SCALING IN DRIVEN FLUIDS

AND THE UNREASONABLE EFFECTIVENESS OF NAVIER-STOKES-FOURIER EQUATIONS

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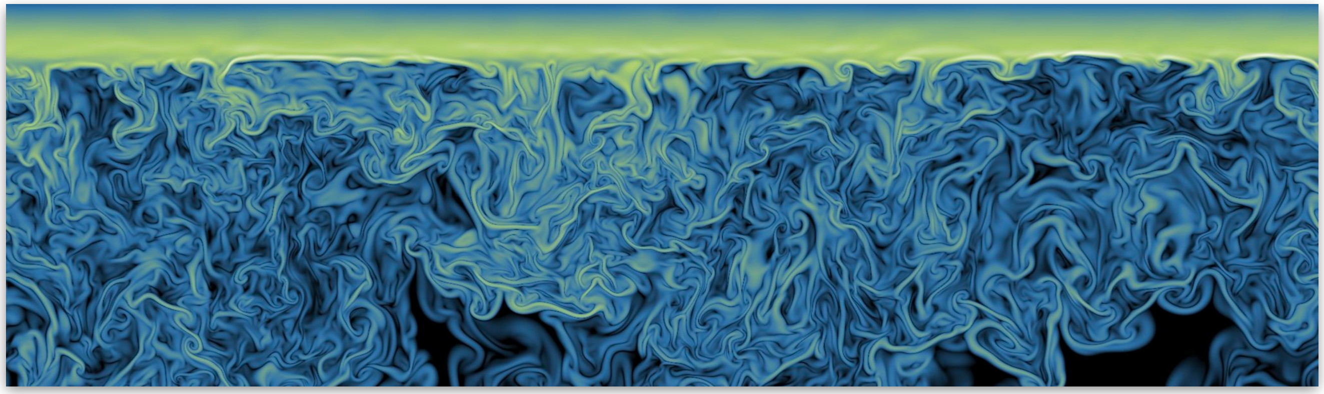
STATIONARY NAVIER-STOKES-FOURIER EQUATIONS

- The **Navier-Stokes-Fourier (NSF) equations** describe flow in compressible, viscous, and heat-conducting fluids
- They are are based on the **local conservation of energy, momentum and mass density**, together with the linear **constitutive laws of Fourier and Newton**
- NSF equations are of fundamental importance in many branches of physics and engineering



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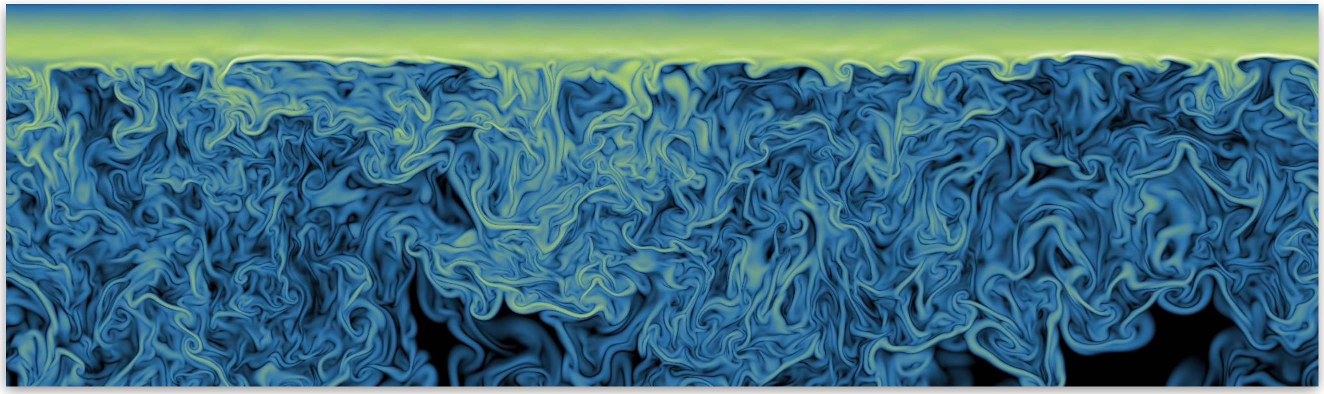


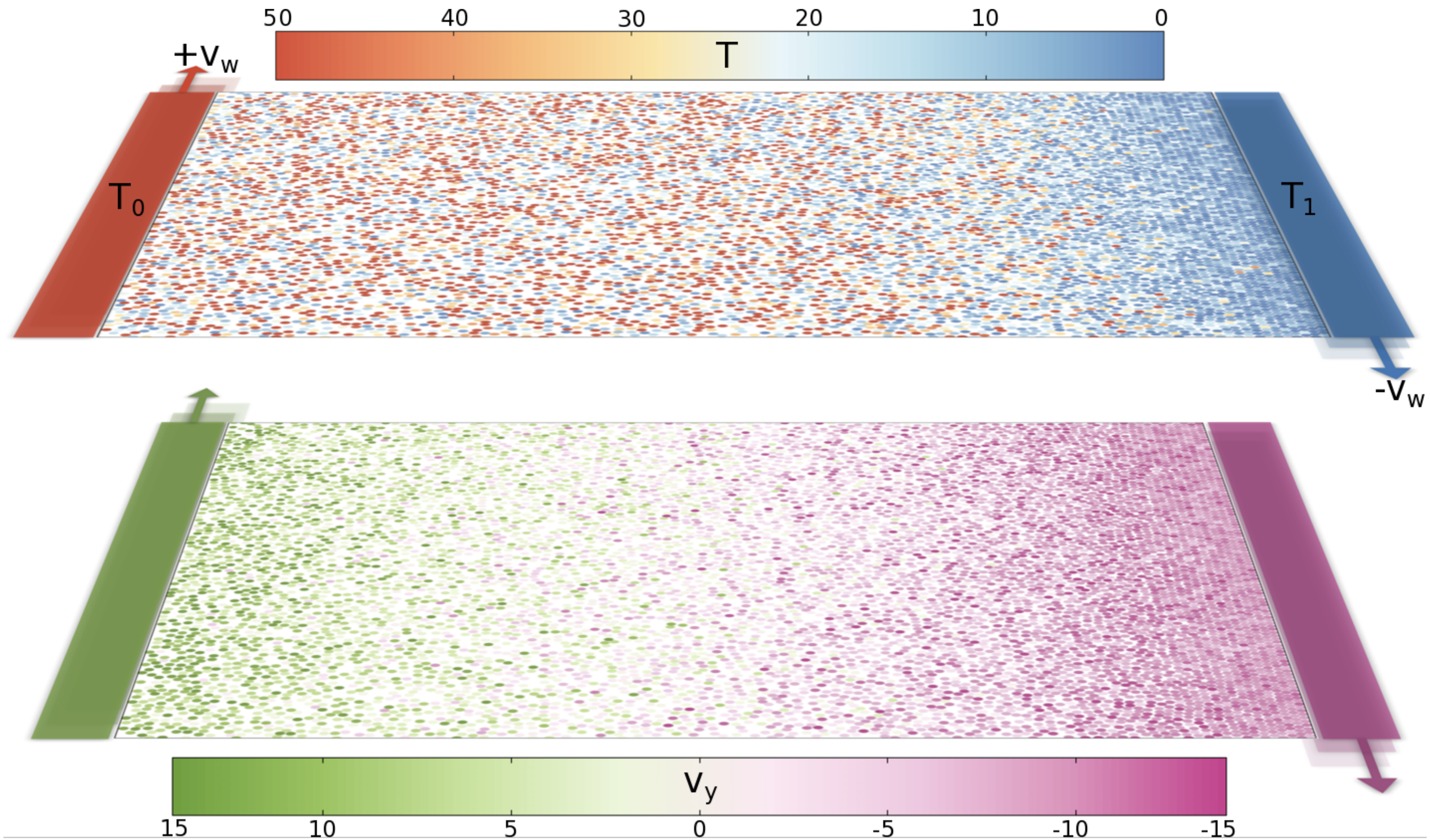
- **Stationary solutions to the NSF equations** are important in fluid dynamics, and describe one of the most challenging examples of a **nonequilibrium steady state**

- The resulting hydrodynamic structure codifies key information on **how the governing macroscopic laws emerge from the complex microscopic dynamics**

- **Aim**: **explore scaling properties of stationary solutions of NSF equations**

NONEQUILIBRIUM STEADY STATE

- We consider a **d-dimensional compressible, viscous and heat-conducting fluid** driven out of equilibrium by **temperature gradient and shear stress** along x-dir.



2d hard disks

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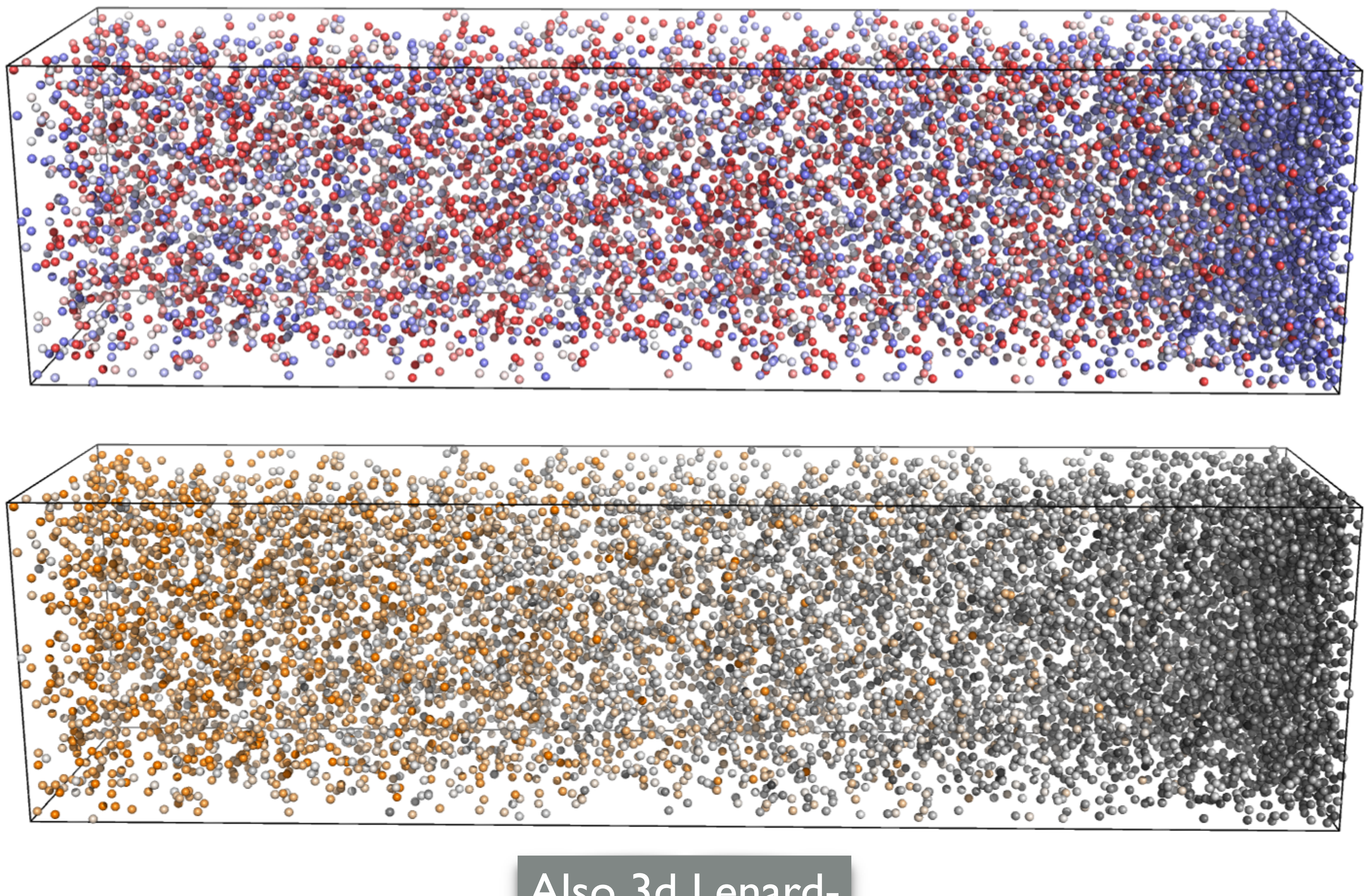

Also 3d Lenard-Jones fluid

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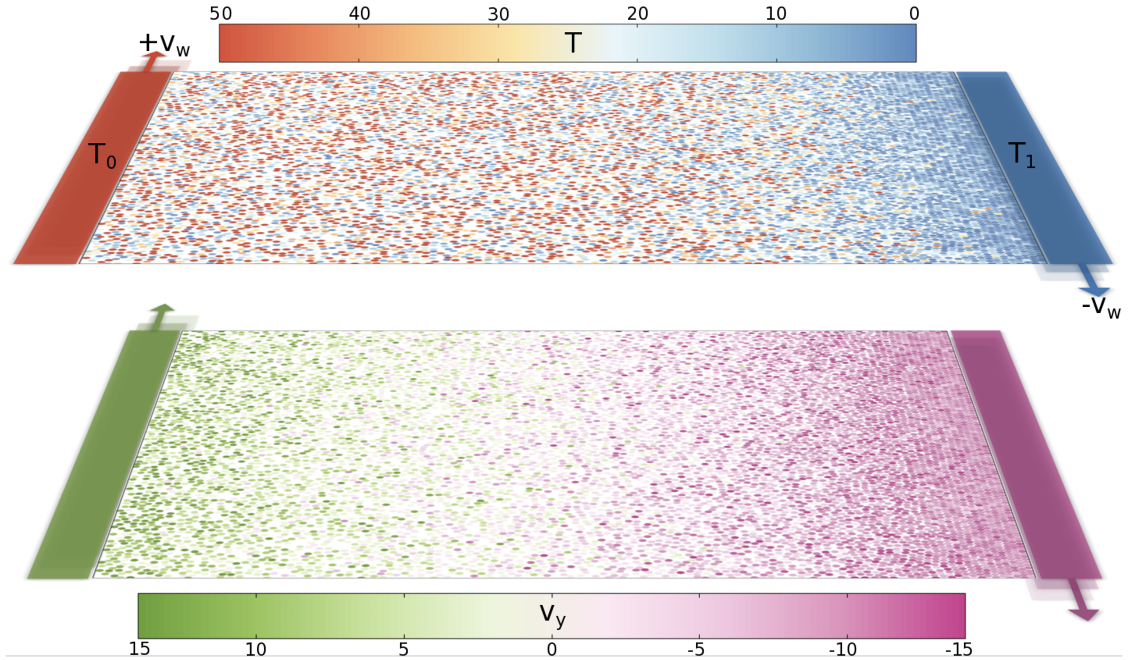
- At the **macroscopic level**, the fluid steady state is described by the **stationary NSF equations** for the density, velocity and temperature fields

$$\frac{d}{dx}\pi(\rho,T)=0 \qquad \frac{d}{dx}\left[\eta(\rho,T)\frac{dv}{dx}\right]=0$$

$$\frac{d}{dx}\left[\kappa(\rho,T)\frac{dT}{dx}\right]+\eta(\rho,T)\left(\frac{dv}{dx}\right)^2=0$$



- **Boundary conditions** are $T(0)=T_0\,,\ T(1)=T_1\,,\ v(0)=v_w\,,\ v(1)=-v_w$ and **periodic along the y-direction**, together with **constraint** $\lambda=\int_0^1\rho(x)dx$

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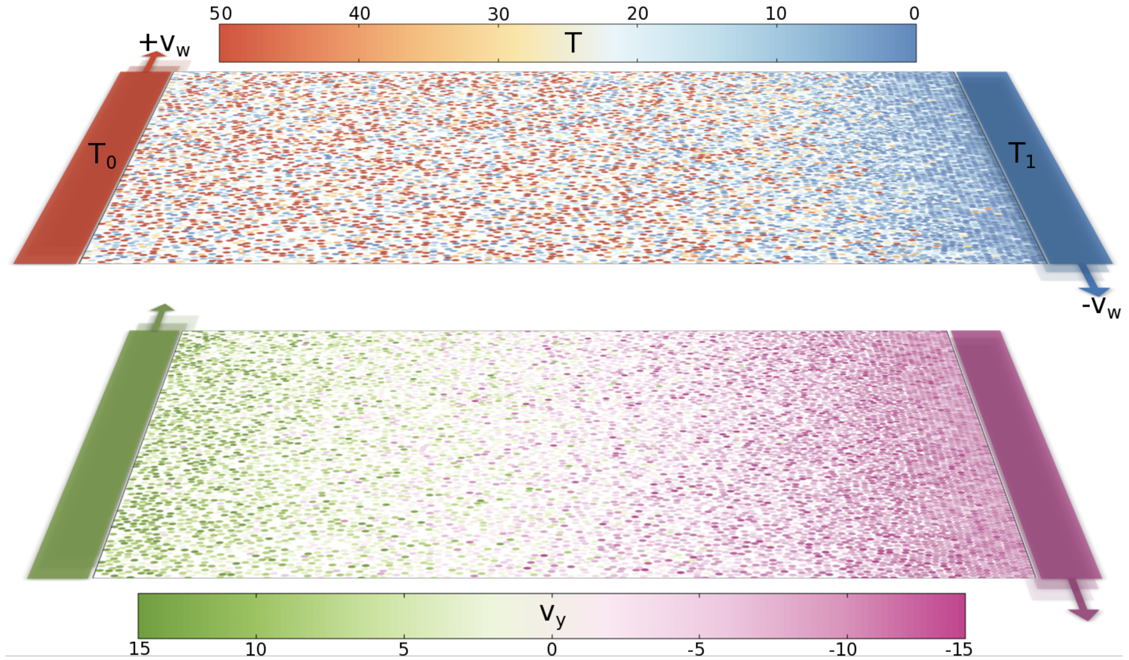

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- It is straightforward to show that

$$\pi(\rho,T)=\underbrace{P}_{\text{Pressure}} \qquad \eta(\rho,T)\frac{dv}{dx}=\underbrace{\sigma}_{\text{Shear stress}} \qquad -\kappa(\rho,T)\frac{dT}{dx}=\underbrace{j(x)}_{\text{Heat current}}=J+\sigma v(x)$$

- Assuming **macroscopic local equilibrium**, $\pi(\rho,T)$ **is given by the fluid's Equation of State (EoS)**

SCALING IN DRIVEN FLUIDS

- **Local equilibrium** can be used to **write $T(x)$ in terms of $\rho(x)$ and P**

$$\pi[\rho, T(x)] = P \quad \Rightarrow \quad T(x) = \tau_P[\rho(x)] \quad \Rightarrow \quad \begin{array}{c} \kappa(\rho, T) \equiv \kappa_P(\rho) \\ \eta(\rho, T) \equiv \eta_P(\rho) \end{array}$$

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- From the **heat equation** and using the (monotonous) velocity as a proxy of space

$$\left.\begin{array}{r} -\kappa_P(\rho)\tau_P'(\rho)\dfrac{d\rho}{dx} = J + \sigma v(x) \\ \dfrac{d\rho}{dx} = \left(\dfrac{d\rho}{dv}\right)\left(\dfrac{dv}{dx}\right) = \dfrac{\sigma}{\eta_P(\rho)}\dfrac{d\rho}{dv} \end{array}\right] \Rightarrow \left[\begin{array}{r} -\dfrac{\kappa_P(\rho)\tau_P'(\rho)}{\eta_P(\rho)}\dfrac{d\rho}{dv} = v + \dfrac{J}{\sigma} \\ \mathcal{G}_P'(\rho)\dfrac{d\rho}{dv} = \dfrac{d\mathcal{G}_P(\rho)}{dv} = v + \dfrac{J}{\sigma} \end{array}\right.$$

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- Therefore, the fields $\rho(x)$ and $T(x)$ are sole functions of the fluid's pressure and a kinetic field $\omega(x)$

$$\left.\begin{array}{l} \mathcal{G}_P(\rho)=\dfrac{1}{2}\left(v+\dfrac{J}{\sigma}\right)^2+\xi \\ \boxed{\omega(x)\equiv\dfrac{1}{2}\left(v(x)+\dfrac{J}{\sigma}\right)^2}\end{array}\right] \xrightarrow{\mathcal{R}_P(\cdot)\equiv\mathcal{G}_P^{-1}(\cdot)} \left[\boxed{\begin{array}{l}\rho(x)=\mathcal{R}_P\left(\omega(x)+\xi\right) \\ T(x)=\mathcal{T}_P(\omega(x)+\xi)\end{array}}\right.$$

- In this way there exist two master surfaces in $\omega - P$ space from which any stationary density and temperature fields follow. Conversely, any measured **density and temperature profiles can be collapsed onto the respective master surfaces**

SCALING IN DRIVEN FLUIDS

$$\omega(x) \equiv \frac{1}{2}\left(v(x) + \frac{J}{\sigma}\right)^2$$

- **The kinetic field obeys in turn a spatial scaling law.** From Newton's law

$$\left.\begin{array}{l} \eta(\rho,T)\dfrac{dv}{dx} = \sigma \\ \dfrac{dv}{dx} = \pm(2\omega)^{-1/2}\dfrac{d\omega}{dx} \end{array}\right] \Rightarrow \left[\begin{array}{l} \overbrace{\boxed{\dfrac{\eta_P[\mathcal{R}_P(\omega+\xi)]}{\sqrt{2\omega}}}}^{\mathcal{H}'_{P,\xi}(\omega)}\dfrac{d\omega}{dx} = \pm\sigma \\ \mathcal{H}_{P,\xi}(\omega) = \pm\sigma x + \zeta \end{array}\right] \xrightarrow{\mathcal{W}_{P,\xi}(\cdot)\equiv\mathcal{H}^{-1}_{P,\xi}(\cdot)} \boxed{\omega(x) = \mathcal{W}_{P,\xi}(\pm\sigma x + \zeta)}$$

- Therefore, there exist a **parametric family of master surfaces $\mathcal{W}_{P,\xi}$ in $x-\xi$ space**, **one for each P**, from which all kinetic profiles $\omega(x)$ follow and where they **collapse**

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- **Density and temperature fields inherit the previous spatial scaling**

$$\left.\begin{array}{l} \rho(x) = \mathcal{R}_P\left[\mathcal{W}_{P,\xi}(\pm\sigma x + \zeta) + \xi\right] \\ T(x) = \mathcal{T}_P\left[\mathcal{W}_{P,\xi}(\pm\sigma x + \zeta) + \xi\right] \end{array}\right] \Rightarrow \left[\begin{array}{l} \rho(x) = \bar{\mathcal{R}}_P(\pm\sigma x + \zeta, \omega + \xi) \\ T(x) = \bar{\mathcal{T}}_P(\pm\sigma x + \zeta, \omega + \xi) \end{array}\right.$$

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- **Inverse power-law fluids** (as hard disks) **exhibit density-temperature separability.** In this case $P = T\pi(\rho)$, $\kappa(\rho,T) = \sqrt{T}\kappa(\rho)$, and $\eta(\rho,T) = \sqrt{T}\eta(\rho)$, simplifying scaling

$$\rho(x) = \mathcal{R}\left(\frac{\omega(x)}{P} + \xi\right) \qquad T(x) = P\,\mathcal{T}\left(\frac{\omega(x)}{P} + \xi\right)$$

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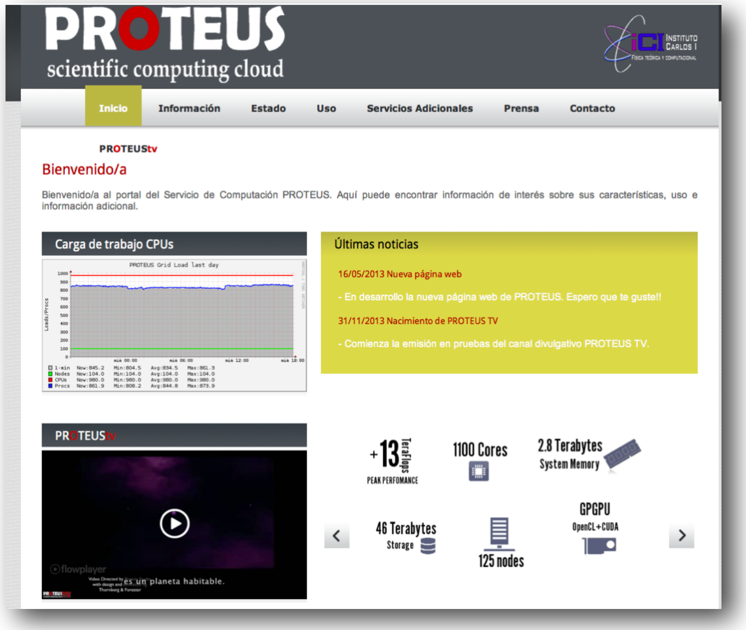
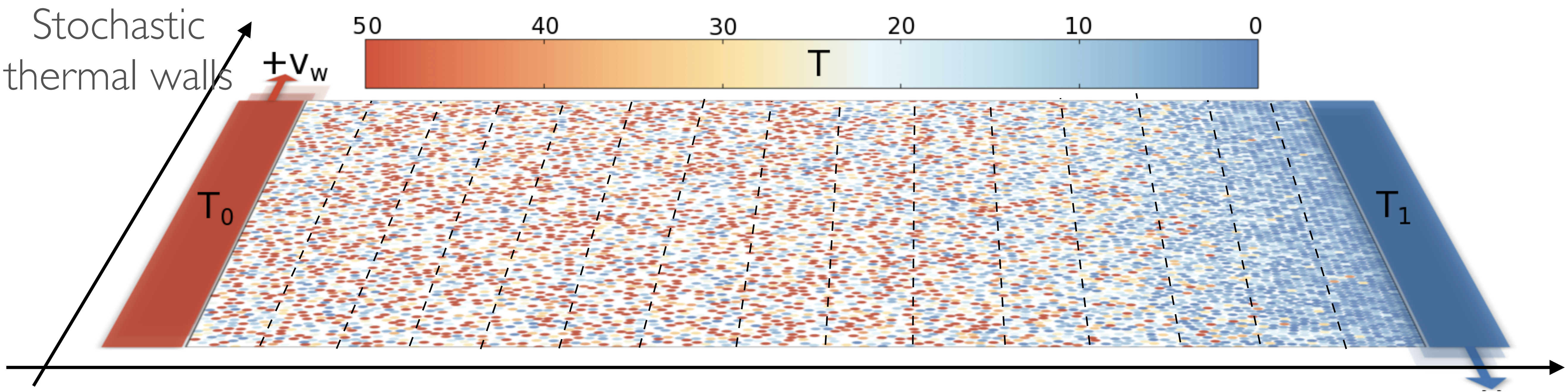
SCALING IN THE HARD DISKS FLUID

~200 simulations ⟶ ~2500 sim. points

- 8 different $N\in[1500,9000]$
- 6 different **constant** ΔT with $T_0\in[1,20]$ ⟶ $r(N)$
- 7 packing fractions $\eta\in[0.05,0.5]$

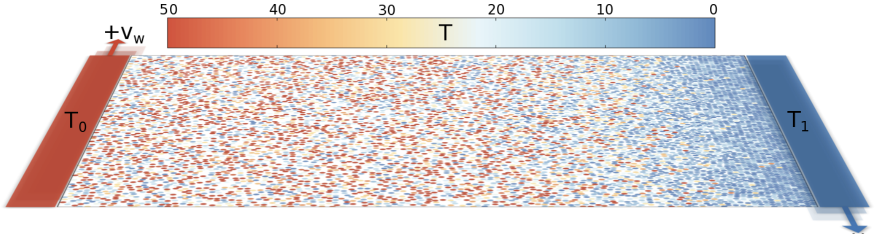


15 (virtual) cells
along gradient direction

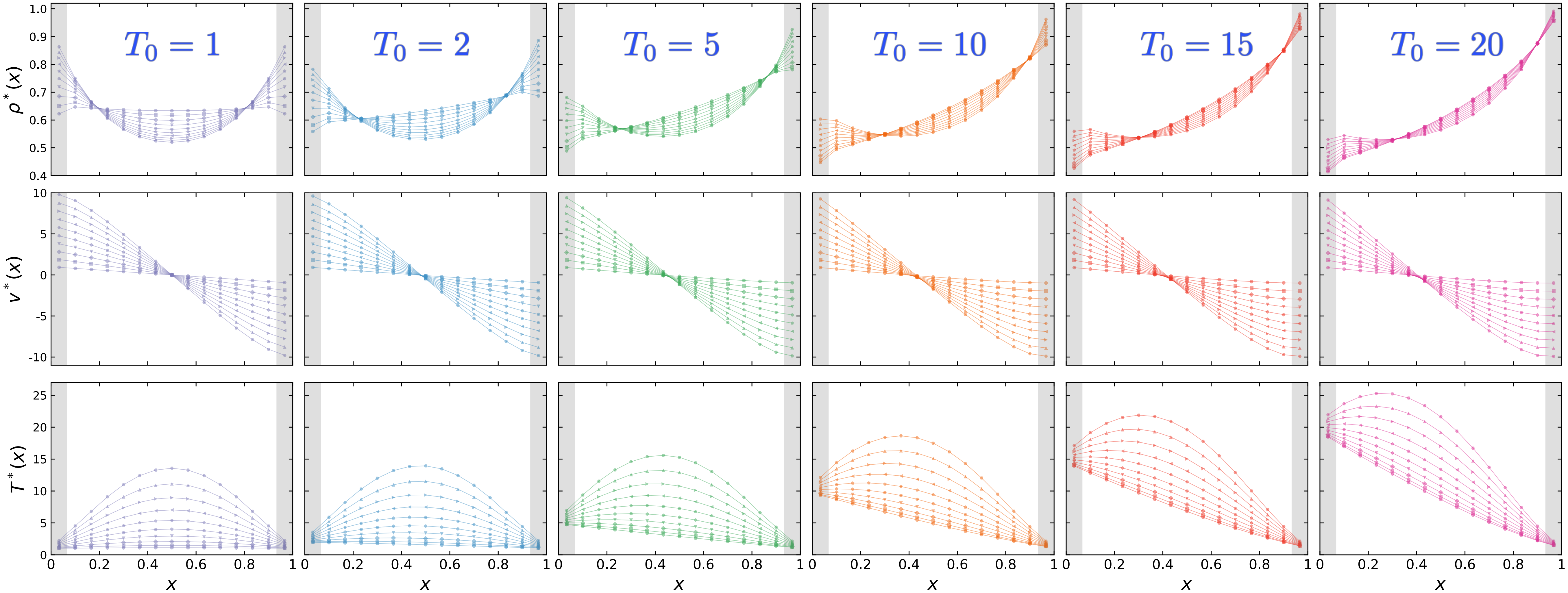


- At the **noneq. steady state**, we measure **density, y-velocity and temperature fields**
- Also **virial pressure, heat current and shear stress profiles**, together with their **wall counterparts**, which **coincide** with the average bulk behavior

HYDRODYNAMIC FIELDS



$N = 1927$ $\lambda = 0.5$



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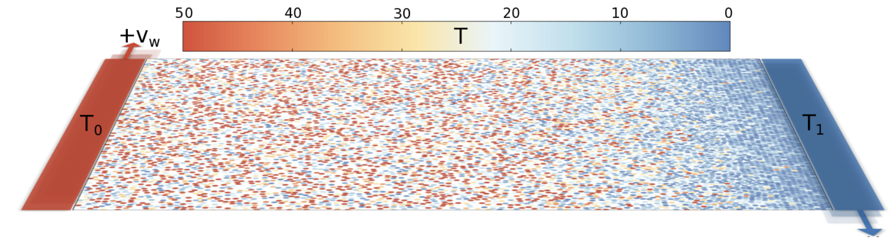

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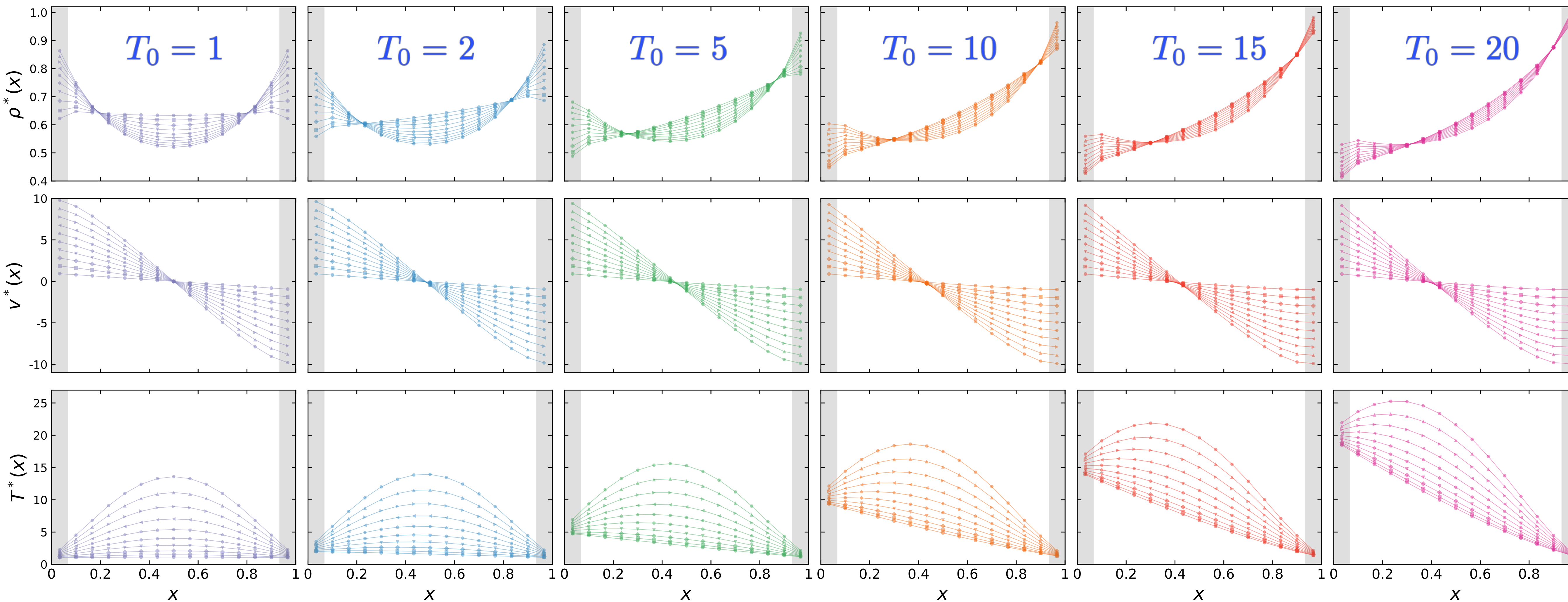
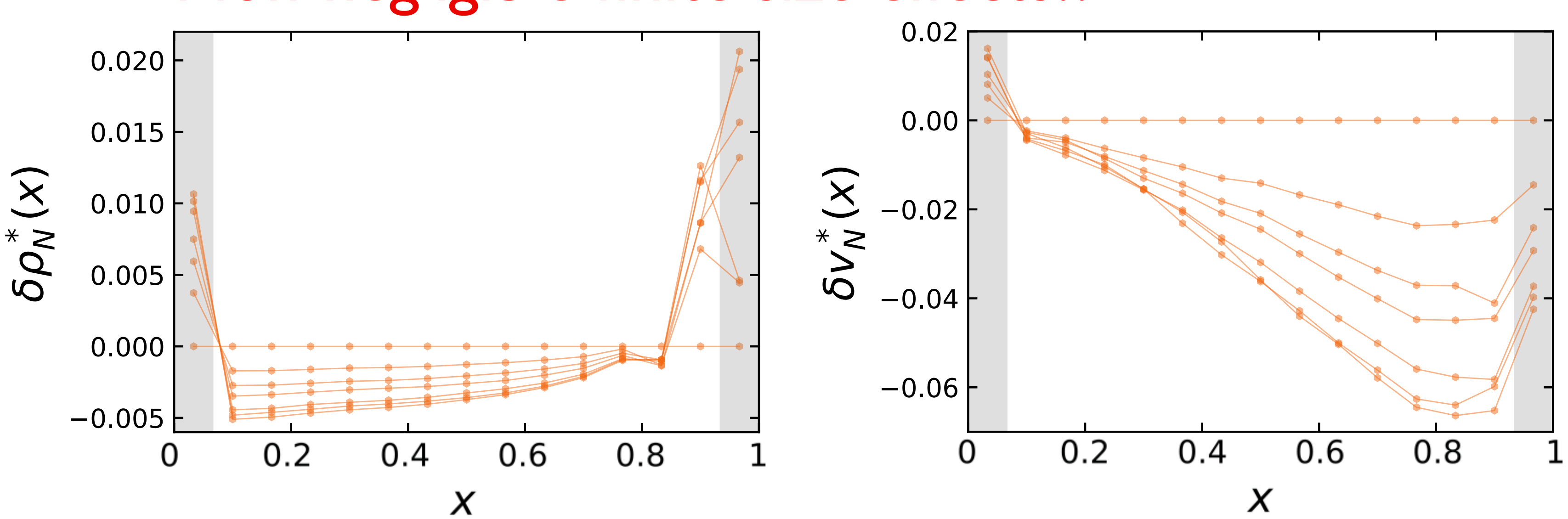
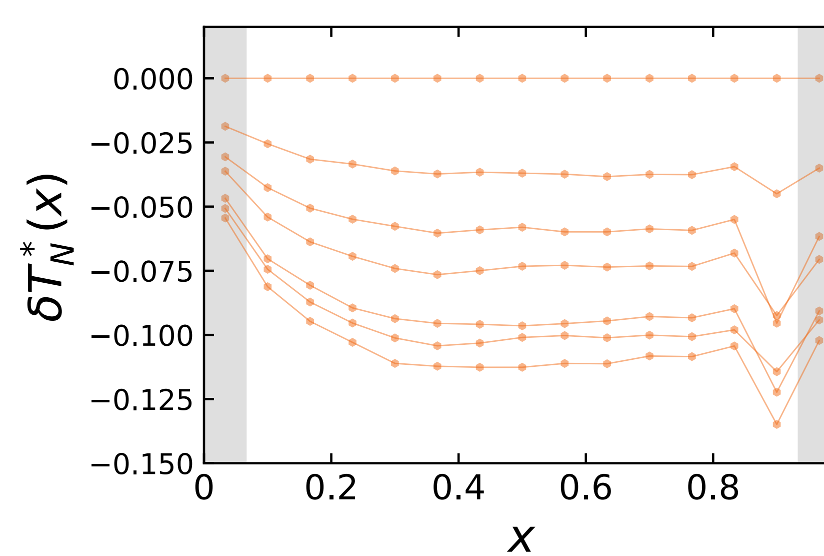


Non-negligible finite size effects!!





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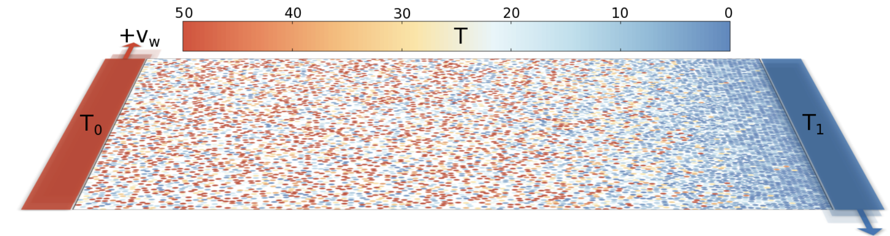

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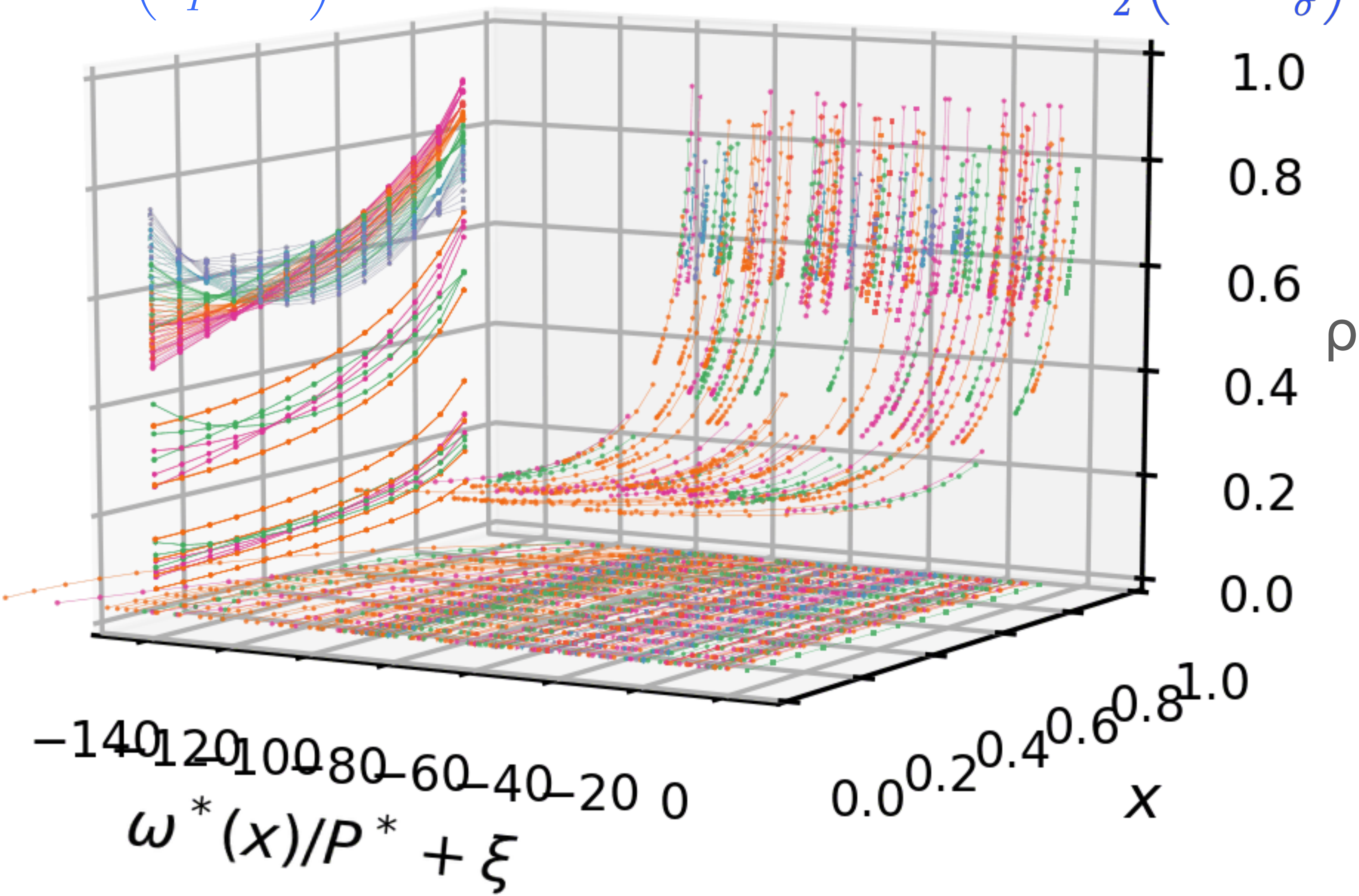

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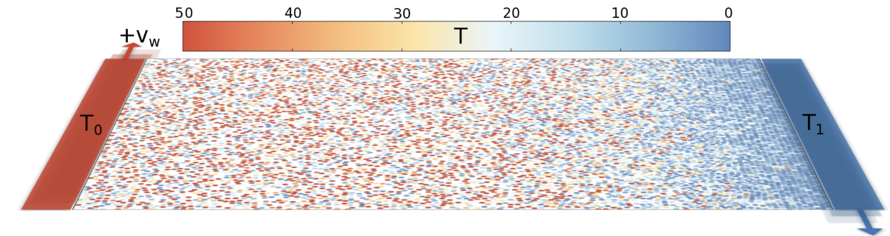

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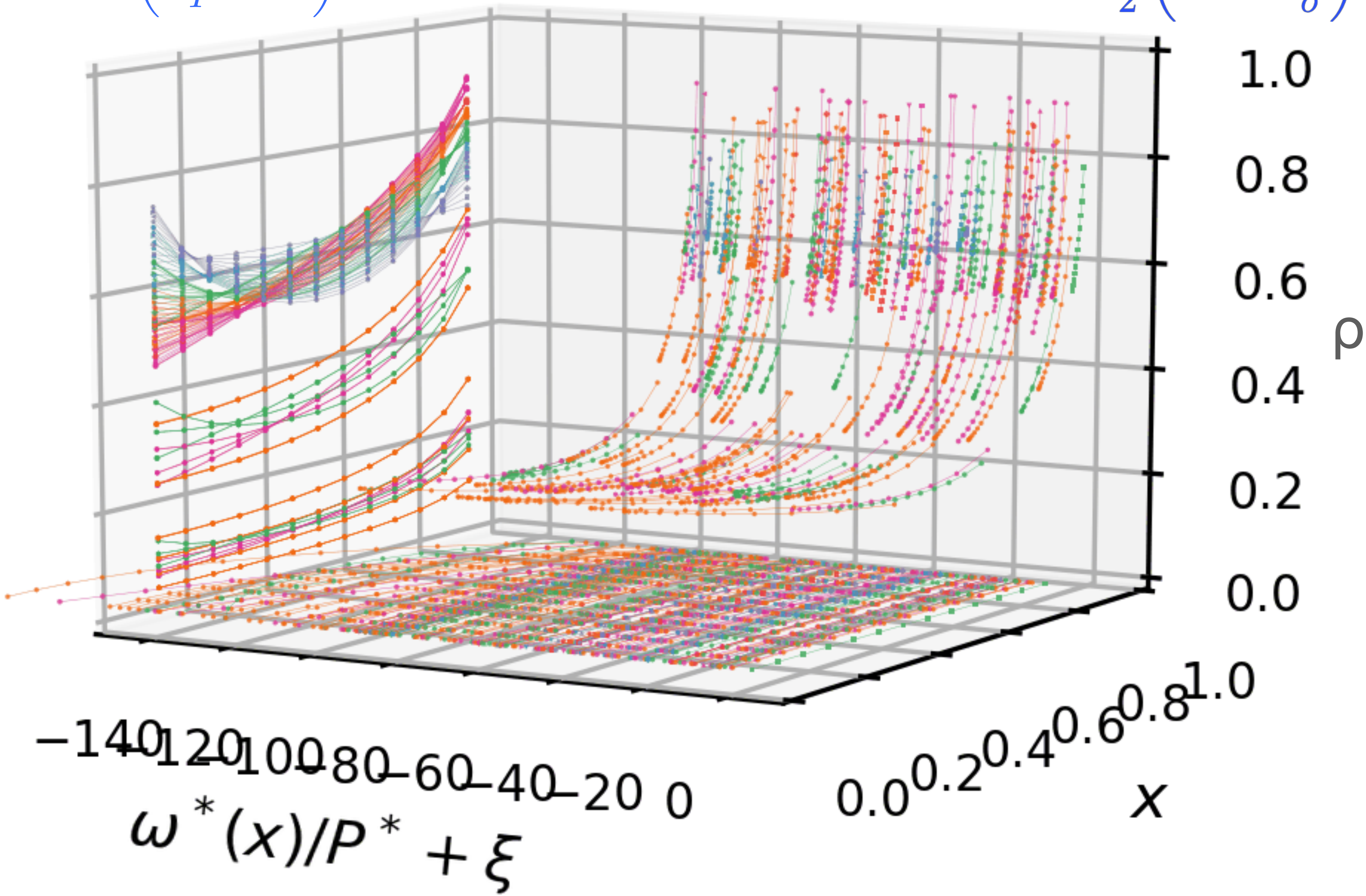

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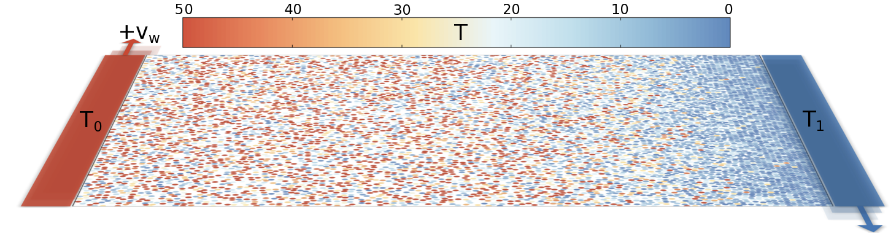

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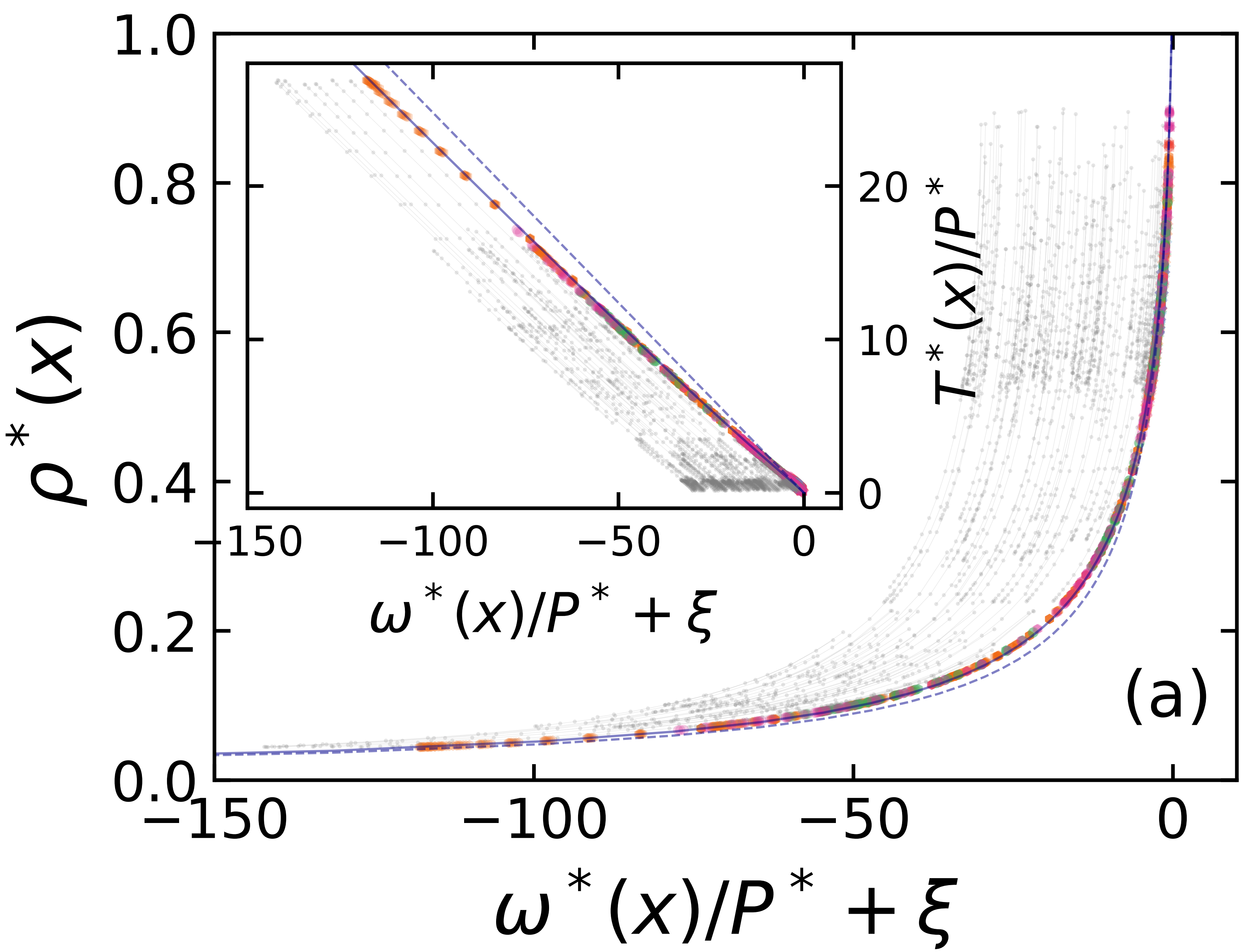

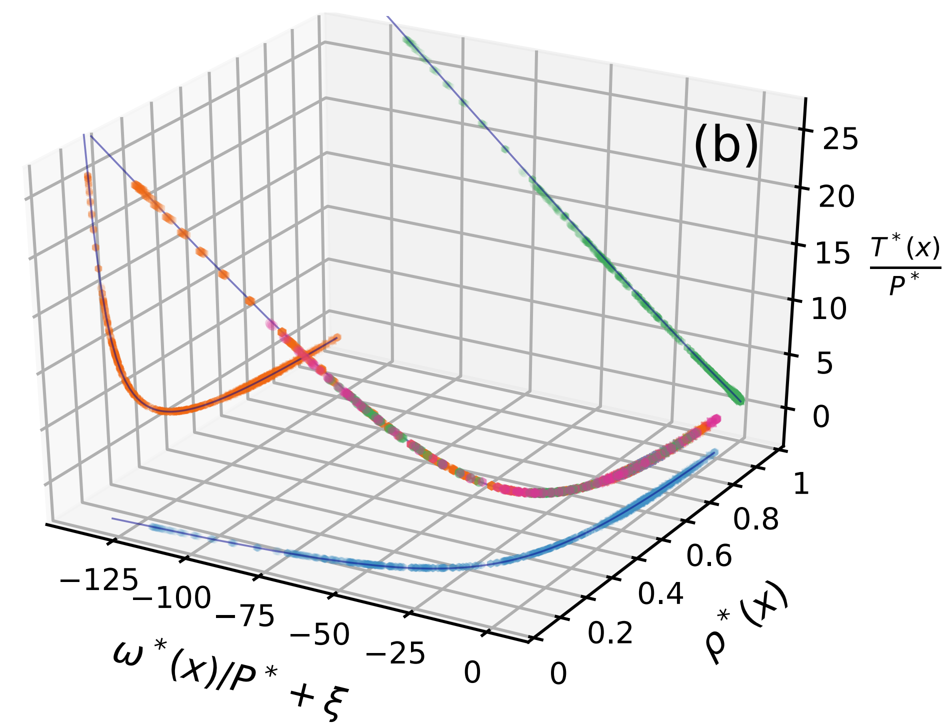

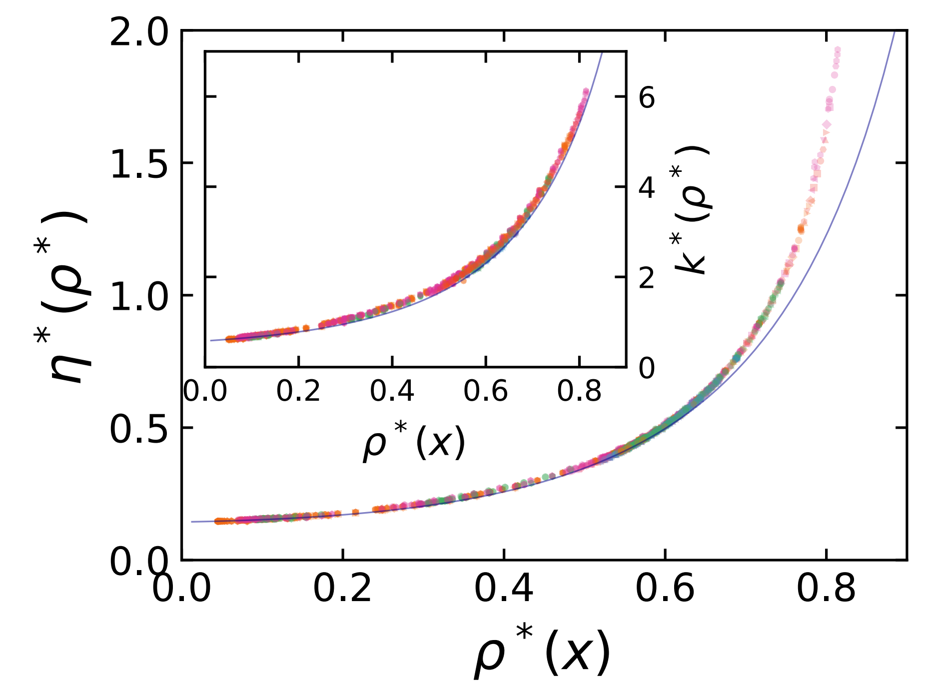

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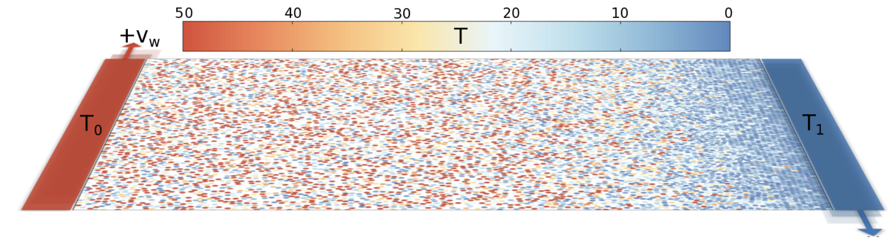

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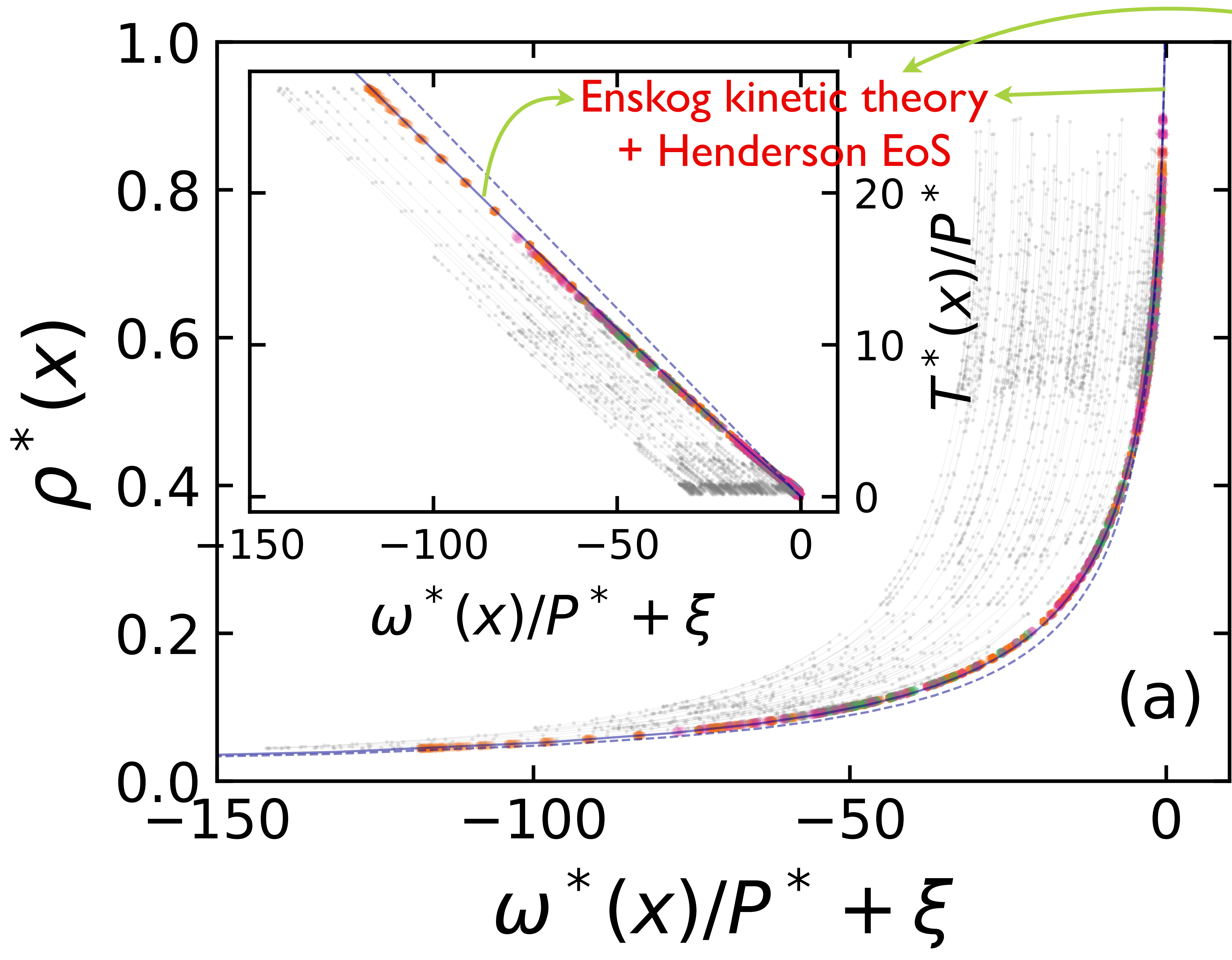

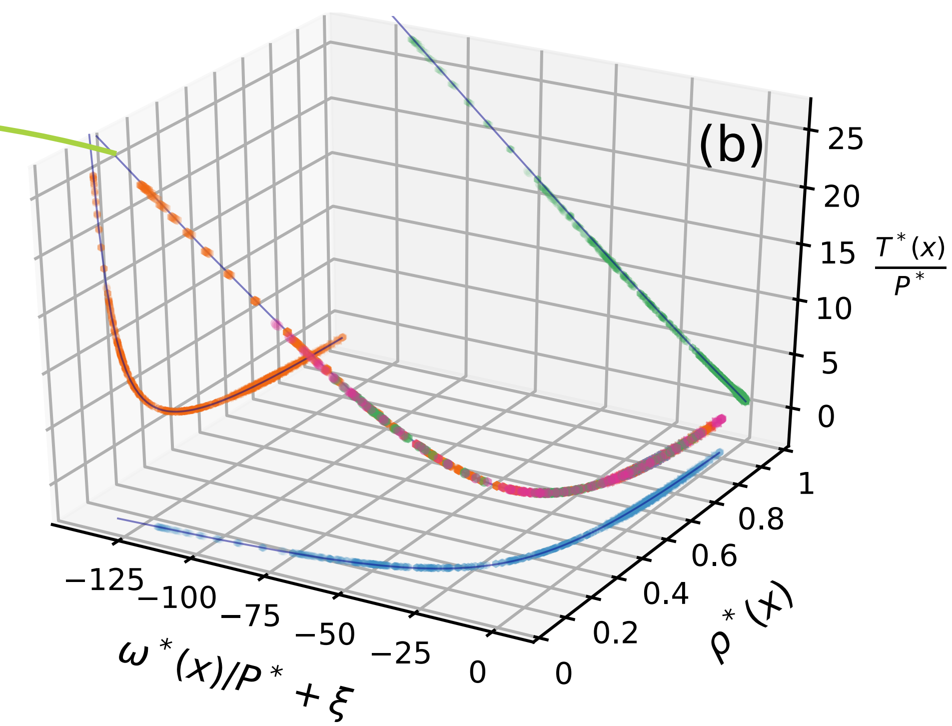

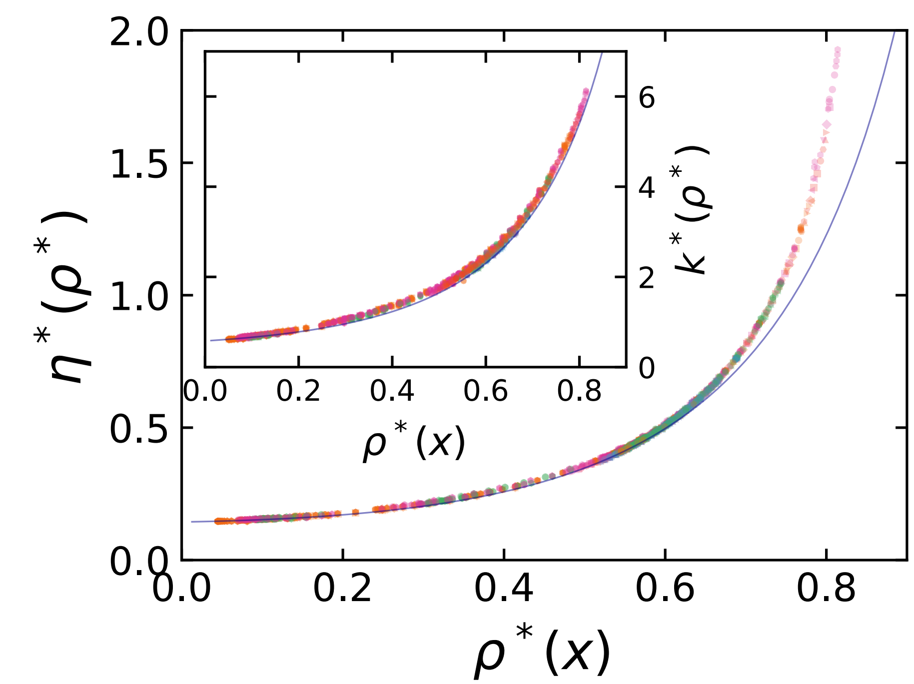

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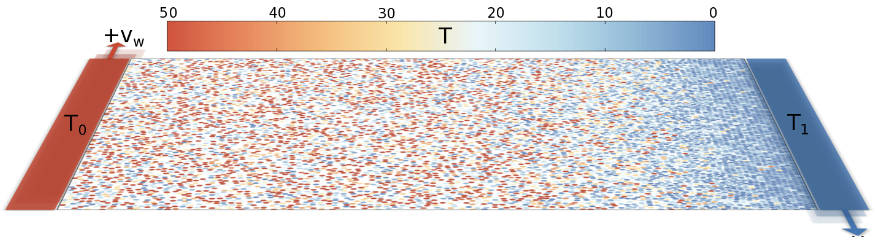

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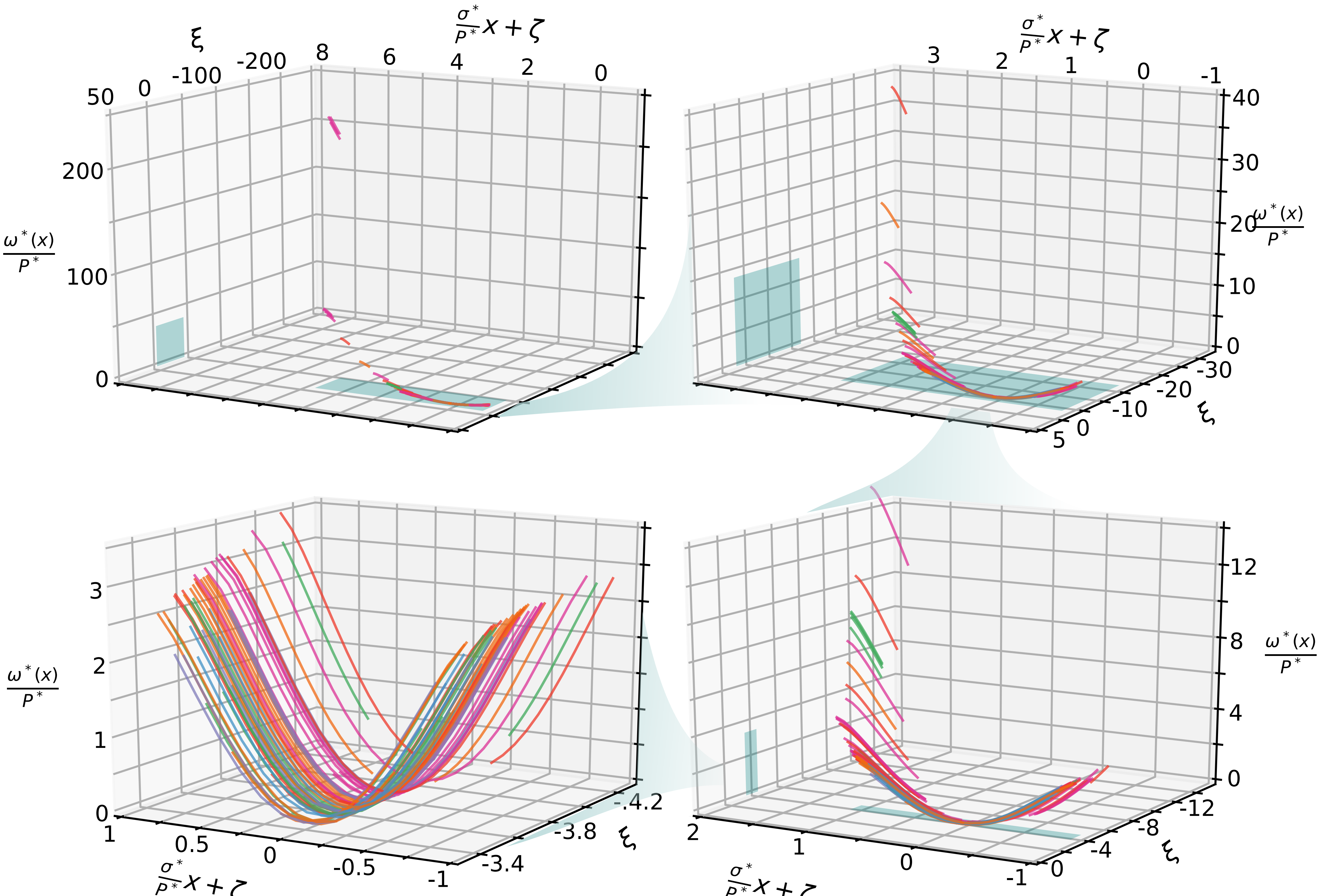

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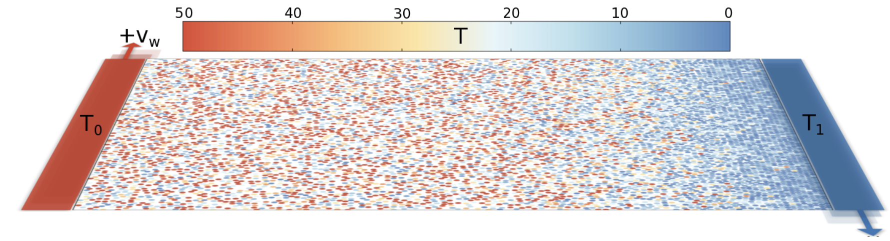

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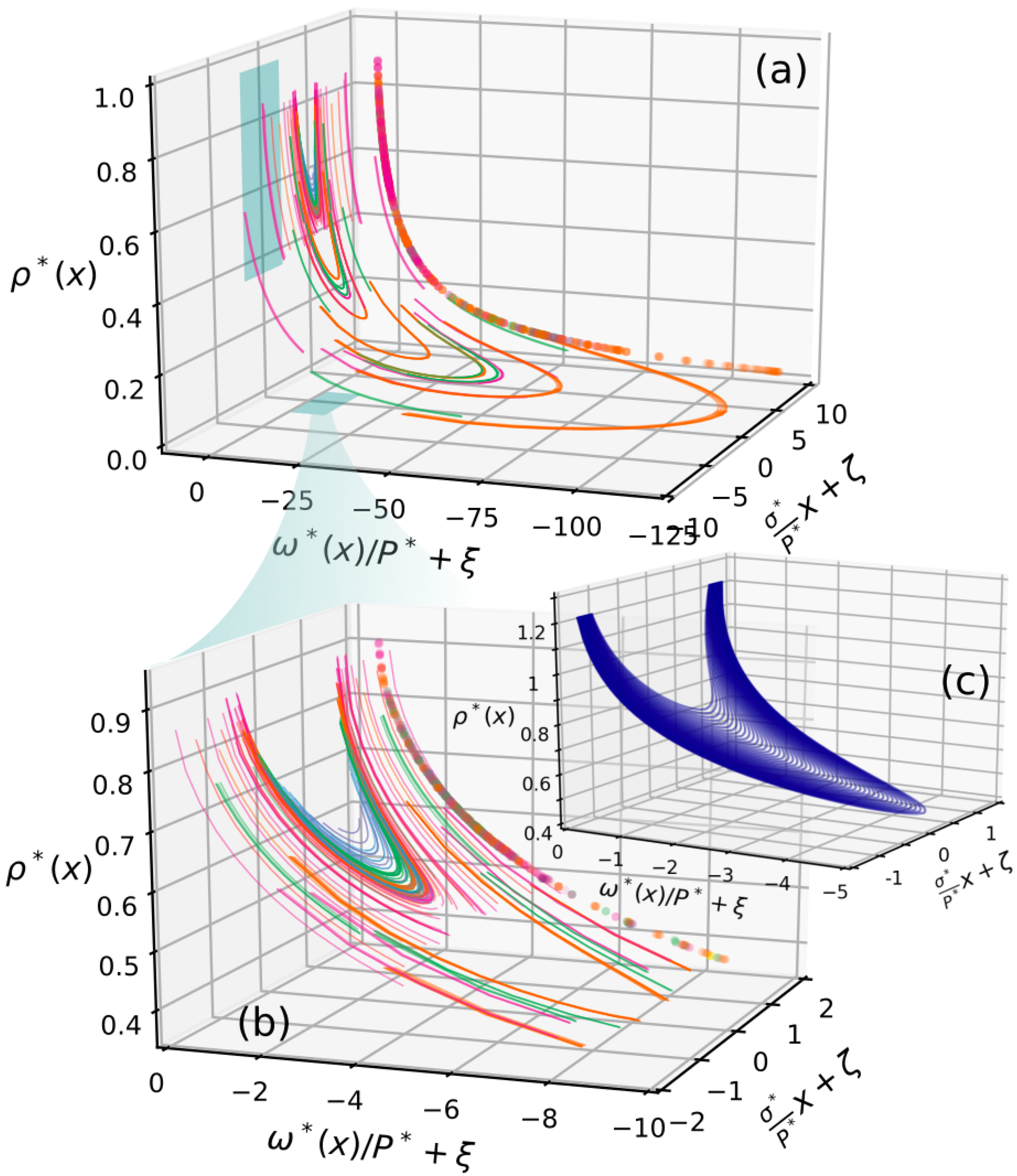

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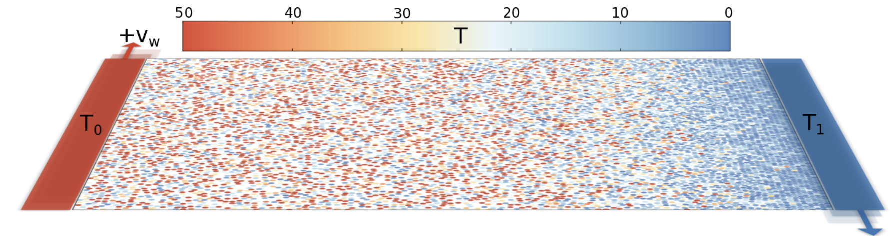

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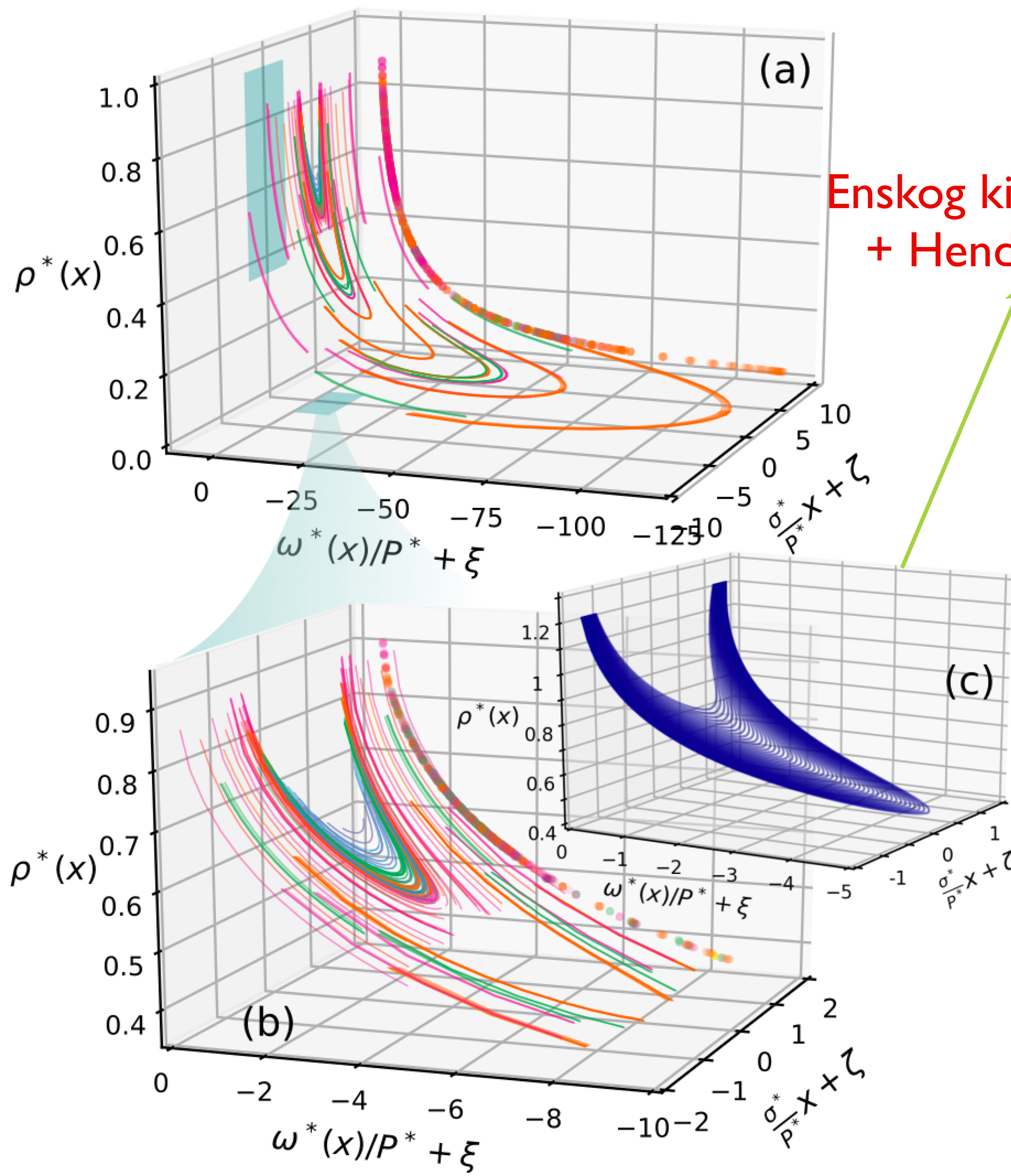
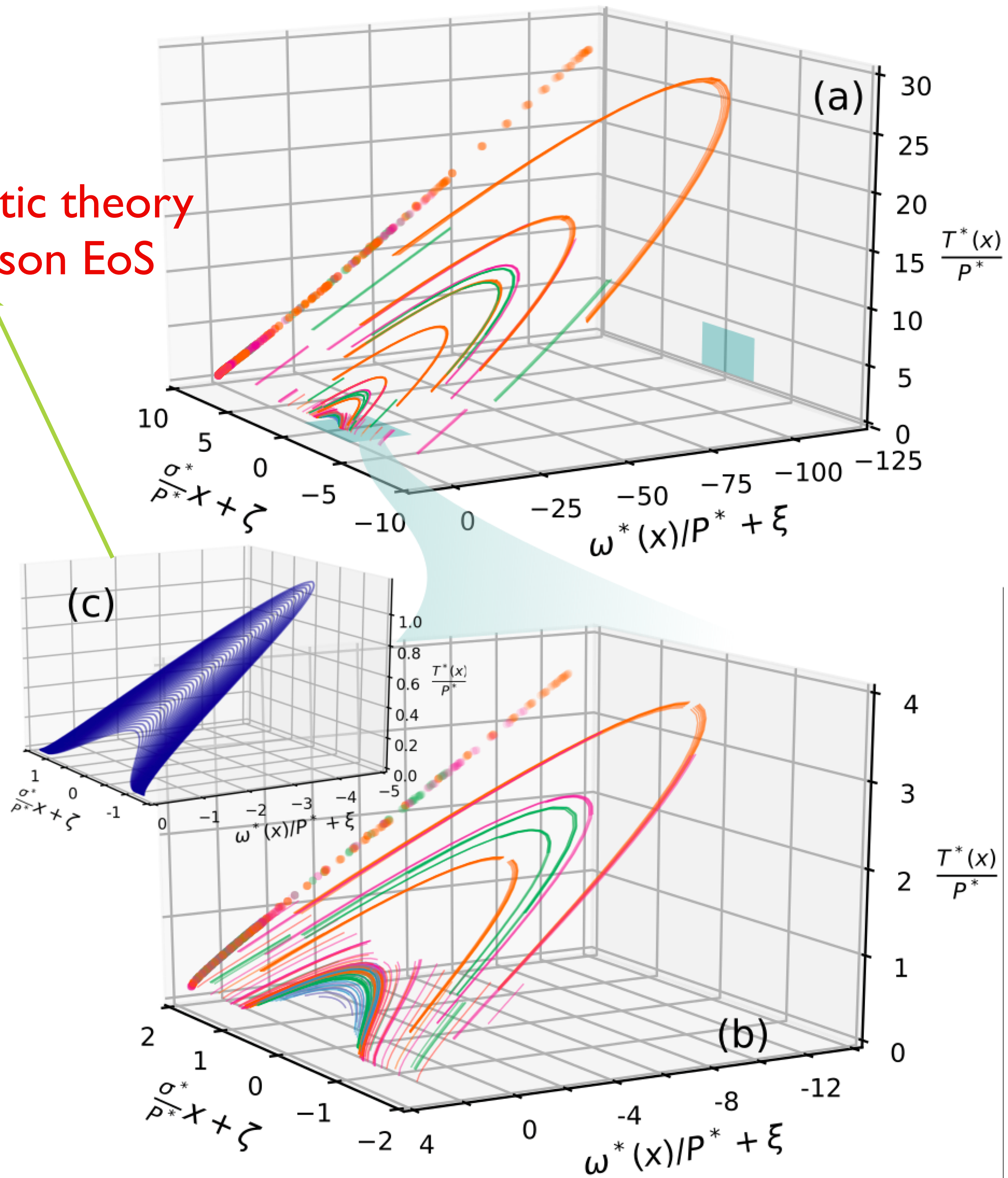
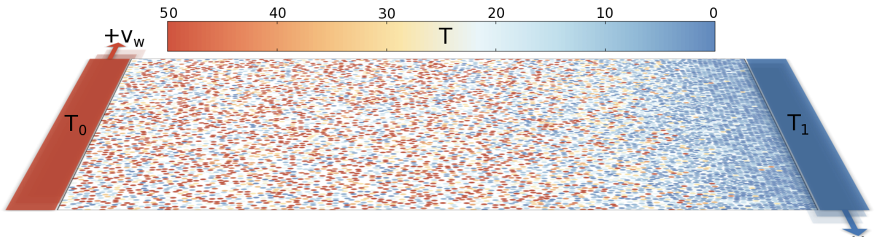
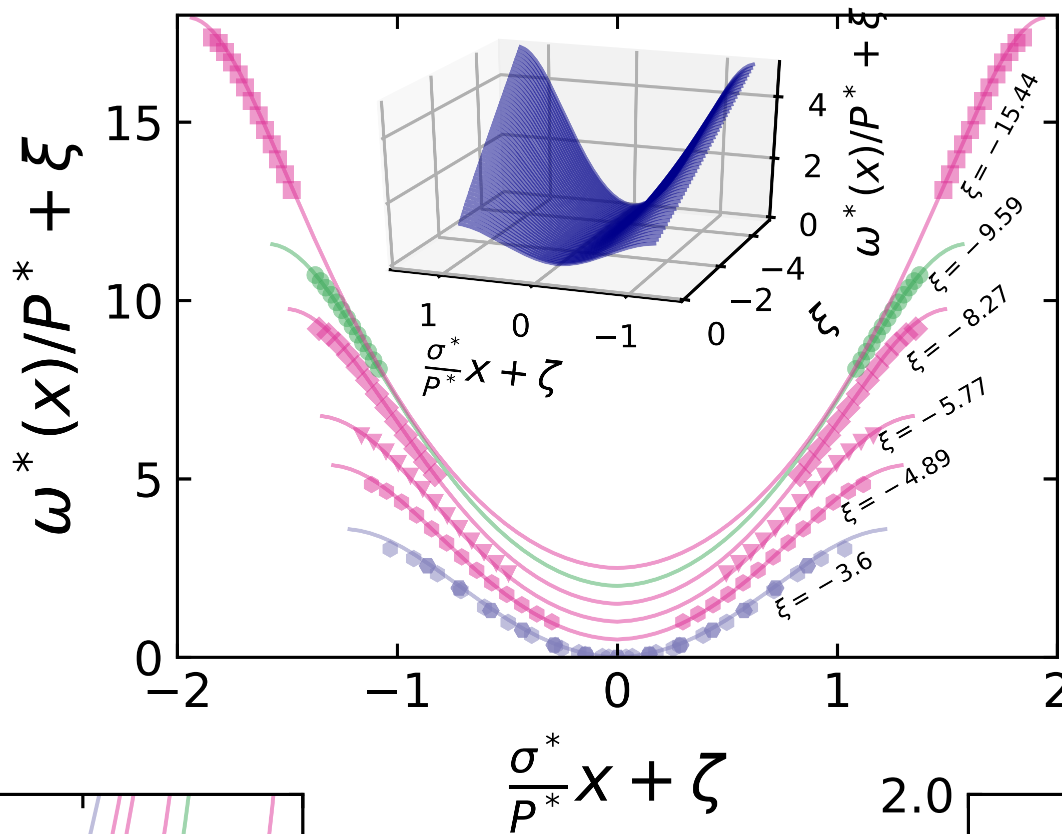


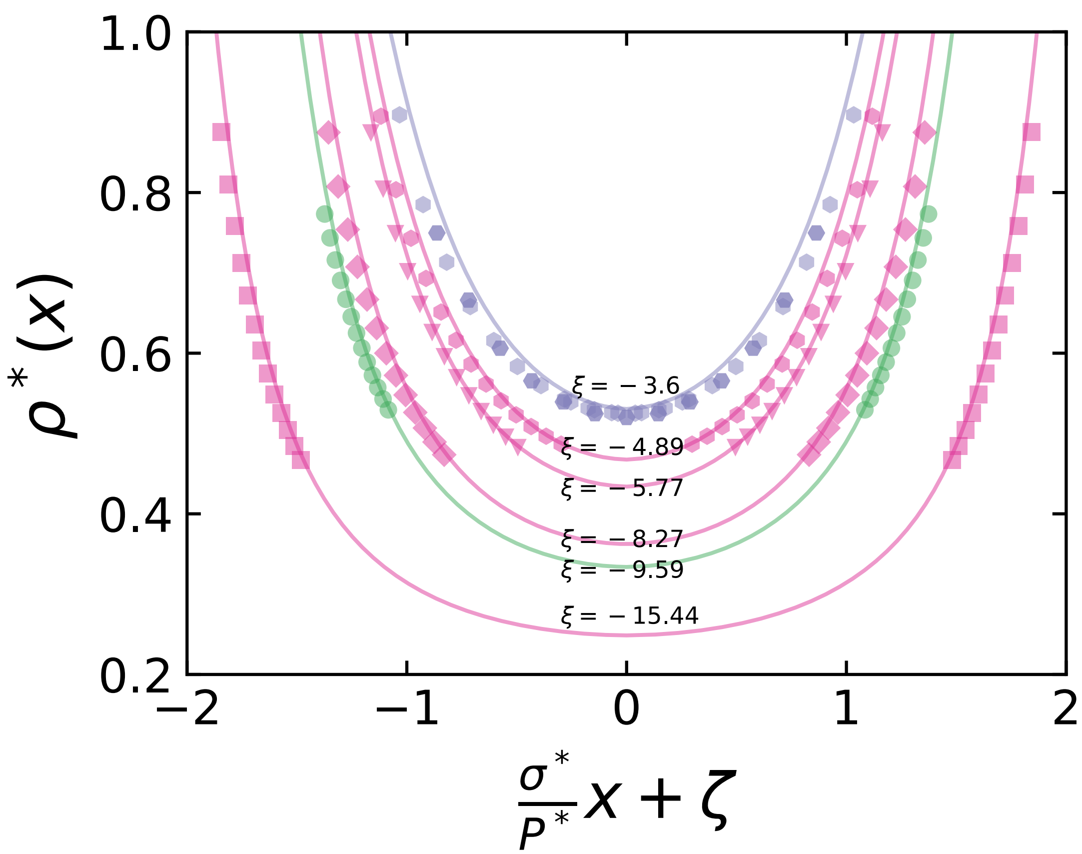
Enskog kinetic theory
+ Henderson EoS

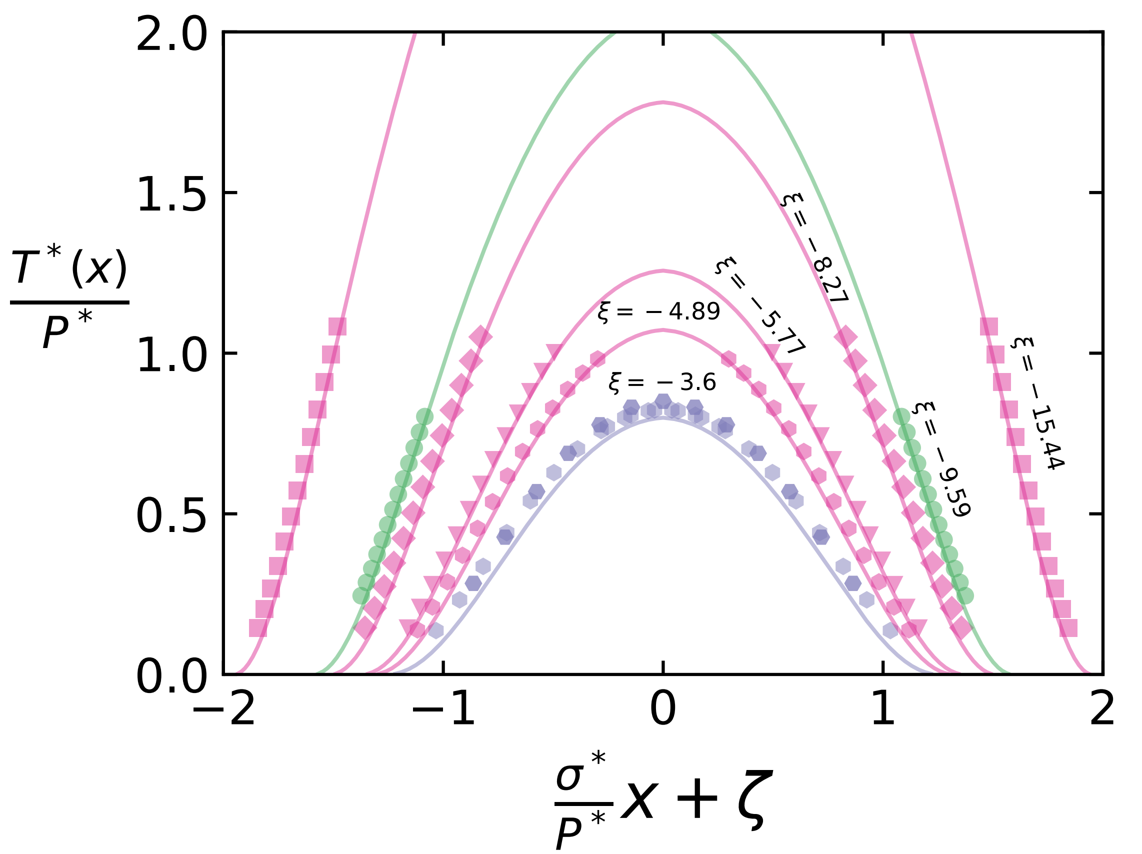


ENSKOG KINETIC THEORY









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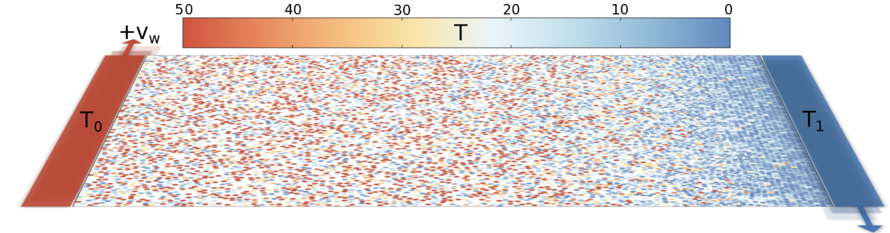
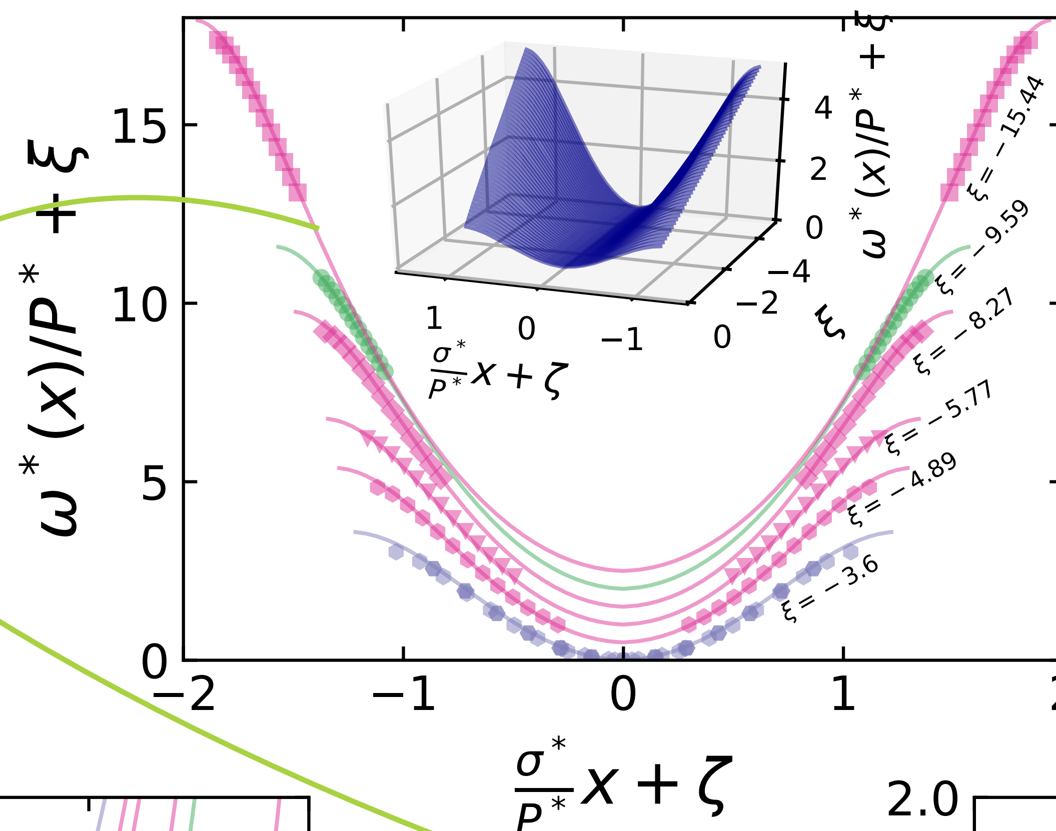
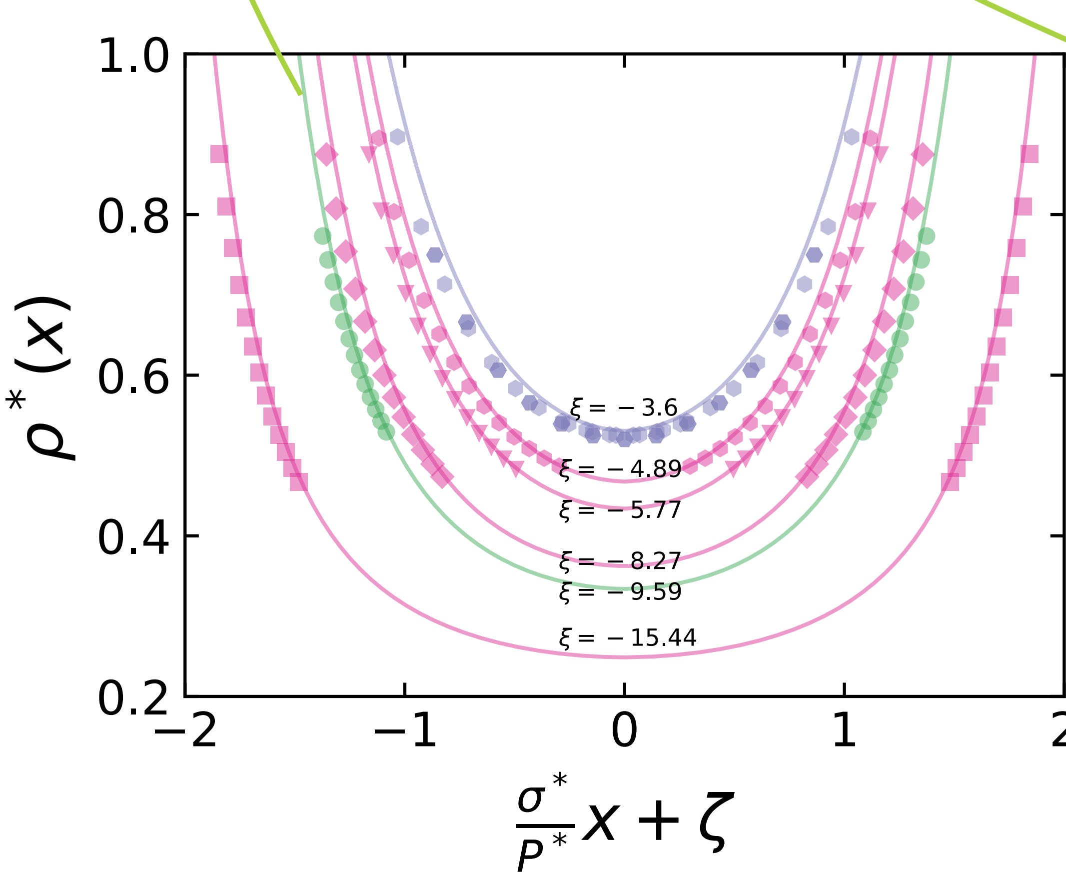
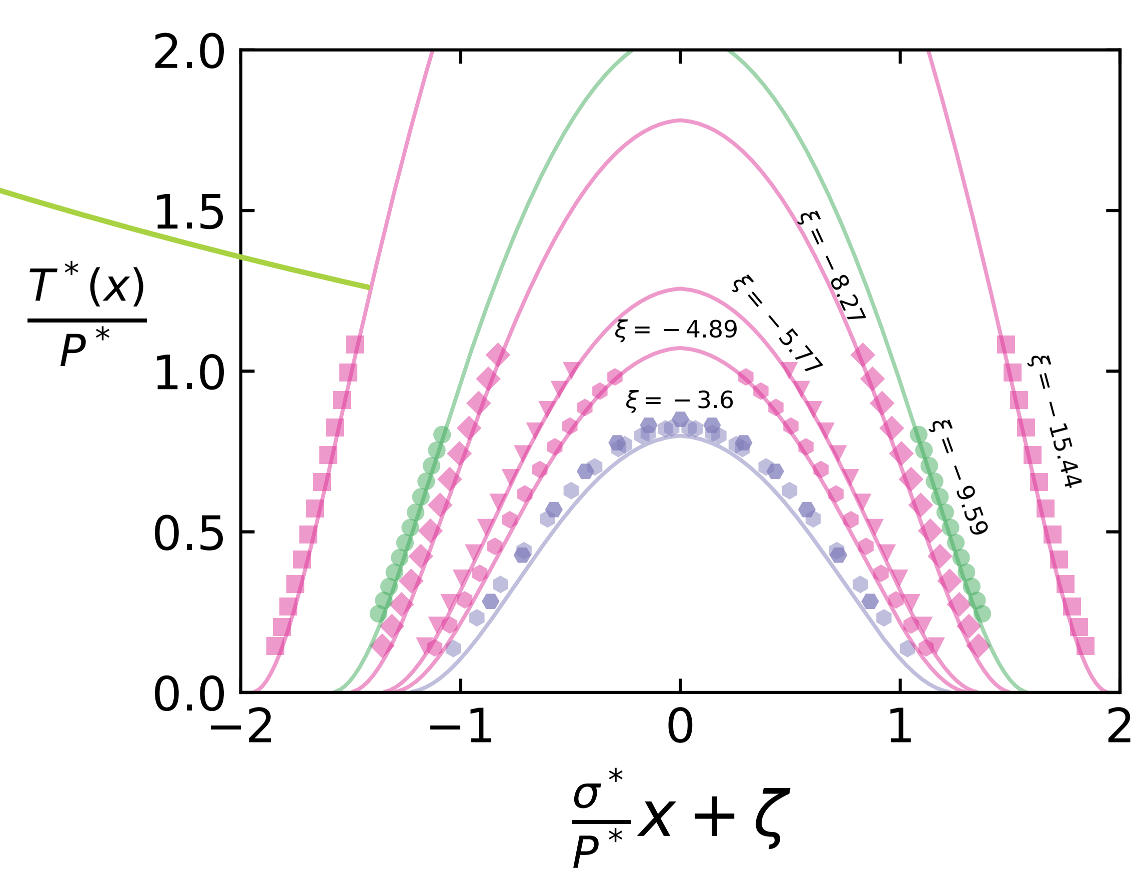


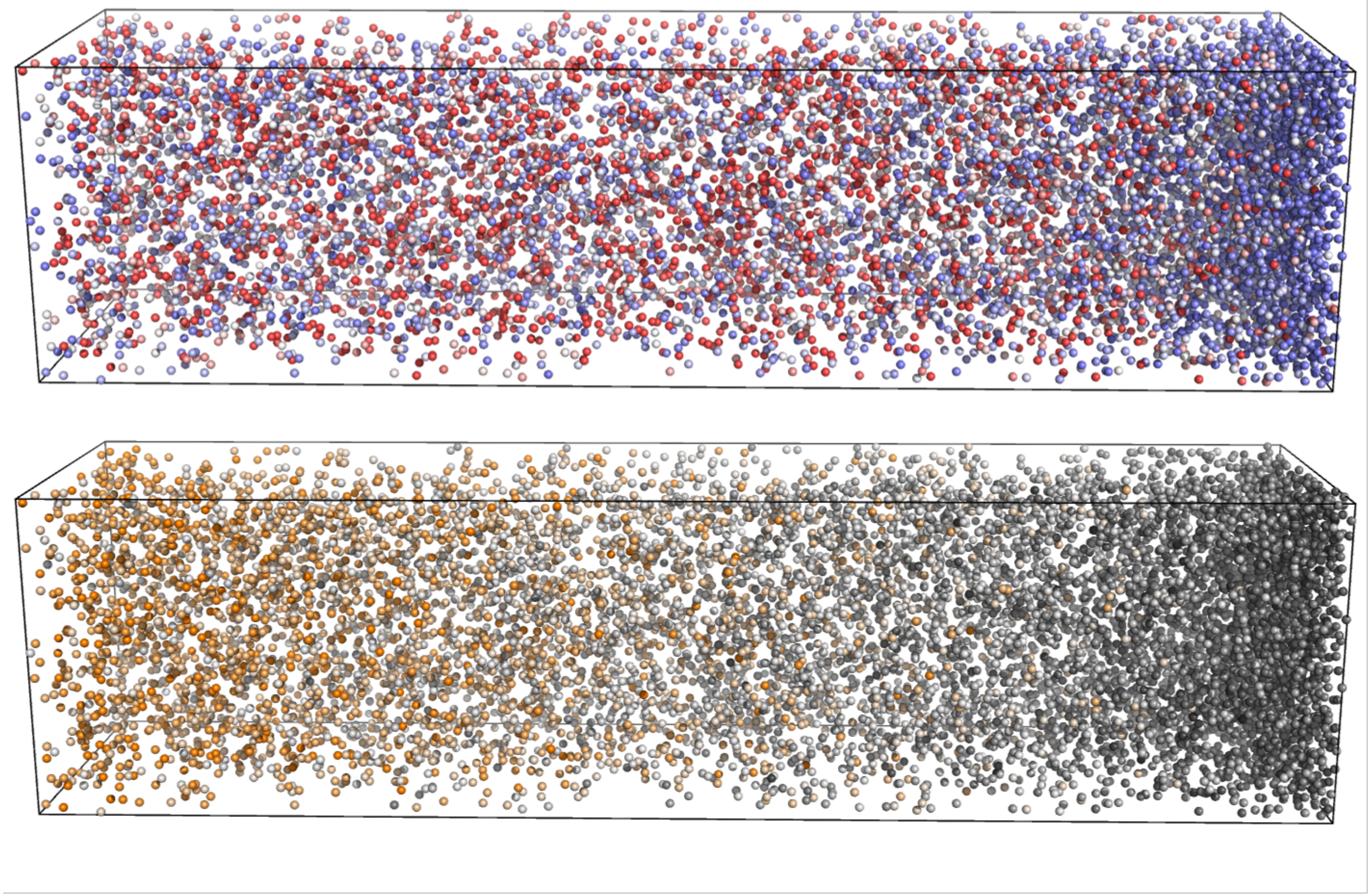


Enskog kinetic theory
+ Henderson EoS

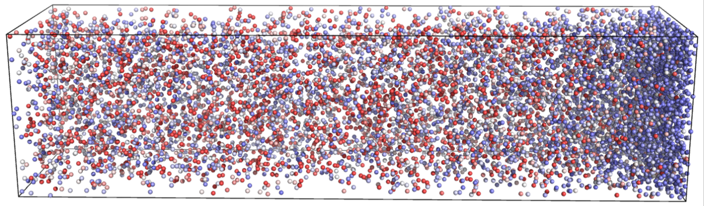


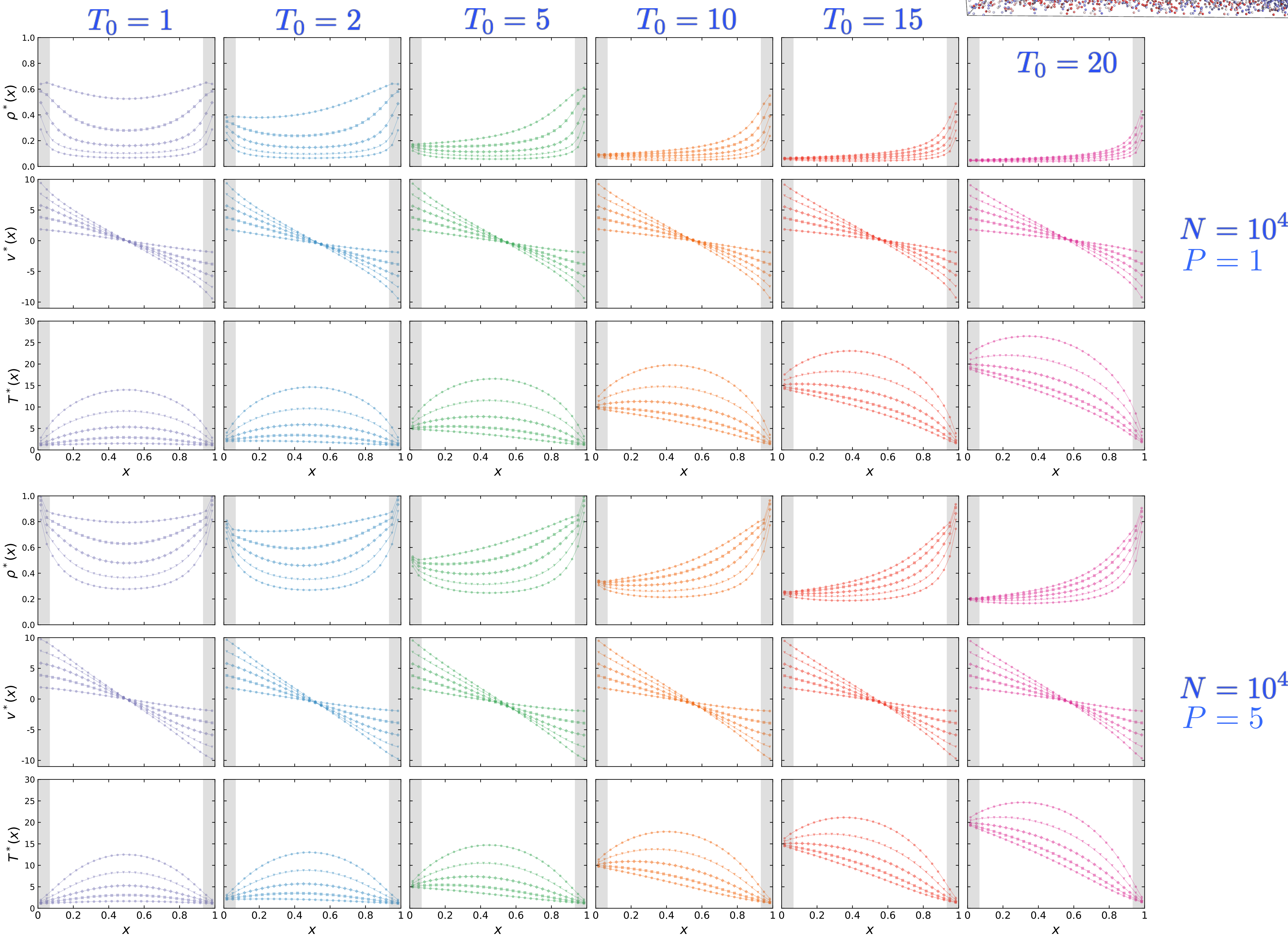


THE LENNARD-JONES FLUID

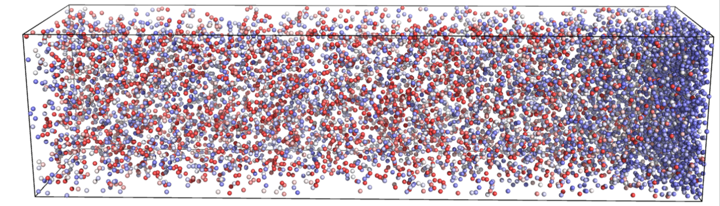


HYDRODYNAMIC FIELDS

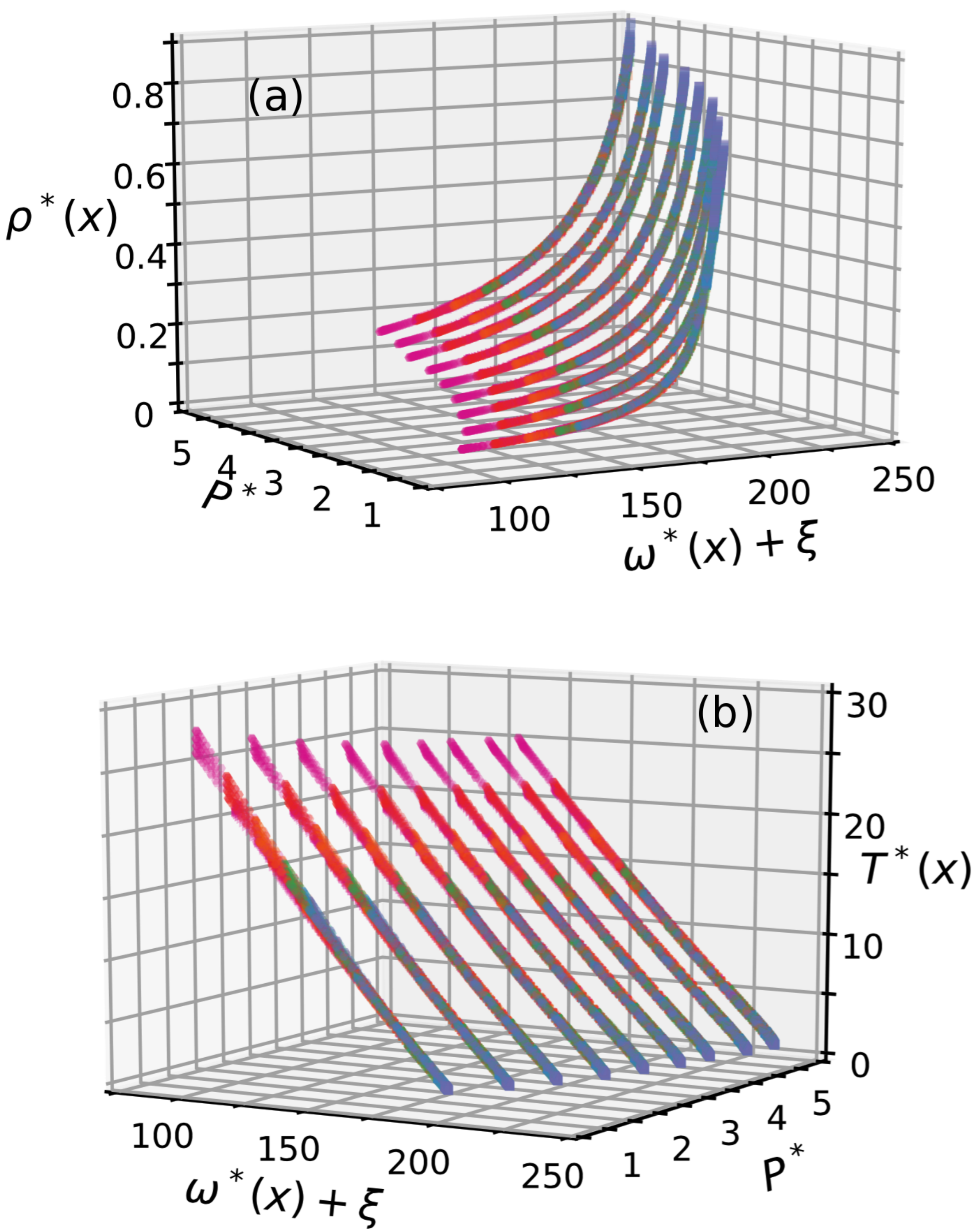


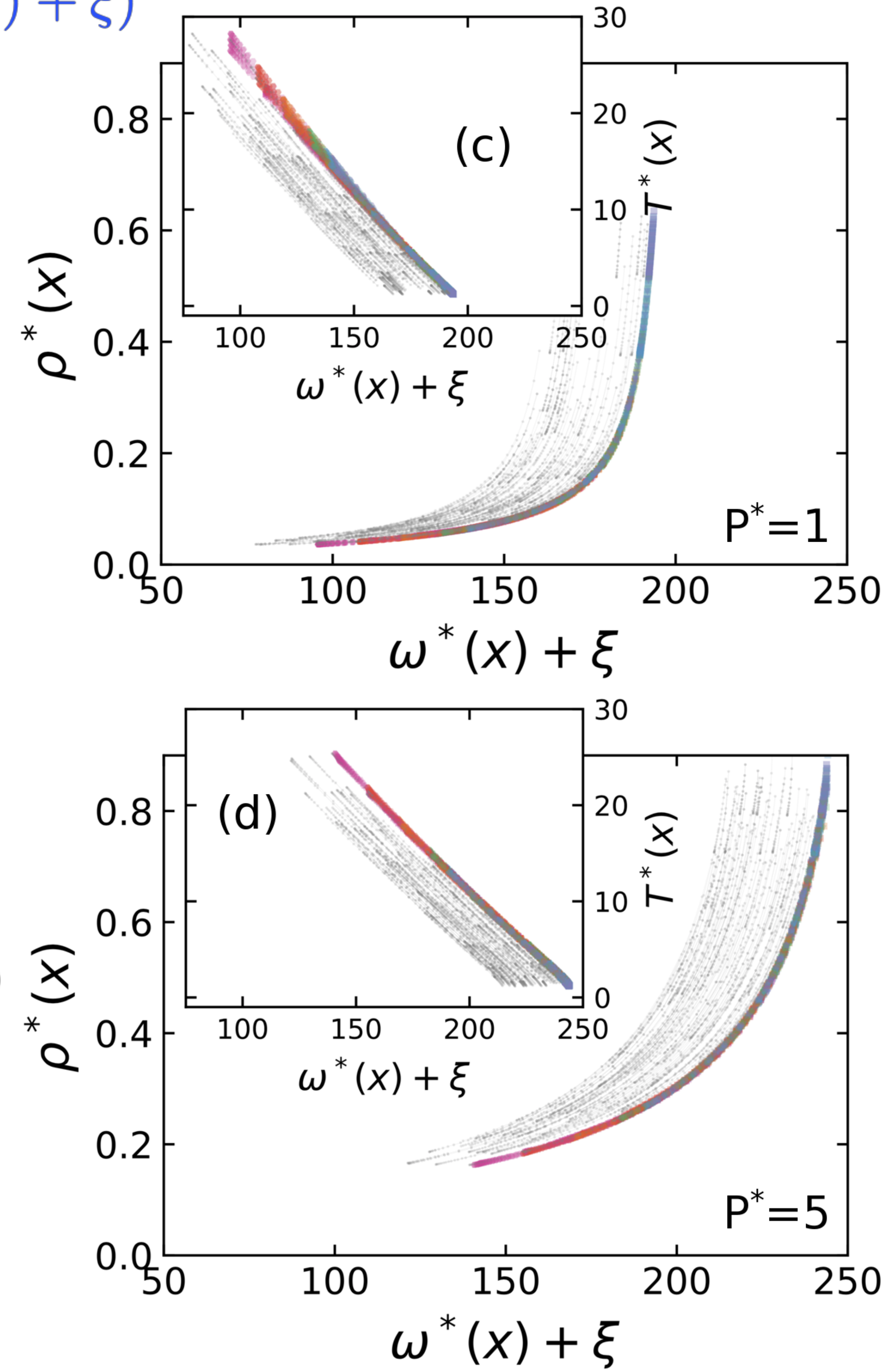


SCALING IN HYDRODYNAMIC FIELDS



$$\rho(x) = \mathcal{R}_P\left(\omega(x) + \xi\right) \qquad T(x) = \mathcal{T}_P(\omega(x) + \xi)$$





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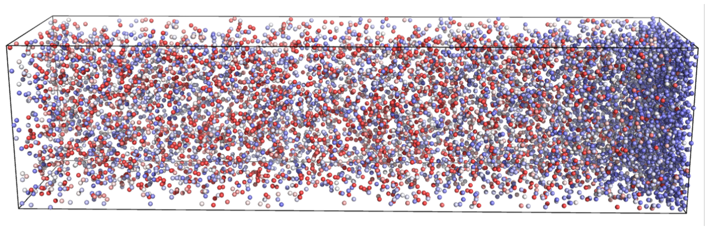
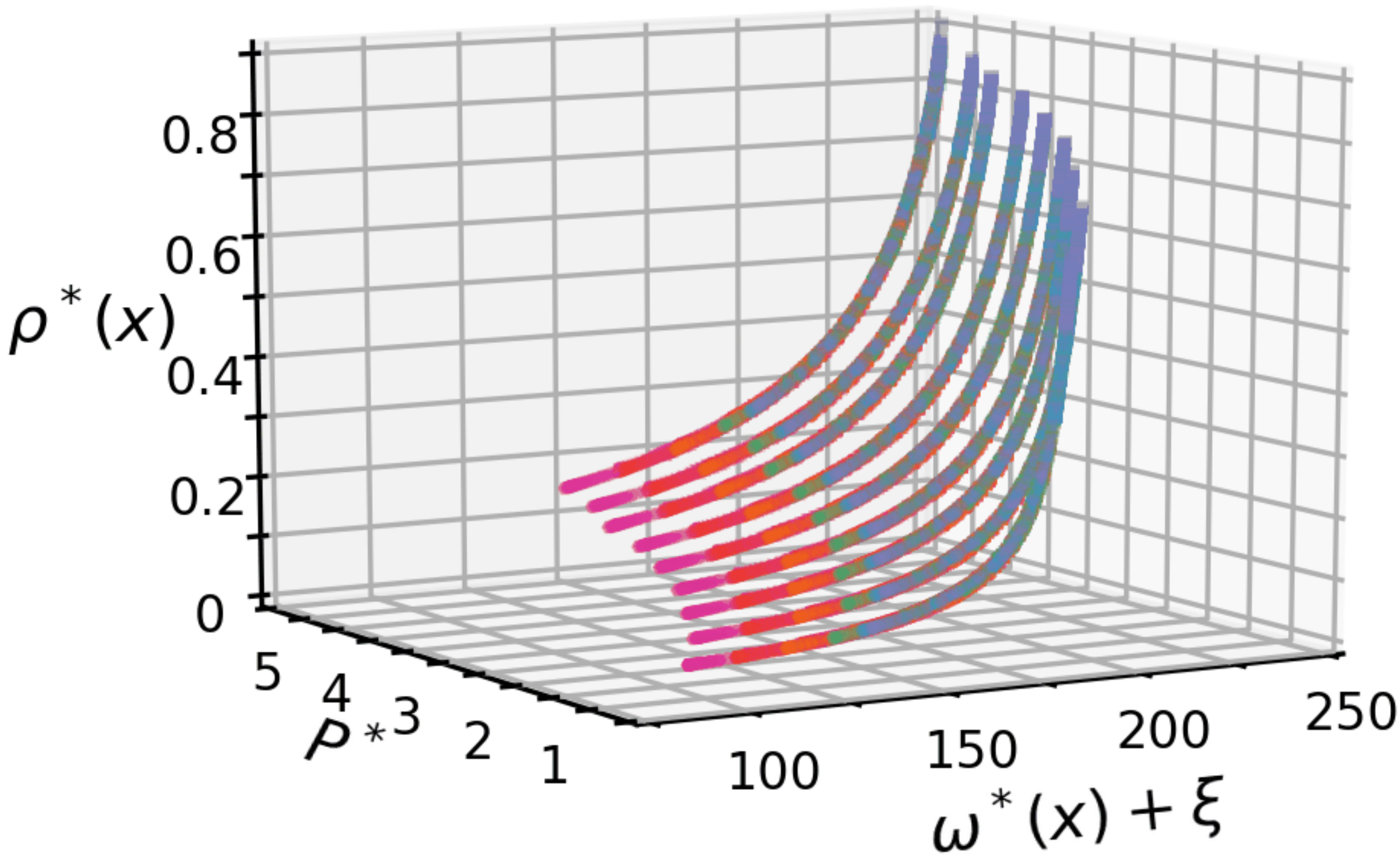


$\rho(x) = \mathcal{R}_P\left(\omega(x) + \xi\right)$ $\qquad$ $T(x) = \mathcal{T}_P(\omega(x) + \xi)$



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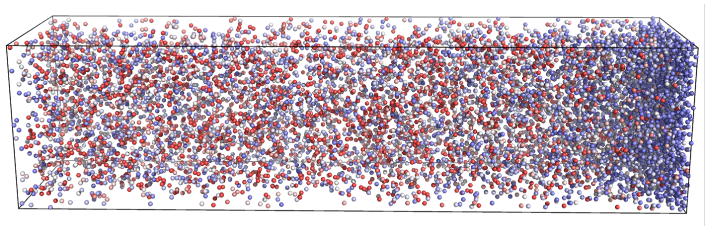

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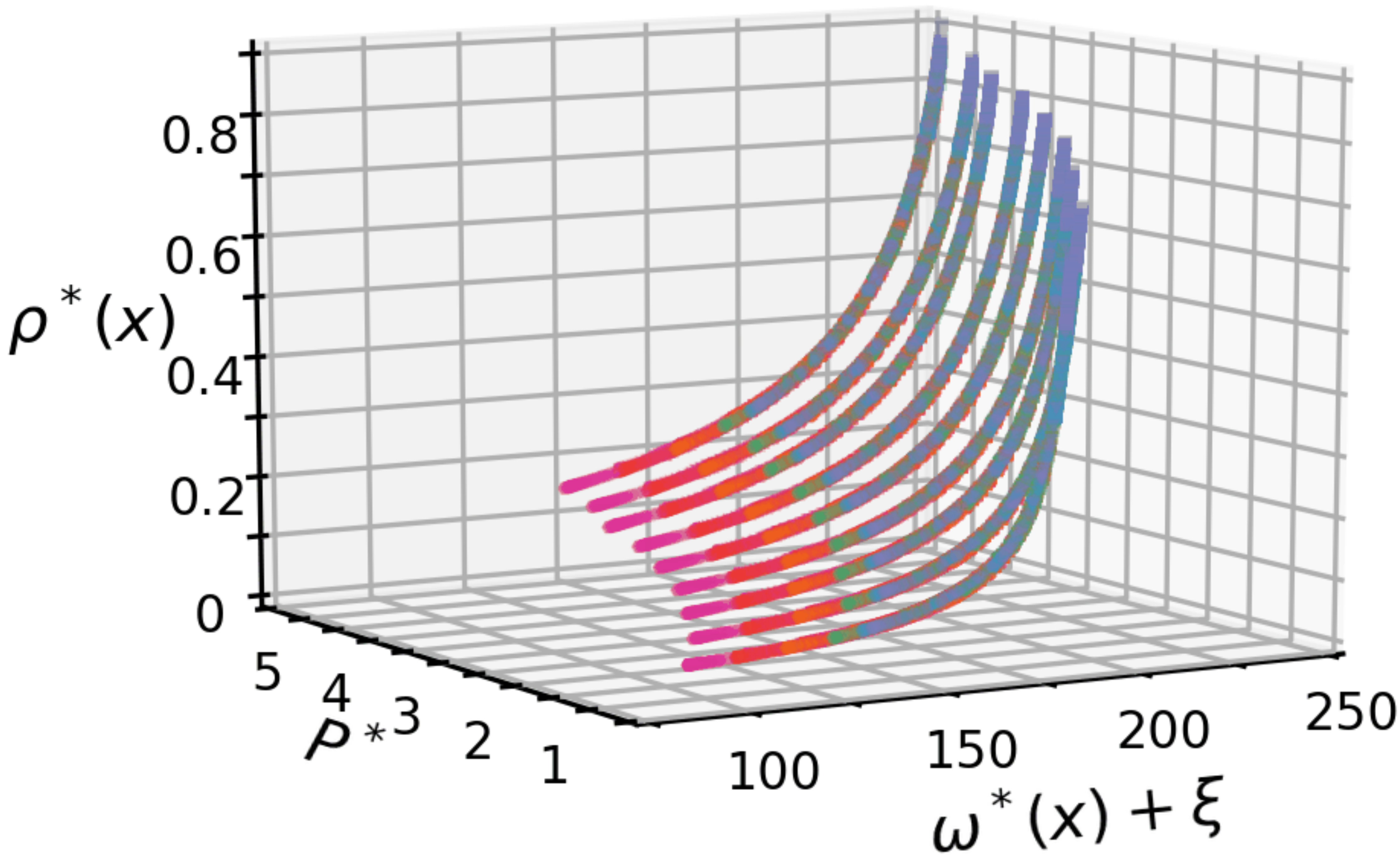

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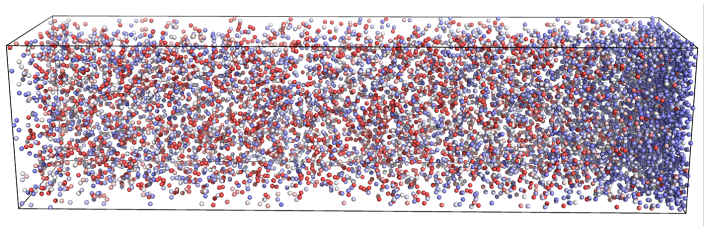
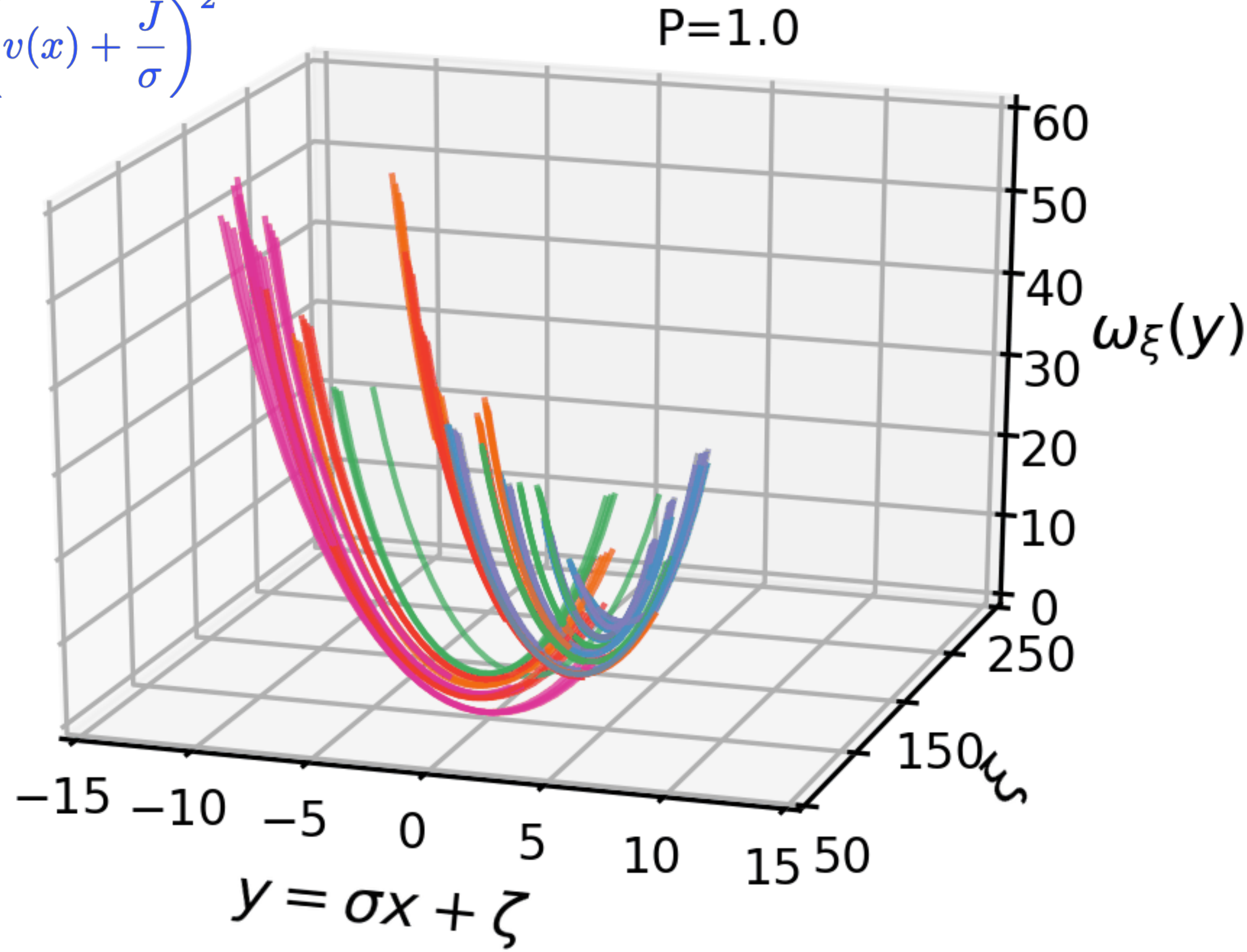
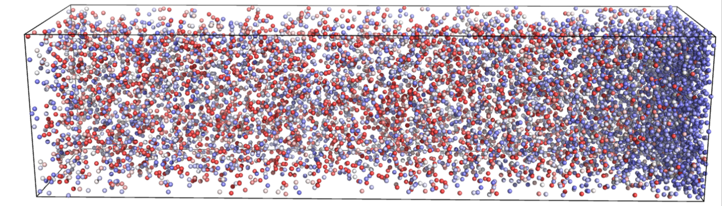


$$\omega(x) = \mathcal{W}_{P,\xi}(\pm\sigma x + \zeta)$$

$$\omega(x) \equiv \frac{1}{2}\left(v(x) + \frac{J}{\sigma}\right)^2$$





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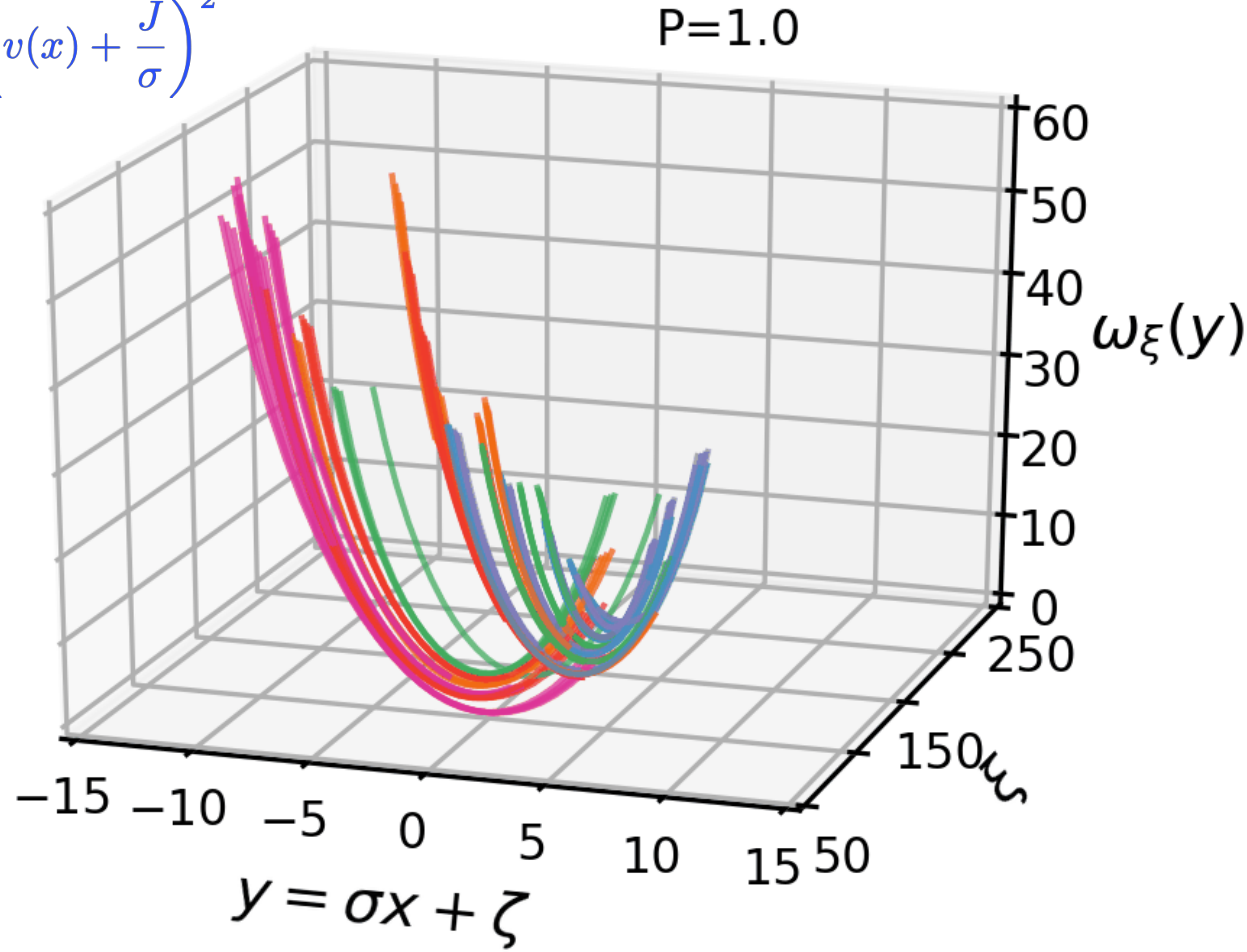

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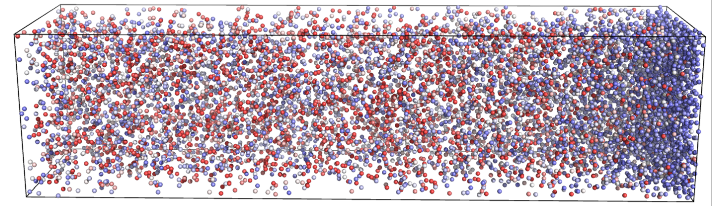
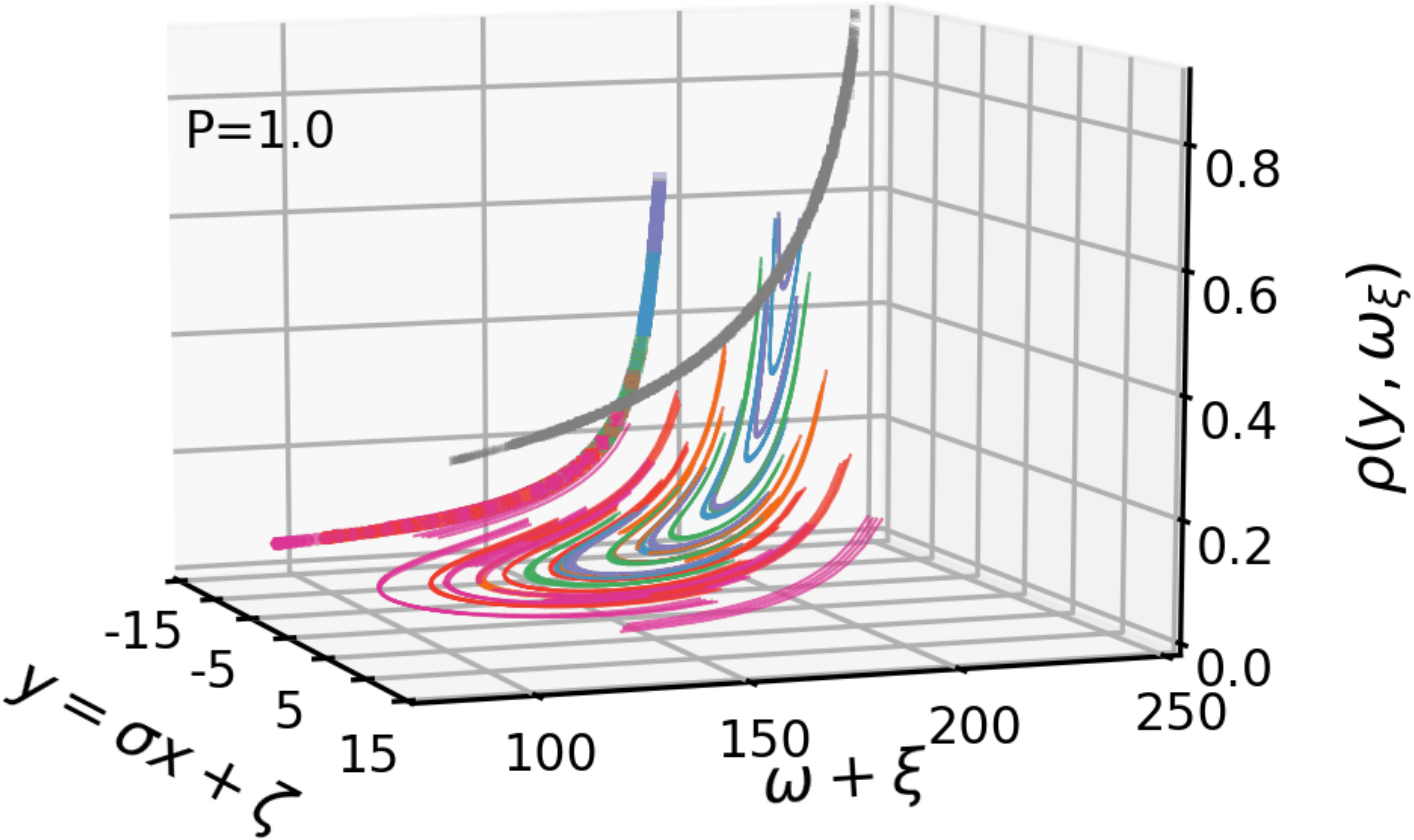


$$\rho(x) = \bar{\mathcal{R}}_P(\pm\sigma x + \zeta, \omega + \xi)$$



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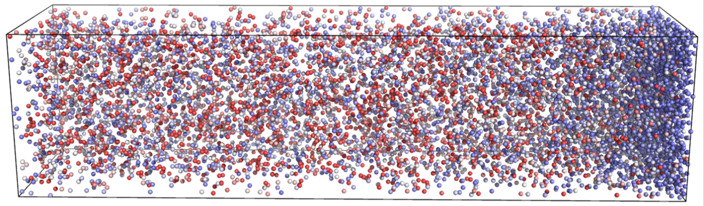

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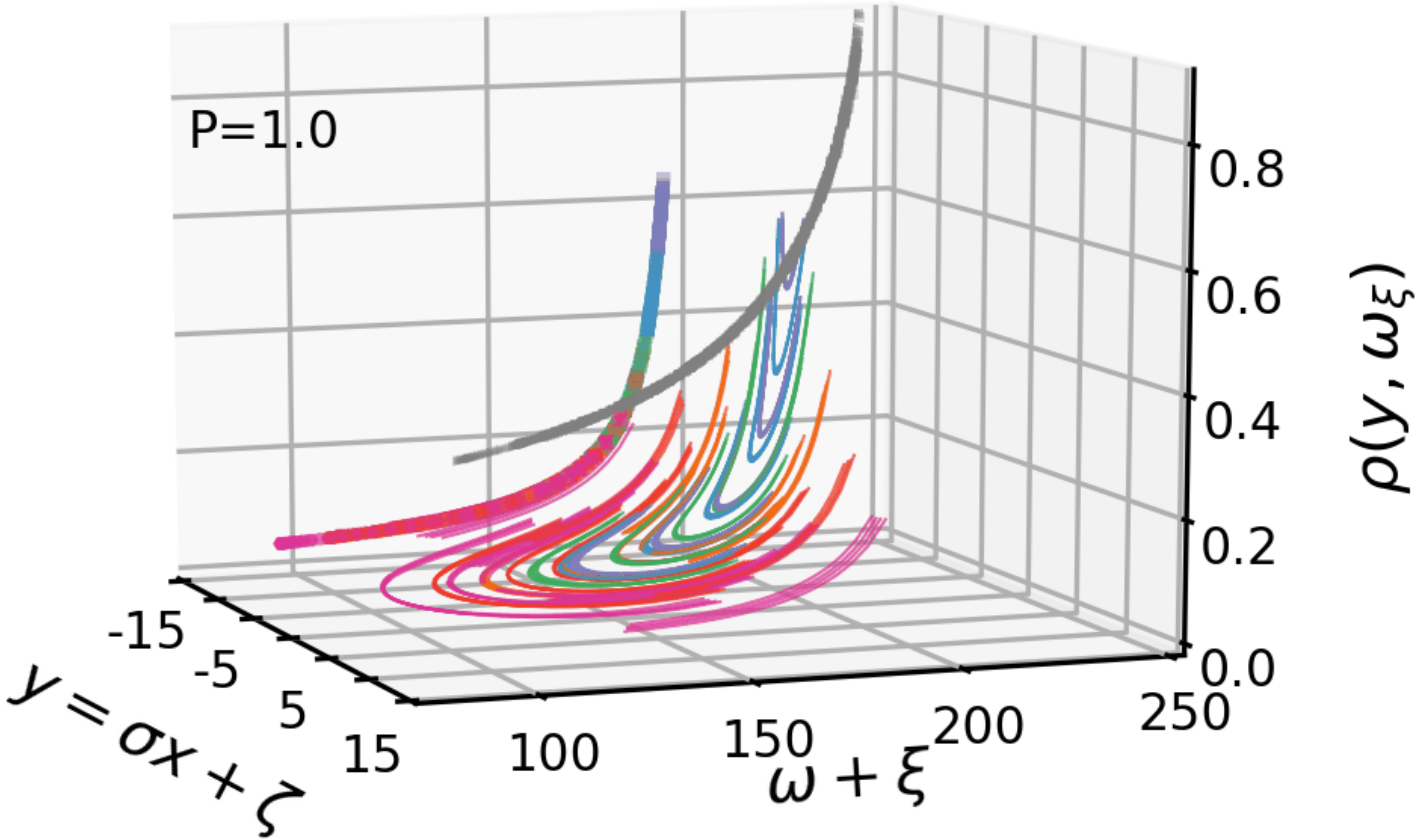

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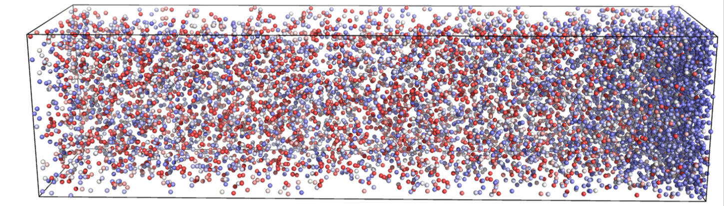

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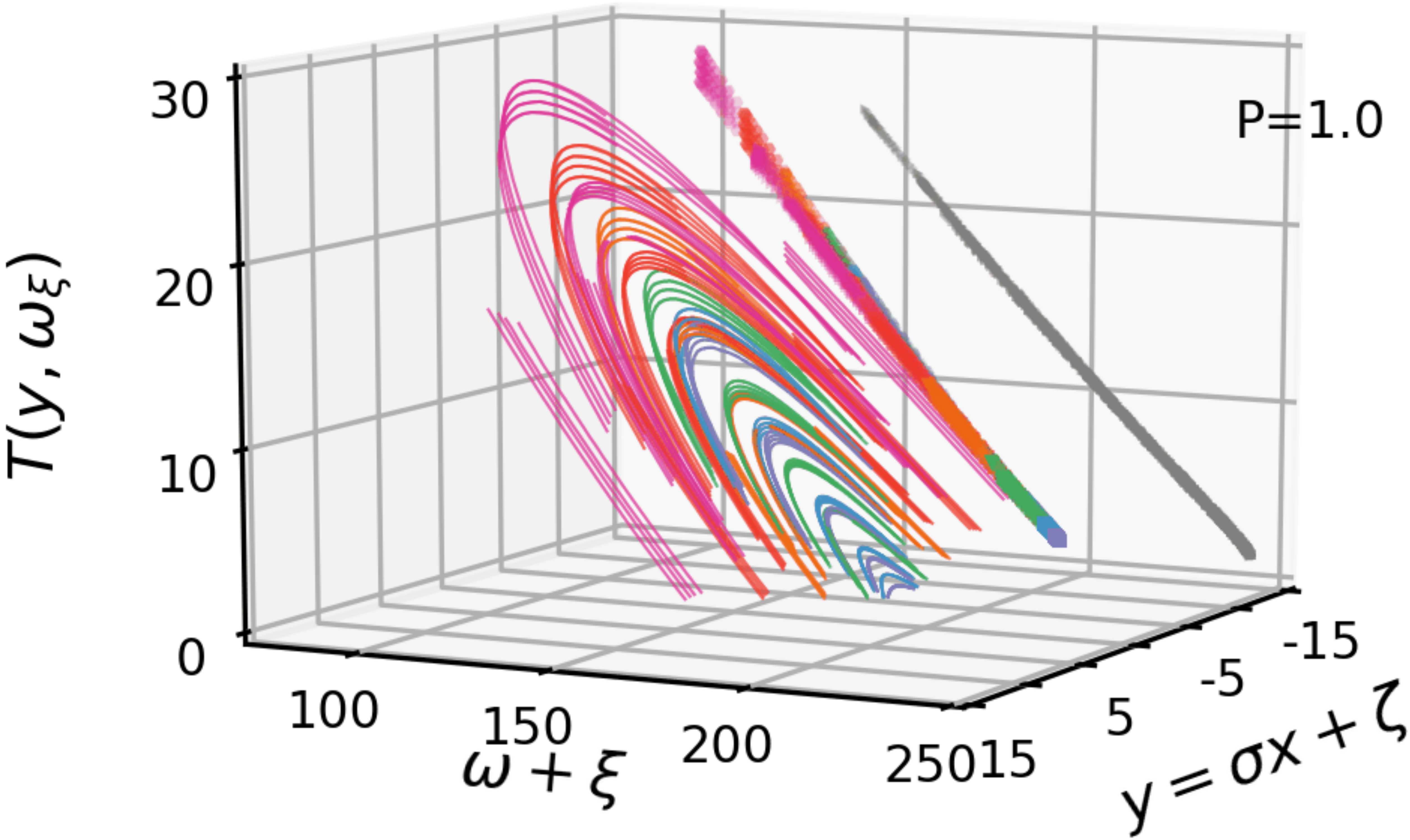
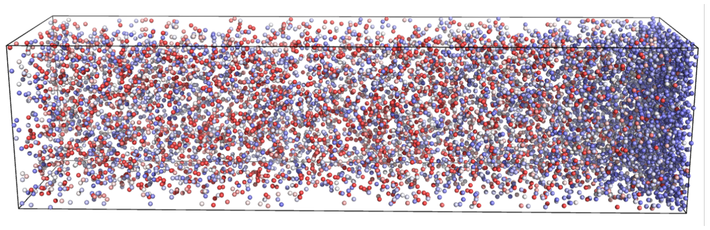


SCALING IN HYDRODYNAMIC FIELDS



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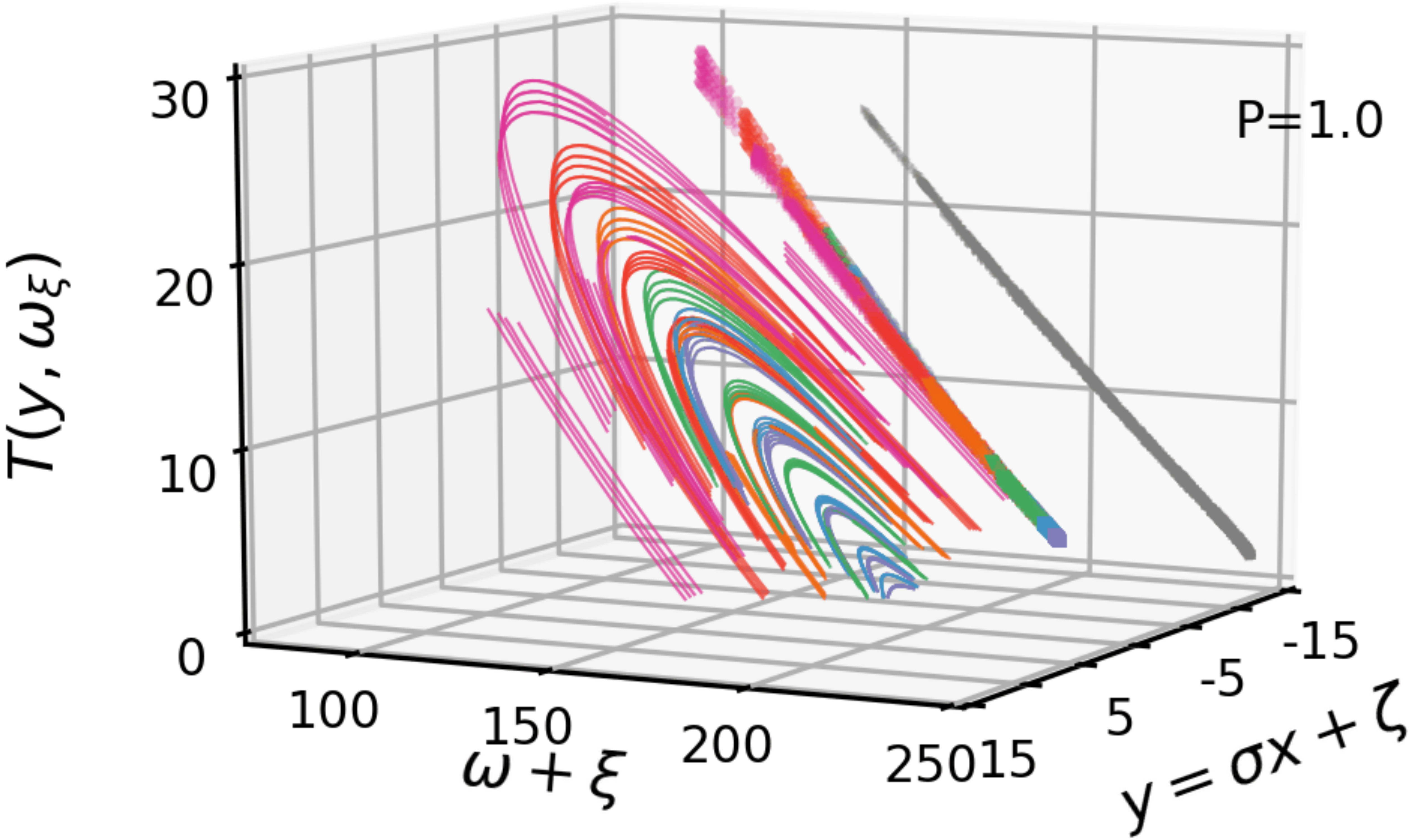

SUMMARY

- We have introduced a **new scaling property for the stationary solutions of the compressible NSF problem** under temperature and velocity gradients
- We find that the **density and temperature fields are local functions of a kinetic field and the fluid's pressure**.
- **This kinetic field obeys a spatial scaling law controlled by the shear stress**, which is inherited by the density and temperature fields.
- We confirm these scaling laws via **compelling data collapses** from massive computer simulations of **two molecular fluids** (hard disks in 2d and Lennard-Jones in 3d).
- The excellent collapses demonstrate the existence of a **bulk-boundary decoupling mechanism** which **enforces the macroscopic laws on the bulk of the finite-sized molecular fluid**.
- When analyzed in terms of scaling, **finite-size molecular fluids do exhibit continuum behavior as predicted by NSF equations**: **novel way to characterize stationary flows?**

Boundary conditions → Bulk constant

$$(T_0, T_1, +v_w, -v_w, P, \lambda) \to (J, \sigma, \xi, \zeta, P, \lambda)$$

COLLABORATORS

P.L. Garrido

J.J. del Pozo

Thank you

ugr Universidad de Granada