Research Centre
for Gas Innovation

Lattice Boltzmann Method: An Introductory Overview

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PME-5429 | Multiscale Methods (2020)

PME-5429 - Lattice Boltzmann Method

Summary of topics

- 20/10: Introduction & Kinetic Theory
- 27/10: Lattice Boltzmann & Hands-On
- 03/11: Dense Fluids & Hands-On

Brief review

Review

$$n_\alpha(\mathbf{r}_k + \mathbf{e}_\alpha \delta t, t + \delta t) = n_\alpha(\mathbf{r}_k, t) + \Omega_\alpha(\mathbf{r}_k, t)$$

- $\Omega_\alpha(\mathbf{r}_k, t) = -\frac{1}{\tau}\big(n_\alpha(\mathbf{r}_k, t) - g_\alpha(\mathbf{r}_k, t)\big)$
- $g_\alpha(\mathbf{r}_k, t) = n_\alpha^{eq}(\mathbf{r}_k, t)\big[1 + 3(\delta t/c^2)\big(\tau - \frac{1}{2}\big)(\mathbf{e}_\alpha - \mathbf{u}_k) \cdot \mathbf{g}_k\big]$
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- $\nu = \frac{1}{3}c^2 \delta t(\tau - \frac{1}{2}), \quad p = \frac{1}{3}c^2\rho, \quad c_s = c/\sqrt{3}$

D2Q9-isothermal Lattice Boltzmann model

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Next steps: dense fluids

Thermodynamic Foundations of Kinetic Theory and Lattice Boltzmann Models for Multiphase Flows

Xiaoyi He[1, 2] and Gary D. Doolen[1]

Received January 16, 2001; accepted October 18, 2001

- Mean-field treatment of long-range intermolecular forces
- Lattice models for non-ideal fluids

Part 3:
Dense fluids

1. Non-ideal gases: long-range forces
2. Shan-Chen models
3. Phase separation
4. Cohesion-adhesion model
5. Hands-on tutorial

Non-ideal gases:
(ii) long-range forces

Inspiration: kinetic theory of plasmas

Neutral plasmas are usually described as a gas of electrons moving in the presence of an uniform positive background charge, with density en_+ [Bhatnagar, Gross, Krook (1954)]

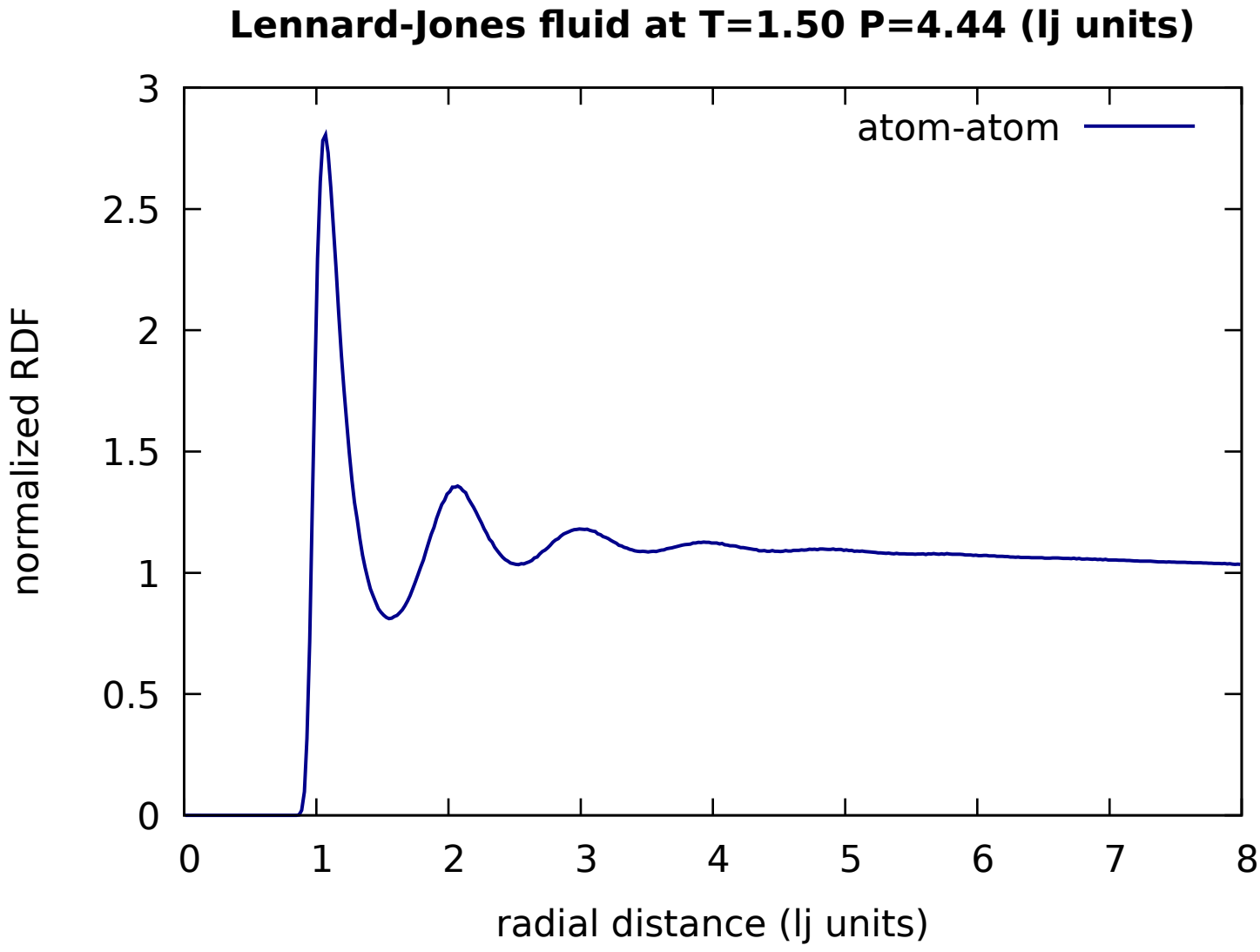
The velocity distribution of electrons $f(\mathbf{r}, \boldsymbol{\xi}, t)$ obeys the Boltzmann equation:

$$\frac{\partial f}{\partial t} + \boldsymbol{\xi} \cdot \frac{\partial f}{\partial \mathbf{r}} - \frac{e\mathbf{E}}{m} \cdot \frac{\partial f}{\partial \boldsymbol{\xi}} = \Omega(f)$$

where the electric field is found by

$$\epsilon_0 \boldsymbol{\nabla} \cdot \mathbf{E}(\mathbf{r}, t) = e\Big[n_+ - \int d\boldsymbol{\xi} f(\mathbf{r}, \boldsymbol{\xi}, t)\Big]$$

RDFs: the long-range region



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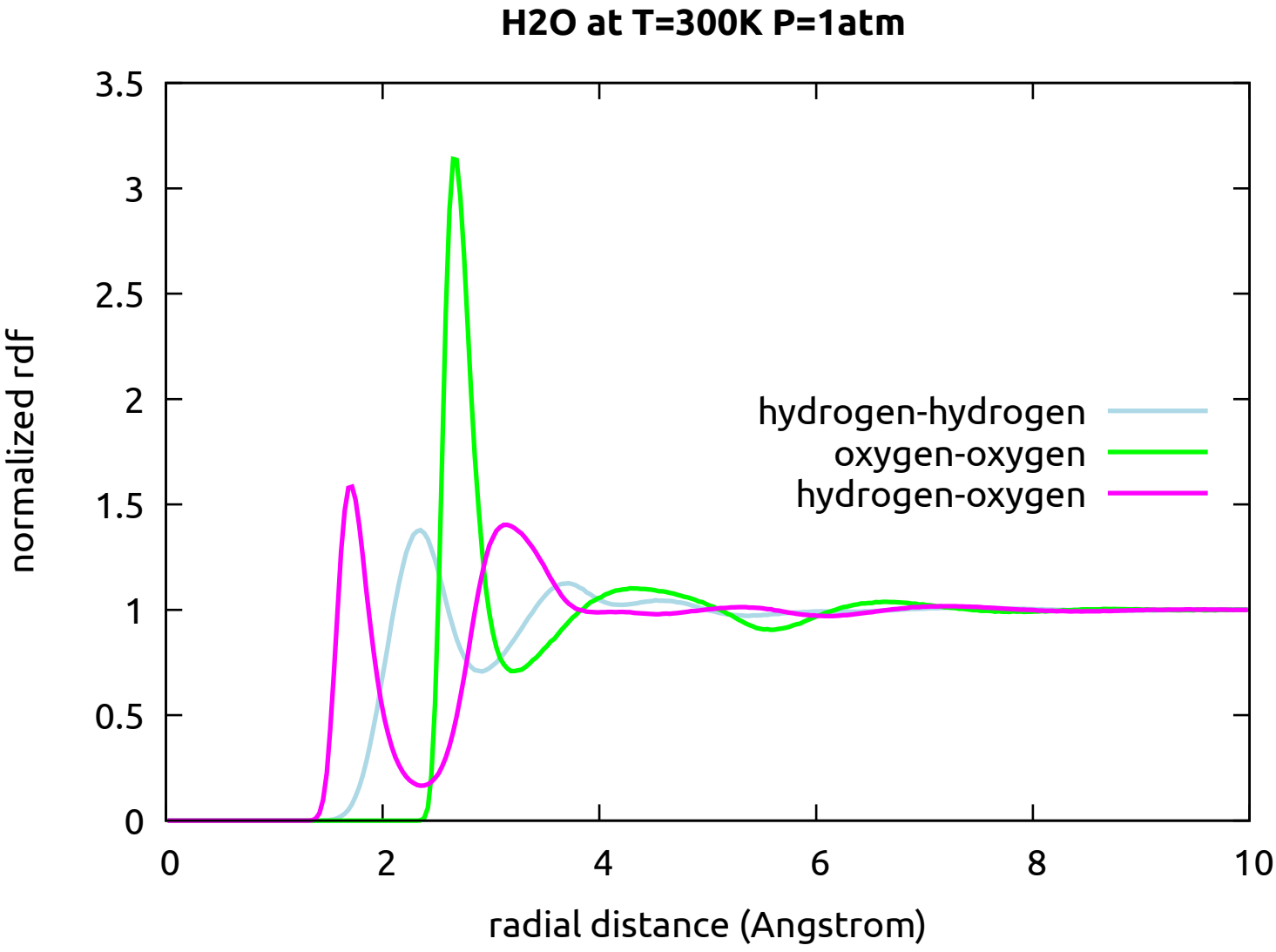

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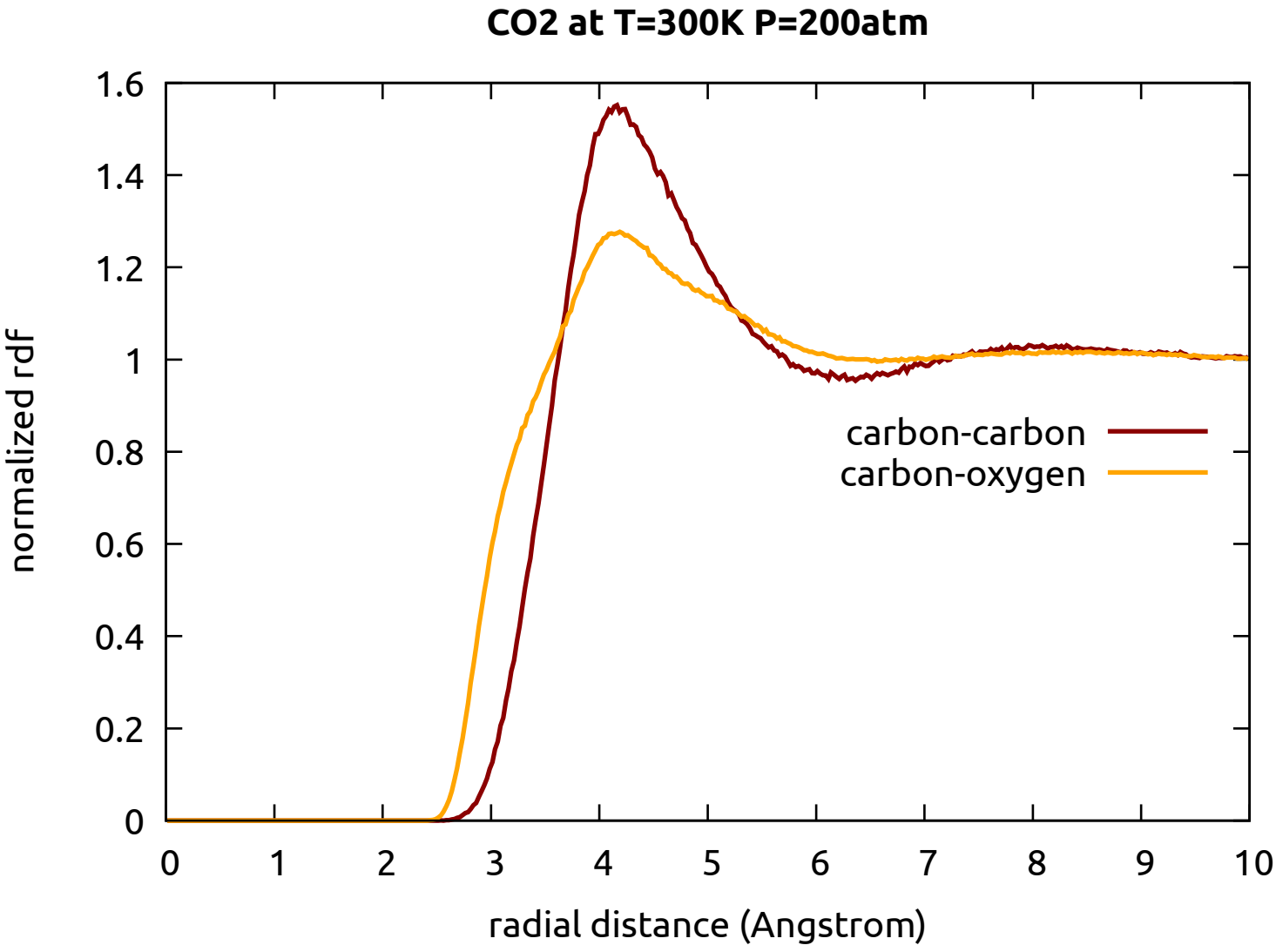

RDFs: the long-range region

In gases and liquids

- RDF is uniform at sufficiently long ranges*
- Long-range forces can be interpreted as if caused by a continuum mass distribution
- Molecules can be treated as test particles moving in a mean-field
- Mean-field implemented as external force per unit mass: $\mathbf{g}$
- * 'long-range' compared to molecular sizes

Mean-field potential and force

Energy due to pairwise forces (molecule-level)

$$E = \tfrac{1}{2} \sum_{a \neq b} U(\mathbf{r}_a, \mathbf{r}_b)$$

The potential energy per unit mass at $\mathbf{r}$ is

$$\varphi(\mathbf{r}, t) = m^{-1} \int_\Lambda U(\mathbf{r}, \mathbf{r}') n(\mathbf{r}', t) d\mathbf{r}'$$

$$[U(\mathbf{r}, \mathbf{r}')] = [\text{energy}]$$

The force per unit mass at $\mathbf{r}$ is

$$\mathbf{g}(\mathbf{r}, t)_\Lambda = -\boldsymbol{\nabla}_{\mathbf{r}} \varphi(\mathbf{r}, t)$$

Mean-field potential and force

Energy due to pairwise forces (continuum)

$$E = \tfrac{1}{2} \iint U(\mathbf{r}, \mathbf{r}')\, n_{\text{pairs}}(\mathbf{r}', \mathbf{r})\, d\mathbf{r}' d\mathbf{r}$$

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Mean-field potential and force

Energy due to pairwise forces (mean-field)

$$n_{\text{pairs}}(\mathbf{r}', \mathbf{r}) \;\to\; n(\mathbf{r}')n(\mathbf{r}) \qquad (\text{if } |\mathbf{r}' - \mathbf{r}| \to \infty)$$

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Mean-field potential and force

Energy due to pairwise forces (mean-field)

$$E = E_{\text{close}} + \tfrac{1}{2} \int \int_{\Lambda} U(\mathbf{r}, \mathbf{r}')\, n(\mathbf{r}') n(\mathbf{r})\, d\mathbf{r}' d\mathbf{r}$$

The potential energy per unit mass at $\mathbf{r}$ is

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Mean-field potential and force

Energy due to pairwise forces (mean-field)

$$E = \underbrace{E_{\text{close}}}_{\tau_c} + \tfrac{1}{2} \int \Big[\int_\Lambda U(\mathbf{r}, \mathbf{r}') \cdot \, n(\mathbf{r}') d\mathbf{r}' \Big] n(\mathbf{r}) d\mathbf{r}$$

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The potential energy per unit mass at $\mathbf{r}$ is

$$\varphi(\mathbf{r}, t) \equiv \int \upsilon(\mathbf{r}, \mathbf{r}') \rho(\mathbf{r}', t) d\mathbf{r}'$$

$$[\upsilon(\mathbf{r}, \mathbf{r}') = U(\mathbf{r}, \mathbf{r}')/m^2] = [\text{energy/mass}^2]$$

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(appears in the transport equation)

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The force per unit volume at $\mathbf{r}$ is

$$\rho(\mathbf{r}, t) \mathbf{g}(\mathbf{r}, t)_\Lambda = -\rho(\mathbf{r}, t) \int_\Lambda [\boldsymbol{\nabla}_{\mathbf{r}} \upsilon(\mathbf{r}, \mathbf{r}')] \rho(\mathbf{r}', t) d\mathbf{r}'$$

(appears in the Navier-Stokes equations)

Mean-field potential and density gradients

A much more convenient expression can be obtained under two assumptions: (a) isotropic interactions

$$v(\mathbf{r}, \mathbf{r}') = v(R), \quad \mathbf{R} = \mathbf{r}' - \mathbf{r}$$

and (b) over the interaction range the following approximation is valid

$$\varphi(\mathbf{r}, t) = \int_\Lambda v(\mathbf{r}, \mathbf{r}')\rho(\mathbf{r}', t)d\mathbf{r}'$$

and inside the integral we take:

$$\rho(\mathbf{r}+\mathbf{R}, t) \approx \rho(\mathbf{r}, t)+\mathbf{R}\cdot\nabla\rho(\mathbf{r}, t)+\tfrac{1}{2}\mathbf{R}\mathbf{R} : \nabla\nabla\rho(\mathbf{r}, t)$$

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Mean-field potential and density gradients

A much more convenient expression can be obtained under two assumptions: (a) isotropic interactions

$$v(\mathbf{r}, \mathbf{r}') = v(R), \quad \mathbf{R} = \mathbf{r}' - \mathbf{r}$$

and (b) over the interaction range the following approximation is valid

$$\varphi(\mathbf{r}, t) = \int_\Lambda v(R)\rho(\mathbf{r} + \mathbf{R}, t)d\mathbf{R}$$

and inside the integral we take:

$$\rho(\mathbf{r}+\mathbf{R}, t) \approx \rho(\mathbf{r}, t)+\mathbf{R}\cdot\nabla\rho(\mathbf{r}, t)+\tfrac{1}{2}\mathbf{R}\mathbf{R} : \nabla\nabla\rho(\mathbf{r}, t)$$

Mean-field potential and density gradients

The resulting expression can then be organized as

$$\varphi(\mathbf{r},t) = -2a\rho(\mathbf{r},t) - \kappa\nabla^2\rho(\mathbf{r},t)$$

with coefficients

$$a = -\tfrac{1}{2}\int_\Lambda v(R)\, d\mathbf{R}$$
$$\kappa = -\tfrac{1}{6}\int_\Lambda R^2 v(R)\, d\mathbf{R}$$

(not independent)

Then, the mean-field force per unit mass at $\mathbf{r}$ is

$$\mathbf{g}_\Lambda = -\boldsymbol{\nabla}\varphi = \boldsymbol{\nabla}(2a\rho + \kappa\nabla^2\rho)$$

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Korteweg's tensor

The transport equation becomes

$$\frac{\partial f}{\partial t} + \boldsymbol{\xi} \cdot \frac{\partial f}{\partial \mathbf{r}} + \mathbf{g}_\Lambda \cdot \frac{\partial f}{\partial \boldsymbol{\xi}} = \Omega(f)$$

A new force per unit volume appears in the momentum equation, which can be written as

$$\rho \mathbf{g}_\Lambda = \rho \boldsymbol{\nabla}(2a\rho + \kappa \nabla^2 \rho) \equiv \boldsymbol{\nabla} \cdot (a\rho^2 \mathbf{I}) + \boldsymbol{\nabla} \cdot \boldsymbol{\Pi}_\kappa$$

where $\boldsymbol{\Pi}_\kappa$ is known as *Korteweg's capillarity tensor*

$$(\Pi_\kappa)_{ij} = \kappa\left(\rho \nabla^2 \rho + \tfrac{1}{2} \boldsymbol{\nabla}\rho \cdot \boldsymbol{\nabla}\rho\right) \delta_{ij} - \kappa \frac{\partial \rho}{\partial x_i} \frac{\partial \rho}{\partial x_j}$$

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Fluid dynamics: organizing terms

Momentum equation:

$$\rho\frac{D\mathbf{u}}{Dt} = \rho\frac{\partial\mathbf{u}}{\partial t} + \rho(\mathbf{u}\cdot\boldsymbol{\nabla})\mathbf{u} = \rho\mathbf{g} - \boldsymbol{\nabla}\cdot\mathbf{P}$$

Organizing terms:

$$\begin{aligned}
\rho\frac{D\mathbf{u}}{Dt} &= \rho\mathbf{g}_\Lambda - \boldsymbol{\nabla}\cdot\mathbf{P} \\
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Fluid dynamics: summary

In summary, inclusion of mean-field intermolecular interactions yields (i) a non-ideal equation of state

$$\boxed{p_e = \rho R\, T - a\rho^2}$$

and (ii) a description of surface tension effects via Korteweg stresses

$$\boxed{\mathbf{\Pi}_\kappa = \kappa(\rho\nabla^2\rho + \tfrac{1}{2}|\boldsymbol{\nabla}\rho|^2)\,\mathbf{I} - \kappa\,\boldsymbol{\nabla}\rho\,\boldsymbol{\nabla}\rho}$$

or, equivalently, Korteweg forces

$$\boxed{\boldsymbol{\nabla}\cdot\mathbf{\Pi}_\kappa = \rho\boldsymbol{\nabla}(\kappa\nabla^2\rho)}$$

Fluid dynamics: remark

Remark: the balance equation for the *total* internal energy per unit mass $\varepsilon_{\text{total}} = \varepsilon + \frac{1}{2}\varphi$, can also be derived:

$$\rho \frac{D\varepsilon_{\text{total}}}{Dt} = \lambda \nabla^2 T - p\, \boldsymbol{\nabla} \cdot \mathbf{u} \; \cdots$$
$$- \left(\boldsymbol{\Pi}_{\text{viscous}} + \kappa \boldsymbol{\nabla}\rho \boldsymbol{\nabla}\rho \right) : \boldsymbol{\nabla}\mathbf{u} \; \cdots$$
$$+ \boldsymbol{\nabla}\mathbf{u} : \left[\kappa \boldsymbol{\nabla}(\rho \boldsymbol{\nabla}\rho) - \tfrac{1}{2}\kappa \boldsymbol{\nabla} \cdot (\rho \boldsymbol{\nabla}\rho)\mathbf{I} \right]$$

where

$$p = p_e - \kappa\rho\nabla^2\rho - \tfrac{1}{2}\kappa \boldsymbol{\nabla}\rho \cdot \boldsymbol{\nabla}\rho$$

- consistent with free-energy formulation [He-Doolen (2002)]

Next step

How the mean-field description can be incorporated into a lattice-based framework?

Potential per unit mass:

$$\varphi(\mathbf{r},t) = \int_{\Lambda} d\mathbf{R}\, \upsilon(R)\rho(\mathbf{r}+\mathbf{R},t)$$

Force per unit volume:

$$\rho(\mathbf{r},t)\mathbf{g}(\mathbf{r},t)_{\Lambda} = -\rho(\mathbf{r},t)\int_{\Lambda} d\mathbf{R}[-\frac{1}{R}\frac{\partial\upsilon(R)}{\partial R}]\rho(\mathbf{r}+\mathbf{R},t)\mathbf{R}$$

- seek lattice versions of these formulas

Shan-Chen models

Shan-Chen models

LB forcing style: shifted velocity

$$n_\alpha^{eq}(\tilde{\mathbf{u}}); \quad \tilde{\mathbf{u}} = \mathbf{u} + \delta t(\tau - \tfrac{1}{2})\mathbf{g};$$

Then

$$\rho\tilde{\mathbf{u}} \equiv \rho\mathbf{u} + \rho\delta t(\tau - \tfrac{1}{2})\mathbf{g}$$

where

$$\rho\mathbf{u} = \sum_\alpha m\mathbf{e}_\alpha n_\alpha + \tfrac{1}{2}\delta t\rho\mathbf{g}$$

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$$\rho\tilde{\mathbf{u}} = \sum_\alpha m\mathbf{e}_\alpha n_\alpha + \tau(\rho\mathbf{g}\delta t)$$

Shan-Chen-type models implement an *impulse per unit volume*, $\mathbf{J} \equiv \rho\mathbf{g}\delta t$, at each point of the fluid.

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Shan-Chen models

The general form of the forcing term is

$$\mathbf{J} = -G\,\psi(\mathbf{r},t)\sum_{\alpha}\omega_{\alpha}\psi(\mathbf{r}+\delta t\mathbf{e}_{\alpha},t)\mathbf{e}_{\alpha}$$

where $\psi(\mathbf{r},t) = \psi(\rho(\mathbf{r},t))$ is an *effective density*.

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X. Shan, H. Chen (1994)

obs: compare with:

$$\rho(\mathbf{r},t)\mathbf{g}(\mathbf{r},t)_{\Lambda} = -\rho(\mathbf{r},t)\int_{\Lambda} d\mathbf{R}[-\frac{1}{R}\frac{\partial v(R)}{\partial R}]\rho(\mathbf{r}+\mathbf{R},t)\mathbf{R}$$

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The functional $\psi(\rho)$ is adjustable, but it should reduce to ρ in the low-density limit – a popular model is

$$\psi(\rho) = \rho_0\big(1-\exp(-\rho/\rho_0)\big)$$

- this functional defines the equation of state

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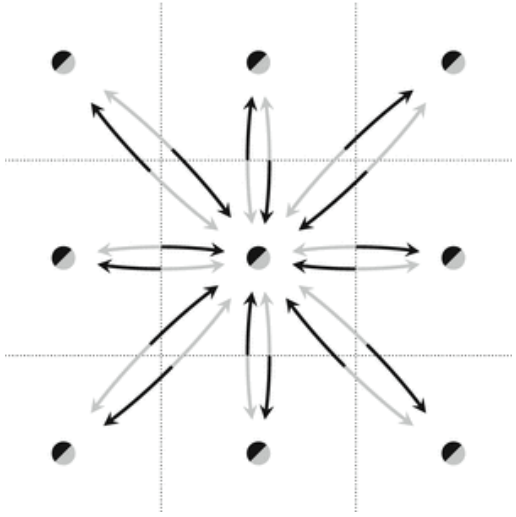
Shan-Chen models

The force per unit volume associated with

$$\mathbf{J} = -G\,\psi(\mathbf{r},t)\sum_{\alpha}\omega_{\alpha}\psi(\mathbf{r}+\delta t\mathbf{e}_{\alpha},t)\mathbf{e}_{\alpha}$$

depends on density gradients. The sign of G determines whether the force is cohesive or anti-cohesive.



from: T. Krüger *et. al.*, The Lattice Boltzmann Method (Springer, 2017)

Shan-Chen models

One way to interpret the Shan-Chen force term is to look at it as resulting from a mean-field force per unit volume computed with the effective density

$$\rho\mathbf{g} = -\psi(\mathbf{r},t)\int d\mathbf{R}[-\frac{1}{R}\frac{\partial\upsilon(R)}{\partial R}]\psi(\mathbf{r}+\mathbf{R},t)\mathbf{R}$$

The lattice expression is recovered by quadrature if we let

$$\upsilon(R) = -\tfrac{1}{3}c^2G(2\pi\gamma^2)^{-\frac{D}{2}}e^{-\frac{R^2}{2\gamma^2}}$$

with a characteristic range of

$$\gamma = c_s\delta t = (\delta x)/\sqrt{3}$$

Shan-Chen models

Then we can show that

$$\rho \mathbf{g} = -\tfrac{1}{3} G c^2 \psi \boldsymbol{\nabla} \psi - \tfrac{1}{18} G c^2 (\delta x)^2 (D/3) \psi \boldsymbol{\nabla} (\nabla^2 \psi)$$

and the model's mean-field coefficients, a and κ, can be identified.

- The equation of state of the model is

$$p = \tfrac{1}{3} \rho c^2 + \tfrac{1}{6} G c^2 [\psi(\rho)]^2$$

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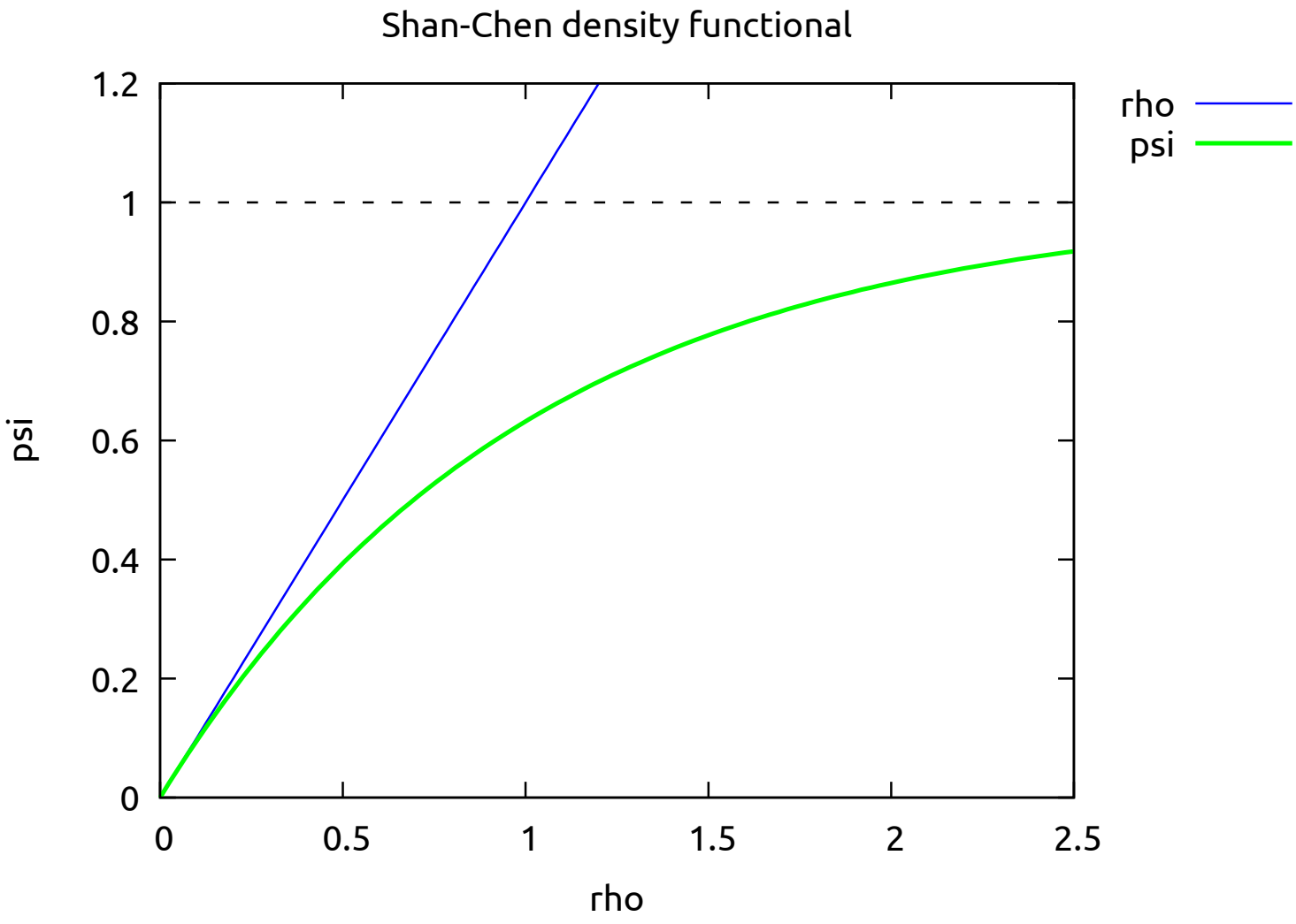
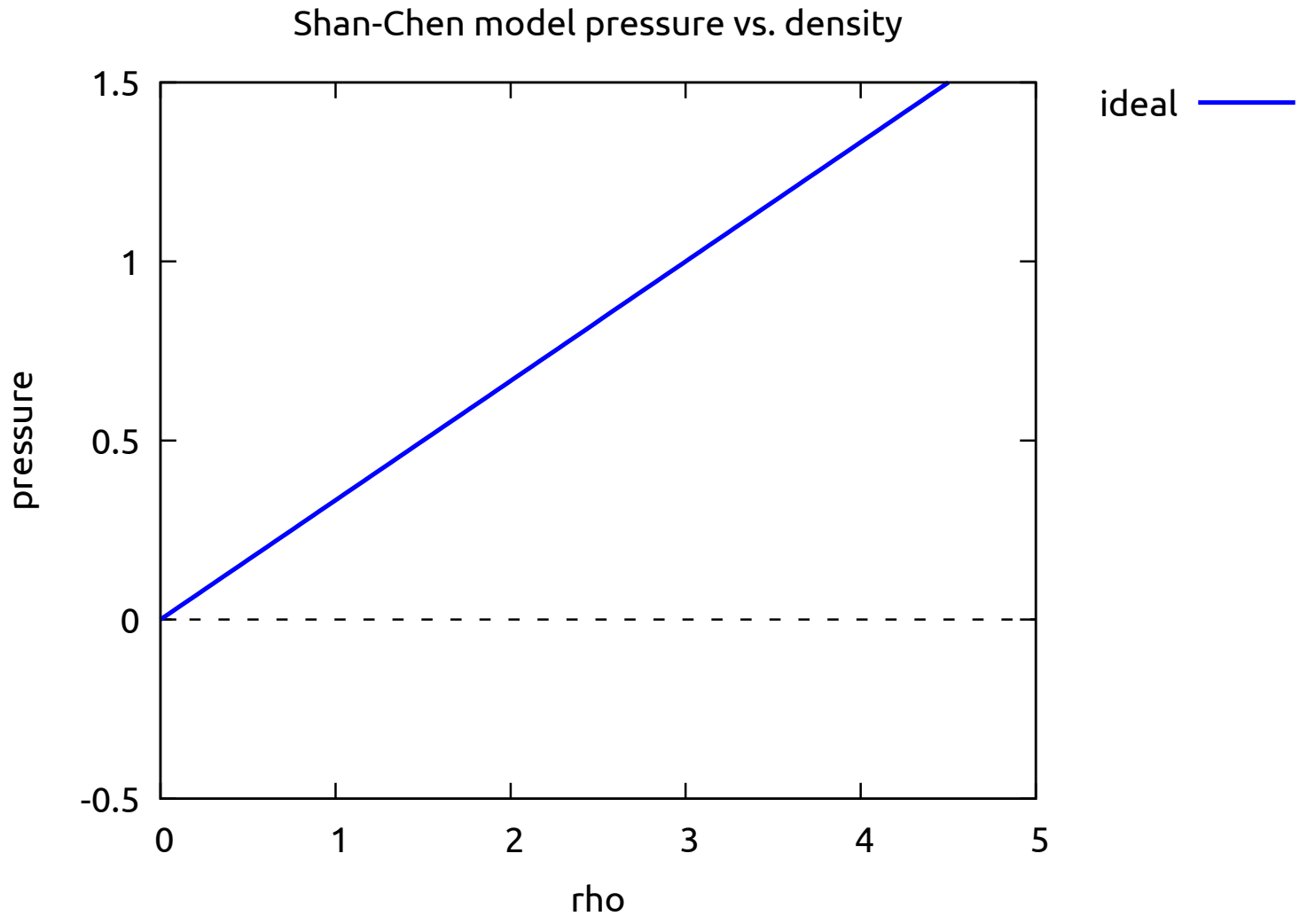
Phase separation

Shan-Chen functional



$$\psi(\rho) = \rho_0(1 - \exp(-\rho/\rho_0)) \quad (\rho_0 = 1.00)$$

Shan-Chen functional



$$p = \frac{1}{3}\rho$$

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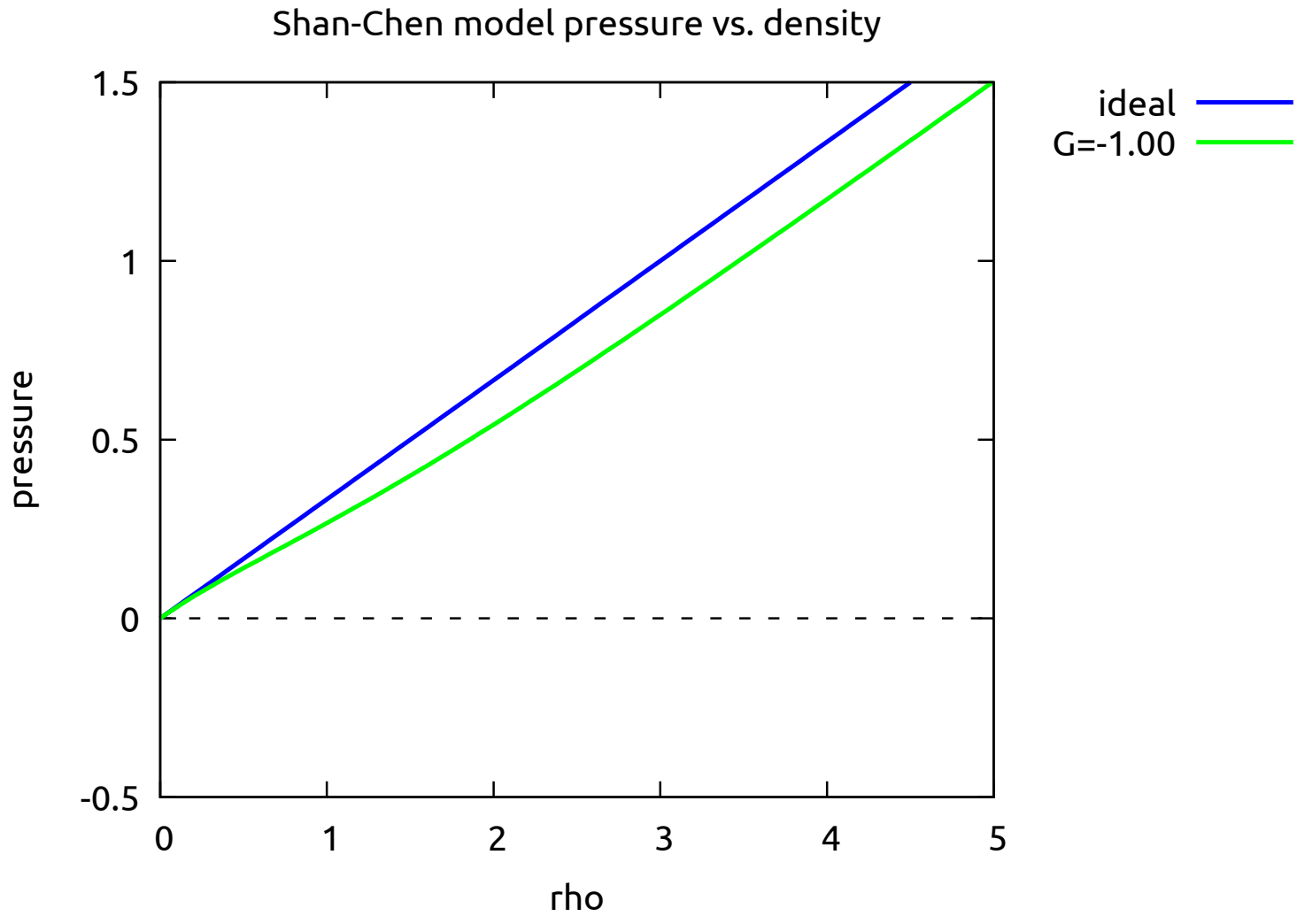
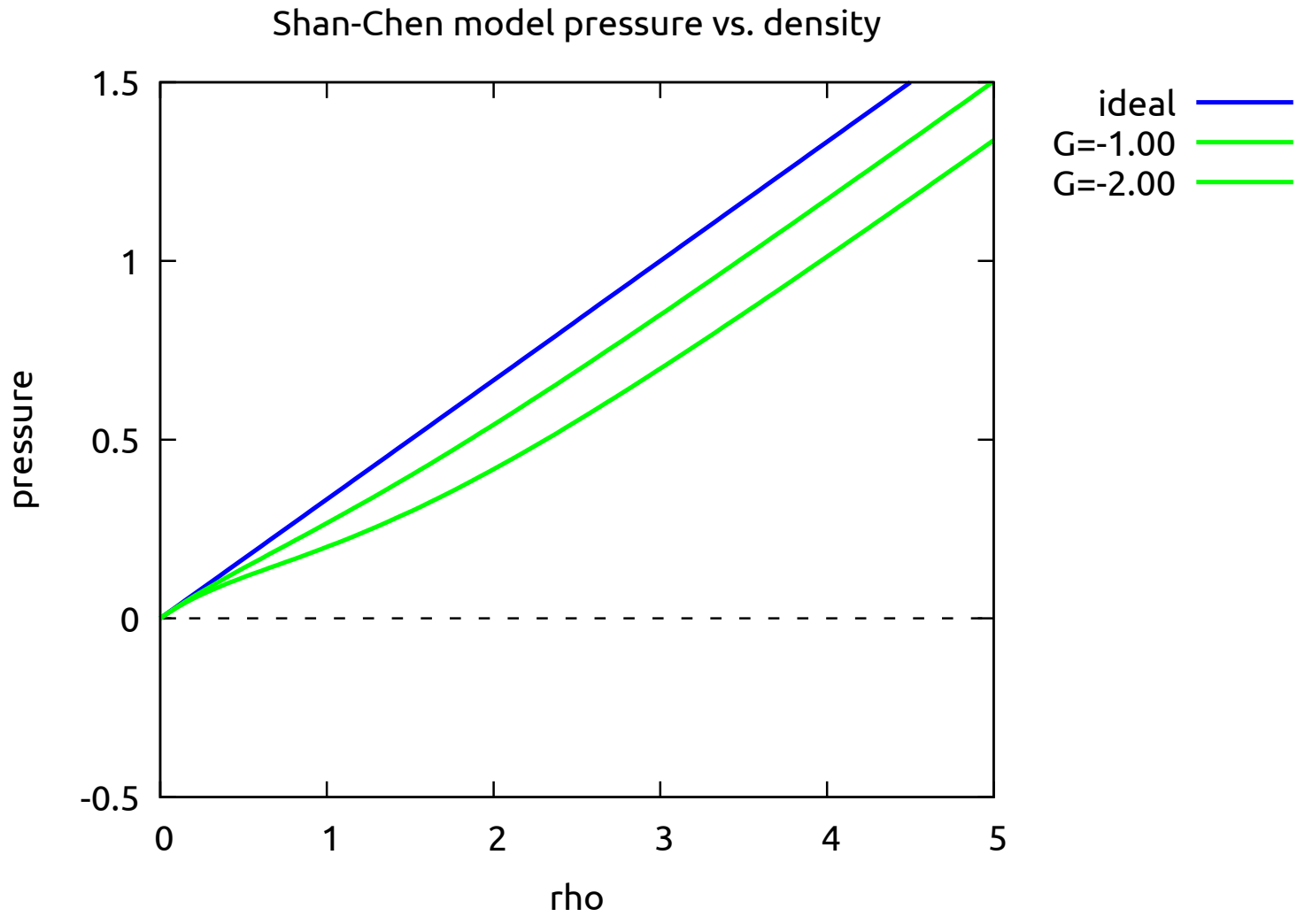


$$p = \frac{1}{3}\rho + \frac{1}{6}G\psi(\rho)^2$$

Shan-Chen functional



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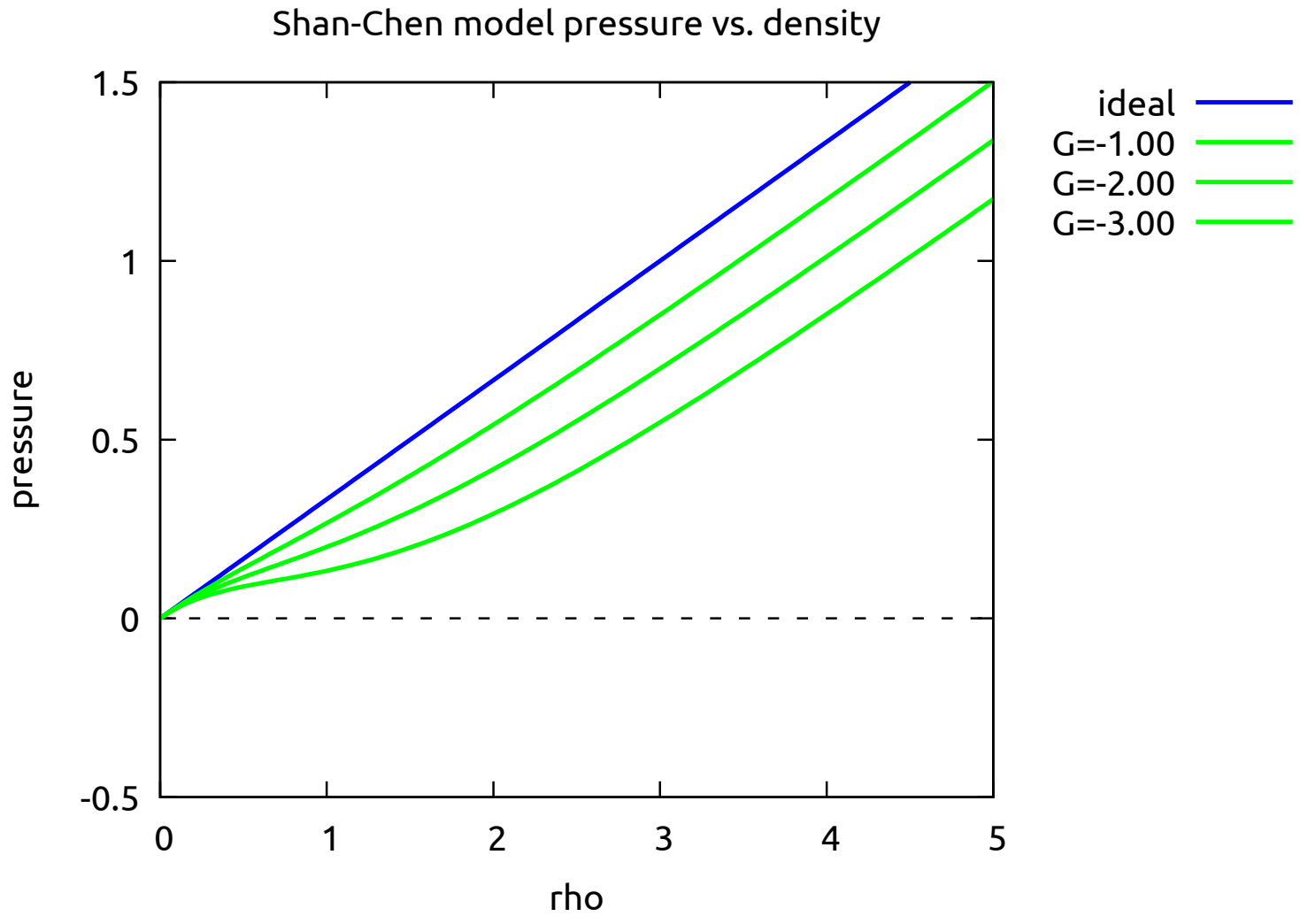

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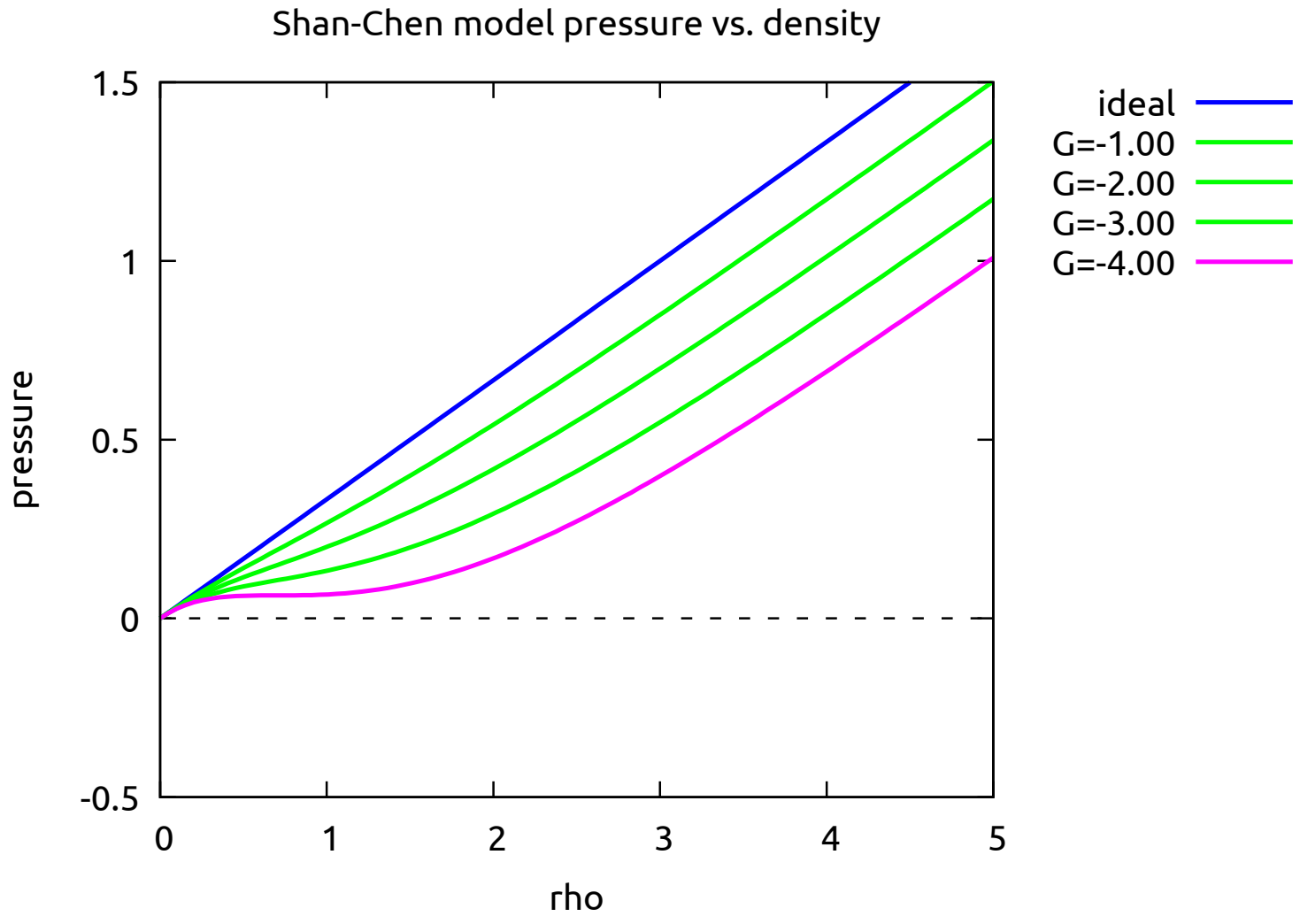

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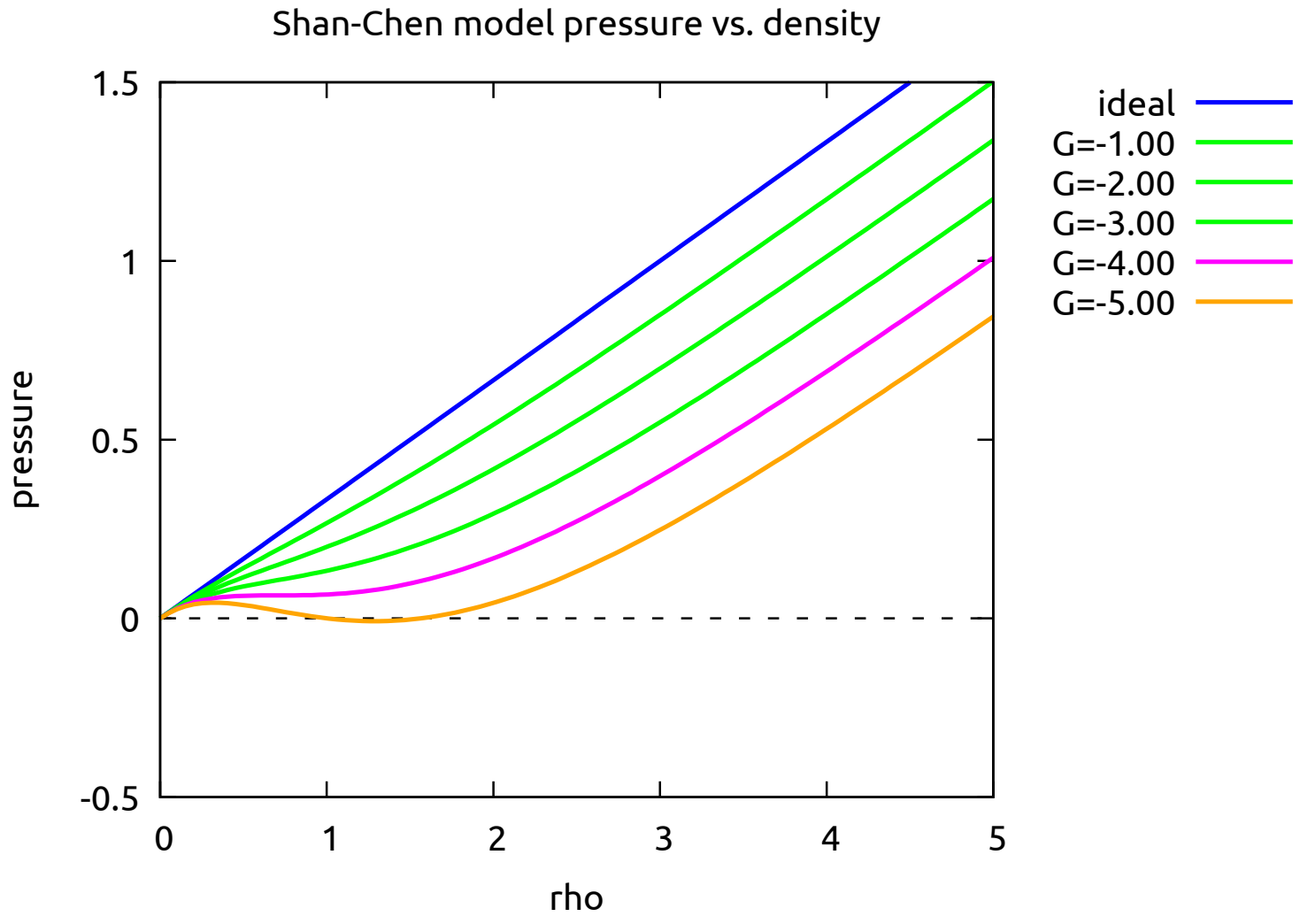

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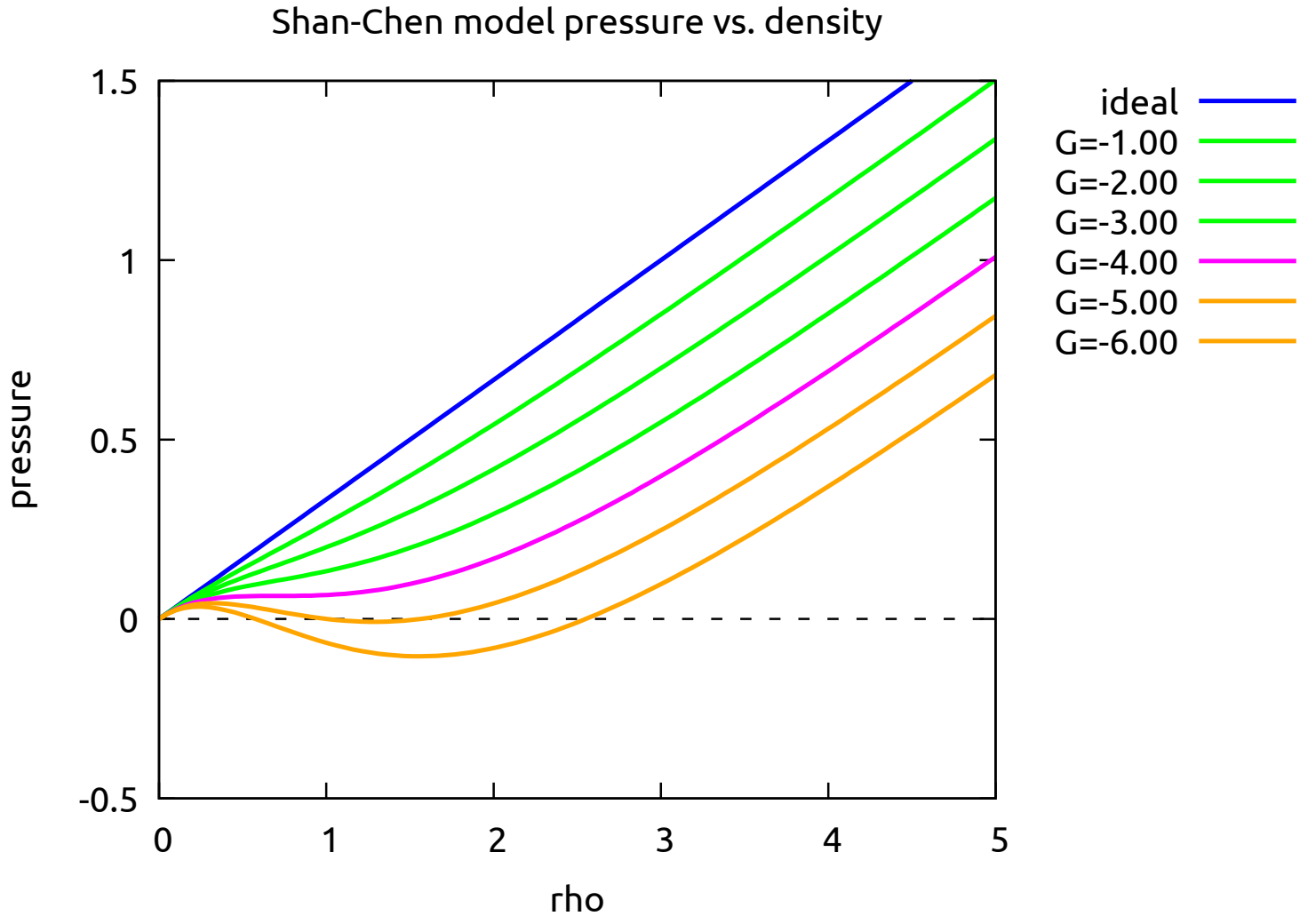

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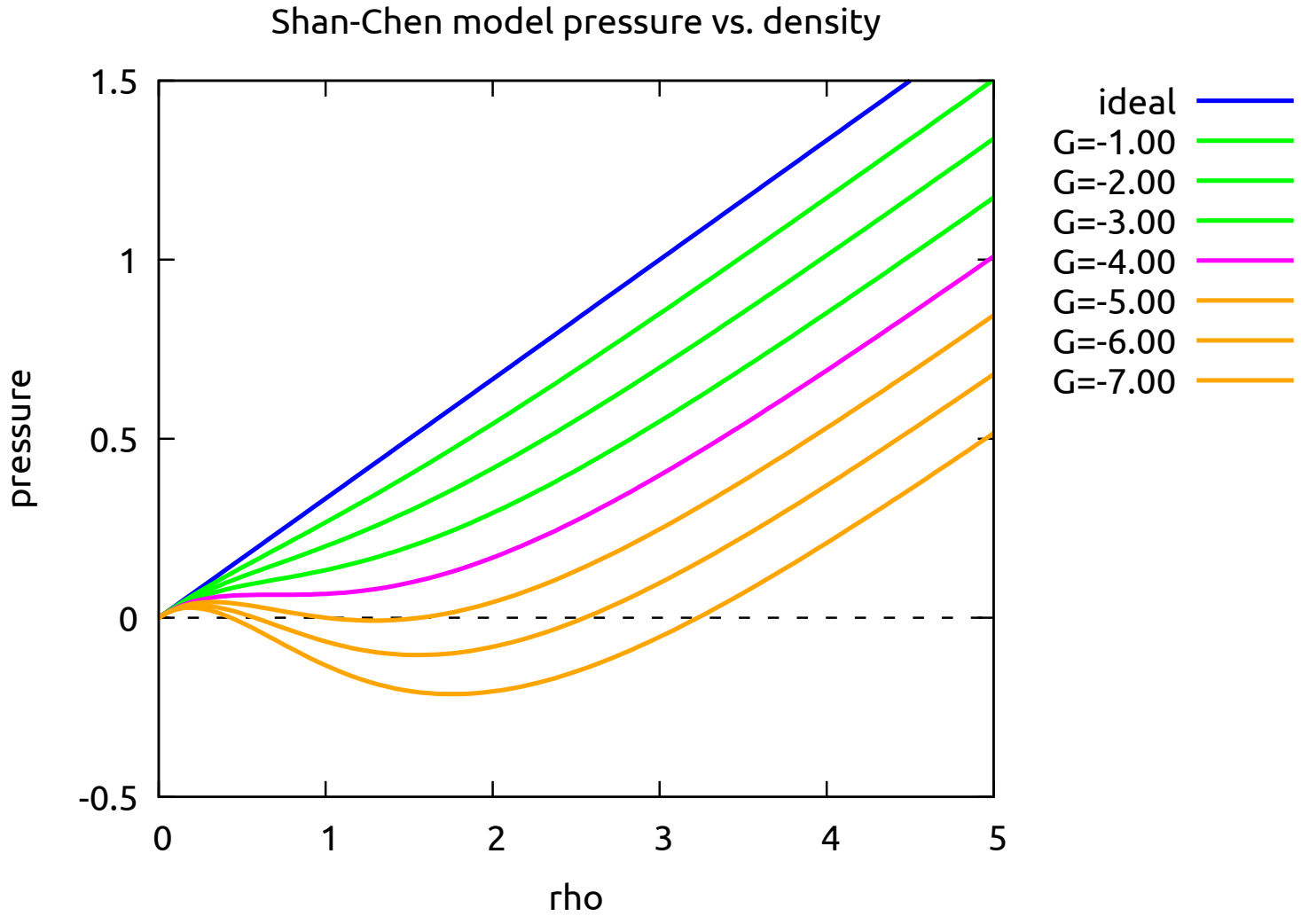

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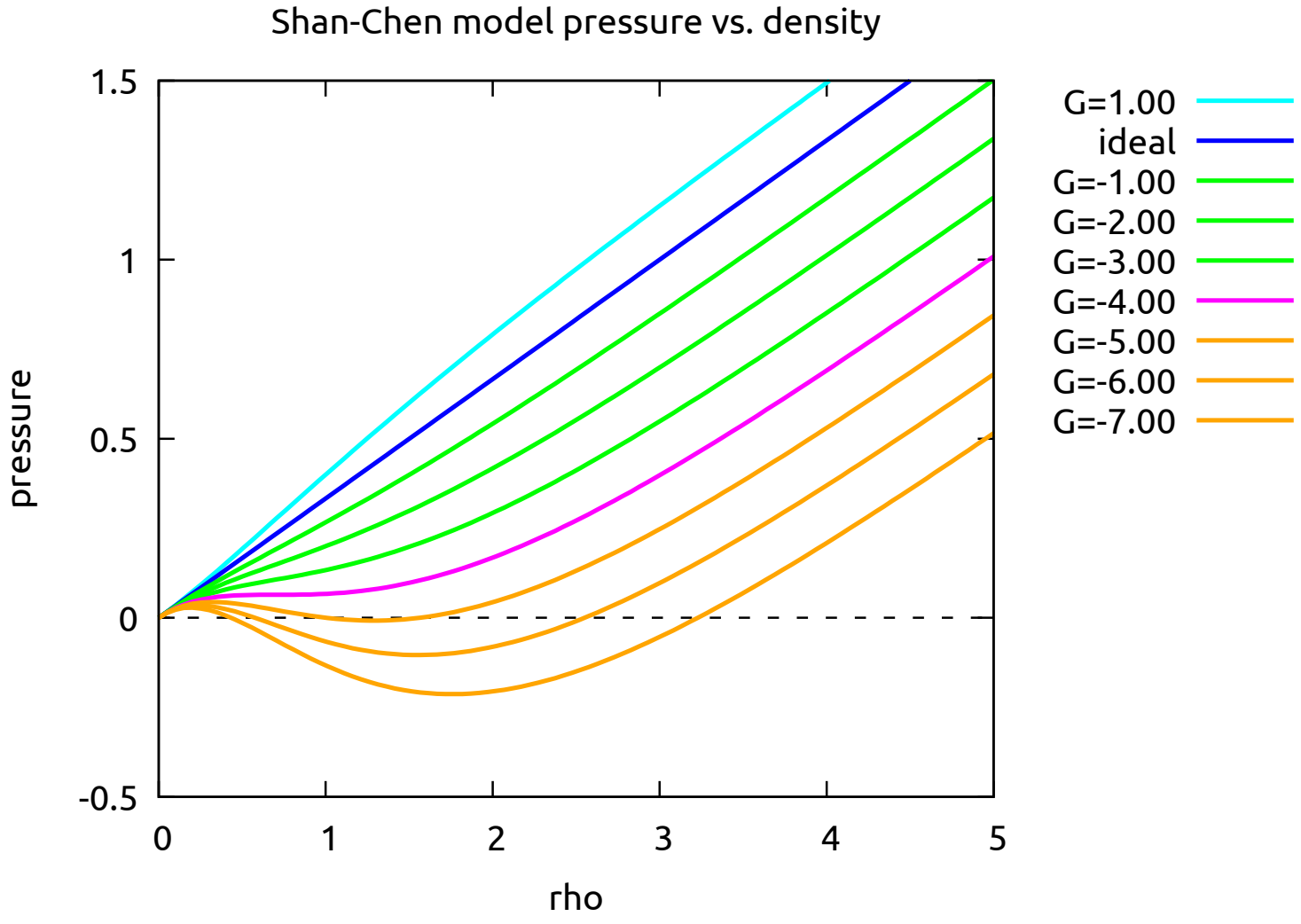

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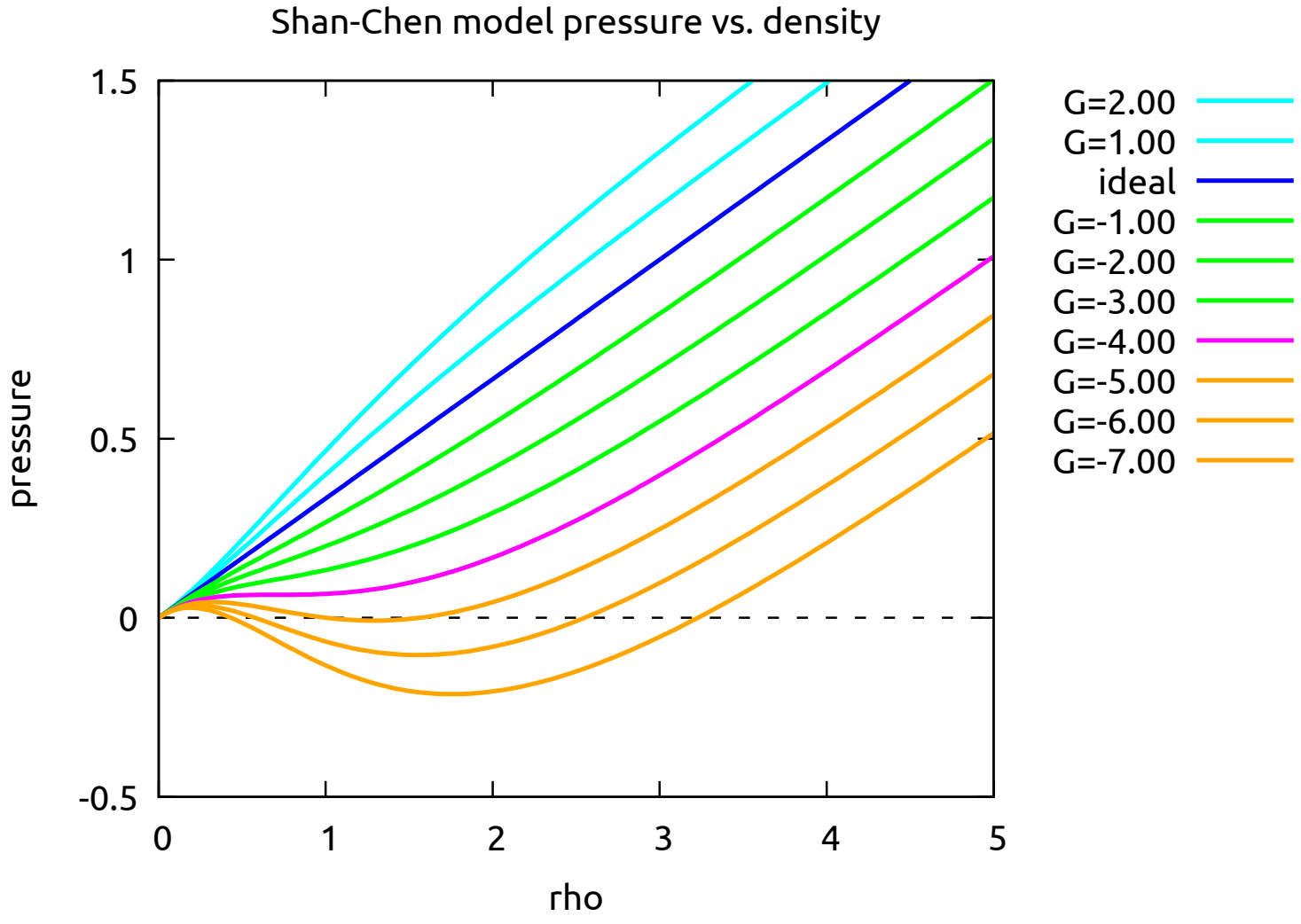

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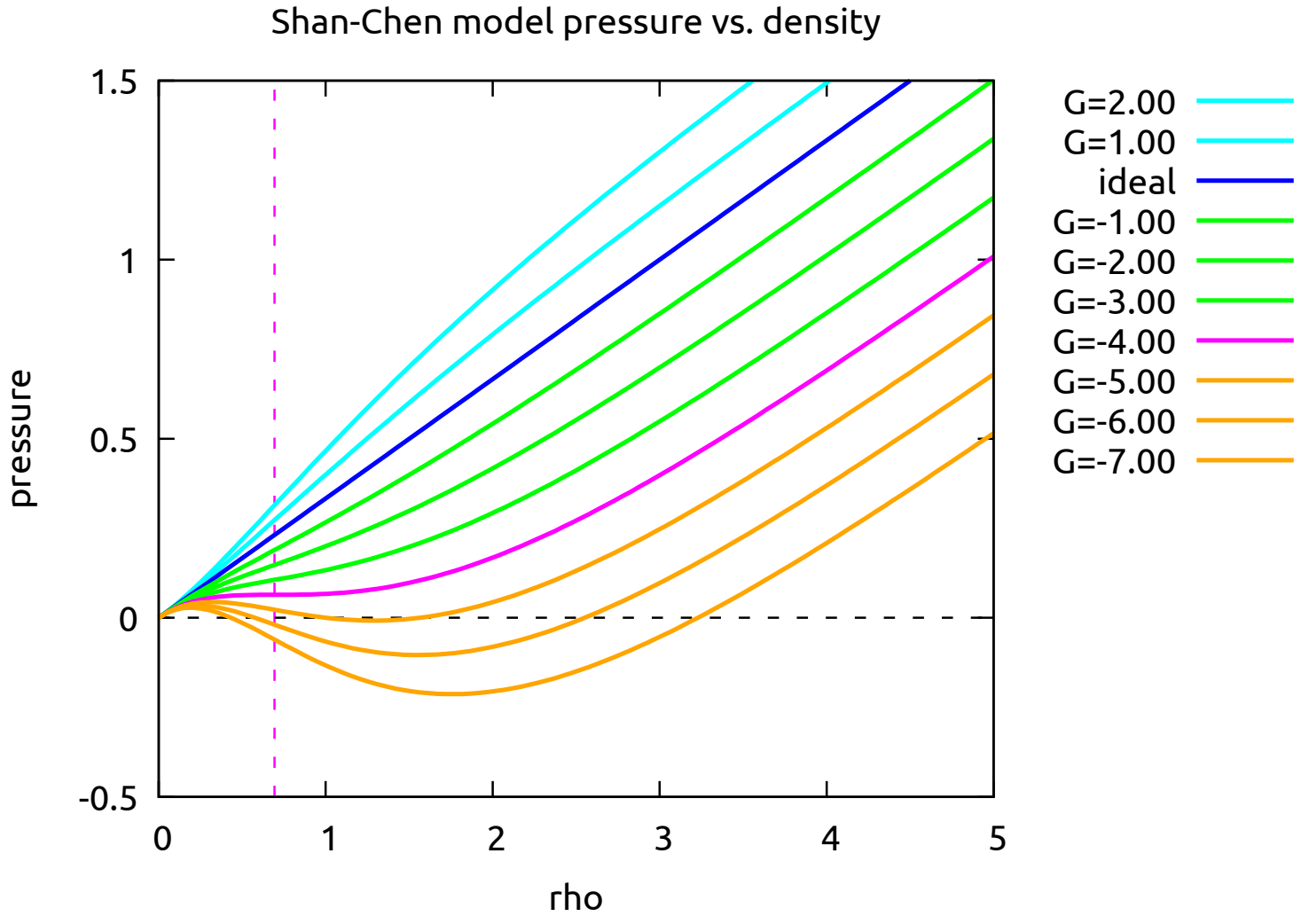

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Phase transition

For a certain range of G values there can be a decrease in pressure with an increase in density: this signals a phase transition.

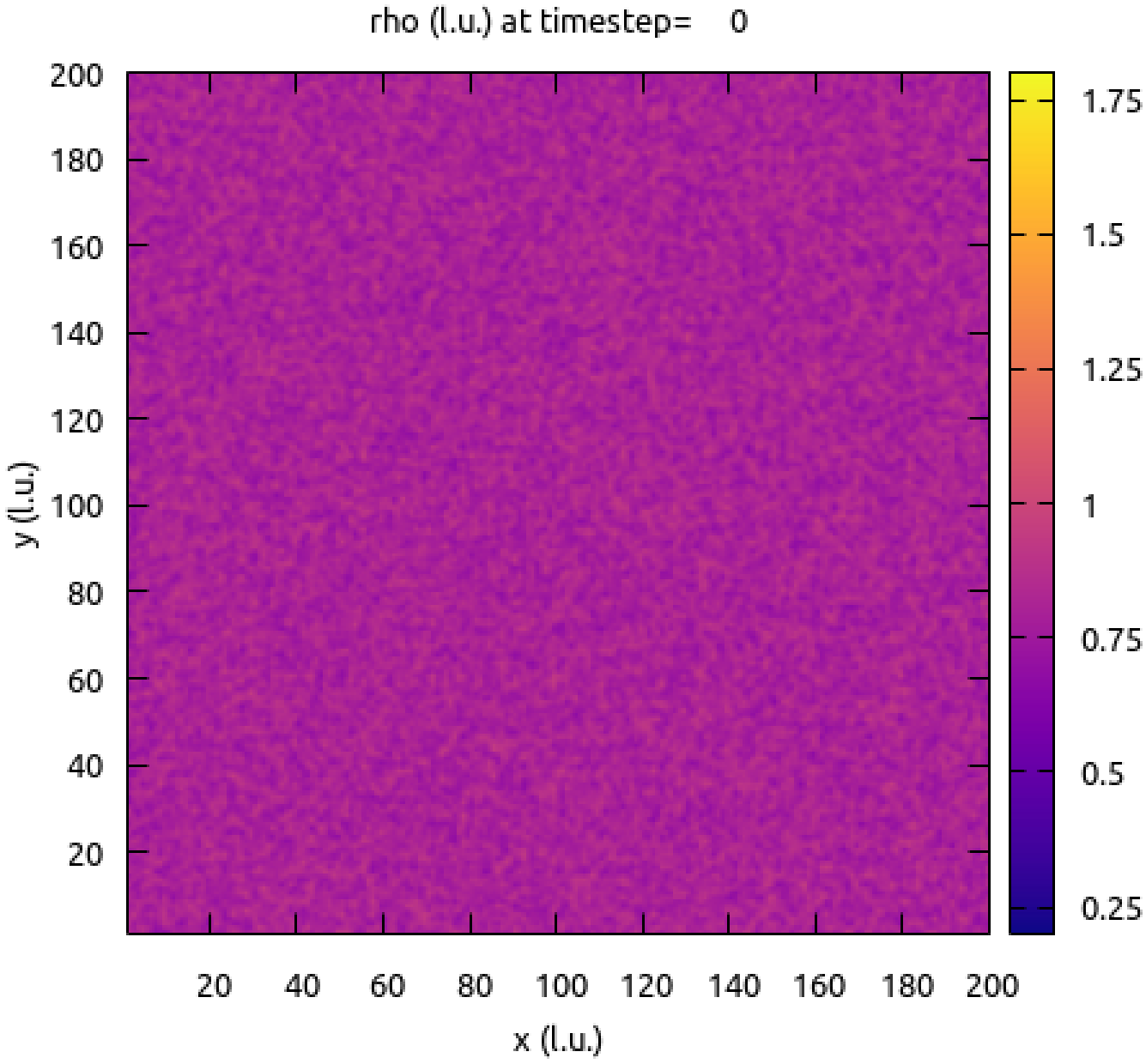
The change in behavior is marked by an inflection of the p vs. ρ curve – the critical values, G_c and ρ_c, are determined by the conditions

$$\left.\frac{dp}{d\rho}\right|_{\rho_c,G_c} = 0; \quad \left.\frac{d^2p}{d\rho^2}\right|_{\rho_c,G_c} = 0$$

A simple calculation gives:

$$\rho_c = \rho_0 \ln 2; \quad G_c = -4.00$$

Phase transition $(G = -5.00)$



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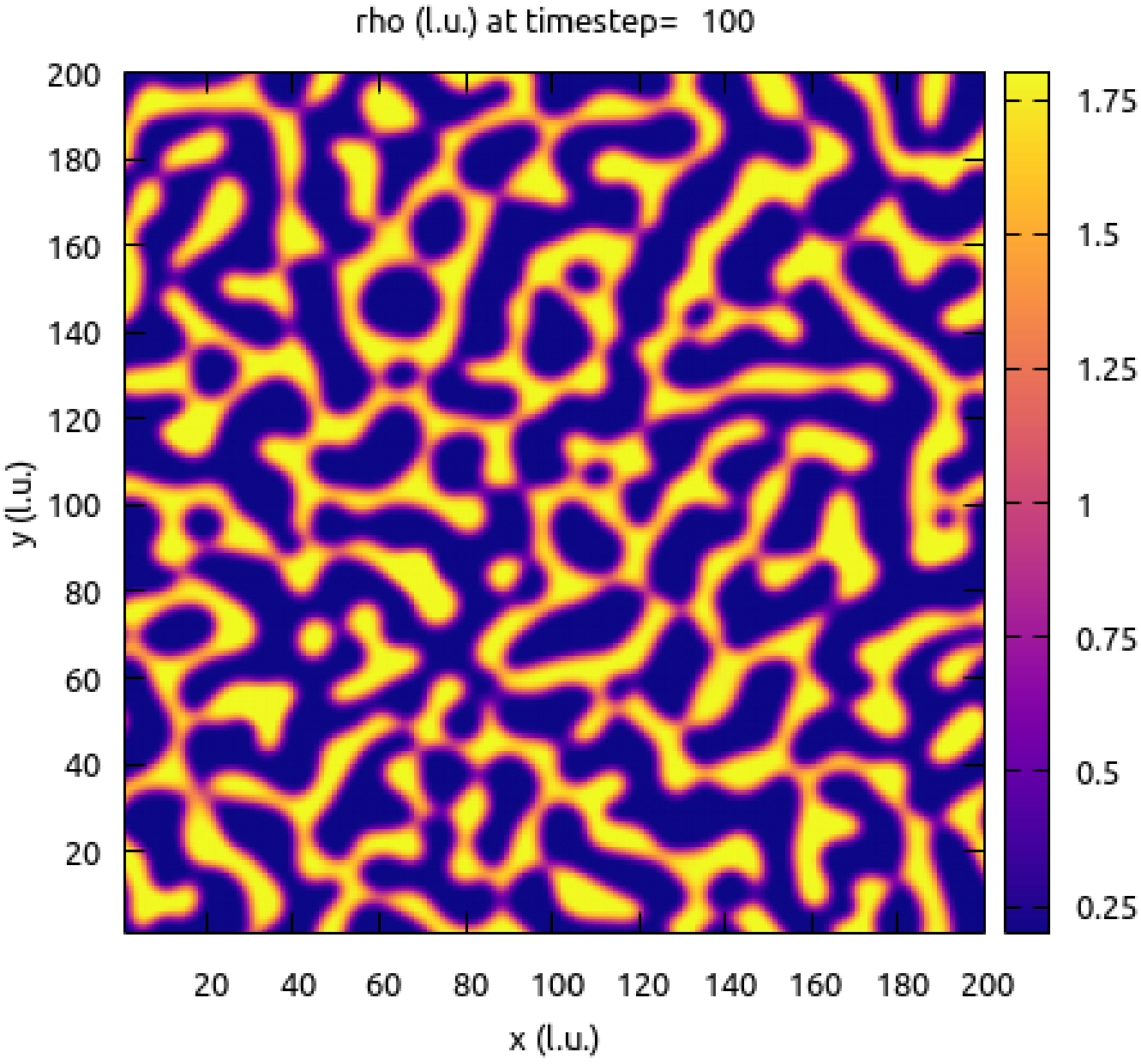

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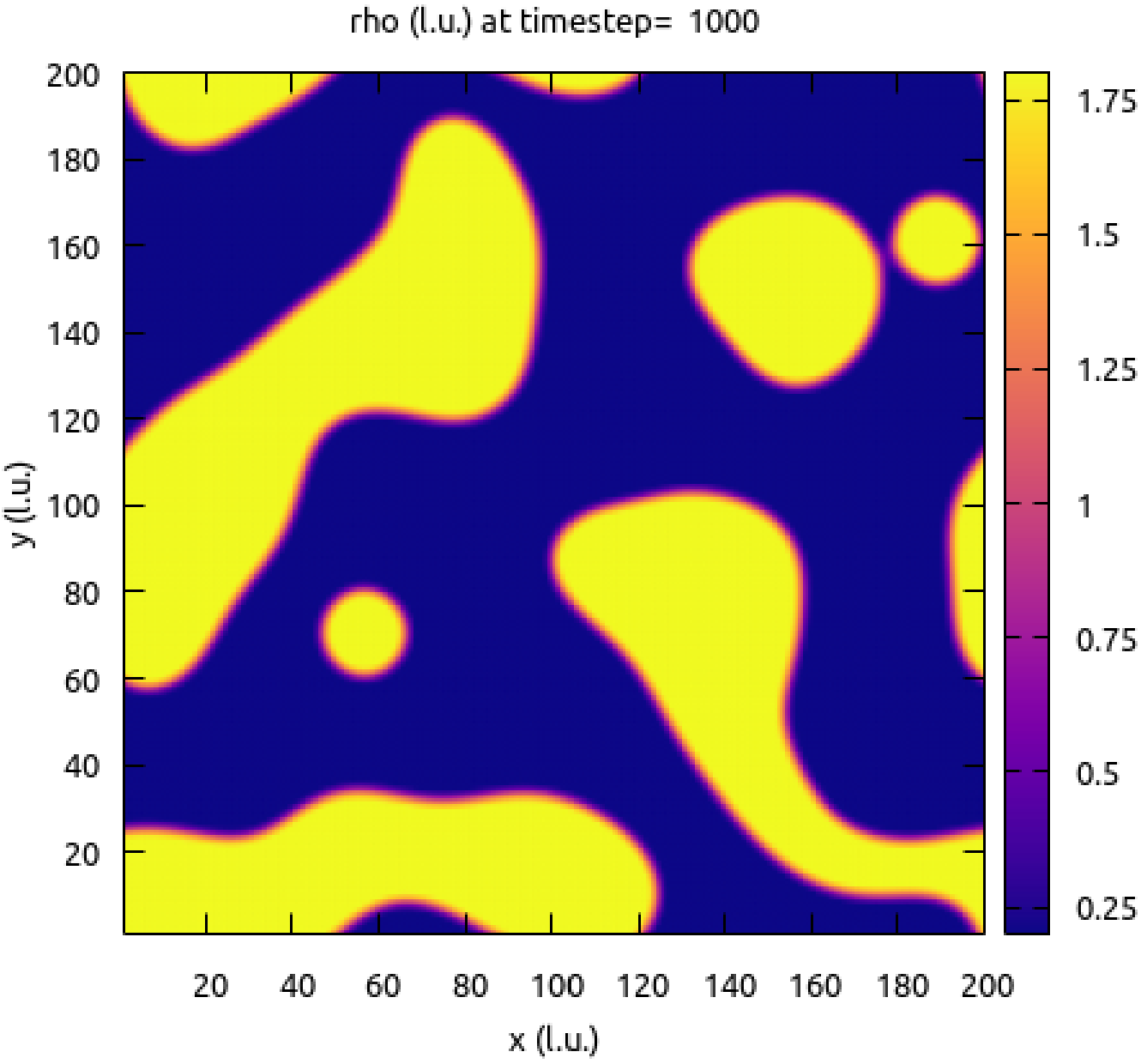

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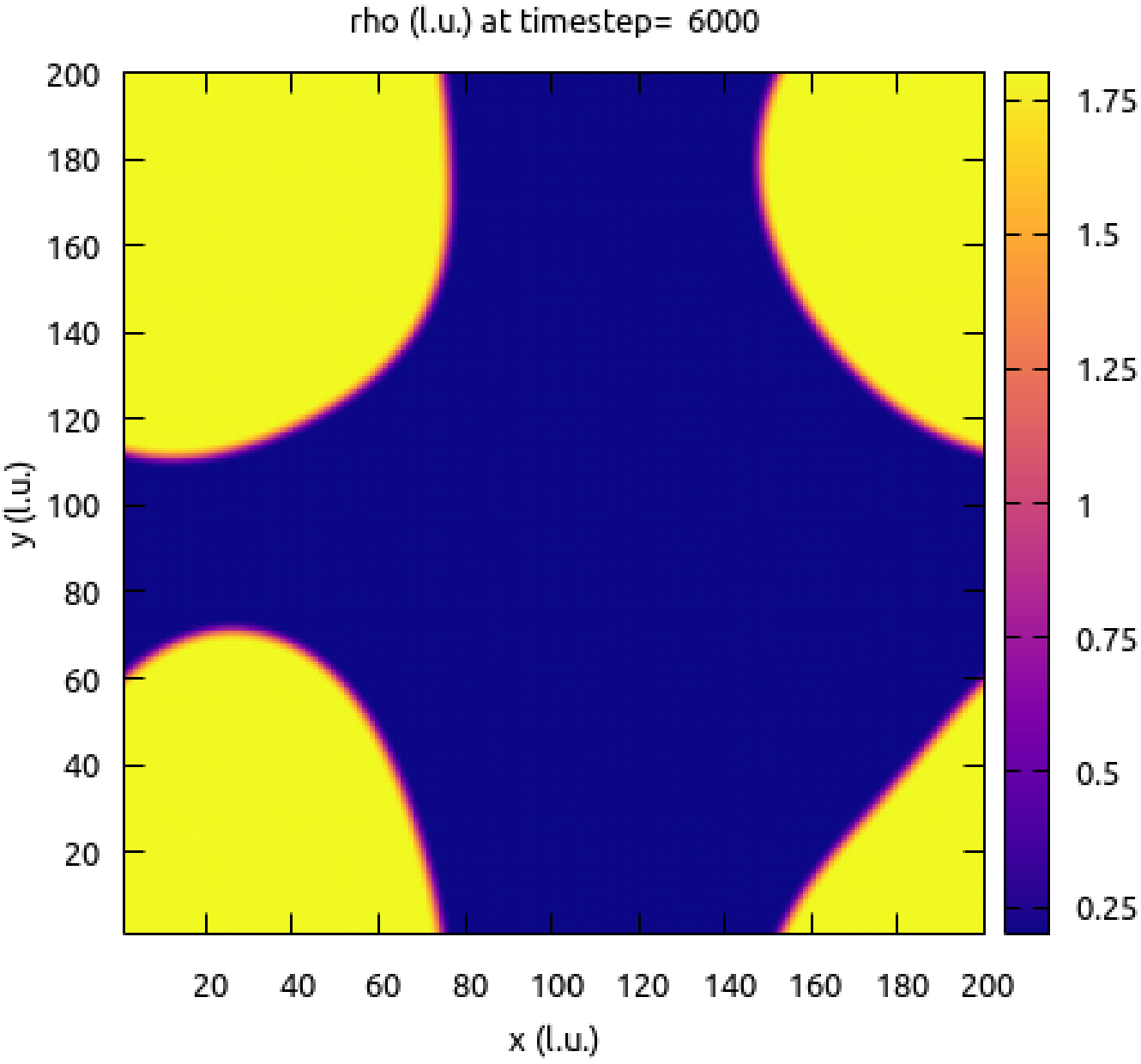
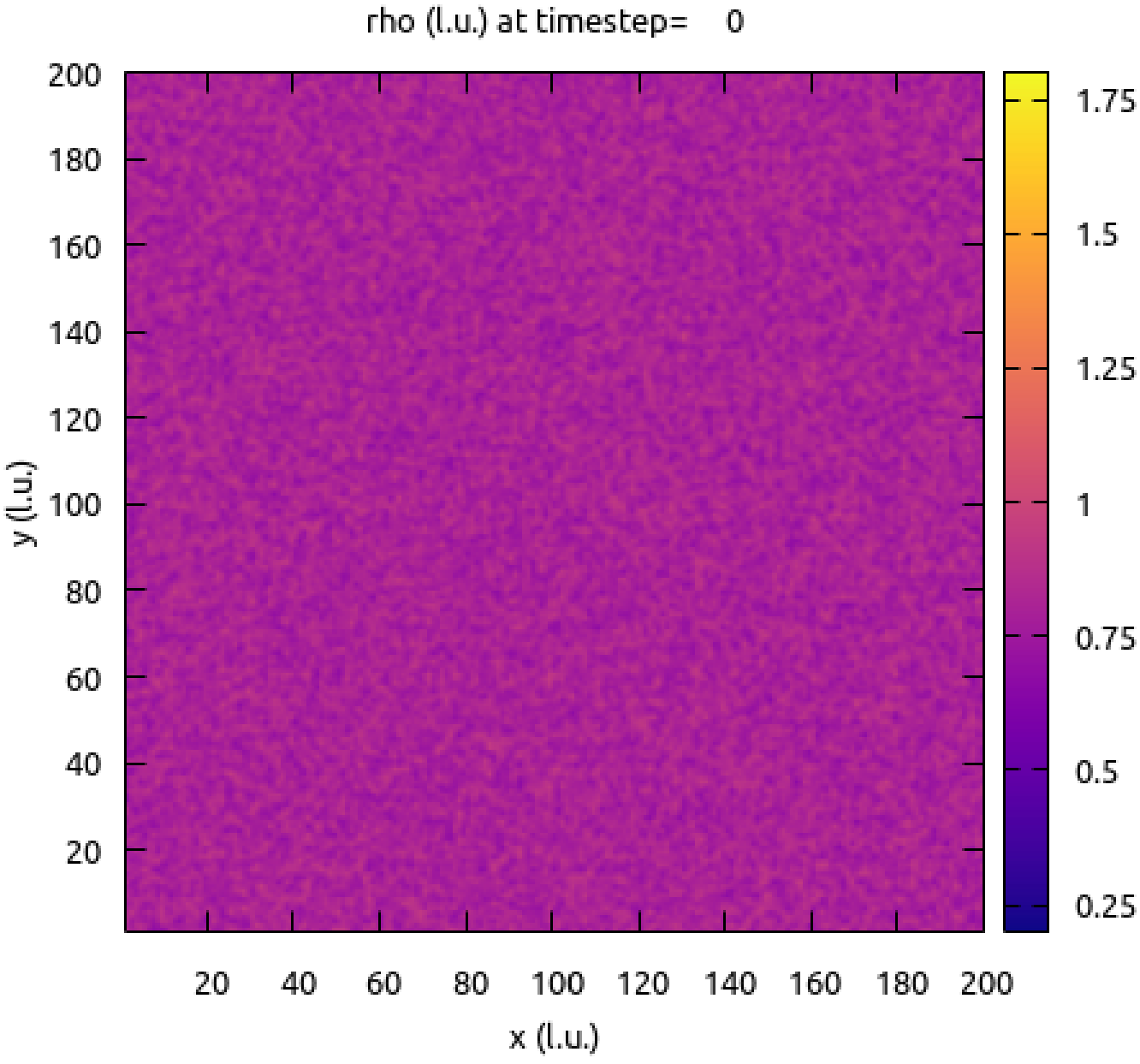


No separation: $(G = -3.00)$



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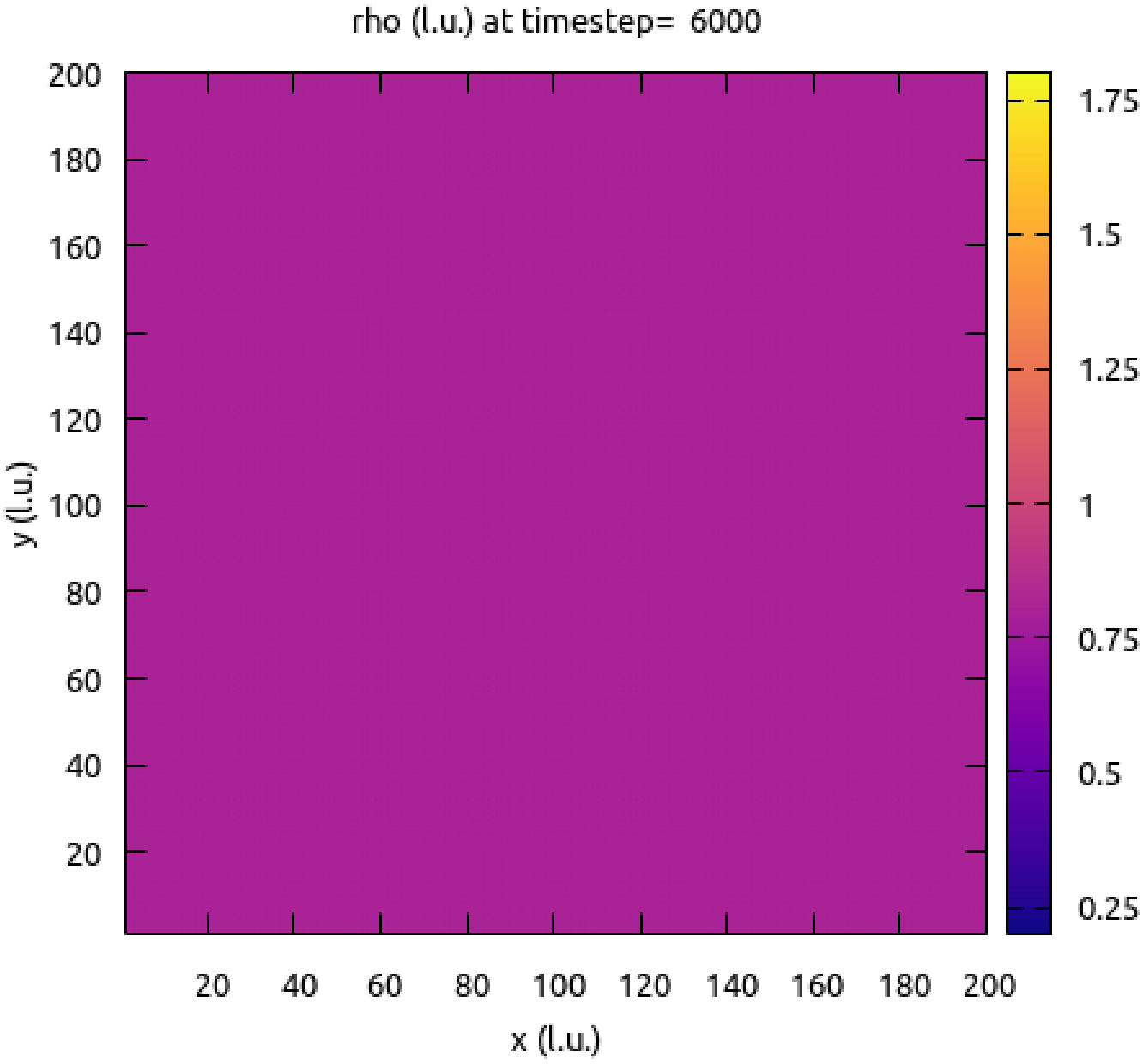

Cohesion-adhesion model

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The Shan-Chen model can be used for modeling multi-component fluid-fluid interactions, e.g.

$$\mathbf{J}_\sigma = -\psi_\sigma(\mathbf{r},t)\sum_\alpha \omega_\alpha \Big[\sum_{\sigma'} G_{\sigma\sigma'}\psi_{\sigma'}(\mathbf{r}+\delta t\mathbf{e}_\alpha)\Big]\mathbf{e}_\alpha$$

and also fluid-solid interactions, e.g.

$$\mathbf{J}_{\mathrm{ff}} = -G_{\mathrm{ff}}\,\psi(\mathbf{r},t)\sum_\alpha \omega_\alpha \psi(\mathbf{r}+\delta t\mathbf{e}_\alpha)\mathbf{e}_\alpha$$

$$\mathbf{J}_{\mathrm{fs}} = -G_{\mathrm{fs}}\,\psi(\mathbf{r},t)\sum_\alpha \omega_\alpha S(\mathbf{r}+\delta t\mathbf{e}_\alpha)\mathbf{e}_\alpha$$

- G_{ff} controls surface tension (cohesion)
- G_{fs} controls wetting (adhesion)

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$$S(\mathbf{r},t) = \begin{cases} 1 \text{ at solid nodes} \\ 0 \text{ at fluid nodes} \end{cases}$$

Hands-on tutorial

Hands on

***LB-lab-3**:*
phase separation

***LB-lab-4**:*
contact angle

***LB-lab-5**:*
heterogeneous surfaces

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