古典統計力学模型と数値計算

Classical Statistical Models and Numerical Simulation

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Background of lecturer

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Research:

Statistical Physics, Condensed matter physics, Magnetism,
(Computational Physics)

- Random packing of disks
- Mean-filed analysis of hierarchical society
- Ordering of (classical) frustrated spin system
  - Z_2-vortex, skyrmion, multiple-Q states, …
- Deconfined quantum criticality
- Tensor network methods
- ….

Outline

- Many-body problems: Quantum or Classical ?
  - When we can use classical “models” ?
  - Target of general calculations and this lecture
- Examples of classical statistical models
- Computational science for (classical) statistical models
  - Statistical ensembles
  - Numerical calculation for ensemble average
    - Time average and relaxation time

Many body problems: Quantum or Classical?

Many-body problems: Quantum or Classical?

Two types of classical many-body problems

1. Approximation of quantum problems

Nature: Elementary particles obey quantum mechanics.

$$i\hbar\frac{\partial}{\partial t}|\Psi\rangle = \mathcal{H}|\Psi\rangle$$

➡ Classical mechanics is an approximation

2. Pure classical problems

Classical problems not necessary based on quantum mechanics

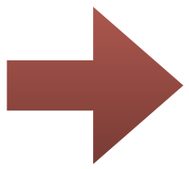
- Percolation, covering, packing, …
- Stochastic process, “dynamical” system, ..
- Critical phenomena
- …

Classical problems as an approximation: molecules

Interaction of molecules:

- Coulomb interactions of charges
- Van der Waals force
- …

For aciculate treatment, we need to consider quantum mechanics



However, we can approximate the system as a set of "classical" point particles

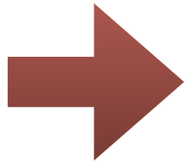
- Lennard-Jones potential for nobel gas
- Effective potential for water
- ….

Classical problems as an approximation: magnetism

Electron Spin: "Quantum" degree of freedom

For aciculate treatment, the spin quantum number S is important

S=1/2, 1, 3/2, …



However, we can approximate the system by taking the limit of $S \to \infty$.
"classical" spin model

- Classical Heisenberg model
- Anisotropy: Ising model, XY model
- ….

Classical problems as an approximation

When a classical approximation becomes accurate?

- High temperature
  - We safely neglect quantum nature compared with thermal fluctuation
- Low density
  - The interaction between particles are small (rare)
- Classical order (magnetism)
  - If the ground state is classical magnetic long range order typically, classical approximation is not so bad

Pure classical problems: Critical phenomena

Critical phenomena:

At the critical point, characteristic length diverges

→ Scale invariance

Several quantities show power-low behaviors

Correlation length : $\xi \sim |T - T_c|^{-\nu}$

Specific heat : $C \sim |T - T_c|^{-\alpha}$

Susceptibility : $\chi \sim |T - T_c|^{-\gamma}$

exponent = critical exponent

Universality

Critical exponents depends only on “symmetry” and “spacial dimensions”

→ A lot of critical phenomena are exactly understood from classical models

Pure classical problems: other examples

- Percolation problem
  - Physics of Bingo game
- Sphere packing
  - What is the most dense packing in a box?
  - Packing structure of poly-disperse systems?
- Stochastic process
  - Dynamics of financial trades
  - Dynamics of population, society, …

Target of studies: Static or Dynamics

Static properties:

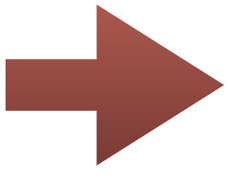
Physical properties independent on time

(free) energy, specific heat, (static) susceptibilities, …

Dynamical properties:

Related to a response to external forces

Time-dependent susceptibilities, Time-Correlations,



By computational science, both types of quantities can be calculated, although the method could depend on the type.

(Typically, dynamical properties are more difficult to be obtained)

Target of studies: Equilibrium or Non-Equilibrium

Equilibrium system:

Systems are described by thermodynamics

Non-Equilibrium system:

Systems are not described by thermodynamics

Steady state:

Its physical quantities are independent of time

Non-steady state:

Its physical quantities are depends on time

Typically, treatment of non-steady state is very difficult.

Target of this lecture

Steady state of classical system (not necessarily in equilibrium)

→ Physical quantities are calculated through steady state distribution $P(\Gamma)$

$$O = \langle \hat{O} \rangle = \mathop{\mathrm{Tr}}_{\Gamma} \left(\hat{O}(\Gamma) P(\Gamma) \right)$$

$$C(\tau) = \langle \hat{A}(t=0) \hat{B}(t=\tau) \rangle = \mathop{\mathrm{Tr}}_{\Gamma} \left(\hat{A}(\Gamma) \hat{B}(\Gamma(\tau)) P(\Gamma) \right)$$

$\Gamma = \{S_i\}, \{q_i, p_i\}, \cdots$:state in the phase space

- 第３回：古典統計力学模型と計算科学
- 第４回：古典モンテカルロ法とその応用
- 第５回：分子動力学法とその応用
- 第６回：拡張アンサンブル法によるモンテカルロ計算

Examples of classical statistical models

Statistical mechanical models:

Models considered in this lecture:

- Classical Spin systems
  - Ising, XY, Heisenberg, …
  - Frustration, DM interactions, Anisotropy, …
- Particle systems
  - Molecules, hard spheres,…

Models related to the methods presented in this lecture:

- Agent models of socio-physics
- Lattice models representing (non-equilibrium) steady state
  - ASEP, lattice gas, …
- Langevin dynamics (Stochastic differential equation)
  - Brownian motion, econophysics, …

Classical spin system: spin model on lattice

Spin systems:

Spin degree of freedoms defined on a lattice and interact each other

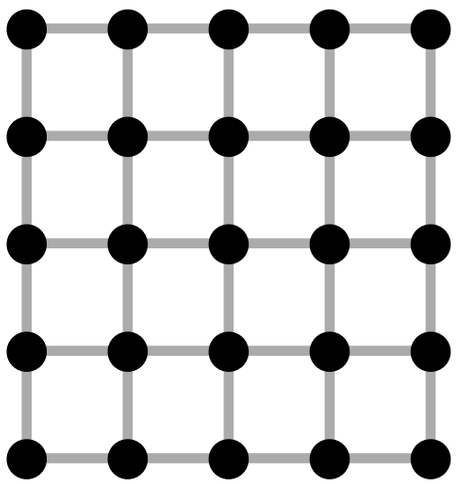
Lattice

1D

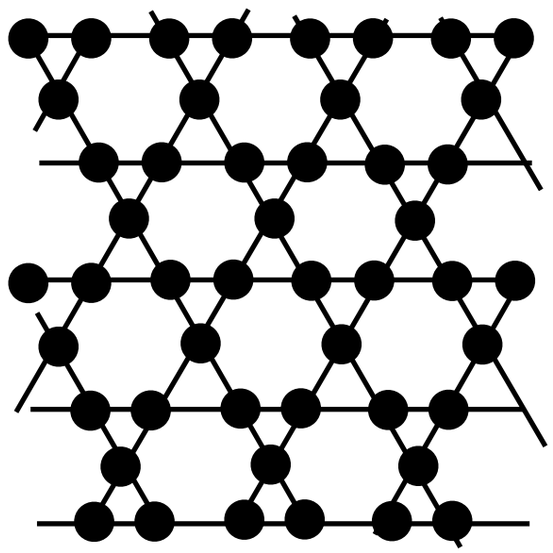
Chain

2D

Square lattice



Kagame lattice



3D simple cubic, FCC lattice, BCC lattice, …

Classical spin degree of freedom

Classical spin:

1. $S \to \infty$ limit of quantum spin
2. simple degree of freedom reflecting symmetry

1. Heisenberg spin $S_i = (S_i^x, S_i^y, S_i^z)$

Three component unit vector: $(S_i^x)^2 + (S_i^y)^2 + (S_i^z)^2 = 1$

A lot of magnetism can be understand through classical Heisenberg spin

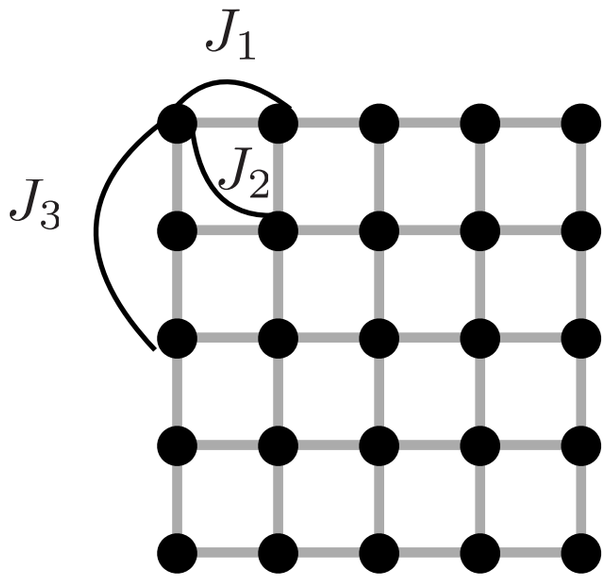
2. Ising spin $S_i = \pm 1 = \uparrow, \downarrow$
   - Strong easy axis anisotropy
   - Representing underlying Z_2 symmetry
3. XY spin $S_i = (S_i^x, S_i^y)$ Two component unit vector: $(S_i^x)^2 + (S_i^y)^2 = 1$
   - Strong easy plane anisotropy
   - Representing underlying U(1) symmetry

Classical spin model: interactions

Heisenberg spin $S_i = (S_i^x, S_i^y, S_i^z)$

Heisenberg interaction:

$$\mathcal{H} = J_1 \sum_{\langle i,j \rangle} S_i \cdot S_j + J_2 \sum_{\langle\langle i,j \rangle\rangle} S_i \cdot S_j$$



Single ion anisotropy

$$D \sum_i (S_i^z)^2 + E \sum_i \left[(S_i^x)^2 - (S_i^y)^2 \right]$$

$D \rightarrow +\infty$: XY spins

$D \rightarrow$ -∞ : Ising spins

Dzyaloshinskii-Moriya interaction

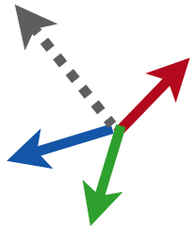
$$\sum_{\langle i,j \rangle} \vec{D} \cdot (S_i \times S_j)$$

A lot of “novel” magnetism appears even in classical spin system

Topological Z_2 vortex

Classical antiferromagnetic Heisenberg model
on triangular lattice

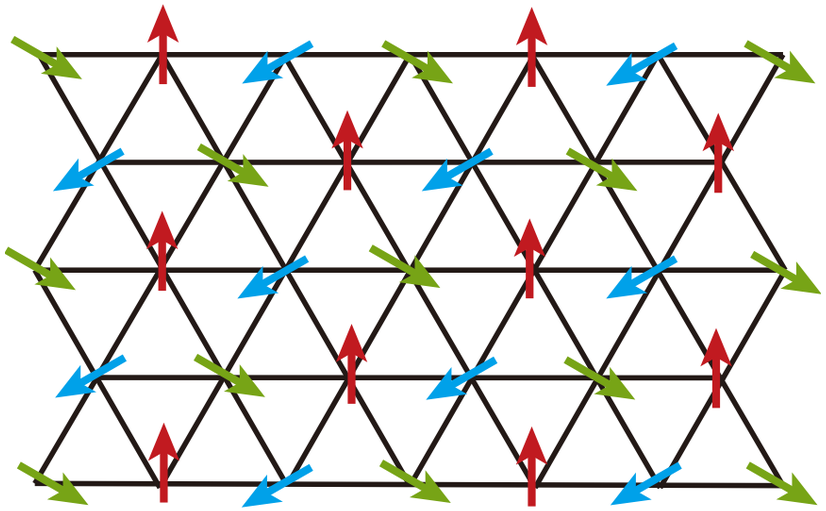
local 120° structure has SO(3) symmetry



Topological excitation

"Z_2 vortex"

120° structure

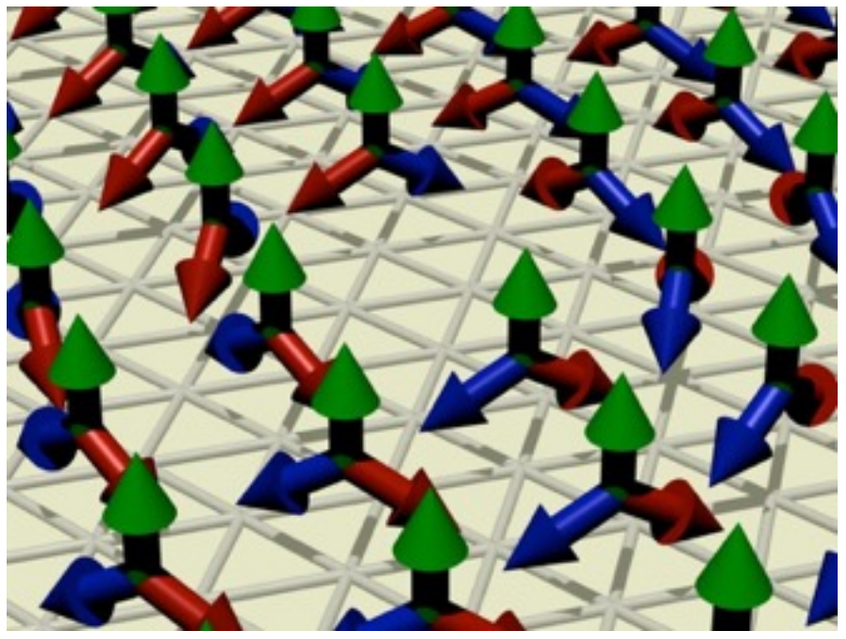


It is characterize by Z_2 value
"exist" or "not-exist"

Possible phase transition with respect to
binding-unbinding of Z_2 vortex

H. Kawamura and S. Miyashita (1984)

My search project using
Monte Carlo simulation using K-computer



Magnetic skyrmion

Classical antiferromagnetic Heisenberg model on triangular lattice under magnetic fields

By considering J_1 and J_2 (or J_3) interaction

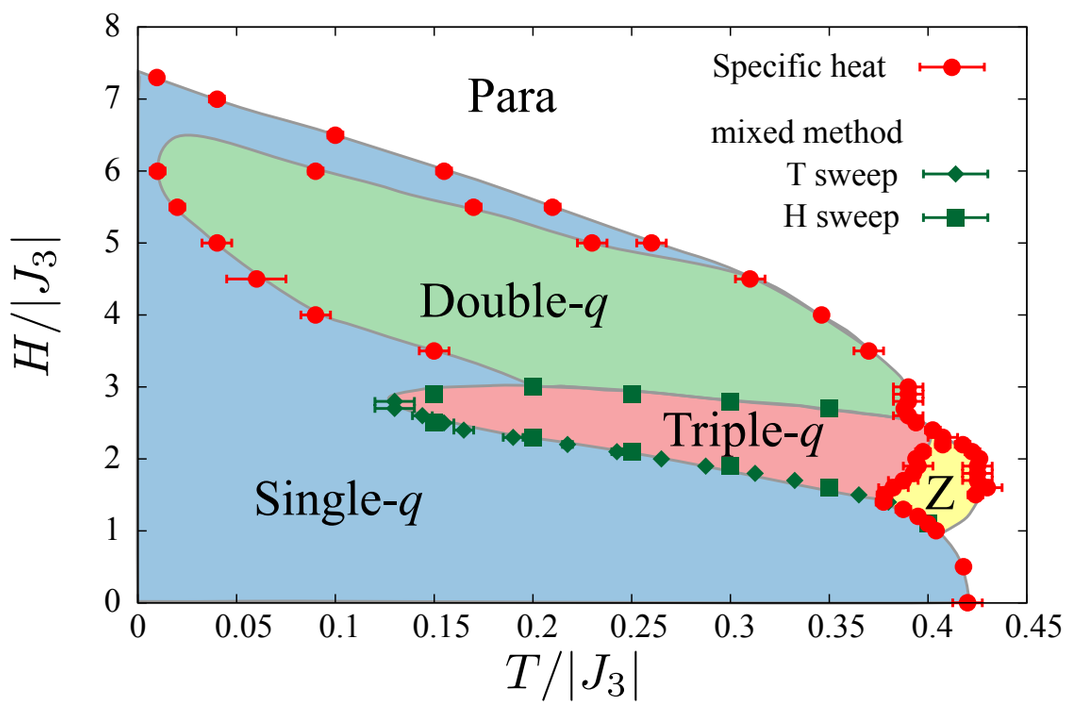
(effective model for $NiGa_2S_4$)

→ Novel multiple-q states are stabilized

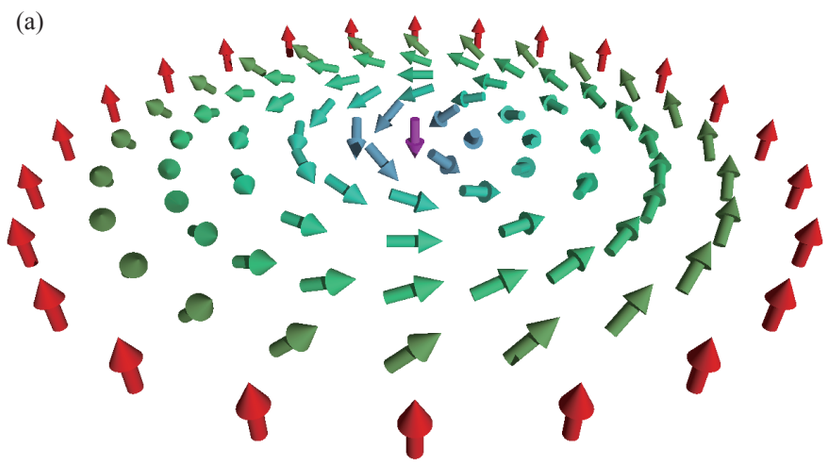
One of them is identical with "magnetic skyrmion"

This has been also investigated by Monte Calro simulation

Phase diagram



Magnetic skyemion



Particle system:

Particle systems:

Particles moving in continuous space by interacting each other

Typically, their degree of freedoms are “positions” and “momentum”

Two components in Hamiltonian

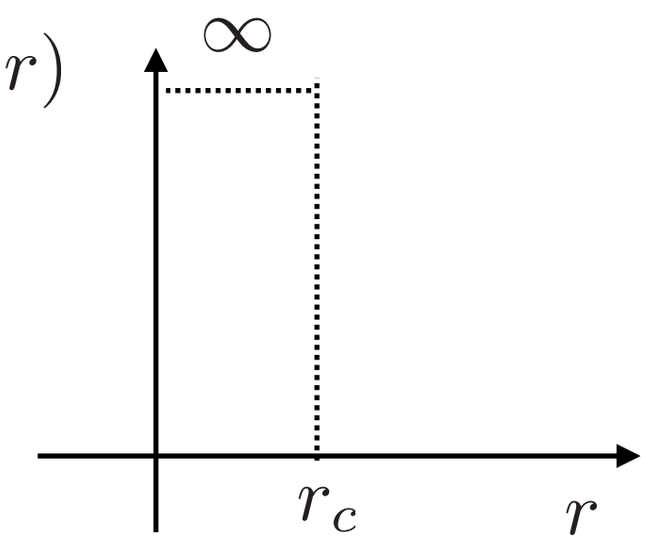
Interacting potential: $V(\boldsymbol{r}_i - \boldsymbol{r}_j)$

Kinetic Energy: $\dfrac{p_i^2}{2m_i}$

Variety of models: variety of interacting potentials

Hard sphere

$$V(\boldsymbol{r}_i - \boldsymbol{r}_j) = \begin{cases} 0 & (r > r_c) \\ \infty & (r \leq r_c) \end{cases} \qquad r = |\boldsymbol{r}_i - \boldsymbol{r}_j|$$

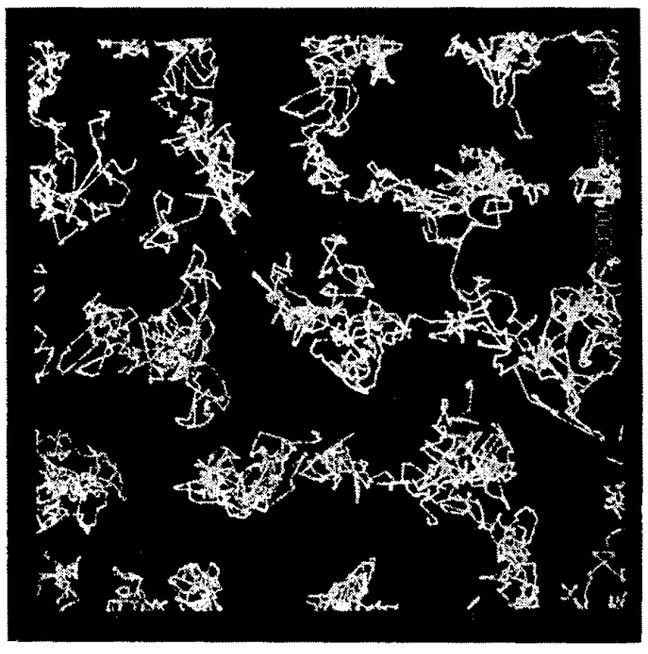


The first application of molecular dynamics

Alder and Wainwright, J. Chem. Phys. **27**, 1208 (1957);**31**, 459 (1959)

- Event driven molecular dynamics simulation

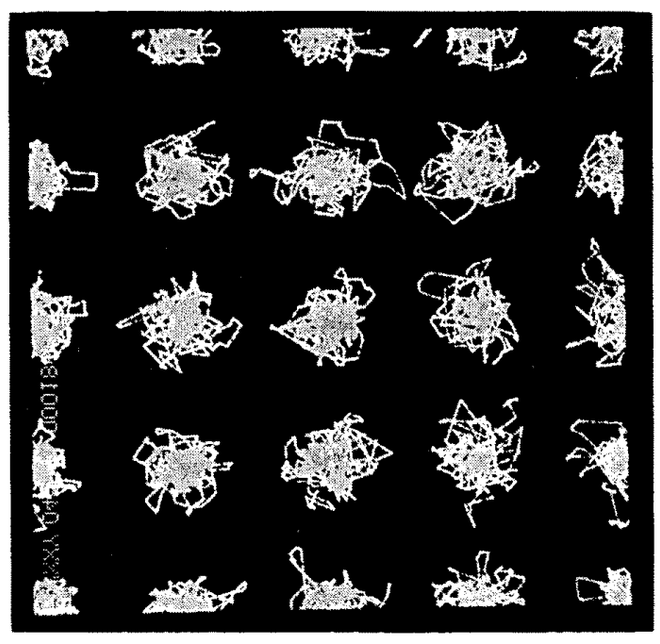
Fluid



Phase transition

(Alder transition)

Crystal

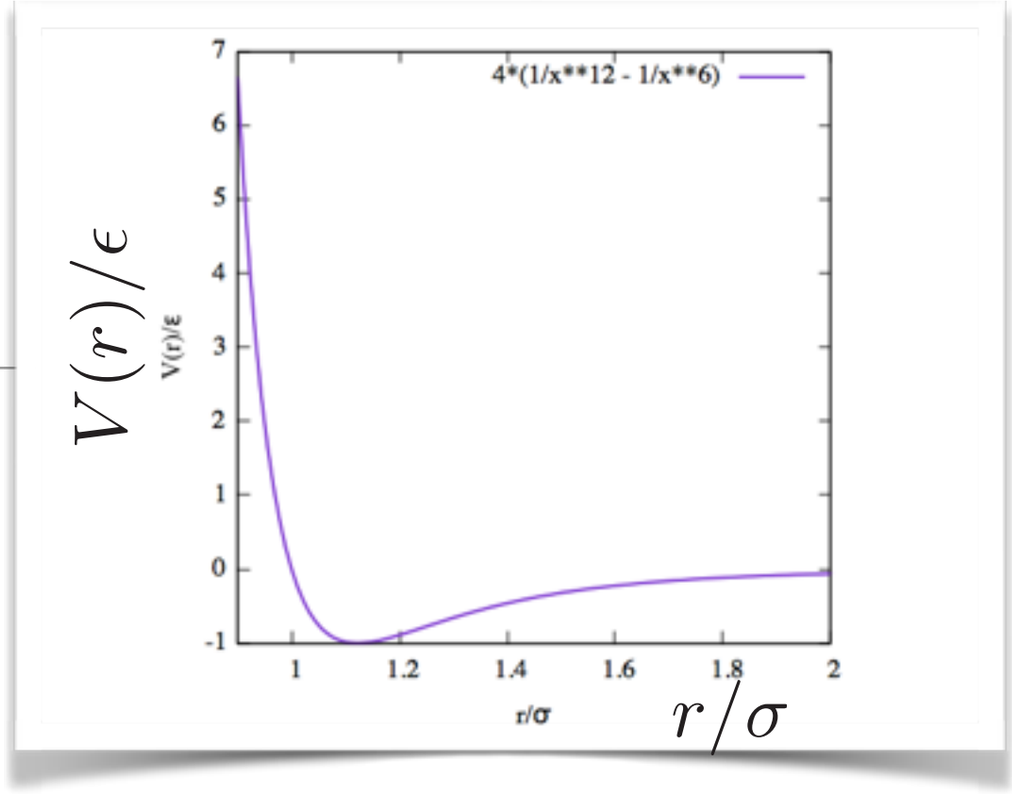


32 particle system

Lennard-Jones potential

$$V(r) = 4\epsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right]$$

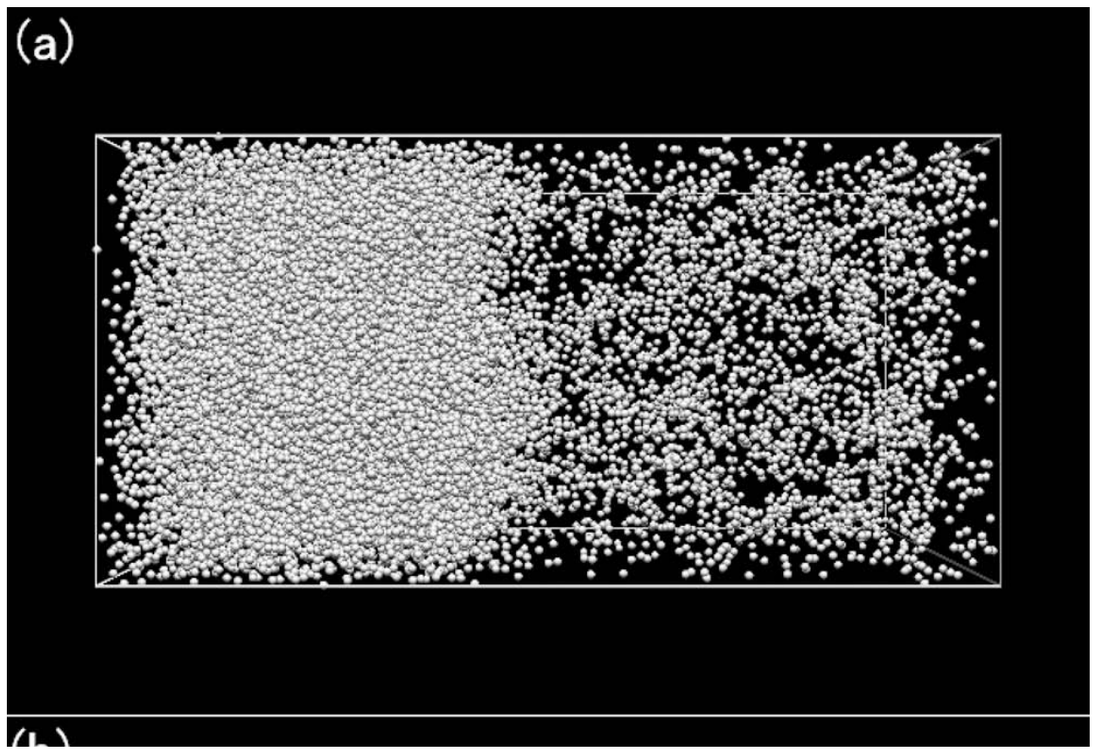
Model potential for nobel gas (Ar, …)



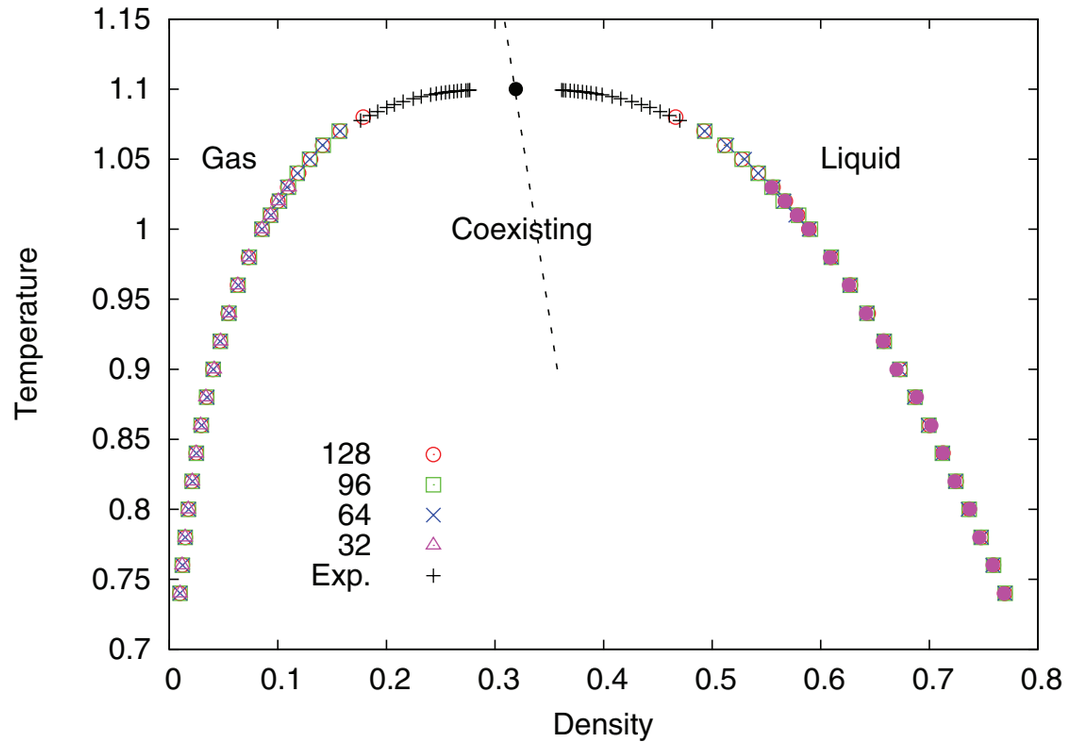
Recent simulation: H. Watanabe et al, J. Chem. Phys. **136**, 204102 (2012).

(~1,000,000 particles)

Gas-Liquid coexistence



Phase diagram



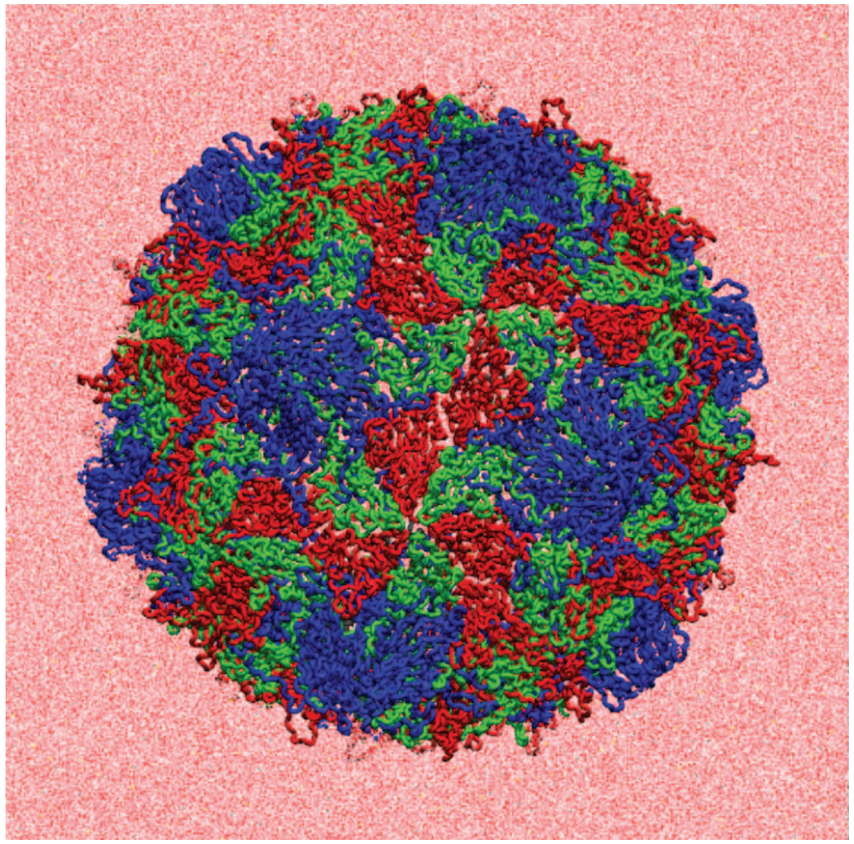
Complex systems

Eg. Poliovirus capsid in electrolyte solution

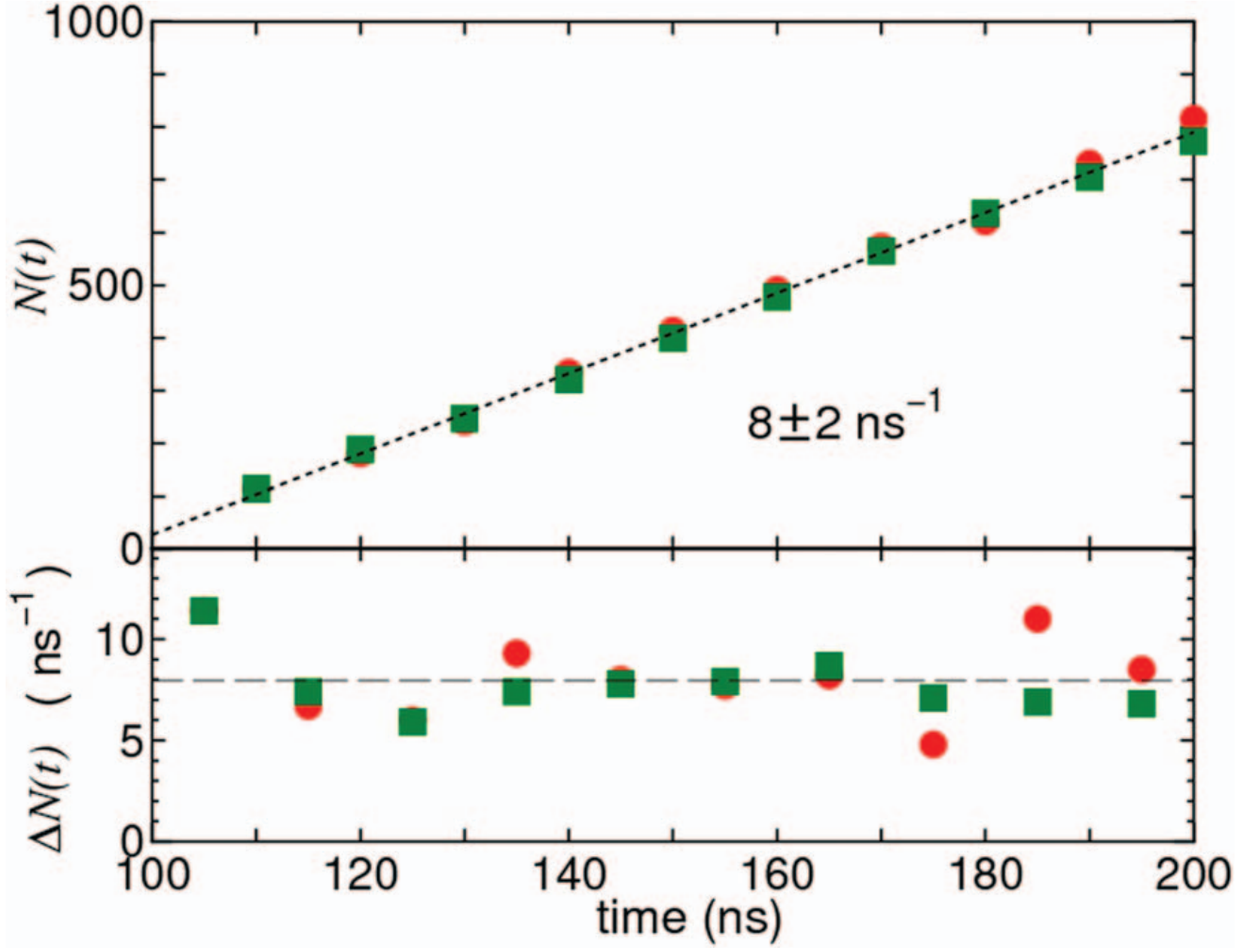
Y. Ando et al, J. Chem. Phys. **141**, 165101(2014).

Long-range coulomb interaction

Poliovirus capsid



Dynamics of water molecules



Computational science for (classical) statistical models

Statistical mechanics: Ensemble

Statistical mechanics:

Connect microscopic models to macroscopic observable

Example: Ising model

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} S_i S_j - h \sum_i S_i \qquad (S_i = \pm 1 = \uparrow, \downarrow)$$

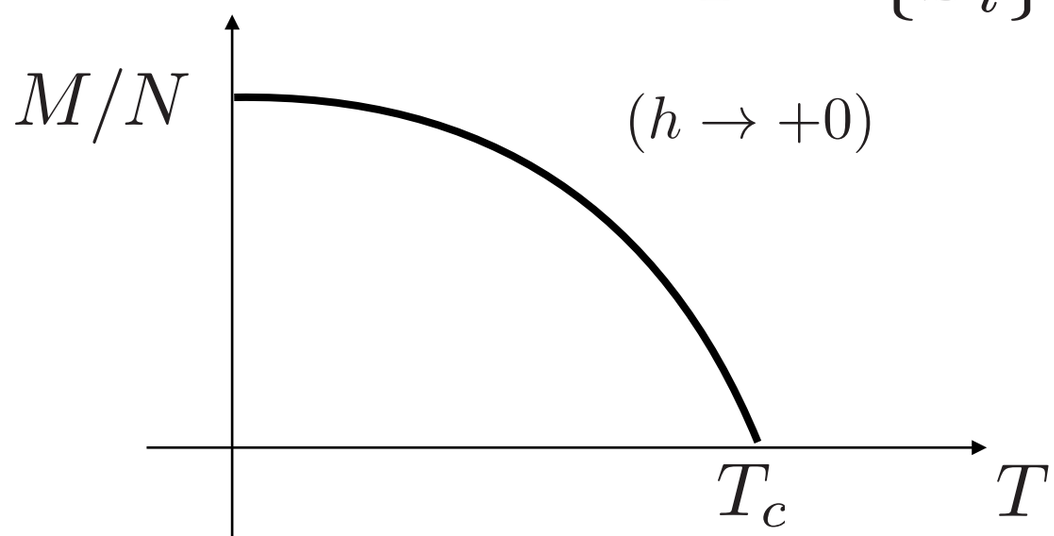
Canonical ensemble (NVT-ensemble) :

$$P(\Gamma; T) = \frac{1}{Z} \exp\left(-\frac{1}{k_B T} \mathcal{H}(\Gamma) \right)$$

Magnetization at T:

$$M(T) = \left\langle \sum_i S_i \right\rangle_T = \sum_\Gamma \sum_i S_i P(\Gamma; T)$$

$$\Gamma = \{S_i\}$$



Statistical mechanics: important ensembles

Micro Canonical ensemble (NVE-ensemble)：

$$P(\Gamma; E) \propto \sum_{\Gamma} \delta(E - \mathcal{H}(\Gamma))$$

E: energy

NPT-ensemble：

$$P(\Gamma; P, T) \propto \int dV e^{-\beta PV} \sum_{\Gamma(V)} e^{-\beta \mathcal{H}(\Gamma)}$$

P: pressure
V: volume

$$\beta = \frac{1}{k_B T}$$

Grand Canonical ensemble (μVT-ensemble)：

$$P(\Gamma; \mu, T) \propto \sum_{N} \frac{1}{N!} e^{\beta \mu N} \sum_{\Gamma(N)} e^{-\beta \mathcal{H}(\Gamma)}$$

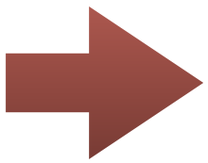
μ: chemical potential

General ensemble：

- Not necessarily related to thermal equilibrium
- But, it may represent a steady state of physical system
  - Non-equilibrium steady state

Computational science for statistical models

Purpose of computational science for statistical models



Calculate ensemble averages numerically

Two types of approaches

- Evaluate ensemble average as a “time average”
  based on a special dynamics
  - Monte Calro (MC) , Molecular Dynamics (MD)
  - Target of this lecture
- Calculate partition function directly
  - Transfer matrix method, Tensor network method
  - It will be treated slightly in “計算科学における情報圧縮”

Time average for ensemble average

States depending on time

$$\Gamma(t) = \{q_i(t), p_i(t)\}, \{S_i(t)\}, \cdots$$

$$\langle \hat{O} \rangle = \lim_{T\to\infty} \frac{1}{T} \int_0^T \hat{O}(\Gamma(t))dt$$

$$= \lim_{T\to\infty} \frac{1}{T} \sum^{T} \hat{O}(\Gamma(t))$$
$$t=1$$

Molecular dynamics:

Dynamics of Γ obeys a differential equation (Newton equation)

$$\frac{d}{dt}\begin{bmatrix} q_i \\ p_i \end{bmatrix} = \begin{bmatrix} \partial\mathcal{H}/\partial p_i \\ -\partial\mathcal{H}/\partial q_i \end{bmatrix}$$

Monte Carlo:

$\rho_t(\Gamma)$:probability distribution

$W_{\Gamma\to\Gamma'}$:transition probability

Dynamics of Γ obeys a master equation

$$\rho_{t+1}(\Gamma) - \rho_t(\Gamma) = \sum_{\Gamma'} W_{\Gamma'\to\Gamma}\rho_t(\Gamma') - \sum_{\Gamma'} W_{\Gamma\to\Gamma'}\rho_t(\Gamma)$$

Time Correlation and relaxation time

Time correlation function

$$C_{AB}(t) \equiv \langle \hat{A}(0)\hat{B}(t)\rangle - \langle \hat{A}\rangle\langle \hat{B}\rangle$$

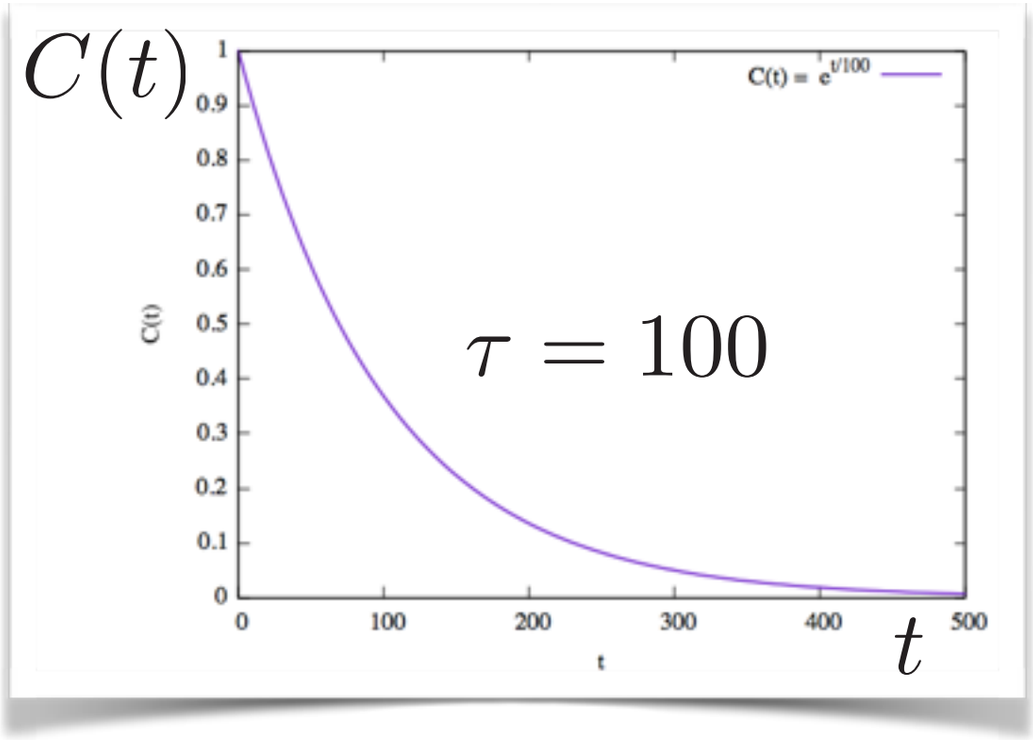
Auto correlation function

$$C_{AA}(t) \equiv \langle \hat{A}(0)\hat{A}(t)\rangle - \langle \hat{A}\rangle^2$$

Typical asymptotic behavior

$$C_{AA}(t) \sim e^{-t/\tau_A}$$ exponential decay

Relaxation time: τ_A



Relaxation time determines efficiency of sampling

smaller τ → higer efficiency

lager τ → lower efficiency

Error estimation

Error due to finite number of sampling

$$\bar{A} \equiv \frac{1}{T}\sum_{t=1}^{T} \hat{A}(\Gamma(t))$$

$\langle \cdots \rangle$:average over trajectories (initial condition)

Standard error: $\epsilon^2 = \langle \bar{A}^2 \rangle - \langle \bar{A} \rangle^2$

$$\epsilon^2 = \left\langle \frac{1}{T^2}\sum_{t_1=1}^{T}\sum_{t_2=1}^{T} A_{t_1}A_{t_2} \right\rangle - \left\langle \frac{1}{T}\sum_{t=1}^{T} A_t \right\rangle^2$$

$$= \frac{1}{T^2}\sum_{t_1=1}^{T}\sum_{t_2=1}^{T} C_{AA}(|t_2 - t_1|)$$

$C_{AA} \sim C_{AA}(0)e^{-t/\tau}$

$$\underset{T\to\infty}{\sim} \frac{2\tau}{T} C_{AA}(0) \quad \Rightarrow \quad \epsilon \propto \sqrt{\frac{\tau}{T}}$$

In order to reduce the error, we want to reduce τ

Phenomena with large relaxation time

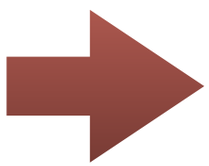
- Critical phenomena
  - $\tau \sim (T\text{-}T_c)^{-\nu z}$ with standard algorithm (critical slowing down)
  - z can be significantly reduced by using "global update"
- Glass transition (structural glass, spin glass), protein folding, first order phase transition
  - $\tau \sim \exp(-a/T)$ or $\exp(-a/(T\text{-}T_c))$
  - exponential can be reduce to polynomial by using extended ensemble methods

Answer to question:

Compiler dependence:

If you use “default” setting, compilers may not use extended instructions

(like SIMD, fused multiply-add, …)



gcc could be much slower than icc.

However, there are several options telling the compilers which extended instructions we can use.

gcc: -march=*architecture-type, cpu-type*
-mtune=*cpu-type*

cpu-type=core2, core-avx2, …

if you use -march=native , it is optimized for “local computer”.

icc, ifort: -x*code*

code=core-avx2, sse4.2, …

if you use -xHost , it is optimized for “local computer”.