Looking at bare transport coefficients in fluctuating hydrodynamics

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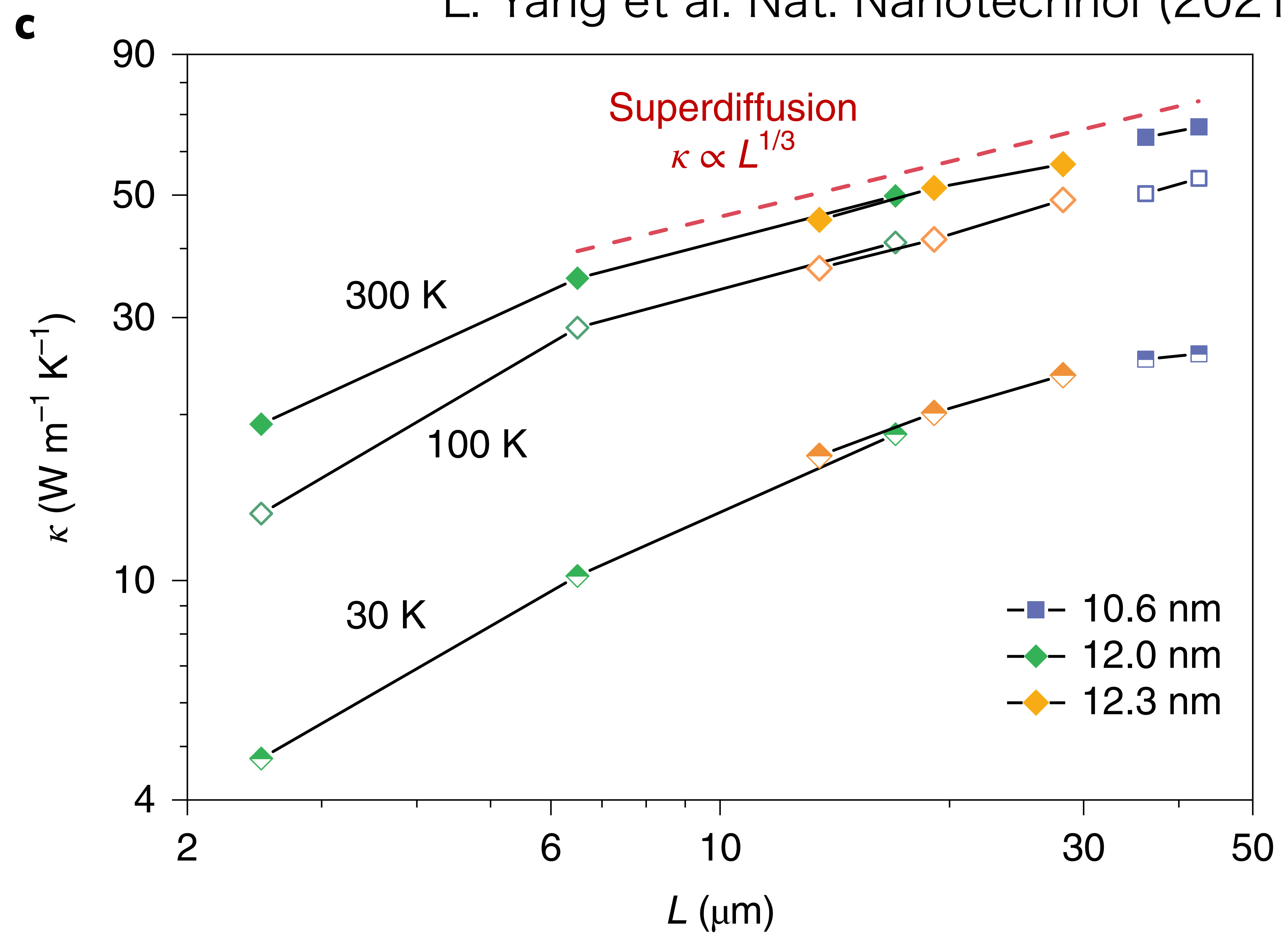
arXiv:2502.15241 (2025)

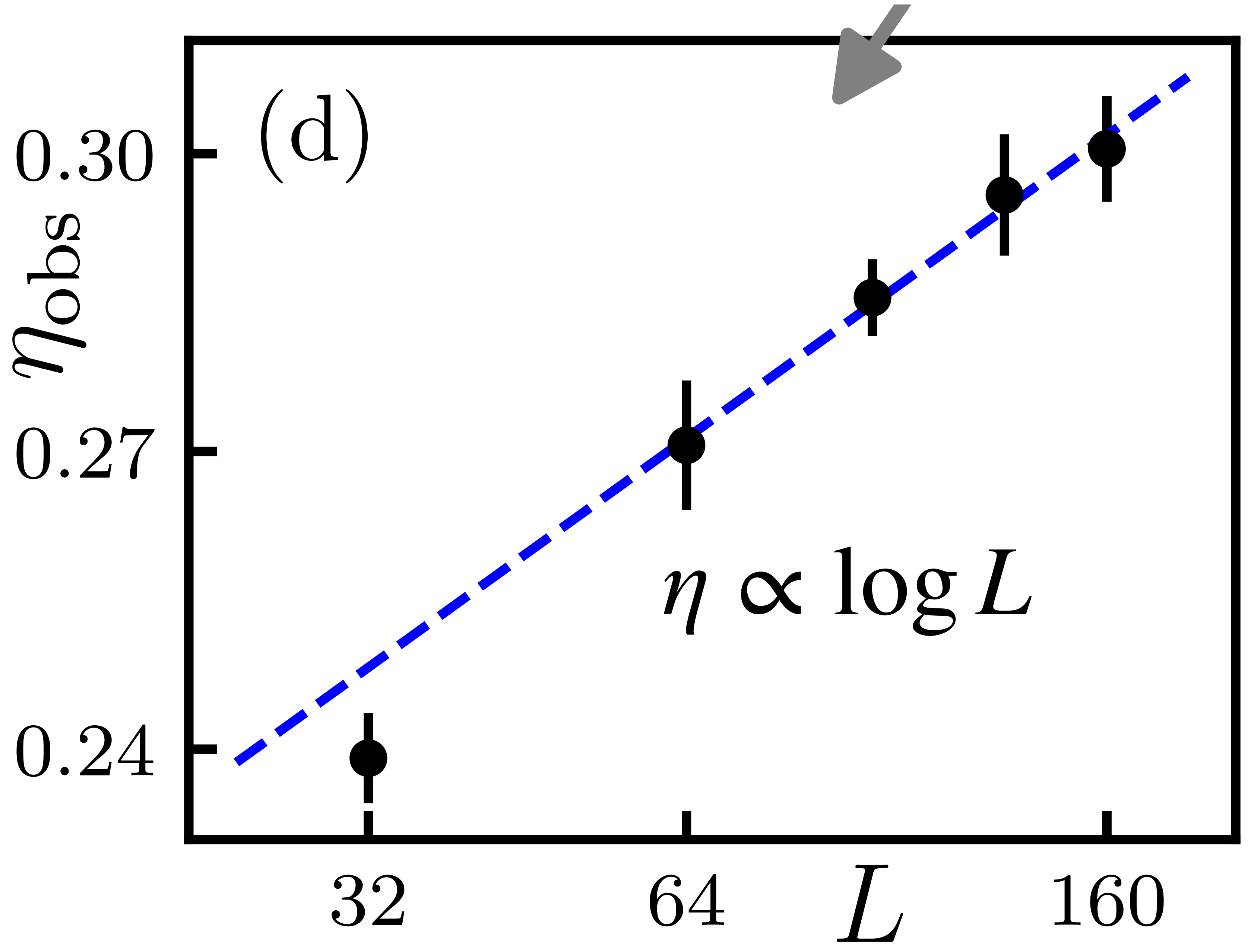
Anomalous Transport in Low-Dimensional Fluids

Key features in low-dimensional systems

- Exhibit **large fluctuations** due to low dimensionality.
- Leads to divergence of transport coefficients with system size (L).

L. Yang et al. Nat. Nanotechnol (2021)





1D Nanowires (Experimental)

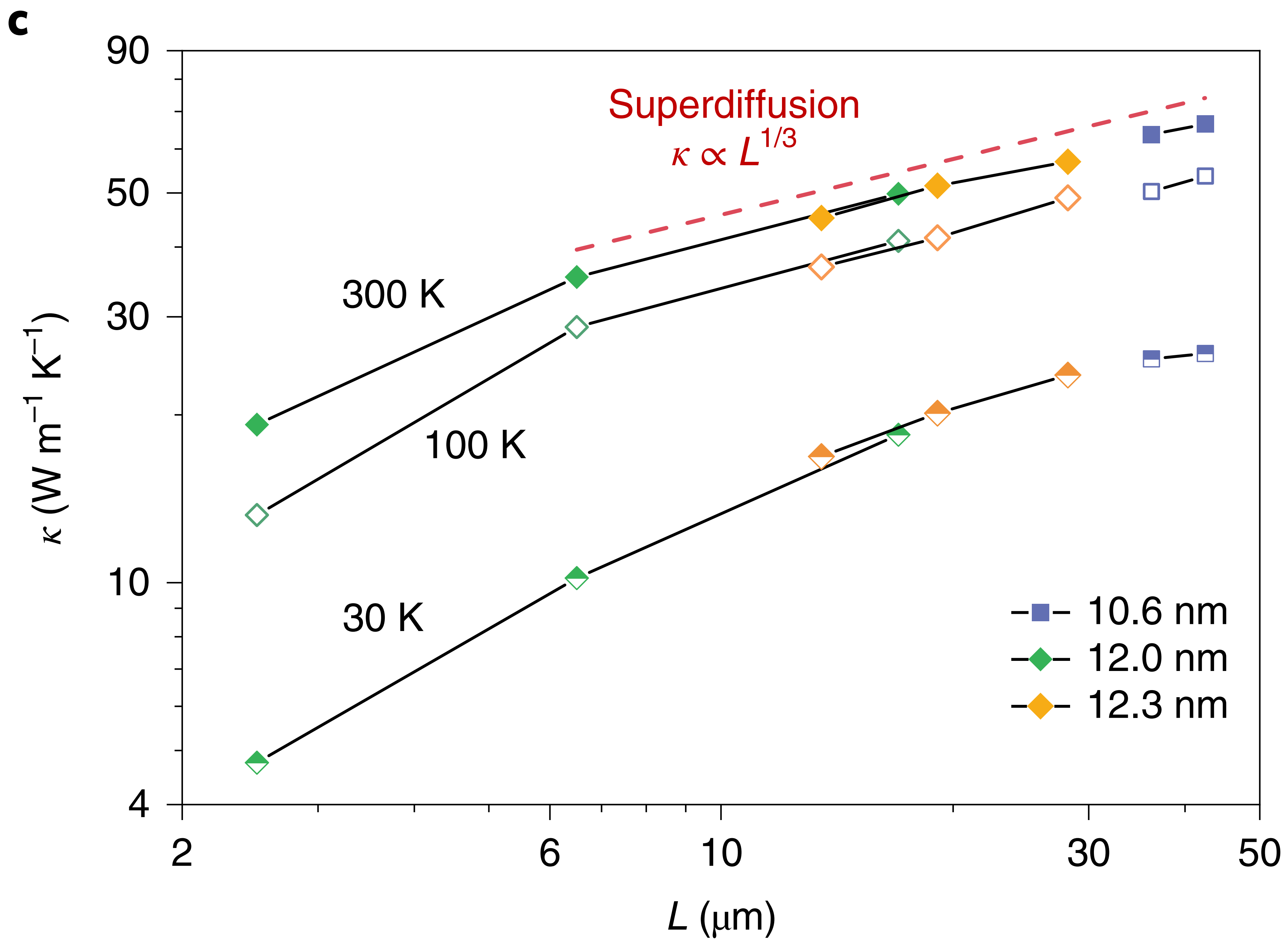
Thermal conductivity (κ) diverges $\sim L^{1/3}$

2D Fluids (Theoretically)

Shear viscosity (η) diverges $\sim \log L$

Our Research Question

L. Yang et al. Nat. Nanotechnol (2021)



Anomalous Transport Research: A Common Focus

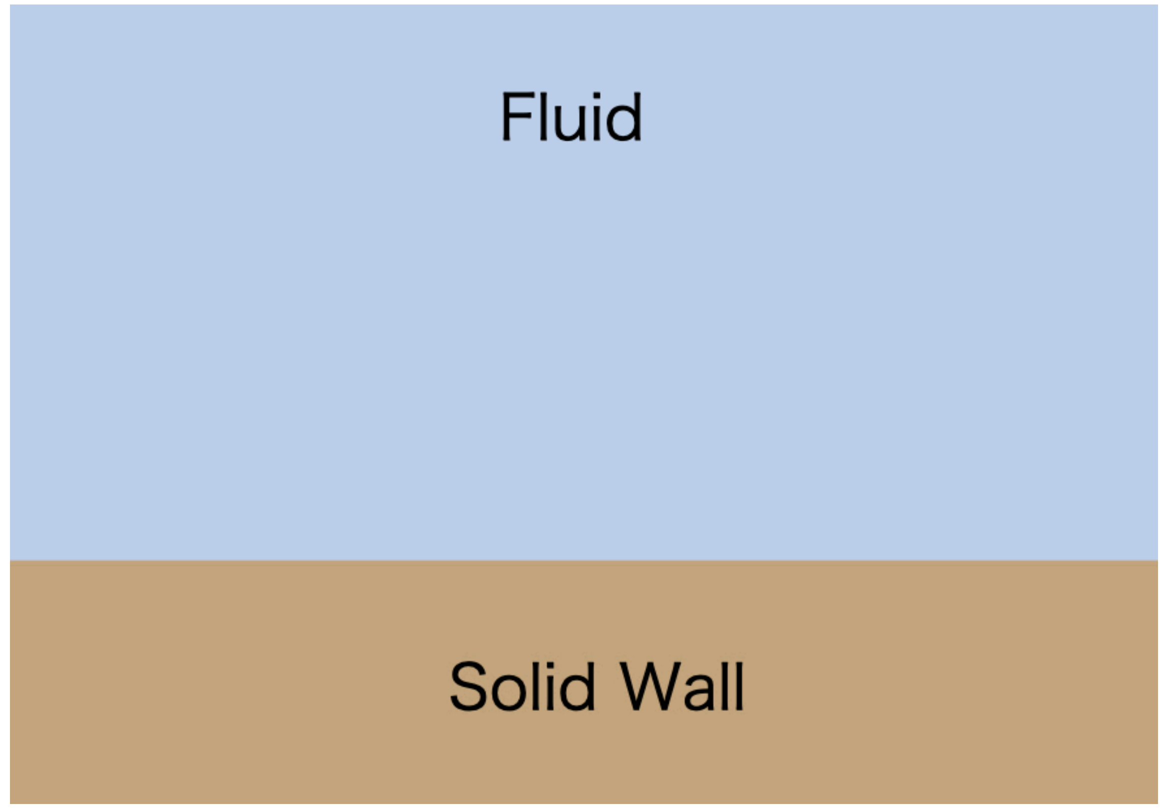
- Establishing **divergence exponents** (e.g., $\kappa \sim L^{1/3}$)
- Understanding scaling laws and universality classes

Our focus: A Different Angle

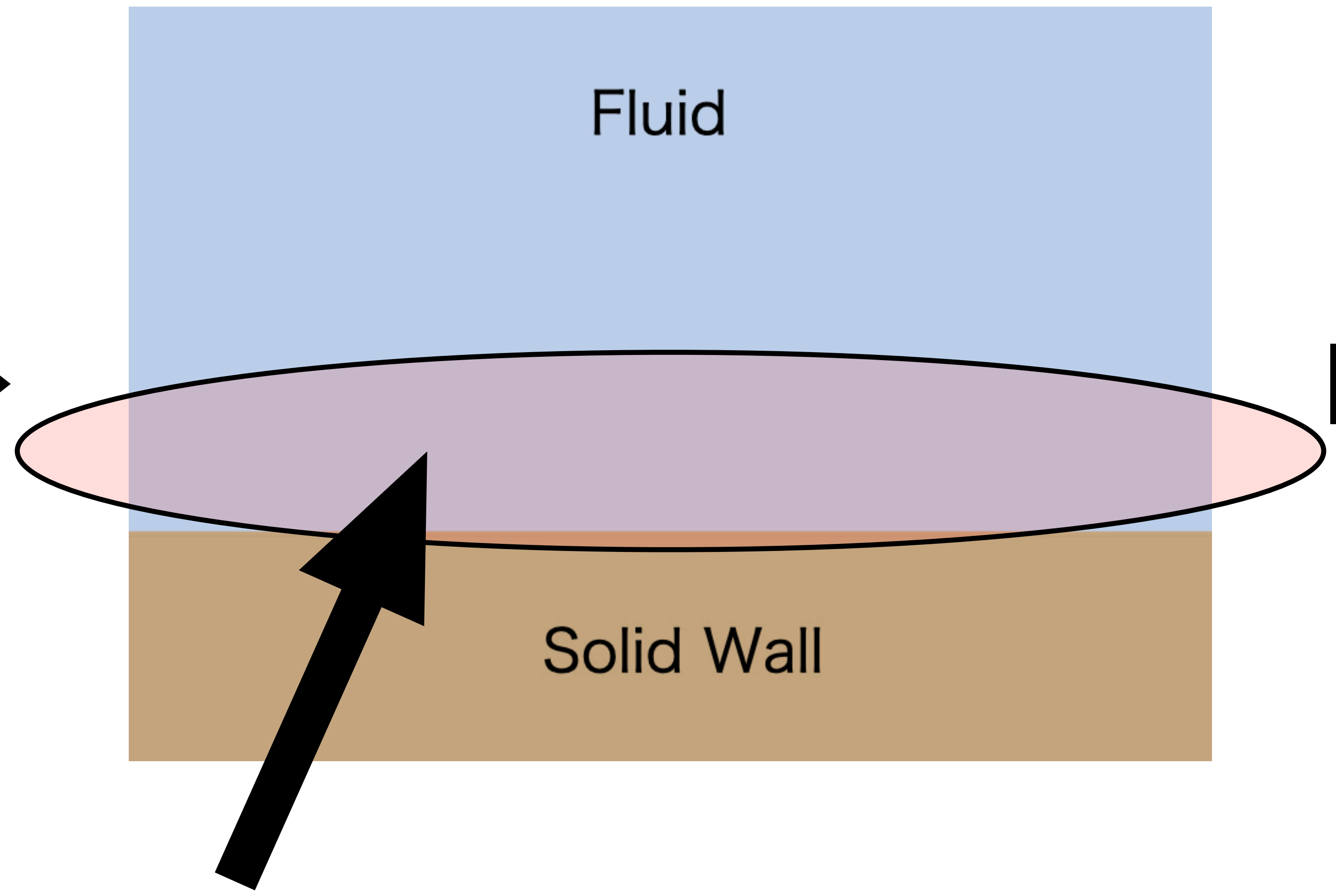
- Can we define system-size-independent transport coefficients in low-dimensional systems?
- If yes, are they useful for predicting fluid flow?

Core Idea: Wall Effects on Fluctuations and Transport

Focus: Fluid behavior near thermalized walls.



Thermalized Wall
(Wall particles follow canonical distribution at temperature)



Fluid particles also tend to thermalize near the walls
(Hydrodynamic fluctuations (or long-time tail) are suppressed near walls?)

Our expectation

Transport coefficients in bulk fluids

$\neq$

Transport coefficients near the wall

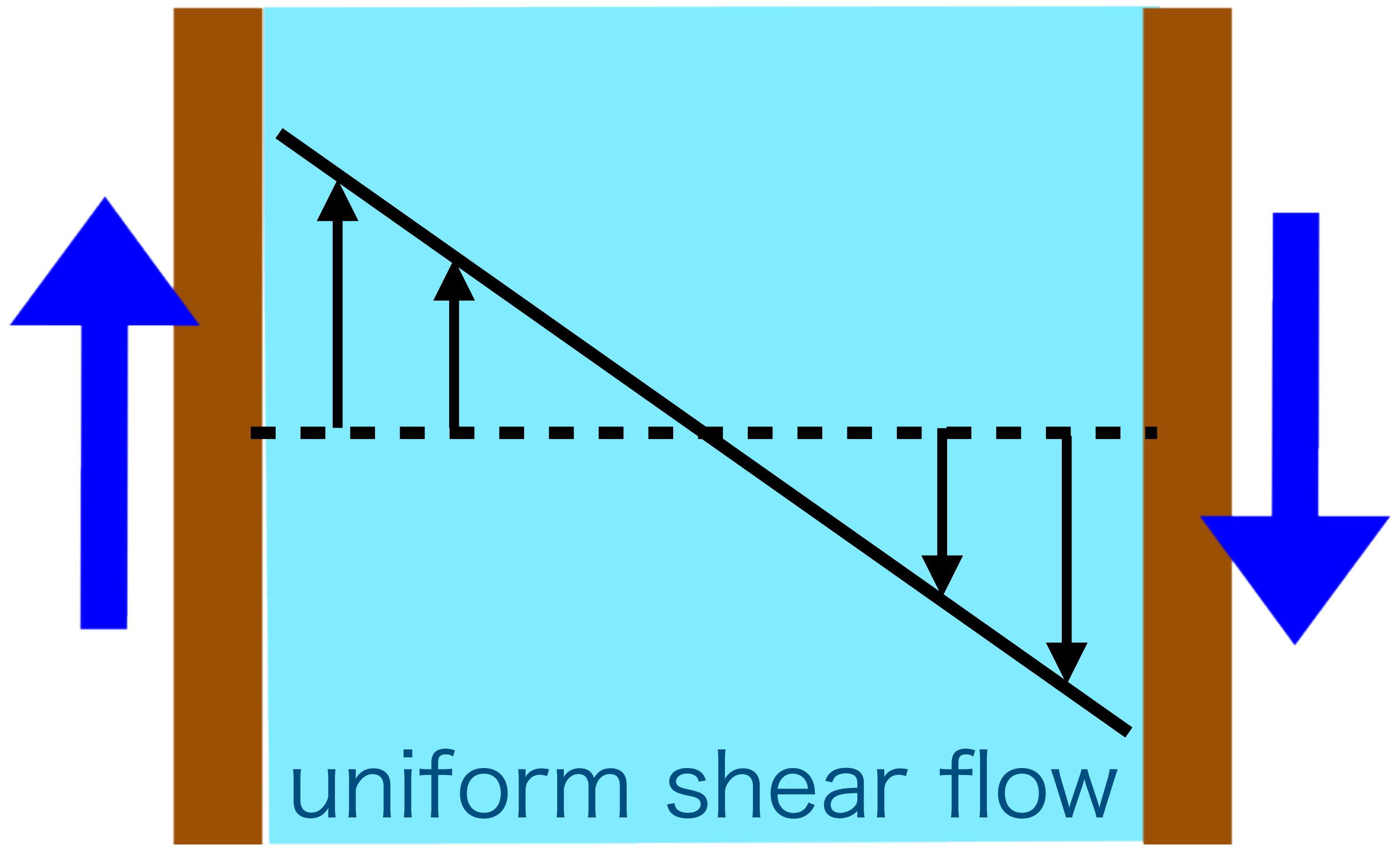
Investigate **fluctuating hydrodynamics** near walls to verify this concept.

Goal of This Talk: The Need for Local Viscosity

System: 2D Fluid under Shear

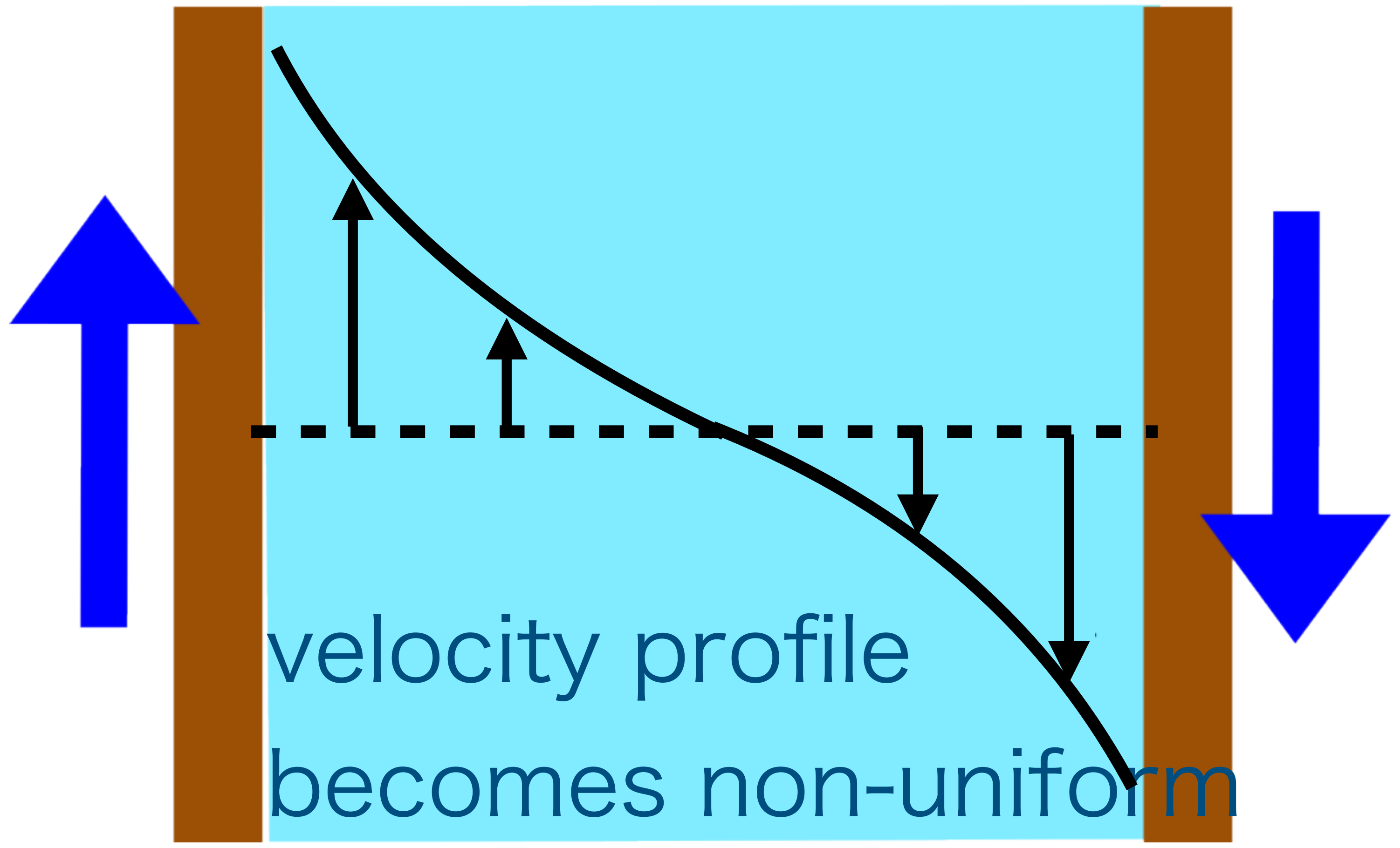
Conventional prediction

Standard Prediction
(Deterministic Hydrodynamics)



Our finding

Impact of Fluctuations (Our Focus)



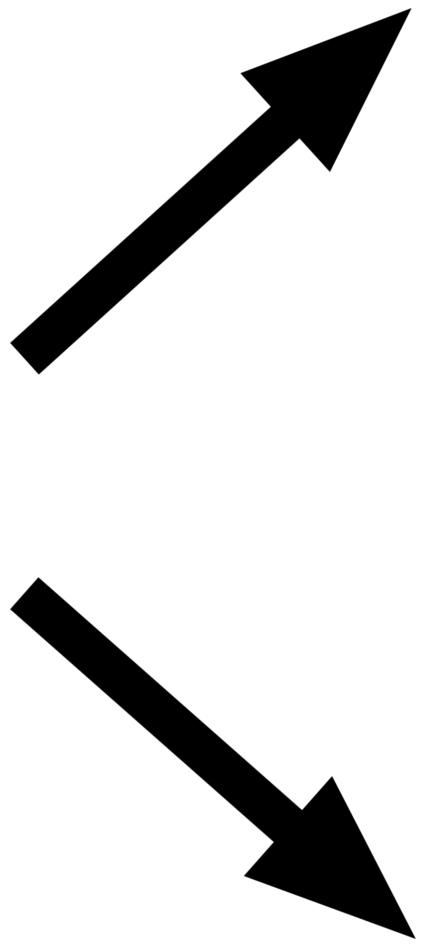
Need for Local Viscosity $\eta(x)$
(where x is distance from wall)

Main Discussion:
System-size (L) dependence of **local viscosity** $\eta(x, L)$.

Goal of This Talk: The Need for Local Viscosity

System: 2D Fluid under Shear

Conventional prediction



Our finding

Standard Prediction
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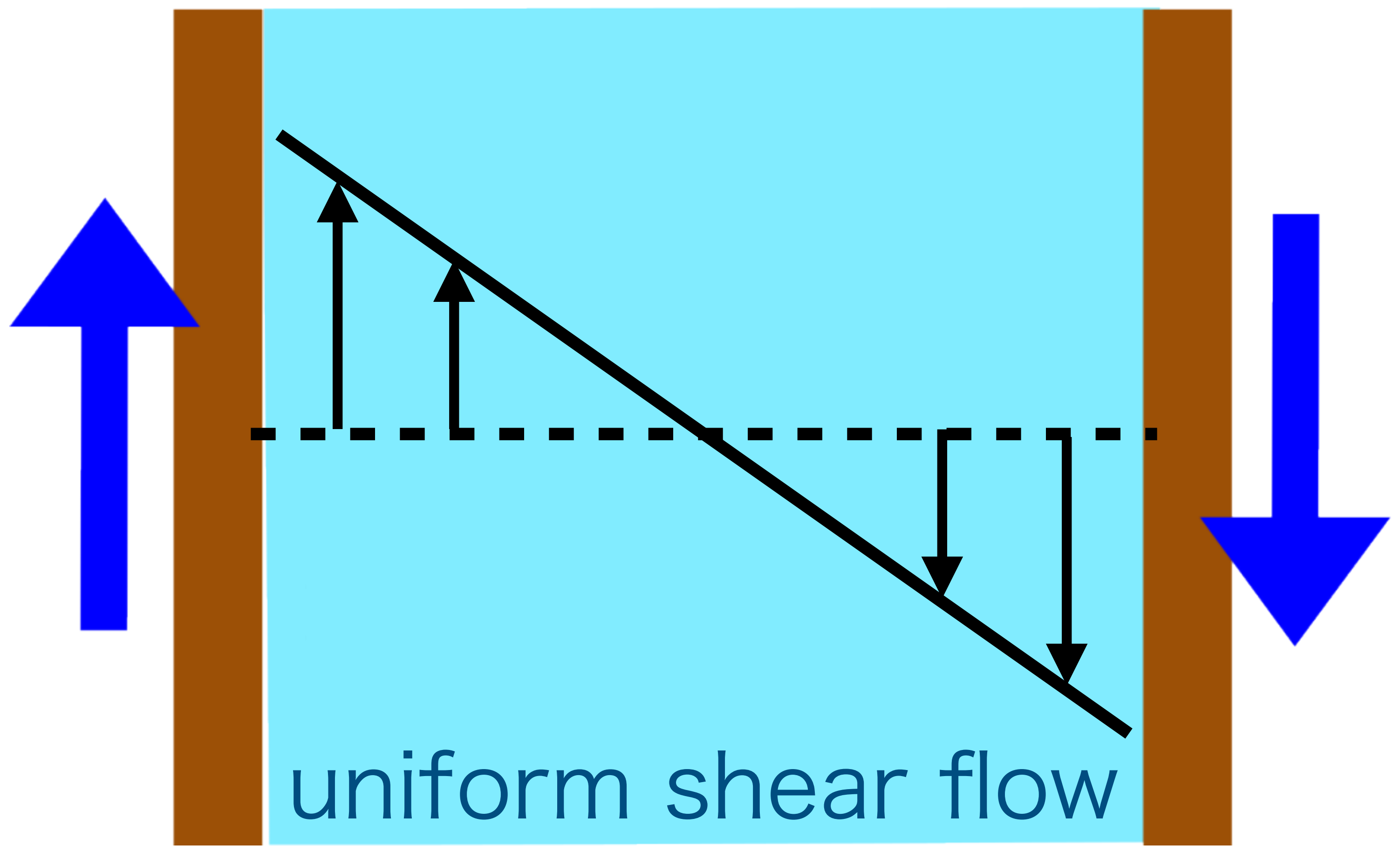
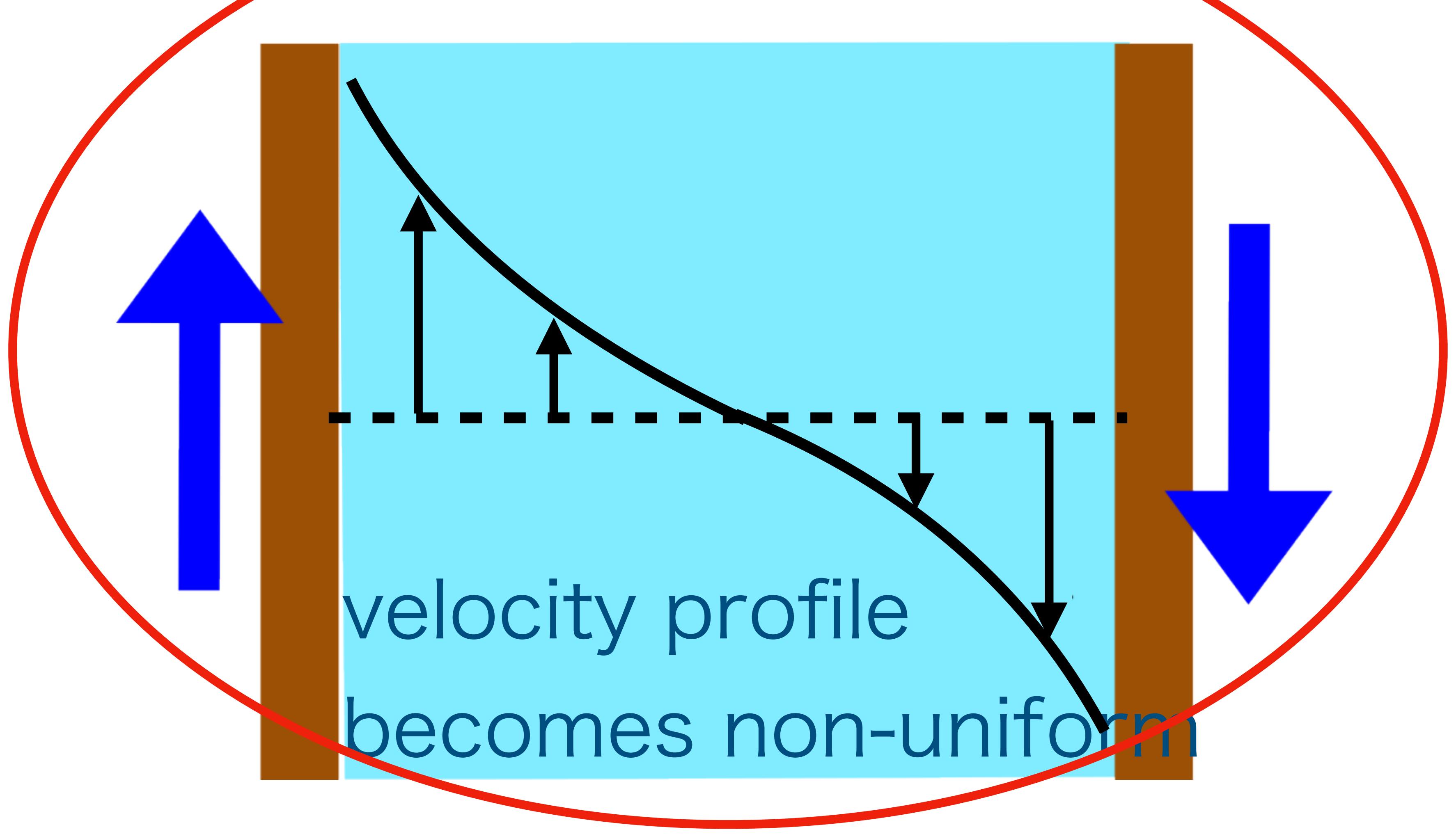


Impact of Fluctuations (Our Focus)



Need for Local Viscosity $\eta(x)$
(where x is distance from wall)

Main Discussion:
System-size (L) dependence of **local viscosity** $\eta(x, L)$.

Content in this talk

1. Discussion based on fluctuating hydrodynamics

2. Observation of microscopic particle system based on the MD simulation

3. Summary (some remarks)

Part 1.
Discussion based on fluctuating hydrodynamics

Fluctuating hydrodynamics: our model

Fluctuating hydrodynamics explains anomalous transport & divergence of transport coefficients.

Our focus: two-dimensional fluids

▶ density and momentum are conserved quantities (energy dynamics is ignored)

2d fluid

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \boldsymbol{v}) \qquad p(\rho) = C_{\text{press}}\rho \qquad c_T := \sqrt{\left(\frac{\partial p}{\partial \rho}\right)_T} = \sqrt{C_{\text{press}}}$$

$$\rho\left[\frac{\partial \boldsymbol{v}}{\partial t} + (\boldsymbol{v}\cdot\nabla)\boldsymbol{v}\right] = -\nabla p + \eta_0 \nabla^2 \boldsymbol{v} + \zeta_0 \nabla(\nabla\cdot\boldsymbol{v}) + \nabla \boldsymbol{\Pi}^{\text{ran}}$$

$$\langle \boldsymbol{\Pi}^{\text{ran}}_{ab}(\boldsymbol{r}, t)\rangle = 0,$$

$$\langle \boldsymbol{\Pi}^{\text{ran}}_{ab}(\boldsymbol{r}, t)\boldsymbol{\Pi}^{\text{ran}}_{cd}(\boldsymbol{r}', t')\rangle = 2k_B T\delta(\boldsymbol{r}-\boldsymbol{r}')\delta(t-t')\left[\eta_0\left(\delta_{ac}\delta_{bd} + \delta_{ad}\delta_{bc}\right) + (\zeta_0 - \eta_0)\,\delta_{ab}\delta_{cd}\right],$$

Fluctuating hydrodynamics: our model

Fluctuating hydrodynamics explains anomalous transport & divergence of transport coefficients.

2d fluid

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \boldsymbol{v}) \qquad p(\rho) = C_{\mathrm{press}}\rho \qquad c_T := \sqrt{\left(\frac{\partial p}{\partial \rho}\right)_T} = \sqrt{C_{\mathrm{press}}}$$

$$\rho\left[\frac{\partial \boldsymbol{v}}{\partial t} + (\boldsymbol{v}\cdot\nabla)\boldsymbol{v}\right] = -\nabla p + \eta_0 \nabla^2 \boldsymbol{v} + \zeta_0 \nabla(\nabla\cdot\boldsymbol{v}) + \nabla \boldsymbol{\Pi}_R$$

For some specific assumptions in our model:

▶ **Pressure**

The pressure follows the equation of state for an ideal gas.

▶ **Low Mach number approximation**

The sound velocity c_T is sufficiently large and the fluids are treated as incompressible.

The ζ_0 term is neglected; we focus on only the η_0 term.

We focus on the dense liquid.

Viscosity in Fluctuating hydrodynamic equation

Fluctuating hydrodynamics explains anomalous transport & divergence of transport coefficients.

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \boldsymbol{v}) \qquad p(\rho) = C_{\mathrm{press}} \rho \qquad c_T := \sqrt{\left(\frac{\partial p}{\partial \rho}\right)_T} = \sqrt{C_{\mathrm{press}}}$$

$$\rho \left[\frac{\partial \boldsymbol{v}}{\partial t} + (\boldsymbol{v} \cdot \nabla) \boldsymbol{v} \right] = -\nabla p + \eta_0 \nabla^2 \boldsymbol{v} + \zeta_0 \nabla (\nabla \cdot \boldsymbol{v}) + \nabla \boldsymbol{\Pi}_R$$

▶ Key assumption of fluctuating hydrodynamics framework

η_0 : system-size-independent quantity

▶ Fluctuating hydrodynamics derives the system-size-dependent "macroscopic" viscosity.

(characterize the overall (macroscopic) fluid dissipation)

$$\eta = \eta_0 + \Delta \eta$$

system-size-dependent quantity

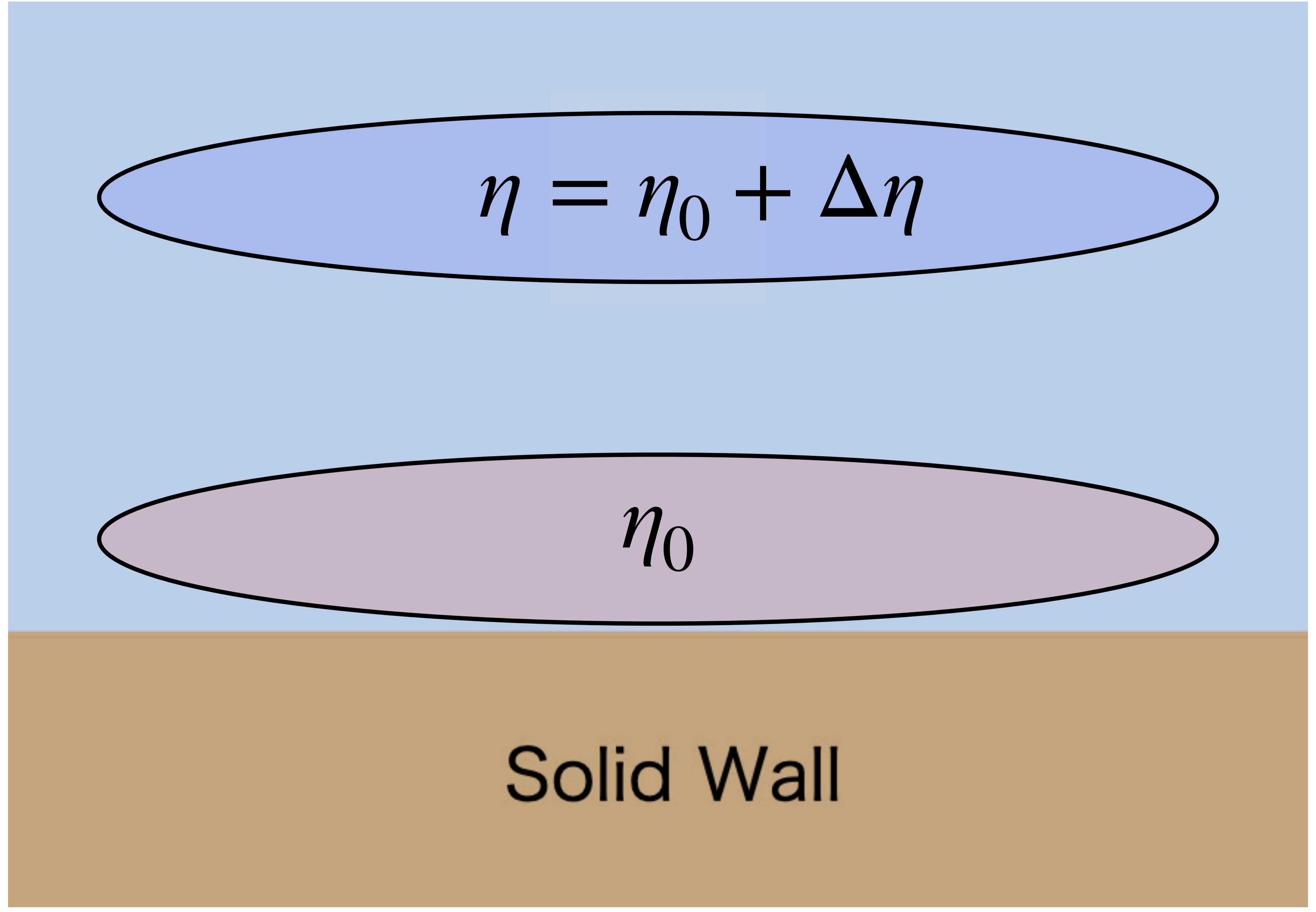
-> divergence of macroscopic viscosity

First main result of our study

2d fluid

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \boldsymbol{v}) \qquad p(\rho) = C_{\text{press}}\rho \qquad c_T := \sqrt{\left(\frac{\partial p}{\partial \rho}\right)_T} = \sqrt{C_{\text{press}}}$$

$$\rho\left[\frac{\partial \boldsymbol{v}}{\partial t} + (\boldsymbol{v}\cdot\nabla)\boldsymbol{v}\right] = -\nabla p + \eta_0 \nabla^2 \boldsymbol{v} + \zeta_0 \nabla(\nabla\cdot\boldsymbol{v}) + \nabla \boldsymbol{\Pi}_R$$



The first main result

η_0 governs the fluid motions near the walls,

while $\eta = \eta_0 + \Delta\eta$ appears only in the bulk region.

Simulation Setup

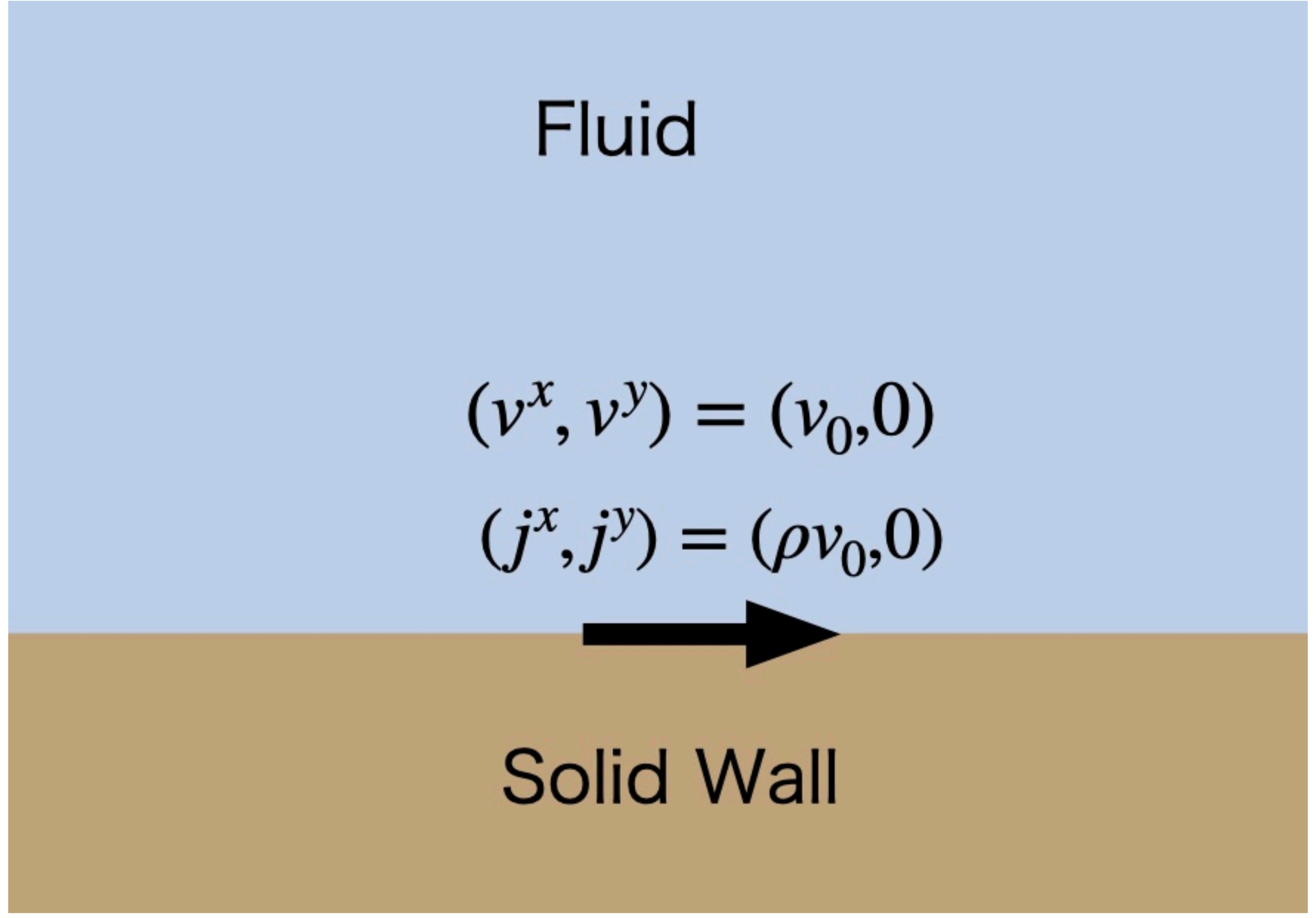
▶ We consider solving fluctuating hydrodynamics numerically

2d fluid

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \boldsymbol{v}) \qquad p(\rho) = C_{\mathrm{press}}\rho \qquad c_T := \sqrt{\left(\frac{\partial p}{\partial \rho}\right)_T} = \sqrt{C_{\mathrm{press}}}$$

$$\rho\left[\frac{\partial \boldsymbol{v}}{\partial t} + (\boldsymbol{v}\cdot\nabla)\boldsymbol{v}\right] = -\nabla p + \eta_0 \nabla^2 \boldsymbol{v} + \zeta_0 \nabla(\nabla\cdot\boldsymbol{v}) + \nabla \boldsymbol{\Pi}_R$$

The sufficiently large C_{press} yields nearly incompressible fluids



We apply a common boundary condition in fluid dynamics

1. The velocity field at the wall is $(v^x, v^y) = (v_0, 0)$
2. The momentum density field at the wall is $(j^x, j^y) = (\rho v_0, 0)$

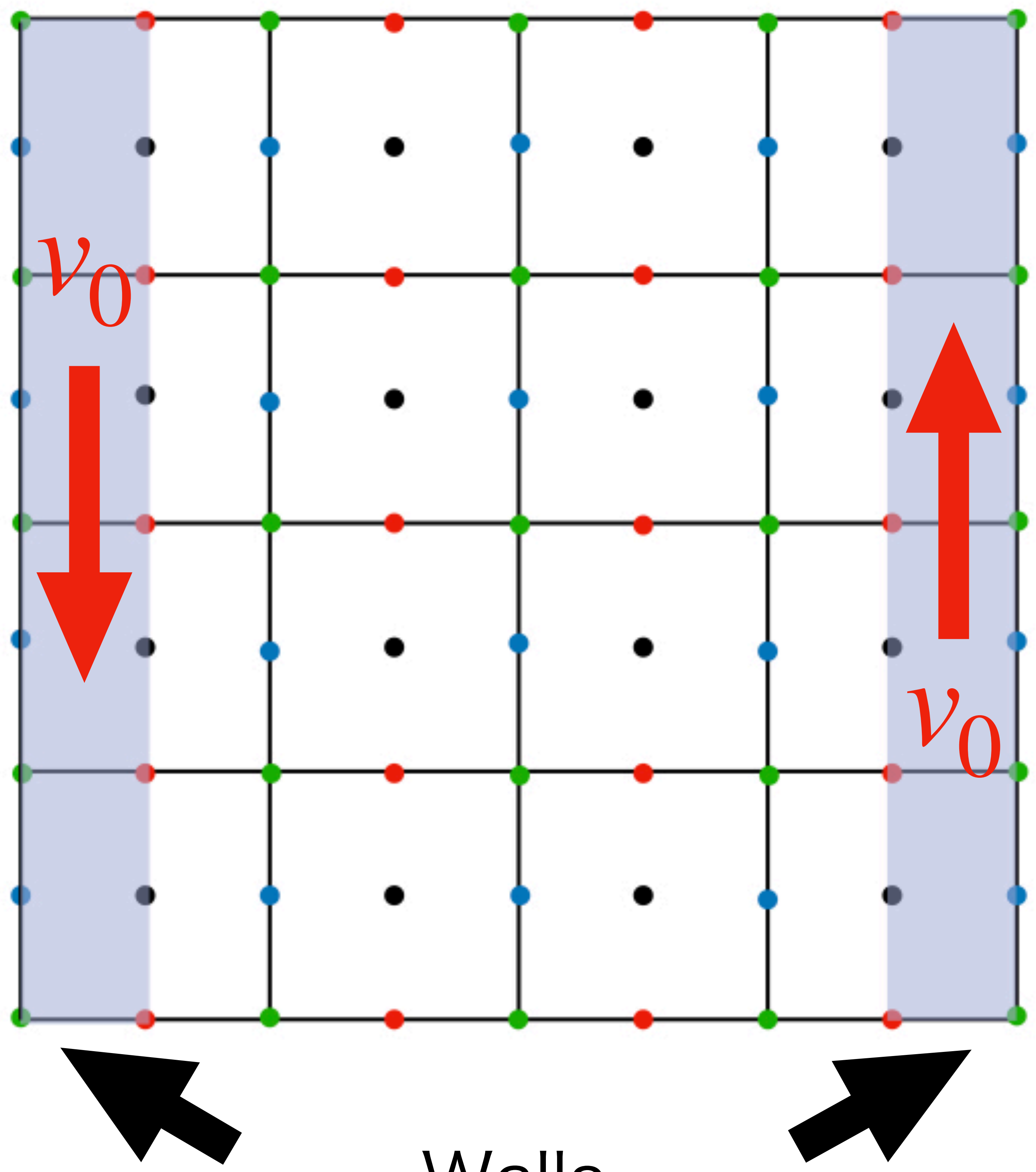
The fluid does not fluctuate at all at the solid walls

Steady-State profile of numerical simulations

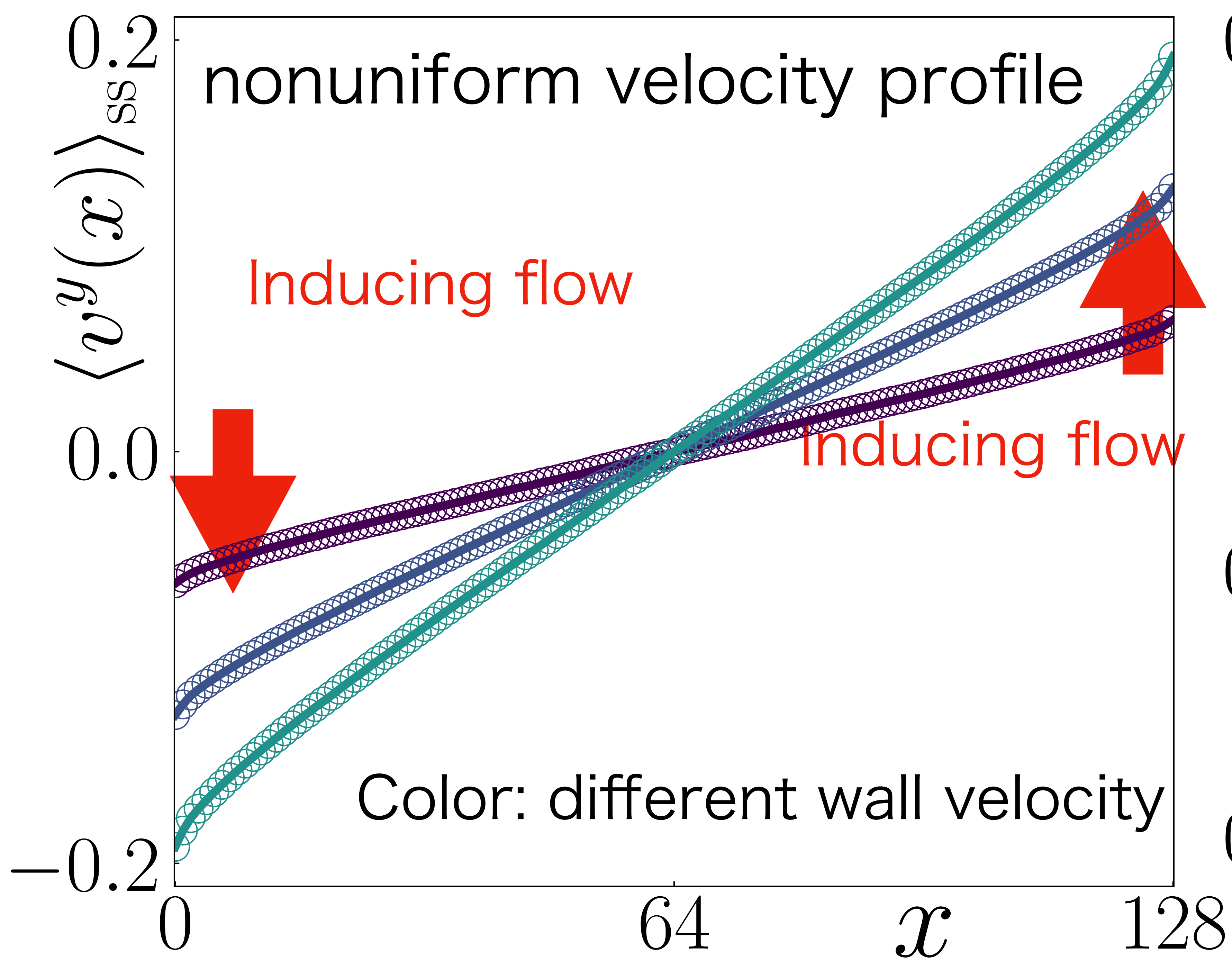
$\eta_0 = 0.1,\ a_{\mathrm{uv}} = 1.0,\ \rho_0 = 0.765,\ k_B T = 1.0,\ L = 128$

(I will explain the units for physical quantities later)

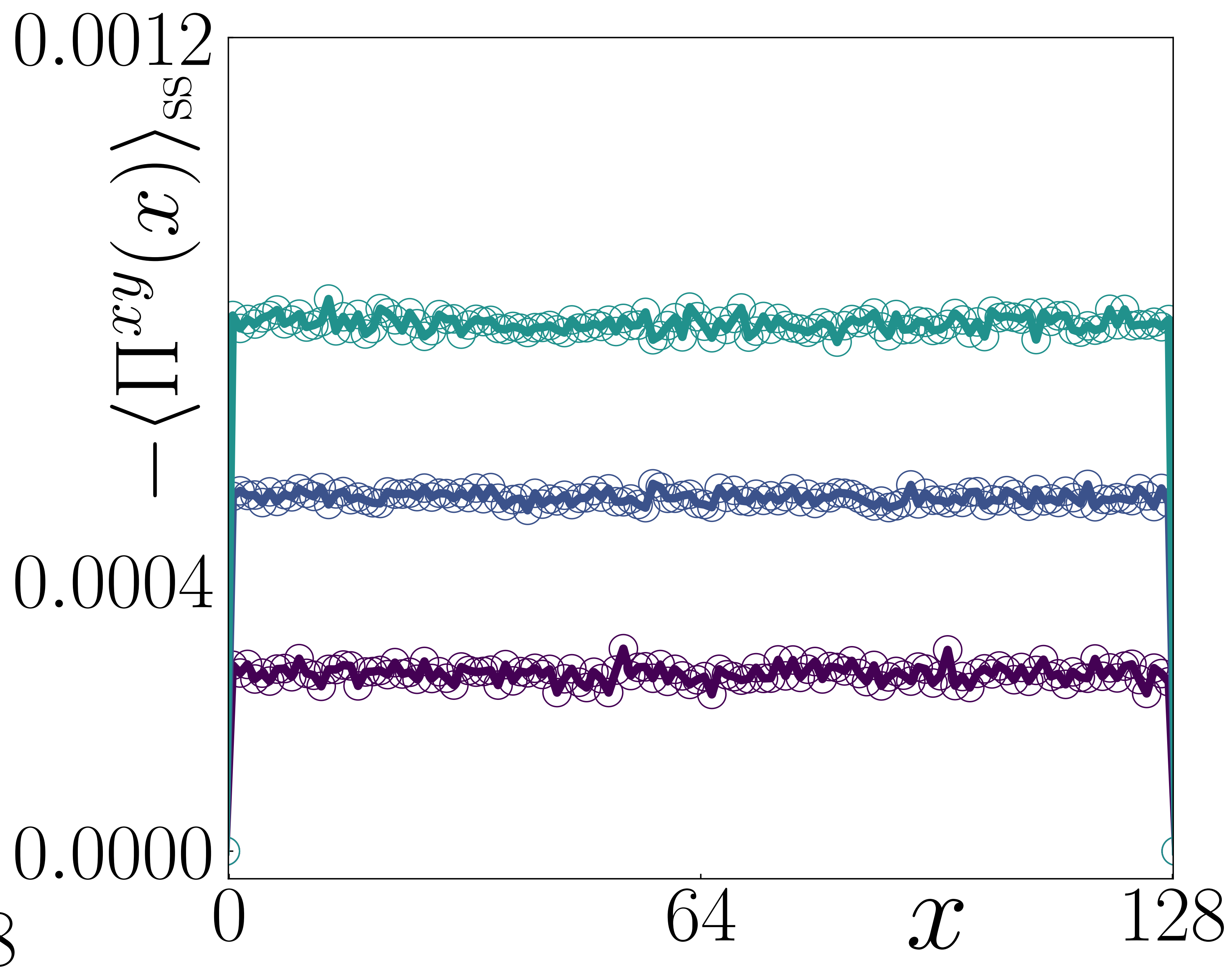
▶ We add wall velocity v_0 of three different magnitudes.



Walls



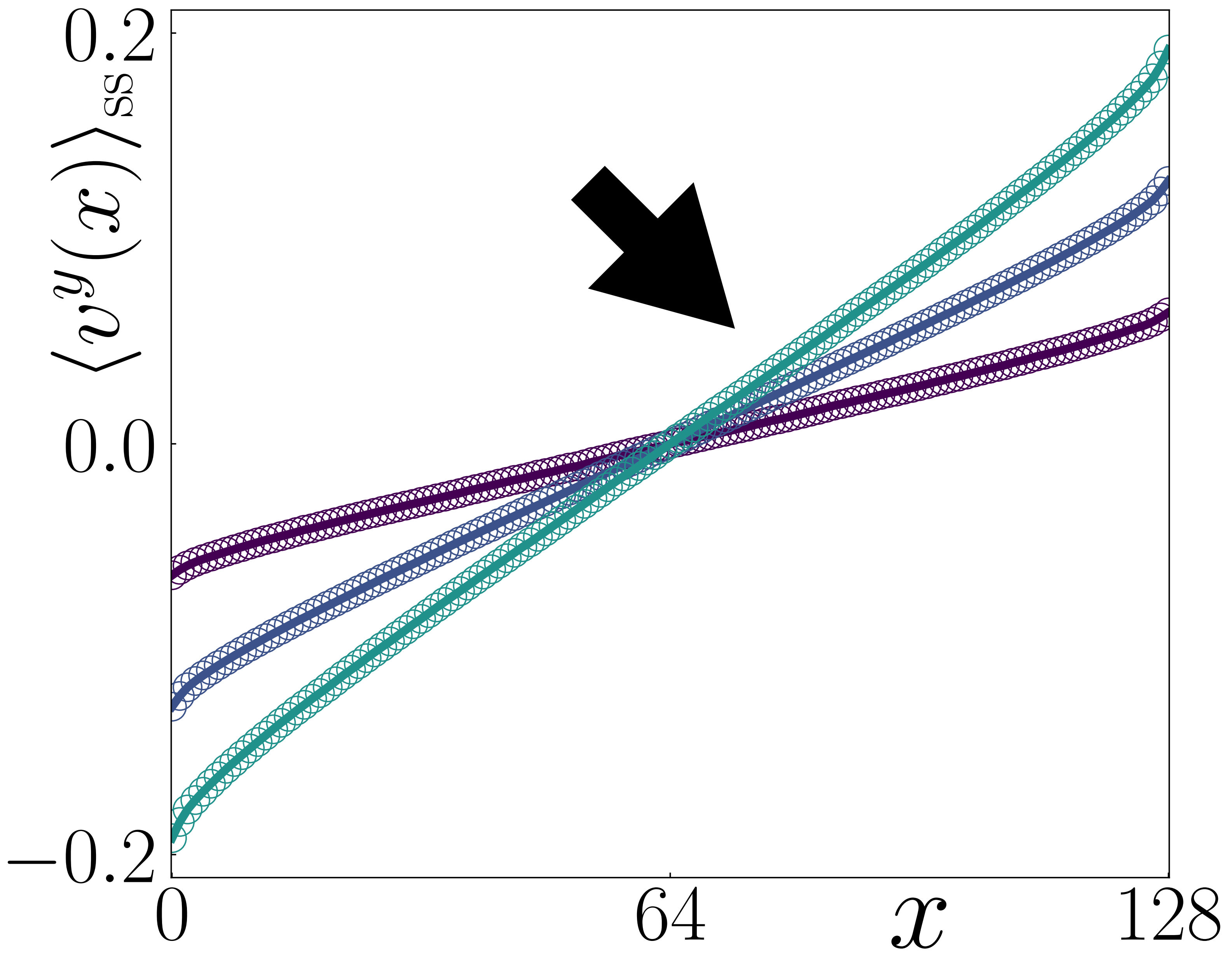
Velocity profile

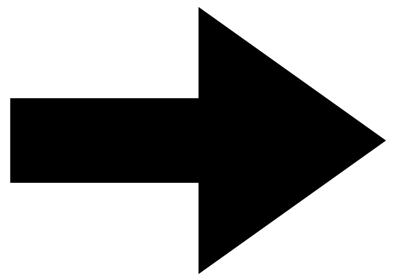


Shear stress profile

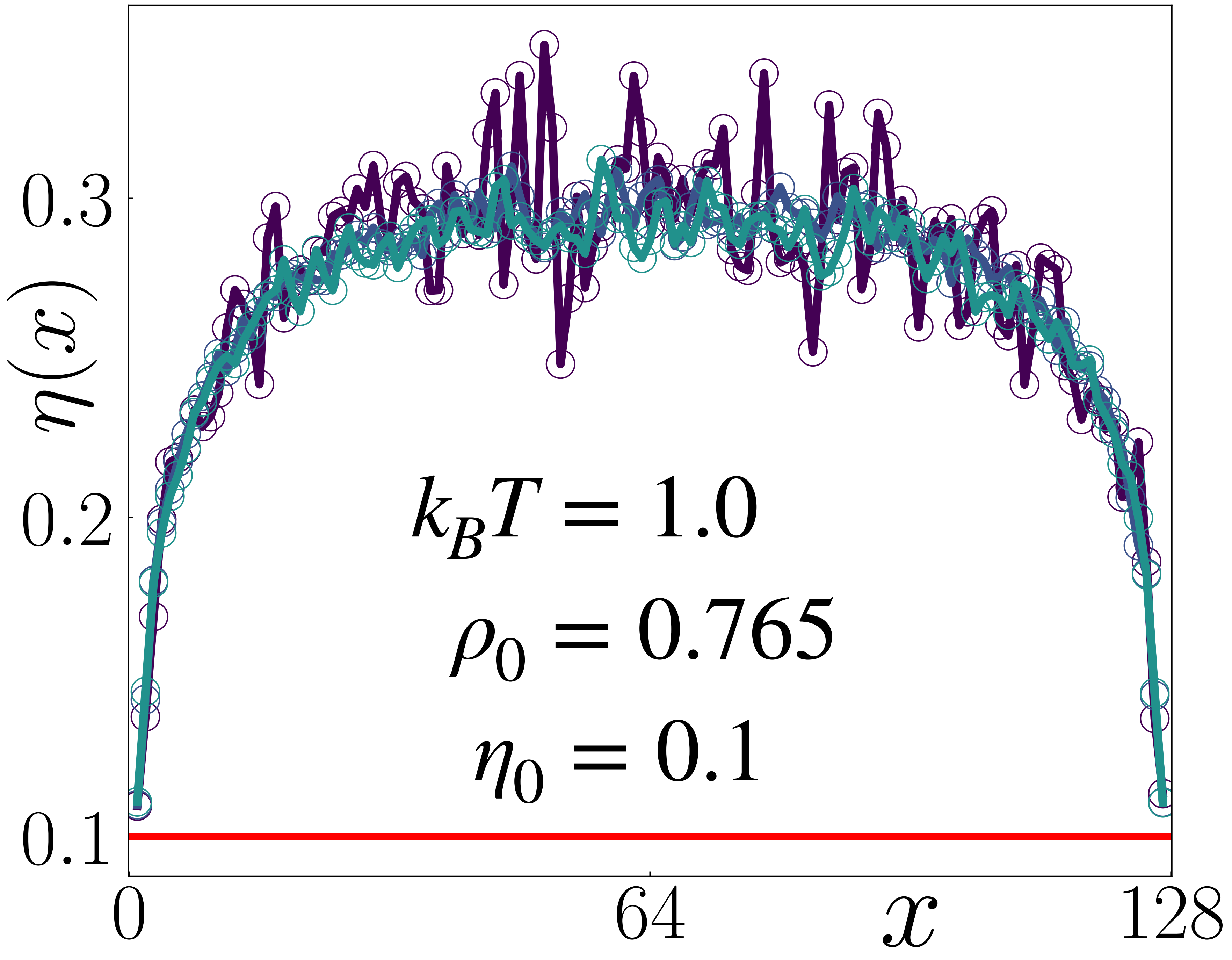
Introduction of Local Viscosity

Velocity gradient is not spatially uniform





Viscosity depends on the spatial coordinate



Local viscosity $-\langle \Pi^{xy} \rangle_{ss} = \eta(x) \dfrac{\partial \langle v^y \rangle_{ss}}{\partial x}$

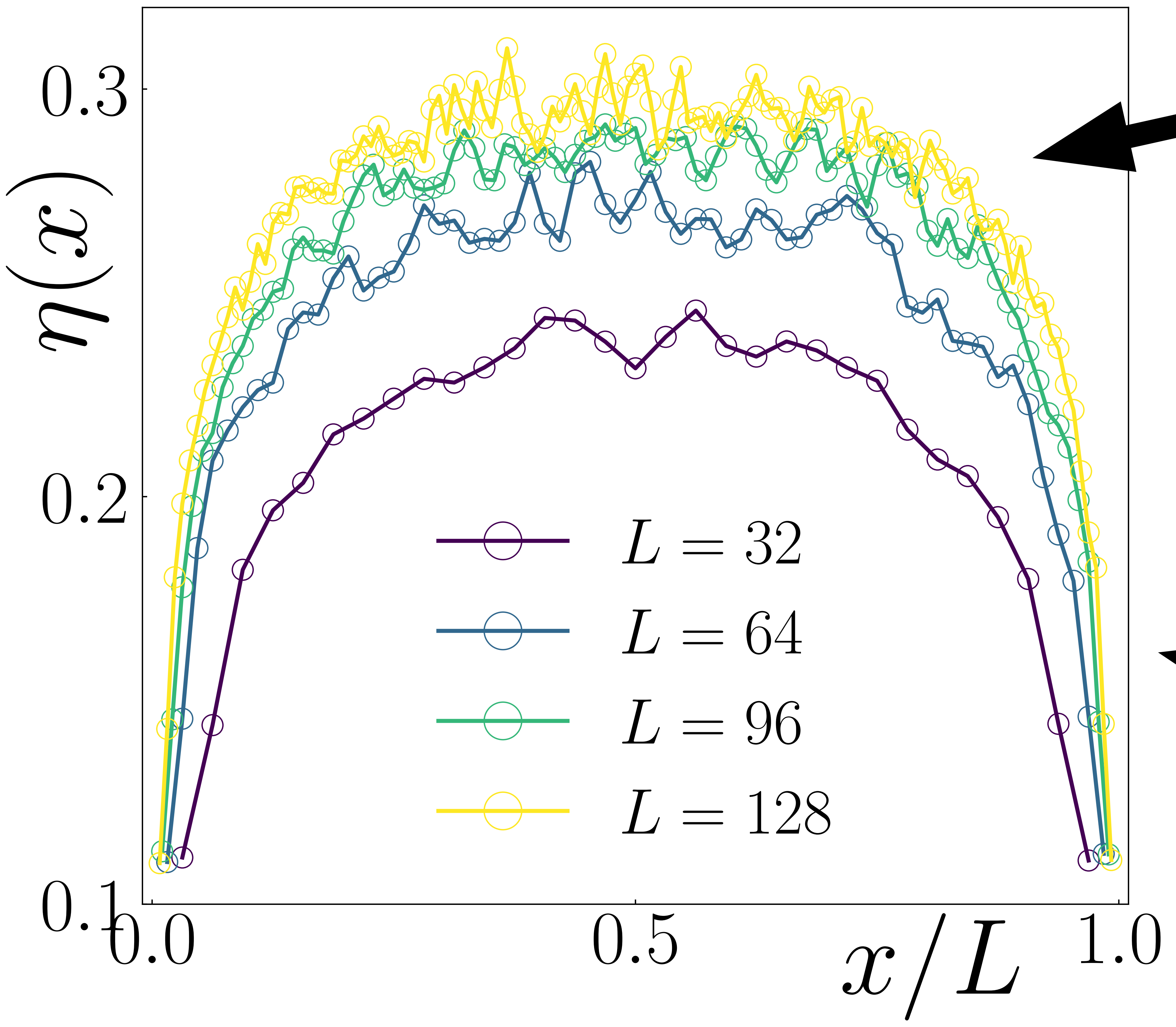
This quantity at each specific position is defined by using the local velocity gradient at that point.

The local viscosity decreases near the solid walls

The input viscosity η_0 is observed near solid walls.

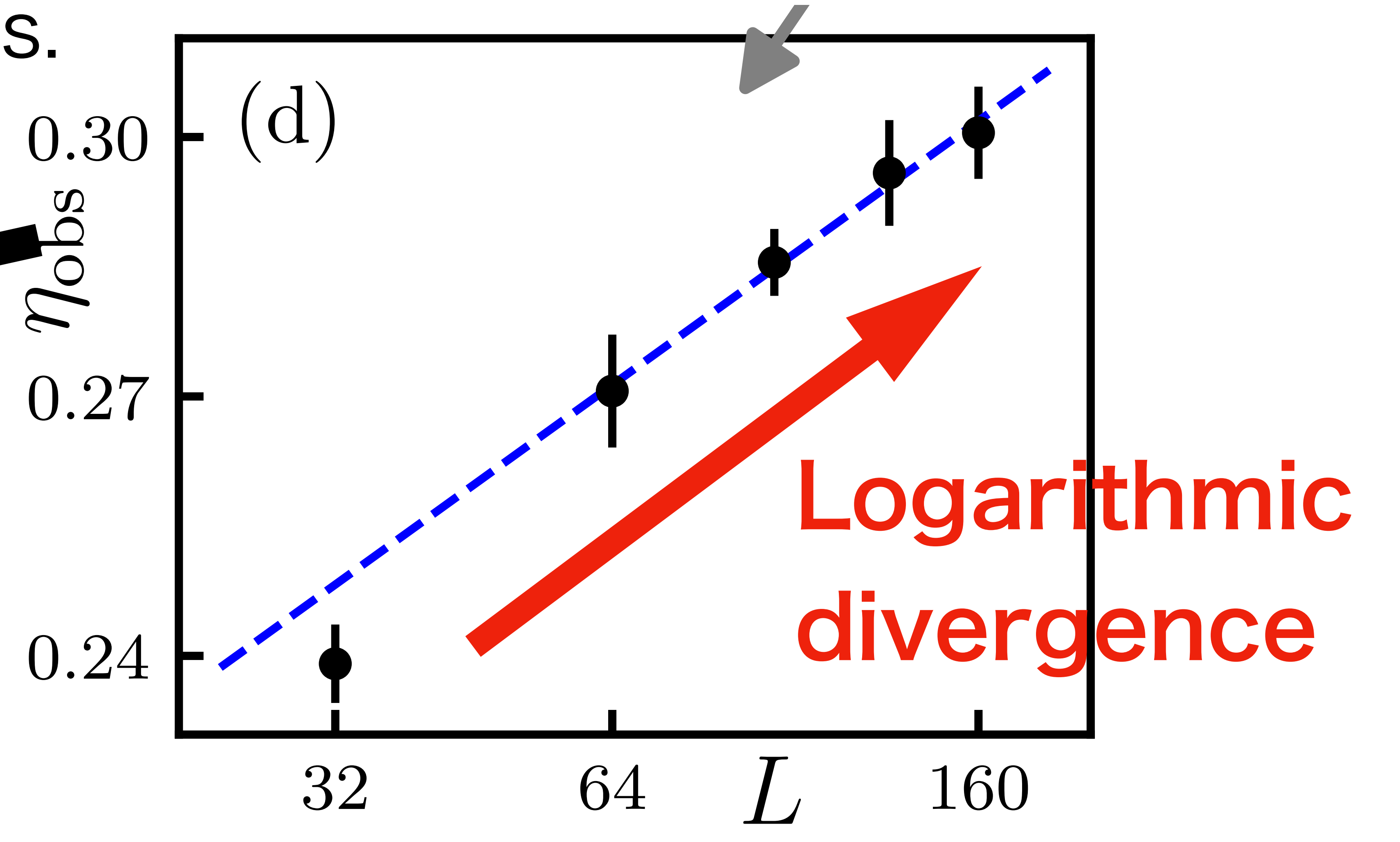
System-Size dependence of Local Viscosity

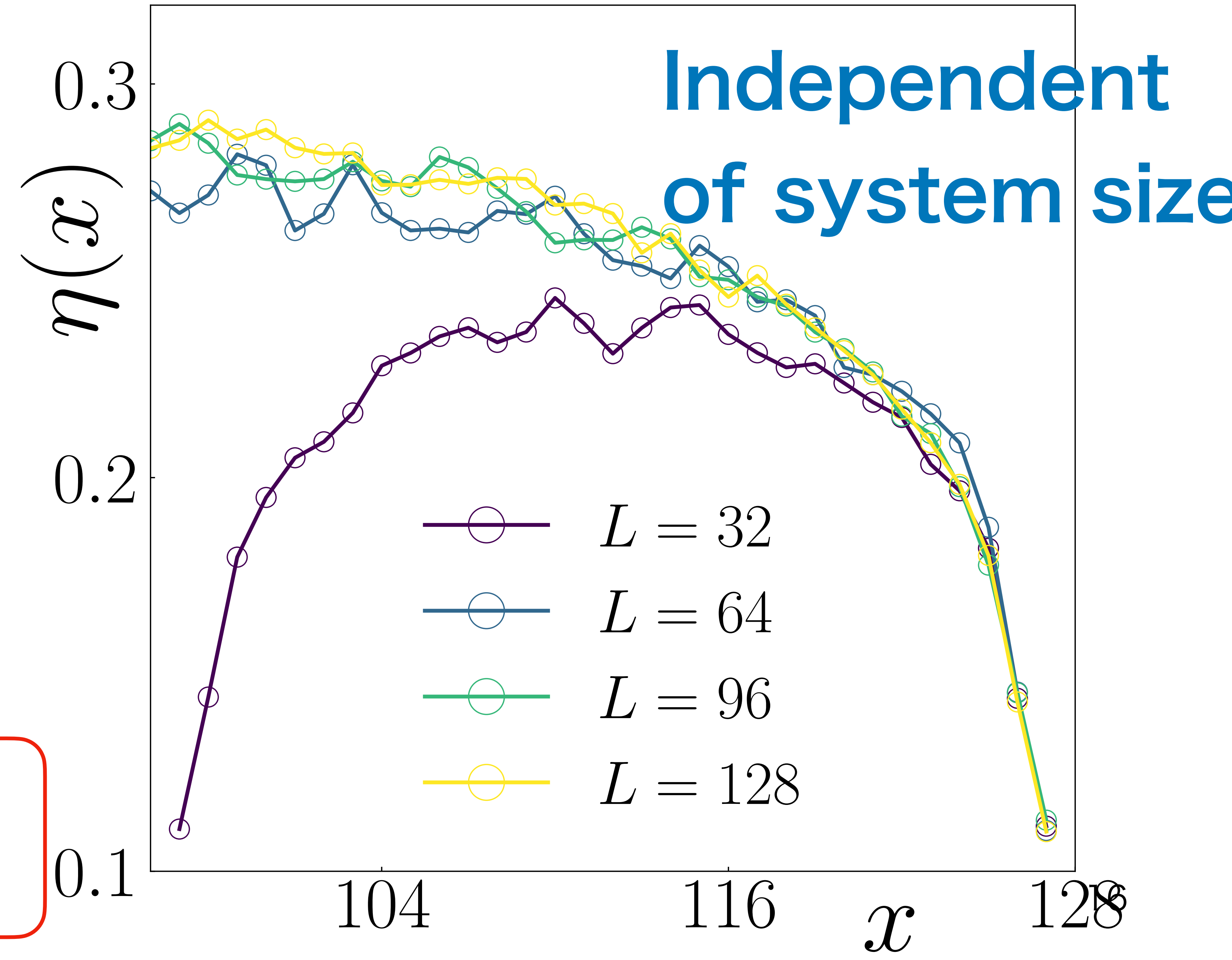
- We change the system size L while fixing to the other parameters.



far from walls

near walls





The anomalous transport does not occur near the walls.

Analytical expression of velocity and local viscosity profile

▶ We can calculate the theoretical expression for the noise-averaged Couette flow.

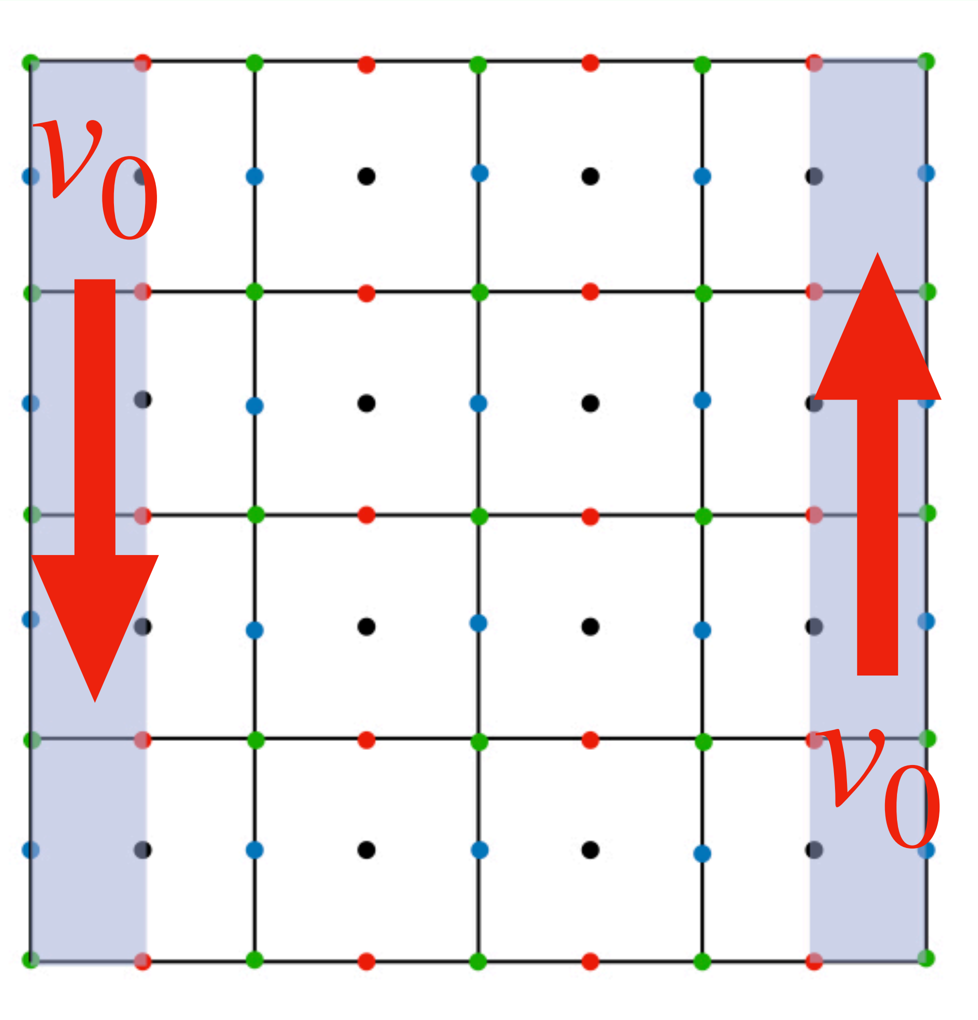
incompressible condition $\nabla \cdot \boldsymbol{v} = 0$

Fluctuating Navier-Stokes eq. $\rho\left[\frac{\partial \boldsymbol{v}}{\partial t} + \epsilon(\boldsymbol{v} \cdot \nabla)\boldsymbol{v}\right] = -\nabla p + \eta_0 \nabla^2 \boldsymbol{v} + \nabla \boldsymbol{\Pi}_R$

Boundary condition

$$v^x\Big|_{y=0} = 0 \qquad v^y\Big|_{y=0} = -v_0$$

$$v^x\Big|_{y=L} = 0 \qquad v^y\Big|_{y=L} = v_0$$



This calculation can be done using a perturbative expansion in ϵ (the nonlinear term).

$$\boldsymbol{v} = \boldsymbol{v}_{(0)} + \epsilon \boldsymbol{v}_{(1)} + \epsilon^2 \boldsymbol{v}_{(2)} + \cdots$$

Several approximations were necessary to complete the calculation (the full details are omitted here)

Analytical expression of velocity profile

$$\langle v^y(x)\rangle = \dot{\gamma}x - \epsilon^2\frac{\dot{\gamma}A}{L}\sum_{k_x}\frac{1}{k_x}\frac{\sin(2k_x x)}{2k_x} \qquad k_x := \frac{\pi}{L}n$$

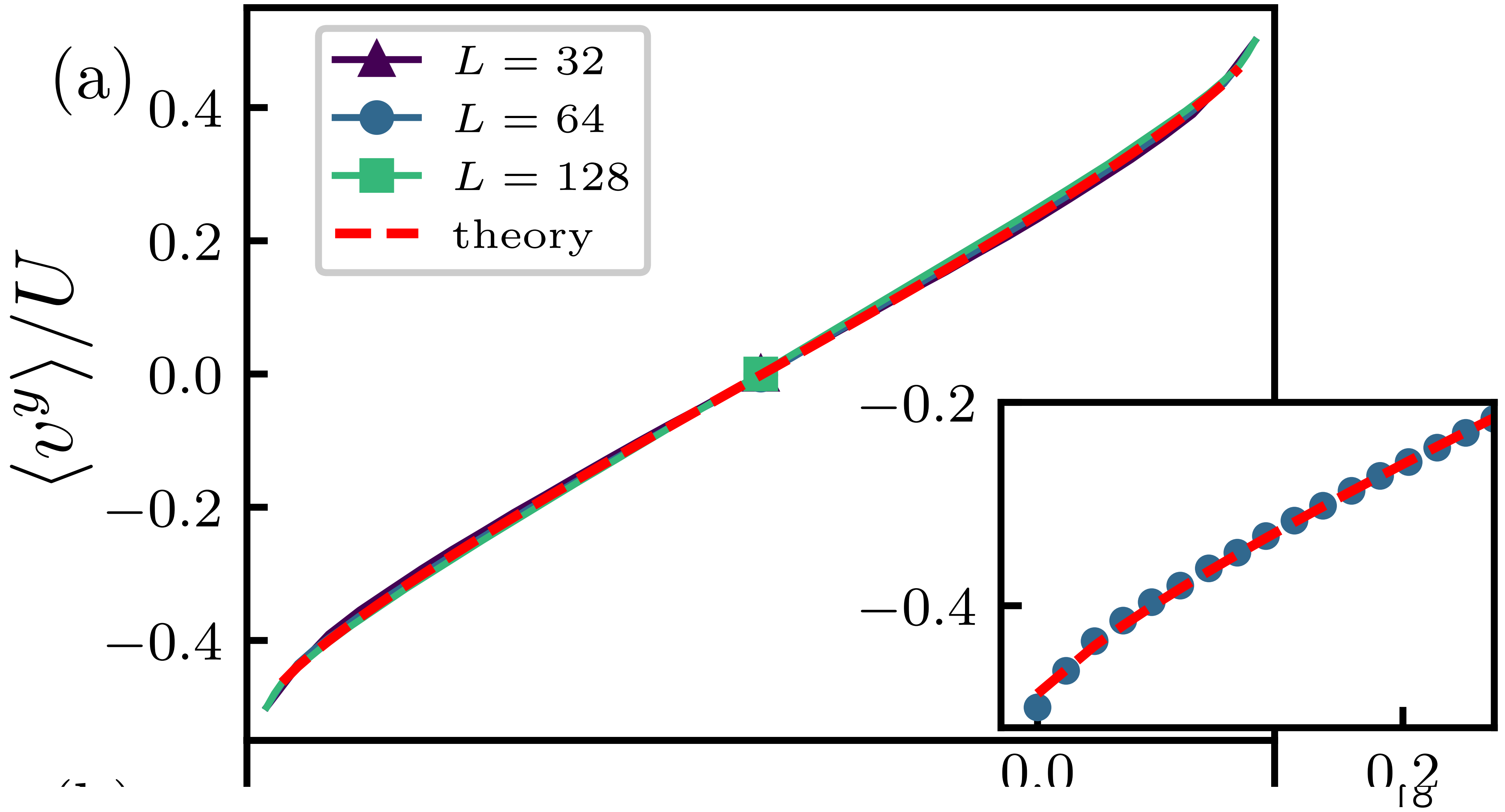
$\dot{\gamma} := 2v_0/L$

A : numerical factor depending on density, temperature⋯.

$$A = \frac{\rho_0 k_B T}{4\eta_0^2}$$ (within our approximation)

For comparison, we treat A as a fitting parameter because this calculated value can deviate from the true value due to the approximations made in the derivation.

Our derived equation accurately captures the functional form of the velocity profile.



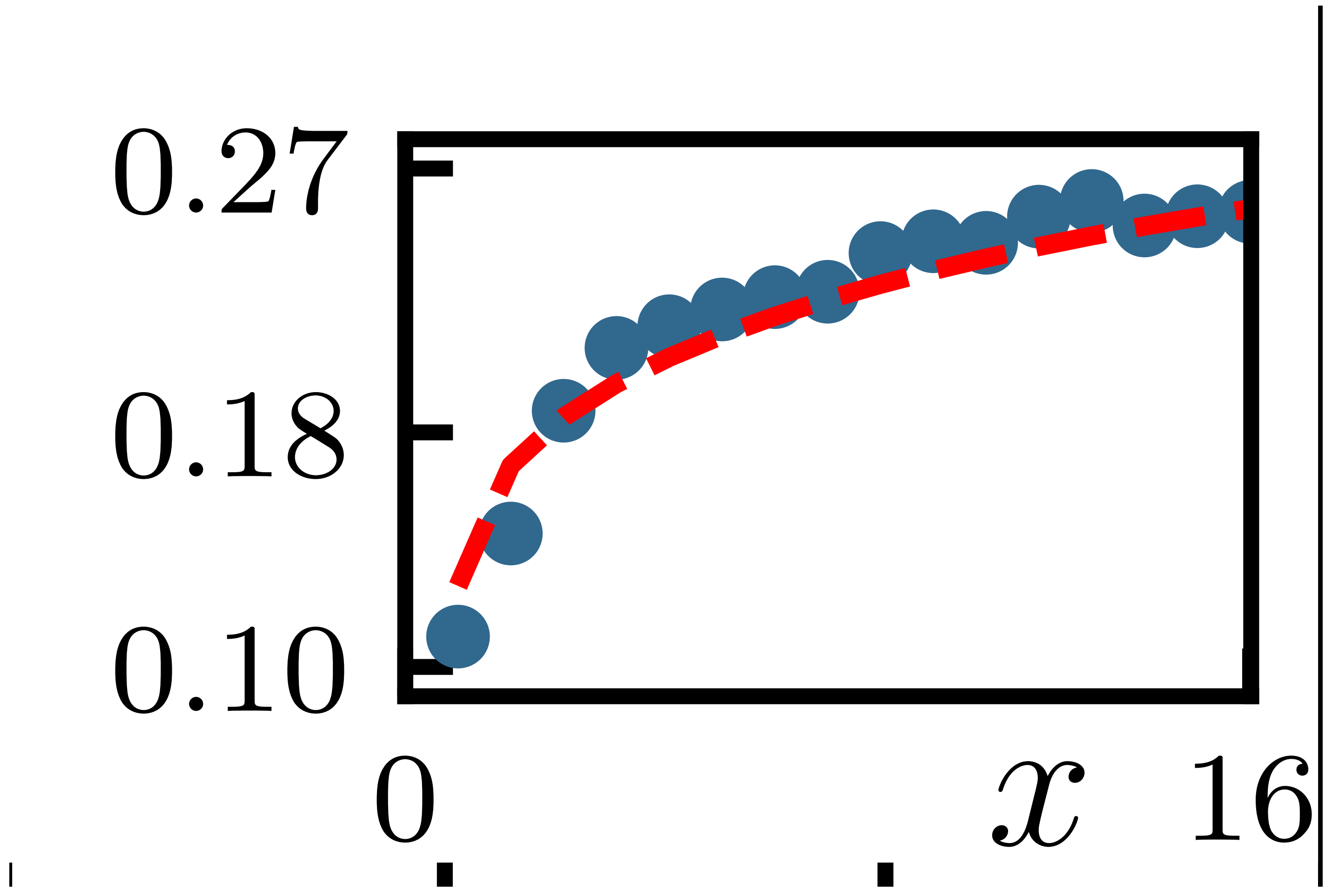
Analytical expression of local viscosity profile

$$\eta(x) = \eta_0\left(1 + \epsilon^2 \frac{2A}{L}\sum_{k_x}\frac{1}{k_x}\sin^2(k_x x)\right) \qquad k_x := \frac{\pi}{L}n$$

$\dot{\gamma} := 2v_0/L$

A : numerical factor depending on density, temperature⋯.

$$A = \frac{\rho_0 k_B T}{4\eta_0^2} \qquad \text{(within our approximation)}$$

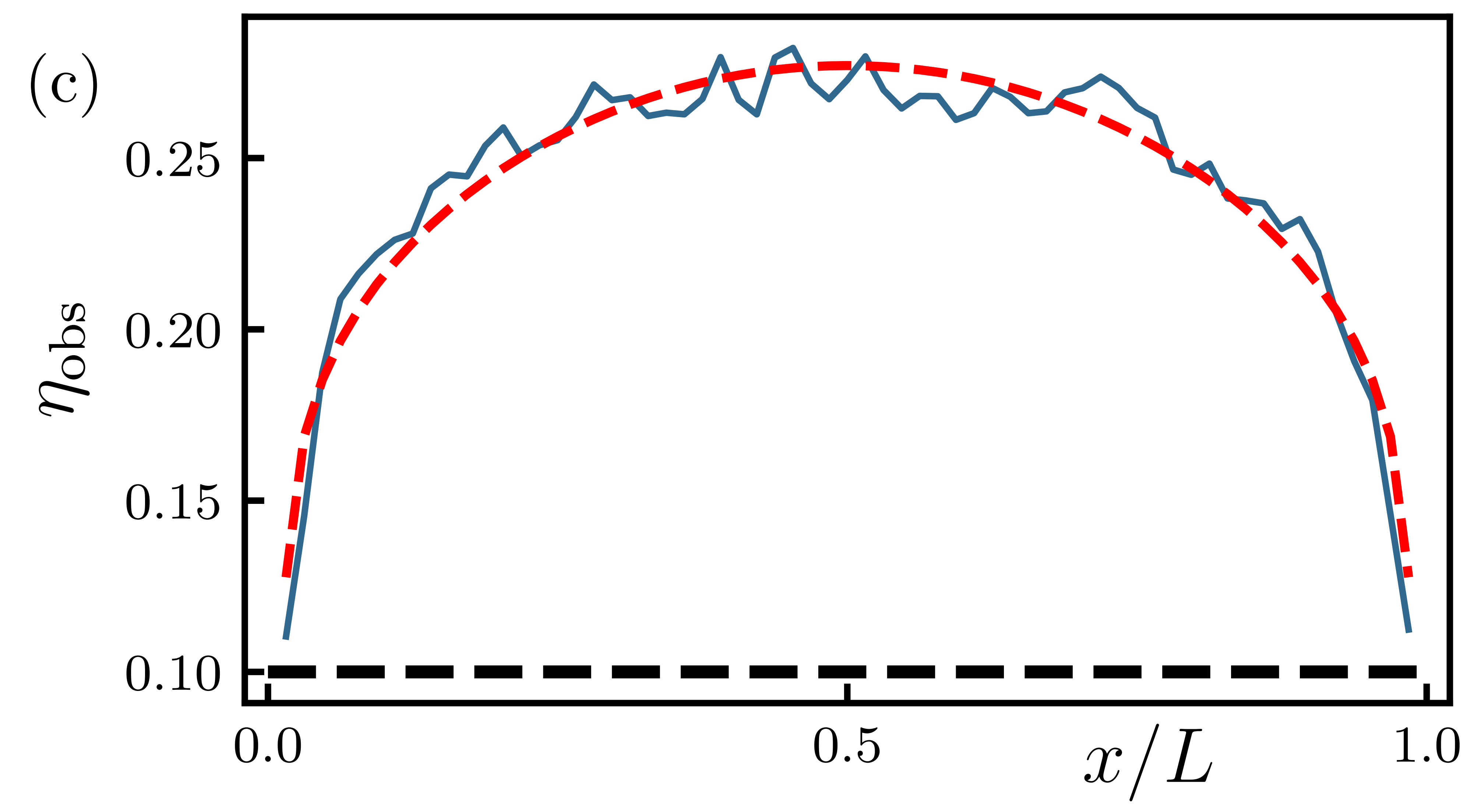


For comparison, we treat A and η_0 as a fitting parameter

$$\eta_0^{\mathrm{sim}} = 0.100 \quad \Rightarrow \quad \eta_0^{\mathrm{fit}} \simeq 0.116$$

This value is very close to the simulation value η_0

demonstrating good accuracy of this expression.



Key insight from the theoretical expression

$$\eta(x) = \eta_0\left(1 + \epsilon^2 \frac{2A}{L} \sum_{k_x} \frac{1}{k_x} \sin^2(k_x x)\right) \qquad k_x := \frac{\pi}{L} n$$

$\dot{\gamma} := 2v_0/L$

A : numerical factor depending on density, temperature⋯.

$$A = \frac{\rho_0 k_B T}{4\eta_0^2}$$ (within our approximation)

▶ This expression provides a key insight into the fluid's behavior

$$\eta(x = 0) = \eta_0$$

near the solid walls

$$\eta(x = L/2) \propto \eta_0 + C \log L$$

in the bulk region

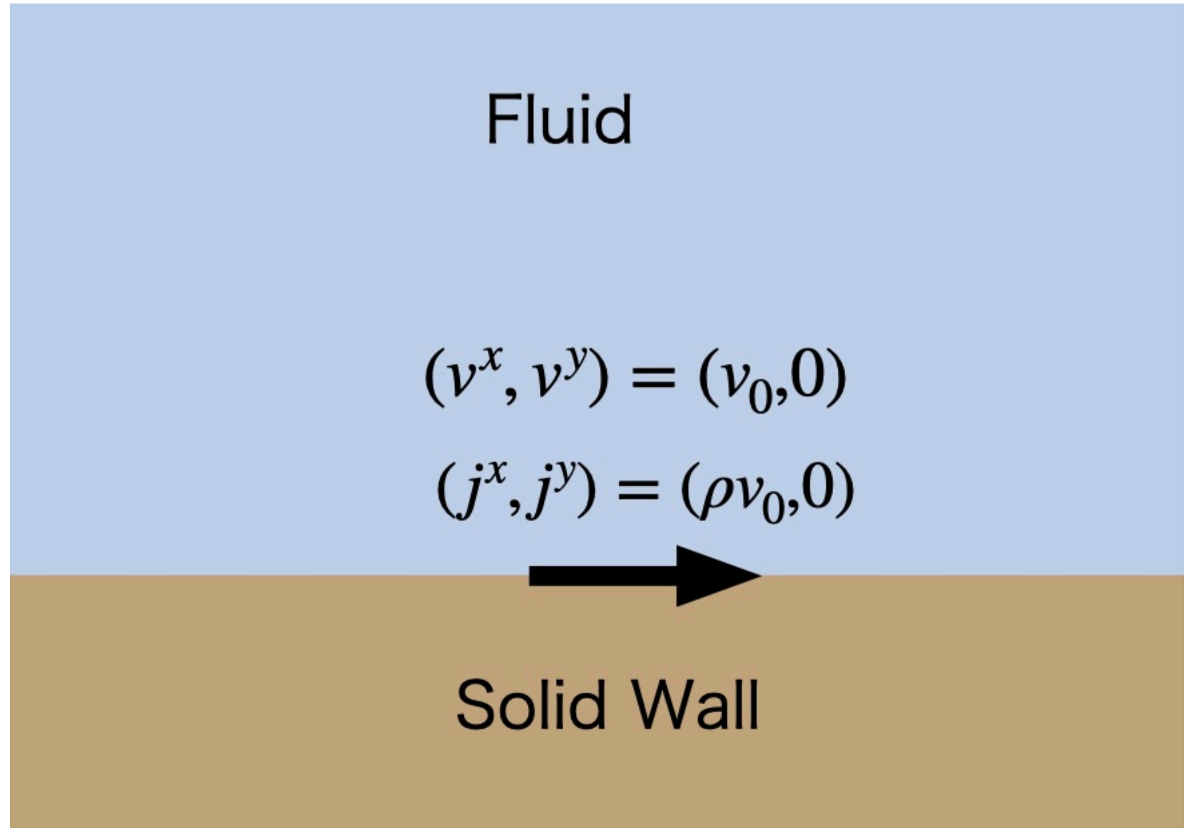
Our local viscosity expression is fundamental for describing the complete flow field.

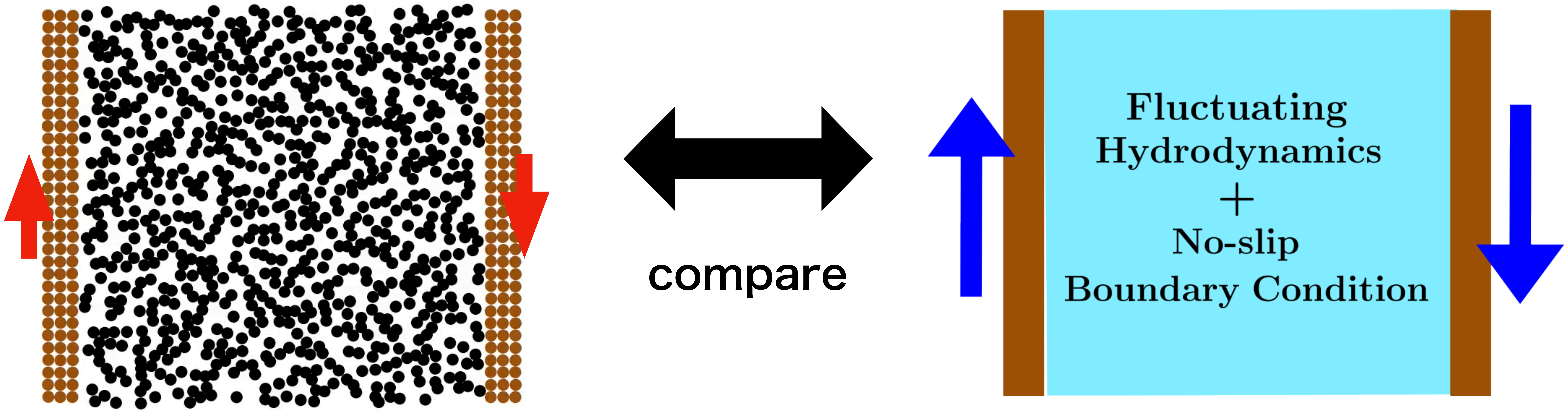
Part 2.
Observation of microscopic particle system based on the MD simulation

Strategy of MD simulation

Can we validate this boundary condition?

The fluid does not fluctuate
at all at the solid walls.

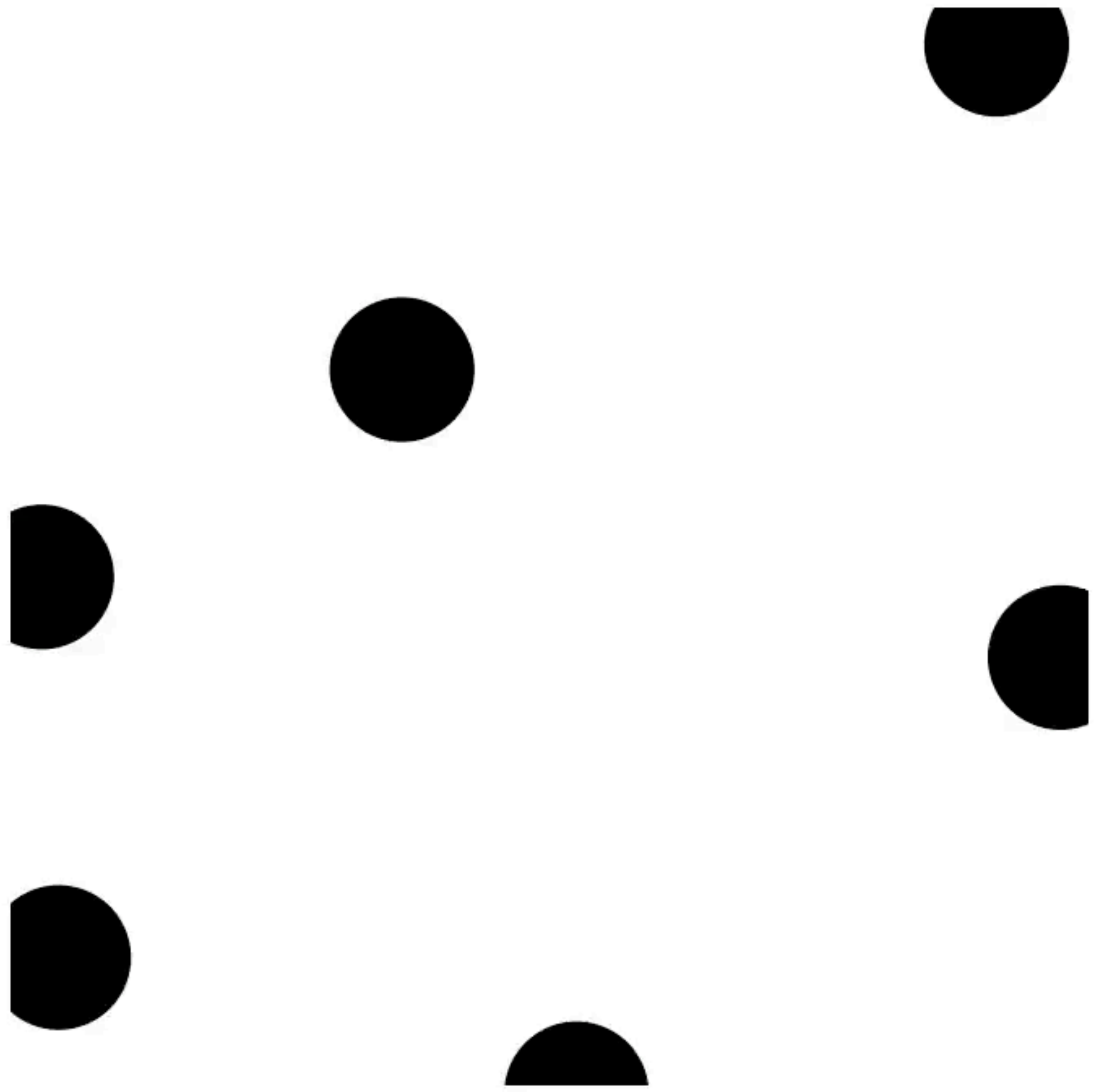




We check whether the MD simulation results can be described by fluctuating hydrodynamics incorporating the no-slip boundary condition **second main result: YES!!**

Setup of MD simulation

▶ We perform molecular dynamics (MD) simulations.



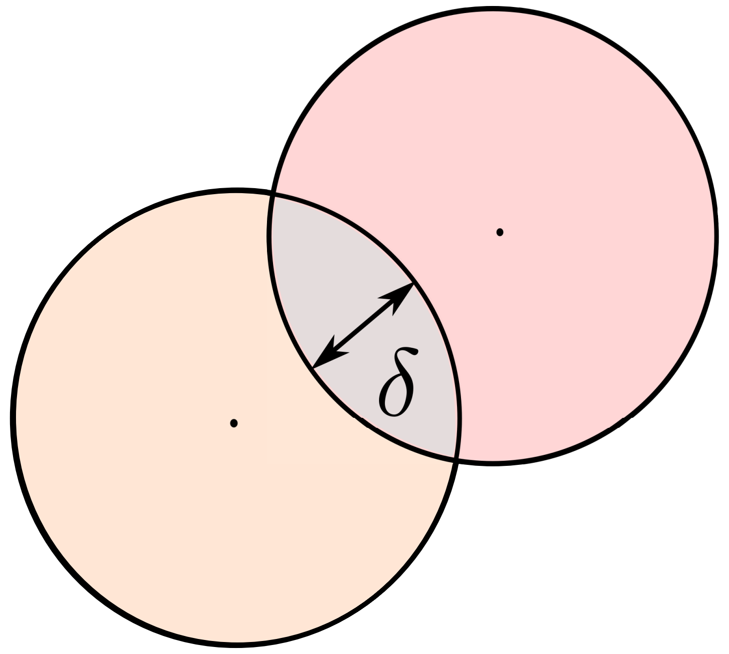
In MD simulations, atoms are represented as particles that follow the classical Hamiltonian dynamics.

$$\frac{d\boldsymbol{r}_i}{dt} = \frac{\boldsymbol{p}_i}{m} \qquad \frac{d\boldsymbol{p}_i}{dt} = -\frac{\partial V}{\partial \boldsymbol{r}_i}$$

▷ simple repulsive potential

$$V(r) = 10\delta^{\alpha} \quad \text{for } \delta > 0$$

$$V(r) = 0 \quad \text{for } \delta < 0$$



(particles only repel each other when they overlap)

Units for the MD simulation

atomic diameter σ

atomic mass m

thermal velocity $v_{th} := \sqrt{k_B T/m}$

(or microscopic time $\tau = \sigma / v_{th}$)

Implementation of solid wall

- Solid walls are implemented as a collection of particles.

1. Solid particles are trapped using an on-site potential.

$$V_{\mathrm{onsite}}(\boldsymbol{q}) = V_0\left[\sin(2\pi q_x) + \sin(2\pi q_y)\right] \qquad V_0 = 50$$

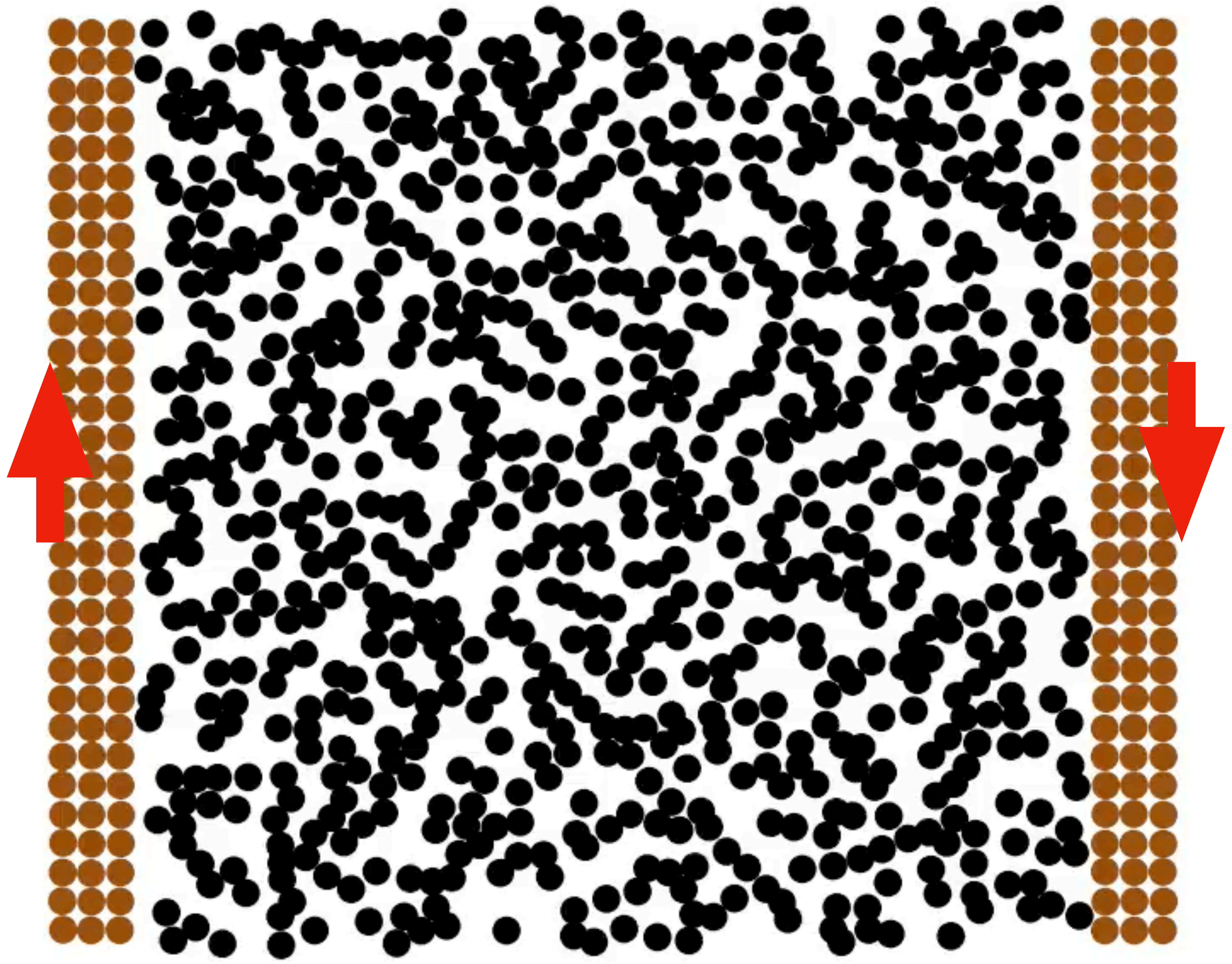
2. Solid particles are thermalized using the Langevin thermostat.

$$\frac{d\boldsymbol{q}_j}{dt} = \frac{\boldsymbol{p}^w}{m}$$

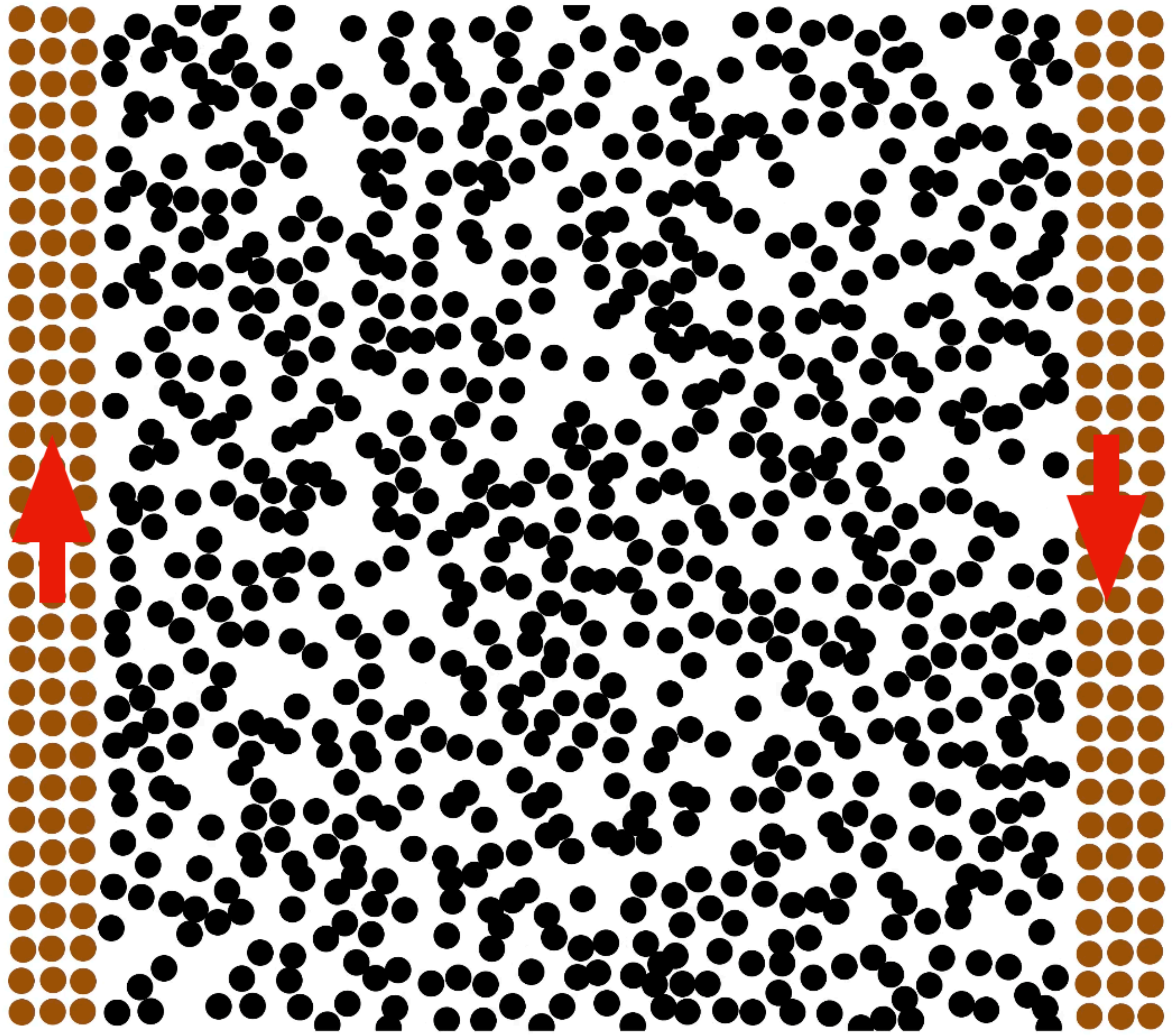
$$\frac{d\boldsymbol{p}_j^w}{dt} = -\frac{\partial V_{\mathrm{onsite}}(\boldsymbol{q}_j - v_0 t \boldsymbol{e}_x)}{\partial \boldsymbol{q}_j} - \sum_{i=1}^{N} \frac{\partial V_{\mathrm{wf}}(|\boldsymbol{r}_i - \boldsymbol{q}_j|)}{\partial \boldsymbol{q}_j} - \gamma \boldsymbol{p}_j^w + \xi_j(t)$$

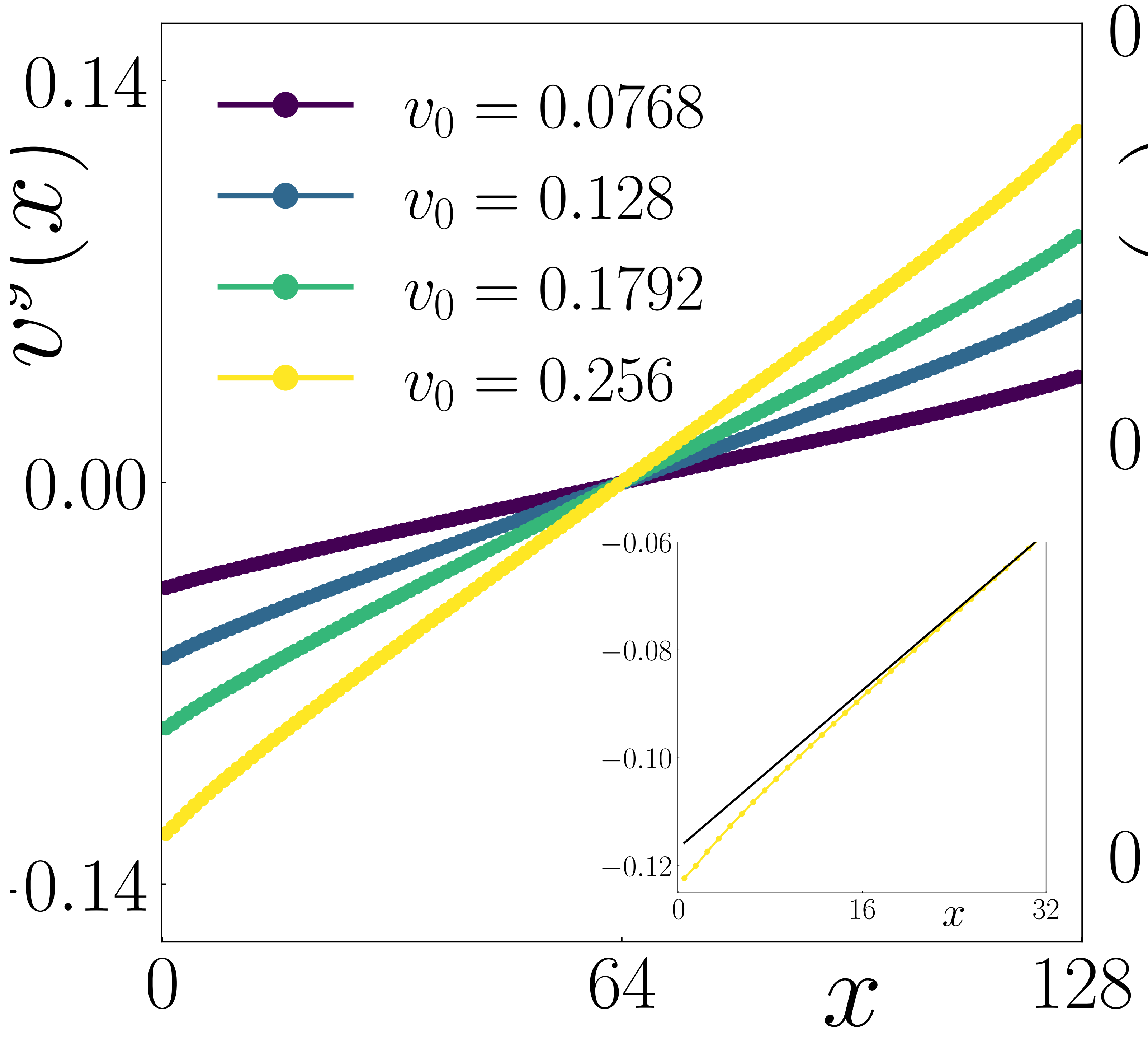
3. Fluid particles interact with solid particles.

4. The motion of the walls is simulated by moving the solid particles (and on-site potential) collectively at a velocity v_0.

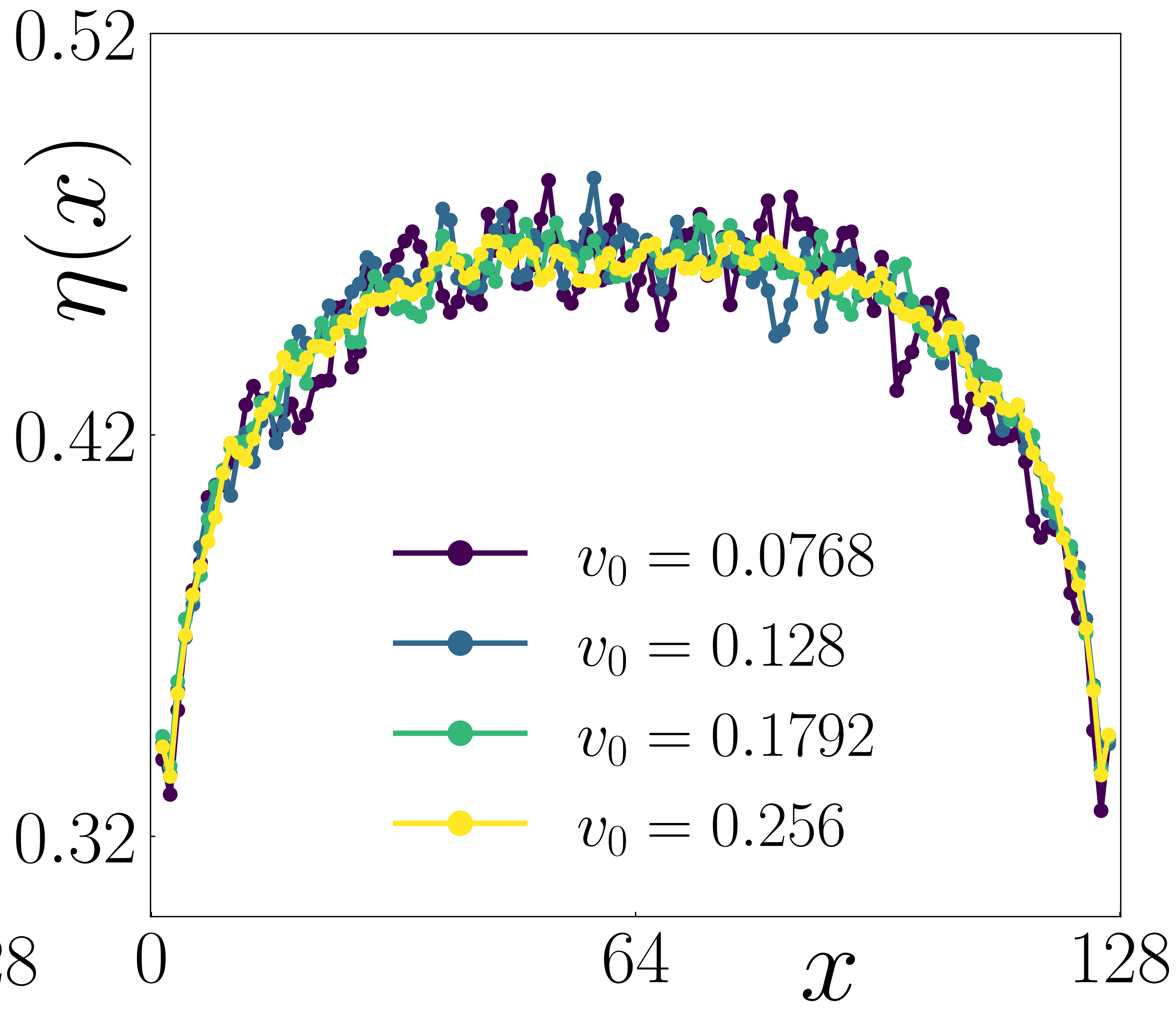


MD simulation results





Color: different wall velocities



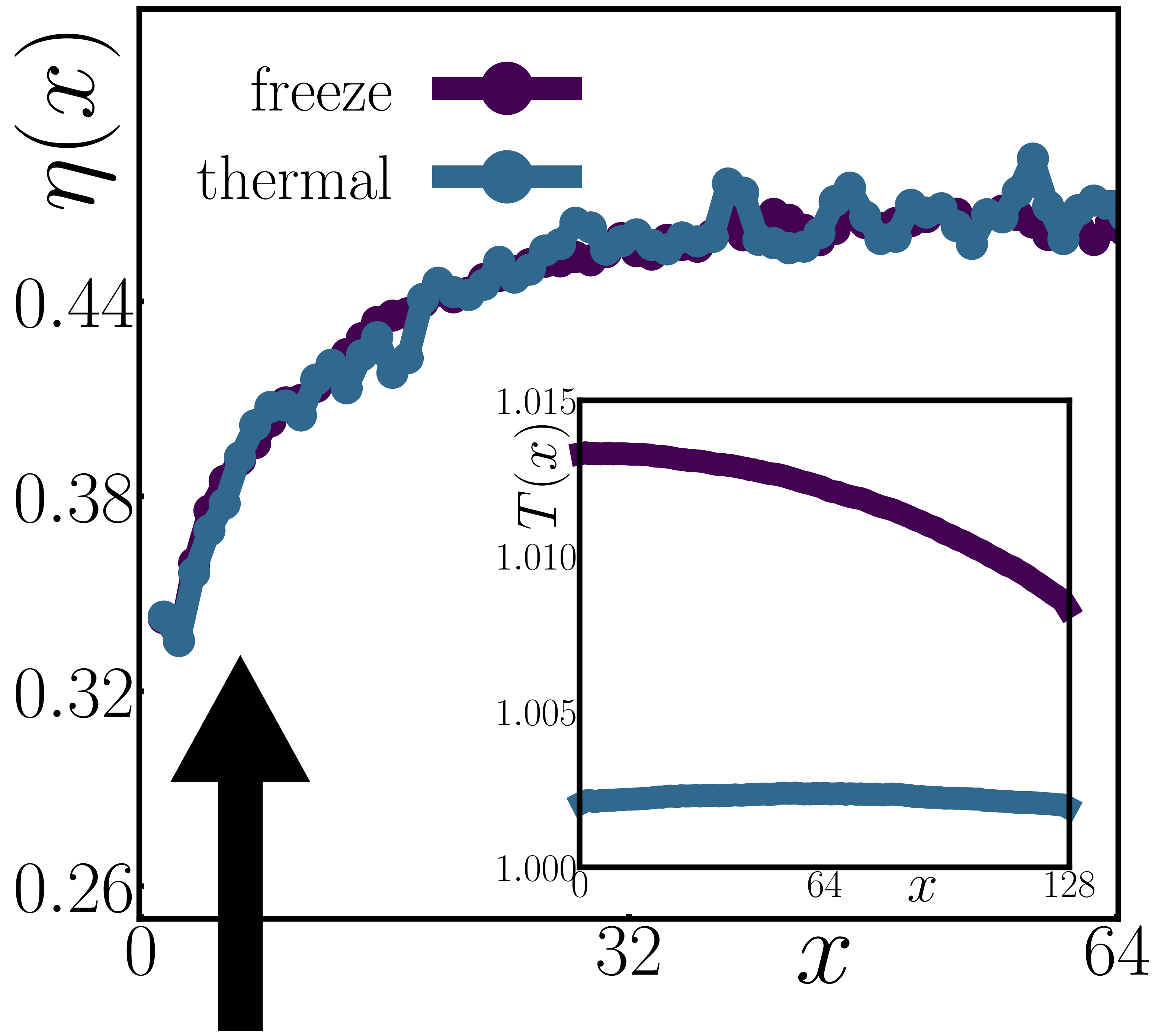
$$-\langle \Pi^{xy}(x) \rangle_{\mathrm{ss}}^{\dot{\gamma}} = \eta(x) \frac{\partial v^y}{\partial x}$$

▶ The local viscosity is observed in the same way as in the fluctuating hydrodynamics.

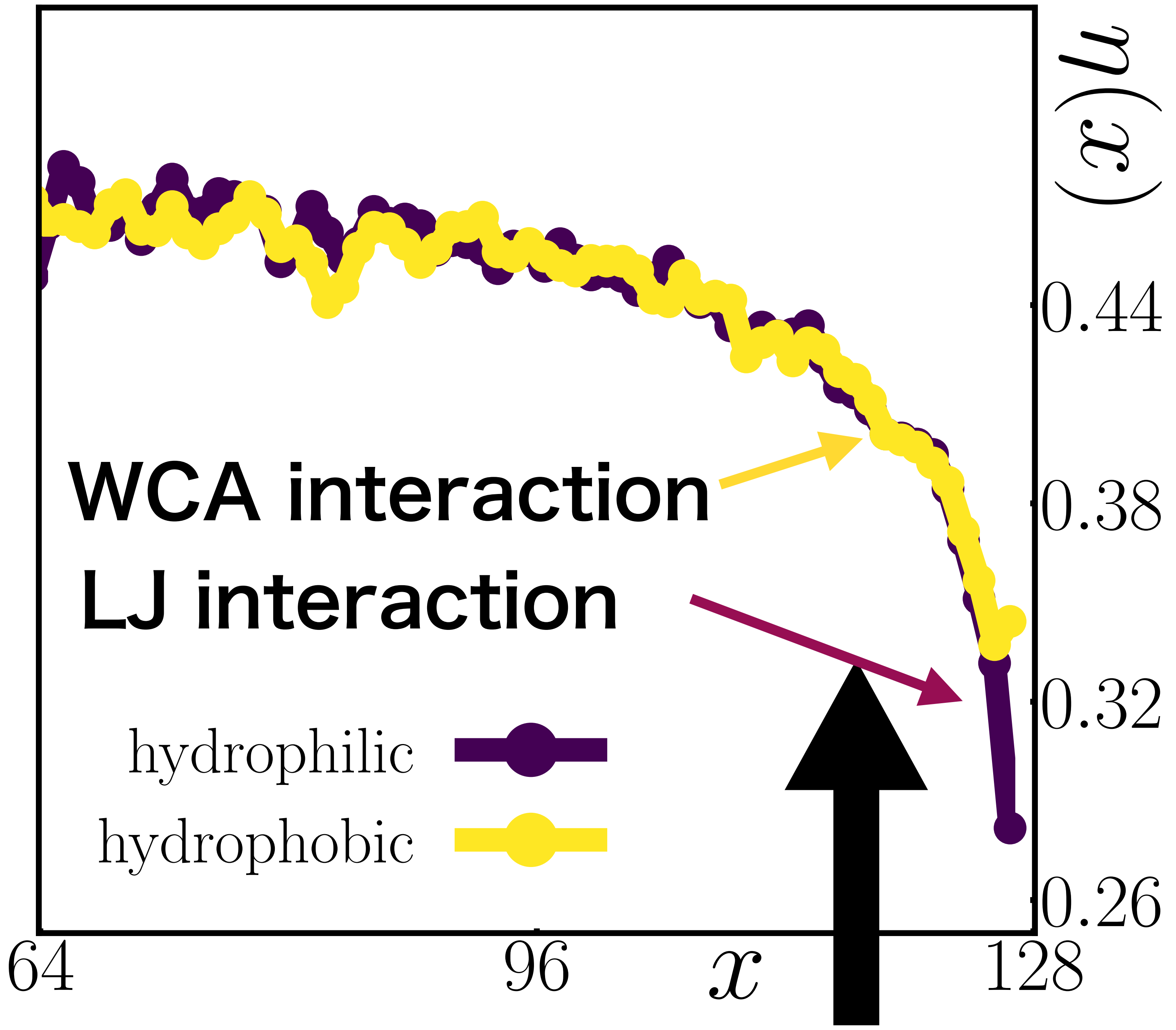
The observed viscosity decreases near solid walls, which is consistent with the behavior in fluctuating hydrodynamics.

Changing microscopic properties of the walls

the effect of wall temperature



the effect of solid-fluid interaction



Freeze: Set the wall temperature to 0.
Thermal: Set the wall temperature to a finite value.

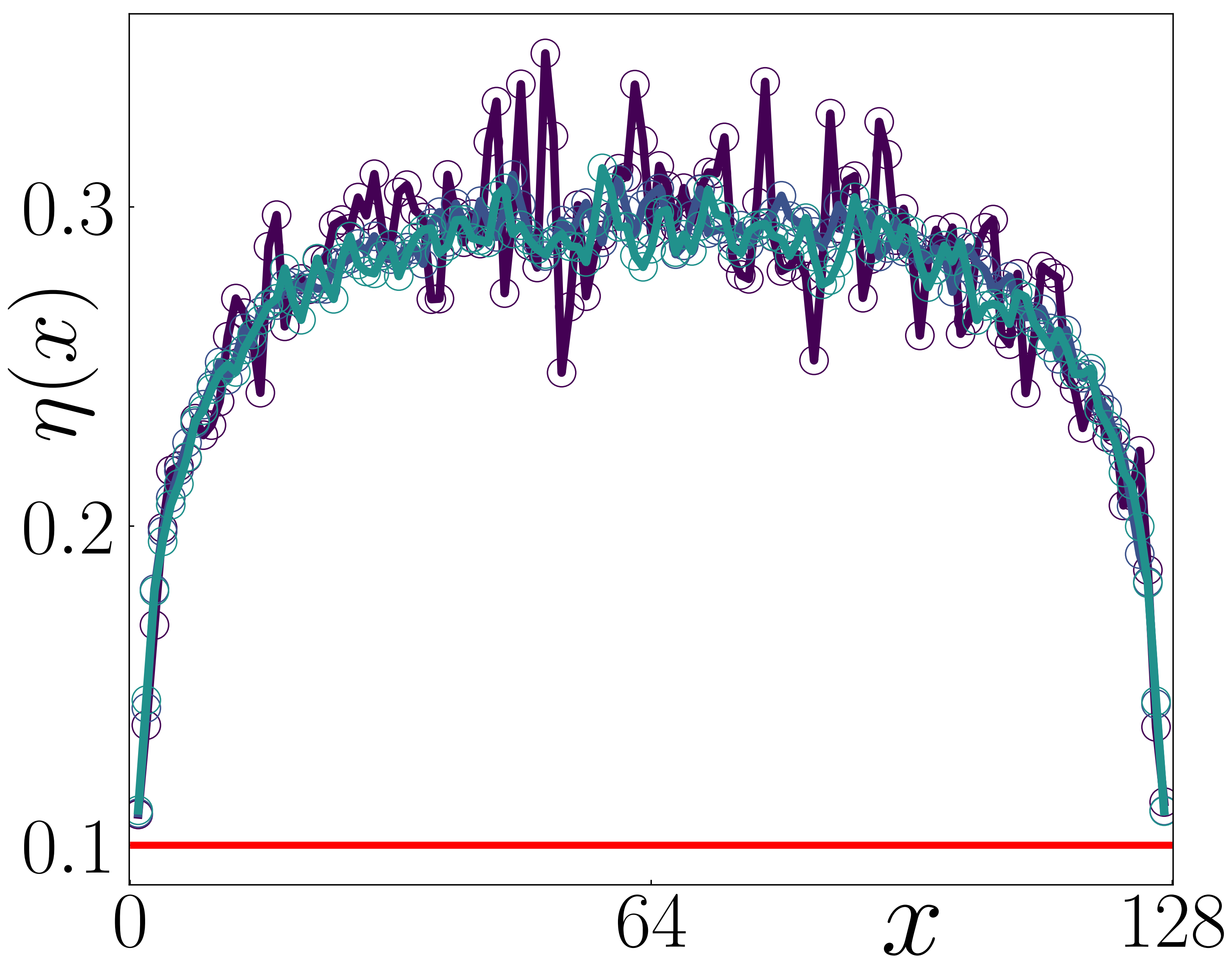
hydrophilic: Use attractive solid-fluid interactions (LJ).
hydrophobic: Use only repulsive solid-fluid interactions (WCA

■ The microscopic properties of walls do not affect the results at the quantitative level.

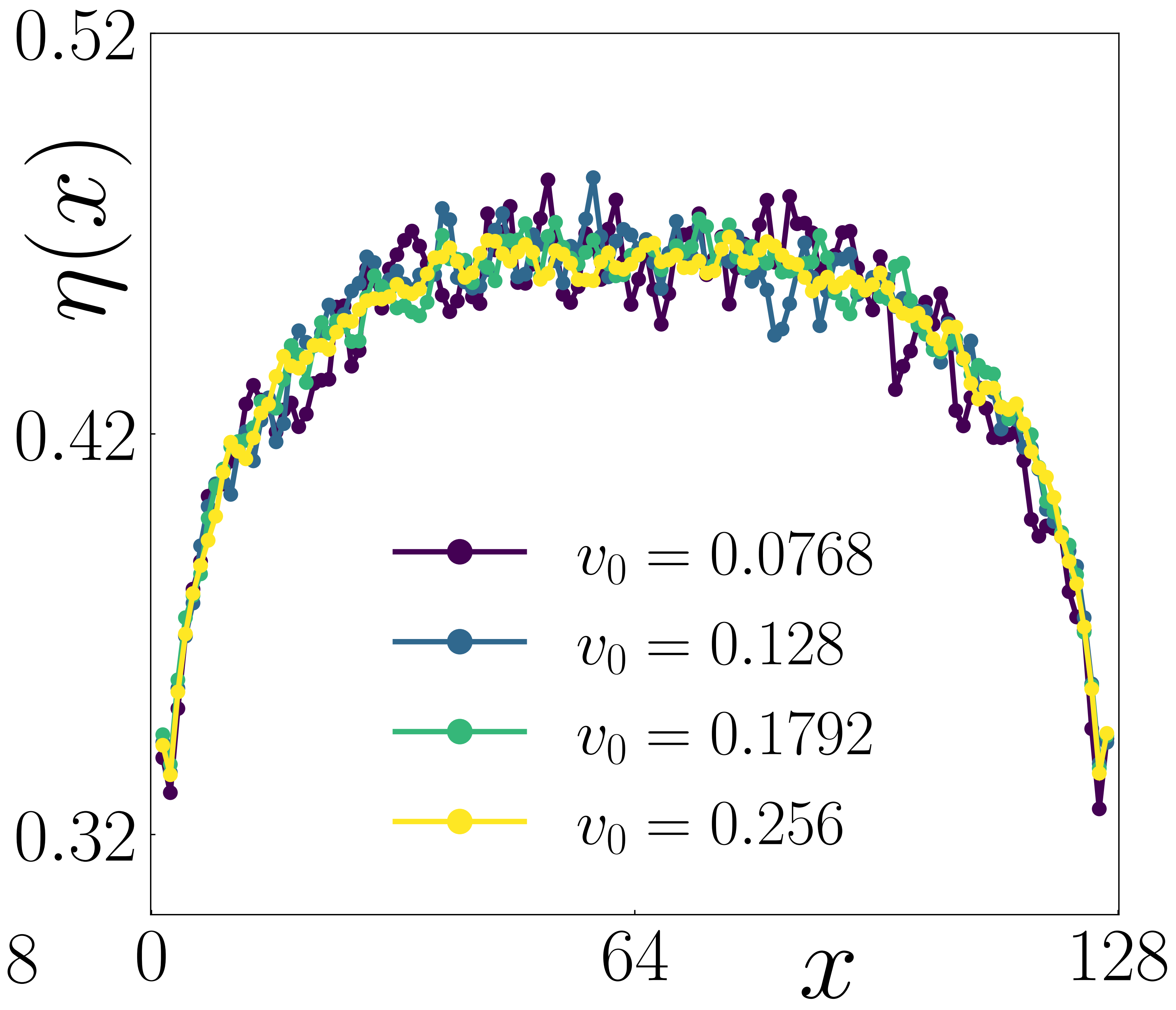
This suggests the robustness of the results of the fluctuating hydrodynamics simulations.

Direct comparison between MD and FH simulation

Fluctuating hydrodynamics



MD(atomic system)



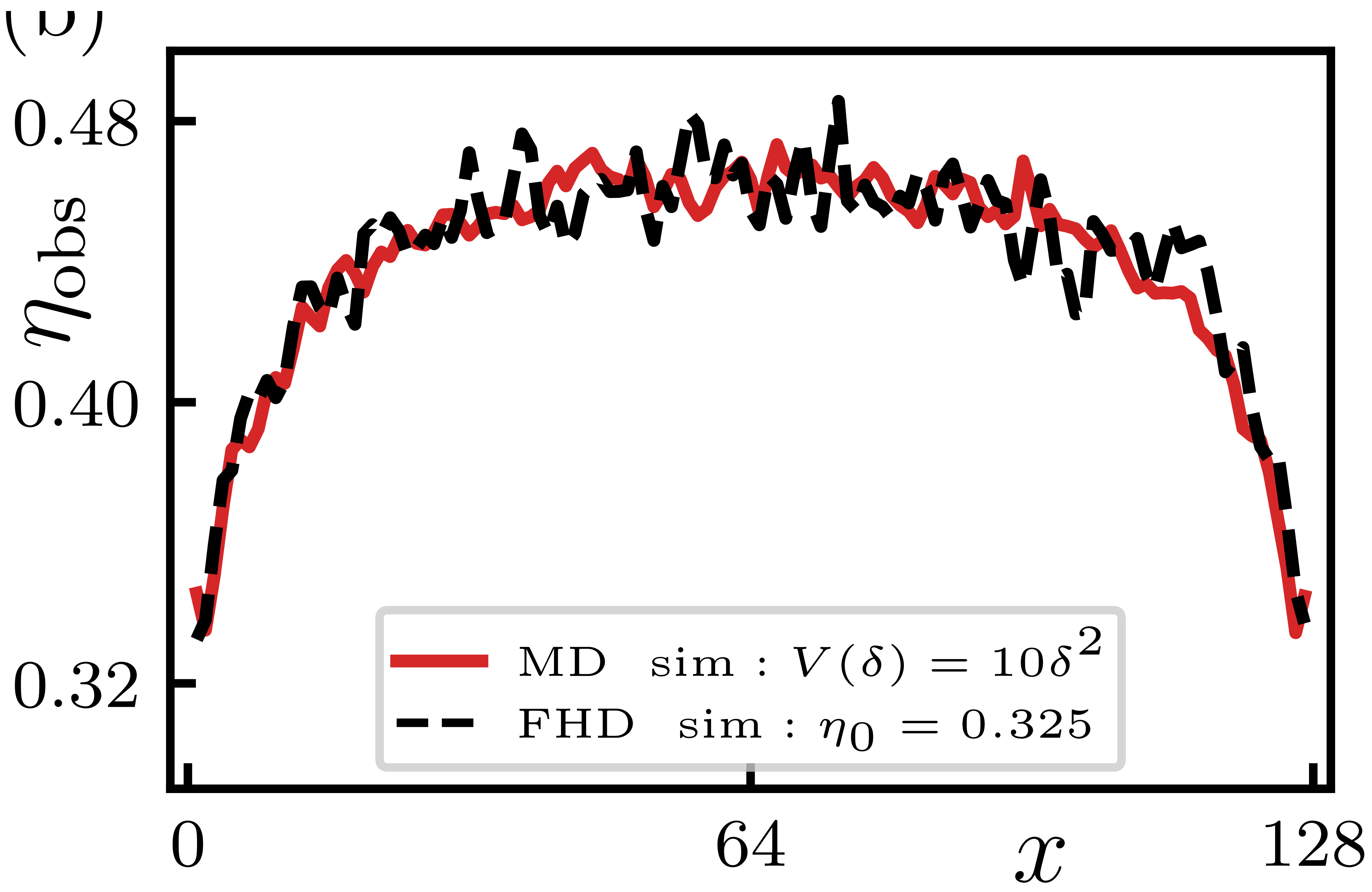
comparison

Set the same system size, density, and temperature to match the units of both models.

Use viscosity parameter η_0 as fitting parameters.

$$\rho\left[\frac{\partial \boldsymbol{v}}{\partial t} + (\boldsymbol{v} \cdot \nabla)\boldsymbol{v}\right] = -\nabla p + \eta_0 \nabla^2 \boldsymbol{v} + \nabla \boldsymbol{\Pi}_R$$

Direct comparison between MD and FH simulation



The fluctuating hydrodynamics with $\eta_0 = 0.325$ reproduces the local viscosity $\eta(x)$ of the MD simulation with high accuracy.

This strongly suggests that even in the atomic systems, η_0 governs the fluid motion near the walls.

The agreement between the two models is observed even at the atomic diameter scale.

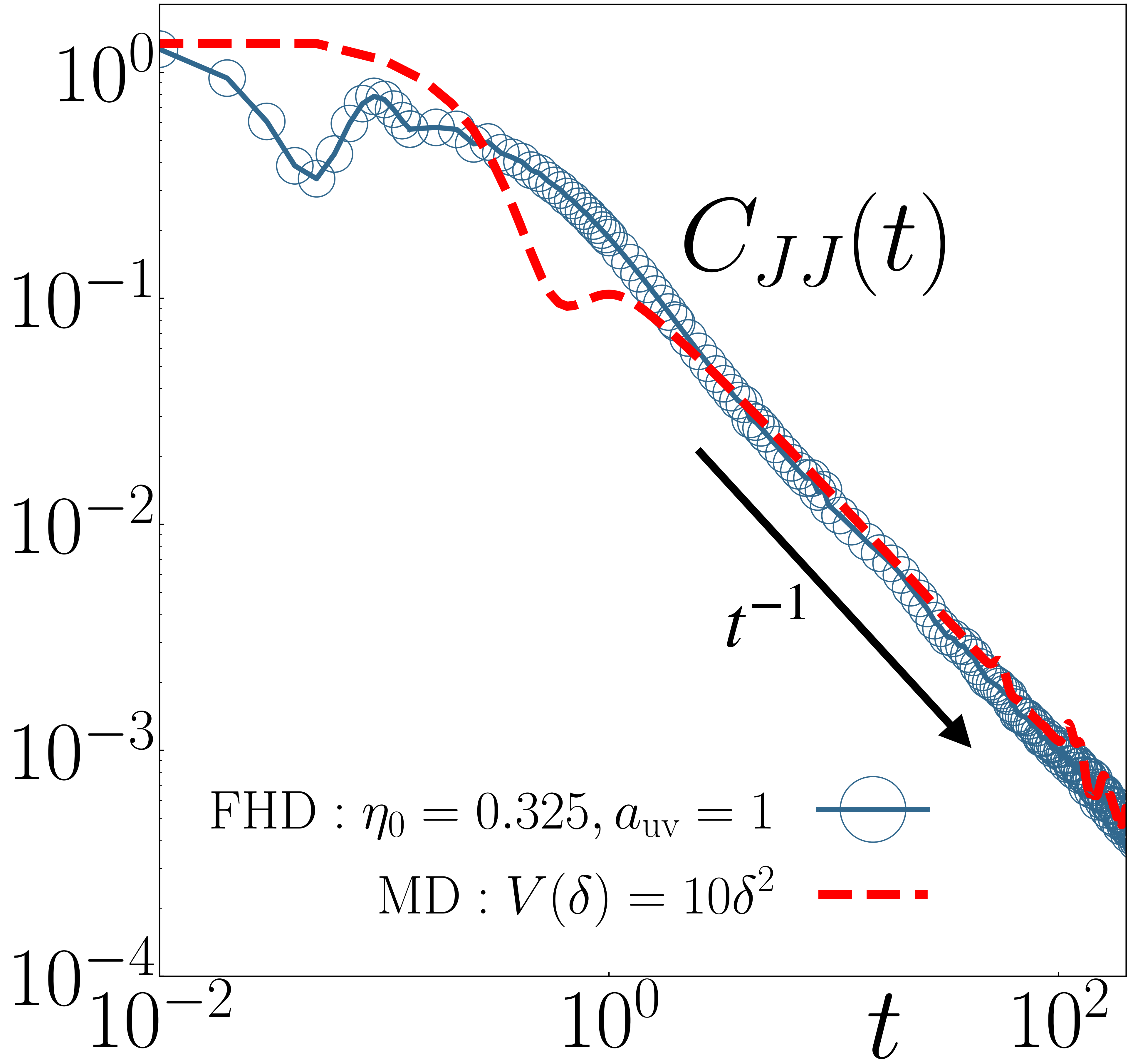
Consistency check of best-fit viscosity parameter 1

▶ To validate our estimate of viscosity η_0, we compare the time correlation of the momentum density field in the bulk region **in equilibrium**.

$$C_{JJ}(t) := \frac{1}{2}\langle \boldsymbol{j}(\boldsymbol{r},t)\cdot \boldsymbol{j}(\boldsymbol{r},0)\rangle_{\mathrm{eq}} \qquad \boldsymbol{j} := \rho \boldsymbol{v}$$

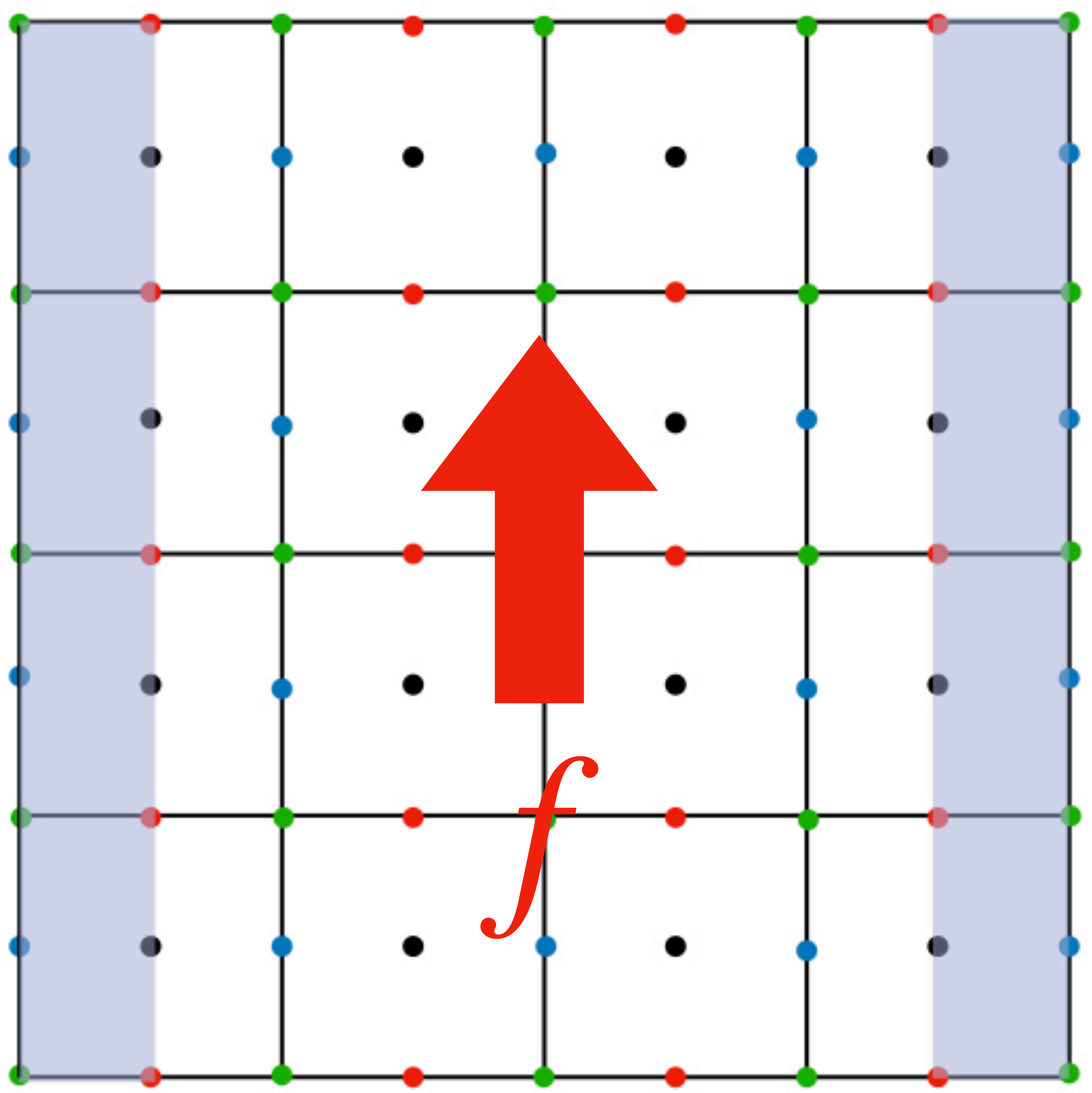
The fluctuating hydrodynamics with $\eta_0 = 0.325$ reproduces the long-time tail of the MD simulation quantitatively with high accuracy.

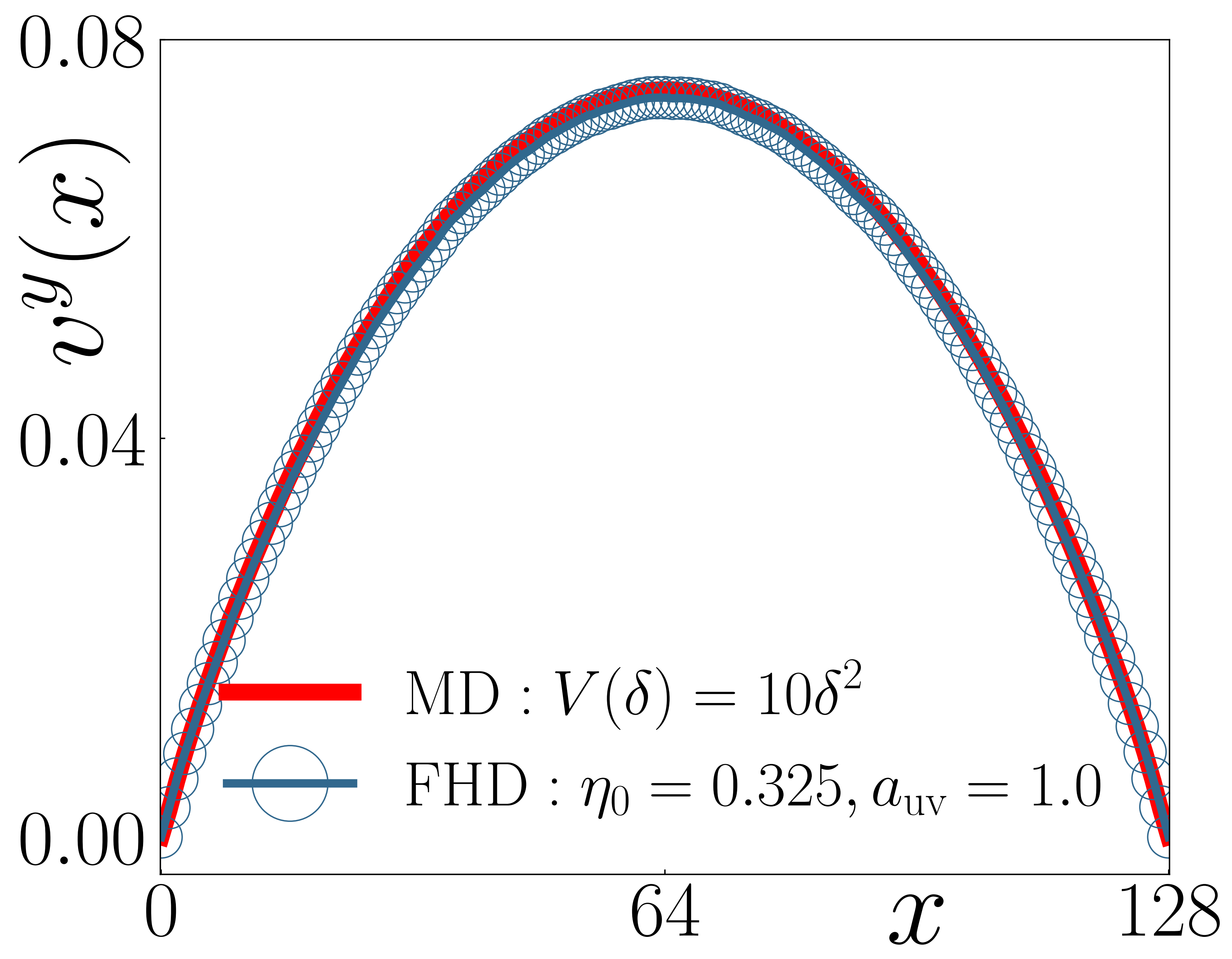
The agreement between the two models is observed even at the atomic time scale.



Consistency check of best-fit viscosity parameter 2

- As another consistency test, we perform the simulation of the Poiseuille flow.



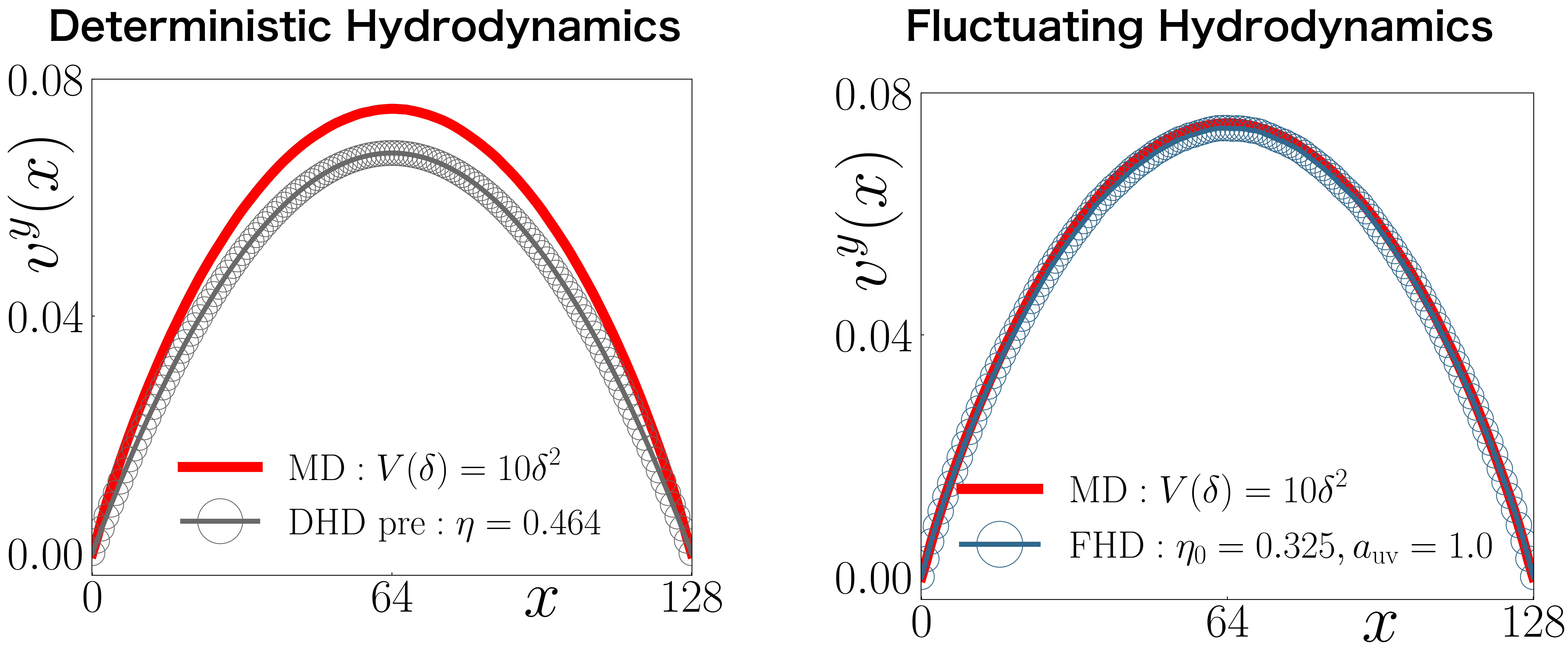


Good agreement!!

The Poiseuille flow is realized by adding a constant force to entire fluids and imposing periodic boundary condition in the flow direction.

Fluctuating hydrodynamics describes the fluid motion both near the walls and in the bulk region

Non-tiviality of the Agreement of Poiseuille Flow

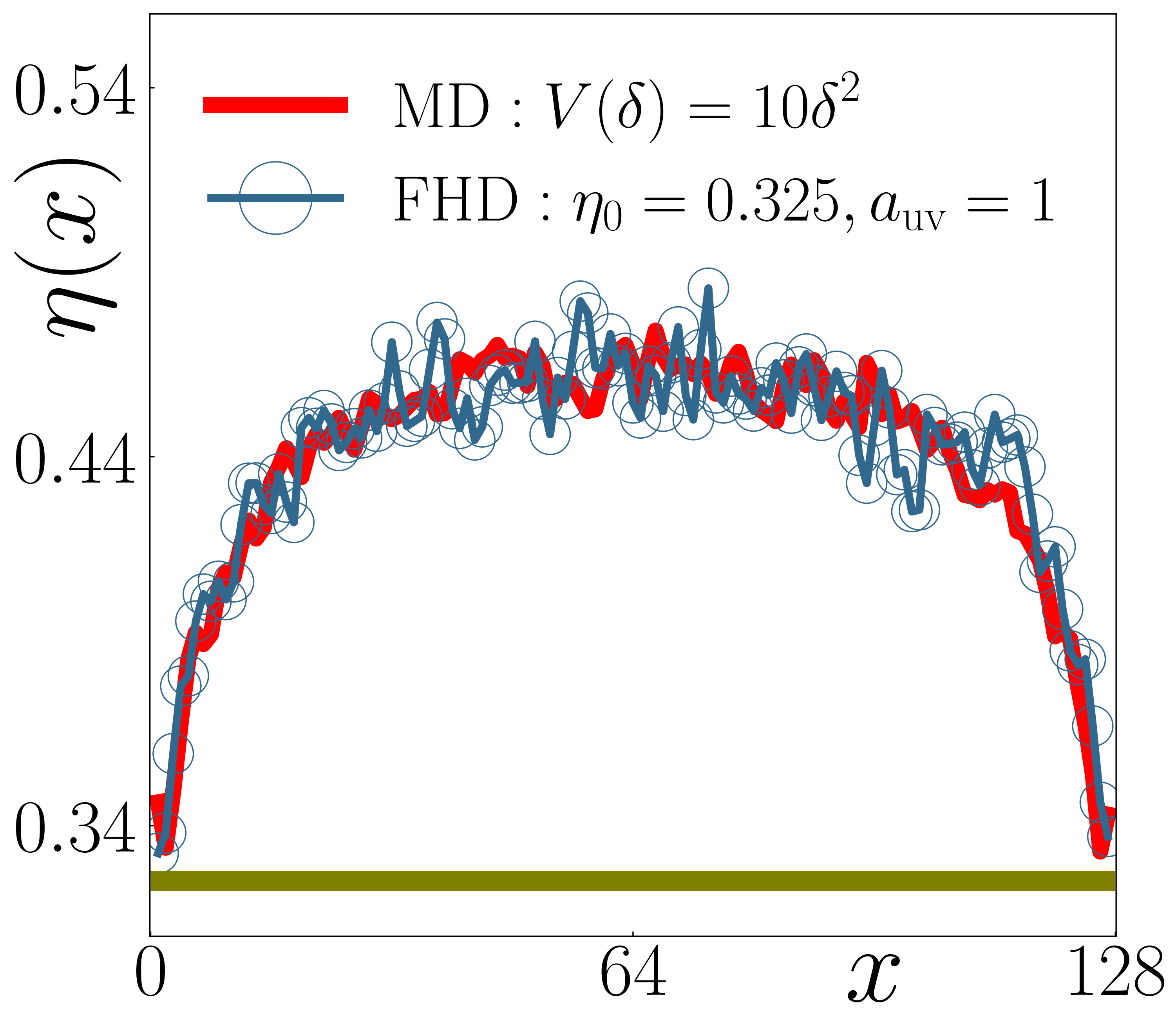


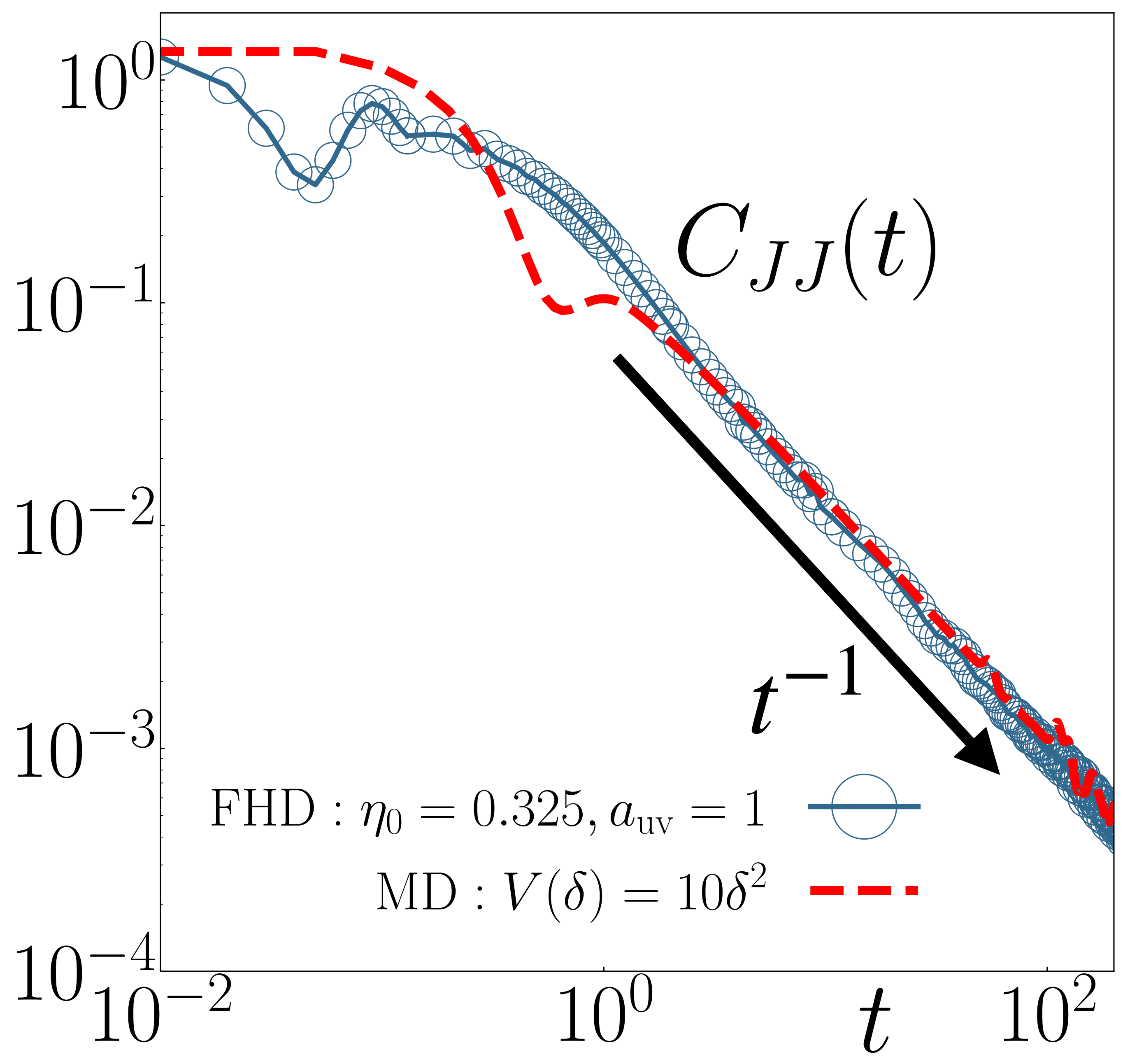
▶ The deterministic hydrodynamics with the viscosity observed in bulk region ($\eta = 0.464$) cannot reproduce the results of MD simulations.

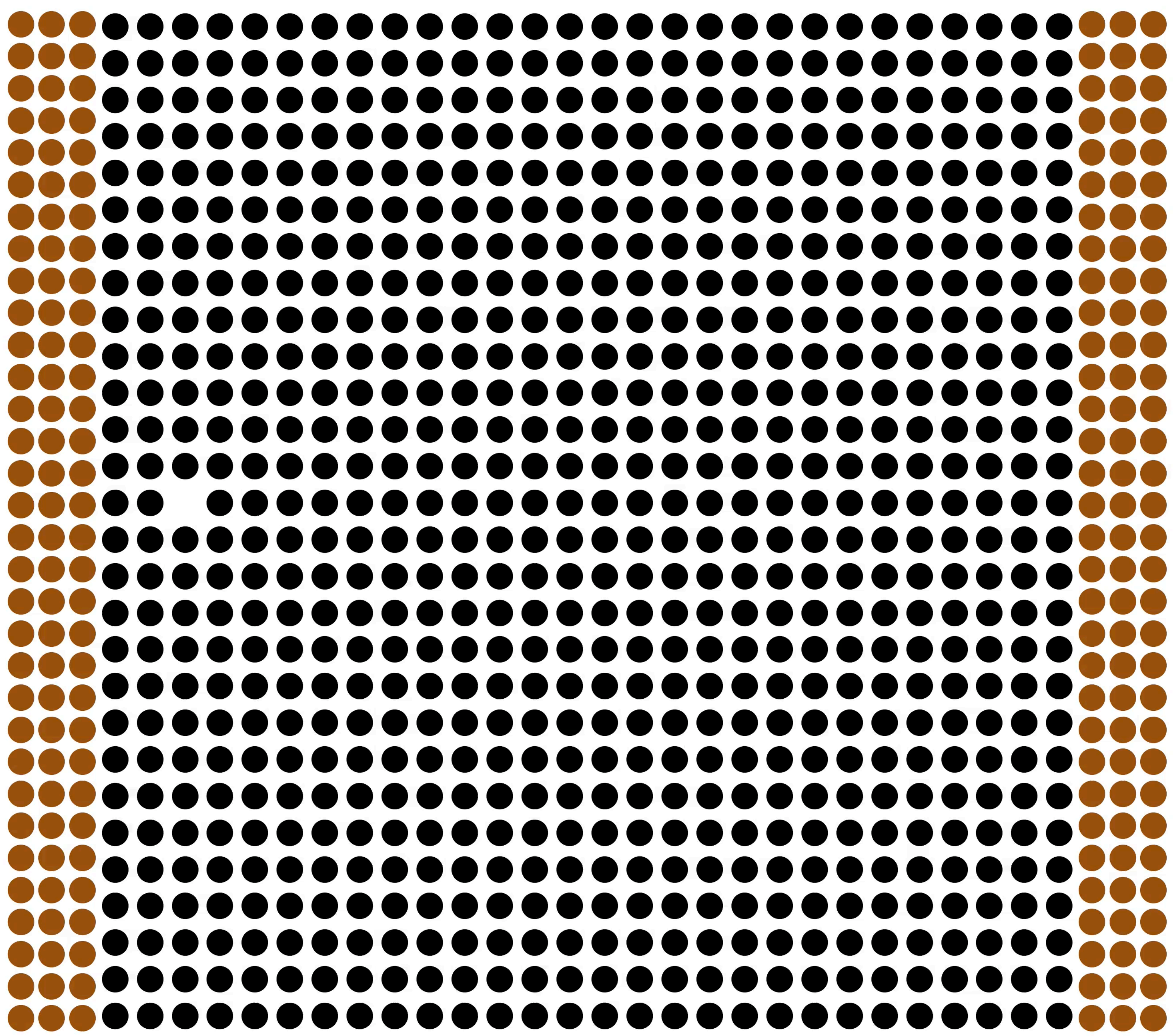
Fluctuating hydrodynamics is necessary to describe fluids near walls (at least in low-dimensional systems).

Description ability of atomic scale behaviors

Fluctuating hydrodynamics can reproduce MD results down to the atomic scale.







The mean free path of our system is roughly a few atomic diameters.

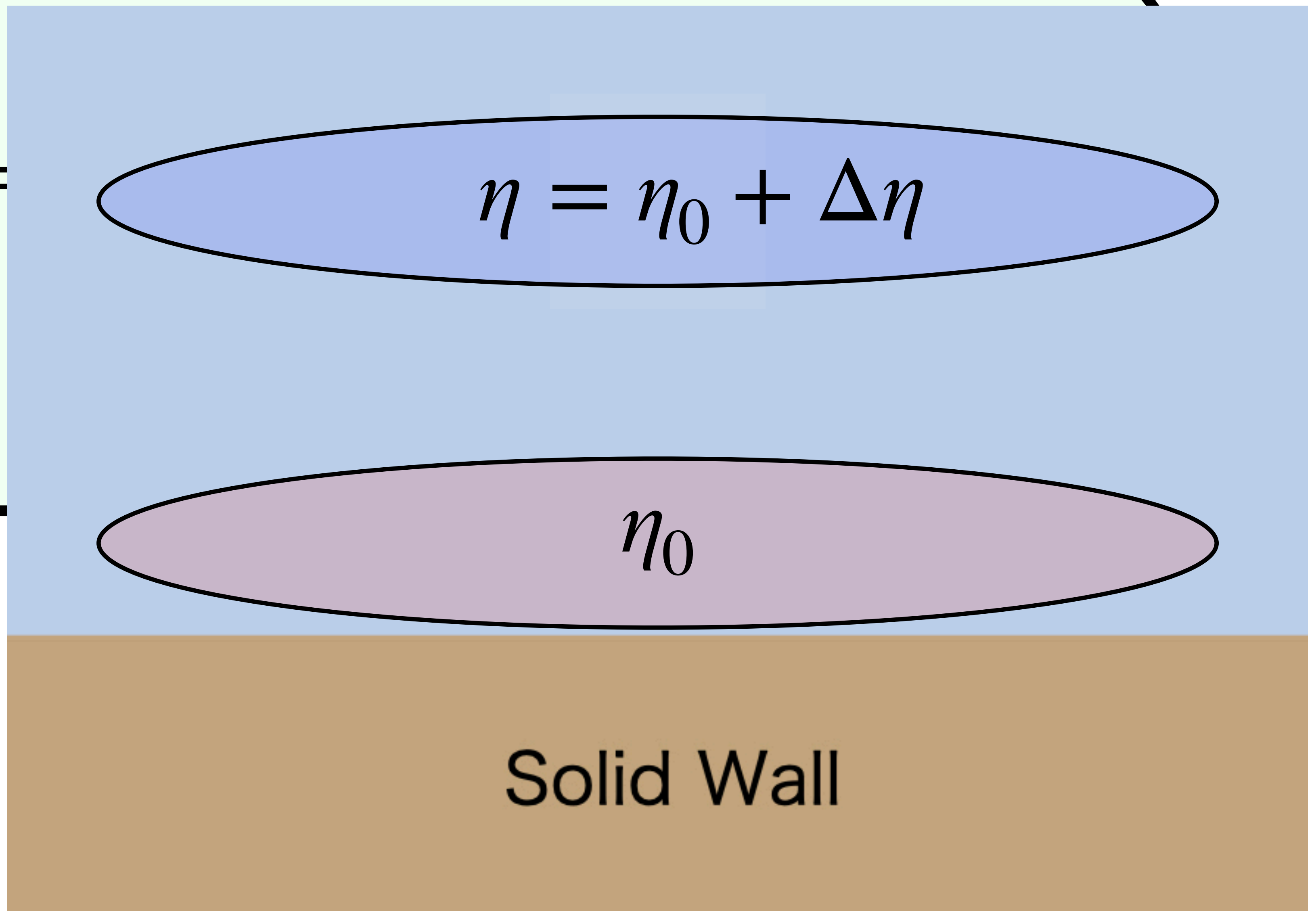
Our results suggest that fluid description is possible at the mean-free path scale in such dense systems.

Summary

2d fluid

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \boldsymbol{v}) \qquad p(\rho) = C_{\mathrm{press}}\rho \qquad c_T :=$$

$$\rho\left[\frac{\partial \boldsymbol{v}}{\partial t} + (\boldsymbol{v}\cdot\nabla)\boldsymbol{v}\right] = -\nabla p + \eta_0 \nabla^2 \boldsymbol{v} + \zeta_0 \nabla(\nabla\cdot\boldsymbol{v}) + \nabla \boldsymbol{\Pi}_R$$



- We focus on the 2d fluids in contact with the solid walls.

  We analyze the fluctuating hydrodynamic equations

  / perform the MD simulations

The first main result

η_0 **governs the fluid motions near the walls,**

while $\eta = \eta_0 + \Delta\eta$ appears only in the bulk region.

The second main result

Even in the atomic systems, **the anomalous transport does not occurs near the walls** and η_0 governs the fluid motion near the walls.

Discussion: Physical Meaning of η_0

2d fluid

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \boldsymbol{v}) \qquad p(\rho) = C_{\mathrm{press}}\rho \qquad c_T := \sqrt{\left(\frac{\partial p}{\partial \rho}\right)_T} = \sqrt{C_{\mathrm{press}}}$$

$$\rho\left[\frac{\partial \boldsymbol{v}}{\partial t} + (\boldsymbol{v}\cdot\nabla)\boldsymbol{v}\right] = -\nabla p + \eta_0 \nabla^2 \boldsymbol{v} + \zeta_0 \nabla(\nabla\cdot\boldsymbol{v}) + \nabla \boldsymbol{\Pi}_R$$

- η_0 is independent of the system size.
- η_0 describes fluid motion at the **microscopic scale**, on the order of a particle diameter.
- η_0 characterizes **microscopic dissipation**, which is fundamentally different from the system-size-dependent **macroscopic dissipation**. $\eta = \eta_0 + \Delta\eta$

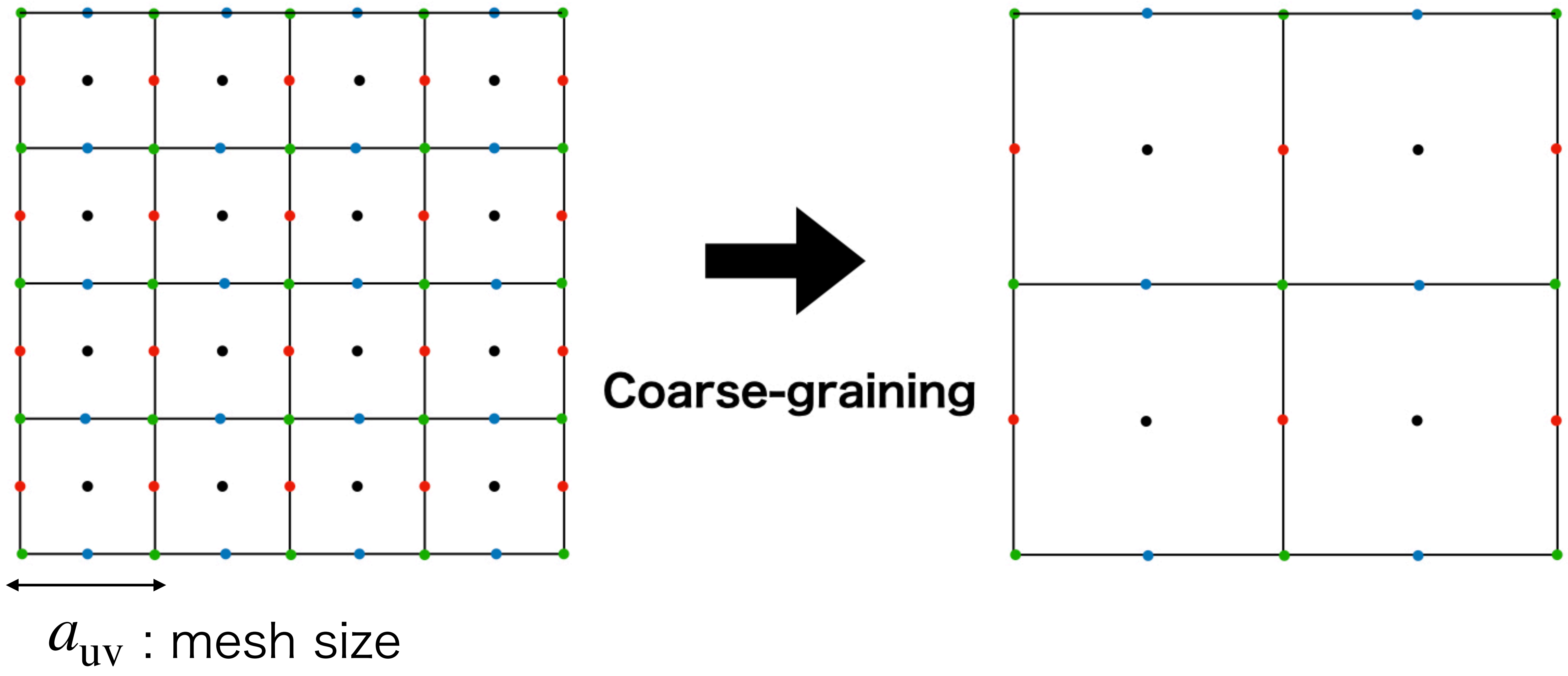
Our proposition : η_0 **is the “bare” viscosity**

This is the fundamental contribution to viscosity from the purely microscopic domain.

Appendix

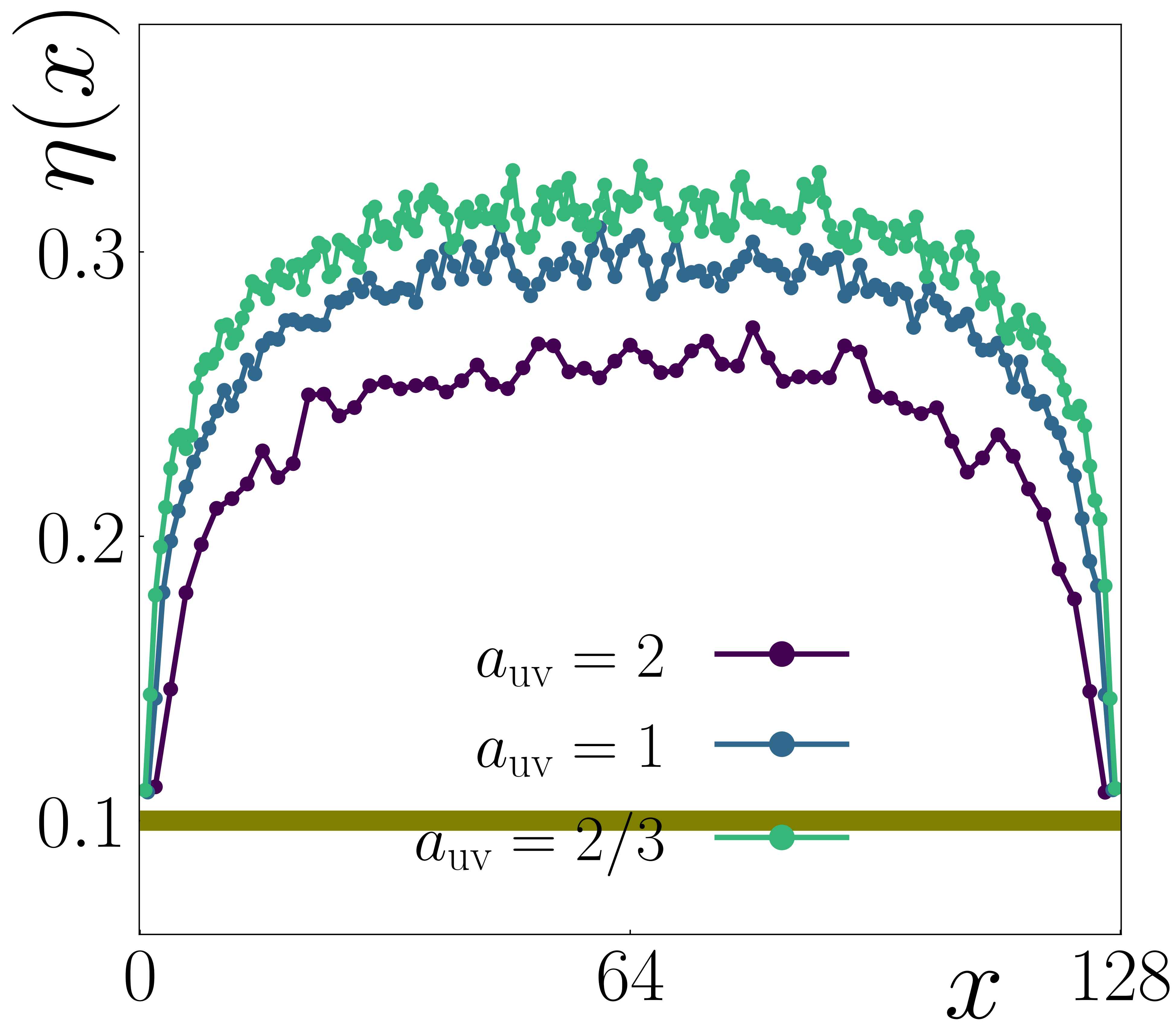
UV cutoff length

- Changing the UV cutoff length is related to coarse-graining process.



UV cutoff length

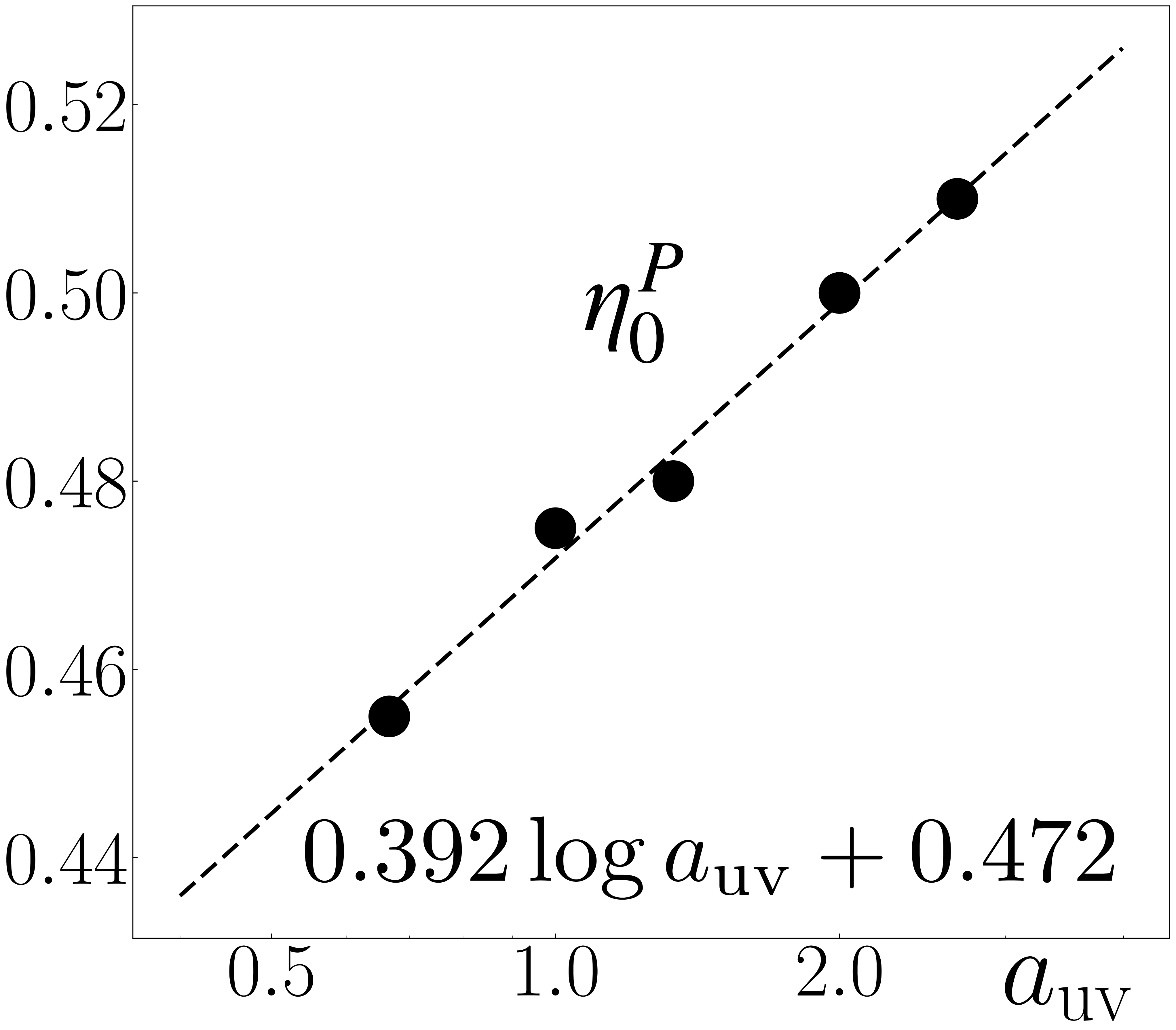
- The predictions of fluctuating hydrodynamics depend on the value of the UV cutoff length a_{uv}.



The observed local viscosity changes by varying only the UV cutoff length a_{uv} with all other parameters including viscosity η_0 fixed at the same value.

Both parameters (η_0, a_{uv}) can be used as adjustable parameters.

Bare viscosity



In practice, the bare viscosity η_0^P is determined to satisfy

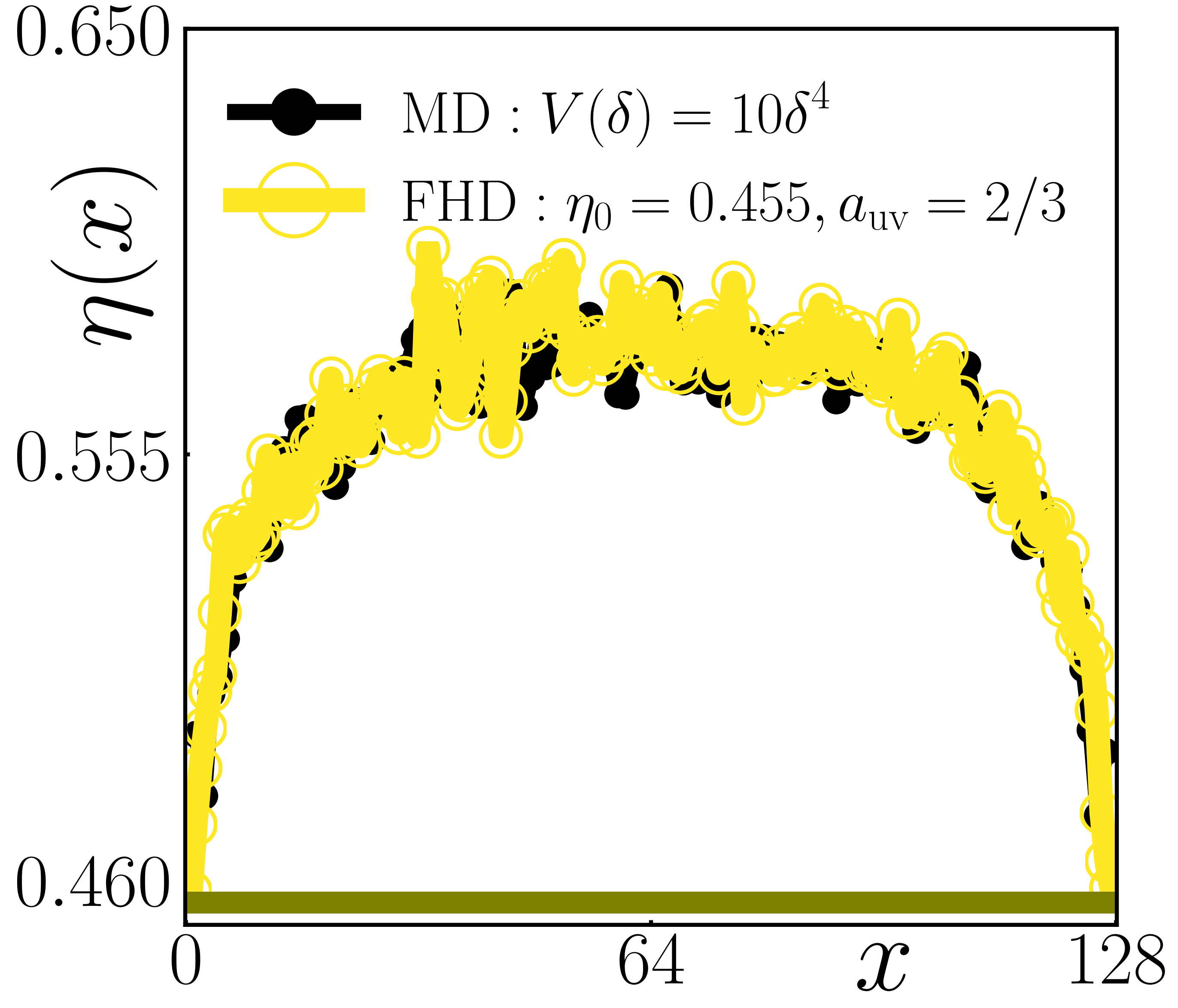
$$\eta_{\mathrm{MD}}(x) = \eta_{\mathrm{FH}}(x : \eta_0^P, a_{\mathrm{uv}})$$

The “practical” bare viscosity η_0^P depends on the UV cutoff length.

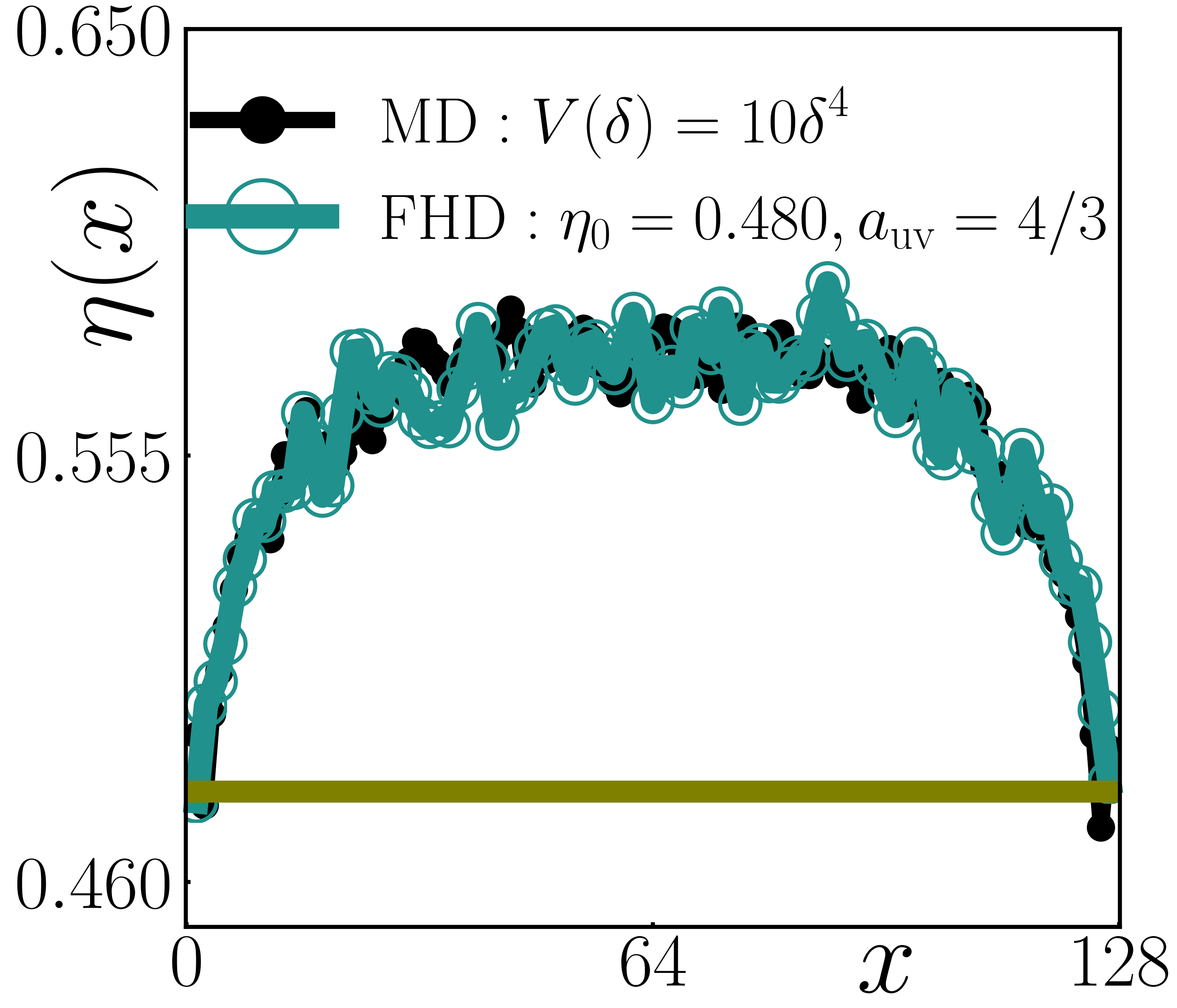
If $(\eta_0, a_{\mathrm{uv}})$ lie on this relationship, any pair will reproduce the macroscopic phenomena well.

Best value of UV cutoff length

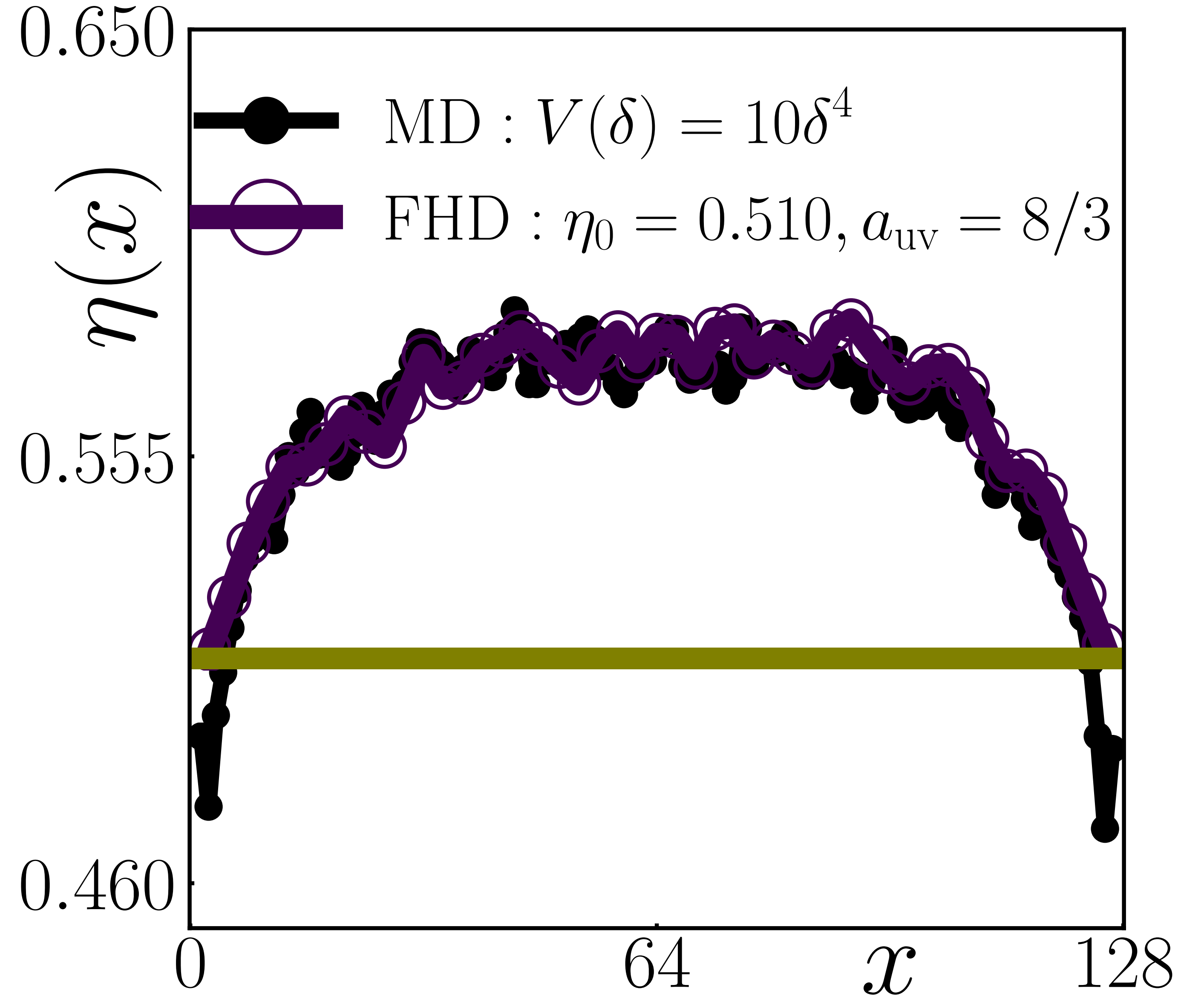
- We investigated the best-fit bare viscosity for different UV cutoff lengths.



$\eta_0 = 0.455$ for $a_{\rm uv} = 2/3$



$\eta_0 = 0.480$ for $a_{\rm uv} = 4/3$



$\eta_0 = 0.510$ for $a_{\rm uv} = 8/3$

Black: MD
(all the same data)

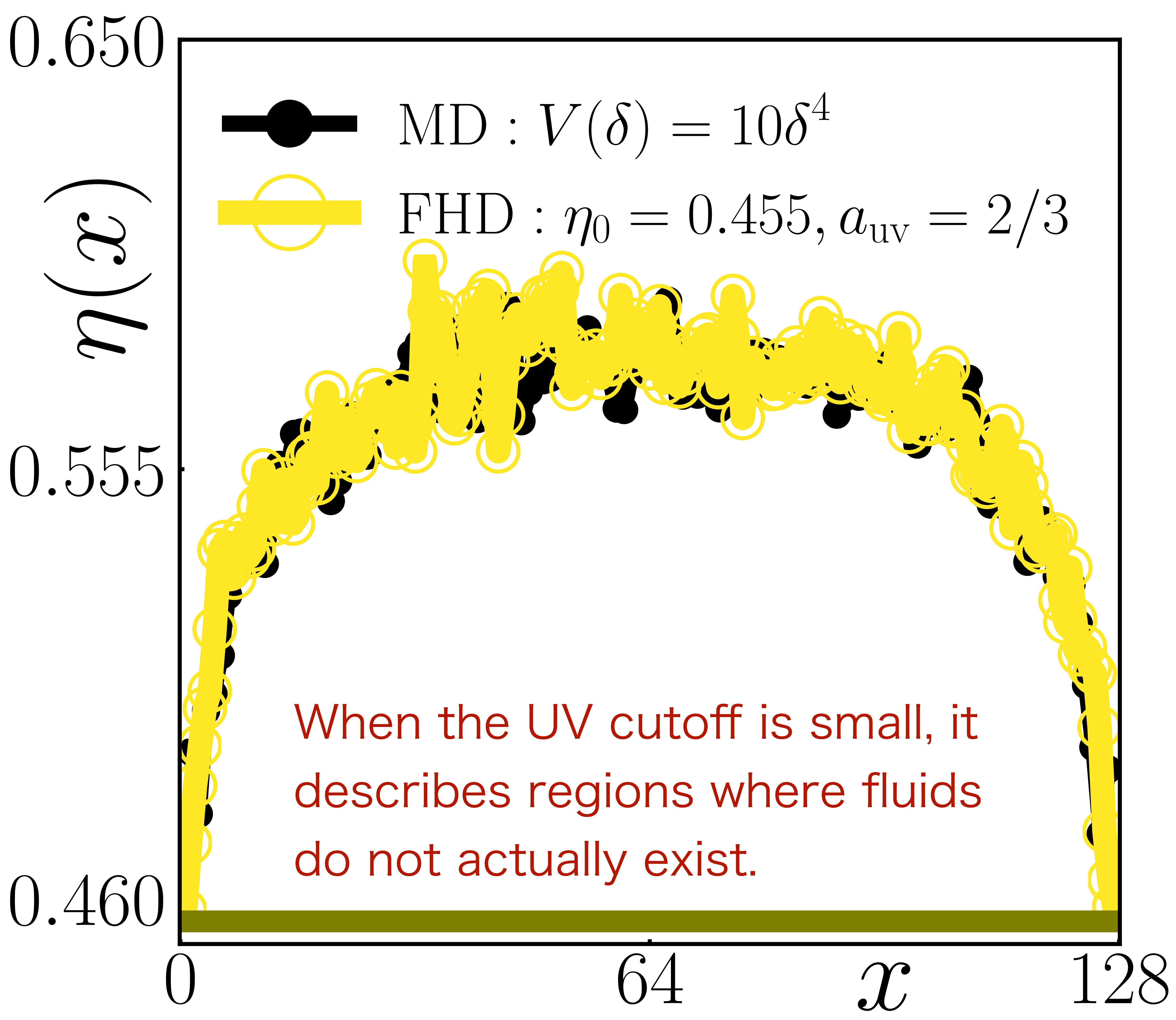
Colored: FHD
(with different $(\eta_0, a_{\rm uv})$)

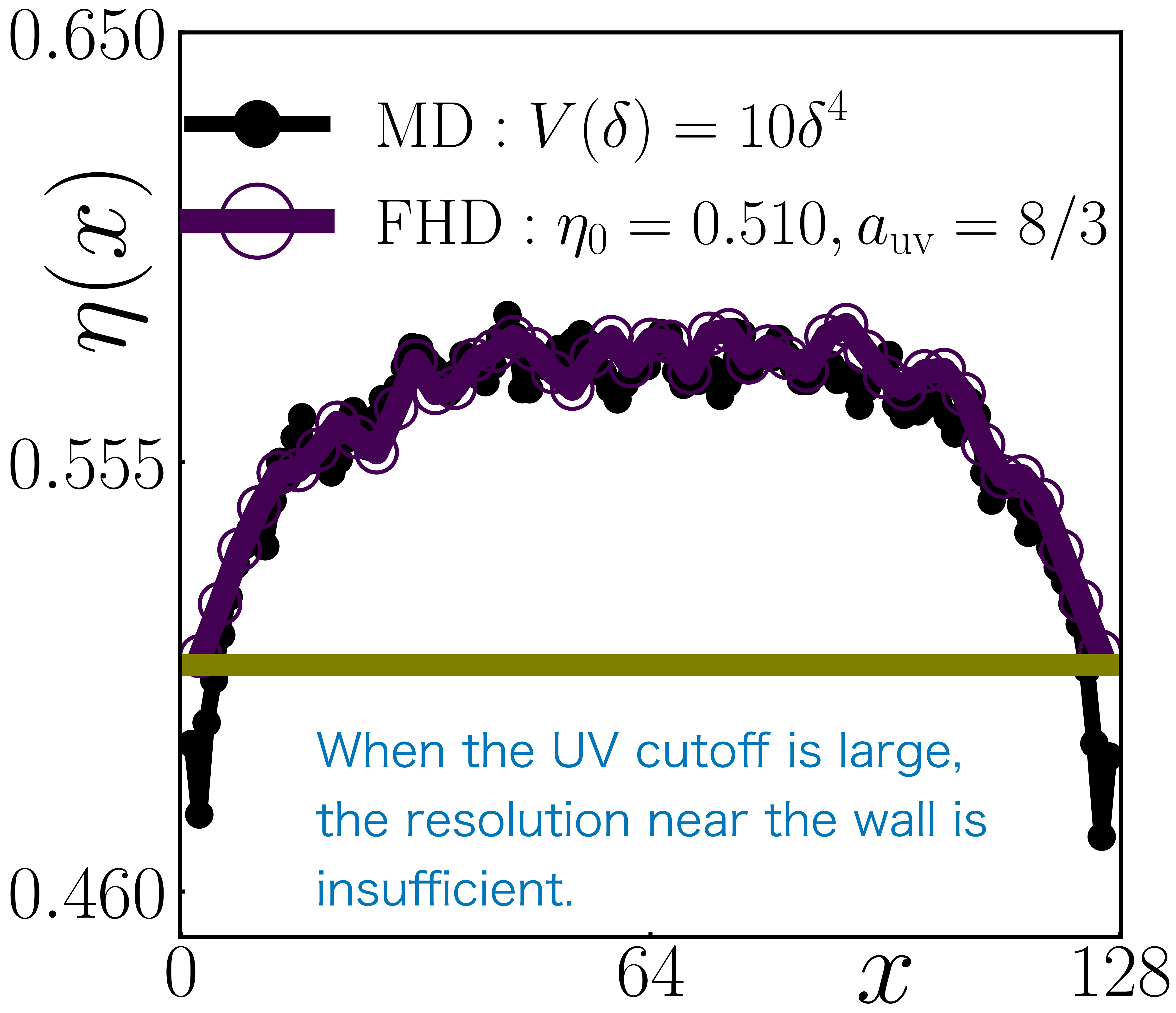
By carefully choosing η_0, the MD results can be well reproduced for any $a_{\rm uv}$.

The best value of UV cutoff length is about mean-free path length?

(in our simulations, it is atomic diameter)

Best value of UV cutoff length





The best value of UV cutoff length is about atomic diameter!!