Effect of viscosity contrast on hydrodynamic coarsenning

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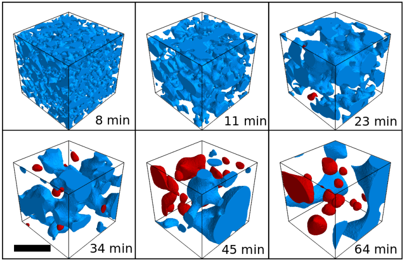
Motivations

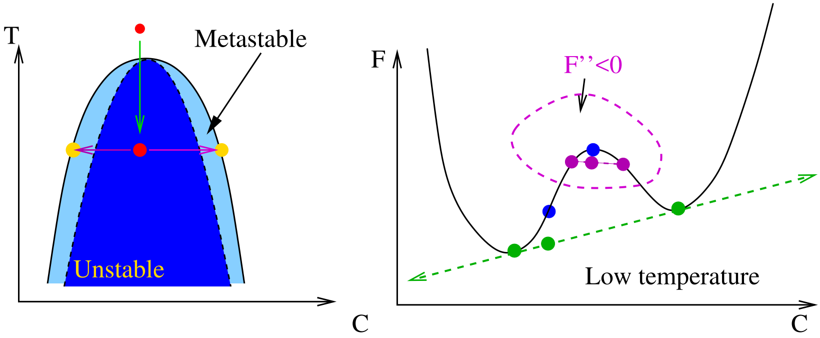
Recent adavances in visualisation techniques and computing.



X-Ray Tomography
Real time observation of 3D structures. D. Bouttes, E. Gouillart, D Vandembrouq

Real space imaging and description of geometrical complexity ?
Effect of the symmetry breaking between the phases in the case of hydrodynamic coarsenning ?
Practical importance : relationship between microstructure and properties

Phase diagramm



- spontaneous phase separation.
- no information about the spatial organization.

Thermodynamics and spatial organisation

Cahn-Hilliard free energy

$$\mathcal{F} = \int \frac{\varepsilon}{2}|\nabla c|^2 + A(c^2(c-1)^2)$$

A>0. Initial composition $c_0 = 0.5$. Double tangent is at $c = 0,\ 1$.

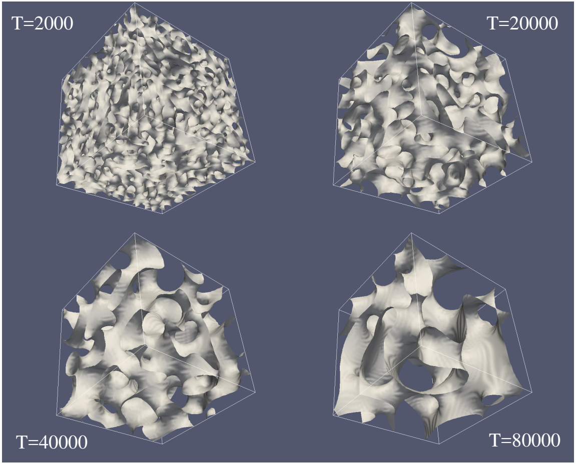
Initial pattern :

Long wavelength favored due to energy
Diffusion favors short wavelength.

initial pattern with short wavelength

Self similar coarsenning

Mechanism that decreases surface energy :



When l is large : flow dominated.

The model equations

Cahn Hilliard

$$\mathcal{F} = \int \frac{\varepsilon}{2}|\nabla c|^2 + A(c^2(c-1)^2) \qquad (1)$$

$$\partial_t C + \mathbf{v}.\nabla c = -\mathrm{div}(+M\nabla\mu), \quad \mu = +\frac{\delta\mathcal{F}}{\delta c} \qquad (2)$$

Navier Stokes

$$\partial_t \mathbf{v} + \nabla\cdot(\mathbf{v}\otimes\mathbf{v}) = \frac{-1}{\rho}(\nabla p + \epsilon\nabla\cdot(\nabla c\otimes\nabla c)) + \nabla\cdot\left(\frac{\nu_{(c)}}{2}(\nabla\mathbf{v}+\nabla\mathbf{v}^T)\right) \qquad (3)$$

$$\nabla\cdot\mathbf{v} = 0 \qquad (4)$$

Motion induced by surface tension.γ. $\nu(c) = \nu_1 c + (1-c)\nu_2$. $VC = \nu_1/\nu_2$.

Numerics

Numerical method

- CH : semi implicit, pseudo-spectral.
- NS : semi implicit, pseudo spectral.
- $div v = 0$: projection on a divergence free field.

details

- mpi-openmp. (Good scaling)
- 512^3 to 1024^3 grids.
- curvatures computed with specific post-processing.
- simulations performed at IDRIS (Turing/ Blue Gene Q)

dimensionless numbers and scaling

A characteristic length l.
Characteristic velocity : balances surface tension and viscosity :
$v_0 = \gamma/(\nu\rho)$ Siggia 1979

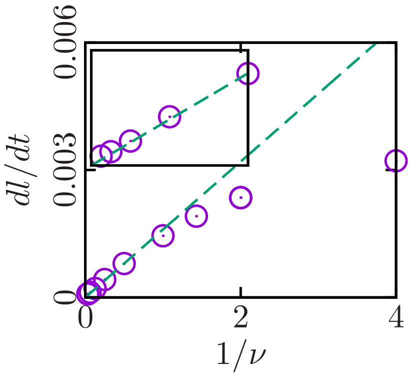
Dimensionless numbers

- Peclet number $Pe = lv_0/D$. Relative importance of diffusive transport vs advection.
- Reynolds number $Re = l/l_0$ with $l_0 = \nu^2/\gamma\rho$. Relative importance of inertial forces vs viscosity.

Non constant during the evolution

What happens to a microstructure when $Pe >> 1$, $Re << 1$?

Isoviscous case : inertial effects



Siggia's prediction :

Constant growth rate of l

$v_0 \propto \gamma/(\nu\rho)$

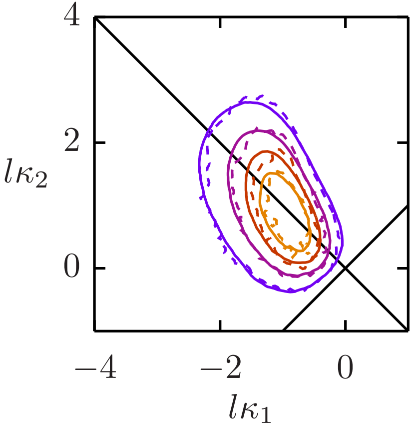
Numerical observation

Valid for $Re < 1$.

Inertial effects are visible earlier than previously estimated (Siggia 79, Kendon 2000).

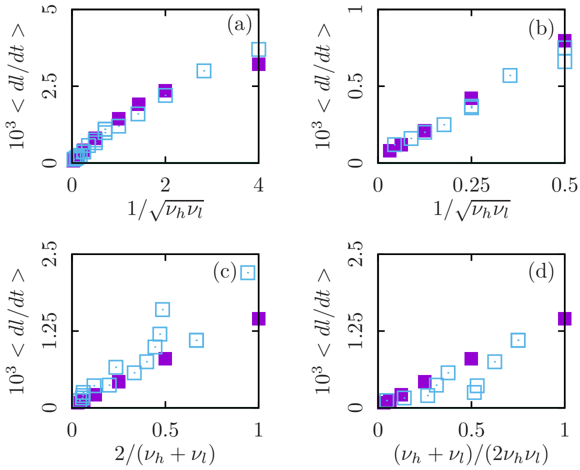
Viscosity contrast effects on the structure

No visible (to the naked eye) effects (not as in experiments) : too small values of VC ?



- Self similarity is preserved.
- Visible effects on the PDFs.
  - Symmetry breaking
  - Significant $\kappa_1\kappa_2 > 0$ region.

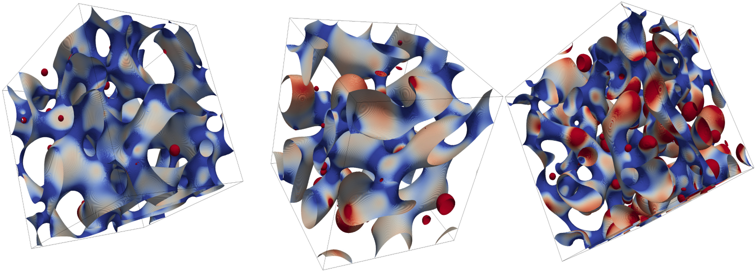
Viscosity contrast and growth velocity



Effective viscosity $\nu_{eff} = \sqrt{\nu_h \nu_l}$

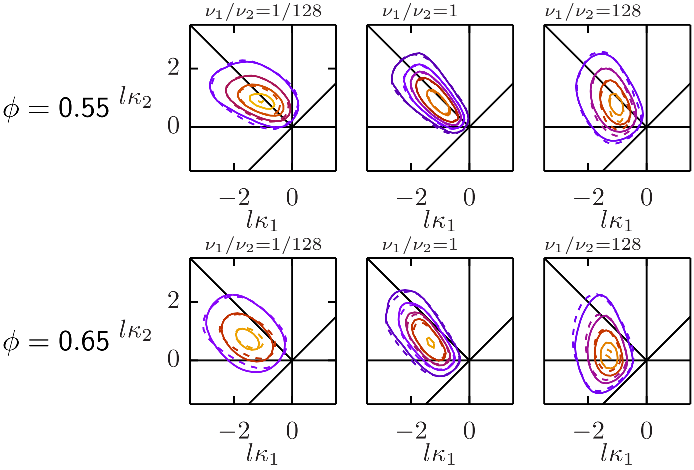
Visible morphological changes ($\phi = 0.7$)

From left to right : decreasing viscoity of minorty phase.

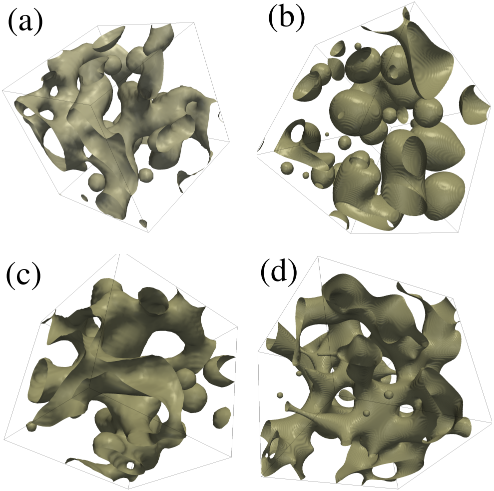


note : bicontinuous structures are relatively easy to obtain up to $\phi = 0.75$.

Self similar cases

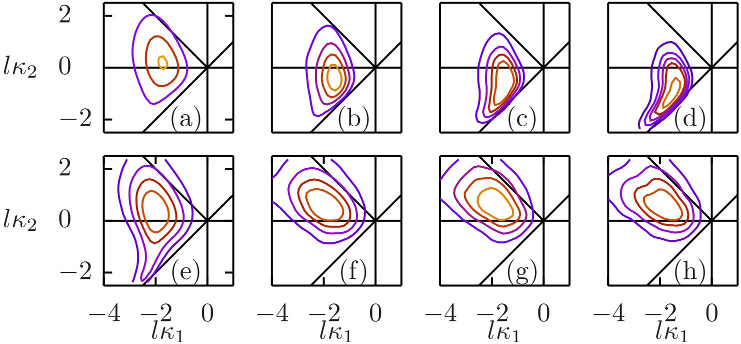


Topological changes. Examples. $\varphi = 0.735$



Effects on the PDF $\varphi = 0.735$

Top : Minorirty (less viscous). Bottom : Minority more viscous.



Minority phase the more viscous $\rightsquigarrow$ Self similarity

Measure the connectivity of the microstructrure

Compute its conductance $\mathcal{G}$. The conductivity is

$$G(c) = 1 \text{ if } c > 0.5\ ,\varepsilon << 1 \text{ otherwise.} \qquad (5)$$

$\rightsquigarrow$ solve

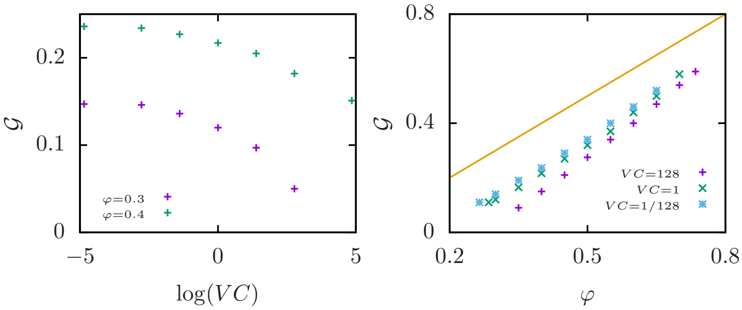
$$0 = \nabla.(G(c)\nabla V) \text{ with } V(z = L) = 1,\ \ V(z = 0) = 0 \qquad (6)$$

Then the flux (independant of z_0)is a measure of the connectivity.

$$\mathcal{G} = \int_{z=z_0} dx\ dy\ \ G(c)\nabla V \qquad (7)$$

Here length scaling by L so that $\varphi = 1 \rightsquigarrow \mathcal{G} = 1$

G vs φ and VC



Conclusions

- Numerical study of the viscous coarsenning
- Confirmation of the self-similar regime predicted by Siggia (1979) in an assymetric case.
- Description of morphological changes induced by symmetry braking.
- For a given ϕ transition from self-similar regime to matrix and inclusions.
- Effective viscosity for mixtures of different mechanical properties.