Morphology And Dynamics of Phase Separation: From Simple to Active fluids

Giuseppe Negro
Supervisor: Prof. G. Gonnella, Dott. Antonio Lamura

November 13, 2017

Dip. Fisica 'M. Merlin' Bari

Table of contents

Framework

Motivations

Research activity has been focused on the dynamics of phase transition in some important classes of fluids systems:

Motivations

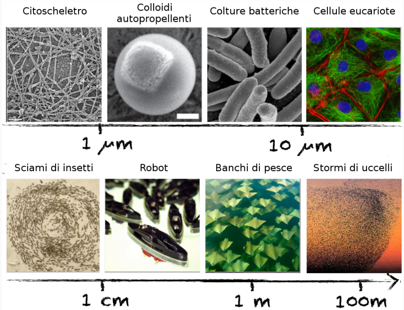
Research activity has been focused on the dynamics of phase transition in some important classes of fluids systems:

- Single component fluids with Liquid-Vapor Transition in $3D$(Never done before) **Power-law growth for domain size expected**

Motivations

Research activity has been focused on the dynamics of phase transition in some important classes of fluids systems:

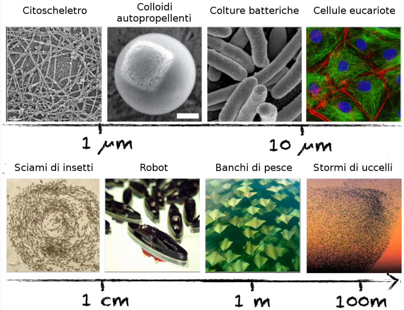
- Single component fluids with Liquid-Vapor Transition in $3D$(Never done before) **Power-law growth for domain size expected**
- Mixtures with an active component :
  Energy supplied at the level of the individual constituents. These are Fluids out of equilibrium



Motivations

Research activity has been focused on the dynamics of phase transition in some important classes of fluids systems:

- Single component fluids with Liquid-Vapor Transition in $3D$(Never done before) **Power-law growth for domain size expected**
- Mixtures with an active component :
  Energy supplied at the level of the individual constituents. These are Fluids out of equilibrium **New mechanisms of self-propulsion**.
  Morphology and dynamics of active emulsions.



Methods

We use a continuum description in terms of a few coarse-grained fields
Dynamics is governed by the Navier-Stokes equation and by equations for the evolution of the order parameter and numerically solved

Methods

We use a continuum description in terms of a few coarse-grained fields

Dynamics is governed by the Navier-Stokes equation and by equations for the evolution of the order parameter and numerically solved

Lattice Boltzmann Method (LB)

Methods

We use a continuum description in terms of a few coarse-grained fields
Dynamics is governed by the Navier-Stokes equation and by equations for the evolution of the order parameter and numerically solved

Lattice Boltzmann Method (LB)

- Discretization of space and velocities introducing a lattice

Methods

We use a continuum description in terms of a few coarse-grained fields Dynamics is governed by the Navier-Stokes equation and by equations for the evolution of the order parameter and numerically solved

Lattice Boltzmann Method (LB)

- Discretization of space and velocities introducing a lattice
- On each point of the lattice a set of velocities $\{\mathbf{e_i}\}$ and distribution functions $\{f_i\}$ are defined which evolve according to the discretized Boltzmann transport equation (BGK approximation):

$$f_i(\mathbf{r} + \mathbf{e}_i \Delta t, t + \Delta t) - f_i(\mathbf{r}, t) = -\frac{\Delta t}{\tau}[f_i(\mathbf{r}, t) - f_i^{eq}(\mathbf{r}, t)]$$

$$\sum_i f_i^{eq} = \rho \quad , \qquad \sum_i f_i^{eq} \mathbf{e_i} = \rho \mathbf{u}$$

Methods

We use a continuum description in terms of a few coarse-grained fields Dynamics is governed by the Navier-Stokes equation and by equations for the evolution of the order parameter and numerically solved

Lattice Boltzmann Method (LB)

- Discretization of space and velocities introducing a lattice
- On each point of the lattice a set of velocities $\{\mathbf{e_i}\}$ and distribution functions $\{f_i\}$ are defined which evolve according to the discretized Boltzmann transport equation (BGK approximation):

$$f_i(\mathbf{r} + \mathbf{e}_i \Delta t, t + \Delta t) - f_i(\mathbf{r}, t) = -\frac{\Delta t}{\tau}[f_i(\mathbf{r}, t) - f_i^{eq}(\mathbf{r}, t)]$$

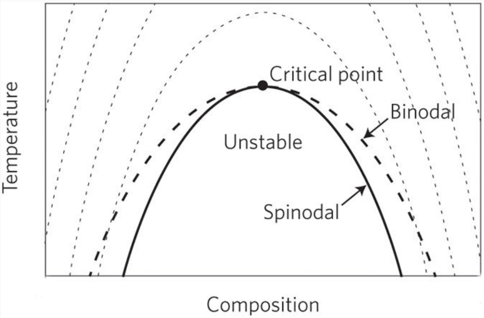
$$\sum_i f_i^{eq} = \rho \quad , \qquad \sum_i f_i^{eq} \mathbf{e_i} = \rho \mathbf{u}$$

- Expansion of the equilibrium distribution functions f_i^{eq} with coefficient chosen in order to regain the correct continuum equations.

Dynamics of Liquid-Vapor Phase Separation

Spinodal decomposition

When a fluid is quenched from an initial disordered state into a regime of two-phase coexistence below the spinodal line, **domains of the two phases are formed and grow with time**



Hydrodynamics is in general relevant and the coupling with the velocity field can change the law of growth

Kinetics of phase separation

Dynamical scaling hypothesis

Growth is a scaling phenomenon: despite a changing in the length scale $l(t)$ there exists self similarity of domain patterns

Kinetics of phase separation

Dynamical scaling hypothesis

Growth is a scaling phenomenon: despite a changing in the length scale $l(t)$ there exists self similarity of domain patterns

The average size of domains $l(t)$ growths in time as a power law

$$l(t) \sim t^{\alpha}$$

Kinetics of phase separation

Dynamical scaling hypothesis

Growth is a scaling phenomenon: despite a changing in the length scale $l(t)$ there exists self similarity of domain patterns

The average size of domains $l(t)$ growths in time as a power law

$$l(t) \sim t^{\alpha}$$

The growth exponent α depends on

- dimensionality d
- morphology
- presence of hydrodynamic effects
- number of order parameters and conservation

Growth Exponents

For binary mixtures three different regimes can be derived, each corresponding to a specific physical mechanism:

- $l(t) \sim t^{1/3}$ (Lifshitz Slyozov)
  Diffusive growth: Diffusion of molecules from smaller higher-curvature domains to larger lower-curvature ones

Growth Exponents

For binary mixtures three different regimes can be derived, each corresponding to a specific physical mechanism:

- $l(t) \sim t^{1/3}$ (Lifshitz Slyozov)
  Diffusive growth: Diffusion of molecules from smaller higher-curvature domains to larger lower-curvature ones
- $l(t) \sim \sigma t/\eta$ (Siggia)
  Viscous growth: Tubes of fluid are unstable to fluctuations of their interfaces, and this results in pinch-off

Growth Exponents

For binary mixtures three different regimes can be derived, each corresponding to a specific physical mechanism:

- $l(t) \sim t^{1/3}$ (Lifshitz Slyozov)
  Diffusive growth: Diffusion of molecules from smaller higher-curvature domains to larger lower-curvature ones
- $l(t) \sim \sigma t/\eta$ (Siggia)
  Viscous growth: Tubes of fluid are unstable to fluctuations of their interfaces, and this results in pinch-off
- $l(t) \sim (\sigma t^2/\rho)^{1/3}$ (Furukawa)
  Inertial growth: Curvature differences induce tangential pressure gradients and hence a velocity field that favours the smoothing of protuberances and dimples from interfaces

Growth Exponents

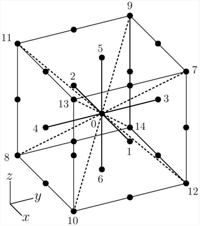
For binary mixtures three different regimes can be derived, each corresponding to a specific physical mechanism:

- $l(t) \sim t^{1/3}$ (Lifshitz Slyozov)
  Diffusive growth: Diffusion of molecules from smaller higher-curvature domains to larger lower-curvature ones
- $l(t) \sim \sigma t/\eta$ (Siggia)
  Viscous growth: Tubes of fluid are unstable to fluctuations of their interfaces, and this results in pinch-off
- $l(t) \sim (\sigma t^2/\rho)^{1/3}$ (Furukawa)
  Inertial growth: Curvature differences induce tangential pressure gradients and hence a velocity field that favours the smoothing of protuberances and dimples from interfaces

For Liquid-Vapor systems exponents are not known but expected similar to binary mixtures
Few 2D numerical studies (Sofonea et al 2009)

Development of a 3D LB scheme

To address the problem we developed a lattice Boltzmann scheme using a $3DQ15$ geometry



and a forcing therm which encodes the properties of a van der Waals fluid

$$f_i(\mathbf{r} + \mathbf{e}_i \Delta t, t + \Delta t) - f_i(\mathbf{r}, t) = -\frac{\Delta t}{\tau}[f_i(\mathbf{r}, t) - f_i^{eq}(\mathbf{r}, t)] - \Delta t F_{\mathrm{int},i}$$

- Expansion of the distributions evaluated on abscissas of Gauss-Hermite quadrature (*Abe and He 2007*)
- New isotropic discretized differential operators (*Succi et al 2012*)

Development of a 3D LB scheme

Continuity equation

$$\partial_t \rho + \partial_\alpha(\rho u_\alpha)$$

Navier-Stokes

$$\partial_t(\rho u_\alpha) + \partial_\beta(\rho u_\alpha u_\beta) = -\partial_\alpha p^i + F_{int,\alpha} + \partial_\beta[\eta(\partial_\alpha u_\beta + \partial_\beta u_\alpha)] + o(u^3)$$

Development of a 3D LB scheme

Continuity equation

$$\partial_t \rho + \partial_\alpha(\rho u_\alpha)$$

Navier-Stokes

$$\partial_t(\rho u_\alpha) + \partial_\beta(\rho u_\alpha u_\beta) = -\partial_\alpha p^i + F_{int,\alpha} + \partial_\beta[\eta(\partial_\alpha u_\beta + \partial_\beta u_\alpha)] + o(u^3)$$

Viscosity

$$\eta = \rho(\tau - \frac{\Delta t}{2})$$

Development of a 3D LB scheme

Continuity equation

$$\partial_t \rho + \partial_\alpha(\rho u_\alpha)$$

Navier-Stokes

$$\partial_t(\rho u_\alpha) + \partial_\beta(\rho u_\alpha u_\beta) = -\partial_\alpha p^i + F_{int,\alpha} + \partial_\beta[\eta(\partial_\alpha u_\beta + \partial_\beta u_\alpha)] + o(u^3)$$

Viscosity

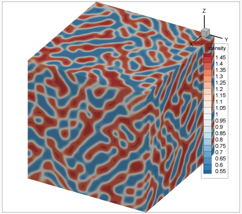
$$\eta = \rho(\tau - \frac{\Delta t}{2})$$

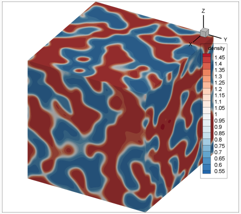
For a van der Waals fluid

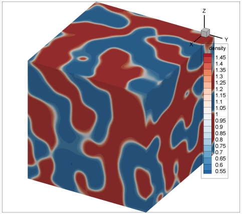
$$F_{int,\alpha} = \partial_\alpha(p^i) - \partial_\beta \Pi_{\alpha\beta}$$

$$\Pi_{\alpha\beta} = \left[p^w - k\rho\nabla^2\rho - \frac{k}{2}(\nabla\rho)^2\right]\delta_{\alpha\beta} + k\partial_\alpha\rho\partial_\beta\rho$$

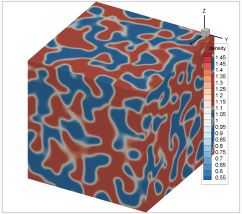
Lattice Boltzmann Simulations of 3D van Der Waals Fluid

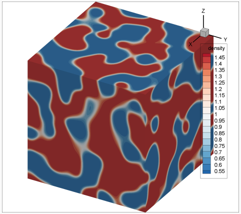


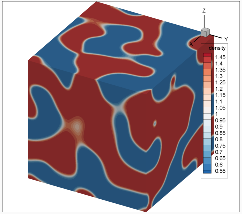




High Viscosity ($\eta = 3$)



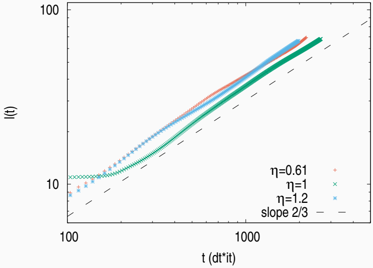




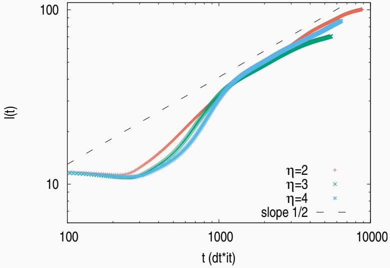
Low Viscosity ($\eta = 1$)

3D Liquid-Vapor Phase Separation

Mean domains size *(Lattice size $L = 256$)* (Typical run one week 60GB RAM (RECAS HPC cluster))



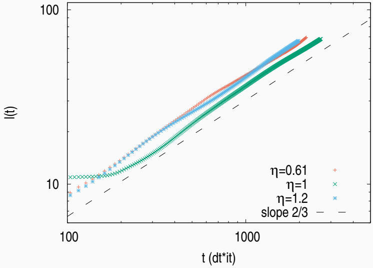
Low viscosity



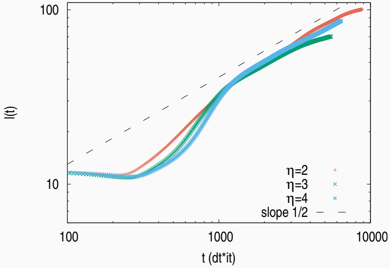
High viscosity

3D Liquid-Vapor Phase Separation

Mean domains size *(Lattice size $L = 256$)* (Typical run one week 60GB RAM (RECAS HPC cluster))



Low viscosity



High viscosity

Evidence of inertial regime $(\alpha = 2/3)$ **at late times**

For different values of viscosity $\alpha \simeq 1/2$

Active Liquid Vapor and Active Mixtures

Cell motility

Motility is the ability to move spontaneously and actively, consuming energy in the process

[1] H. Kelleret al 2002

Cell motility

Motility is the ability to move spontaneously and actively, consuming energy in the process

- The mechanistic understanding of *cell crawling* has been described in various successful model based on:
  Actin Polymerization
  Myosin contractility

[1]H. Kelleret al 2002

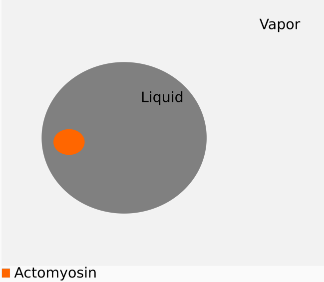
Cell motility

Motility is the ability to move spontaneously and actively, consuming energy in the process

- The mechanistic understanding of *cell crawling* has been described in various successful model based on:
  Actin Polymerization
  Myosin contractility
- Some cells can move also without substrate adhesion
  Recent experimental results suggest the possibility of motion solely guided buy myosin contraction[1]
  Our goal is to provide a model and a mechanism for cell motility in bulk both minimal and generic

[1] H. Kelleret al 2002

Active force



Interaction therm

$$F_{int,\alpha} = F_{active,\alpha} + \partial_\alpha p^i - \partial_\beta \Pi_{\alpha\beta}$$

Pressure tensor for van der Waals fluid

$$\Pi_{\alpha\beta} = \left[p^w - k\rho\nabla^2\rho - \frac{k}{2}(\nabla\rho)^2\right]\delta_{\alpha\beta} + k\partial_\alpha\rho\partial_\beta\rho$$

Active force

$$F_{active,\alpha} = -\zeta\partial_\alpha\phi$$

Free energy model

Free energy

$$\mathcal{F} = \int dr \left\{ WD + \frac{1}{2}\phi^2 - b(\rho - \rho_{av})\phi^2 + k(\nabla\phi)^2 + c\phi(\nabla\rho)^2 \right\}$$

Dynamics equations

$$\partial_t(\rho u_\alpha) + \partial_\beta(\rho u_\alpha u_\beta) = -\partial_\alpha p^i + F_{int,\alpha} + \partial_\beta\left[\eta(\partial_\alpha u_\beta + \partial_\beta u_\alpha)\right]$$

$$\partial_t\phi + \partial_\alpha(\phi u_\alpha) = \Gamma\nabla^2\left(\frac{\delta\mathcal{F}}{\delta\phi}\right)$$

Free energy model

Free energy

$$\mathcal{F} = \int dr \left\{ WD + \frac{1}{2}\phi^2 - b(\rho - \rho_{av})\phi^2 + k(\nabla\phi)^2 + c\phi(\nabla\rho)^2 \right\}$$

Dynamics equations

$$\partial_t(\rho u_\alpha) + \partial_\beta(\rho u_\alpha u_\beta) = -\partial_\alpha p^i + F_{int,\alpha} + \partial_\beta\left[\eta(\partial_\alpha u_\beta + \partial_\beta u_\alpha)\right]$$

$$\partial_t\phi + \partial_\alpha(\phi u_\alpha) = \Gamma\nabla^2\left(\frac{\delta\mathcal{F}}{\delta\phi}\right)$$

Our LB simulations in 2D show contractility alone is able to catch the origin of cell motility

Model for active polar emulsion

Free energy functional

$$
\begin{aligned}
F \quad [\phi, \mathbf{P}] &= \int d\mathbf{r} \, \{ \frac{a}{4\phi_{cr}^4} \phi^2 (\phi - \phi_0)^2 + \frac{k}{2} \left| \nabla \phi \right|^2 + \frac{c}{2} (\nabla^2 \phi)^2 \\
- \quad & \frac{\alpha}{2} \frac{(\phi - \phi_{cr})}{\phi_{cr}} \left| \mathbf{P} \right|^2 + \frac{\alpha}{4} \left| \mathbf{P} \right|^4 + \frac{\kappa}{2} (\nabla \mathbf{P})^2 + \beta \mathbf{P} \cdot \nabla \phi \}
\end{aligned}
$$

Model for active polar emulsion

Free energy functional

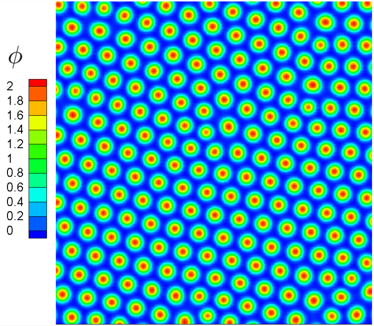
$$
\begin{aligned}
F \quad [\phi, \mathbf{P}] &= \int d\mathbf{r}\, \{ \frac{a}{4\phi_{cr}^4}\phi^2(\phi-\phi_0)^2 + \frac{k}{2}\left|\nabla\phi\right|^2 + \frac{c}{2}(\nabla^2\phi)^2 \\
- \quad & \frac{\alpha}{2}\frac{(\phi-\phi_{cr})}{\phi_{cr}}\left|\mathbf{P}\right|^2 + \frac{\alpha}{4}\left|\mathbf{P}\right|^4 + \frac{\kappa}{2}(\nabla\mathbf{P})^2 + \beta\mathbf{P}\cdot\nabla\phi \}
\end{aligned}
$$

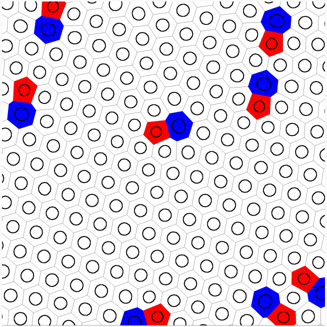
Dynamics equations

$$
\begin{aligned}
\rho\left(\frac{\partial}{\partial t} + \mathbf{v}\cdot\nabla\right)\mathbf{v} &= -\nabla p + \nabla\cdot\underline{\underline{\sigma}}^{total}\ , \quad \sigma_{\alpha\beta}^{active} = -\zeta\phi\left(P_\alpha P_\beta - \frac{1}{3}|\mathbf{P}|^2\delta_{\alpha\beta}\right) \\
\frac{\partial\phi}{\partial t} + \nabla\cdot(\phi\mathbf{v}) &= \nabla\cdot\left(M\nabla\frac{\delta F}{\delta\phi}\right) \\
\frac{\partial\mathbf{P}}{\partial t} + (\mathbf{v}\cdot\nabla)\,\mathbf{P} &= -\underline{\underline{\Omega}}\cdot\mathbf{P} + \xi\underline{\underline{D}}\cdot\mathbf{P} - \frac{1}{\Gamma}\frac{\delta F}{\delta\mathbf{P}},
\end{aligned}
$$

Passive Emulsion

Asymmetric emulsion (10:90) **In absence of activity**

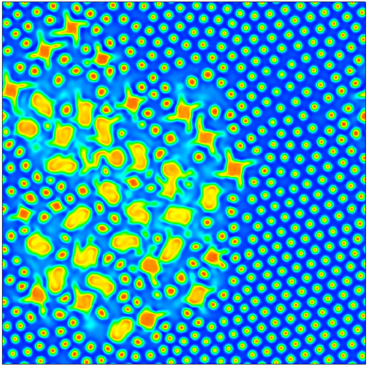




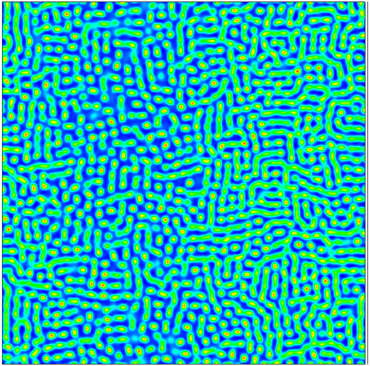
Hexatic order

Morphology of active polar emulsion

Activity greatly effects the morphology of the emulsion[2]



Extensile activity $\zeta = 0.0080$



Contractile activity $\zeta = -0.02$

[2] *G.Negro et al., Submitted to Physica A*

Future perspectives

Future perspectives

Liquid-Vapor phase separation

- Systems of size $L \geq 512$ (Parallel version of our LB scheme)
- New LB scheme in order to consider quenches at lower temperatures

Active Liquid-Vapor and Active Mixtures

- Extend the study to $d = 3$ in order to compare our results with real systems and study changes in cell shape
- 3D Active Emulsions

- **Flowing matter 2017**, Porto, Poster contribution.
- **FPSP 2018**, Bruneck: International summer school in Foundamental problems in Statistical Physics.

Esami sostenuti:

- C++ del Prof. Cafagna (Superato)
- Programming with Python Prof. Diacono (Superato)
- Inglese Prof. White (Superato)
- Progettazione europea Prof. D'orazio (Superato)
- Renormalization of field theories Prof. Defazio (Superato)
- Linear stability analysis Prof. Gonnella (Da sostenere)
- Interpolation Methods and techniques for Experimental Data Analysis Prof. Pompili (Superato)
- Processi di Levy Prof. Cufaro (Da sostenere)

Morphology and flow patterns in highly asymmetric active emulsions, *G. Negro, L.N. Carenza, P. Digregorio, G. Gonnella,A. Lamura*, **Submitted to Physica A**.