Nonequilibrium Thermodynamics for one-dimensional system

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- Nonequilibrium thermodynamics

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  b) Thermodynamic potential equilibrium/nonequilibrium

- One-dimensional system

  a) convenience

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Classic nonequilibrium thermodynamics

1) Equilibrium, state function

Isolated System in Equilibrium

$(P,T) \rightarrow (E,V)$

$$\frac{P}{T} = f(E,V)$$

$$\frac{1}{T} = G(E,V)$$

$$\frac{\partial f}{\partial E} = \frac{\partial G}{\partial V}$$

$$\int_{E_0,V_0}^{E_1,V_1} dS = S(E,V)$$

Thermodynamic potential

Entropy

$$dS = f dV + G dE \qquad dS = \frac{P}{T} dV + \frac{1}{T} dE$$

Classic nonequilibrium thermodynamics

1) Equilibrium

Isolated System in Equilibrium
$(P,T) \rightarrow (E,V)$

Isolated unitary System in equilibrium
$(S,V) \rightarrow (P,T)$

$$-S = f(P,T)$$

$$V = g(P,T)$$

$$\frac{\partial f}{\partial P} = \frac{\partial g}{\partial T}$$

$$dG = f dT + g dP$$

$$\int dG = G(P,T)$$

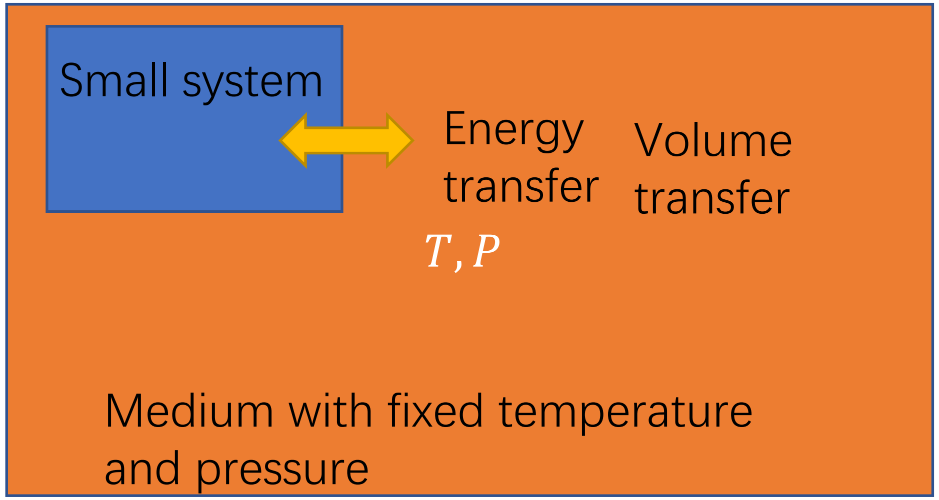
Thermodynamic potential

Gibbs function

$$dG = -S dT + V dP$$

Isolated System in equilibrium

$(P,T) \rightarrow (E,V)$



$$S_{total} = S_{small} + S_{medium}$$

$$E_{small} \ll E_{medium} \qquad V_{small} \ll V_{medium}$$

$$dS = \frac{P}{T} dV + \frac{1}{T} dE$$

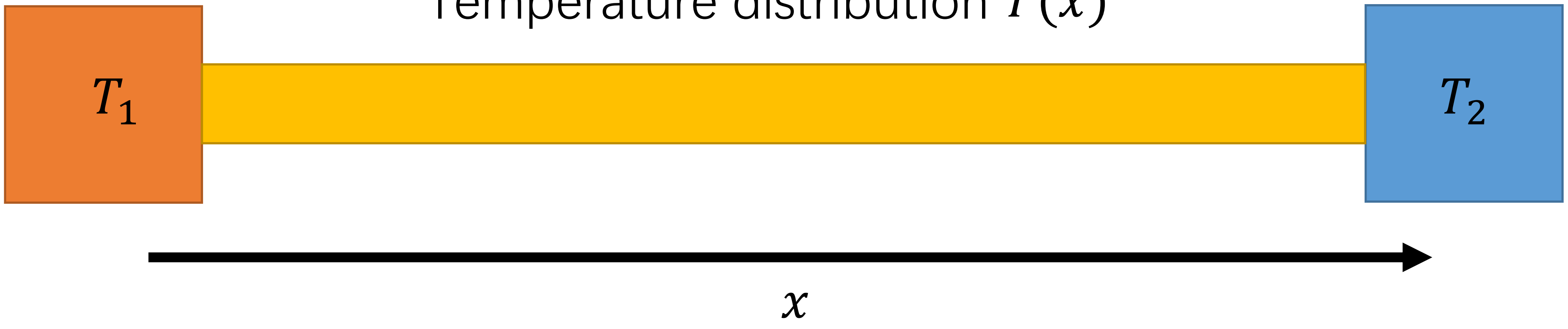
$$S_{medium} = \frac{-E_{small} - PV_{small}}{T}$$

$$S_{total} = \frac{TS_{small} - E_{small} - PV_{small}}{T} = -\frac{G}{T}$$

$$S \uparrow \qquad G \downarrow$$

2) Nonequilibrium

Temperature distribution $T(x)$



thermodynamic potential is additive in nonequilibrium system.

$$G(T,P) \propto V \quad g(T,P) = G/V$$

$$\dot{G} = 0 \rightarrow \dot{S} > 0$$

$$G = \int g(T(x),P)dx$$

Steady state corresponds to extremum of entropy production.

The framework of nonequilibrium thermodynamics

State function

$$dG = -S(T,P)dT + V(T,P)dP$$

Thermodynamic potential(minimum or maximum)

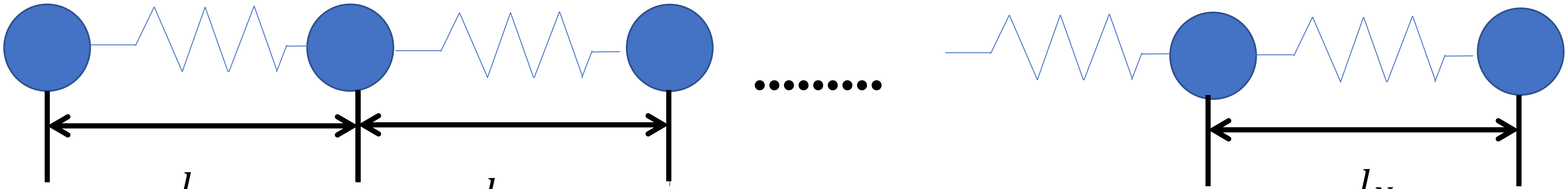
$$G(T,P)$$

Local thermodynamic equilibrium (minimum loss or production)

$$G = \int g(T(x),P)dx$$

The validity of the three components in one-dimensional system

Convenience



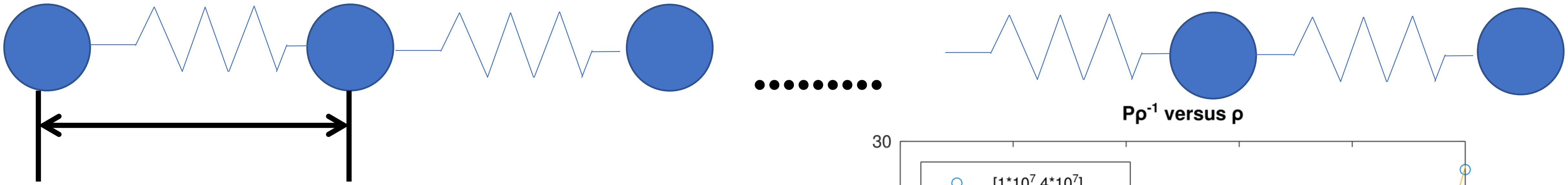
$$dG = -S(T,P)dT + V(T,P)dP$$

$$V_i = \langle l_i \rangle \qquad P_i = \langle F_{i,i+1} \rangle$$

$$T_i = \left\langle \frac{p_i^2}{m_i} \right\rangle$$

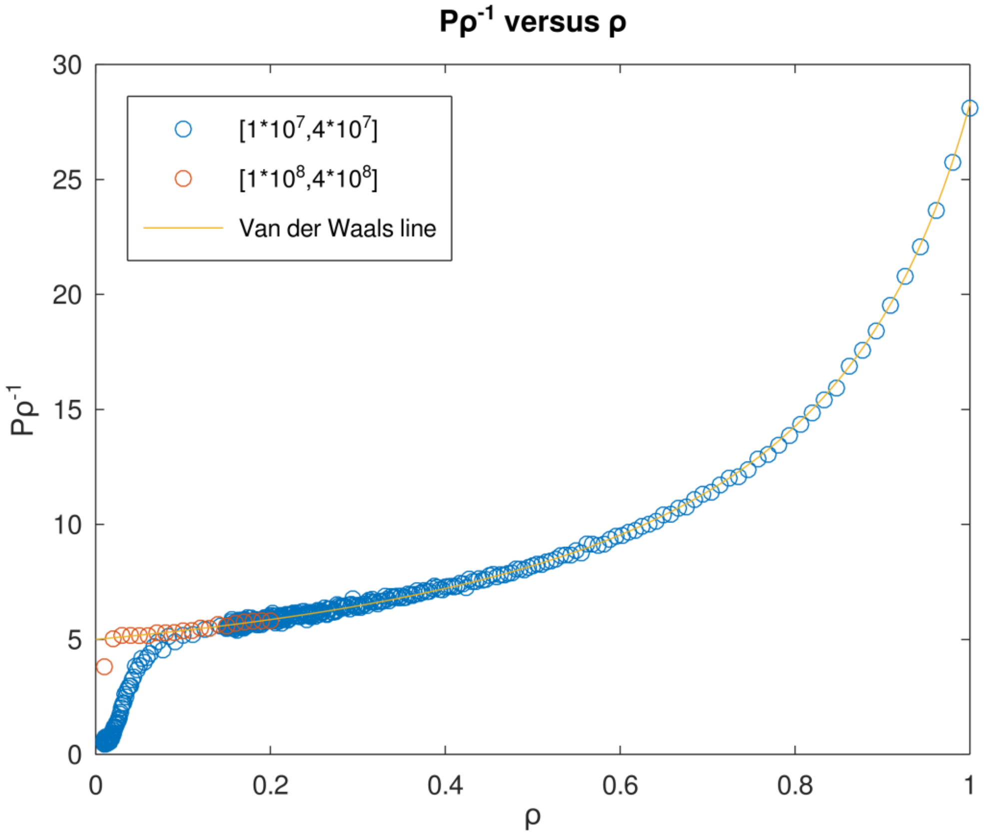
$$\mathbf{P}(\mathbf{r},t) = \sum_i m_i \mathbf{c}_i(t)\mathbf{c}_i(t)\delta(\mathbf{r}-\mathbf{r}_i) - \frac{1}{2}\sum_i \sum_{j\neq i} \mathbf{r}_{ij}\mathbf{F}_{ij}^{\emptyset}(t)\int_0^1 ds\,\delta(\mathbf{r}-\mathbf{r}_i - s\mathbf{r}_{ij})$$

Vander Waals equation



Lennard Jones potential

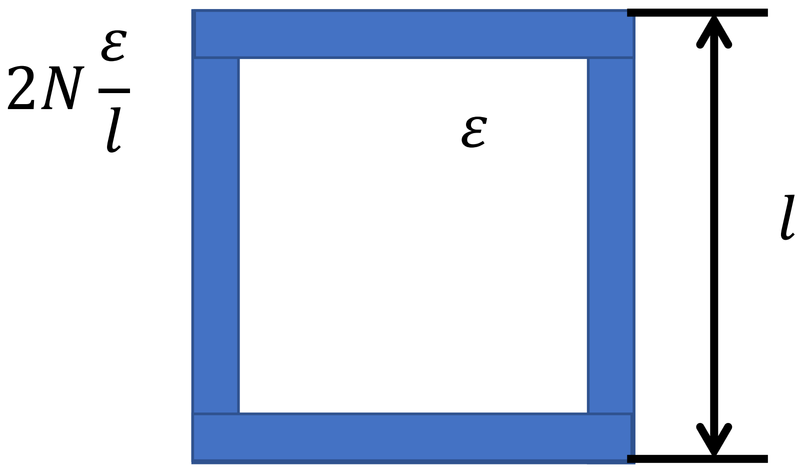
Mean field approximation is much more applicable



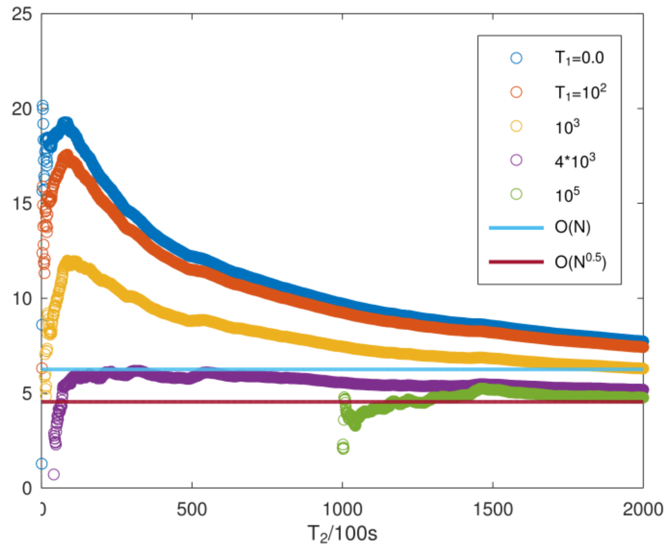
Challenge

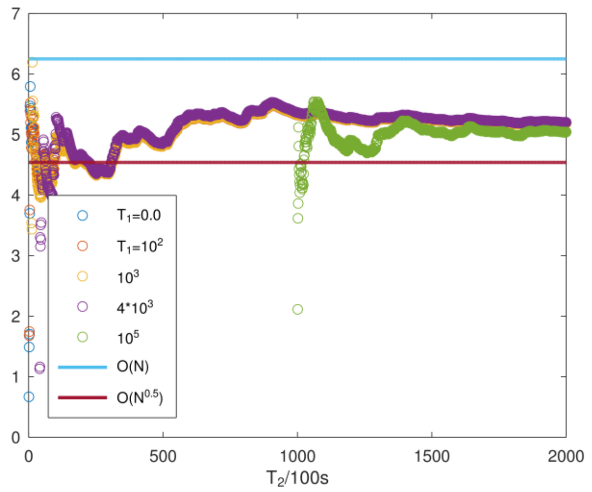
1) Slow convergence, sensitive to initial states

Boundary region for N-dimensional cube



$$G_{in} = G_{out}$$

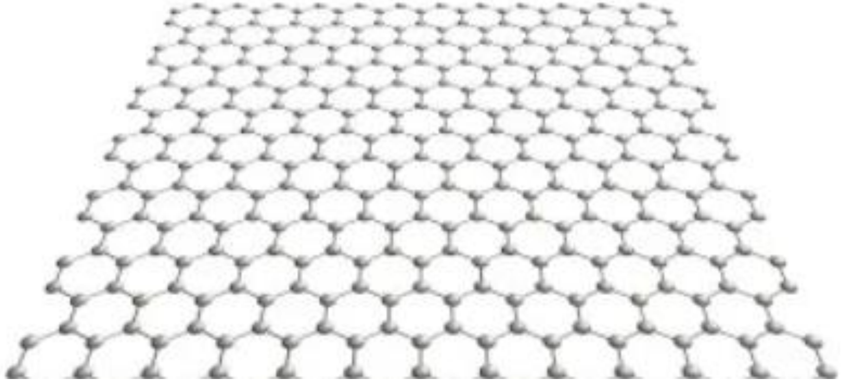


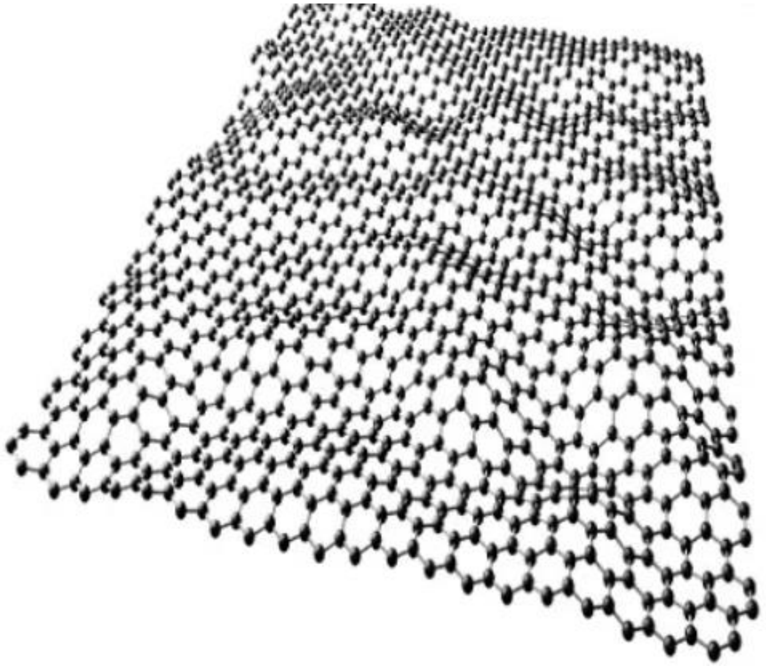


Challenge

2) Semi-one-dimensional system

There is no pure one-dimensional





Thank you