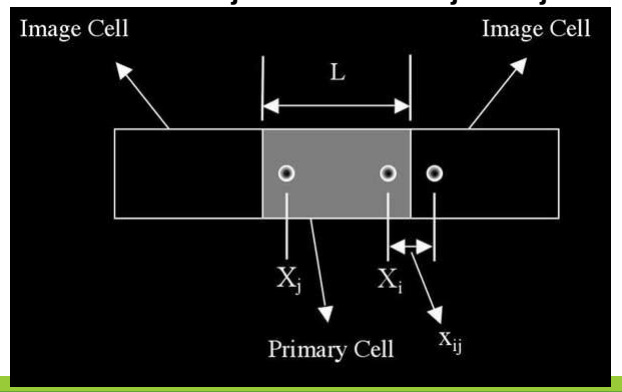
Case B: $x_{ij} < -0.5L$ $x_{ij} = x_{ij} + L$



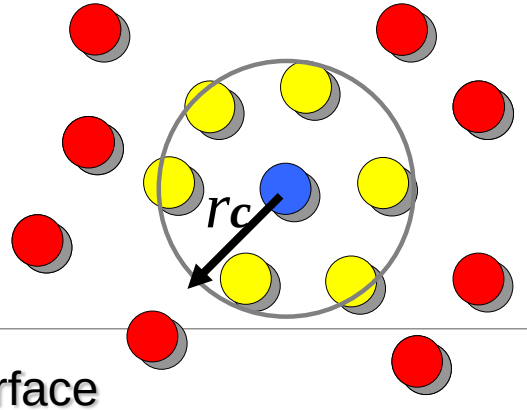
Case B: $x_{ij} < -0.5L$ ➔ $x_{ij} = x_{ij} + L$



Case C: $x_{ij} > 0.5L$ ➔ $x_{ij} = x_{ij} - L$



Force Truncation



- **Truncation**

$$U(r) = \begin{cases} U(r) & r < R_C \\ 0 & r \geq R_C \end{cases}$$

- **Shift function:** modifies the entire potential energy surface

$$U_{nb}(r) = \begin{cases} U_{nb}(r)\left(1-(\frac{r}{R_c})^2\right)^2 & r < R_C \\ 0 & r \geq R_C \end{cases} \quad \cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots \text{ Brook et. al.}$$

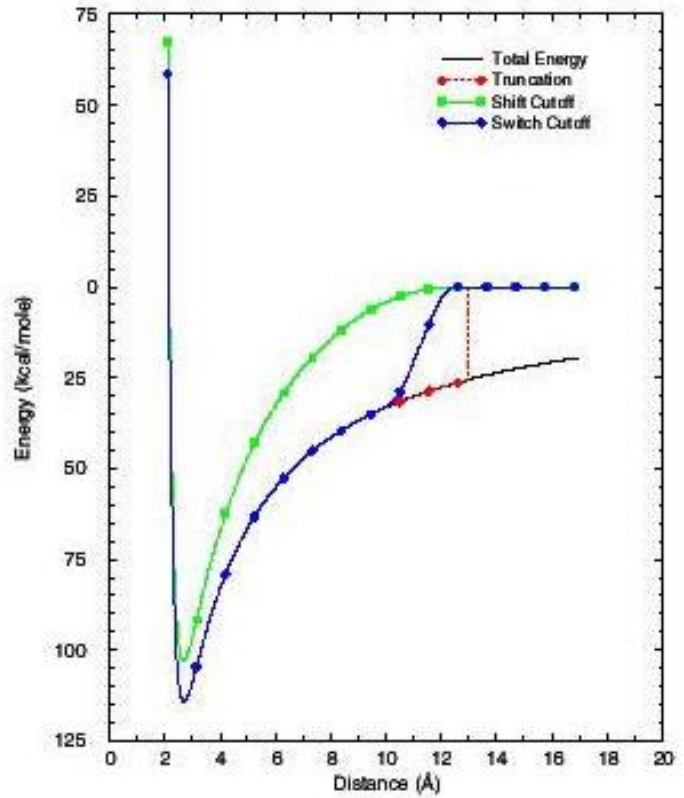
$$U_{nb}(r) = \begin{cases} U_{nb}(r) - \left[U_{nb}(R_C) + (r-R_C)\left[\frac{dU_{nb}(R_C)}{dr}\right]\right] & r < R_C \\ 0 & r \geq R_C \end{cases} \quad \cdots\cdots\cdots\cdots \text{ Levitt et. al.}$$

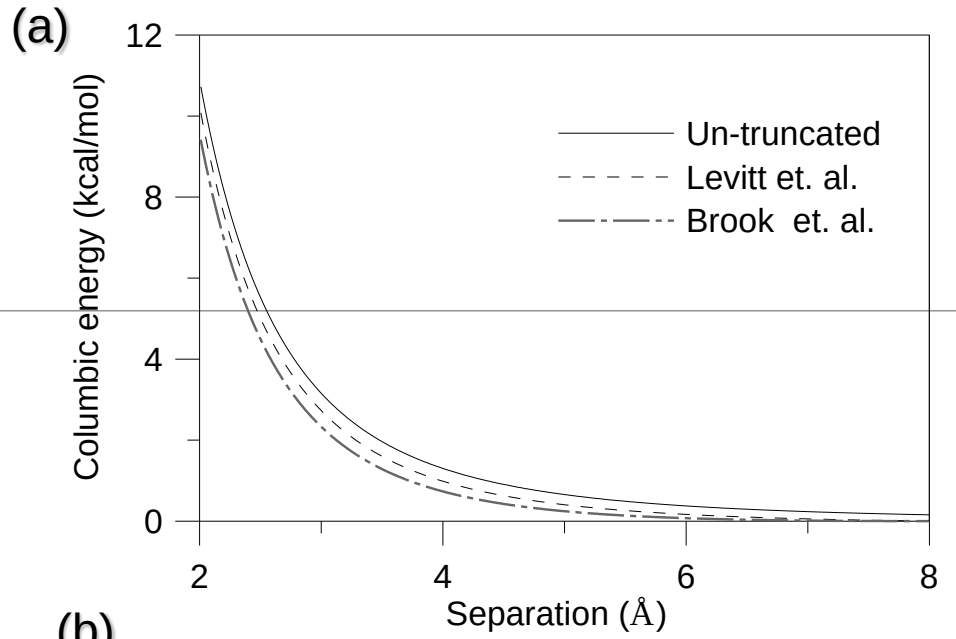
- **Switch function:** modifies the interaction potential over a predefined range of distances

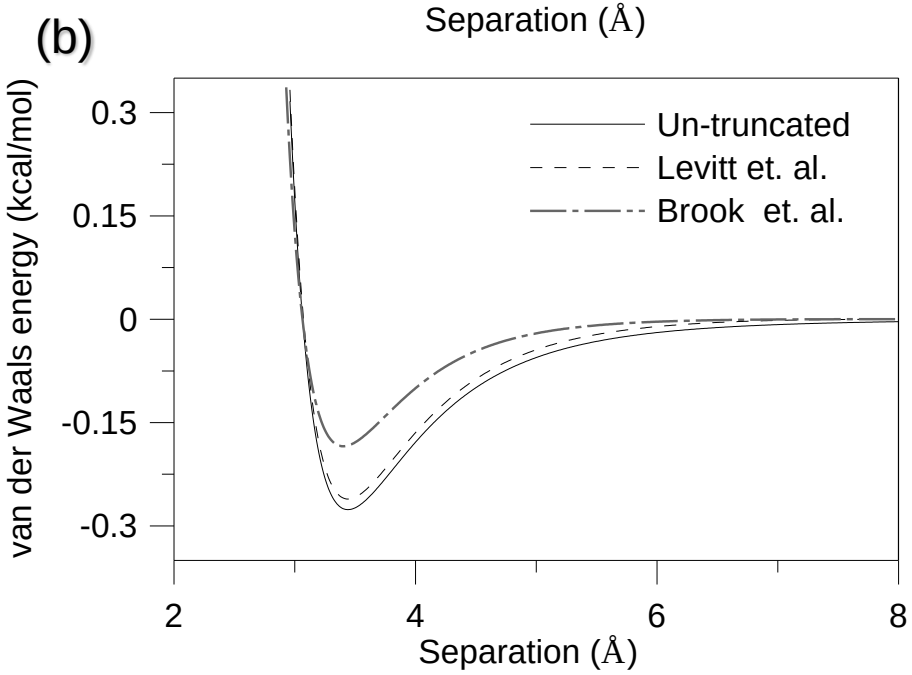
$$U_{nb}(r) = \begin{cases} U_{nb}(r) & r < r_l \\ U_{nb}(r)\left\{\frac{(r_c-r)^2(r_c+2r-3r_l)}{(r_c-r_l)^3}\right\} & r_l \leq r < r_C \\ 0 & r_C \leq r \end{cases} \quad \cdots\cdots \text{ CHARMm}$$

- **The Ewald summation technique**

(a)Columbic energy profile between two water molecules and (b) the van der Waals energy profile between oxygen atom in C=O group and nitrogen atom in N-H group with and without truncation methods.

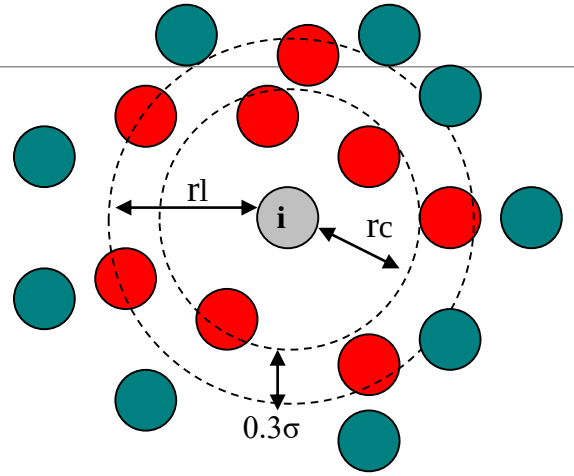




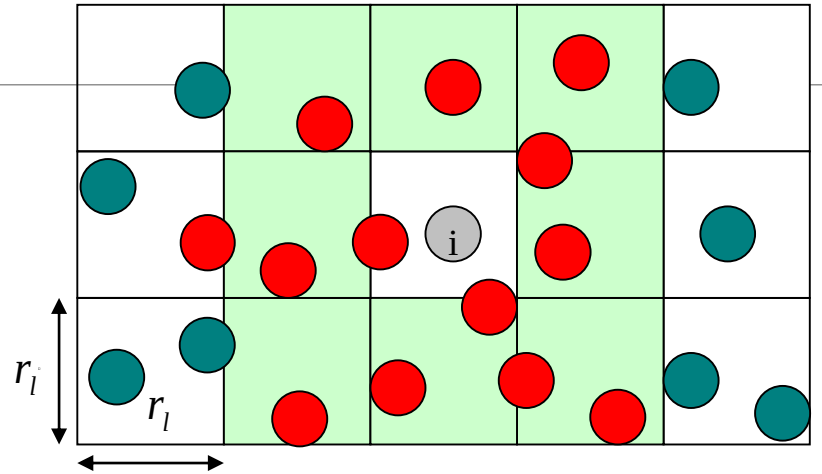


Efficient Neighbours List

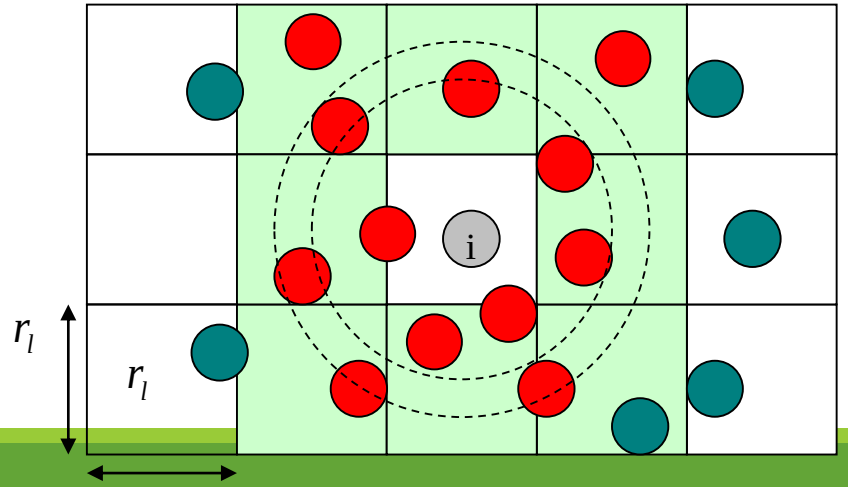
- **Verlet List**



- **Cell Link**



- **Verlet List + Cell Link**



Packages for molecular modeling

Package Name	Developer	Features
LAMMPS	Sandia National Labs	atomic, polymeric, biological, metallic, granular, and coarse-grained systems
NAMD	Parallel Programming Labs	structural biology
GROMACS	Science for Life Labs	general purpose
DL_POLY	Daresbury Labs	general purpose
Desmond	D. E. Shaw Research	biological and chemical systems
AMBER	Peter Kollman et. Al.	biomolecules
SPaSM	Los Alamos National Labs	Large scale simulation

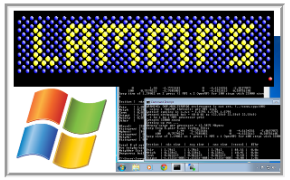
Installation of Windows pre-built binary (ICMS version)

LAMMPS Windows Installer Repository

https://packages.lammps.org/windows.html

webpage screenshot

LAMMPS-ICMS Windows Installer Repository



This repository is hosting pre-compiled Windows installers of the LAMMPS molecular dynamics simulation software package. The binaries are built semi-automaticall with MinGW64 Linux to Windows cross compilers using up-to-date snapshots of the LAMMPS-ICMS git repository hosted at the Institute for Computational Molecular Science at Temple University. The LAMMPS binaries contain **all** optional packages included in the source distribution **except**: KIM (license is not GPL compatible), USER-CUDA (CUDA does not support cross compilation), KOKKOS (does not support cross-compilation), and REAX (superseded by the USER-REAXC package).

OpenCL

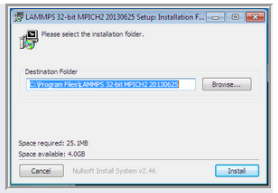
Some Notes on GPU Support
These Windows binaries include (experimental on Windows) GPU acceleration via the GPU package. This is achieved through compiling the GPU package in OpenCL mode and linking to an OpenCL v1.2 compatible ICD loader. This means the executables do not contain any vendor provided code and should be compatible with GPUs from both AMD and Nvidia. The GPU package has been compiled for mixed precision computation and is currently somewhat tuned for Nvidia (Fermi generation) GPUs. It does not yet work with OpenCL drivers for CPUs (like those included in the Intel and AMD OpenCL SDKs). Work is under way to improve and expand OpenCL support in LAMMPS and particularly provide means so that the individual kernels are optimized for specific platforms at runtime. Please watch Mike Brown's LAMMPS accelerator library web page for status updates.

When reporting problems, please always include the exact version of the installer and the output of the `ocl_get_devices` tool.

Looking for pre-compiled Linux binary RPMs? They are just a mouse click away.

Installing LAMMPS on Windows

There are installer packages for 32-bit and 64-bit versions of Windows available.



- Latest version for 32-bit Windows / 32-bit Windows download area
- Latest version for 64-bit Windows / 64-bit Windows download area

The respective download directory will contain installer packages that are labeled with the date they were compiled on and one package labeled as *latest*. It is usually recommended to download and install the latest package via the link above. The other packages are provided in case there is a problem with it. Download the installer executable suitable for your machine, execute it, and follow the instructions in the dialogs. Each version will install into a different directory, so it is possible to have multiple versions installed at the same time. Both kinds of packages contain:

- A regular multi-threaded LAMMPS executable called `lmp_serial`. This should always work.
- A multi-threaded LAMMPS executable that also supports parallel execution via MPI message passing. This executable is called `lmp_mpi` and requires installation of a suitable MPICH2 package to work.
- the LAMMPS manual in PDF format
- the colvars reference manual in PDF format
- the potential files bundled with the LAMMPS source code
- most of the example inputs, reference outputs and related files
- the benchmark inputs and reference outputs
- the tools `restart2data, binary2txt, chain, msi2lmp, ocl_get_devices`

Both executables will run in serial when executed directly. Please see below for instructions on how to perform parallel runs. To use the MPI based parallelism, you also need to install MPICH2 from Argonne lab. For 32-bit Windows you have to download and install mpich2-1.4.1p1-win-ia32.msi or any compatible version. Correspondingly, for 64-bit Windows you have to download and install mpich2-1.4.1p1-win-x86-64.msi or any compatible version.

Running LAMMPS on Windows

General Comments

http://rpm.lammps.org/windows.html Fri Aug 15 2014 10:35:07 GMT+0800 (台北標準時間)

Choose executable file based on the architecture of your PC, then double click on it to install.
If you want to run LAMMPS in parallel mode, mpich2-1.4.1p1-win-x86-64.msi is also needed.

Run LAMMPS on Windows

1. Install lammps on your windows system, put the path of lammps exe file(Ex. lmp_serial.exe) in the PATH environment variable (Ex. C:\Program Files\LAMMPS 64-bit 16Aug2018\bin) .
2. Put input file(Ex. in.**xxx**), potential file or coordinate file (optional)in project folder (X:\project_folder).
3. Open cmd , and change directory to project folder(“X:” then “cd project_folder”).
4. Or press shift and right click to open cmd in the project_folder.
5. Use the following command to run lammps “C:\Program Files\LAMMPS 64-bit 16Aug2018\bin\lmp_serial.exe -in in.**xxx**”
6. Use the following command to run lammps with multi-threading parallelization “C:\Program Files\LAMMPS 64-bit 16Aug2018\bin\lmp_serial.exe -in in.**xxx** -pk omp 4 -sf omp”

LAMMPS Command-line options

lmp_serial.exe -in in.xxx -pk omp 4 -sf omp -v rseed 46

- -i or -in Specify a file to use as an input script.
- -pk or -package Invoke the package command with style and args
- -sf or -suffix Use variants of various styles if they exist. The specified style can be gpu, intel, kk, omp, opt, or hybrid.
- -v or -var Specify a variable that will be defined for substitution purposes when the input script is read. (referenced as $abc or ${abc} in the input script)
- …

LAMMPS input script

- LAMMPS executes by reading commands from a input script (text file).
- One line at a time.
- The input script is read one line at a time and each command takes effect when it is read.
- Some commands are only valid when they follow other commands.

```
timestep 0.5
run      100
run      100
```

```
run      100
timestep 0.5
run      100
```

LAMMPS input script

- All characters from the first “#” character onward are treated as comment and discarded.
- If the last printable character on the line is a “&” character, the command is assumed to continue on the next line.
- The input script is read one line at a time and each command takes effect when it is read.
- The line is broken into “words” separated by white-space (tabs, spaces).
- The first word is the command name. Other words in the line are arguments.
- If you want text with spaces to be treated as a single argument, it can be enclosed in either single or double or triple quotes.
- If you want multiple lines of an argument to retain their line breaks, the text can be enclosed in triple quotes.

LAMMPS input script structure

設定檔可區分為4個部分

Initialization

Atom Definition

Settings

Run a Simulation

Settings

Run a Simulation

...

命令可以分類成9群

1. Initialization
2. Atom Definition
3. Force Fields
4. Settings
5. Fixes
6. Computes
7. Outputs
8. Actions
9. Miscellaneous

LAMMPS	Commands
INITIALIZATION	atom_modify, atom_style, boundary, dimension, newton, processors, units
ATOM DEFINITION	create_atoms, create_box, lattice, read_data, read_dump, read_restart, region, replicate
SETTINGS	
Force fields	angle_coeff, angle_style, bond_coeff, bond_style, dielectric, dihedral_coeff, dihedral_style, improper_coeff, improper_style, kspace_modify, kspace_style, pair_coeff, pair_modify, pair_style, pair_write,special_bonds
Parameters	neighbor, neigh_modify, group, timestep, reset_timestep, run_style, min_style, min_modify.
Fixes	fix, fix_modify, unfix
Computes	compute, compute_modify, uncompute
Output	dump, dump image, dump_modify, dump movie, restart, thermo, thermo_modify, thermo_style, undump, write_data, write_dump, write_restart
RUN	run, temper, minimize, neb prd, rerun
Actions	delete_atoms, delete_bonds, displace_atoms, change_box
Miscellaneous	clear, echo, if, include, jump, label, log, next, print, shell, variable

Command Format

- ✓ *COMMAND* (+ group-ID) (+args…) (style (+args…))(+其它(+ values …)) (+ keyword (+ values …))

  Example:

  neb etol ftol N1 N2 Nevery file-style arg

  - etol = stopping tolerance for energy (energy units)
  - ftol = stopping tolerance for force (force units)
  - N1 = max # of iterations (timesteps) to run initial NEB
  - N2 = max # of iterations (timesteps) to run barrier-climbing NEB
  - Nevery = print replica energies and reaction coordinates every this many timesteps
  - file-style= *final* or *each* or *none*

  final arg = filename
  filename = file with initial coords for final replica coords for intermediate replicas are linearly interpolated between first and last replica
  each arg = filename
  filename = unique filename for each replica (except first) with its initial coords
  none arg = no argument
  all replicas assumed to already have their initial coords

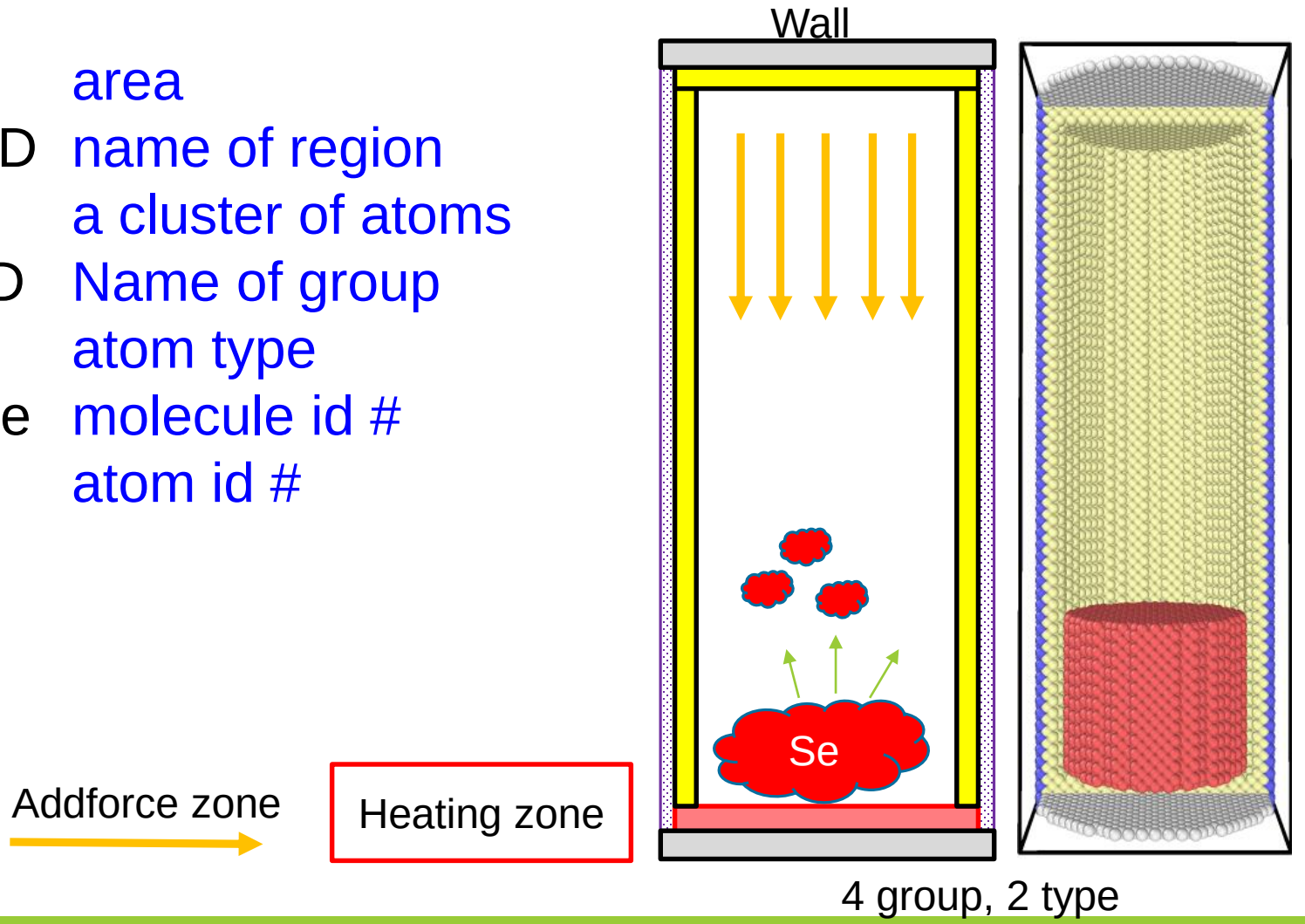
- ✓ fix +ID + group-ID + style (+args…) (+ keyword (+ values …))
- ✓ compute +ID + group-ID + style (+args…) (+ keyword (+ values …))
- ✓ variable+name + style_name +args…

※若arg 或value為斜字體即為字元(*yes, no, final* …)，若非則為數字

command參數	說　明
style(+arg)	擁有多重功能參數之command 會有style參數 ✓ 功能參數 -style ，名稱有特定 -arg，部份名稱為特定，部份由使用者給數據，可為數字或字元 ✓ 無指定群組，e.g.: min_style (選擇能量最小化方法) lattice (選擇晶格) pair_style (選擇勢能函數) ✓ 指定群組，e.g.: fix (+ID + group - ID + style_name) compute (+ID + group - ID + style_name)
ID, group-ID, region-ID, fix-ID,	參數中的指定代號,指定群組代號,指定區間代號 , fix代號 (使用者給定)
keyword (+value)	可額外選用之子功能/子條件之參數(可給可不給) -keyword，名稱有特定 -value，部份名稱為特定，部份由使用者給數據，可為數字或字元
file	檔案名稱，e.g.: dump ID group-ID style N file args
name	名稱，e.g.: variable name
其它	以上參數以外的名稱通常為供特定功能所設置之參數名稱，其定義請閱讀manual

You should know about this

region	area
region-ID	name of region
group	a cluster of atoms
group-ID	Name of group
type	atom type
molecule	molecule id #
id	atom id #



compute command --diagnostics

centro/atom - centro-symmetry parameter for each atom
cna/atom - common neighbor analysis (CNA) for each atom
com - center-of-mass of group of atoms
com/molecule - center-of-mass for each molecule
coord/atom - coordination number for each atom
group/group - energy/force between two groups of atoms
gyration/molecule - radius of gyration for each molecule
heat/flux - heat flux through a group of atoms
inertia/molecule - inertia tensor for each molecule
ke - translational kinetic energy
msd - mean-squared displacement of group of atoms
msd/molecule - mean-squared displacement for each molecule
pe - potential energy
pe/atom - potential energy for each atom
pressure - total pressure and pressure tensor
rdf - radial distribution function g(r) histogram of group of atoms
reduce - combine per-atom quantities into a single global value
reduce/region - same as compute reduce, within a region
stress/atom - stress tensor for each atom
temp - temperature of group of atoms
voronoi/atom - Voronoi volume and neighbors for each atom

fix command (1/2) --Operations

addforce - add a force to each atom
ave/atom - compute per-atom time-averaged quantities
ave/time - compute/output global time-averaged quantities
deform - change the simulation box size/shape
deposit - add new atoms above a surface
efield - impose electric field on system
freeze - freeze atoms in a granular simulation
gravity - add gravity to atoms in a granular simulation
gcmc - grand canonical insertions/deletions
heat - add/subtract momentum-conserving heat
indent - impose force due to an indenter
langevin - Langevin temperature control
momentum - zero the linear and/or angular momentum of a group of atoms
move - move atoms in a prescribed fashion
neb - nudged elastic band (NEB) spring forces
npt - constant NPT time integration via Nose/Hoover
npt/asphere - NPT for aspherical particles
npt/sphere - NPT for spherical particles
nve - constant NVE time integration
nvt - constant NVT time integration via Nose/Hoover

fix command (2/2) --Operations

nvt - constant NVT time integration via Nose/Hoover
press/berendsen - pressure control by Berendsen barostat
print - print text and variables during a simulation
restrain - constrain a bond, angle, dihedral
rigid - constrain many small clusters of atoms to move as a rigid body with NVE integration
setforce - set the force on each atom
shake - SHAKE constraints on bonds and/or angles
srd - stochastic rotation dynamics (SRD)
temp/berendsen - temperature control by Berendsen thermostat
temp/rescale - temperature control by velocity rescaling
thermal/conductivity - Muller-Plathe kinetic energy exchange for thermal conductivity calculation
viscosity - Muller-Plathe momentum exchange for viscosity calculation
viscous - viscous damping for granular simulations
wall/lj93 - Lennard-Jones 9-3 wall
wall/reflect - reflecting wall(s)

Data Visualization for Atomistic/Molecular Simulations

These are high-quality visualization packages we have used and recommend.
LAMMPS can either write output files directly in an input format recognized by these programs

VMD

AtomEye

OVITO

ParaView

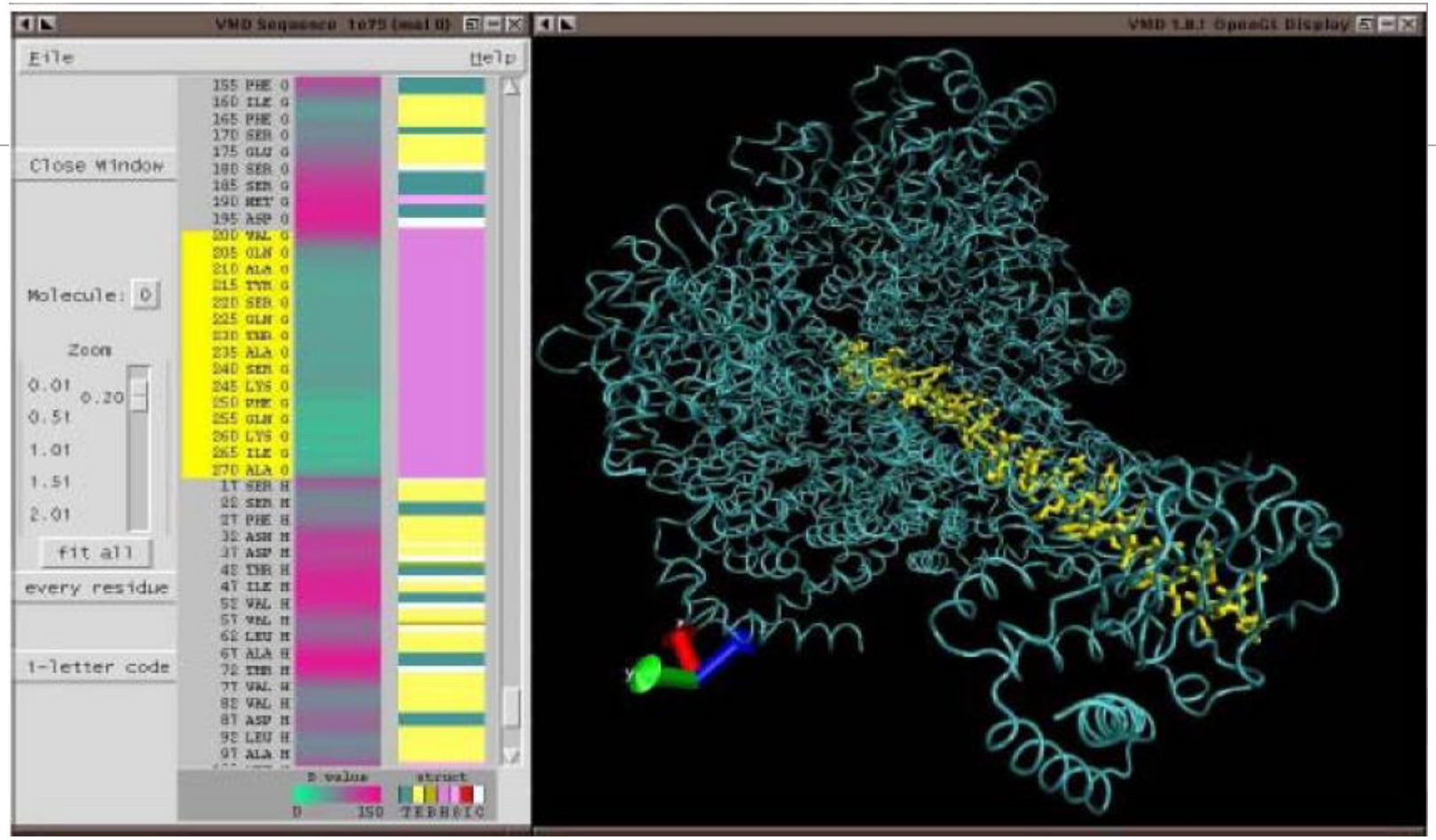
PyMol

Raster3d

RasMol

VMD

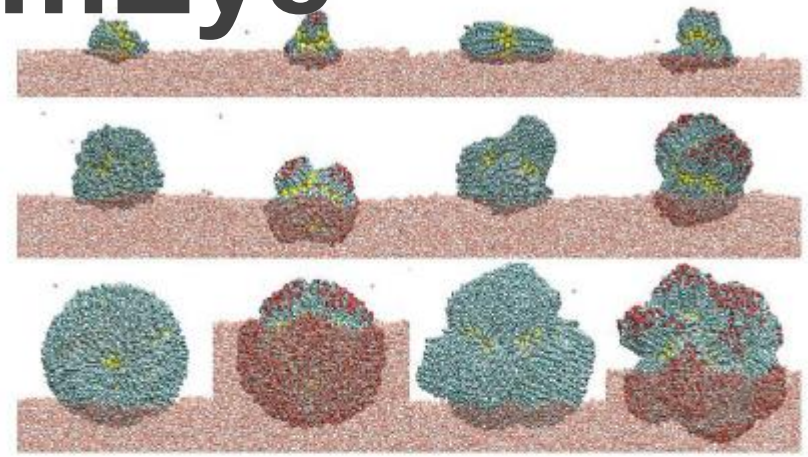
http://www.ks.uiuc.edu/Research/vmd

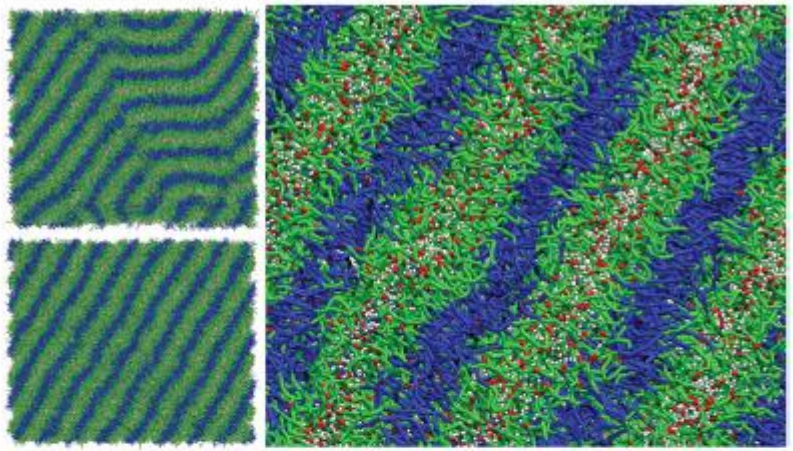


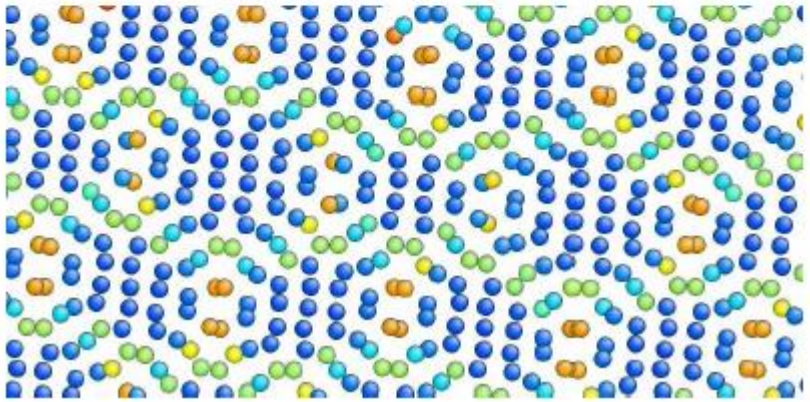
- Feature : surface, electronic density, hydrogen bond…
- Format : .pdb, mol, xyz, POSCAR, gjf …

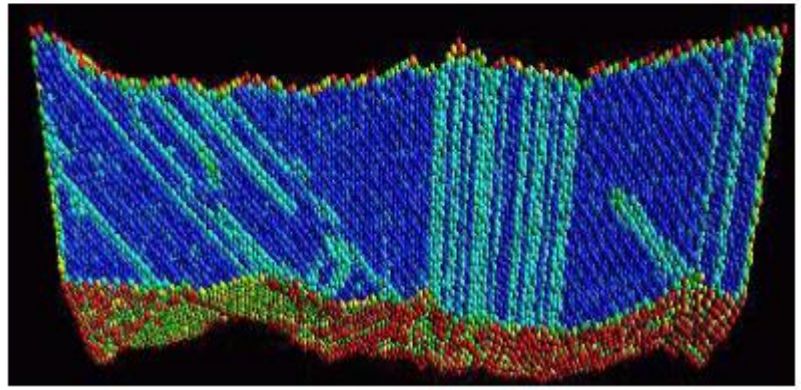
AtomEye

http://li.mit.edu/Archive/Graphics/A/





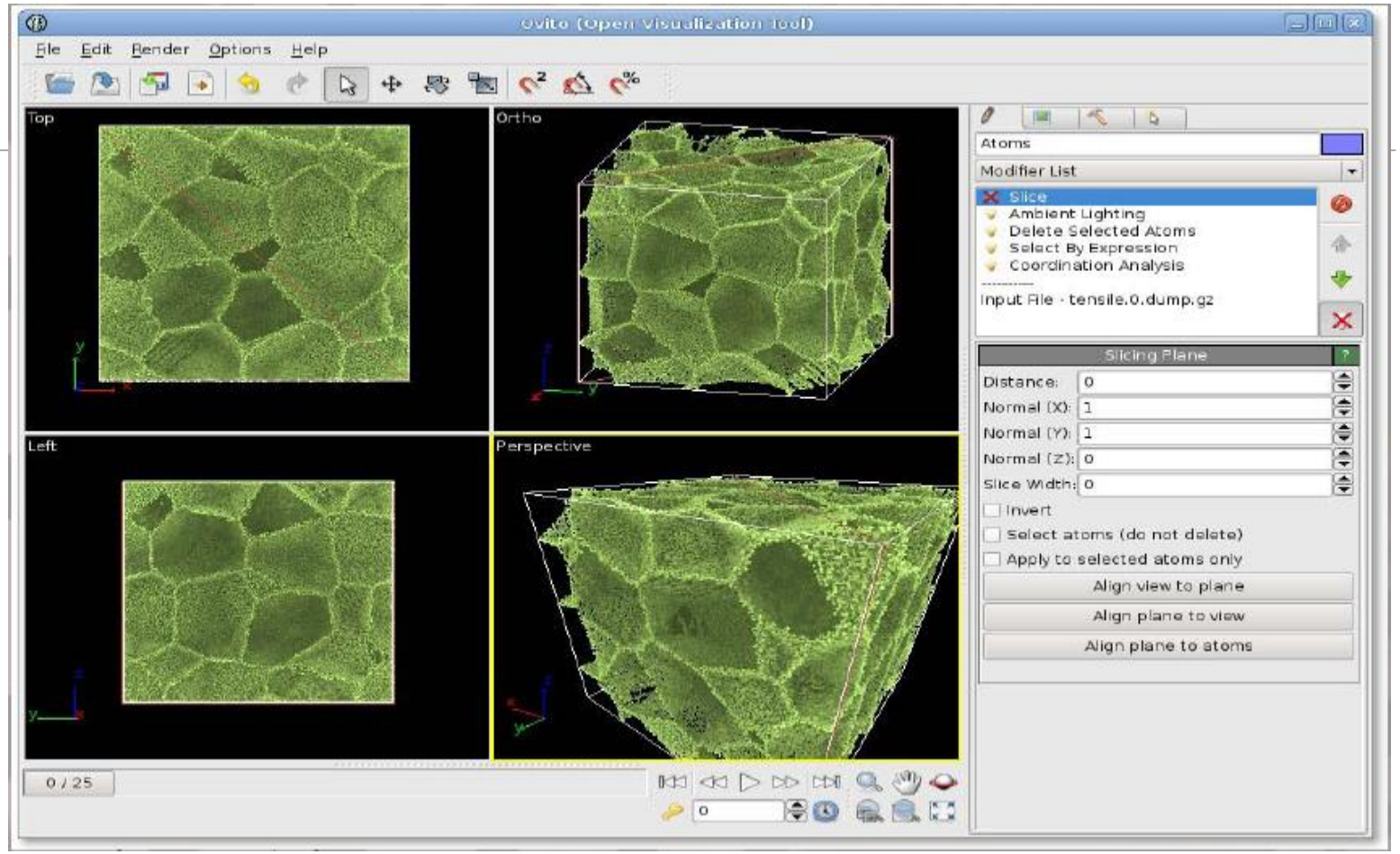




- Feature : default ➔ coordination number, central symmetry parameter, local von Mises shear strain
- Format : cfg

Ovito

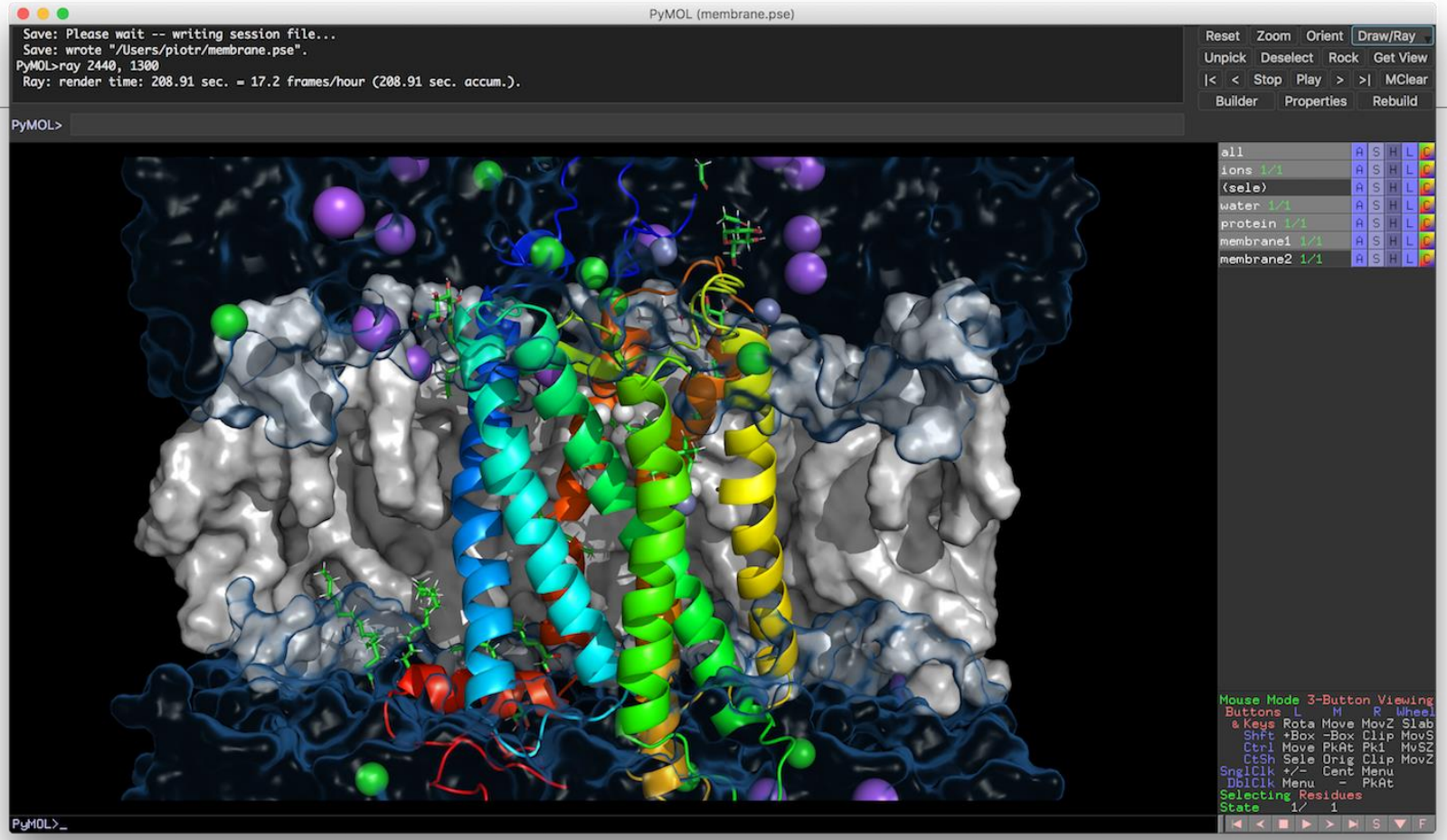
http://www.ovito.org/



- Feature : A fast analyzing configuration viewer for crystal structures ➔ FCC BCC HCP ….
- Format : xyz, cfg

Pymol

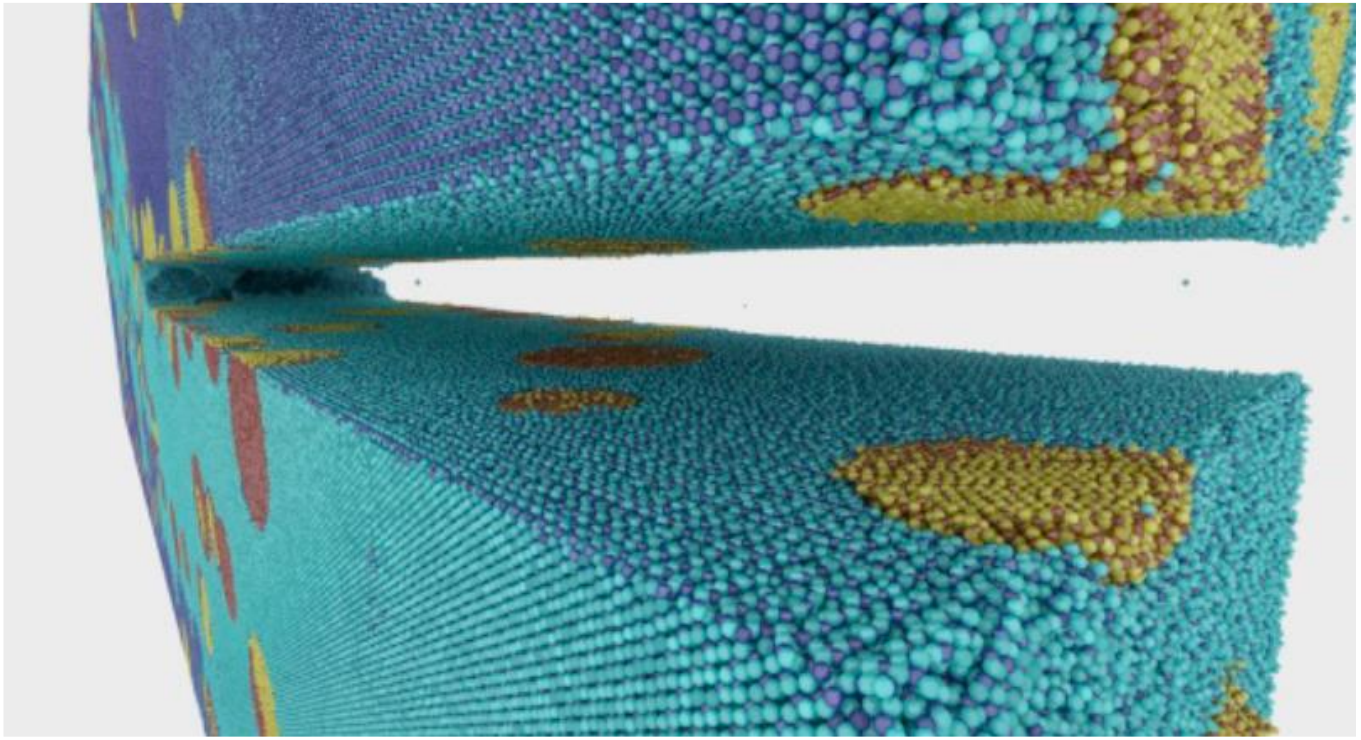
https://pymol.org/2/

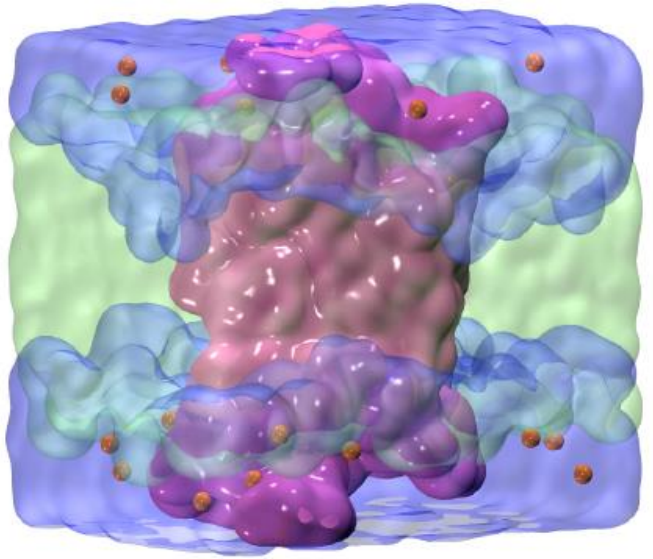


- Feature : surface, electronic density, hydrogen bond…
- Format : .pdb, mol, xyz, POSCAR, gjf …

https://www.paraview.org/

paraview





- Feature : Highly customized analyze tool and large scale visualization.
- Format : xyz, cfg, vtk,…

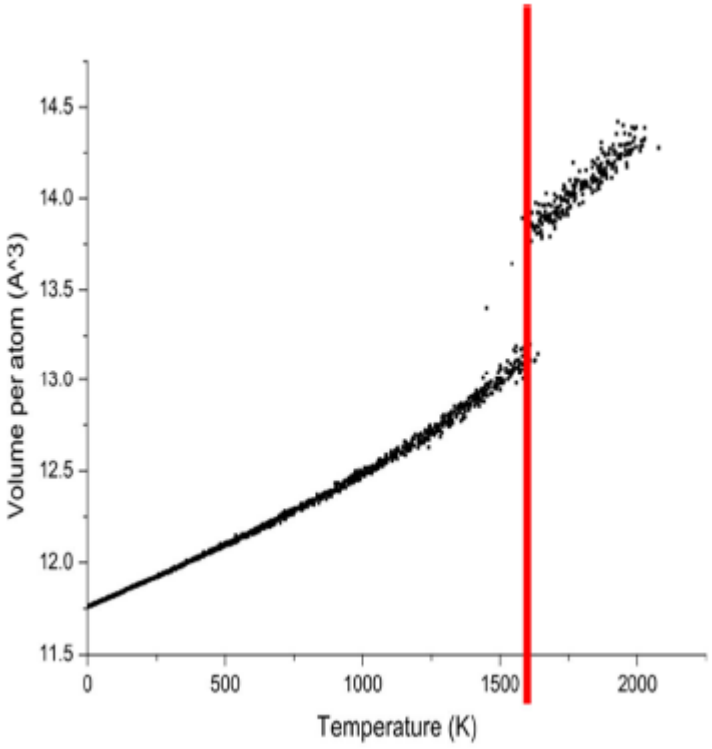
Melting-Cu

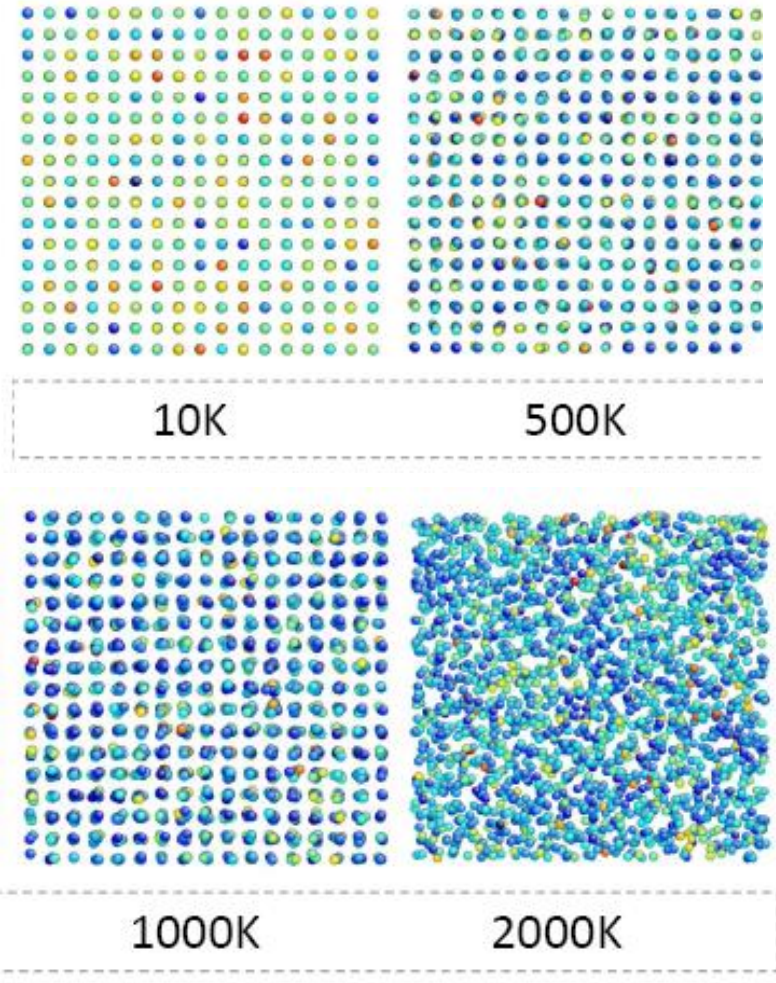
Model system Cu
Initial conditions T, P…
Supercell number of atoms, PBCs …
Interatomic potentials EAM
Ensembles NPT (Nosé-Hoover thermostat)

input script

```
# Melting
units           metal
boundary        p p p
atom_style      atomic
lattice         fcc 3.61
region          box block 0 4 0 4 0 4
create_box      1 box
create_atoms    1 box
pair_style      eam
pair_coeff      * * Cu_u3.eam
timestep        0.01
thermo          1000
variable         N equal step
variable        pote equal pe
variable        T equal temp
variable        Press equal press
variable        V equal vol
velocity        all create 10 825577 dist gaussian
fix             extra all print 100 "${N} ${T} ${V} ${pote} ${Press}" file data
dump            1 all cfg 10000 a*.cfg id type xs ys zs c_ke
dump_modify     1 element Cu
fix             1 all npt temp 10 2000 1 iso 0 0 10
run             120000
```

若超過三組輸出參數 需使用{}


Volume per atom (A^3)
14.5
14.0
13.5
13.0
12.5
12.0
11.5
0
500
1000
1500
2000
Temperature (K)


10K
500K
1000K
2000K

Initialization

- units metal

  設定模擬使用的單位，有metal, lj(default), real, si, cgs, electron, micro, nano等選擇。

- boundary p p p

  設定模擬空間三個方向週期邊界條件，p 代表週期邊界，f 代表固定邊界，

- atom_style atomic

  設定原子的型態，有angle or atomic(default) or body or bond or charge or dipole or dpd or edpd or mdpd or tdpd or electron or ellipsoid or full or line or meso or molecular or peri or smd or sphere or spin or tri or template or hybrid，需要跟據模擬的需求自己選擇。

Atom definition

- lattice fcc 3.615

定義長度，方便在模擬中做度量，我們要件晶格結構，所以用lattice constant作單位很方便。

- region cubic block 0 10 0 10 0 10

定義區域，後面可以用來做其他的操作，像是選取或是建立範圍。

- create_box 1 cubic

跟據前一行建立的區域建立模擬空間，還有其他的建立方式。

- create_atoms 1 box

在前一行的模擬空間中(晶格點上)，建立原子，1代表原子種類的數目。

- mass 1 63.55

定義原子的質量，偶而在勢能函數也會有定義，但明確寫出比較好。

Atom definition

- print ${rseed}

  從command-line option 的-v rseed xxx讀入值，作為亂數種子。

- velocity all create 300.0 ${rseed} mom yes rot yes dist gaussian

  設定所有原子的的速度，使速度滿足300K時的高斯分布，並且動量、角動量都為0。

- pair_style eam

  設定使用eam勢能函數來描述原子間作用力，為了移植性，不明確寫出sufix，改用command-line option 的-pk –sf來控制是否使用加速套件。

- pair_coeff 1 1 "C:\Program Files\LAMMPS 64-bit 16Aug2018\Potentials\Cu_u3.eam“

  明確指出勢能函數檔案的位置，沒有指明路徑就會在兩個地方依序搜尋1. in.xxx同一個資料夾。2. LAMMPS_POTENTIALS這個變數定義的位置。

Setting

- neighbor 2.0 bin

  設定鄰近表列的建立方式，2.0表示以比截斷半徑多2.0(長度單位)的長度建立表列，bin代表用長度來建立表列，nsq代表用數量來建立表列。

- neigh_modify every 2 delay 20 check yes ## 20+1 step=>check

  設定更新表列的頻率，every 2代表每隔2 step更新一次表列， delay 20 代表離上次更新表列超過20 steps後也強制更新， check yes 代表檢查每個原子的位移有無超過0.5 skin厚度。

- timestep 0.001 #1fs

  設定每次疊代的時間長度，單位是跟據先前unit的選擇。

- thermo 1000

  輸出熱力性質的頻率。

- thermo_style custom step time temp press vol pe ke etotal enthalpy

  調整想要監控的性質。

- thermo_modify flush yes

  強迫從記憶體中輸出到螢幕。

Setting

- variable a1 equal step
- variable a2 equal time
- variable a3 equal temp
- variable a4 equal press
- variable a5 equal vol
- variable a6 equal "pe/atoms"
- variable a7 equal "ke/atoms"
- variable a8 equal etotal
- variable a9 equal enthalpy
- fix tdo all print 1000 "${a1} ${a2} ${a3} ${a4} ${a5} ${a6} ${a7} ${a8} ${a9}" file tdo.txt title "Step Time Temp Press Volume PotEng KinEng TotEng Enthalpy" screen no
- min_style cg

- minimize 0.0 1.0e-6 20000 200000

Run a simulation

- fix 1 all nve
- fix 2 all temp/rescale 10 300.0 300.0 10.0 0.8
- write_dump all cfg initial.cfg mass type xs ys zs vx vy vz modify element Cu
- dump 1 all cfg 10000 dump.*.cfg mass type xs ys zs vx vy vz fx fy fz
- dump_modify 1 element Cu pad 6
- run 100000

Run a simulation

- unfix 1
- unfix 2
- fix 3 all npt temp 300.0 1200.0 100.0 iso 1.01325 1.01325 1000.0
- run 100000

Melting-Si

Model system Si
Initial conditions T, P…
Supercell number of atoms, PBCs …
Interatomic potentials Tersoff
Ensembles NPT (Nosé-Hoover thermostat)

input script-1

```
units                   metal
atom_style              atomic

lattice                 diamond  5.431
region                  cubic block 0 3 0 3 0 5
create_box              1 cubic
create_atoms    1 box
mass                    1 28.0855
pair_style              tersoff
pair_coeff              * * Si.tersoff Si


velocity                all create 300.0 456236 sum yes mom
yes dist gaussian
neighbor                1 bin
neigh_modify    every 1 delay 20 check yes   ## 20+1
step=>check
thermo                  1000
timestep                0.002
```

input script-2

```
variable                Pot equal " pe/atoms"
variable                kee equal "ke/atoms"
variable                tstep equal "step*dt"
fix                     eng all print 200 "${tstep} ${Pot} ${kee}" file Energy.dat screen no
variable        vv atom "(vx*vx+vy*vy+vz*vz)^(1/2)  “
##############compute average energy/atom################
#compute                        pe_a      all pe/atom
#fix                    vva all ave/atom 10 70 1000 vx vy vz
#fix                    pe_a all ave/atom 10 70 1000 c_pe_a
#dump                   id all custom 1000 dump.melt x y z mass f_pe_a
##############compute average energy/atom################

fix                             1 all nvt temp 300 300 1
run                             500
unfix                   1

#fix                    1 all nve
#fix                    2 all temp/rescale 10 300.0 300.0 10.0 1.0
fix                     2 all npt temp 2000 4000 1 x 1 1 1 y 1 1 1
##############deform################
#fix                    3 all deform 1 z erate 0.005 units box

run                             200000
```