Investigation of the dynamics in a nanoconfined Lennard-Jones fluid

by

NEMD simulations and linear hydrodynamics

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01.06.2023
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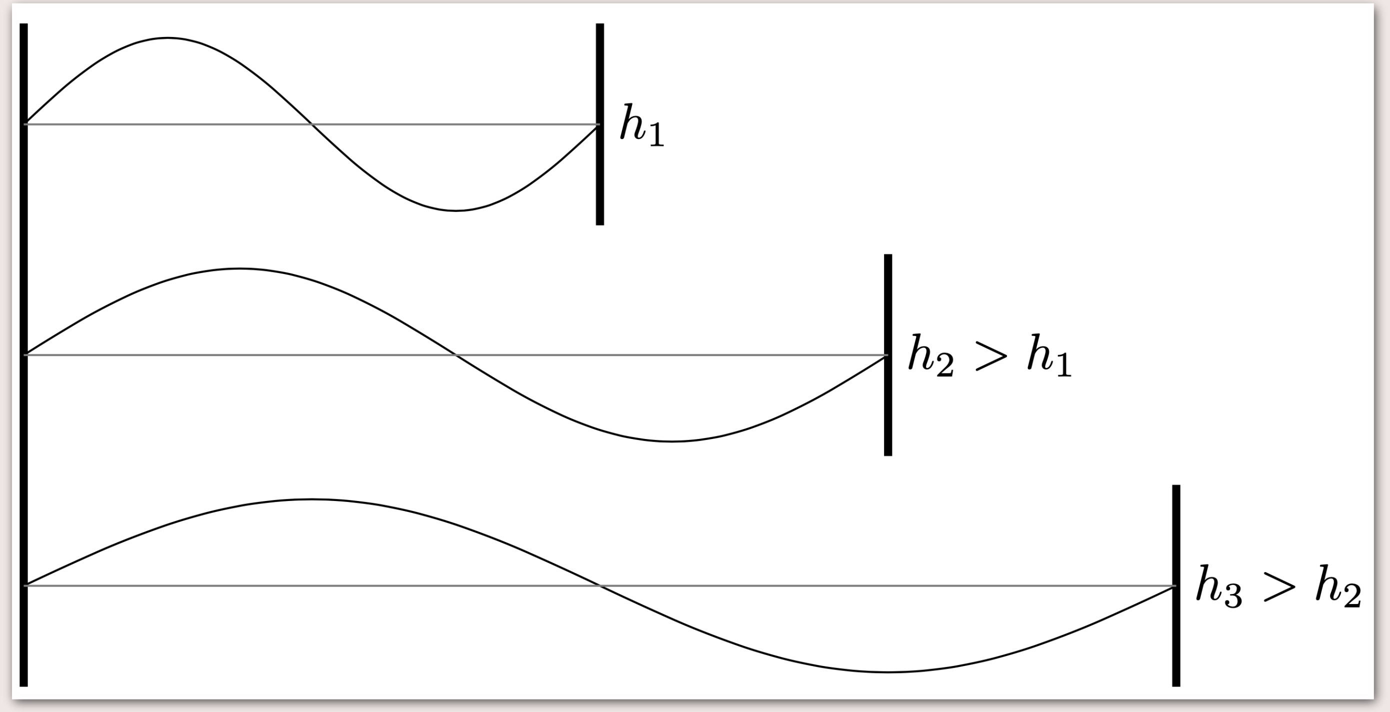
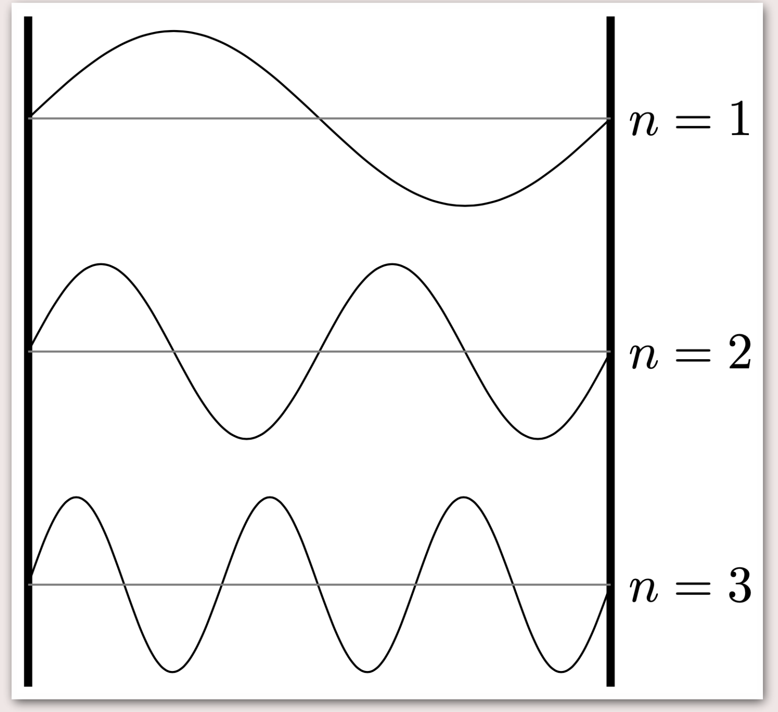
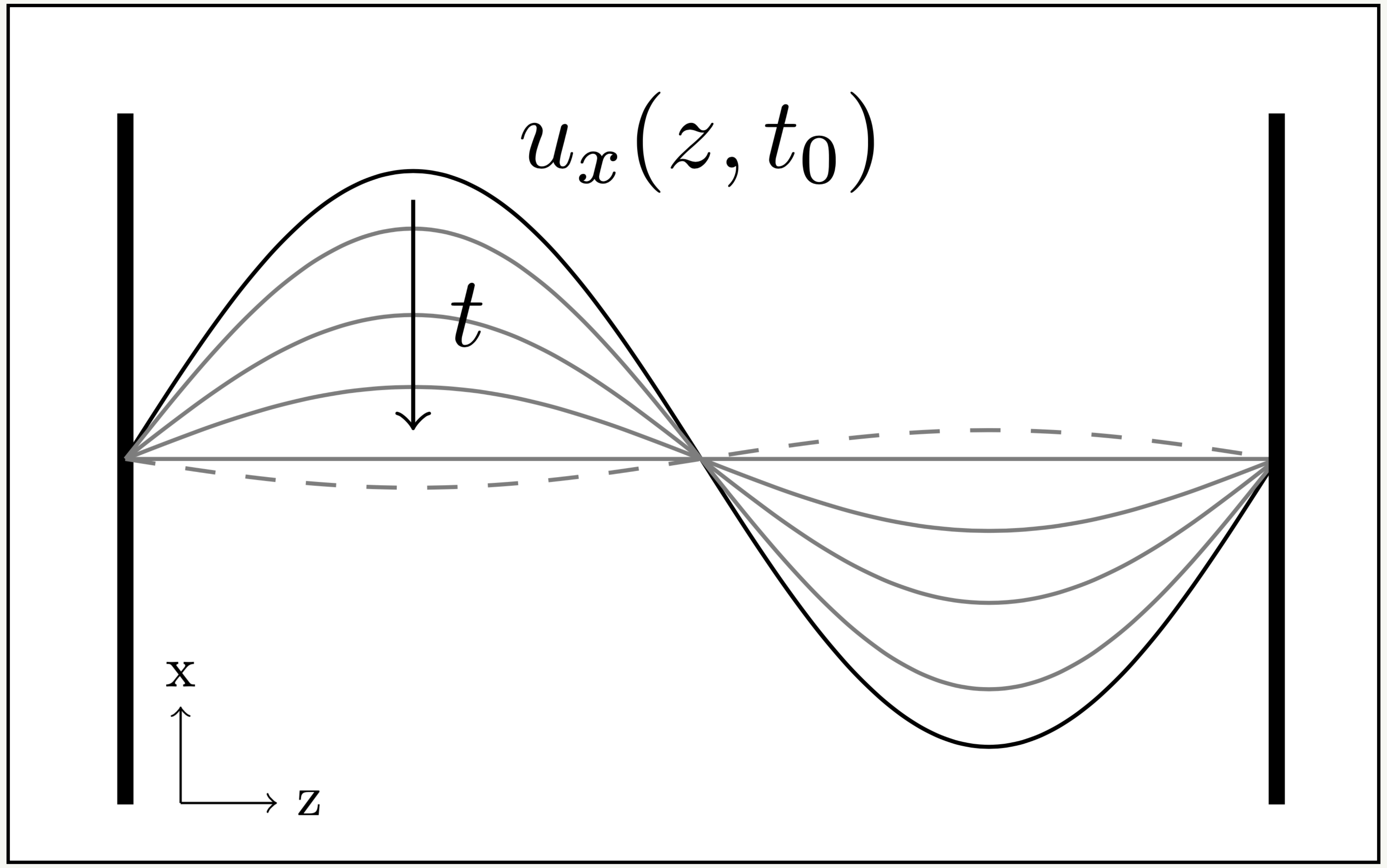
UNIVERSITAS ROSKILDENSIS · IN FLUCTU VITA · IN TRANQUILLO MORS ·

Basic idea

- Relaxing a sinusoidal velocity profile
- Two setups: height and sine mode







$$u_x(z) = \frac{A_n}{\eta_0 \chi_n^2} \sin(\chi_n z)$$

$$\chi_n = 2\pi n/h$$

$$n \in \mathcal{N}$$

Hydrodynamic derivations

Boundary conditions

$$u_x(0,t) = u_x(h,t) = 0$$

Definitions

$$\nu_0 = \eta_0/\rho$$

$$\mu = \nu_0 \chi_n^2$$

Two variants: i) simple ii) viscoelastic

$$\rho \frac{\partial u_x}{\partial t} = -\frac{\partial P_{xz}}{\partial z}$$

+

$$P_{xz} = -\eta_0 \frac{\partial u_x}{\partial z}$$

Newton's law of viscosity

→

$$u_x^i(z,t) = \frac{A_n}{\eta_0 \chi_n^2} \sin(\chi_n z) \exp\left(-\nu_0 \chi_n^2 t\right)$$

+

$$\frac{\partial u_x}{\partial z} = -\frac{1}{\eta_0}\left(1 + \tau_M \frac{\partial}{\partial t}\right) P_{xz}$$

Maxwell's model

→

$$\hat{u}_x^{ii}(z,t) = \frac{A_n}{\eta_0 \chi_n^2} \sin(\chi_n z) \Lambda^{ii}(t)$$

$$\Lambda^{ii}(t) = \begin{cases} e^{-\frac{t}{2\tau_M}} \left(\frac{(1-2\tau_M\mu)}{\sqrt{1-4\tau_M\mu}} \sinh\left(\frac{t\sqrt{1-4\tau_M\mu}}{2\tau_M}\right) + \cosh\left(\frac{t\sqrt{1-4\tau_M\mu}}{2\tau_M}\right)\right), & \tau_M < 1/4\mu \\ e^{-\frac{t}{2\tau_M}}, & \tau_M = 1/4\mu \\ e^{-\frac{t}{2\tau_M}} \left(\frac{1-2\tau_M\mu}{\sqrt{|1-4\tau_M\mu|}} \sin\left(\frac{t\sqrt{|1-4\tau_M\mu|}}{2\tau_M}\right) + \cos\left(\frac{t\sqrt{|1-4\tau_M\mu|}}{2\tau_M}\right)\right), & \tau_M > 1/4\mu \end{cases}$$

Boundary conditions

$u_x(0,t) = u_x(h,t) =$

$\rho \frac{\partial u_x}{\partial t} = -\frac{\partial}{}$

$\frac{\partial u_x}{\partial z} = -\frac{1}{\eta_0}\Big($

Maxwell

Definitions

$\nu_0 = \eta_0/\rho$

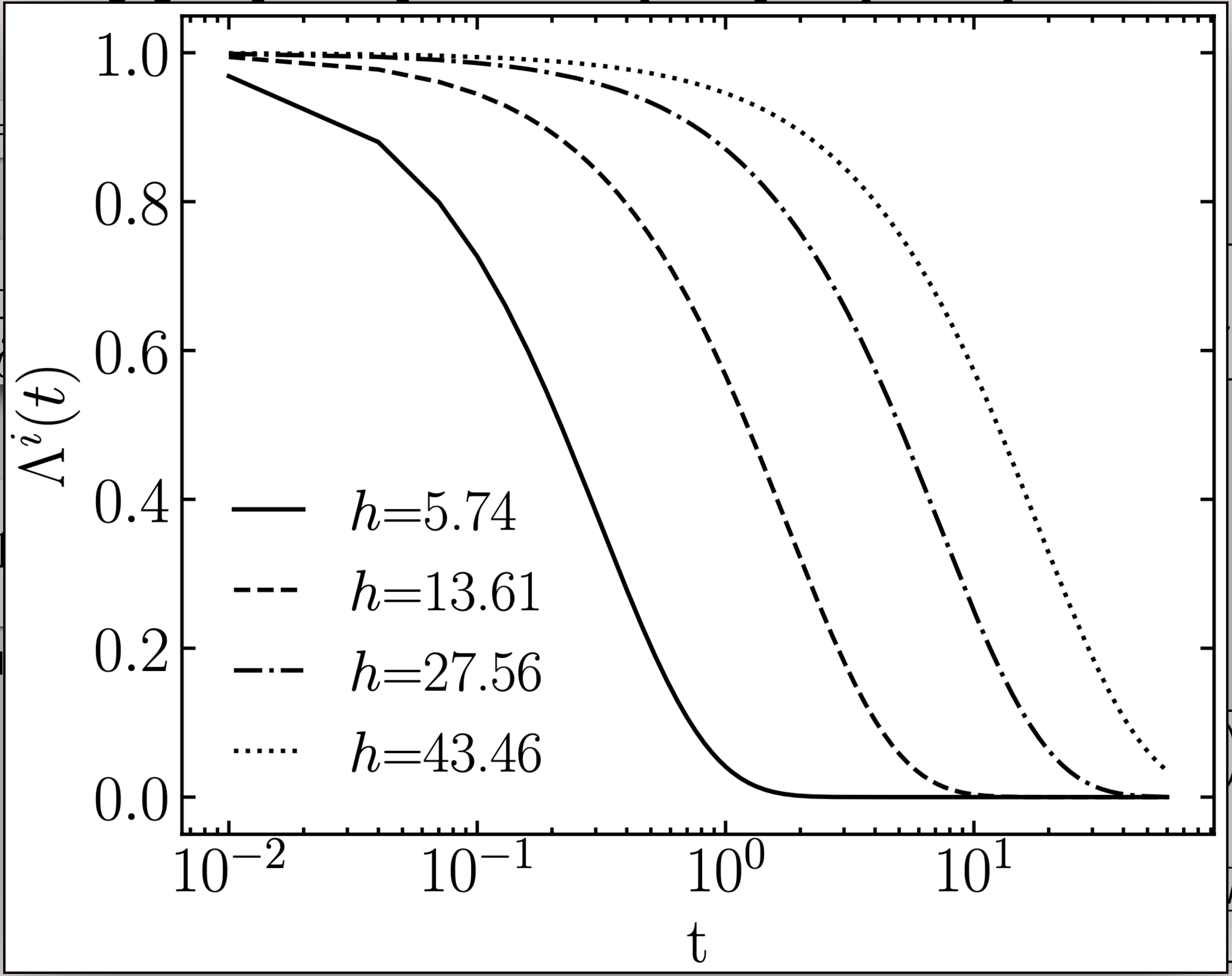
$\mu = \nu_0 \chi_n^2$

$z)\exp(-\nu_0\chi_n^2 t)$

$\Big)\Big), \quad \tau_M < 1/4\mu$

$\tau_M = 1/4\mu$

$\overline{\mu|}\Big)\Big), \quad \tau_M > 1/4\mu$



Boundary conditions

$u_x(0,t) = u_x(h,t) =$

Definitions

$\nu_0 = \eta_0/\rho$

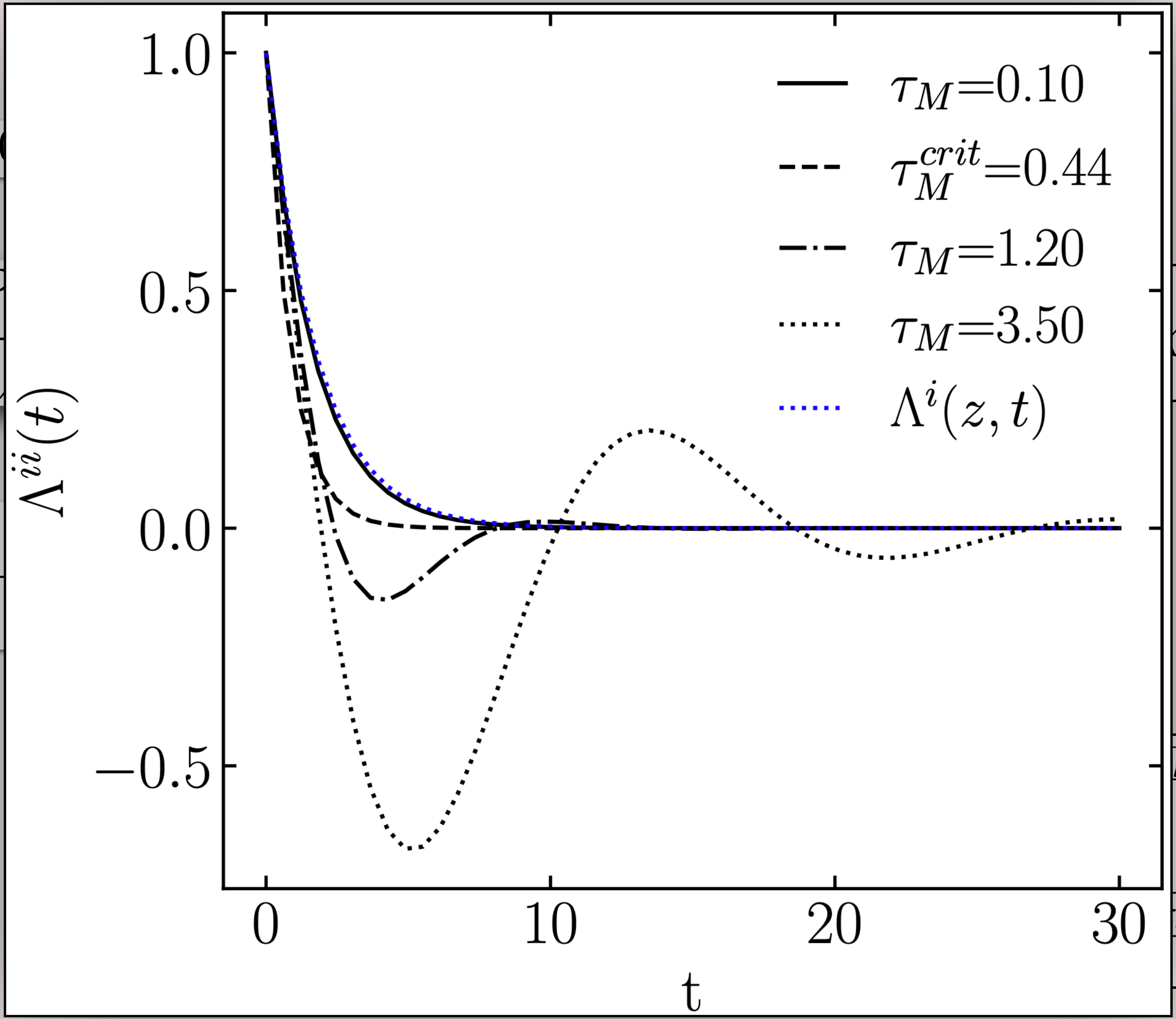
$\mu = \nu_0 \chi_n^2$

$\rho \frac{\partial u_x}{\partial t} = -\frac{\partial P}{\partial}$

$\chi_n z) \exp(-\nu_0 \chi_n^2 t)$

$\frac{\partial u_x}{\partial z} = -\frac{1}{\eta_0} \left(1 \right.$

Maxwell's

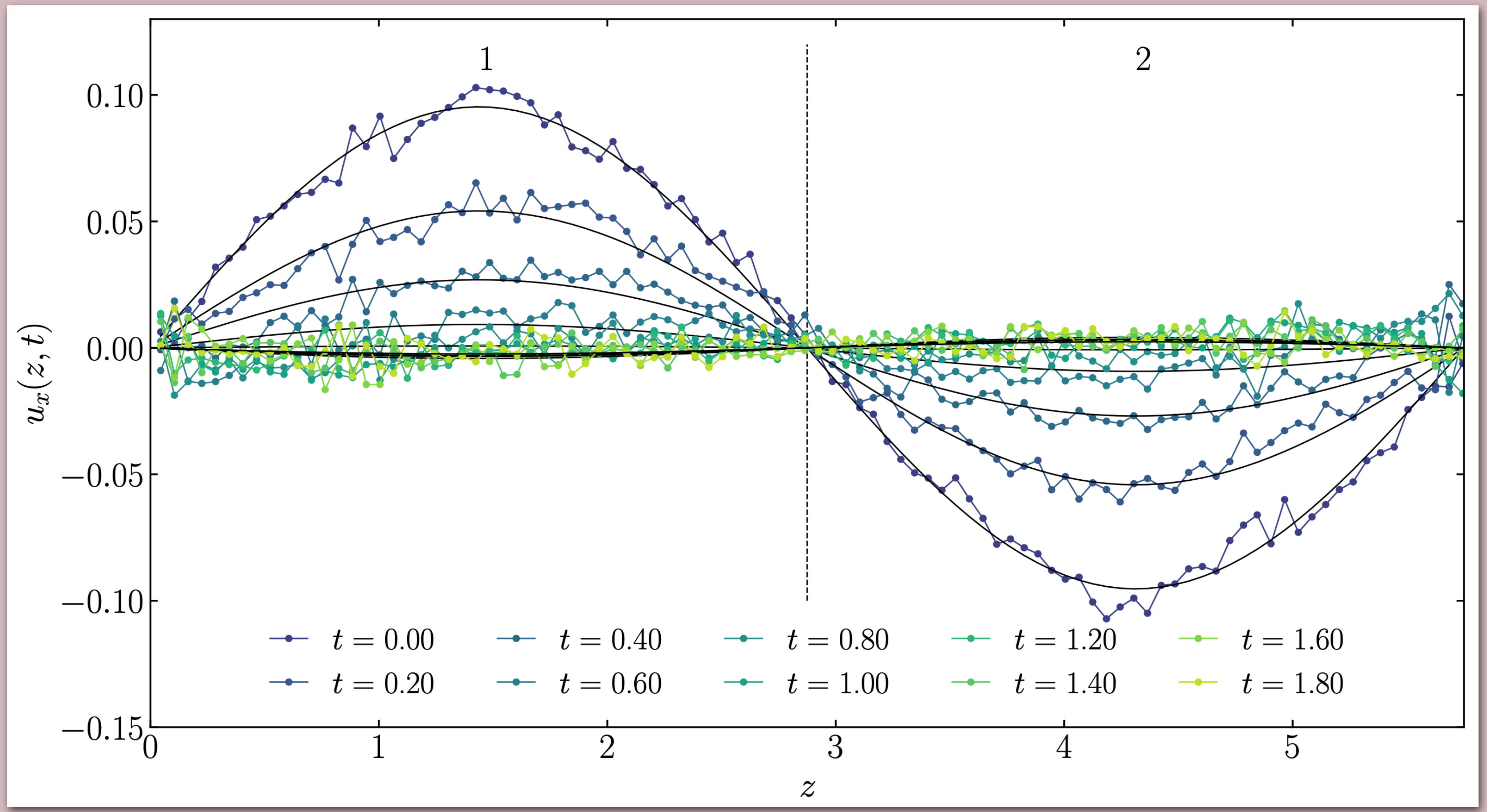


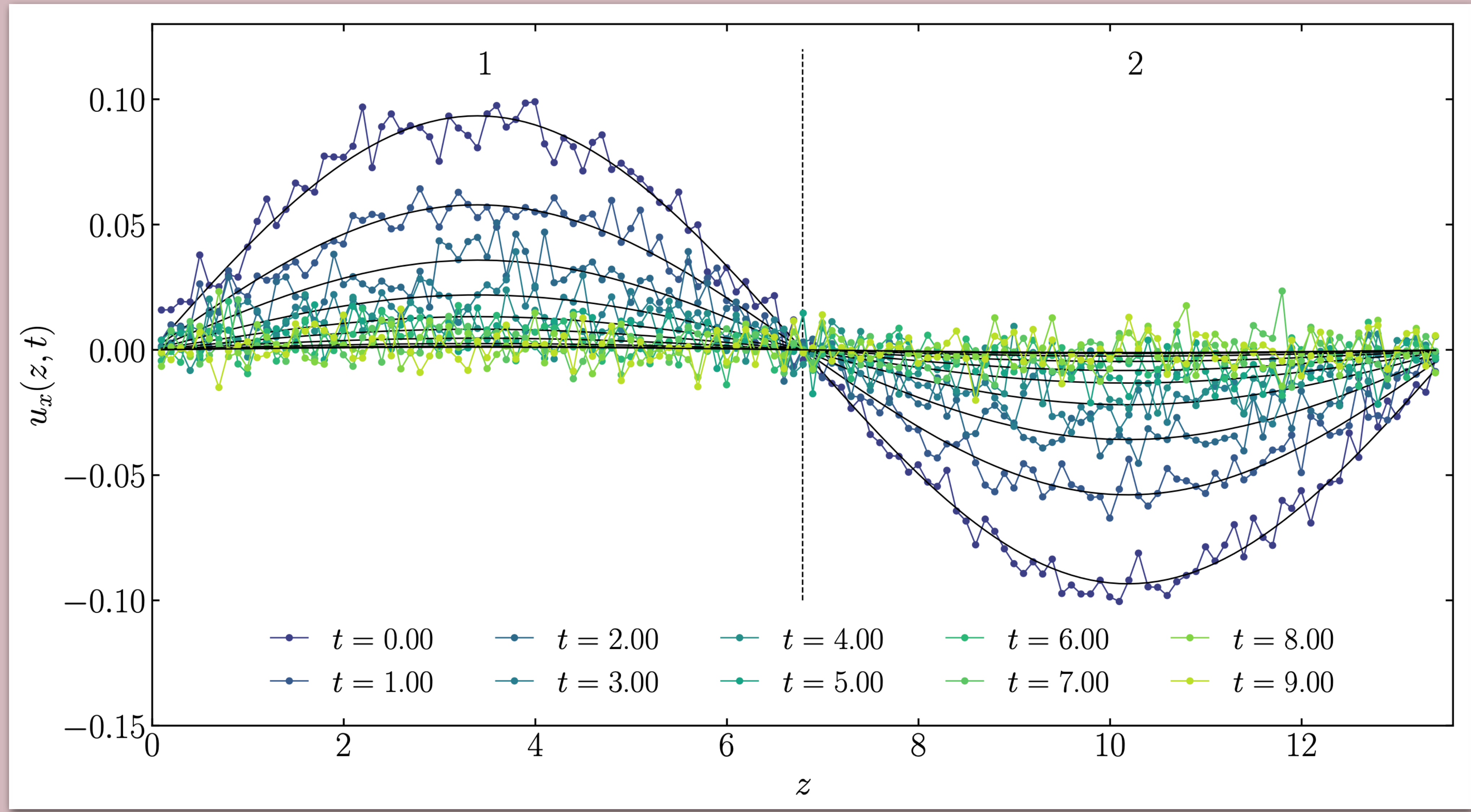
$\tau_M < 1/4\mu$

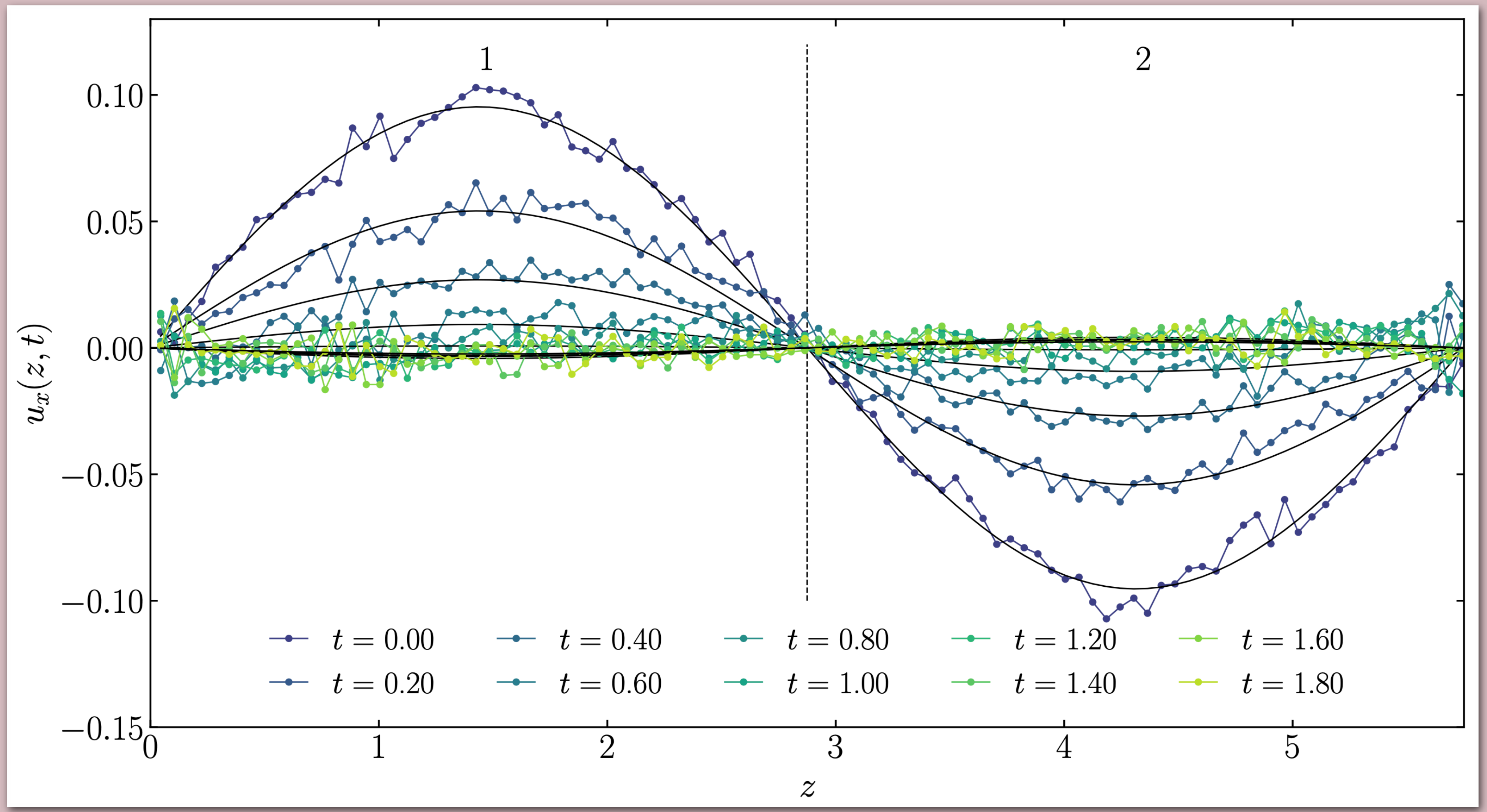
$\tau_M = 1/4\mu$

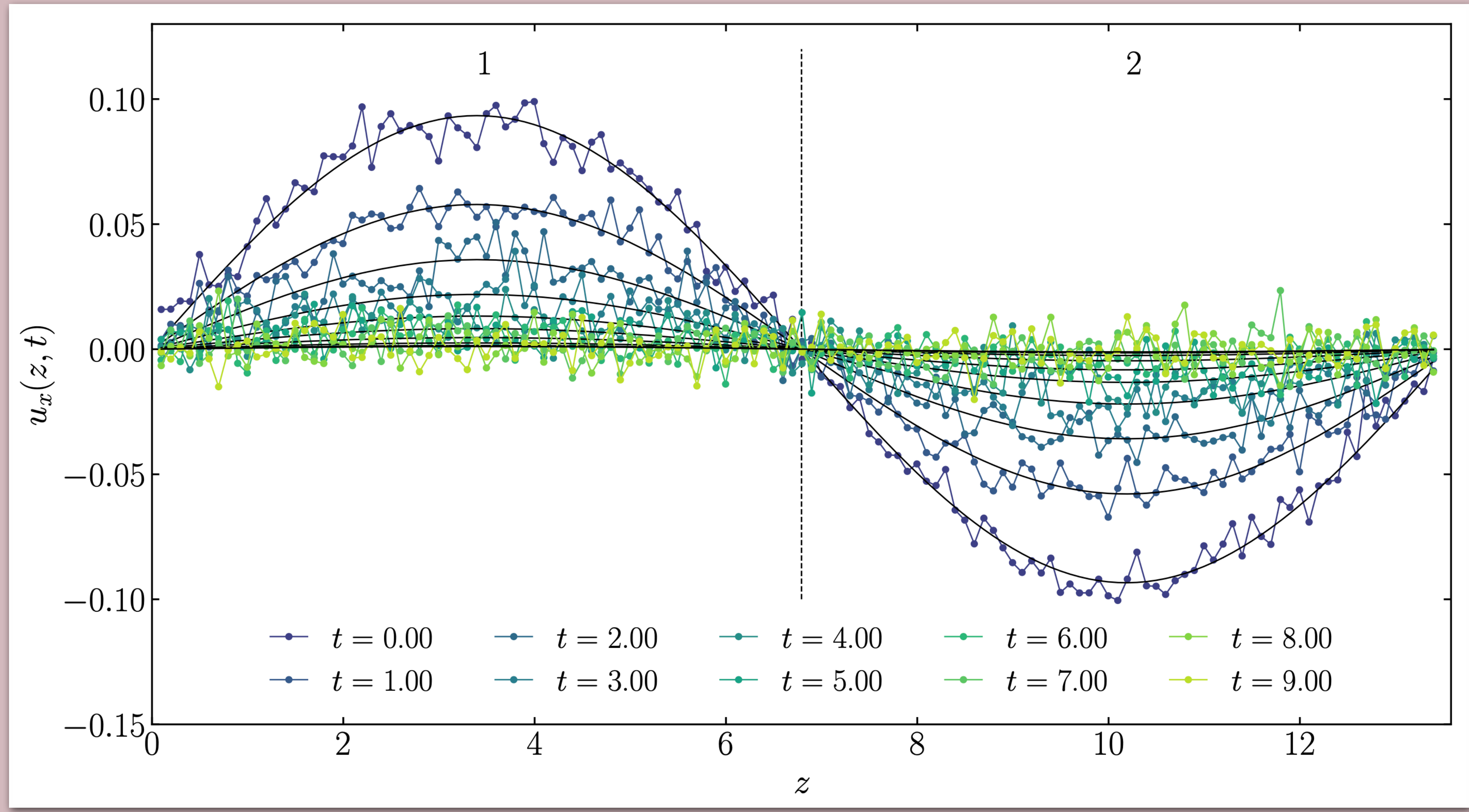
$\tau_M > 1/4\mu$

Channel heights

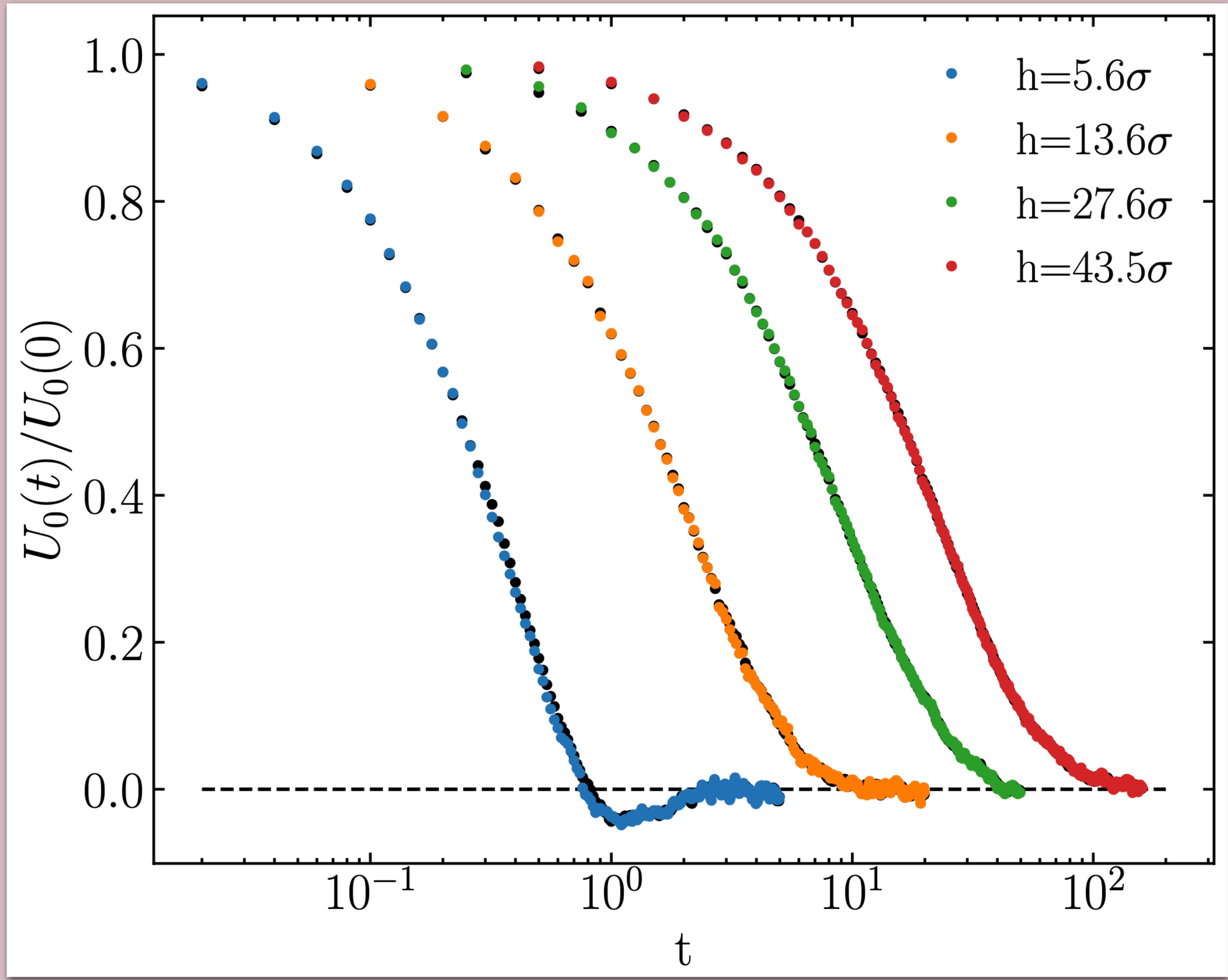




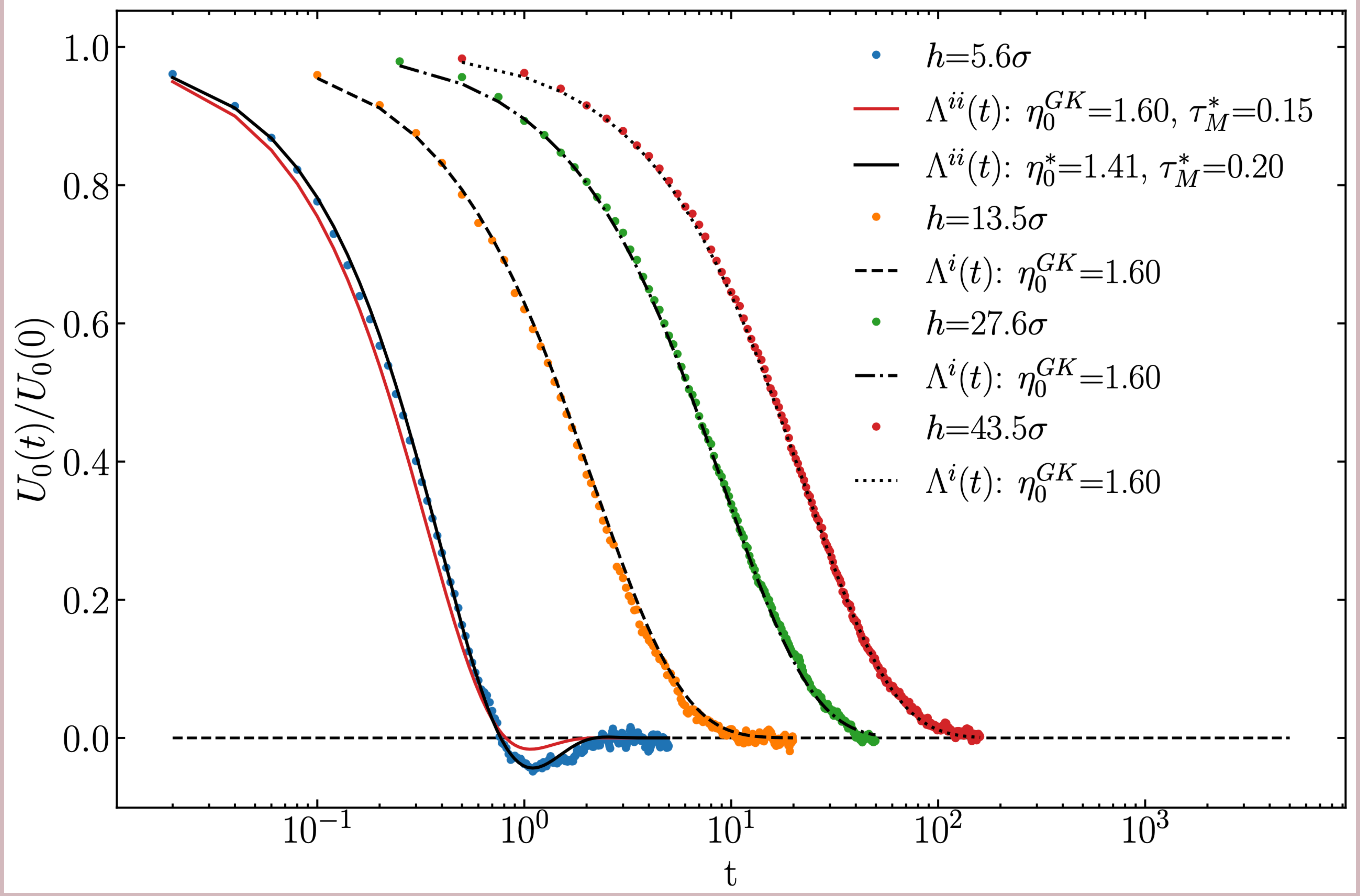




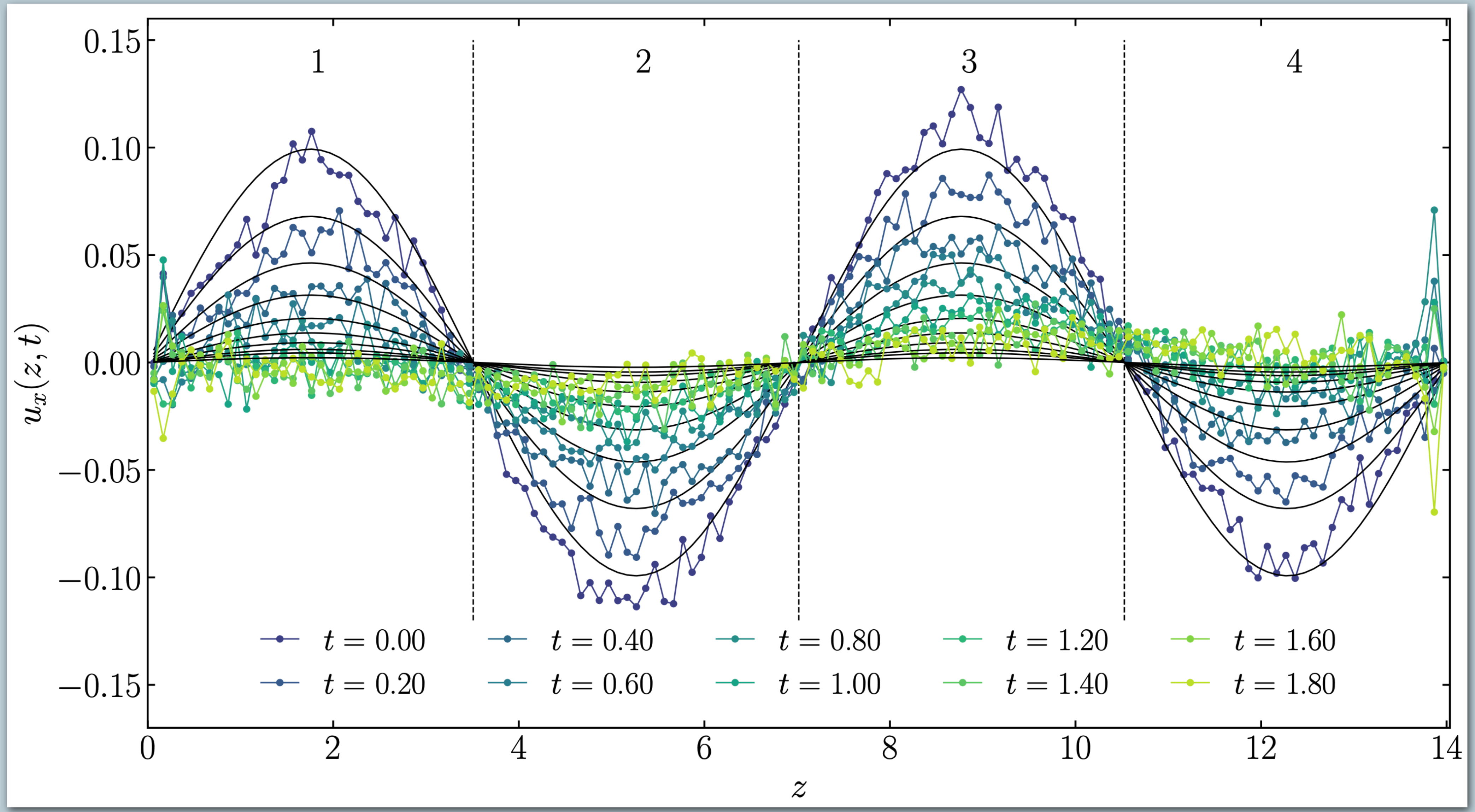
Channel heights



Comparison

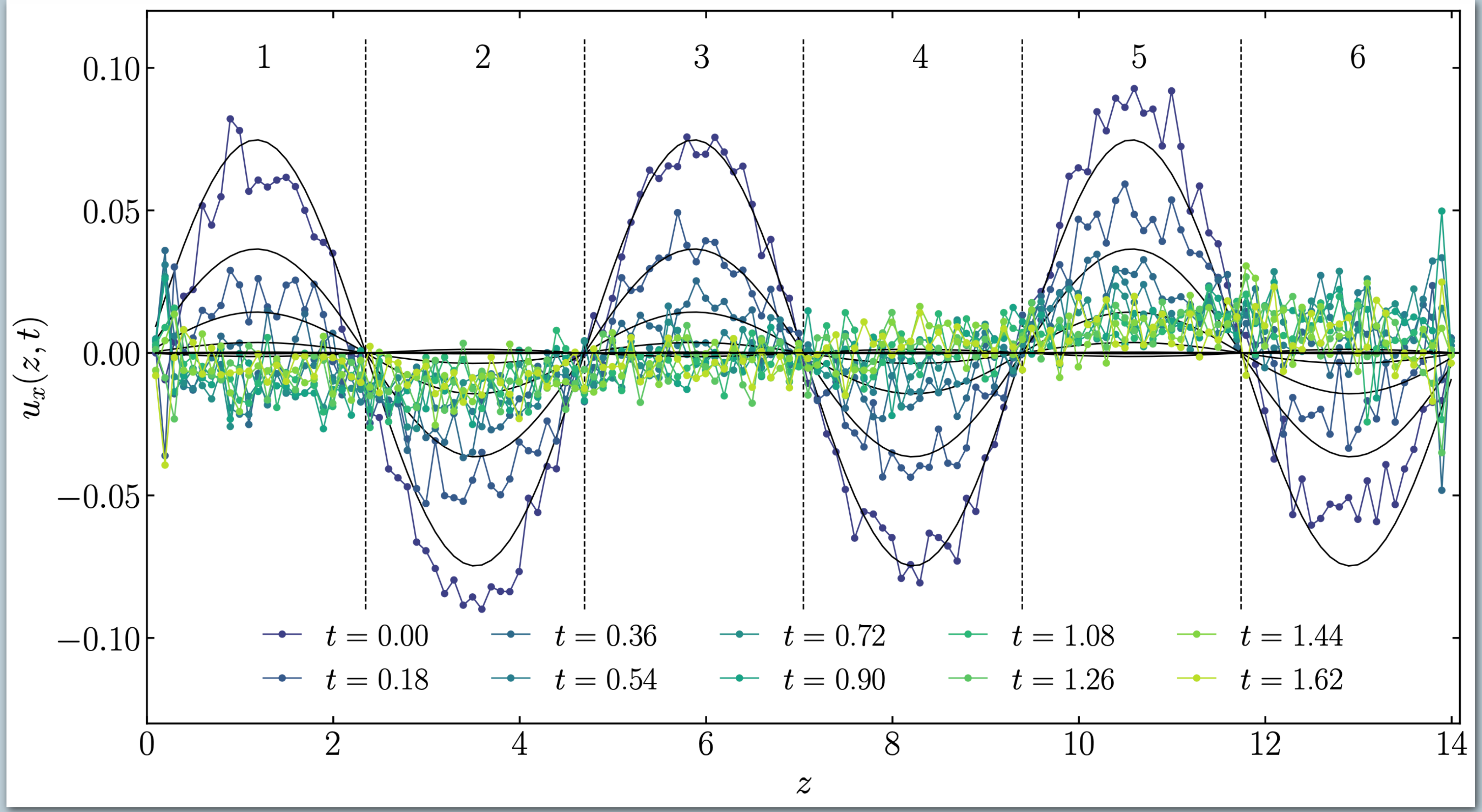


h=5.6σ
$\Lambda^{ii}(t)$: η_0^{GK}=1.60, τ_M^*=0.15
$\Lambda^{ii}(t)$: η_0^*=1.41, τ_M^*=0.20
h=13.5σ
$\Lambda^{i}(t)$: η_0^{GK}=1.60
h=27.6σ
$\Lambda^{i}(t)$: η_0^{GK}=1.60
h=43.5σ
$\Lambda^{i}(t)$: η_0^{GK}=1.60
$U_0(t)/U_0(0)$
1.0
0.8
0.6
0.4
0.2
0.0
10^{-1}
10^0
10^1
10^2
10^3
t



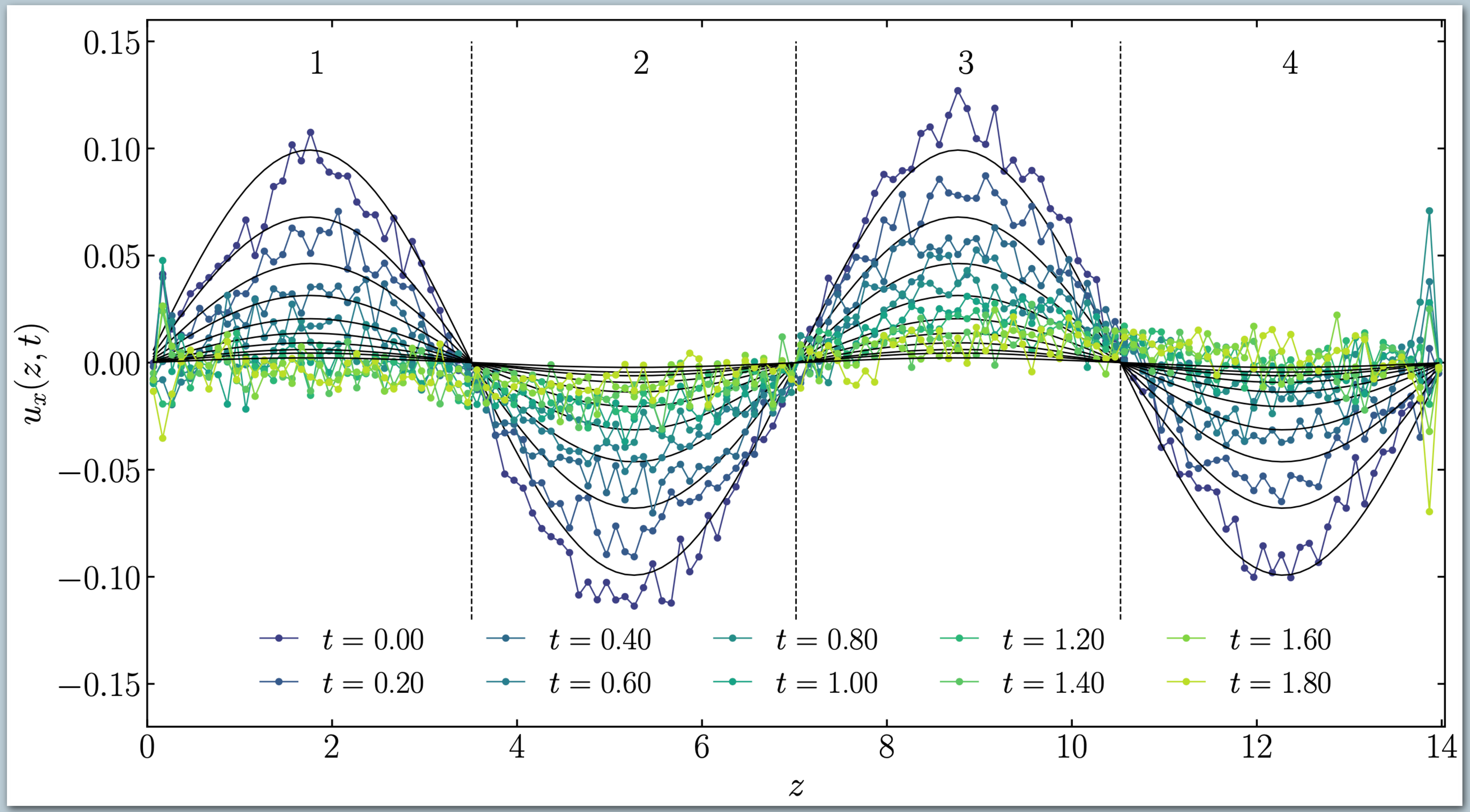
n = 2

Sine modes

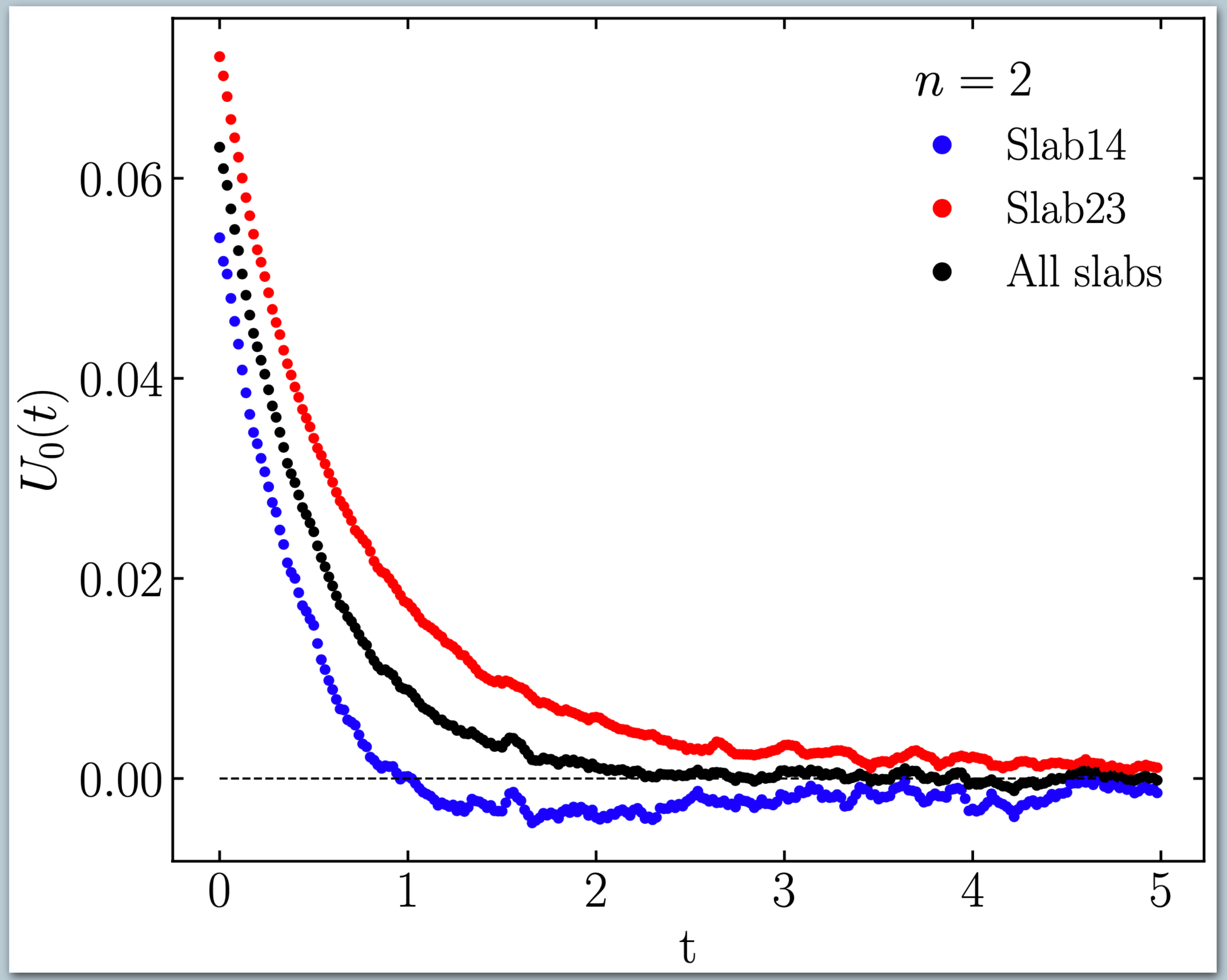


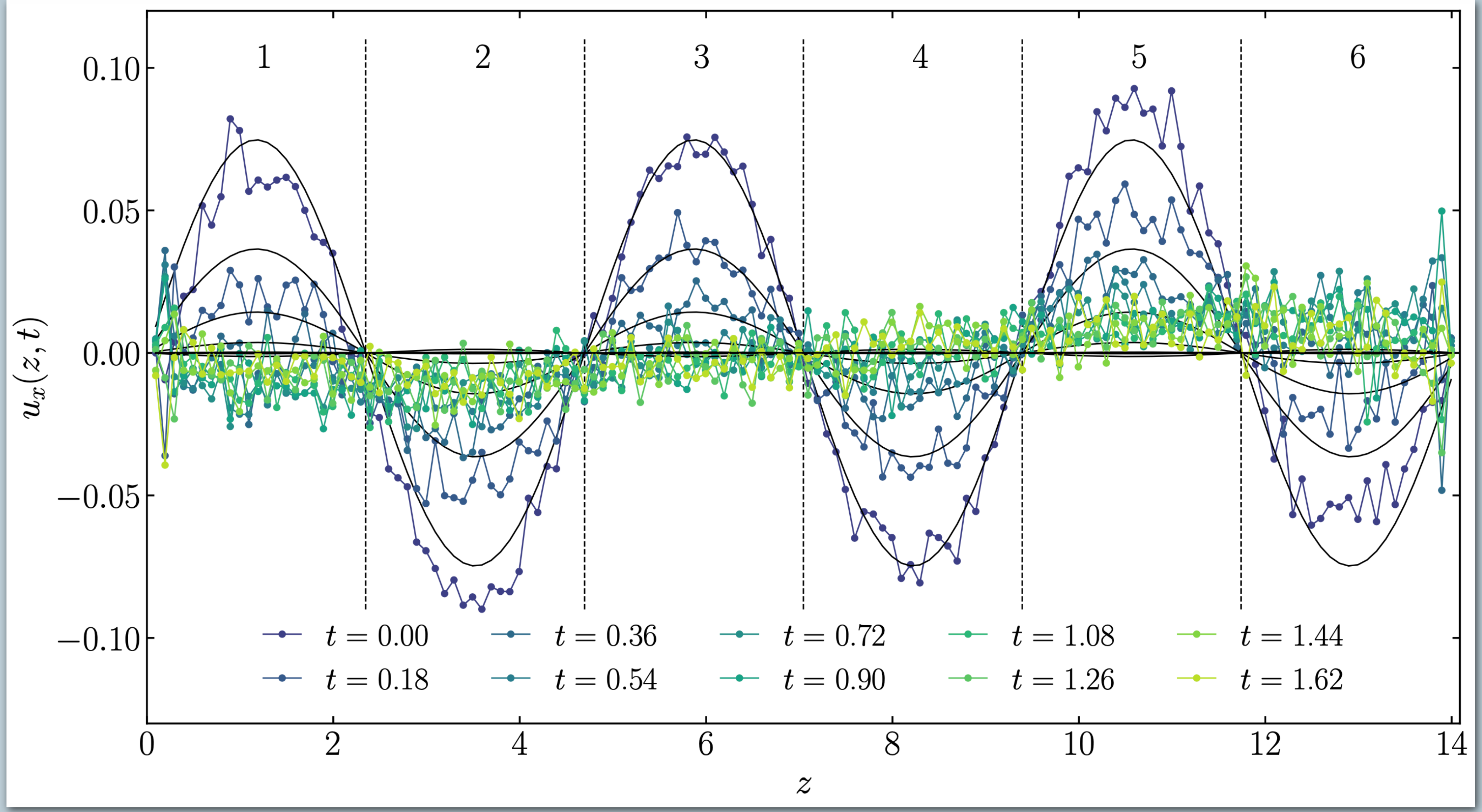
n = 3

Sine modes

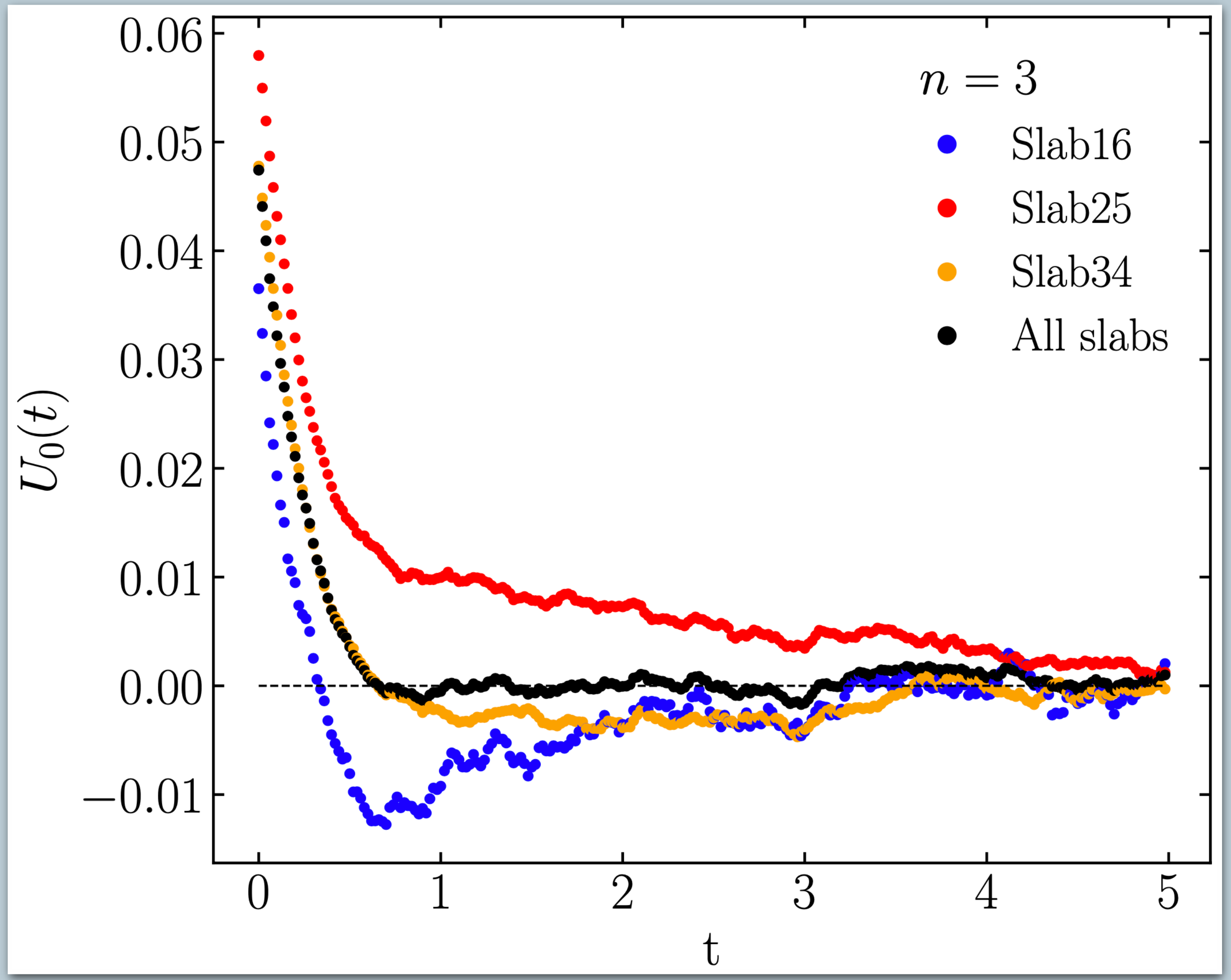


n = 2

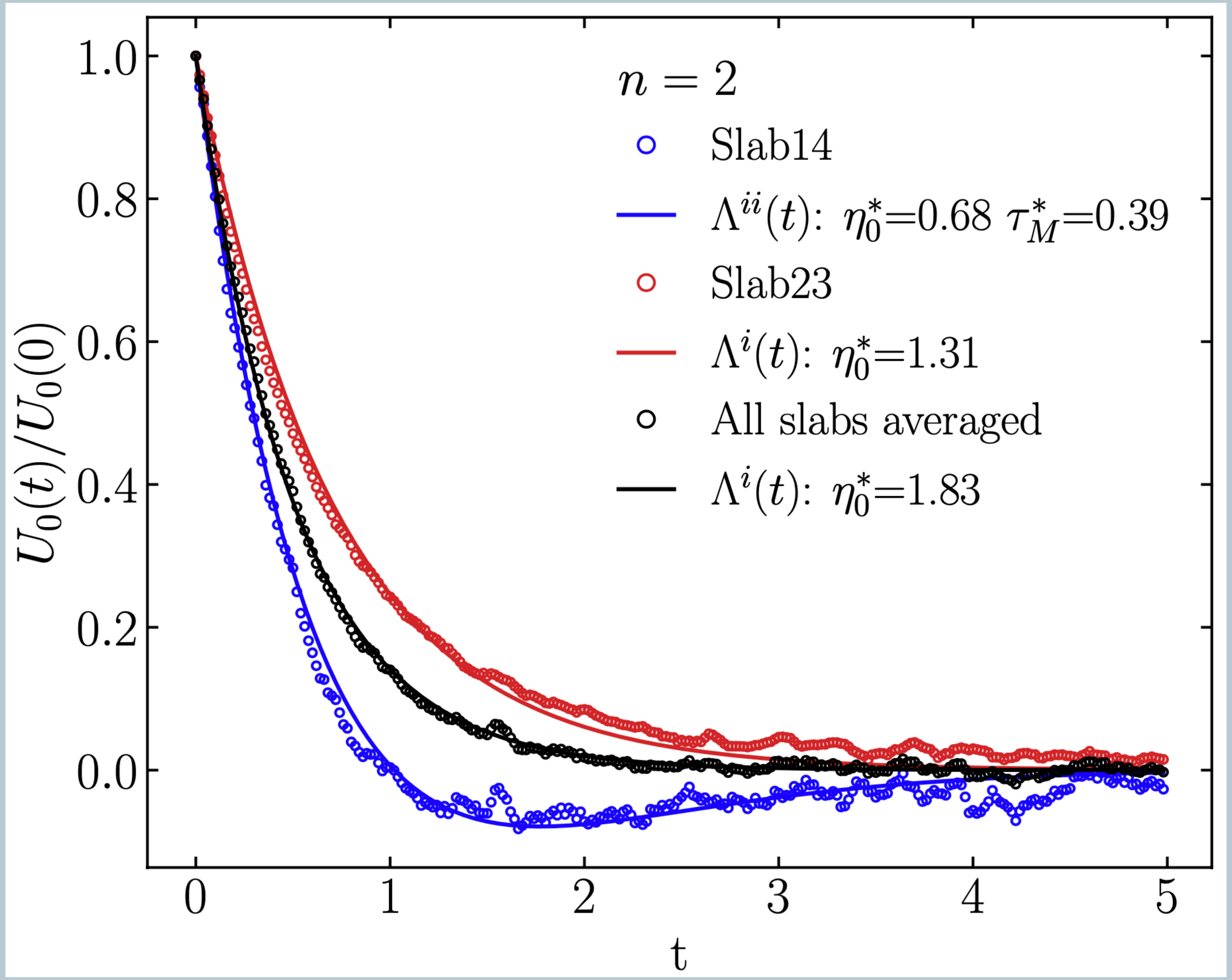




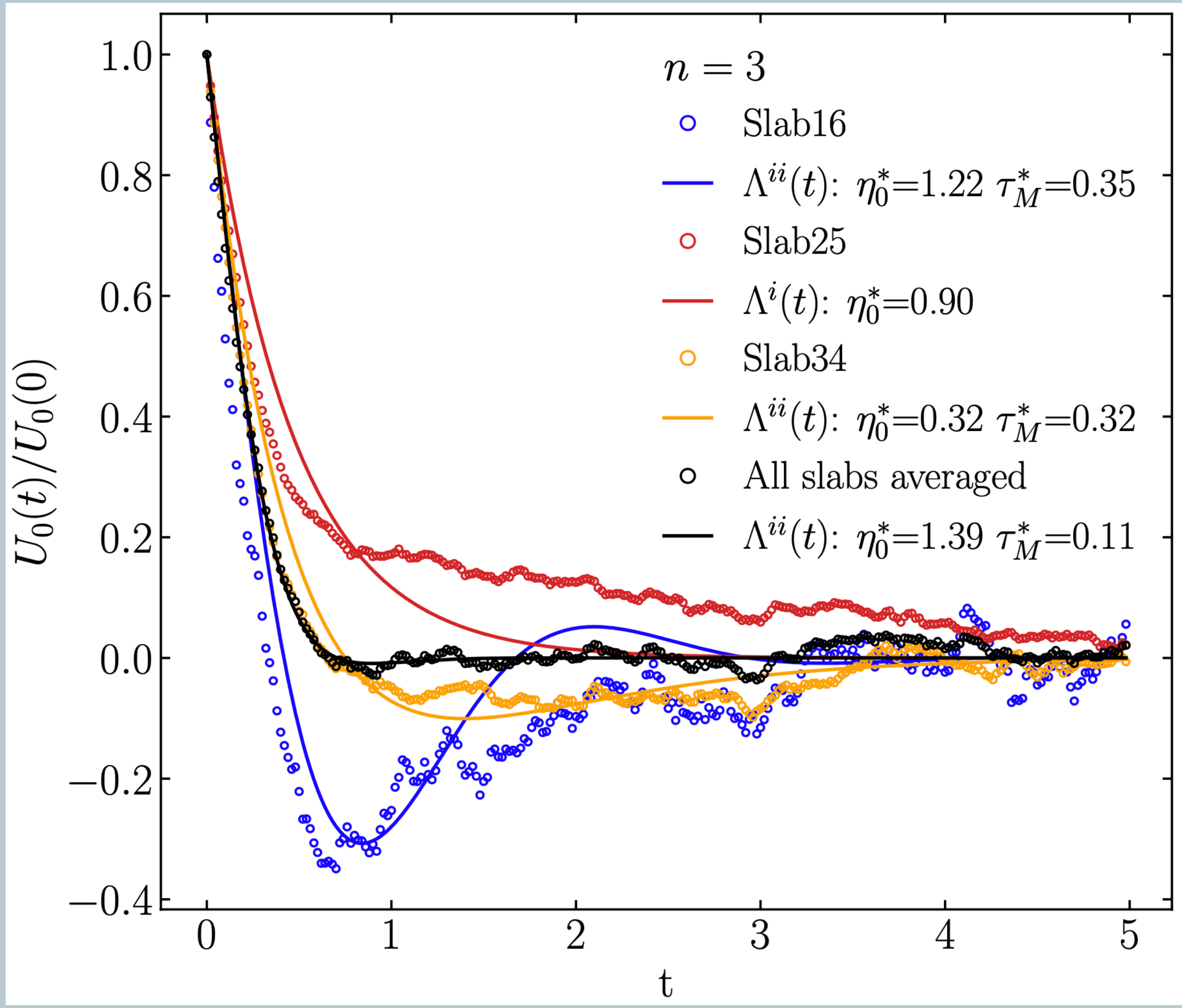
n = 3



Comparison



$n = 2$
Slab14
$\Lambda^{ii}(t)$: η_0^*=0.68 τ_M^*=0.39
Slab23
$\Lambda^{i}(t)$: η_0^*=1.31
All slabs averaged
$\Lambda^{i}(t)$: η_0^*=1.83
$U_0(t)/U_0(0)$
t



$n = 3$
Slab16
$\Lambda^{ii}(t)$: η_0^*=1.22 τ_M^*=0.35
Slab25
$\Lambda^{i}(t)$: η_0^*=0.90
Slab34
$\Lambda^{ii}(t)$: η_0^*=0.32 τ_M^*=0.32
All slabs averaged
$\Lambda^{ii}(t)$: η_0^*=1.39 τ_M^*=0.11
$U_0(t)/U_0(0)$
t

Thank you!