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van der Waals-like transition in Fluidized Granular Matter

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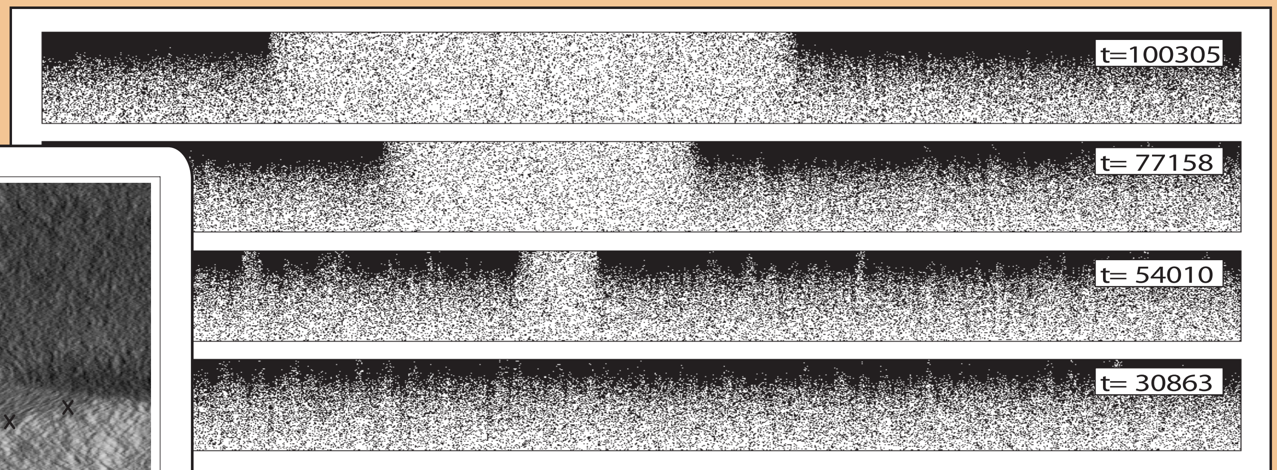
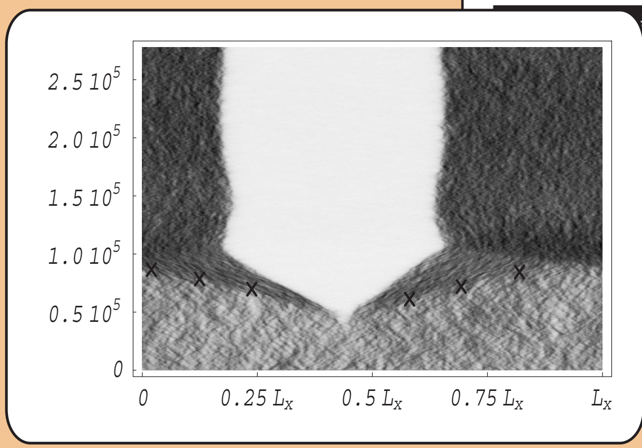
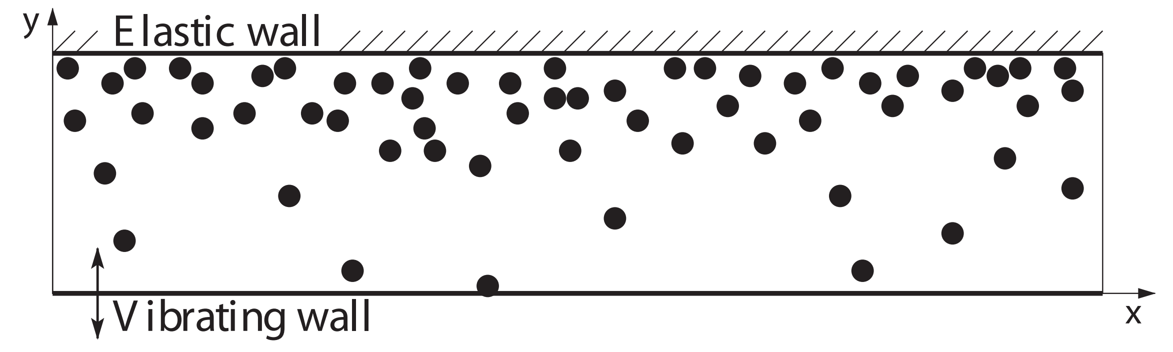




Configuration

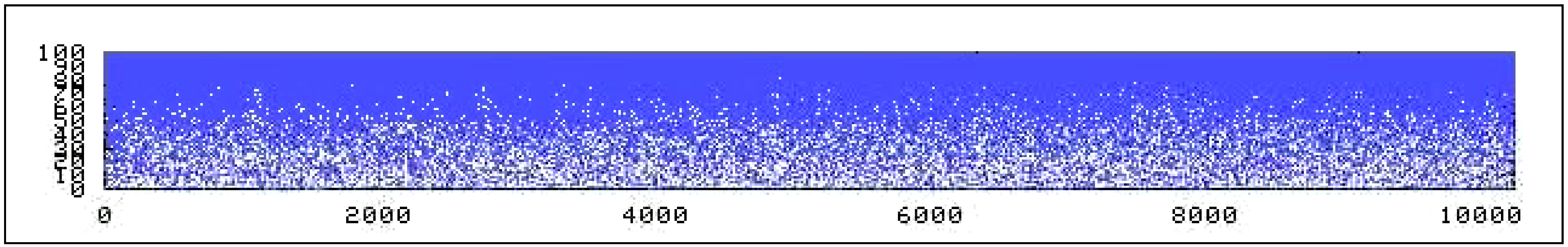
- Box with sand ($L_x >> L_y$).
- No gravity $g=0$.
- Bottom wall: vibrating
  ($\omega \to \infty$; $A \to 0.0$).



- Top wall: perfect elastic.
- Horizontal diractions: periodic boundary conditions.

Molecular dynamics simulations

- Inelastic Hard Sphere model. Restitution coefficient (r=1-2q).
- Molecular dynamics simulation.
- Bottom wall modeled by an stochastic wall.
- Units: diameter $\sigma=1$, mass m=1, $T_{wall}=1$.
- Expected: (blue dots are grains)



vertical gradients: bottom hot and dilute, top cold and dense.

Analysis of molecular dynamic simulations

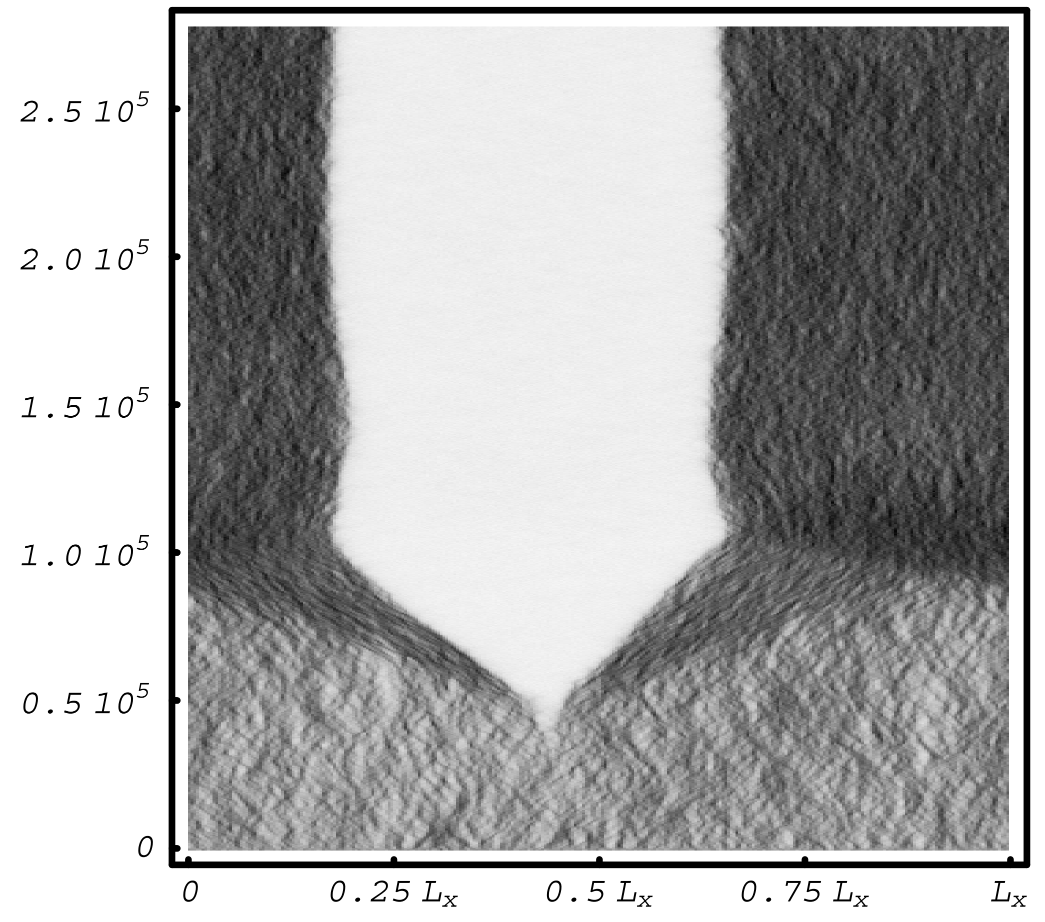
Introducing the coarse-graned density

$$\rho(x,y) = \frac{1}{L_y}\int dy\; n\,(x,y)$$

and

$$N = 153600,\; q = 0.02,$$

$$n_o = \frac{N}{L_x L_y} = 0.15, L_y = 100.$$



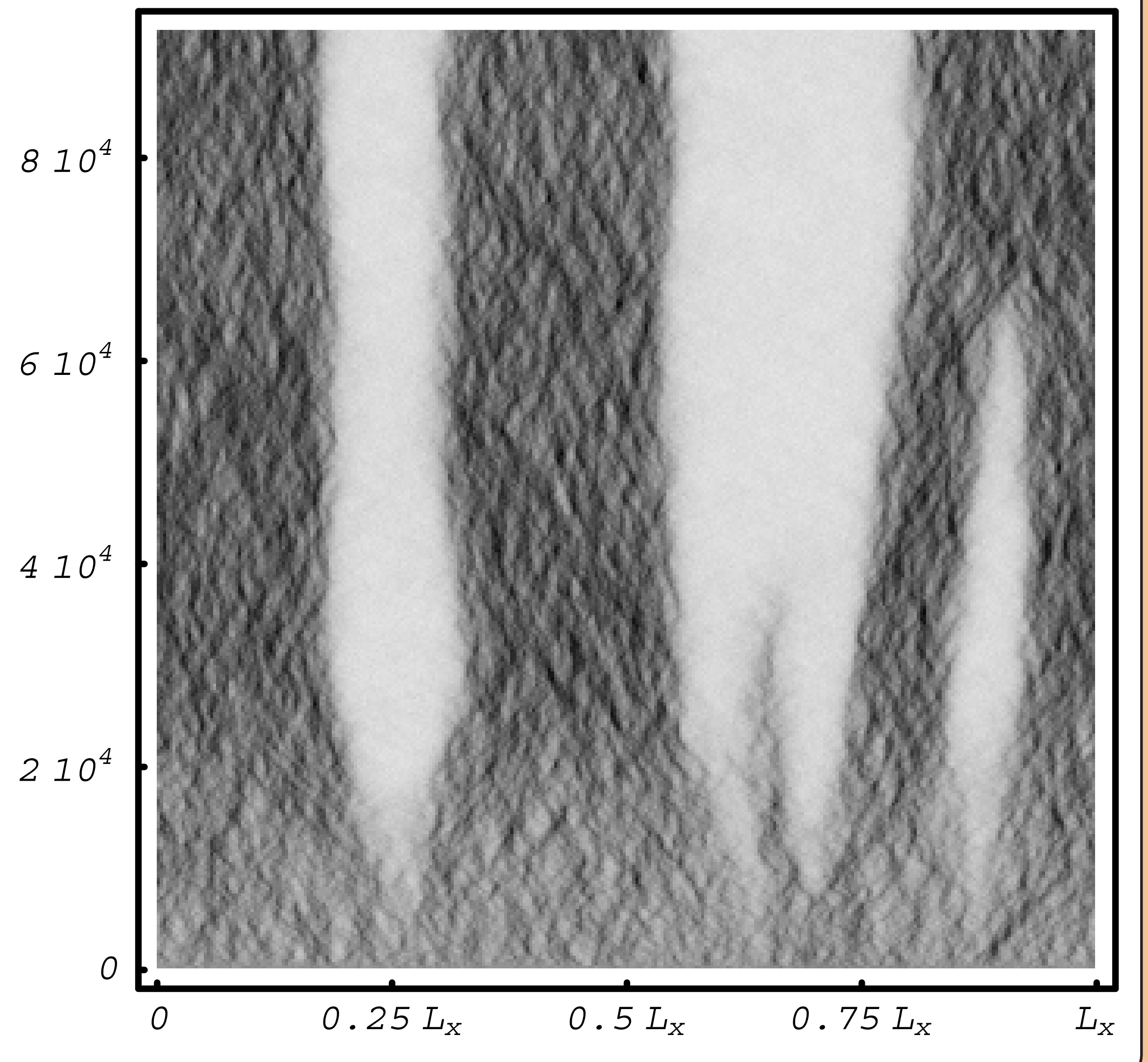
Observations:

- Metastablility
- Constant velocity expansion
- Shock and rarifaction waves
- Bubble oscillations
- Slow dynamics

Molecular dynamics simulation with small dissipation q=0.01

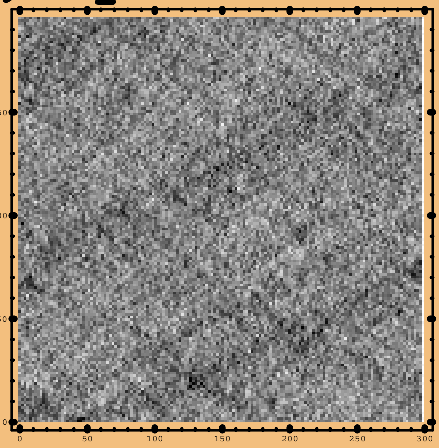
Observations:

- No Metastablility
- Many bubbles
- Interactions mediated by waves
- Evaporation
- Coagulation

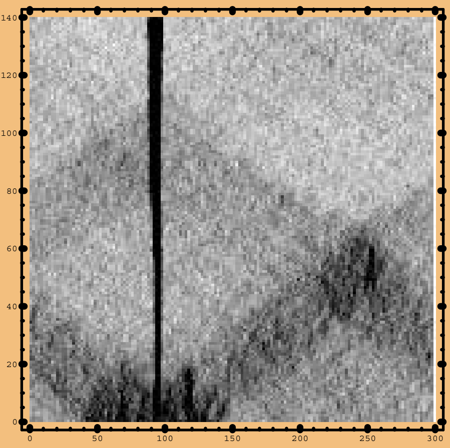


Phenomenology: changing the restitution coefficeints

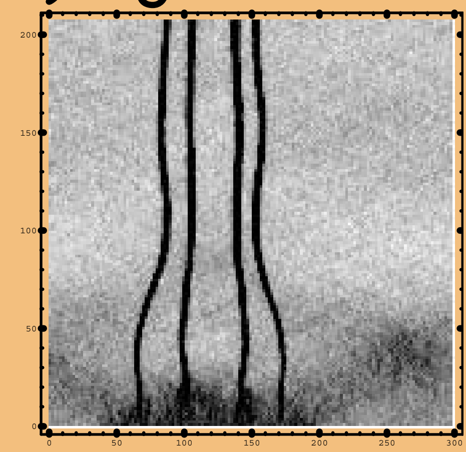
a) r_1



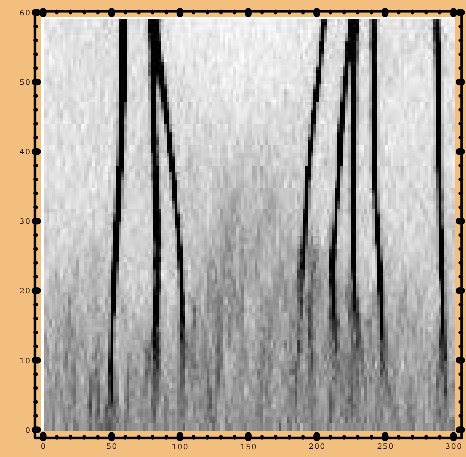
b) r_2



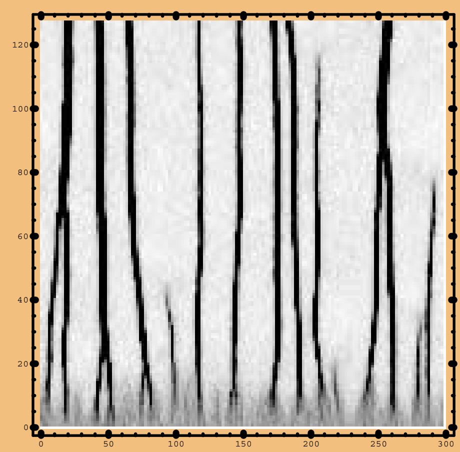
c) r_3



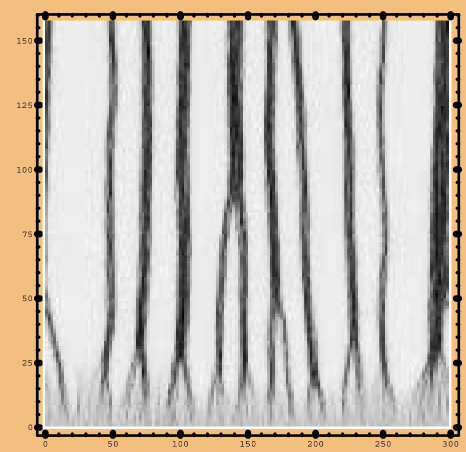
d) r_4



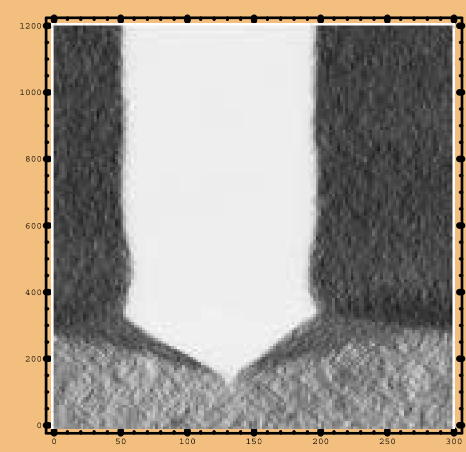
e) r_5



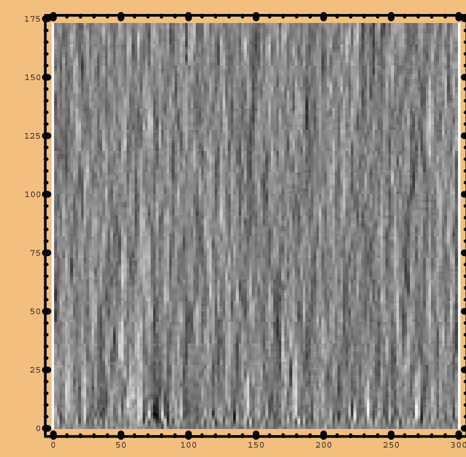
f) r_6



g) r_7



h) r_8



with $r_1 > r_2 > \ldots\ldots > r_8$.

Theoretical description

ingredients:

- $L_x >> L_y$.
- mass ρ and J horizontal momentum are conserved.
- Energy T and vertical monentum are not conserved.

fast evolution in y, slow in x.

Energy and vertical momentum evolve fast, they are slave variables of ρ and J.

Thus,

$$\partial_t \rho(x,t) = -\partial_x J(x,t), \\ \partial_t J(x,t) = -\partial_x \Phi,$$

Symmetries: reflection, spatio-temporal homogeneity, the horizontal momentum flux is a function

$$\Phi = \Phi\left[\rho, \partial_x^{2n}\rho, j^2, \partial_x^{2n-1} j, n = 1, 2, \cdots\right]$$

The stationary homogeneous state: ρ=n_o, J=0.0 and Φ the hydrostatic pressure is the trivial solution of

$$\partial_t \rho(x,t) = -\partial_x J(x,t)\,,$$
$$\partial_t J(x,t) = -\partial_x \Phi,$$

The fluctuations of this state are describe by wave equation

$$\partial_{tt}\rho(x,t) = \frac{\partial \Phi[n_o,0,0]}{\partial \rho}\partial_{xx}\rho(x,t)$$

Φ is proportional to ρ and T, but T is a slave variable and decrease when ρ increase. Then, the pressure can be non-monotonous in the density.

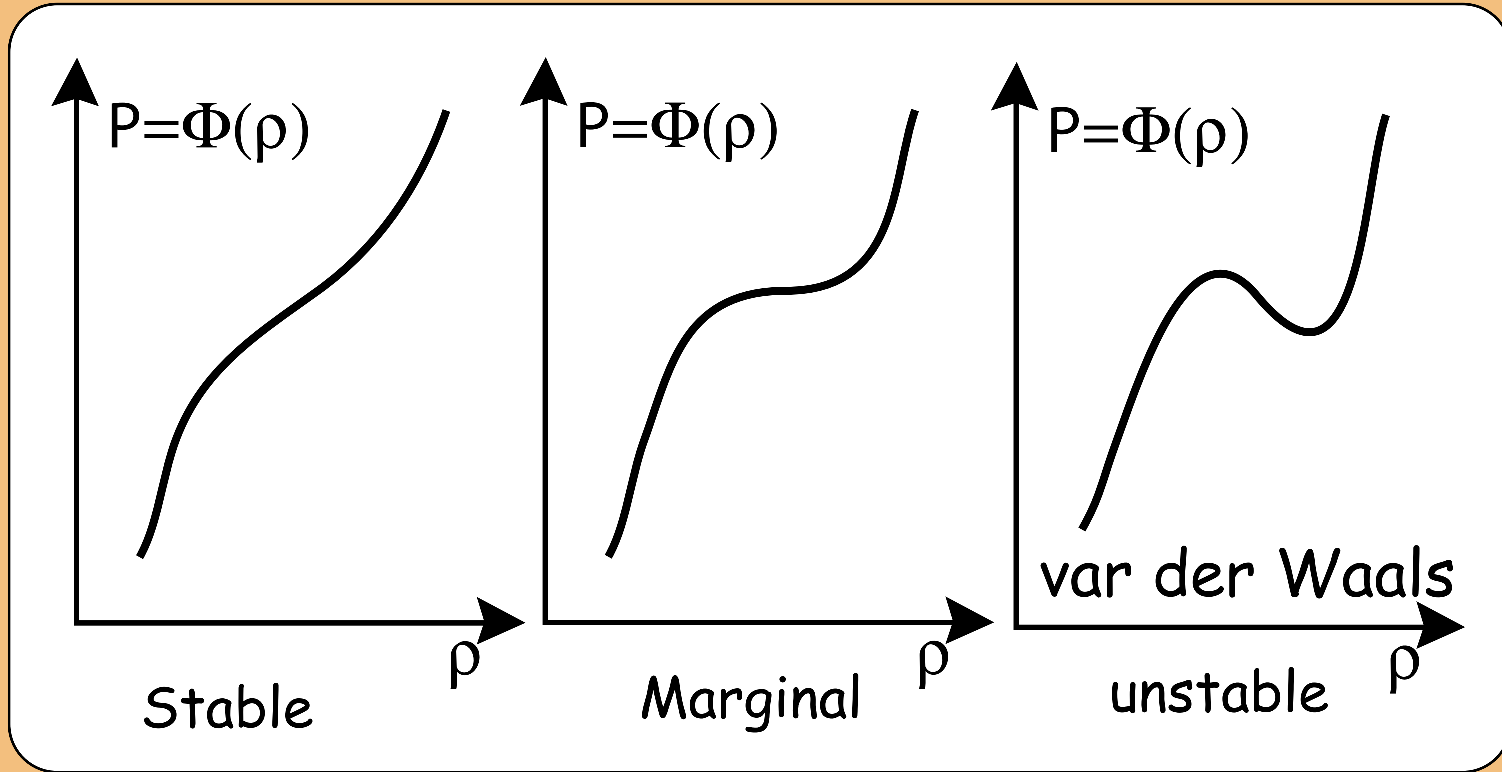
Negative compressibility ⟶ Mechanical instability

Close to inflextion point (ρo)

$$\frac{\partial \Phi}{\partial \rho} = 0,$$

$$\frac{\partial^2 \Phi}{\partial \rho^2} = 0,$$

The horizontal momentum



$$\begin{aligned}\Phi \quad &\approx \quad \Phi_o + \frac{\partial \Phi}{\partial \rho}\bar{\rho} + \frac{\partial^2 \Phi}{\partial^2 \rho}\frac{\bar{\rho}^2}{2} + \frac{\partial^3 \Phi}{\partial^3 \rho}\frac{\bar{\rho}^3}{6} + \frac{\partial \Phi}{\partial j^2} j^2 \\ &+ \frac{\partial \Phi}{\partial \rho_{xx}}\bar{\rho}_{xx} + \frac{\partial \Phi}{\partial j_x} j_x,\end{aligned}$$

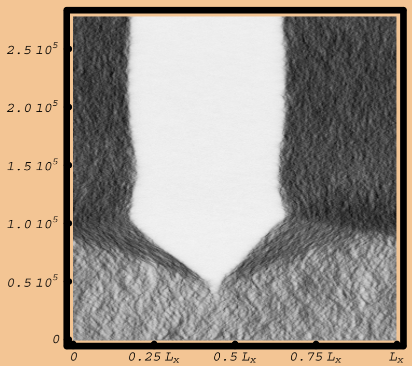
The evolution of the system close to this critical point is described by van der Waals Normal form.

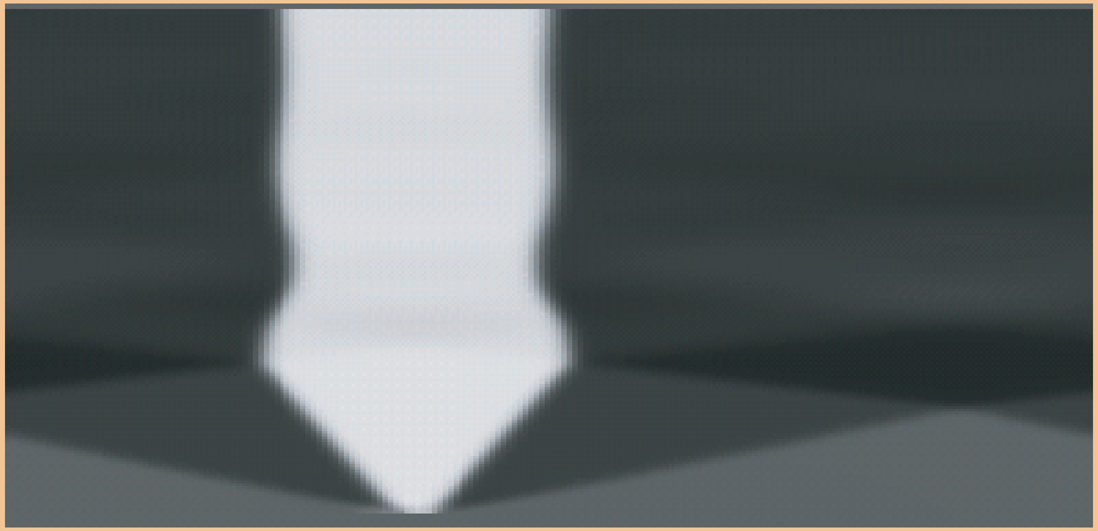
$$\begin{aligned} \partial_{tt} u &= \partial_{xx}\left(\varepsilon u + u^3 - \partial_{xx} u + \nu \partial_t u\right), \\ &= \partial_{xx} \frac{\delta \mathcal{F}}{\delta u} + \nu \partial_{xxt} u, \end{aligned}$$

where

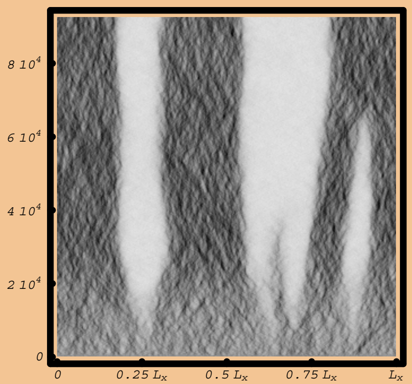
$$\mathcal{F} = \int dx \left\{ \varepsilon \frac{u^2}{2} + \frac{u^4}{4} + \frac{(\partial_x u)^2}{2} \right\}.$$

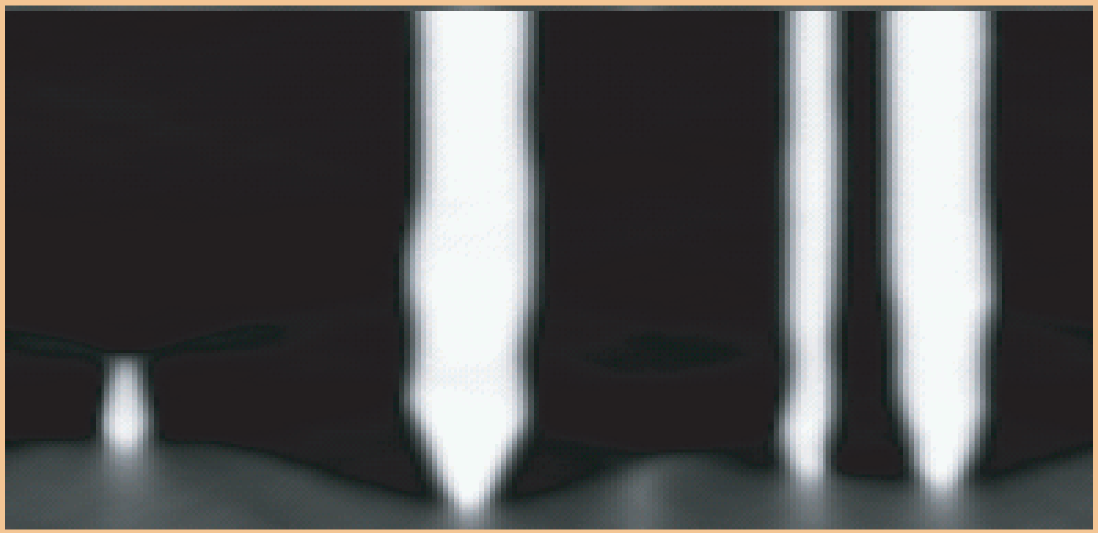
Simulations of the van der Waals normal form





Bistability





Spinodal decomposition

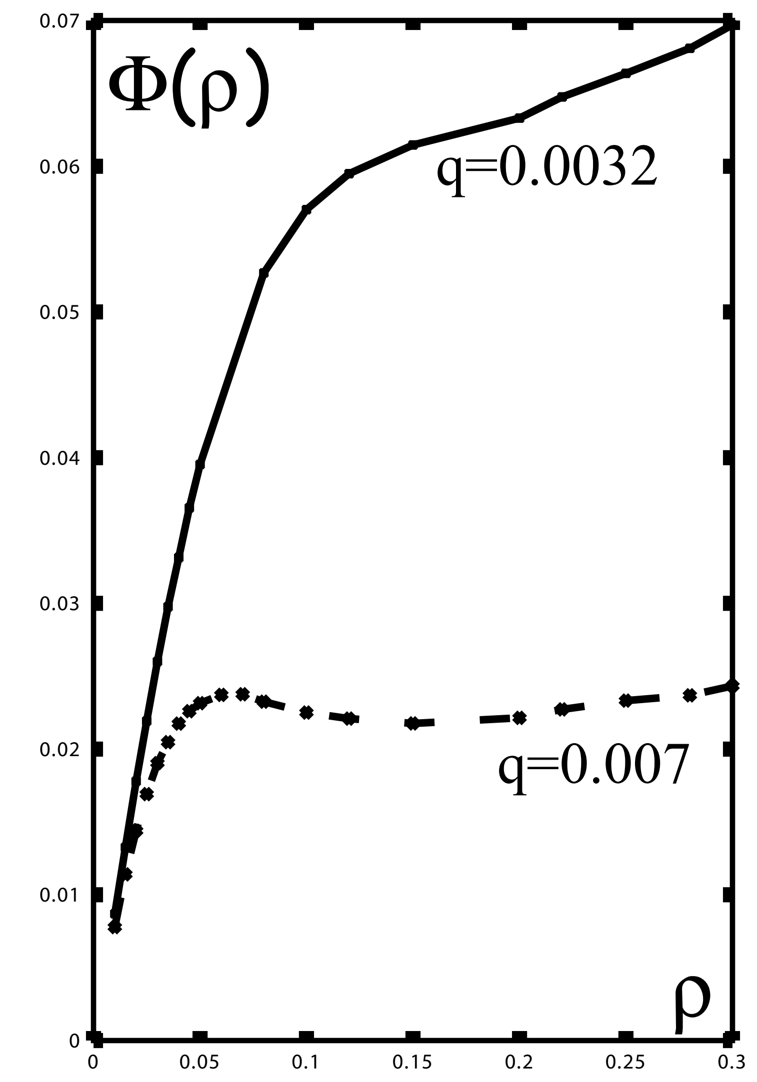
Molecular dynamic simulation (parallel computer)

Interactive simulation (DimX)

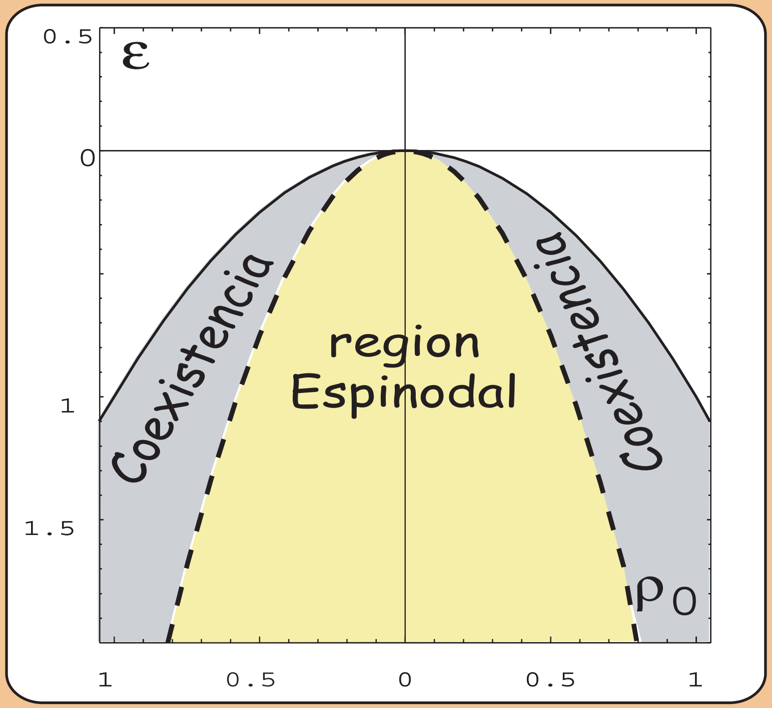
Molecular dynamics simulations of thin columns

- Measure of $\Phi(\rho)$ in simulations of thin columns ($L_x \ll L_y$) to avoid the spatial instability.

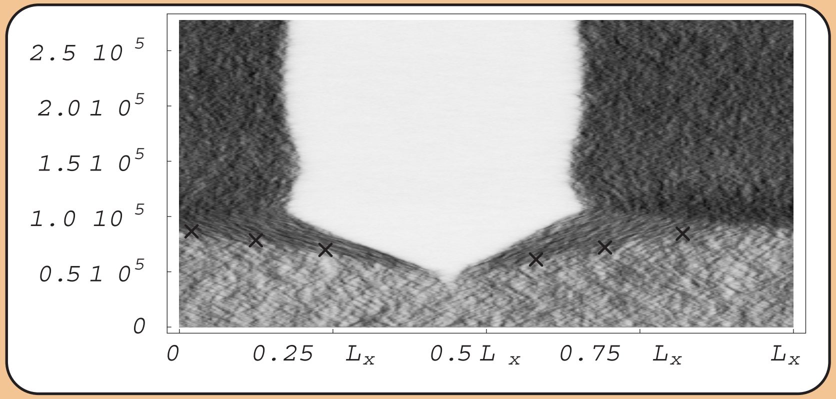
- The Critical point $q=0.0047$ and $\rho o=0.15$



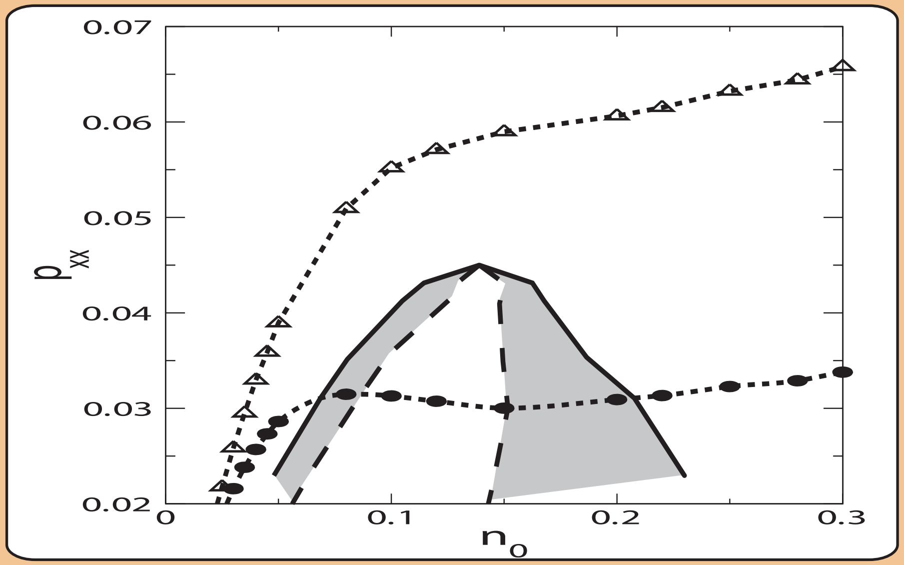
Phase diagram of van der Waals normal form



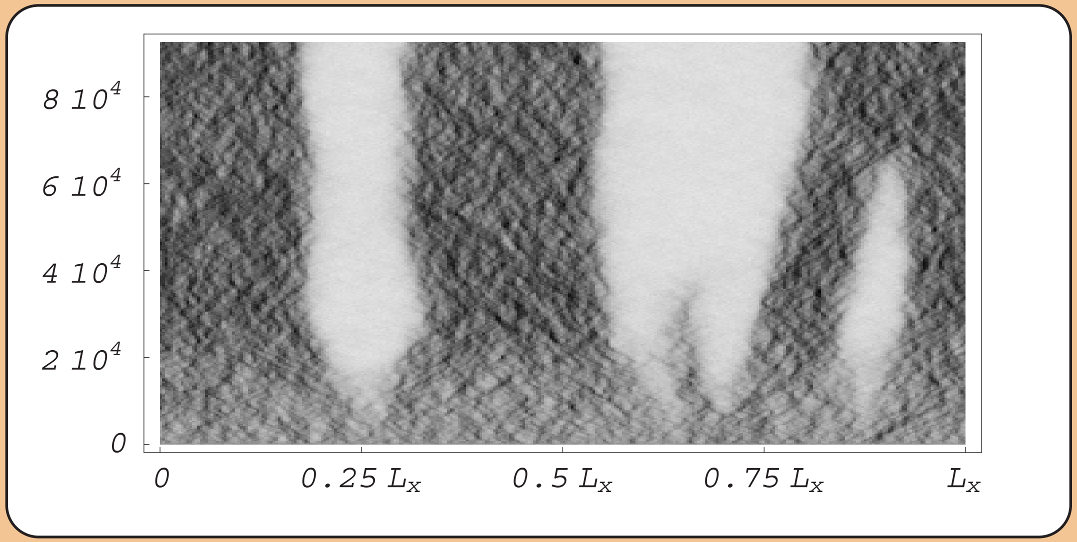
- Metastability



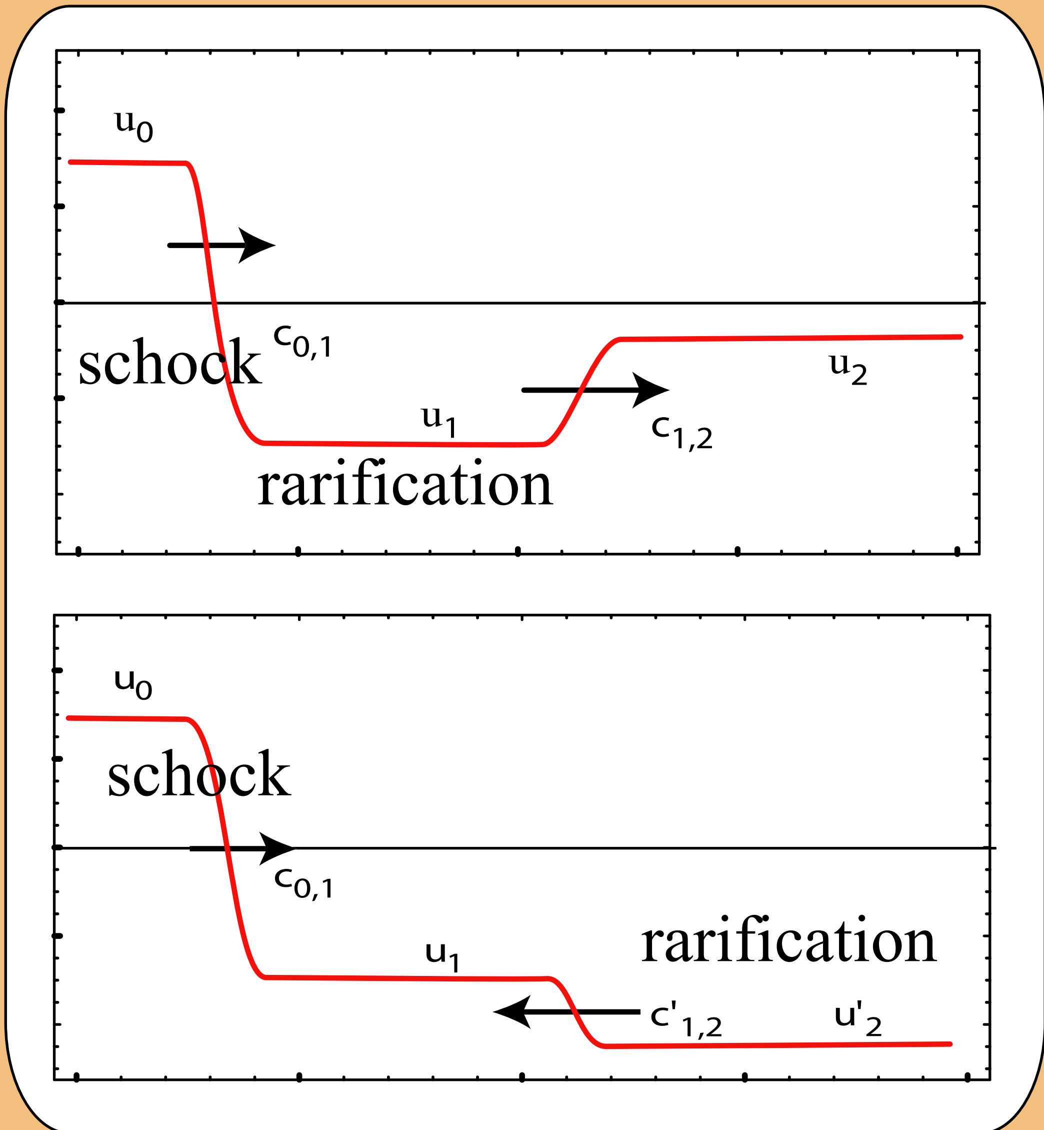
Molecular dynamics simulations



- coarsenig dynamics bubbles



analytical expression of the velocity of densification waves



$$c_{01} = \sqrt{\varepsilon + u_0^2 + u_1^2 + u_0 u_1}$$

$$c_{12} = \sqrt{\varepsilon + u_1^2 + u_2^2 + u_1 u_2}$$

conservation of number of particle

$$(u_0 - u_1)\, c_{01} = (u2 - u_1)\, c_{12}$$

quantity	Numerical	P1	P2
u_2	-0.5	-0.5	-0.5
u_1	-0.713	-0.715	-0.717
u_0	0.719	0.719	0.717
c_{01}	$0.119 \pm 2\, 10^{-3}$	0.118	0.117
c_{12}	$0.783 \pm 4\, 10^{-3}$	0.786	0.786

Hydrodynamic model of fluidized granular matter

For slow dissipation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0$$
$$\rho \left(\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{v} \right) = -\nabla \cdot \mathbb{P}$$
$$\rho \left(\frac{\partial T}{\partial t} + (\mathbf{v} \cdot \nabla) T \right) = -\nabla \cdot \mathbf{Q} - \mathbb{P} : \nabla \mathbf{v} - \omega$$

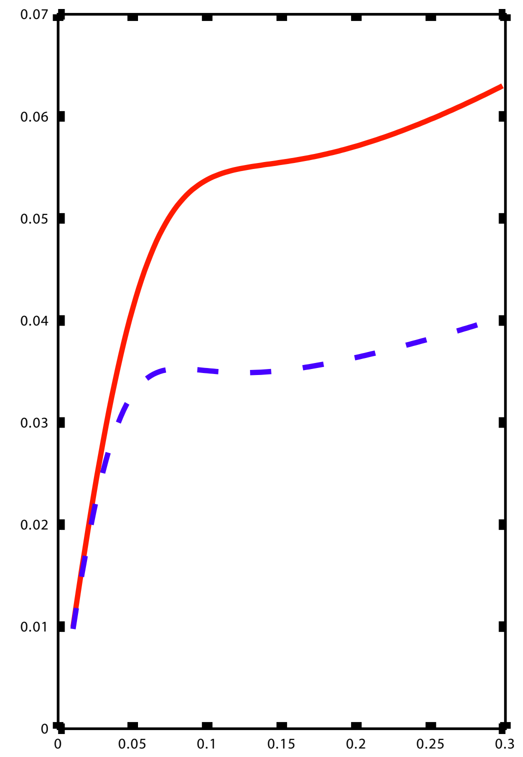
Time scale separation between x and y directions.

$$\frac{\partial \rho}{\partial t} + \frac{\partial j}{\partial x} = 0$$
$$\frac{\partial j}{\partial t} = -\frac{\partial p[\rho, j]}{\partial x}$$

with

$$\frac{\partial p}{\partial y} = 0$$
$$\frac{\partial Q}{\partial y} + \omega = 0$$

critical point
q=0.0085,
ρ=0.11



Conclusions

- Granular fluid exhibits van derWaals-like phase separation.
- Metastability, spinodal decomposition, bubble and droplets nucleation, evaporation, and coagulation.
- Inertial dynamics: waves and shock waves.
- Universal theoretical description. Ingredients: two conservations and negative compressibility region.
- Mechanism verified in molecular dynamics simulations and hydrodynamic model.
- Successful theoretical description.