Theoretical formulations

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General form of empirical potential functions

- In classical molecular dynamics, the **total potential energy** U of a system can be written as the sum of **site potentials** U_i:

$$U = \sum_{i=1}^{N} U_i(\{\vec{r}_{ij}\}_{j \neq i}).$$

- Here

$$\vec{r}_{ij} \equiv \vec{r}_j - \vec{r}_i$$

is the **position difference vector** used throughout this online manual.

General form of interatomic forces

- Recently, a well-defined force expression for **general many-body potentials** that explicitly respects (the weak version of) **Newton's third law** has been derived as [Fan 2015]:

$$\vec{F}_i = \sum_{j \neq i} \vec{F}_{ij};$$

$$\vec{F}_{ij} = -\vec{F}_{ji} = \frac{\partial U_i}{\partial \vec{r}_{ij}} - \frac{\partial U_j}{\partial \vec{r}_{ji}} = \frac{\partial \left(U_i + U_j\right)}{\partial \vec{r}_{ij}}.$$

- Here, $\partial U_i / \partial \vec{r}_{ij}$ is a shorthand notation for a vector with cartesian components $\partial U_i / \partial x_{ij}$, $\partial U_i / \partial y_{ij}$, and $\partial U_i / \partial z_{ij}$.

Starting from the above force expression, one can derive expressions for the stress tensor and the heat current.

Stress tensor

- **Stress tensor** is an important quantity in MD simulations. It consists of two parts: a virial part which is related to the force and an ideal-gas part which is related to the temperature. The virial part must be calculated along with force evaluation.
- The validity of Newton's third law is crucial to derive the following expression of the **virial tensor** [Fan 2015]:

$$\mathbf{W} = \sum_i \mathbf{W}_i;$$

$$\mathbf{W}_i = -\frac{1}{2} \sum_{j \neq i} \vec{r}_{ij} \otimes \vec{F}_{ij},$$

where only relative positions $\vec{r}_{ij}$ are involved.

- After a little algebra, we can also express the virial as [Gabourie 2020]

$$\mathbf{W} = \sum_i \mathbf{W}_i;$$

$$\mathbf{W}_i = \sum_{j \neq i} \vec{r}_{ij} \otimes \frac{\partial U_j}{\partial \vec{r}_{ji}}.$$

- The ideal-gas part of the stress is isotropic, which is given by the ideal-gas pressure:

$$p_{\mathrm{ideal}} = \frac{N k_{\mathrm{B}} T}{V},$$

where N is the number of particles, k_{B} is Boltzmann's constant, T is the absolute temperature, and V is the volume of the system.

- The total stress tensor is thus

$$\sigma^{\alpha\beta} = -\frac{1}{2V} \sum_i \sum_{j \neq i} r_{ij}^{\alpha} F_{ij}^{\beta} + \frac{N k_{\mathrm{B}} T}{V} \delta^{\alpha\beta}.$$

Heat current

- Using the force expression, one can derive the following expression for the **heat current** for the whole system (E_i is the total energy of atom i) [Fan 2015]:

$$\vec{J} = \vec{J}^{\mathrm{pot}} + \vec{J}^{\mathrm{kin}} = \sum_i \vec{J}_i^{\mathrm{pot}} + \sum_i \vec{J}_i^{\mathrm{kin}};$$

$$\vec{J}_i^{\rm kin} = \vec{v}_i E_i;$$

$$\vec{J}_i^{\rm pot} = -\frac{1}{2}\sum_{j\neq i} \vec{r}_{ij} \left(\frac{\partial U_i}{\partial \vec{r}_{ij}} \cdot \vec{v}_j - \frac{\partial U_j}{\partial \vec{r}_{ji}} \cdot \vec{v}_i \right).$$

- The potential part of the per-atom heat current can also be written in the following equivalent forms [Fan 2015]:

$$\vec{J}_i^{\rm pot} = -\sum_{j\neq i} \vec{r}_{ij} \left(\frac{\partial U_i}{\partial \vec{r}_{ij}} \cdot \vec{v}_j \right);$$

$$\vec{J}_i^{\rm pot} = \sum_{j\neq i} \vec{r}_{ij} \left(\frac{\partial U_j}{\partial \vec{r}_{ji}} \cdot \vec{v}_i \right).$$

- Therefore, the per-atom heat current can also be expressed in terms of the per-atom virial [Gabourie 2020]:

$$\vec{J}_i^{\rm pot} = \mathbf{W}_i \cdot \vec{v}_i.$$

where the per-atom virial tensor cannot be assumed to be symmetric and the fully tensor with 9 components should be used [Gabourie 2020]. This result has actually been clear from the derivations in [Fan 2015], but it was **wrongly stated** there that the potential part of the heat current **cannot** be expressed in terms of the per-atom virial.

- One can also derive the following expression for the heat current from a subsystem A to a subsystem B [Fan 2017]:

$$Q_{A\to B} = -\sum_{i\in A}\sum_{j\in B} \left(\frac{\partial U_i}{\partial \vec{r}_{ij}} \cdot \vec{v}_j - \frac{\partial U_j}{\partial \vec{r}_{ji}} \cdot \vec{v}_i \right).$$

Integration by one step

- The aim of time evolution is to find the **phase trajectory**

$$\{\vec{r}_i(t_1),\, \vec{v}_i(t_1)\}_{i=1}^N,\, \{\vec{r}_i(t_2),\, \vec{v}_i(t_2)\}_{i=1}^N,\, \cdots$$

starting from the **initial phase point**

$$\{\vec{r}_i(t_0),\, \vec{v}_i(t_0)\}_{i=1}^N.$$

- The time interval between two time points $\Delta t = t_1 - t_0 = t_2 - t_1 = \cdots$ is called the **time step**.
- The algorithm for integrating by one step depends on the ensemble type and other external conditions. There are many ensembles used in MD simulations, but we only consider the following 3 in the current version:

The NVE ensemble

- This is also called the **micro-canonical ensemble**. We use the **velocity-Verlet** integration method with the following equations:

$$\vec{v}_i(t_{m+1}) \approx \vec{v}_i(t_m) + \frac{\vec{F}_i(t_m) + \vec{F}_i(t_{m+1})}{2m_i}\Delta t;$$

$$\vec{r}_i(t_{m+1}) \approx \vec{r}_i(t_m) + \vec{v}_i(t_m)\Delta t + \frac{1}{2}\frac{\vec{F}_i(t_m)}{m_i}(\Delta t)^2.$$

Explanations:

- $\vec{v}_i(t_m)$ is the velocity vector of particle i at time t_m.
- $\vec{r}_i(t_m)$ is the position vector of particle i at time t_m.
- $\vec{F}_i(t_m)$ is the force vector of particle i at time t_m.
- m_i is the mass of particle i.
- Δt is the time step for integration.

The NVT ensemble

This is also called the **canonical ensemble**. We have implemented quite a few thermostats for the NVT ensemble.

The Berendsen thermostat

- The velocities are scaled in the **Berendsen thermostat** [Berendsen 1984] in the following way:

$$\vec{v}_i^{\text{scaled}} = \vec{v}_i \sqrt{1 + \alpha_T \left(\frac{T_0}{T} - 1 \right)}.$$

- Here, α_T is a dimensionless parameter, T_0 is the target temperature, and T is the instant temperature calculated from the current velocities. The parameter α_T should be positive and not larger than 1.
- When $\alpha_T = 1$, the above formula reduces to the simple velocity-scaling formula:

$$\vec{v}_i^{\text{scaled}} = \vec{v}_i \sqrt{\frac{T_0}{T}}.$$

- A smaller α_T represents a weaker coupling between the system and the thermostat. Practically, any value of α_T in the range of $[0.01, 1]$ can be used.
- The above re-scaling is applied at each time step after the velocity-Verlet integration.
- This thermostat is usually used for reaching equilibrium and is **not good** for sampling the canonical ensemble.

The Nose-Hoover chain thermostat

- In the **Nose-Hoover chain** method [Tuckerman 2010], the equations of motion for the particles in the thermostatted region are (those for the thermostat variables are not presented):

$$\frac{d\vec{r}_i}{dt} = \frac{\vec{p}_i}{m_i};$$

$$\frac{d\vec{p}_i}{dt} = \vec{F}_i - \frac{\pi_0}{Q_0}\vec{p}_i.$$

- Here,
  - $\vec{r}_i$ is the position of atom i.
  - $\vec{p}_i$ is the momentum of atom i.
  - m_i is the mass of atom i.
  - $\vec{F}_i$ is the total force on atom i resulting from the potential model used.

  - $Q_0 = N_{\rm f} k_{\rm B} T \tau^2$ is the *mass* of the thermosat variable directly coupled to the system and π_0 is the corresponding *momentum*.
    - $N_{\rm f}$ is the degree of freedom in the thermostatted region.
    - $k_{\rm B}$ is Boltzmann's constant and T is the target temperature.
    - τ is a time parameter, and we suggest a value from 0.01 ps to 1 ps.
- We used a fixed chain length of 4.

The Langevin thermostat

- In the **Langevin** method, the equations of motion for the particles in the thermostatted region are

$$\frac{d\vec{r}_i}{dt} = \frac{\vec{p}_i}{m_i};$$

$$\frac{d\vec{p}_i}{dt} = \vec{F}_i - \frac{\vec{p}_i}{\tau} + \vec{f}_i,$$

- Here,
  - $\vec{r}_i$ is the position of atom i.
  - $\vec{p}_i$ is the momentum of atom i.
  - m_i is the mass of atom i.
  - $\vec{F}_i$ is the total force on atom i resulted from the potential model used.
  - $\vec{f}_i$ is a random force with a variation determined by the fluctuation-dissipation relation to recover the canonical ensemble distribution with the target temperature.
  - τ is a time parameter. We suggest a value from 0.01 ps to 1 ps.
- We implemented the integrator proposed in [Bussi 2007a].

The Bussi-Donadio-Parrinello thermostat

- The Berendsen thermostat does not generate a true NVT ensemble. As an extension of the Berendsen thermostat, the **Bussi-Donadio-Parrinello** (BDP) thermostat [Bussi 2007b] incorporates a proper randomness into the velocity re-scaling factor and generates a true NVT ensemble.

- In the BDP thermostat, the velocities are scaled in the following way:

$$\vec{v}_i^{\rm scaled} = \alpha \vec{v}_i;$$

$$\alpha^2 = e^{-\Delta t/\tau} + \frac{T_0}{TN_f}\left(1 - e^{-\Delta t/\tau}\right)\left(R_1^2 + \sum_{i=2}^{N_f} R_i^2\right) + 2e^{-\Delta t/2\tau} R_1 \sqrt{\frac{T_0}{TN_f}\left(1 - e^{-\Delta t/\tau}\right)}.$$

- Here,
  - $\vec{v}_i$ is the velocity of atom i before the re-scaling.
  - $N_{\rm f}$ is the degree of freedom in the thermostatted region.
  - T is instant temperature and T_0 is the target temperature.
  - Δt is the time step for integration.
  - τ is a time parameter, and we suggest a value from 0.01 ps to 1 ps.
  - $\{R_i\}_{i=1}^{N_f}$ are $N_{\rm f}$ Gaussian distributed random numbers with zero mean and unit variance.

The NPT ensemble

- This is also called the isothermal-isobaric ensemble. We have only implemented the **Berendsen barostat** [Berendsen 1984].

- In the Berendsen barostat algorithm, the particle positions and box length in a given direction are scaled if periodic boundary conditions are applied to that direction.
- For example, the scaling of the positions in the x direction reads

$$x_i^{\text{scaled}} = x_i \left[1 - \alpha_p (p_{x0} - p_x)\right].$$

- Here, p_{x0} (p_x) is the target (instant) pressure in the x direction.
- The parameter α_p is not dimensionless, and it requires some trial-and-error to find a good value of it for a given system. A harder/softer system requires a smaller/larger value of α_p. In the unit system adopted by `GPUMD`, it is recommended that $\alpha_p = 10^{-4} \sim 10^{-2}$.
- Only directions with periodic boundary conditions will be affected by the barostat. The target pressure in a non-periodic direction is thus irrelevant, although the code requires you to set one. You can just set it to zero.

Heat transport

The EMD method for heat transport

- In MD simulations, a popular approach of computing the lattice thermal conductivity is to use the Green-Kubo formula. In this method, the running lattice thermal conductivity along the x-direction (similar expressions apply to other directions) can be expressed as an integral of the heat current autocorrelation (HAC):

$$\kappa_{xx}(t) = \frac{1}{k_B T^2 V} \int_0^t dt' \mathrm{HAC}_{xx}(t').$$

- Here, k_B is Boltzmann's constant, V is the volume of the simulated system, T is the absolute temperature, and t is the correlation time. The HAC is

$$\mathrm{HAC}_{xx}(t) = \langle J_x(0) J_x(t) \rangle,$$

where $J_x(0)$ and$J_x(t)$ are the total heat current of the system at two time points separated by an interval of t. The symbol $\langle\rangle$ means that the quantity inside will be averaged over different time origins.

- **Related keyword** in the run.in file: compute_hac
- **Related output file**: hac.out
- **Related tutorial**: Tutorial: Thermal conductivity from EMD
- We only used the potential part of the heat current. If you are studying fluids, you need to output the heat currents (potential and kinetic part) using the compute keyword and calculated the HACs by yourself.
- We have decomposed the potential part of the heat current into in-plane and out-of-plane components [Fan 2017]. If you do not need this decomposition, you can simply sum up some components in the hac.out file.

The NEMD method for heat transport

- Nonequilibrium molecular dynamics (NEMD) can be used to study thermal transport. In this method, two local thermostats at different temperatures are used to generate a nonequilibrium steady state with a constant heat flux.
- If the temperature difference between the two thermostats is ΔT and the heat flux is Q/S, the **thermal conductance** G between the two thermostats can be calculated as

$$G = \frac{Q/S}{\Delta T}.$$

Here, Q is the energy transfer rate between the thermostat and the thermostated region and S is the cross-sectional area perpendicular to the transport direction.

- We can also calculate an **effective thermal conductivity** (also called **apparent thermal conductivity**) $\kappa(L)$ for the finite system:

$$\kappa(L) = GL = \frac{Q/S}{\Delta T/L}.$$

where L is the length between the heat source and the heat sink. This is to say that the temperature gradient should be calculated as $\Delta T/L$, rather than that extracted from the linear part of the temperature profile away from the local thermostats. This is an important conclusion in Ref. [Li 2019].

- To generate the nonequilibrium steady state, one can use a pair of local thermostats. Based on Ref. [Li 2019], the Langevin thermostatting method is recommended. Therefore, the ensemble keyword with the first parameter of `heat_lan` should be used to generate the heat current.
- The compute keyword should be used to compute the temperature profile and the heat transfer rate Q.
- **Related output file**: compute.out
- **Related tutorial**: Tutorial: Thermal transport from NEMD and HNEMD

The HNEMD method for heat transport

- The homogeneous nonequilibrium molecular dynamics (HNEMD) method for heat transport by Evans has been recently generalized to general many-body potentials [Fan 2019]. This method is physically equivalent to the Green-Kubo (EMD) method but is computationally much faster.
- In this method, an external force of the form [Fan 2019]

$$\vec{F}_i^{\text{ext}} = E_i \vec{F}_{\text{e}} + \sum_{j \neq i} \left(\frac{\partial U_j}{\partial \vec{r}_{ji}} \otimes \vec{r}_{ij} \right) \cdot \vec{F}_{\text{e}}$$

is added to each atom i, driving the system out of equilibrium. According to [Gabourie 2020], it can also be written as

$$\vec{F}_i^{\text{ext}} = E_i \vec{F}_{\text{e}} + \vec{F}_{\text{e}} \cdot \mathbf{W}_i$$

- Here,
  - E_i is the total energy of particle i.
  - U_i is the potential energy of particle i.
  - $\mathbf{W}_i$ is the per-atom virial.
  - $\vec{r}_{ij} \equiv \vec{r}_j - \vec{r}_i$, and $\vec{r}_i$ is the position of particle i.
  - The parameter $\vec{F}_{\text{e}}$ is of the dimension of inverse length and should be small enough to keep the system within the linear response regime.
- The driving force will induce a nonequilibrium heat current $\left\langle \vec{J} \right\rangle_{\text{ne}}$ linearly related to $\vec{F}_{\text{e}}$:

$$\frac{\left\langle J^\mu(t) \right\rangle_{\text{ne}}}{TV} = \sum_\nu \kappa^{\mu\nu} F_{\text{e}}^\nu,$$

where $\kappa^{\mu\nu}$ is the thermal conductivity tensor, T is the system temperature, and V is the system volume.

- A global thermostat should be applied to control the temperature of the system. For this, we recommend using the Nose-Hoover chain thermostat. So one should use the ensemble keyword with the first parameter of `nvt_nhc`.
- The compute_hnemd keyword should be used to add the driving force and calculate the thermal conductivity.
- The computed results are saved to the kappa.out file.
- **Related tutorial**: Tutorial: Thermal transport from NEMD and HNEMD

Spectral heat current

- In the framework of the NEMD and HNEMD methods, one can also calculate spectrally decomposed thermal conductivity (or conductance). In this method, one first calculates the following virial-velocity correlation function [Gabourie 2020]:

$$\vec{K}(t) = \sum_i \left\langle \mathbf{W}_i(0) \cdot \vec{v}_i(t) \right\rangle,$$

which reduces to the nonequilibrium heat current when $t = 0$.

- Then one can define the following Fourier transform pairs [Fan 2017]:

$$\tilde{\vec{K}}(\omega) = \int_{-\infty}^{\infty} dt e^{i\omega t} K(t)$$

$$\vec{K}(t) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{-i\omega t} \tilde{\vec{K}}(\omega)$$

- By setting $t = 0$ in the equation above, we can get the following spectral decomposition of the nonequilibrium heat current:

$$\vec{J} = \int_0^{\infty} \frac{d\omega}{2\pi} \left[2\tilde{\vec{K}}(\omega) \right].$$

- From the spectral decomposition of the nonequilibrium heat current, one can deduce the spectrally decomposed thermal conductance in the NEMD method:

$$G(\omega) = \frac{2\tilde{\vec{K}}(\omega)}{V \Delta T} \quad \text{with} \quad G = \int_0^{\infty} \frac{d\omega}{2\pi} G(\omega).$$

where ΔT is the temperature difference between the two thermostats and V is the volume of the considered system or subsystem.

- One can also calculate the spectrally decomposed thermal conductivity in the HNEMD method:

$$\kappa(\omega) = \frac{2\tilde{\vec{K}}(\omega)}{V T F_{\mathrm{e}}} \quad \text{with} \quad \kappa = \int_0^{\infty} \frac{d\omega}{2\pi} \kappa(\omega).$$

where F_{e} is the magnitude of the driving force parameter in the HNEMD method.

- This calculation is invoked by the compute_shc keyword and the results are saved to the shc.out file.
- **Related tutorial**: Tutorial: Thermal transport from NEMD and HNEMD

Modal Analysis Methods

- A system with N atoms will have $3N$ vibrational modes. Using lattice dynamics, the vibrational modes (or eigenmodes) of the system can be found. The heat flux can be decomposed into contributions from each vibrational mode and the thermal conductivity can be written in terms of those contributions [Lv 2016].
- To calculate the modal heat current in GPUMD, the velocities must first be decomposed into their modal contributions:

$$\vec{v}_i(t) = \frac{1}{\sqrt{m_i}} \sum_n \vec{e}_{i,n} \cdot \dot{\vec{X}}_n(t)$$

Here,

- $\dot{\vec{X}}_n$ is the normal mode coordinates of the velocity of mode n
- m_i is the mass of atom i
- $\vec{e}_{i,n}$ is the eigenvector that gives the magnitude and direction of mode n for atom i
- $\vec{v}_i$ is the velocity of atom i

- The heat current in GPUMD can be rewritten in terms of the modal velocity to be:

$$\vec{J}^{\rm pot} = \sum_i \mathbf{W}_i \cdot \left[\frac{1}{\sqrt{m_i}} \sum_n \vec{e}_{i,n} \cdot \dot{\vec{X}}_n(t) \right] = \sum_n \left(\sum_i \frac{1}{\sqrt{m_i}} \mathbf{W}_i \cdot \vec{e}_{i,n} \right) \cdot \dot{\vec{X}}_n(t)$$

- This means that the modal heat current can be written as:

$$\vec{J}_n^{\rm pot} = \left(\sum_i \frac{1}{\sqrt{m_i}} \mathbf{W}_i \cdot \vec{e}_{i,n} \right) \cdot \dot{\vec{X}}_n(t)$$

- This modal heat current can be used to extend the capabilities of the EMD and HNEMD methods. The extended methods are called Green-Kubo Modal Analysis (GKMA) [Lv 2016] and Homogeneous Nonequilibrium Modal Analysis (HNEMA) [Gabourie 2020].

GKMA

- The Green-Kubo Modal Analysis (GKMA) calculates the modal contributions to thermal conductivity by using [Lv 2016][Gabourie 2020]:

$$\kappa_{xx,n}(t) = \frac{1}{k_B T^2 V} \int_0^t dt' \left\langle J_{x,n}(t') J_x(0) \right\rangle.$$

Here, $k_{\rm B}$ is Boltzmann's constant, V is the volume of the simulated system, T is the absolute temperature, and t is the correlation time. $J_x(0)$ is the total heat current and and$J_{x,n}(t')$ is the mode-specific heat current of the system at two time points separated by an interval of t'. The symbol $\left\langle \right\rangle$ means that the quantity inside will be averaged over different time origins.

- **Related input file**: eigenvector.in
- **Related keyword** in the run.in file: compute_gkma
- **Related output file**: heatmode.out
- For the GKMA method, we only used the potential part of the heat current.

HNEMA

- The Homogeneous Nonequilibrium Modal Analysis (HNEMA) method calculates the modal contributions of thermal conductivity using [Gabourie 2020]:

$$\frac{\left\langle J_n^\mu(t) \right\rangle_{\rm ne}}{TV} = \sum_\nu \kappa_n^{\mu\nu} F_{\rm e}^\nu,$$

Here, $\kappa_n^{\mu\nu}$ is the thermal conductivity tensor of mode n, T is the system temperature, and V is the system volume. The mode-specific nonequilibrium heat current is $\left\langle J_n^\mu(t) \right\rangle_{\rm ne}$ and the driving force parameter is $\vec{F}_{\rm e}$.

- **Related input file**: eigenvector.in
- **Related keyword** in the run.in file: compute_hnema
- **Related output file**: kappamode.out
- For the HNEMA method, we only used the potential part of the heat current.

- A global thermostat should be applied to control the temperature of the system. For this, we recommend using the Nose-Hoover chain thermostat. So one should use the ensemble keyword with the first parameter of `nvt_nhc`.

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