Relaxation time approximation for ultrarelativistic and multiphase flows

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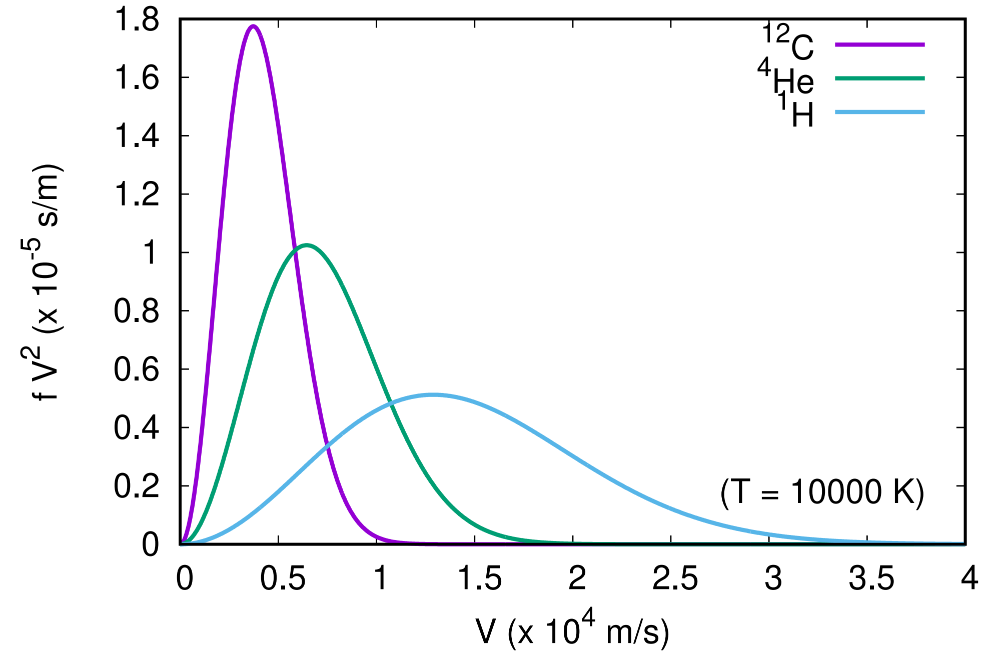
Outline

Introduction

Boltzmann equation

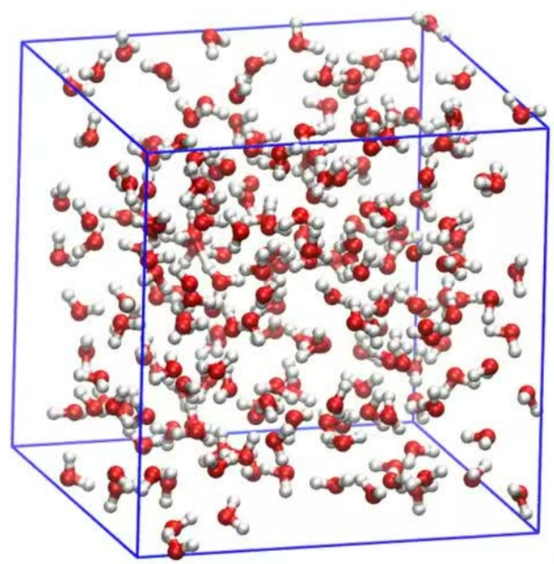
Mesoscale approach

Macroscopic: n, $\boldsymbol{u}$, T
(Navier-Stokes-Fourier)



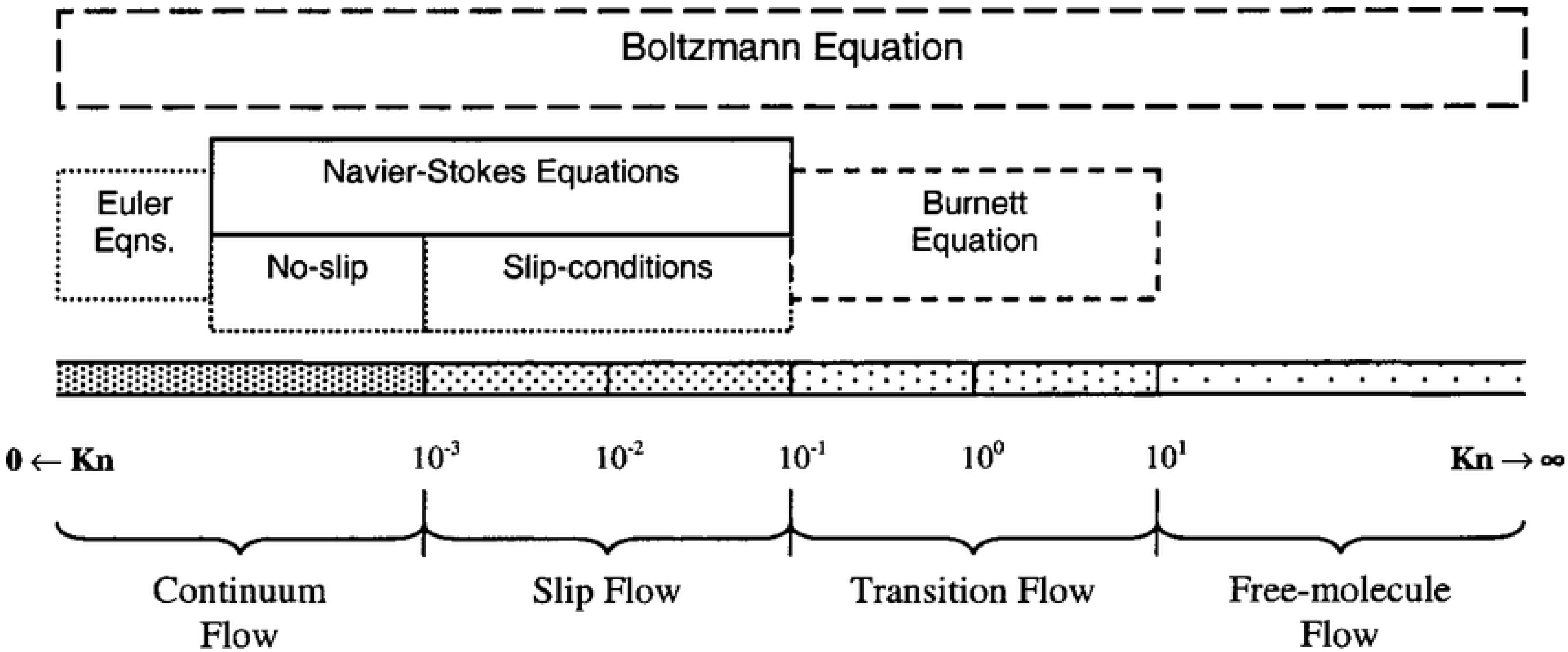
Mesoscopic: $f(\boldsymbol{x}, \boldsymbol{p}, t)$
(Boltzmann)

N_A =
6.02×10^{23}



Microscopic: $(\boldsymbol{x}_i, \boldsymbol{p}_i)$
(MD)

Rarefied flows: Knudsen number (Kn)



- $\mathrm{Kn} = \lambda_{\mathsf{mfp}}/(\text{System size } L)$.
- Hydordynamic regime (NSF): $\mathrm{Kn} \to 0$.
- Ballistic (free-streaming) regime (Vlasov): $\mathrm{Kn} \to \infty$.

Boltzmann Equation

- The Boltzmann eq. governs the evolution of $f \equiv f(x, \boldsymbol{k})$:

$$k^\mu \partial_\mu f = C[f], \qquad C[f] \simeq C_{\rm A-W}[f] = -\frac{k \cdot u}{\tau}[f - f^{(\rm eq)}]. \tag{1}$$

- The macroscopic quantities are obtained as moments of f,

$$\begin{pmatrix} J^\mu \\ T^{\mu\nu} \end{pmatrix} = \int \frac{d^3k}{k^t} f \begin{pmatrix} k^\mu \\ k^\mu k^\nu \end{pmatrix}. \tag{2}$$

- A-W requires the Landau frame ($T^\mu{}_\nu u^\nu = \epsilon u^\mu$) in order to ensure

$$\partial_\mu J^\mu = 0, \qquad \partial_\nu T^{\mu\nu} = 0. \tag{3}$$

- In the Landau frame, $T^{\mu\nu}$ and J^μ admit the decomposition:

$$T^{\mu\nu} = \epsilon u^\mu u^\nu - (p + \varpi)\Delta^{\mu\nu} + \pi^{\mu\nu}, \qquad J^\mu = n u^\mu + V^\mu. \tag{4}$$

Chapman-Enskog expansion

- Within RTA, the hydro limit is achieved when $\tau/L \sim \mathrm{Kn} \ll 1$.
- Writing $f = f^{(\mathrm{eq})} + \delta f$, the Boltzmann–A-W eq. gives

$$\delta f \simeq -\frac{\tau}{k \cdot u} k^\mu \partial_\mu f^{(\mathrm{eq})}. \tag{5}$$

- At leading order in Kn, we have

$$\begin{aligned} V^\mu &= \int \frac{d^3k}{k^t} \delta f\, k^\mu = \kappa_n \Delta^{\mu\nu} \partial_\nu \alpha, \\ \varpi &= -\frac{1}{3} \Delta_{\mu\nu} \int \frac{d^3k}{k^t} \delta f\, k^\mu k^\nu = -\zeta \partial_\mu u^\mu, \\ \pi^{\mu\nu} &= \int \frac{d^3k}{k^t} \delta f\, k^{\langle\mu} k^{\nu\rangle} = 2\eta \partial^{\langle\mu} u^{\nu\rangle}, \end{aligned} \tag{6}$$

  where $A^{\langle\mu\nu\rangle} = (\Delta^\mu{}_\lambda \Delta^\nu{}_\kappa - \frac{1}{3}\Delta^{\mu\nu}\Delta_{\lambda\kappa})A^{\lambda\kappa}$.
- CE can be continued to higher orders to derive 2nd order hydro etc.
- LB quest: recover dissipative hydro with minimum computational effort.

Quadrature-based FDLB

FDLB in a nutshell

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Ingredients:

1. Discretisation of the momentum space (Gauss quadratures);
2. Suitable representation of $f^{(\mathrm{eq})}$ in $C[f]$;
3. Numerical method for time evolution and spatial advection.
4. ...

Scope:

- Focusses primarily on macroscopic moments;
- Exact recovery of the conservation eqs;
- Accurate results with minimal "velocity sets."

From now one, we focus only on the massless case!

Spherical model

- J^μ and $T^{\mu\nu}$ can be computed using spherical coordinates, $k^\mu = k(1, \boldsymbol{v})$:

$$N^\mu = \int_0^\infty dk\, k^2 \int d\Omega_k\, f\, v^\mu, \qquad T^{\mu\nu} = \int_0^\infty dk\, k^3 \int d\Omega_k\, f\, v^\mu v^\nu. \tag{7}$$

- Assuming

$$f = \frac{e^{-k/T_0}}{T_0^3} \sum_{\ell=0}^\infty \frac{\mathcal{F}_\ell(\boldsymbol{v}) L_\ell^{(2)}(k/T_0)}{(\ell+1)(\ell+2)}, \tag{8}$$

the k integration can be performed automatically:

$$N^\mu = \int d\Omega_k v^\mu\, \mathcal{F}_0, \qquad T^{\mu\nu} = \int d\Omega_k v^\mu v^\nu (3\mathcal{F}_0 - \mathcal{F}_1). \tag{9}$$

- Dividing $k^\mu \partial_\mu f = C_{\rm A-W}[f]$ by k gives

$$\partial_t f + \boldsymbol{v} \cdot \nabla f = -\frac{\gamma(1 - \boldsymbol{\beta} \cdot \boldsymbol{v})}{\tau_R}[f - f^{\rm (eq)}]. \tag{10}$$

- The projection on Laguerre polynomials gives:

$$(\partial_t + \boldsymbol{v} \cdot \nabla)\mathcal{F}_\ell = -\frac{\gamma(1 - \boldsymbol{\beta} \cdot \boldsymbol{v})}{\tau_R}[\mathcal{F}_\ell - \mathcal{F}_\ell^{\rm (eq)}]. \tag{11}$$

- Only $\mathcal{F}_0$ and $\mathcal{F}_1$ are required for J^μ and $T^{\mu\nu}$.

Radial quadrature

- Formally, the k integral can be performed exactly when applying the Gauss-Laguerre quadrature (GLQ) prescription:

$$\int_0^\infty dx\, e^{-x} x^2\, P(x) \simeq \sum_{q=1}^{Q} w_q^L P(x_q). \qquad (12)$$

  - The quadrature sum is exact if $P(x)$ is a polynomial of degree $< 2Q$.
  - $x_q = k_q/T_0$ are the roots of $L_Q^{(2)}(x)$.
  - $w_q^L = \dfrac{(Q+2)x_q}{(Q+1)[L_{Q+1}^{(2)}(x_q)]^2}$ are the weights of the GLQ.
- Minimal quadrature for J^μ and $T^{\mu\nu}$ uses $Q = 2$ and

$$f_q(\boldsymbol{v}) = \frac{T_0^3 w_q^L}{e^{-k_q/T_0}} f(k_q, \boldsymbol{v}) \Rightarrow \int_0^\infty dk\, k^2 f\, P(k) = \sum_{q=1}^{Q} f_q(\boldsymbol{v}) P(k_q). \qquad (13)$$

- For $f_{\rm MJ}^{(\rm eq)}$, the projection on $L_\ell^{(2)}$ with $0 \le \ell \le Q - 1 = 1$ reads

$$f_q^{(\rm eq)} = \frac{n}{8\pi (v\cdot u)^3}\left[4 - \frac{k_q}{T_0} - \frac{T/T_0}{v\cdot u}\left(3 - \frac{k_q}{T_0}\right)\right]. \qquad (14)$$

Angular quadrature

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- The angular integral can be performed separately for φ_k and $\xi = k^z/k$.
- The φ_k integral can be performed using the Mysovskikh quadrature,

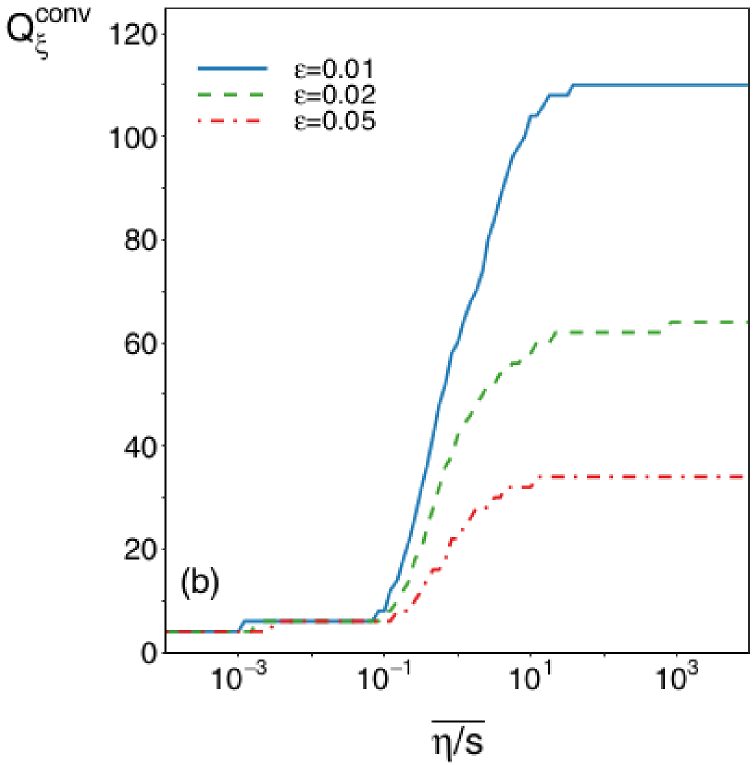
$$\int_0^{2\pi} d\varphi f(\varphi) \simeq \frac{2\pi}{M} \sum_{i=1}^{M} f(\varphi_i), \qquad \varphi_i = \varphi_0 + \frac{2\pi(i-1)}{M}, \tag{15}$$

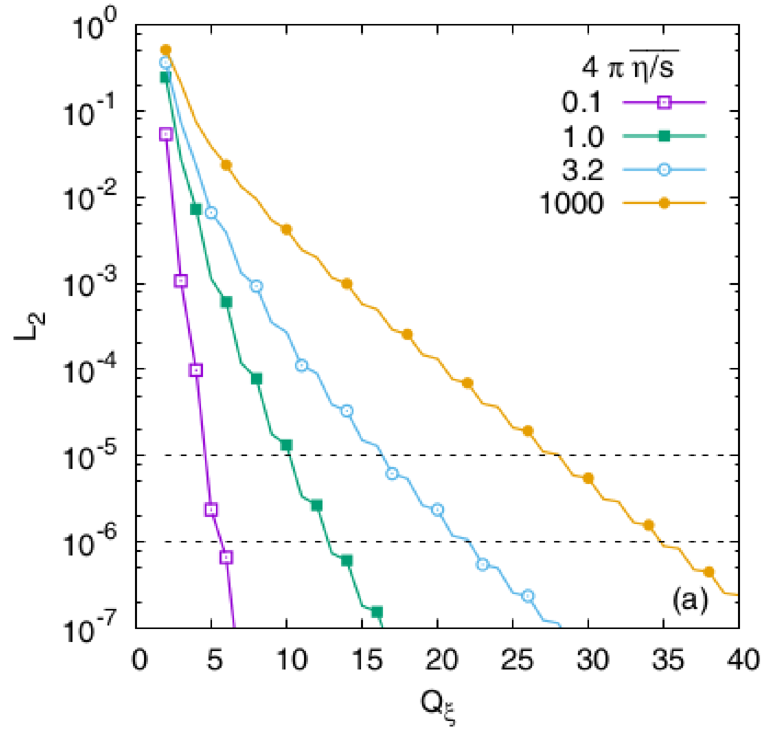
  where the equality is exact if f is a trigonometric polynomial of order $< 2M$.
- The ξ integral can be performed using the Gauss-Legendre quadrature,

$$\int_{-1}^{1} d\xi\, f(\xi) \simeq \sum_{j=1}^{P} w_j^P f(\xi_j), \tag{16}$$

  where the equality is exact if
  - $f(\xi)$ is a polynomial of order $< 2P$;
  - $P_P(\xi_j) = 0$;
  - $w_j^P = 2(1-\xi_j^2)/[(P+1)P_{P+1}(\xi_j)]^2$ are the Gauss-Legendre q. weights.
- Exact recovery of the moments of $f^{(\rm eq)}$ when

$$f_{ijk}^{(\rm eq)} = \frac{2\pi}{M} w_j^P w_q^L \sum_{\ell=0}^{N_L} \frac{L_\ell^{(2)}(k_q/T_0)}{(\ell+1)(\ell+2)} \sum_{m=0}^{N_\Omega} \frac{2m+1}{2} a_{\ell,m}^{(\rm eq)} P_m[\cos\gamma(\boldsymbol{v}_{ij}, \boldsymbol{u})].$$





- $Q = 2$ guarantees exact recovery of J^μ and $T^{\mu\nu}$.
- For $1+1$D systems, $\partial_t f + \xi \partial_z f = -\tau_R^{-1} \gamma (1 - \beta\xi)[f - f^{(\text{eq})}]$.
- $M = 1$ is exact when f is independent of φ_k.
- ξ couples the moments w.r.t. $P_s(\xi)$ [s couples with $s-1$ and $s+1$].
- For $\tau_R \to 0$, evol. of $T^{\mu\nu}$ [$0 \le s \le 2$] requires integrals of $\xi^3 f \Rightarrow P \ge 4$.
- "Higher-order dynamics" requires increasing P.

Waves

Validation 1: Sound waves

[VEA, PRC **97** (2018) 024914]

- Consider a longitudinal wave propagating along z.
- $\nabla_\mu J^\mu = \nabla_\nu T^{\mu\nu} = 0$ can be linearized w.r.t $\delta n = n - n_0$, $\delta P = P - P_0$ and $\beta = u^z/u^0$:

$$\begin{aligned} \partial_t \delta n + n_0 \partial_z \beta &= 0, \\ 3\partial_t \delta P + 4P_0 \partial_z \beta + \partial_z q &= 0, \\ 4P_0 \partial_t \beta + \partial_t q + \partial_z \delta P + \partial_z \Pi &= 0. \end{aligned} \tag{17}$$

- In the (2nd order) hydrodynamic regime, the following constitutive eqs. can be written for q and Π: [W. A. Hiscock, L. Lindblom, Ann. Phys. **151** (1983) 466]

$$\begin{aligned} \tau_q \partial_t q + q &= -\frac{\lambda P_0}{4n_0}\left(\frac{3\partial_z \delta P}{P_0} - \frac{4\partial_z \delta n}{n_0}\right), \\ \tau_\Pi \partial_t \Pi + \Pi &= -\frac{4\eta}{3}\partial_z\left(\beta + \frac{q}{4P_0}\right). \end{aligned} \tag{18}$$

First order hydro

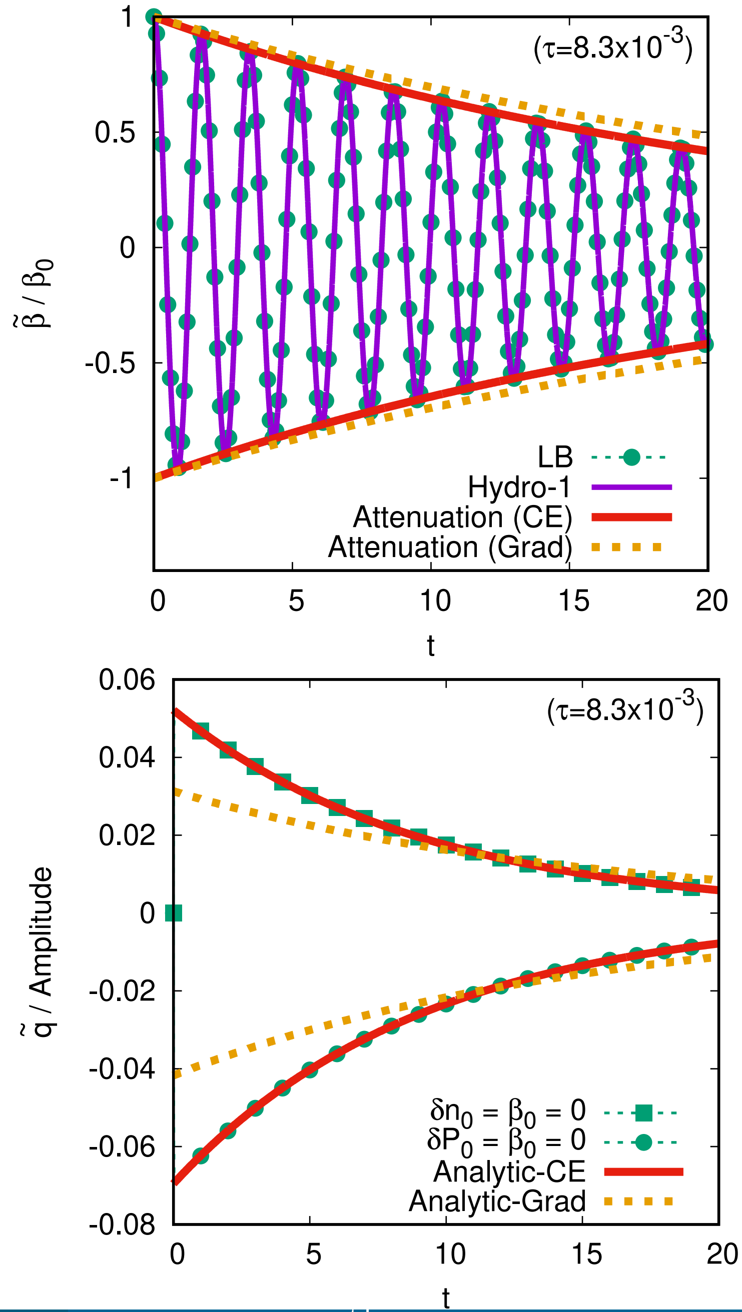
[VEA, PRC **97** (2018) 024914]

- Writing $M(t,z) = \widetilde{M}(t) \times \cos(kz)$ or $\sin(kz)$, the solution of 1st order hydro ($\tau_q = \tau_\Pi = 0$) is:

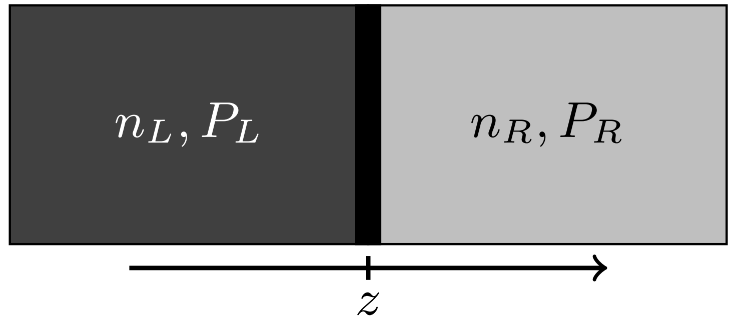
$$\begin{pmatrix} \widetilde{\beta} \\ \widetilde{\delta n} \\ \widetilde{\delta P} \\ \widetilde{q} \\ \widetilde{\Pi} \end{pmatrix} = e^{-\nu_\lambda k t} \begin{pmatrix} \beta_\lambda \\ \delta n_\lambda \\ 0 \\ q_\lambda \\ 0 \end{pmatrix} + e^{-\nu_d k t} \times \left[\begin{pmatrix} \beta_c \\ \delta n_c \\ \delta P_c \\ 0 \\ \Pi_c \end{pmatrix} \cos \nu_o k t + \begin{pmatrix} \beta_s \\ \delta n_s \\ \delta P_s \\ 0 \\ \Pi_s \end{pmatrix} \sin \nu_o k t \right],$$

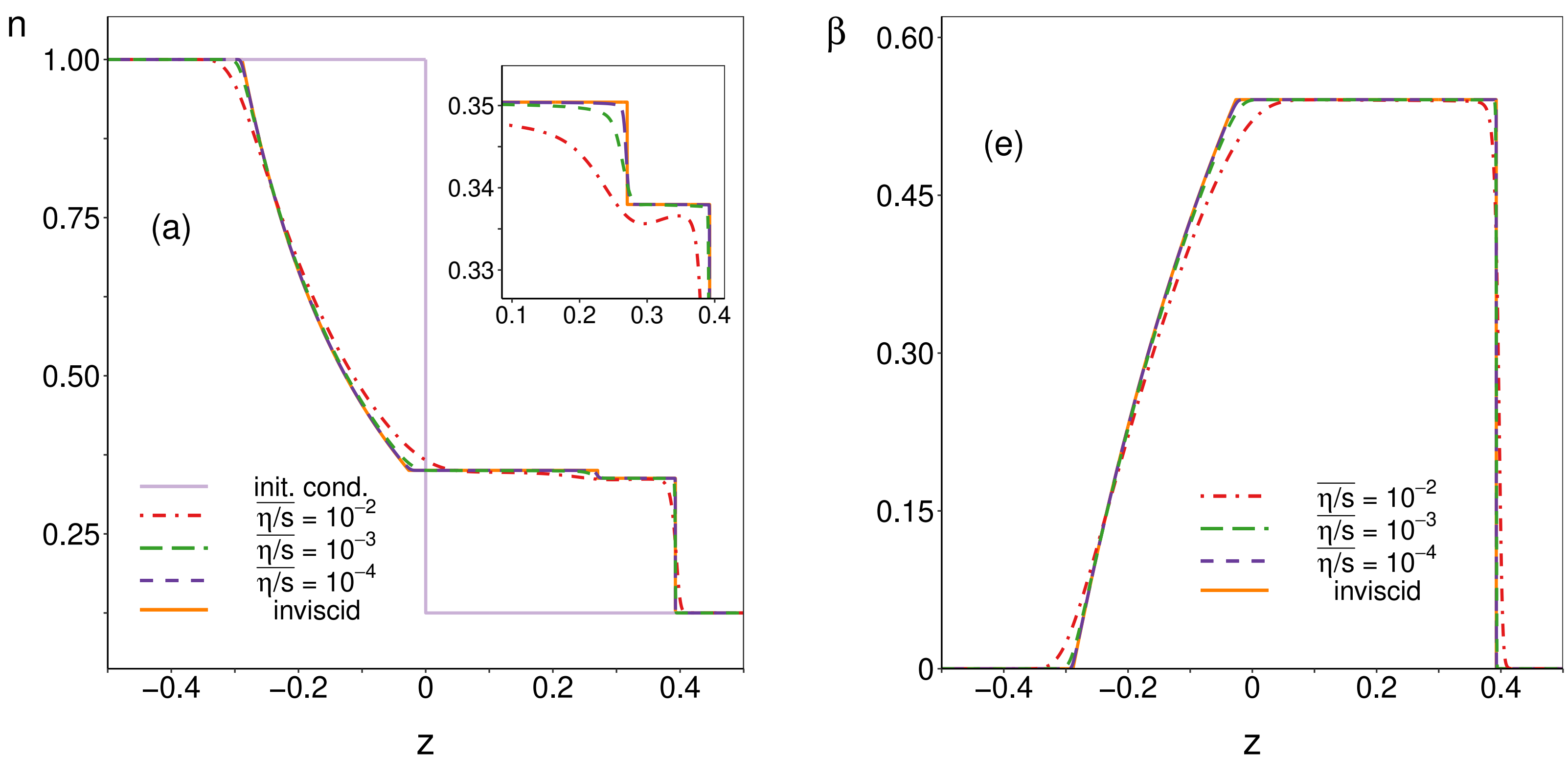
where $\nu_\lambda = k\lambda / 4n_0$, $\nu_d = k\eta / 6P_0$ and $\nu_o \simeq \frac{1}{\sqrt{3}}$ is the speed of sound.

- $(Q = 2) \times (P = 6) \times (M = 1) = 12$ velocities were employed.



Validation 2: Sod shock tube [VEA, R. Blaga, PRC **98** (2018) 035201]





- Inviscid limit smoothly approached as $\eta/s \to 0$.
- Only $Q = 2 \times P = 3 - -4 \times M = 1 = 6 - -8$ velocities required.

Validation against BAMPS [I. Bouras *et al*, PRL **103** (2009) 032301]

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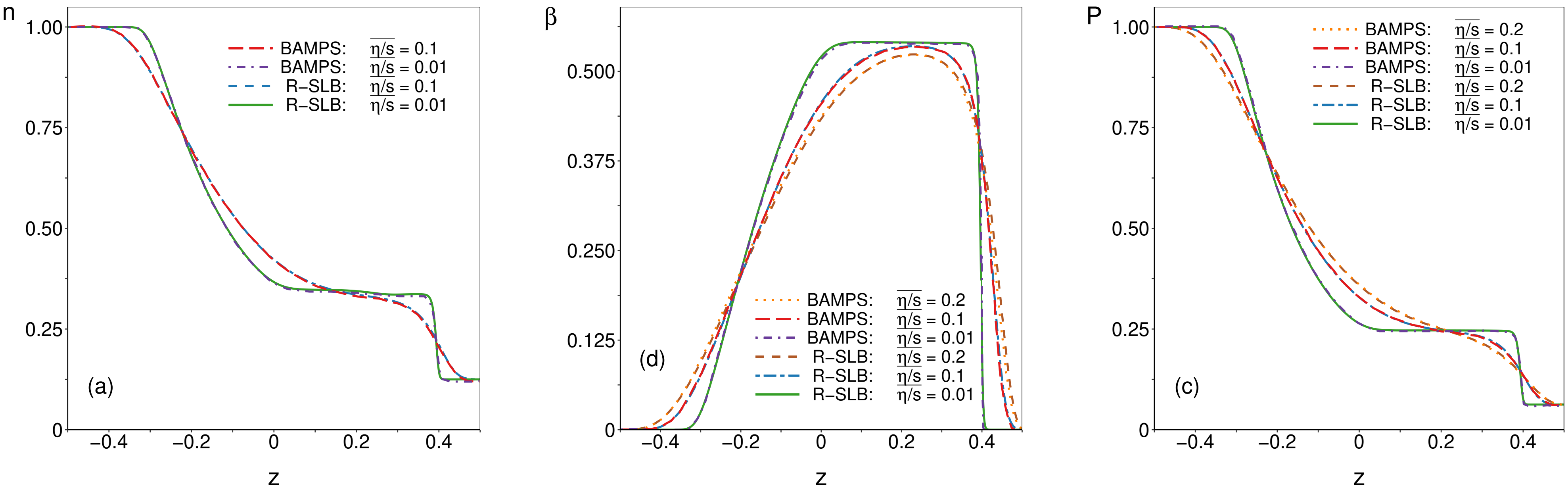
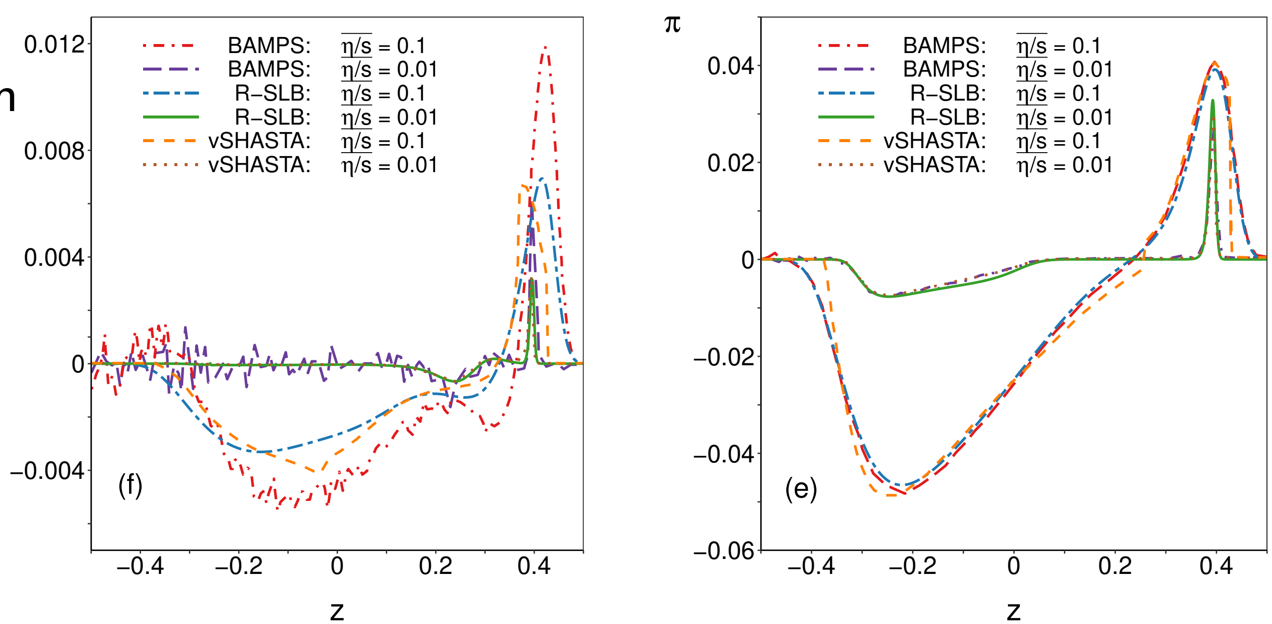


- BAMPS = Boltzmann q Approach to Multiparton Scattering
- vSHASTA = viscous Sharp And Smooth Transport Algorithm
- Good agreement with BAMPS and vSHASTA is observed.



Bjorken flow

Curvilinear coordinates and vielbeins

- For curvilinear coordinates, it is convenient to work with $\omega^{\hat{\alpha}} = \omega^{\hat{\alpha}}_\mu dx^\mu$:

$$ds^2 = g_{\mu\nu} dx^\mu dx^\nu, \qquad g_{\mu\nu} = \eta_{\hat{\alpha}\hat{\beta}} \omega^{\hat{\alpha}}_\mu \omega^{\hat{\beta}}_\nu, \tag{19}$$

- The dual vierbein vectors $e_{\hat{\alpha}} = e^\mu_{\hat{\alpha}} \partial_\mu$ satisfy

$$e^\mu_{\hat{\alpha}} \omega^{\hat{\beta}}_\mu = \delta^{\hat{\beta}}{}_{\hat{\alpha}}, \qquad e^\mu_{\hat{\alpha}} \omega^{\hat{\alpha}}_\nu = \delta^\mu{}_\nu, \qquad g_{\mu\nu} e^\mu_{\hat{\alpha}} e^\nu_{\hat{\beta}} = \eta_{\hat{\alpha}\hat{\beta}}. \tag{20}$$

- Since $k^2 = g_{\mu\nu} k^\mu k^\nu = \eta_{\hat{\alpha}\hat{\beta}} k^{\hat{\alpha}} k^{\hat{\beta}} = m^2$, the mass-shell condition is x-independent:

$$k^{\hat{0}} = \sqrt{\boldsymbol{k}^2 + m^2}. \tag{21}$$

Covariant form

- $\boldsymbol{k} \equiv (k^{\hat{1}}, k^{\hat{2}}, k^{\hat{3}})$ can be parametrised e.g. via spherical coordinates:

$$\boldsymbol{k} \equiv \boldsymbol{k}(k^{\tilde{\imath}}), \qquad k^{\tilde{\imath}}(k, \cos\theta_k, \varphi_k). \tag{22}$$

- Setting $f \equiv f(x^\mu, k^{\tilde{\imath}})$, the Boltzmann eq. can be written in covariant form:[1]

$$\frac{1}{\sqrt{-g}}\partial_\mu(\sqrt{-g}e^\mu_{\hat{\alpha}} k^{\hat{\alpha}} f) - \frac{k^{\hat{\tau}}}{\sqrt{\lambda}} \frac{\partial}{\partial k^{\tilde{\imath}}} \left(K^{\tilde{\imath}}{}_{\hat{\imath}} \Gamma^{\hat{\imath}}{}_{\hat{\alpha}\hat{\beta}} \frac{k^{\hat{\alpha}} k^{\hat{\beta}}}{k^{\hat{\tau}}} f \sqrt{\lambda} \right) = C[f], \tag{23}$$

where $\lambda^{-1/2} = |\mathrm{det} K^{\tilde{\jmath}}{}_{\hat{\imath}}|$ and $K^{\tilde{\jmath}}{}_{\hat{\imath}} = \partial k^{\tilde{\jmath}} / \partial k^{\hat{\imath}}$ is

$$K^{\tilde{\jmath}}{}_{\hat{\imath}} = \begin{pmatrix} \cos\varphi\sqrt{1-\xi^2} & \sin\varphi\sqrt{1-\xi^2} & \xi \\ -\frac{\xi}{k}\cos\varphi\sqrt{1-\xi^2} & -\frac{\xi}{k}\sin\varphi\sqrt{1-\xi^2} & \frac{1-\xi^2}{k} \\ -\frac{\sin\varphi}{k\sqrt{1-\xi^2}} & \frac{\cos\varphi}{k\sqrt{1-\xi^2}} & 0 \end{pmatrix}. \tag{24}$$

- The connection coefficients $\Gamma^{\hat{\imath}}{}_{\hat{\alpha}\hat{\beta}}$ are determined by

$$\nabla_{\hat{\alpha}} e_{\hat{\beta}} = \Gamma^{\hat{\rho}}{}_{\hat{\beta}\hat{\alpha}} e_{\hat{\rho}}. \tag{25}$$

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[1] C. Y. Cardall, E. Endeve, and A. Mezzacappa, Phys. Rev. D **88** (2013) 023011.

Bjorken coordinates

- For boost-invariant expansion, $(t, z) \to (\tau, \eta_s)$ and

$$ds^2 = d\tau^2 - d\mathbf{x}_\perp{}^2 - \tau^2 d\eta_s. \tag{26}$$

- The only non-trivial vierbein vector is $e_{\hat{\eta}_s} = \tau^{-1}\partial_{\eta_s}$, leading to

$$\frac{1}{\tau}\frac{\partial(f\tau)}{\partial\tau} + \boldsymbol{v}_\perp \cdot \nabla f - \frac{\xi^2}{\tau k^2}\frac{\partial(fk^3)}{\partial k} - \frac{1}{\tau}\frac{\partial[\xi(1-\xi^2)f]}{\partial\xi} = -\frac{v \cdot u}{\tau_R}[f - f^{(\mathrm{eq})}]. \tag{27}$$

- $\partial_k[\dots]$ can be evaluated by projection onto the Laguerre polynomials:

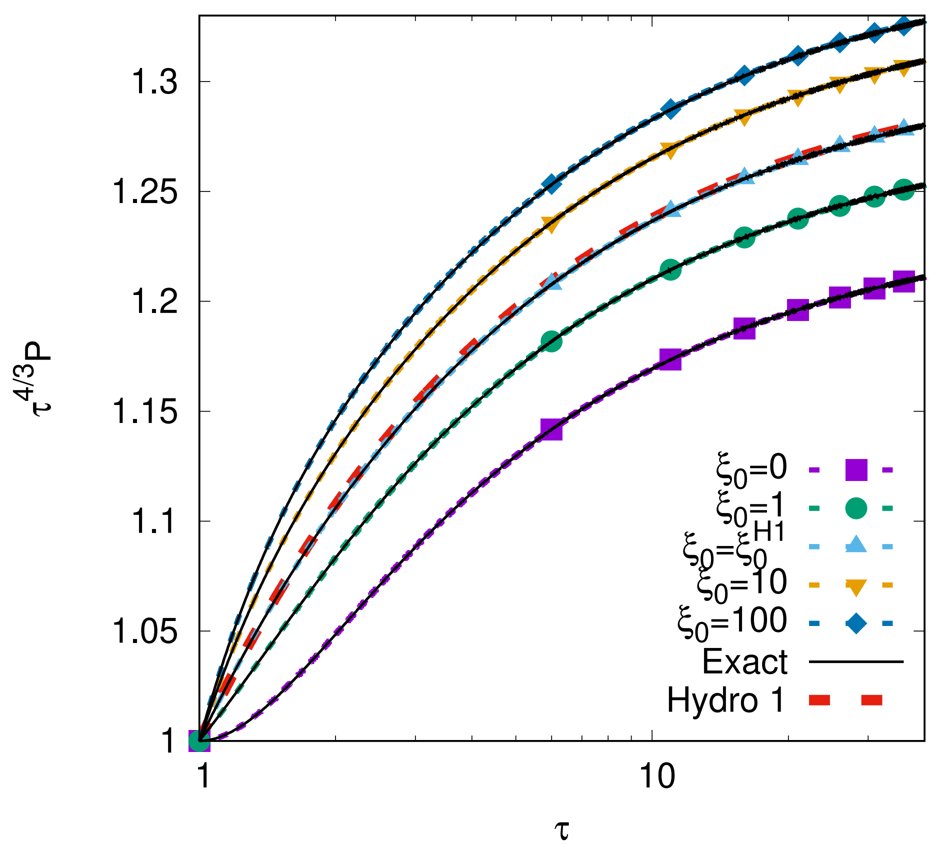
$$f = \frac{e^{-k/T_0}}{T_0^3}\sum_{\ell=0}^{\infty}\frac{\mathcal{F}_\ell L_\ell^{(2)}(k/T_0)}{(\ell+1)(\ell+2)} \Rightarrow \frac{1}{k^2}\frac{\partial(fk^3)}{\partial k} = \frac{e^{-k/T_0}}{T_0^3}\sum_{\ell=0}^{\infty}\frac{L_\ell^{(2)}(k/T_0)}{\ell+1}\left[\mathcal{F}_{\ell-1} - \frac{\ell}{\ell+2}\mathcal{F}_\ell\right],$$

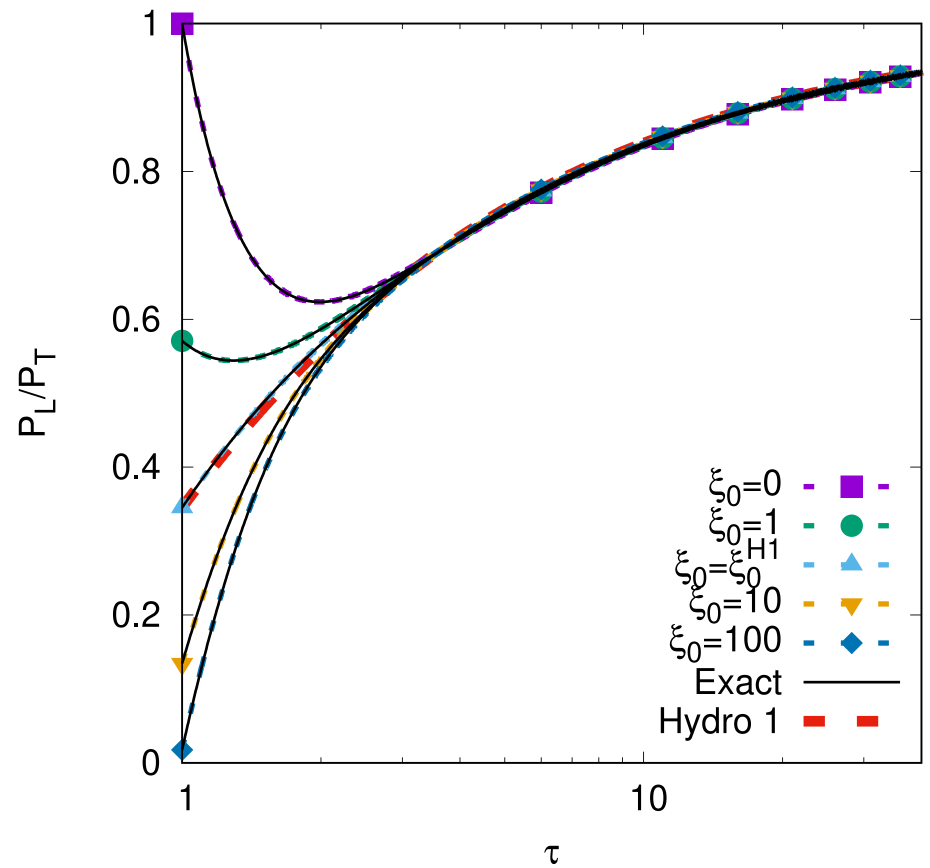
  and similarly for $\partial_\xi[\dots]$.
- More generally, after discretisation, we have

$$\left[\frac{1}{k^2}\frac{\partial(fk^3)}{\partial k}\right]_{ijq} = \sum_{q'=1}^{L}\mathcal{K}^L_{q,q'} f_{ijq'}, \qquad \left[\frac{\partial[\xi(1-\xi^2)f]}{\partial\xi}\right]_{ijk} = \sum_{j'=1}^{P}\mathcal{K}^P_{j,j'} f_{ij'q}, \tag{28}$$

  where $\mathcal{K}^L_{q,q'}$ and $\mathcal{K}^P_{j,j'}$ depend solely on quadrature.

$0 + 1$-D case: conformal fluid

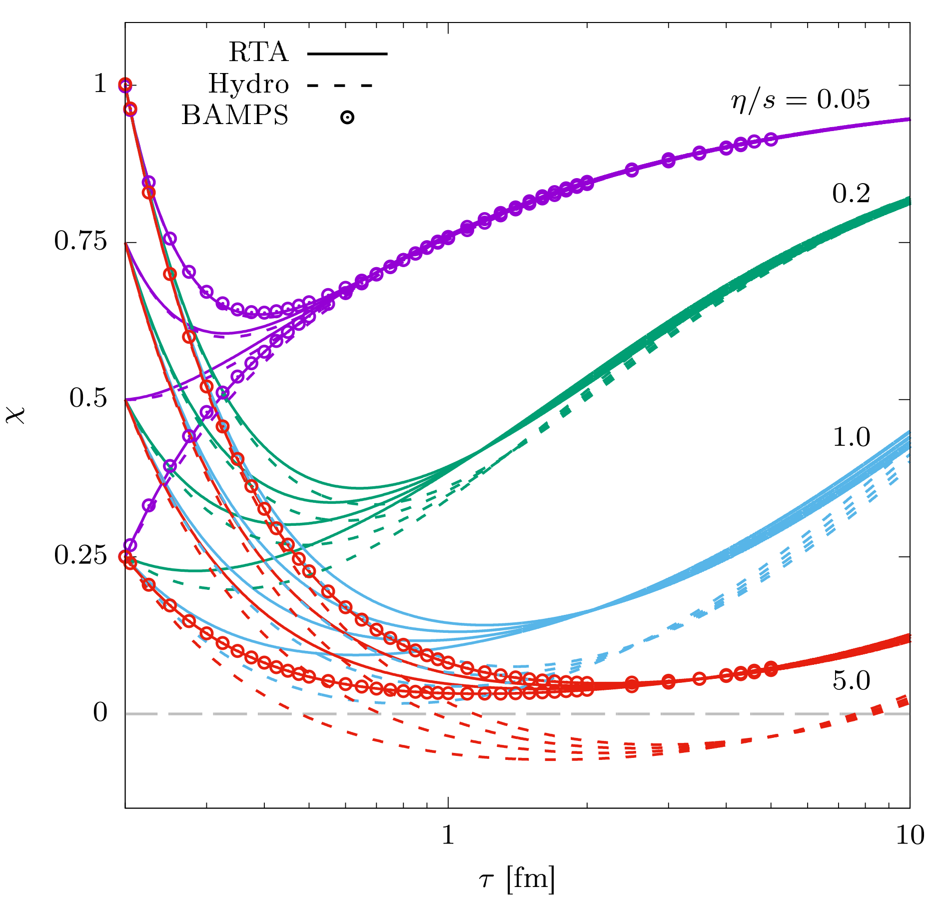




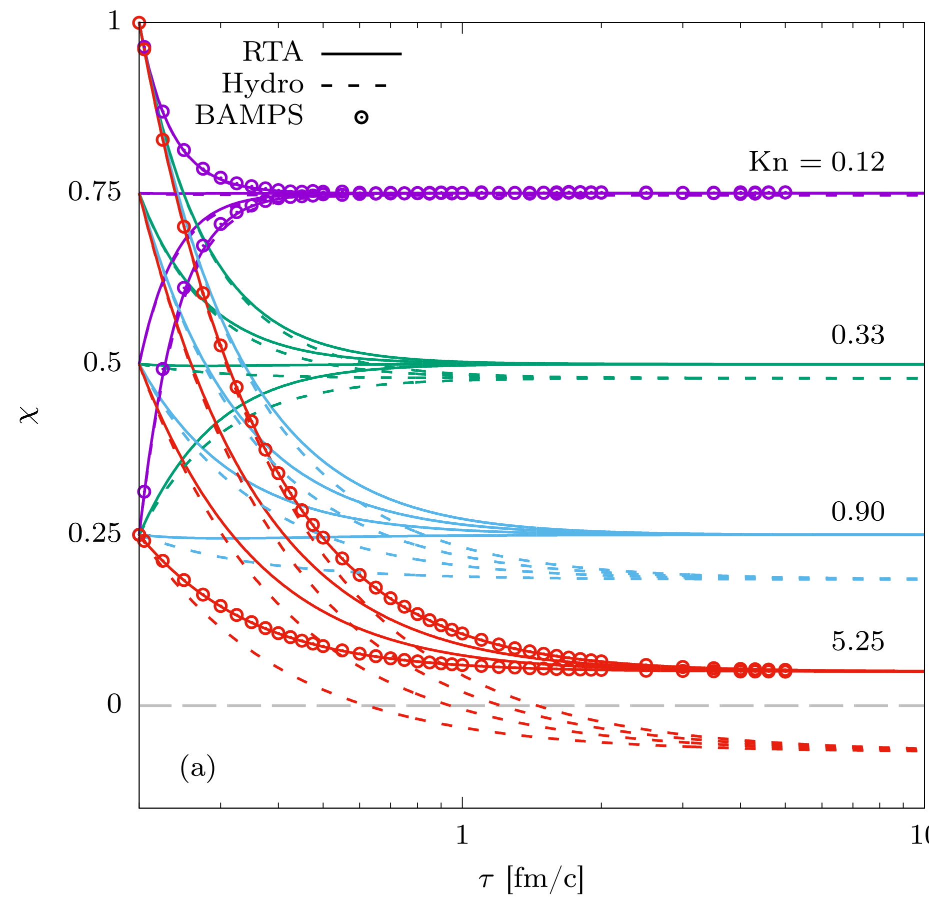
- For conformal fluids, $\mu = 0$ and $T^{\mu\nu}$ can be tracked using $Q = 1$.
- The numerical results are validated against a semi-analytic solution.

[W. Florkowski *et al*, PRC **88** (2013) 024903]

$0 + 1$-D case: non-conformal fluid



(constant η/s)

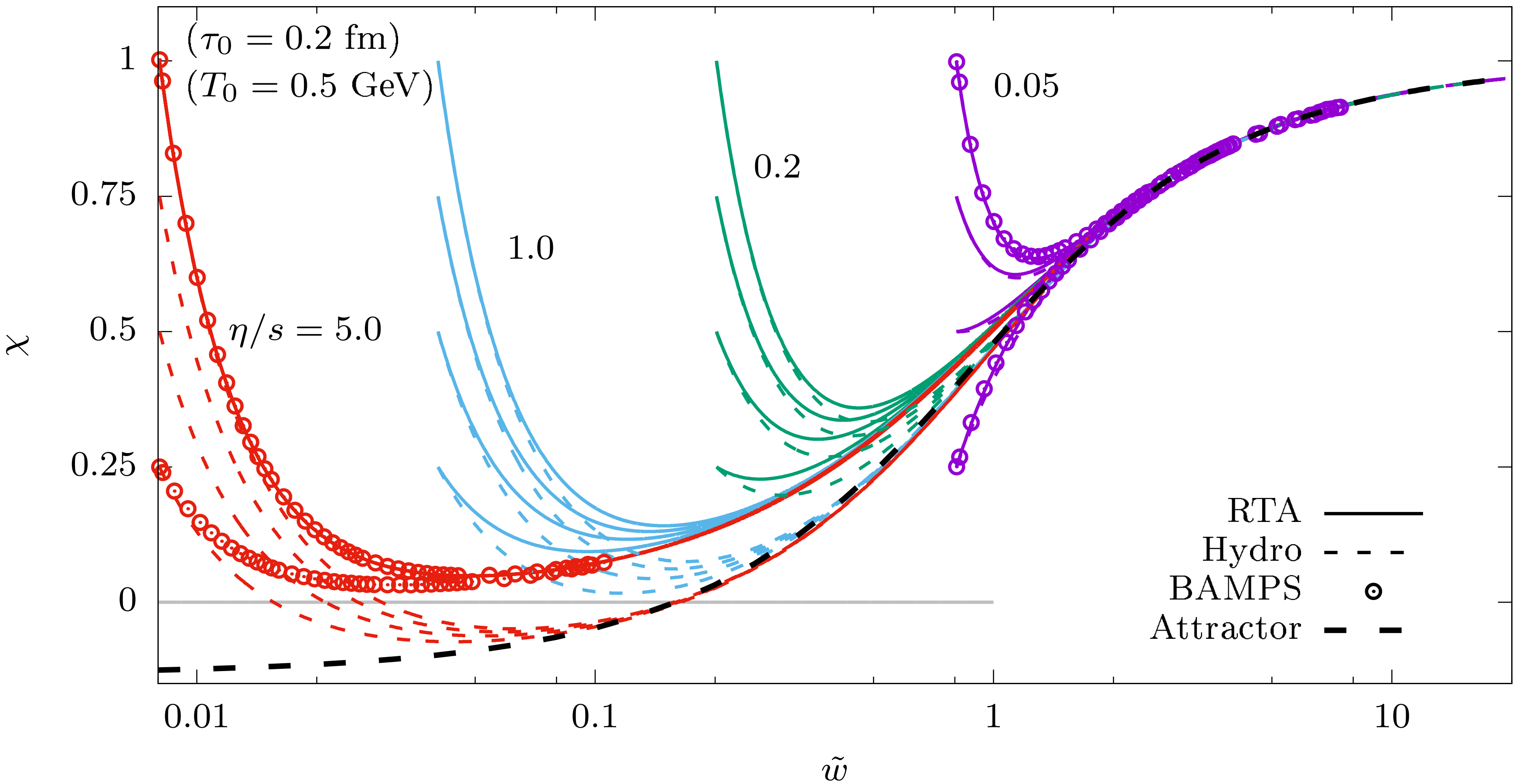


(Hard spheres with $\mathrm{Kn} = 1/n\tau\sigma$)

- $M = 1$ (0 + 1D); $Q = 2$ ($\mu \neq 0$); $P = 40$.
- Good agreemet with hydro & BAMPS.

[VEA *et al*, arXiv:2102.11785]

$0 + 1$-D case: (non-conformal) attractor



- Attractor validated for $\chi = \mathcal{P}_L/\mathcal{P}_T$ when $\tilde{w} = \tau T/(4\pi\eta/s)$ is generalized to

$$\tilde{w}_{\rm nc} = \frac{\tau T}{4\pi\eta/s}\left[1 + \ln\left(\frac{\tau P^{3/4}}{\tau_0 P_0^{3/4}}\right)\right]^{-1}. \qquad (29)$$

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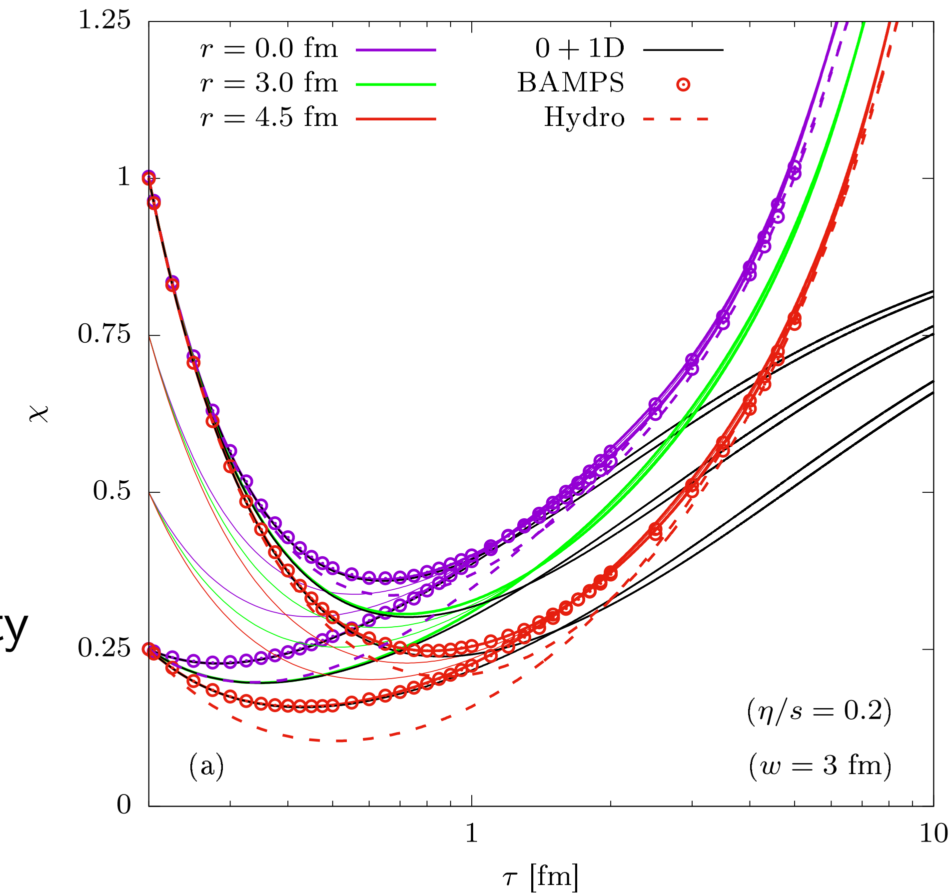


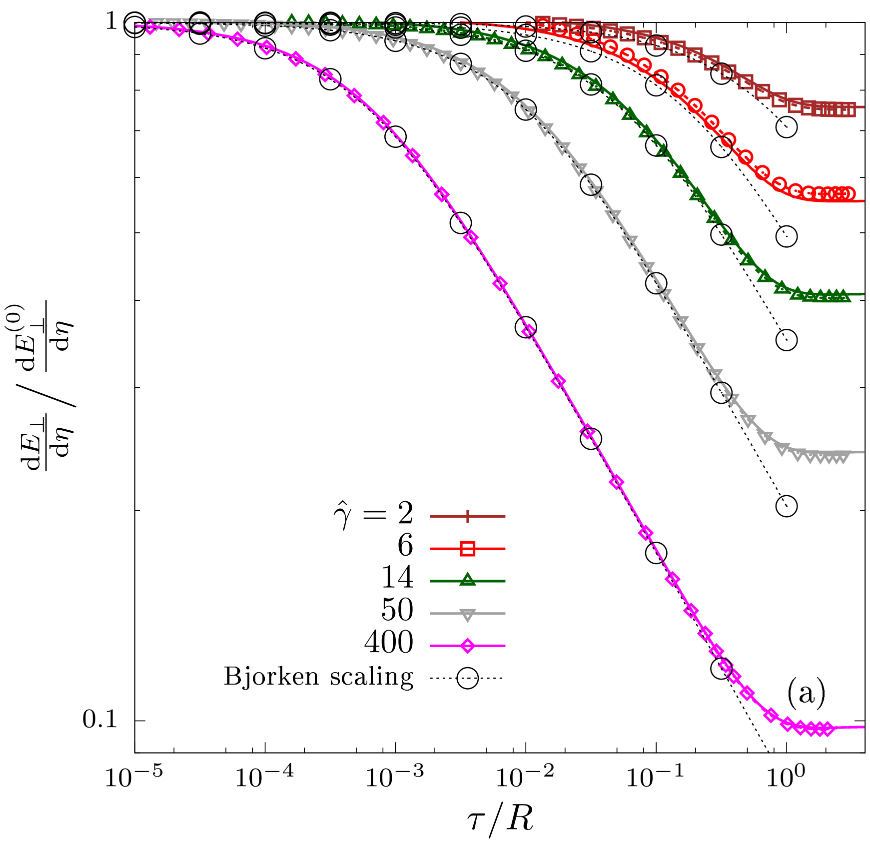
- Initial transverse plane energy density set to

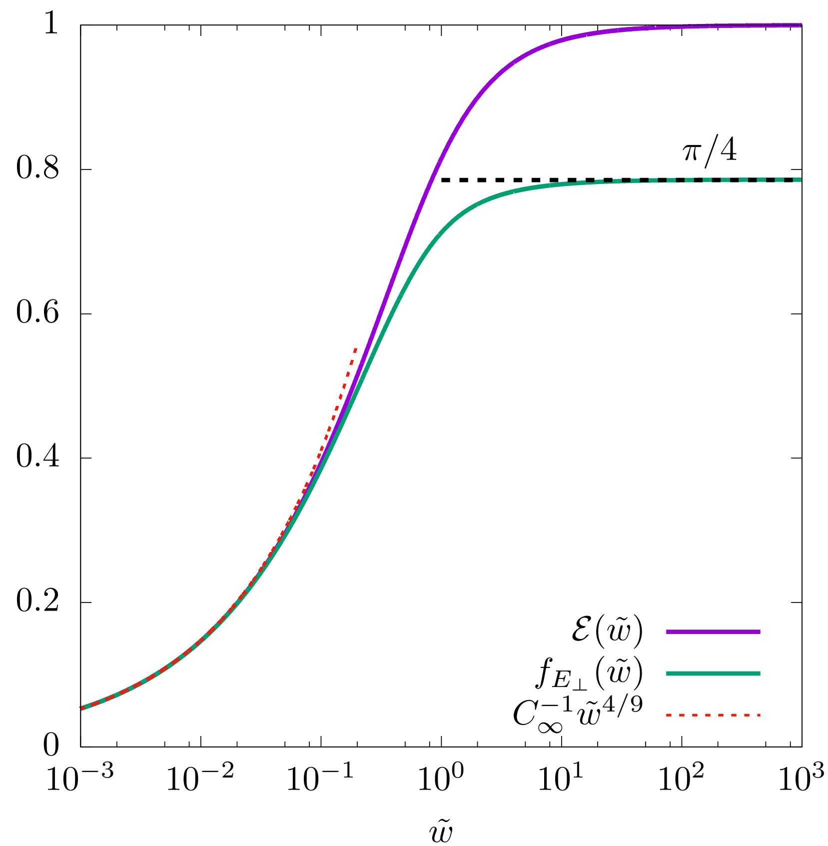
$$\bar{\epsilon}(\tau_0, r) = \epsilon_0 e^{-r^2/R^2},$$

with $R = w\sqrt{3}/2$.

- At early times, the longitudinal expansion is dominant.
- At late times ($\tau > R$), transverse expansion becomes dominant.
- Good agreement with hydro & BAMPS.
- $Q = 2$, $M = 40$ and $P = 160$ due to $\beta \to 1$ at large τ.

$2 + 1$-D case: cooling





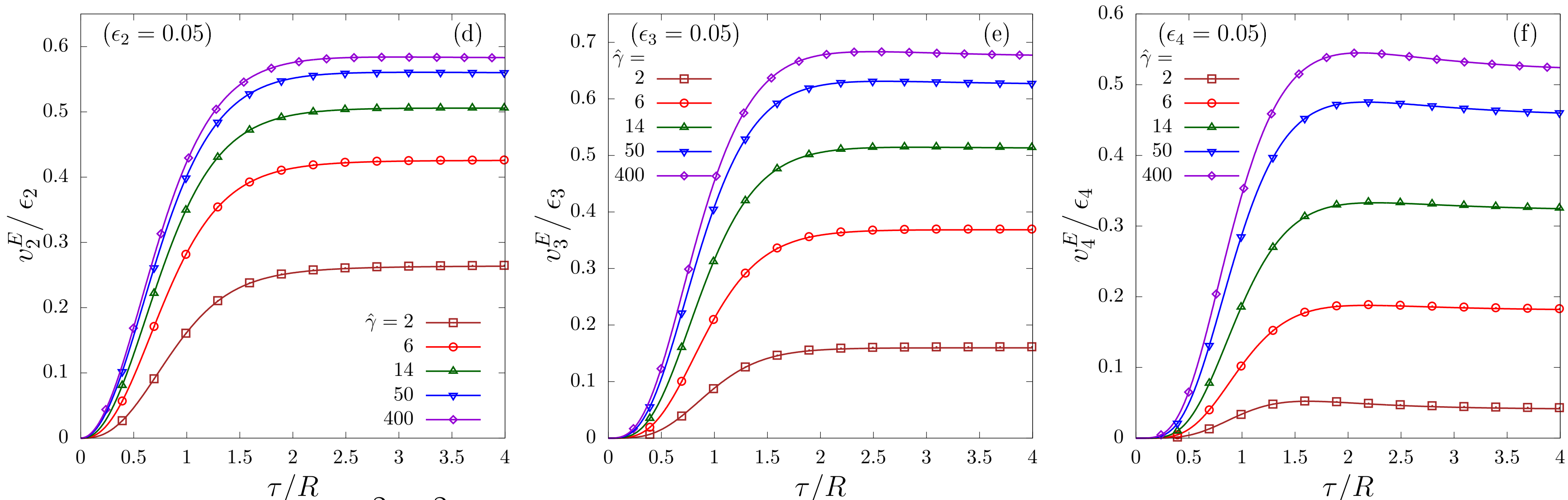
- Early time cooling described by local Bjorken scaling [Giacalone *et al*, PRL **123** (2019) 262301]

$$\tau^{1/3}\frac{dE_\perp}{d^2\mathbf{x}_\perp d\eta} = \left(\frac{4\pi\eta}{s}\right)^{4/9}\left(\frac{\epsilon}{T^4}\right)^{1/9}(\epsilon_0\tau_0)^{8/9}C_\infty f_{E_\perp}(\tilde{w})$$

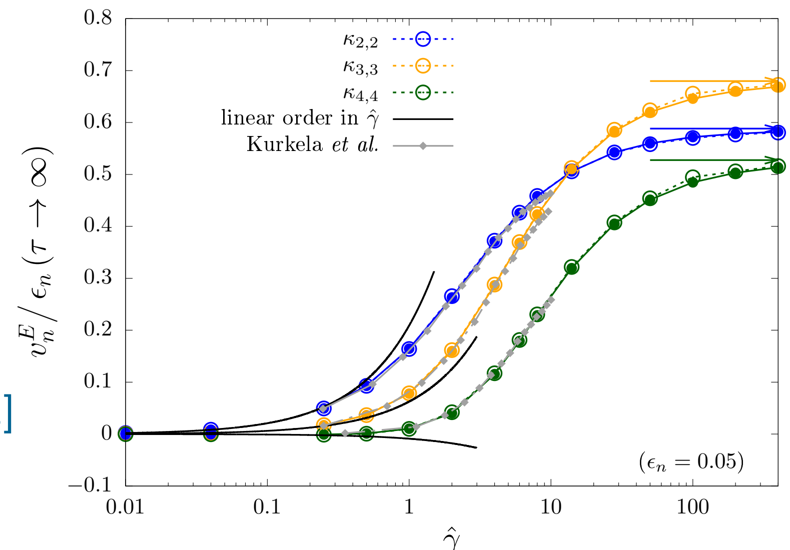
- $f_{E_\perp}$ can be obtained from Bjorken flow and satisfies $[\hat{\gamma} \sim \tau_0^{1/4}R^{3/4}T_0(\eta/s)^{-1}]$

$$f_{E_\perp}(\tilde{w} \ll 1) = C_\infty^{-1}\tilde{w}^{4/9}, \qquad f_{E_\perp}(\tilde{w} \gg 1) = \frac{\pi}{4}.$$

$2 + 1$-D case: Flow harmonics



$$\epsilon(\tau_0, \mathbf{x}_\perp) = \epsilon_0 e^{-r^2/R^2} \times \left\{1 + \delta_n e^{-r^2/2R^2} \left(\frac{r}{R}\right)^n \cos(n\phi)\right\}$$



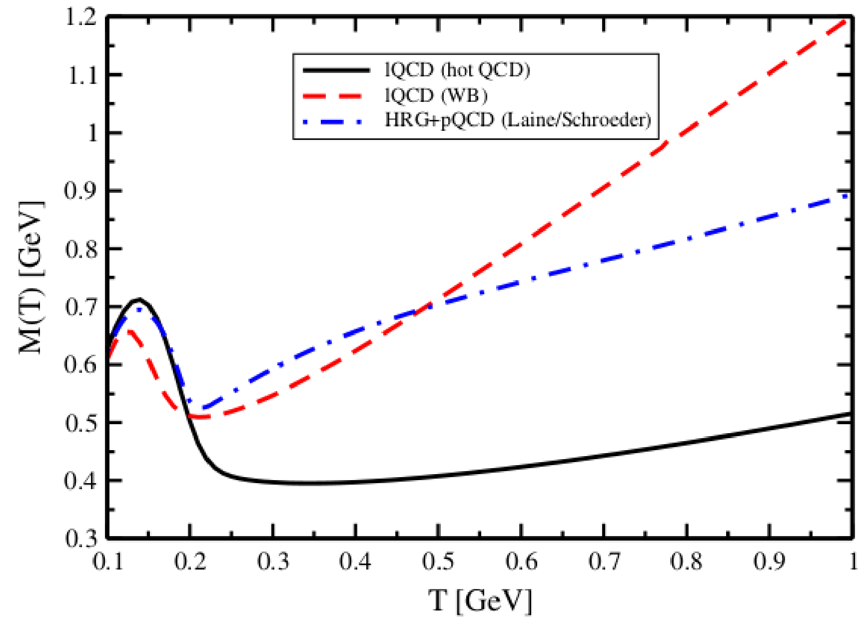
- Good agreement for v_n/ϵ_n vs. τ/R.
- Good agreement of $\tau \to \infty$ limit vs. prev. results. [Kurkela *et al*, PLB **811** (2020) 135901]
- $\hat{\gamma} \sim \tau_0^{1/4} R^{3/4} T_0 (\eta/s)^{-1}$.

Extension: Non-ideal EOS? [P. Romatschke, PRD **85** (2012) 065012]

- Basic idea: allow for medium-dependent M:

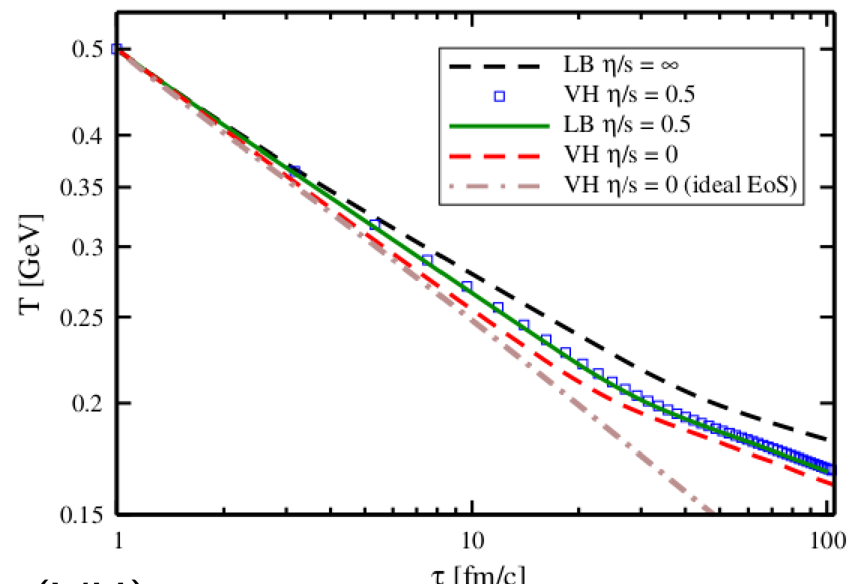
$$\partial_\mu \left(\frac{K^\mu f}{E}\right) + \frac{1}{2}\frac{\partial M^2}{\partial x^i}\frac{\partial (f/E)}{\partial K_i} = \frac{K^\mu U_\mu}{\tau_R E}(f - f^{(\text{eq})}).$$

where $K^2 = M^2(T,\mu)$.



- While $f^{(\text{eq})}$ is still MJ (ideal), the non-ideal EOS is implemented via

$$\begin{aligned}\epsilon =& \epsilon_{\text{MJ}} + B(T,\mu),\\ p =& p_{\text{MJ}} - B(T,\mu),\\ n =& n_{\text{MJ}}.\end{aligned}$$



- Phase transition affects $T(\tau)$.
- Good agreement between LB and hydro (VH).

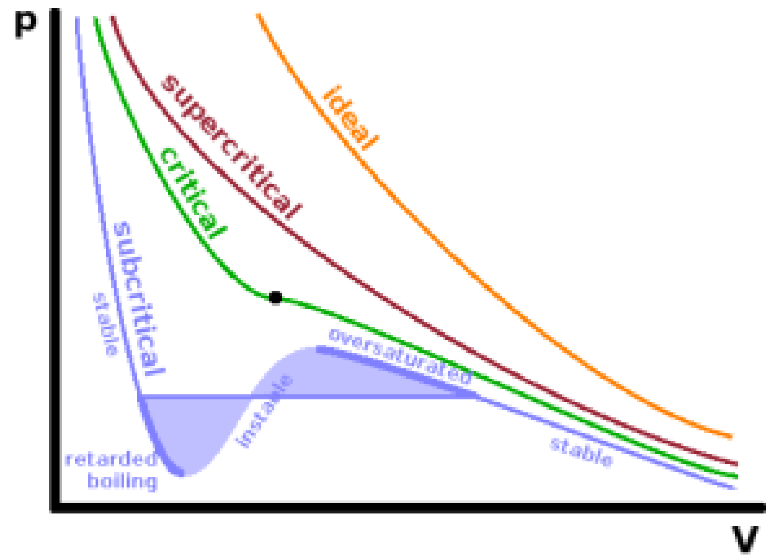
Multiphase flows: Van der Waals fluid (non-relativistic)

Van der Waals EOS

- Step back to non-relativistic fluids.
- $P = nT$ replaced by vdW EOS:

$$P_{\rm Waals} = \frac{3nT}{3-n} - \frac{9}{8}n^2,$$

where $(n = 1, T = 1, P = 3/8) \equiv$ CP.



- A standard (minimal) way to incorporate non-ideal EOS is to introduce the vdW interaction via an external force:

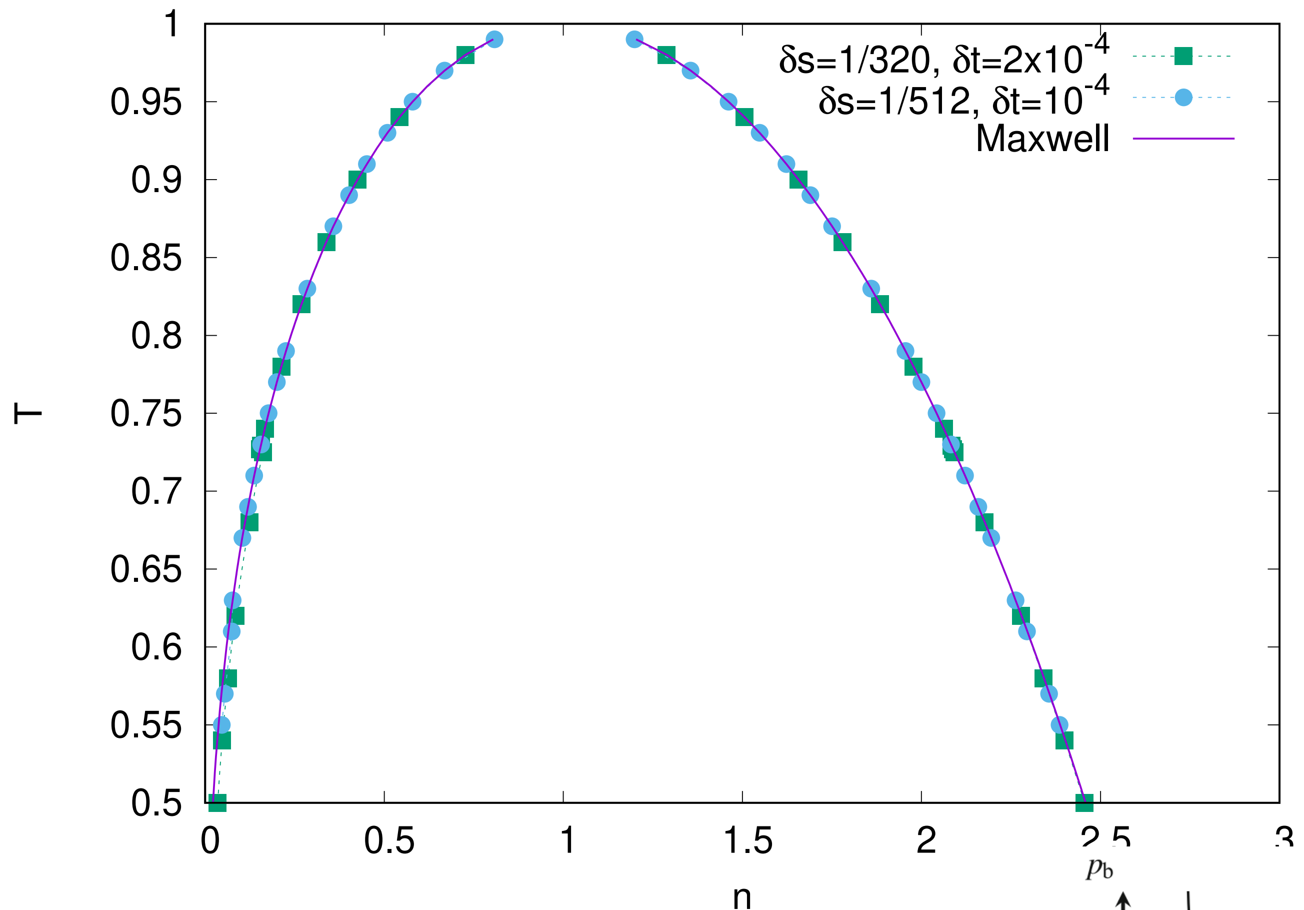
$$\partial_f + \boldsymbol{v} \cdot \nabla f + \frac{\boldsymbol{F}}{m} \cdot \nabla_{\boldsymbol{v}} f = -\frac{1}{\tau}(f - f^{(\rm eq)}),$$
$$\boldsymbol{F} = n\sigma_s \nabla(\Delta n) - \nabla(P_{\rm Waals} - P_{\rm ideal}). \tag{30}$$

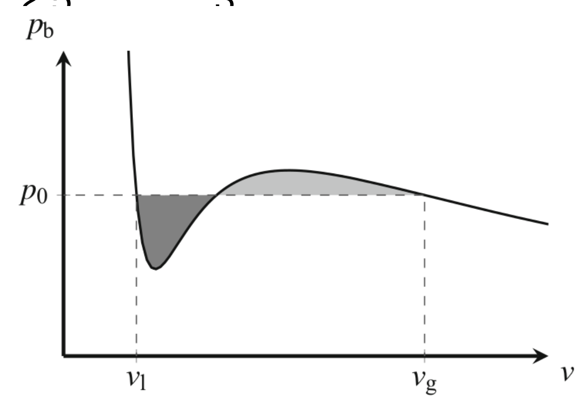
- In the momentum eq. $\rho \frac{D\boldsymbol{u}}{Dt} = n\boldsymbol{F} - \nabla P - \nabla \cdot \overleftrightarrow{\boldsymbol{\sigma}}$ one obtains

$$\rho \frac{D\boldsymbol{u}}{Dt} = n\sigma_s \nabla(\Delta n) - \nabla P_{\rm waals} - \nabla \cdot \overleftrightarrow{\boldsymbol{\sigma}}, \tag{31}$$

where σ_s controls the surface tension.

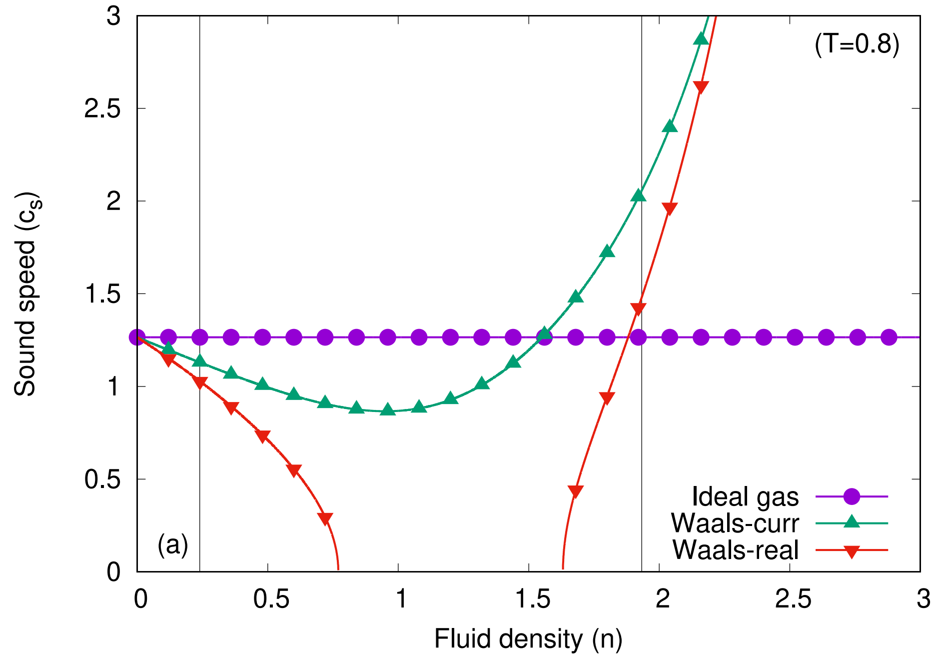
Phase diagram





n_g and n_l are given through the Maxwell construction:

$$\int_{n_l^{-1}}^{n_g^{-1}} [P_{\rm Waals} - P^0_{\rm Waals}] dn^{-1} = 0.$$

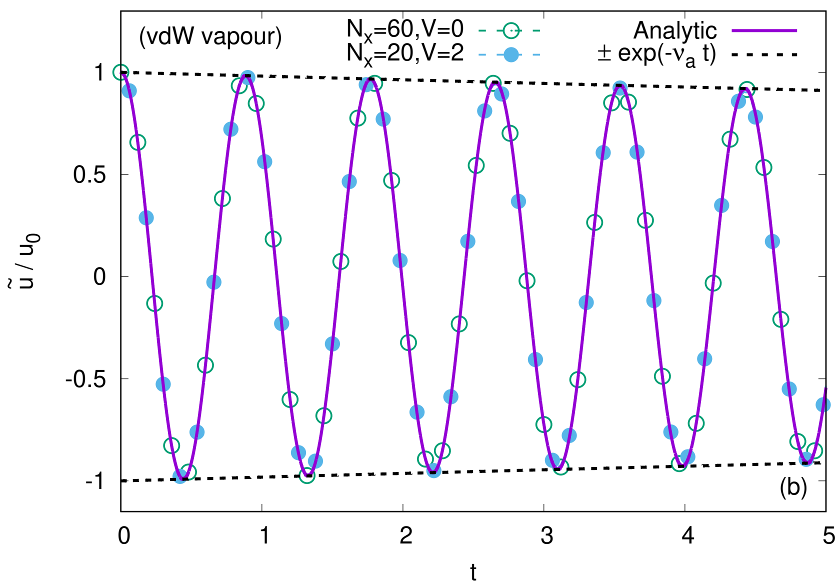


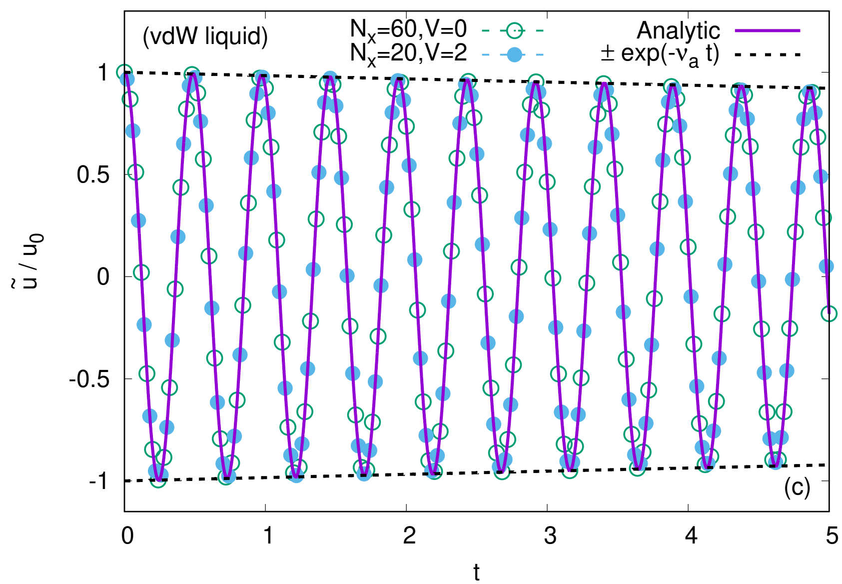
- Spinodal region when $\kappa_T \sim \partial P_{\rm Waals}/\partial n < 0$,

$$n^3 - 6n^2 + 9n - 4T > 0.$$

- Sound speed can become imaginary:

$$c_s^2 = \frac{\partial P_{\rm Waals}}{\partial \rho} + \frac{P_{\rm ideal}}{n\rho}\frac{\partial P_{\rm waals}}{\partial T}.$$





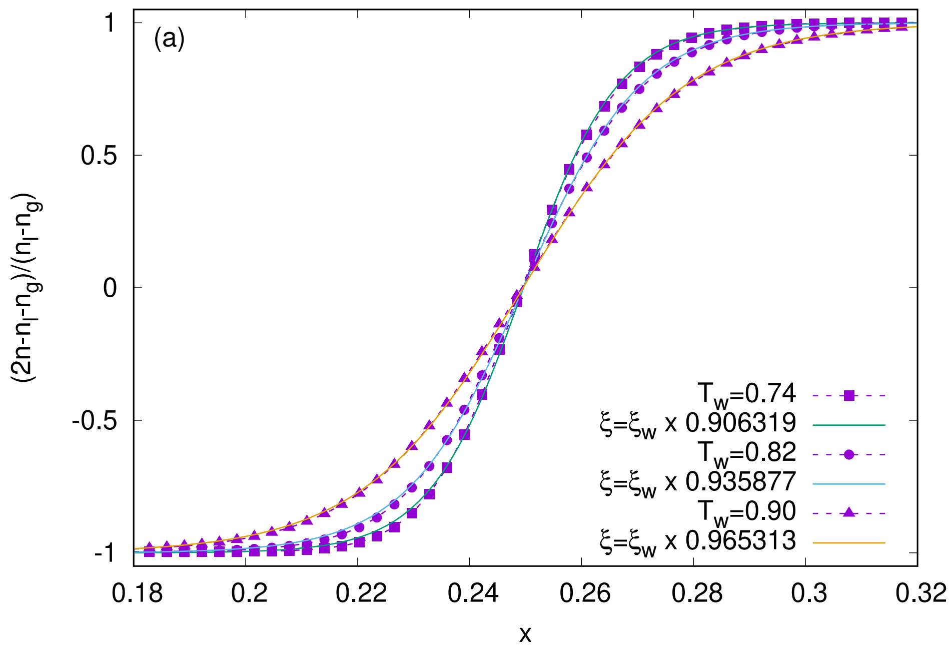
Planar interface

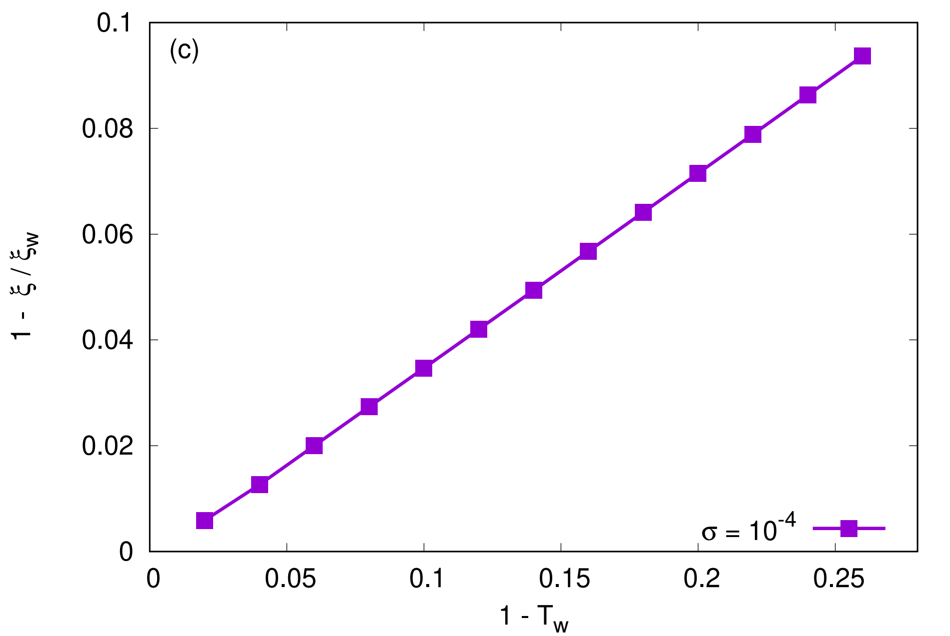
- The fluid is enclosed between two plates at $T_w = 0.8$ and $\pm x_w$.
- The system is hom. w.r.t. y.
- The interfaces are initialised at $\pm x_w/2$.
- Approximate formula (valid when $T \to 1$):

$$n(x) = n_g + \frac{n_l - n_g}{2} \times \left[1 + \tanh\frac{(x - x_0)}{\xi}\right],$$

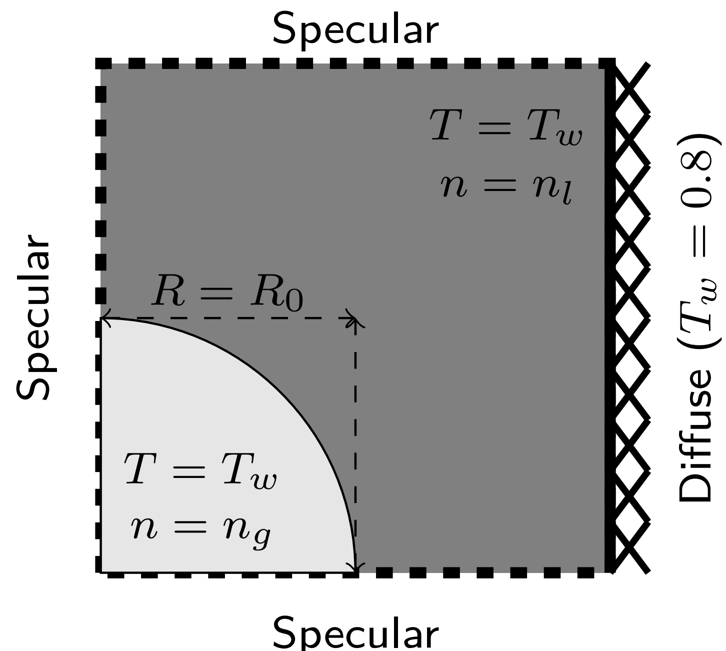
$$\xi_w = \sqrt{\frac{8\sigma}{9(1 - T_w)}}.$$

[Wagner, Pooley, PRE **76** (2007) 045702(R)]





Surface tension

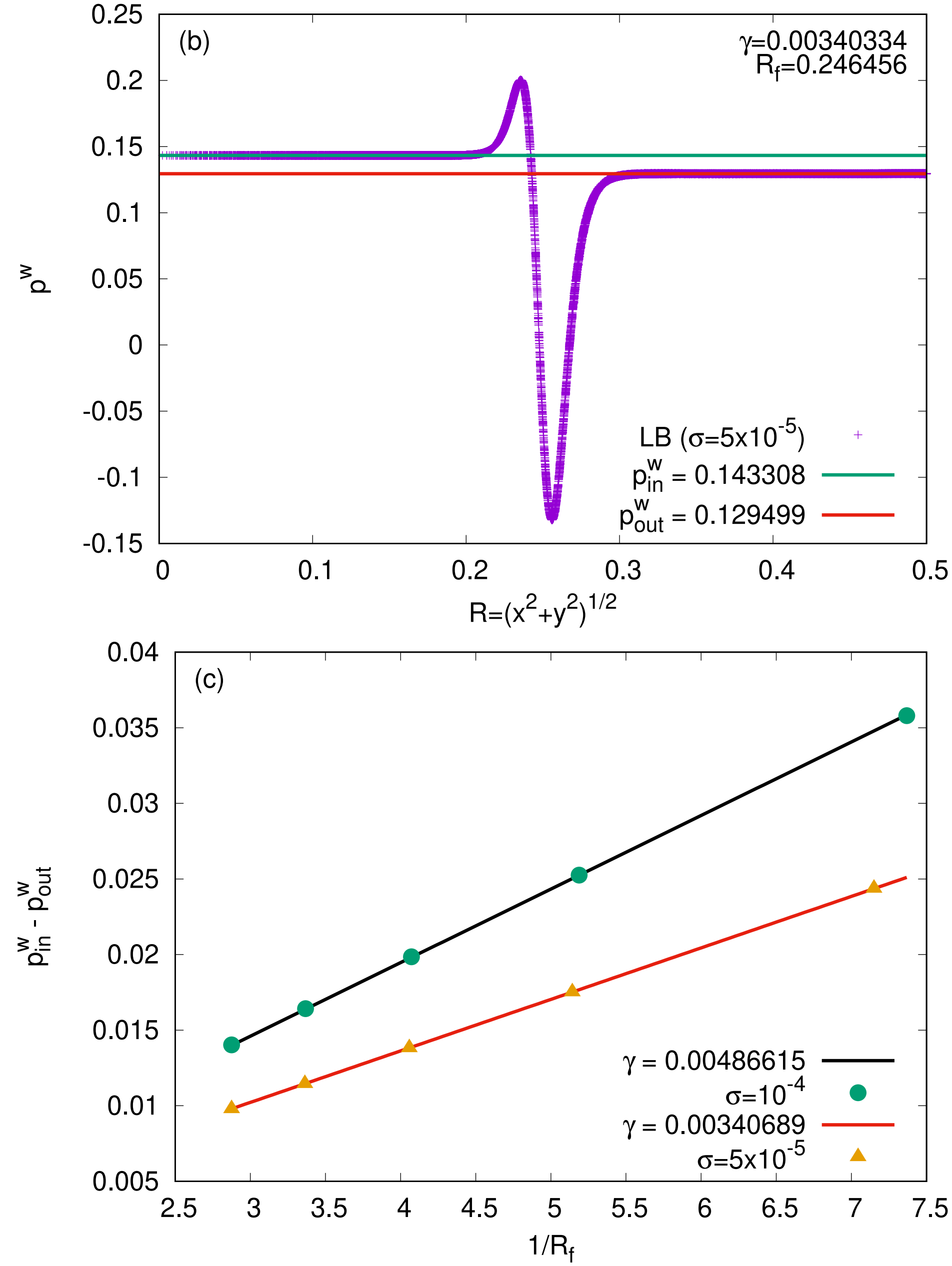


- Laplace's law:

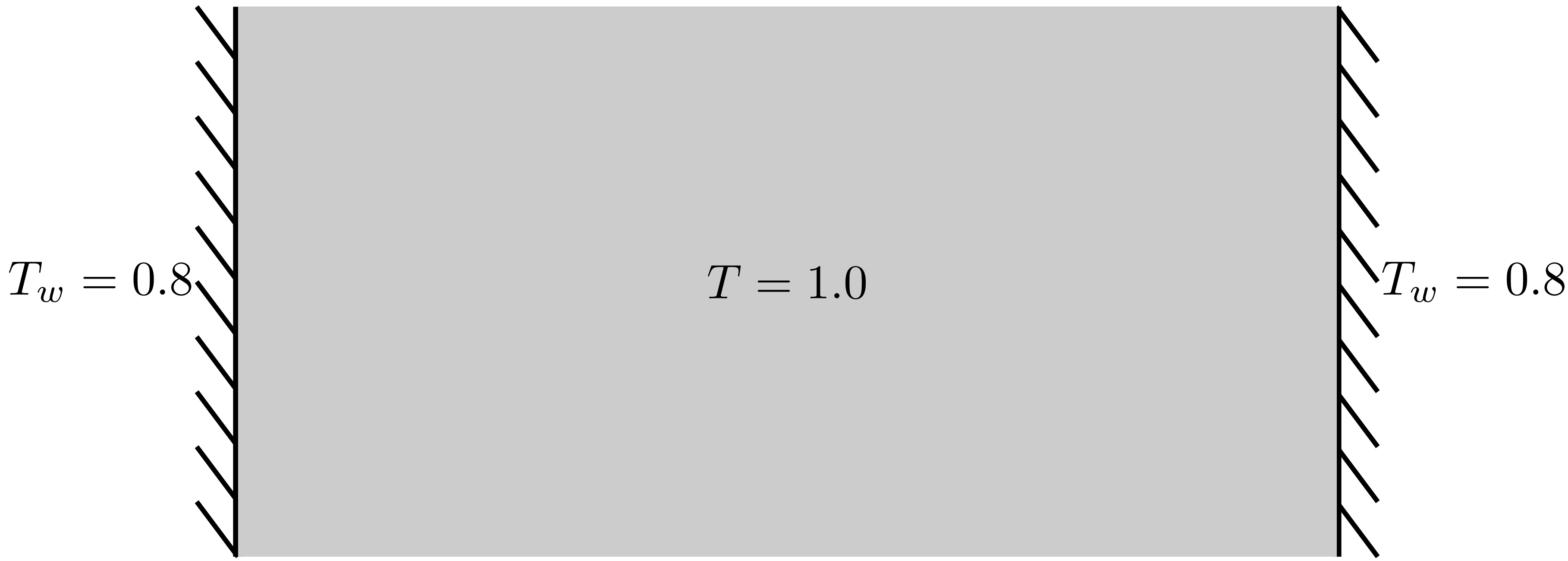
$$P^{\rm w}_{\rm in} - P^{\rm w}_{\rm out} = \frac{\gamma_{\rm Lap}}{R}.$$

- For the planar interface:

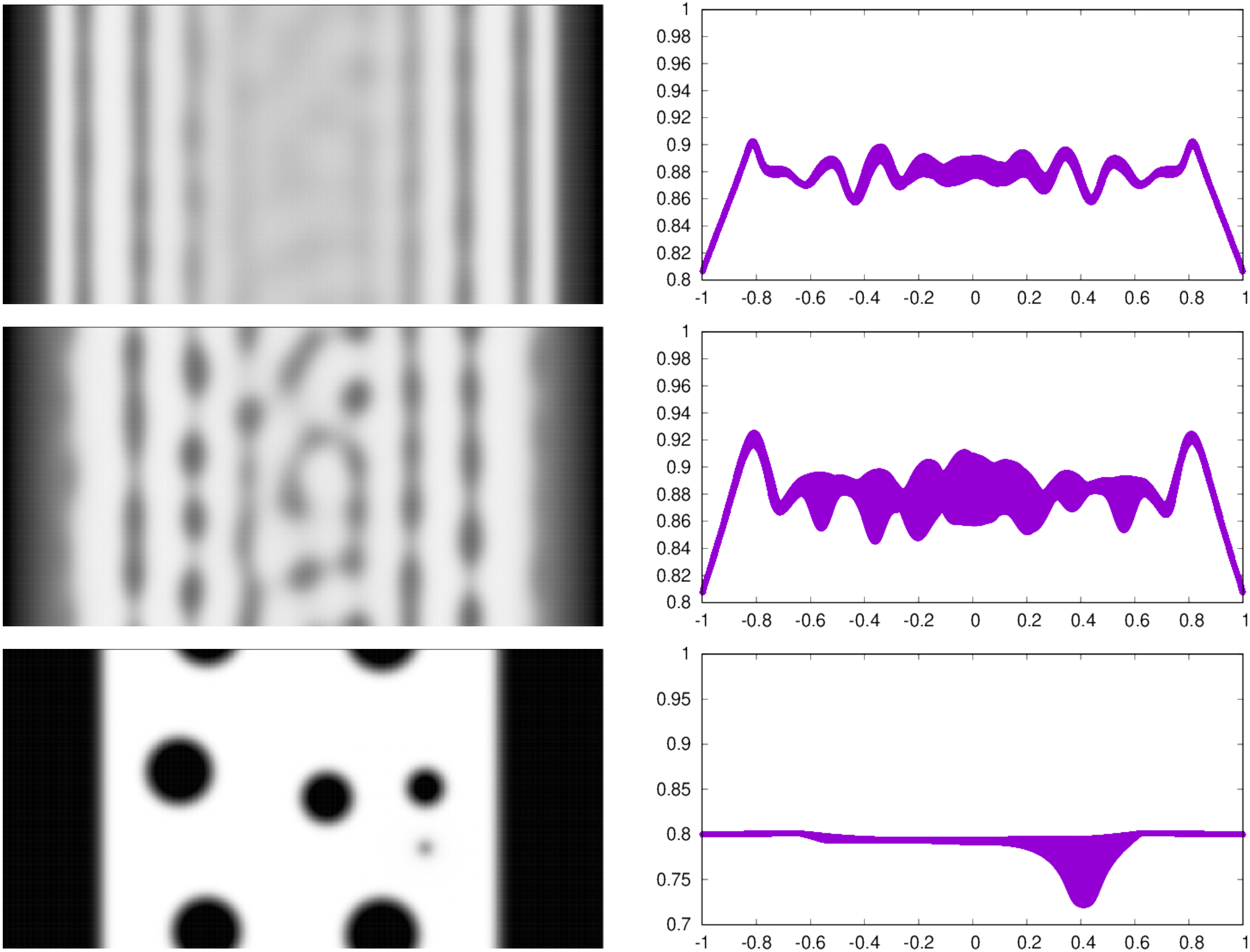
$$\gamma_{\rm pl} = \sigma \int dx \left(\frac{dn}{dx}\right)^2.$$



Phase separation between parallel plates



- The fluid is initially at the critical temperature.
- Small fluctuations ($\sim 1\%$) are present in the initial density.
- The system is quenched due to walls at $0.8 T_c$.



(density) (temperature)

Multicomponent systems: Cahn Hilliard model

Multicomponent flows [Krüger *et al*, LBM: Principles and Practice, Springer, 2

- Multicomponent flows contain two (*binary*) or more (ternary, etc) different substances which do not interconvert.
- The distinction between the components is made using an order parameter ϕ, e.g. (for binary fluids):
$$\phi = \frac{\rho^{(1)} - \rho^{(2)}}{\rho^{(1)} + \rho^{(2)}},$$
where $\rho^{(1)}$ and $\rho^{(2)}$ are the *local* densities of components 1 and 2.
- The bulk phase densities $\rho_b^{(1)}$ and $\rho_b^{(2)}$ correspond to the case of pure components, such that:
$$\phi = \begin{cases} 1, & \text{component 1}, \rho^{(1)} = \rho_b^{(1)}, \rho^{(2)} = 0, \\ -1, & \text{component 2}, \rho^{(1)} = 0, \rho^{(2)} = \rho_b^{(2)}. \end{cases}$$
- *Immiscible fluids* form regions of pure phases separated by internal interfaces characterised by surface tension.

Landau free energy model

[A. J. Bray, Adv. Phys. **51** (2002) 481]

- Assuming that $\rho_b^{(1)} = \rho_b^{(2)} = \rho_b$, the simplest model for multicomponent systems is the Landau free energy model:

$$\Psi = \int_V (\psi_b + \psi_g) dV = \int_V \left[c_s^2 \rho \ln \rho + \frac{A}{4}(\phi^2 - 1)^2 + \frac{\kappa}{2}(\nabla\phi)^2 \right] dV,$$

  where ψ_b and ψ_g are responsible for the bulk and interface properties, respectively.
- $A > 0$ for immiscible fluids.
- ψ_b has two minima: $\phi = \pm 1$, corresponding to the pure phases.
- The fluid evolution must lead to the minimisation of Ψ.
- At equilibrium, the chemical potential μ reaches a constat value:

$$\mu = \frac{\delta(\psi_b + \psi_g)}{\delta\phi} = -A\phi(1 - \phi^2) - \kappa\Delta\phi = \text{const}.$$

Advection-diffusion model

- The time evolution of ϕ is given by the Cahn-Hilliard equation:

$$\partial_t \phi + \nabla \cdot (\boldsymbol{u}\phi) = \nabla \cdot (M \nabla \mu).$$

- The C-H equation governs the advection of ϕ along $\boldsymbol{u}$ and the diffusion of ϕ due to inhomogeneities in μ (M is the mobility parameter).
- The fluid itself evolves according to the Navier-Stokes equations:

$$\partial_t \rho + \nabla \cdot (\boldsymbol{u}\rho) = 0, \qquad \rho(\partial_t u^i + u^j \nabla_j u^i) = -\nabla_j (P^{ij} + \sigma^{ij}),$$

where the non-ideal stress P_{ij} is

$$P_{ij} = \left[P_b - \frac{\kappa}{2} (\nabla \phi)^2 - \kappa \phi \Delta \phi \right] \delta_{ij} + \kappa (\nabla_i \phi)(\nabla_j \phi).$$

- The bulk pressure is

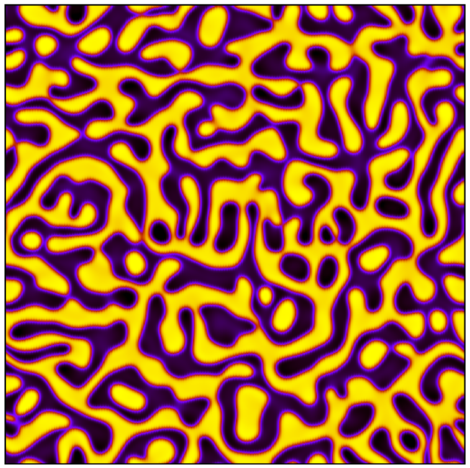
$$P_b = P_{\rm ideal} + A \left(-\frac{1}{2}\phi^2 + \frac{3}{4}\phi^4 \right),$$

where $P_{\rm ideal} = n K_B T$ is the ideal gas pressure.
- The surface tension is governed by the κ term.

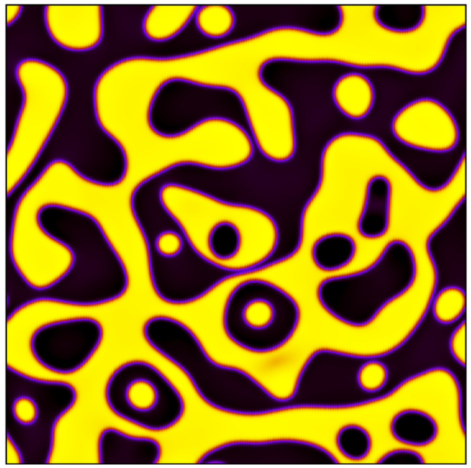
Spinodal decomposition [VEA *et al*, PRE **100** (2019) 063306]

$\phi(t=0,x,y) = delta\phi(x,y)$, $-0.1 < \delta\phi < 0.1$ randomly distributed.

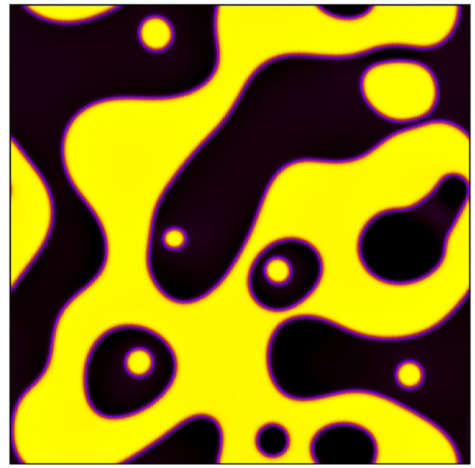
With hydro:



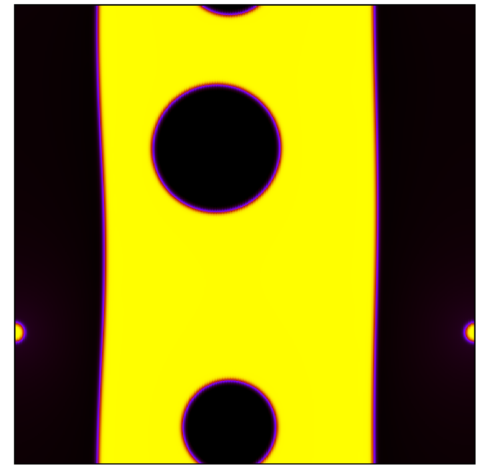
$t = 40$



$t = 100$

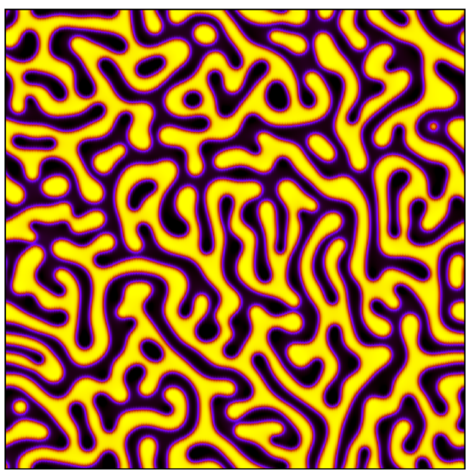


$t = 250$

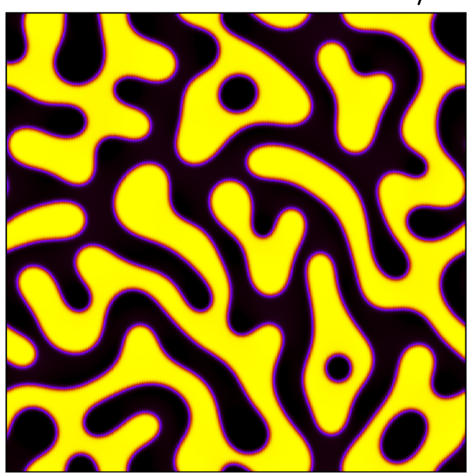


$t = 3000$

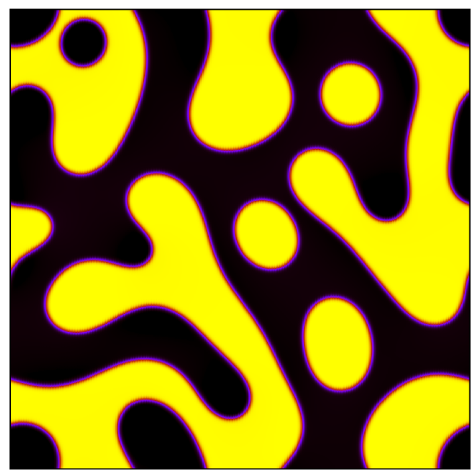
W/o hydro:



$t = 300$



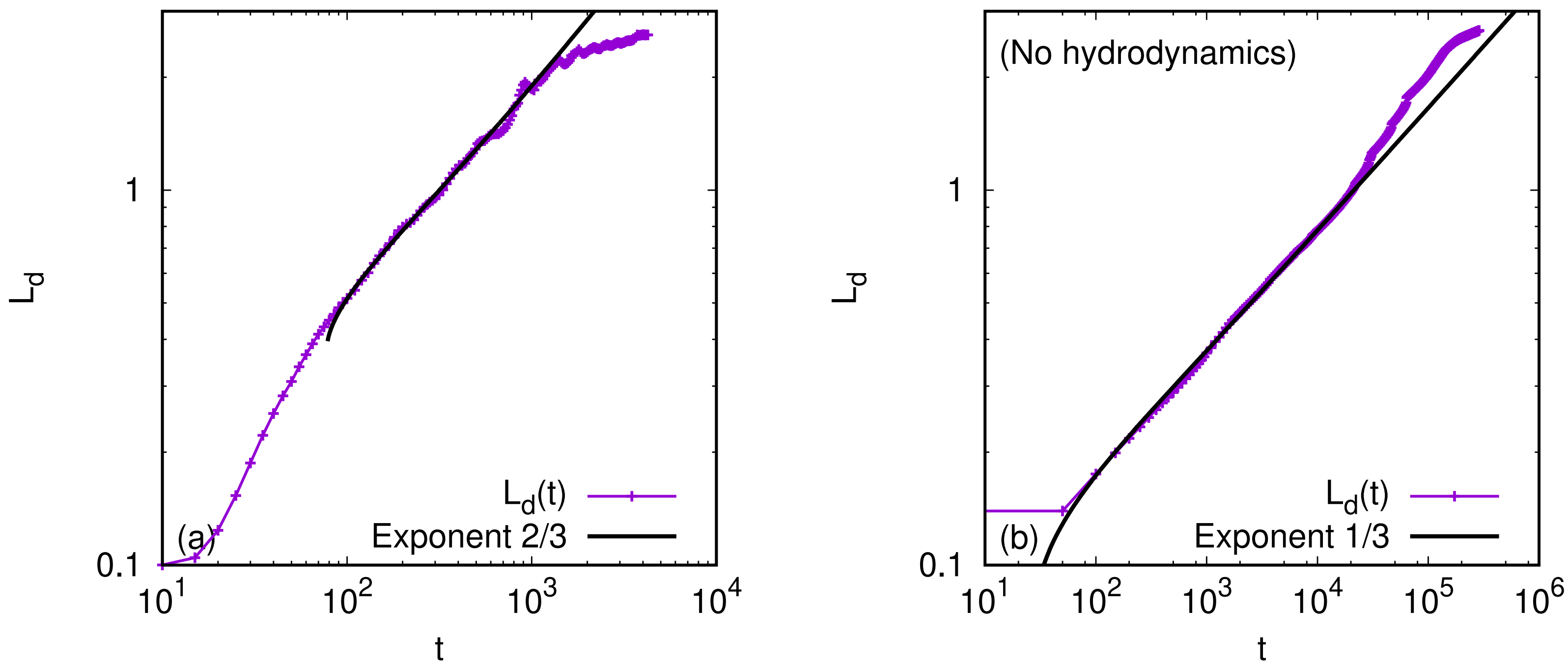
$t = 2700$



$t = 15000$

$t = 168000$

Growth exponents



- The domain sizes can be characterised by the interface length ℓ.
- $L_d = L_x L_y / \ell$ is an increasing function of time.
- $L_d \sim t^{2/3} \Rightarrow$ inertial regime.
- $L_d \sim t^{1/3} \Rightarrow$ diffusive regime.

Curved surface: torus

- A torus can be parametrised using θ and φ:

$$x = (R + r\cos\theta)\cos\varphi, \qquad y = (R + r\cos\theta)\sin\varphi, \qquad z = r\sin\theta,$$

giving rise to the line element:

$$ds^2 = \left[dx^2 + dy^2 + dz^2\right]_{\text{torus}} = (R + r\cos\theta)^2 d\varphi^2 + r^2 d\theta^2.$$

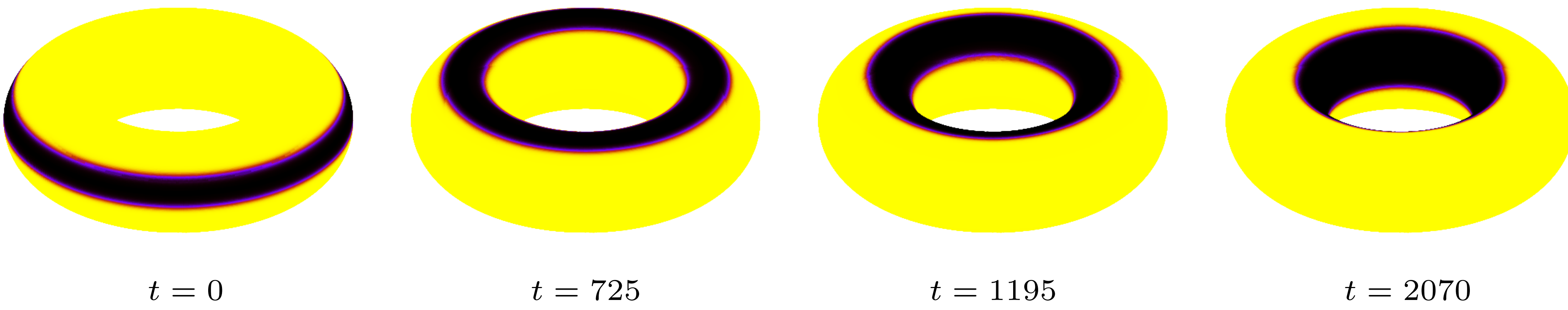
- It is convenient to employ the following vielbein field:

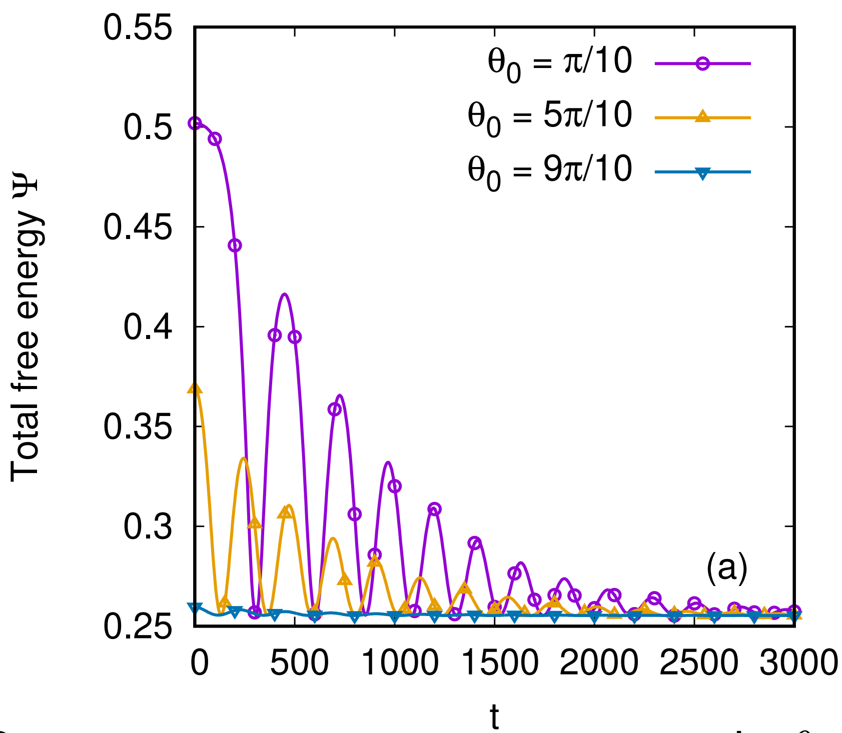
$$e_{\hat{\varphi}} = \frac{\partial_\varphi}{R + r\cos\theta}, \qquad e_{\hat{\theta}} = r^{-1}\partial_\theta,$$

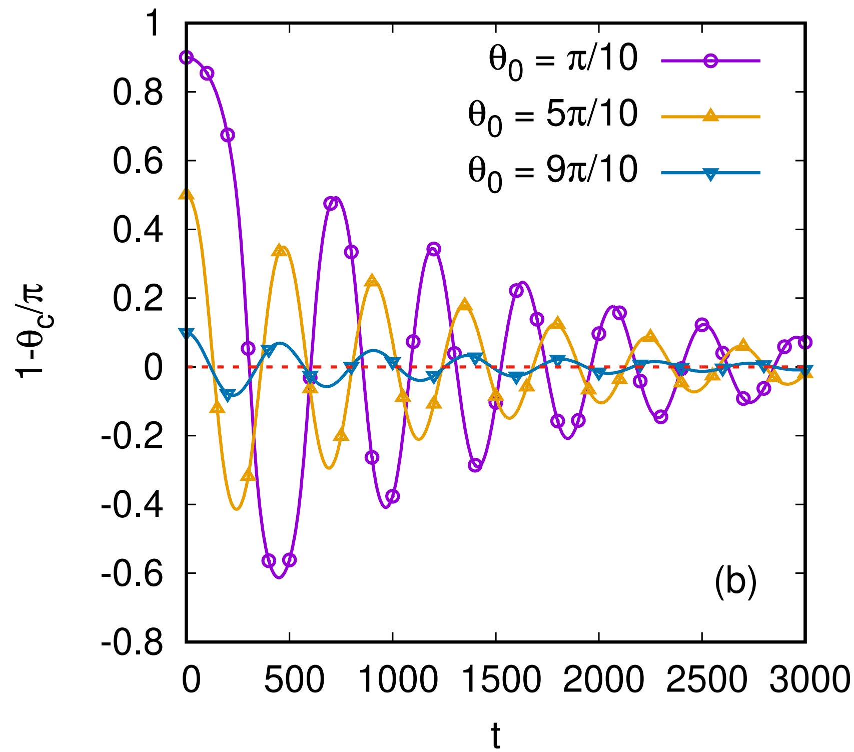
with respect to which $p^i = e^i_{\hat{a}} p^{\hat{a}}$.

- The momentum space is discretised with respect to $p^{\hat{\theta}}$ and $p^{\hat{\varphi}}$.[2]

[2] V. E. Ambruș, S. Busuioc, arXiv: 1708.05944 [physics.flu-dyn].



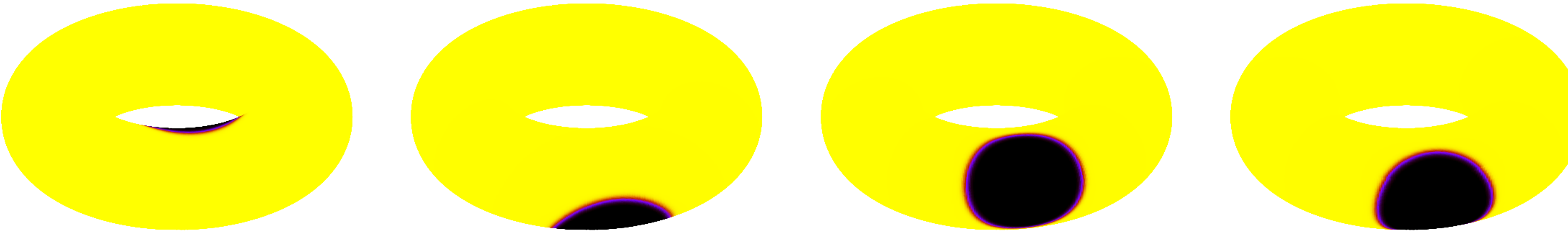




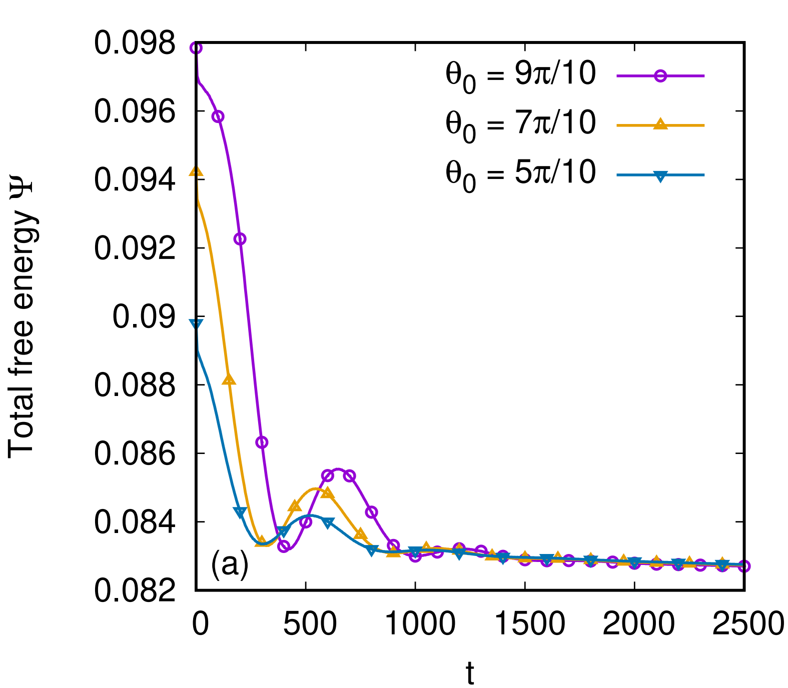
Due to γ, stripes migrate towards $\theta = \pi$.

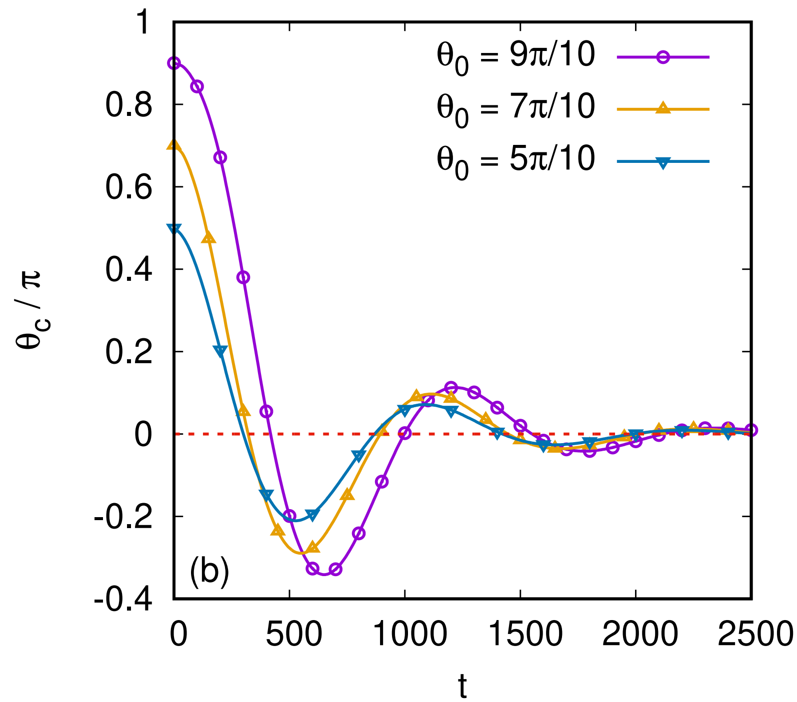
Droplets migration

CRC-TR 211



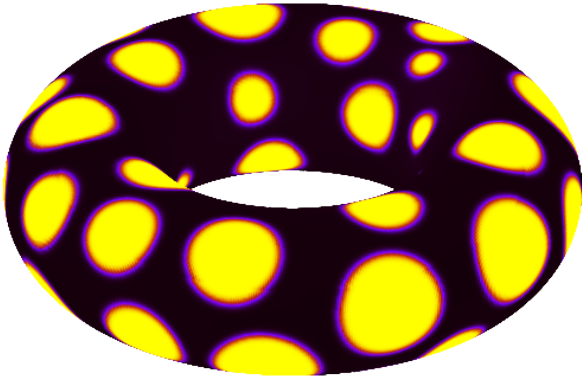
$t = 0$ $t = 650$ $t = 1220$ $t = 1775$



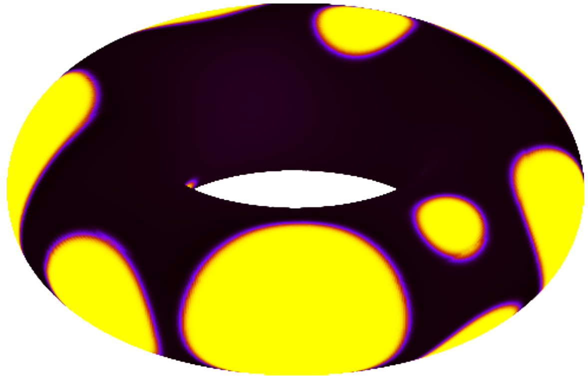


Droplets migrate towards lowest curvature ($\theta = 0$).

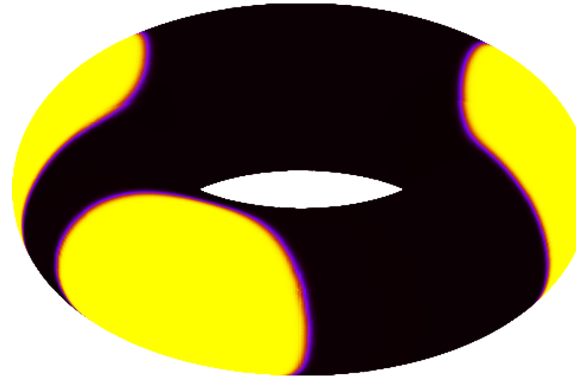
Separation to droplets



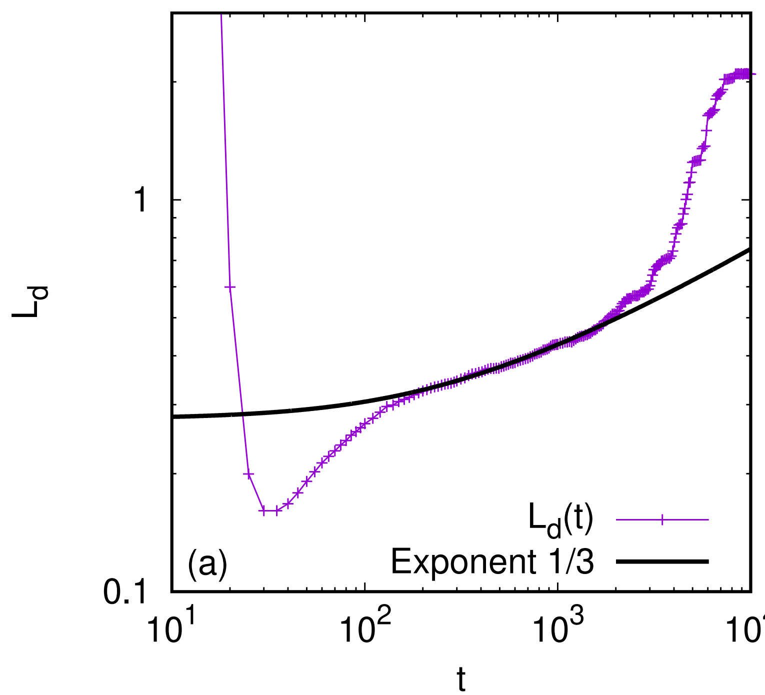
$t = 2500$

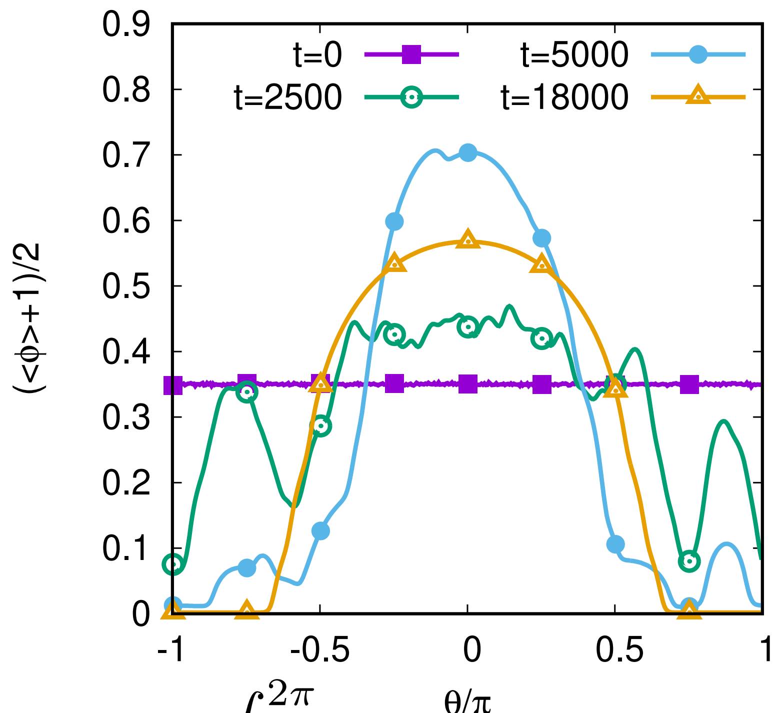


$t = 5000$



$t = 18000$





Droplet migration can be quantified using $\langle \phi \rangle = \int_0^{2\pi} d\varphi\, \phi$.

Conclusions

- LB is a versatile tool for non-eq. flows from hydro to free-streaming.
- Extensions for non-ideal EOS are possible.
- Non-relativistic LB: vdW & Cahn-Hilliard models are extensively studied.
- Relativistic LB: medium dependent mass possible.
- Next: Coupling to Langevin? Relativistic Model H?...

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- THANK YOU FOR YOUR ATTENTION!