Phase-field Models and Isogeometric Analysis

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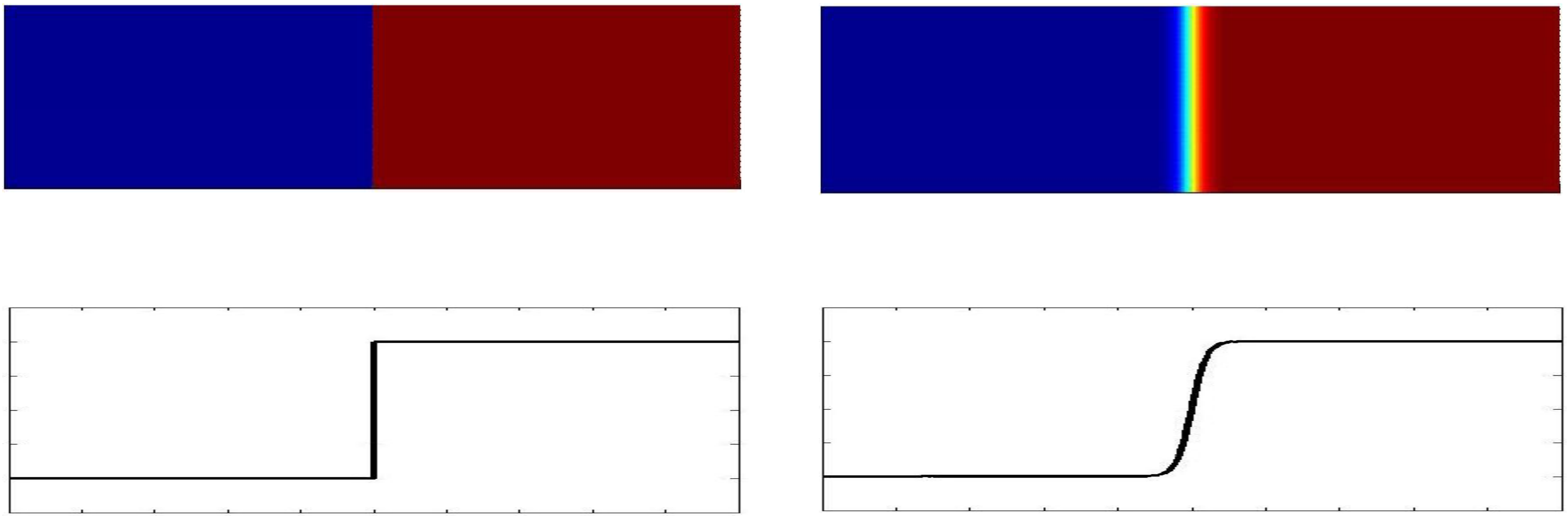
Outline

- Phase-field modeling
- Isogeometric Analysis of phase-field models
  - Navier-Stokes-Korteweg equations
  - Tumor growth equations
- Provably unconditionally stable methods
- Conclusions

Phase-field modeling

- Initiated for phase evolution/transition problems
  - Vaporization and condensation (van der Waals)
  - Phase separation of immiscible fluids (Cahn, Hilliard)
  - Solidification (Kobayashi, Karma, Caginalp)
- Sound mathematics and thermodynamics
- Successfully applied to other phenomena
  - Crack propagation
  - Thin liquid films
  - Porous media flow
  - Cancer growth

Phase-field modeling



Sharp interface

Phase field

Phase-field for phase transition

- Sharp-interface models
  - Partial differential equations of the individual phases are coupled through interface boundary conditions
  - Very difficult numerically

- Phase-field models
  - Sharp interfaces approximated by thin layers described by *higher-order* differential operators
  - All variables are *continuous* across the interface
  - Examples:
    - Navier-Stokes-Korteweg equations
    - Cahn-Hilliard equation

Navier-Stokes-Korteweg equations

- A phase-field model for water/water-vapor two phase flow
- Density is the phase-field parameter
- Simplest model is the isothermal version
- Spatial derivatives of order three
- Very few numerical solutions (see D. Diehl, PhD thesis)

Applications of the NSK equations

- Simulation of cavitating flows
- Simulation of implosion
- Simulation of renal calculi removal by ultrasound
- Simulation of penetrating head injury

Isothermal Navier-Stokes-Korteweg Equations

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \left(\rho u \right) = 0$$

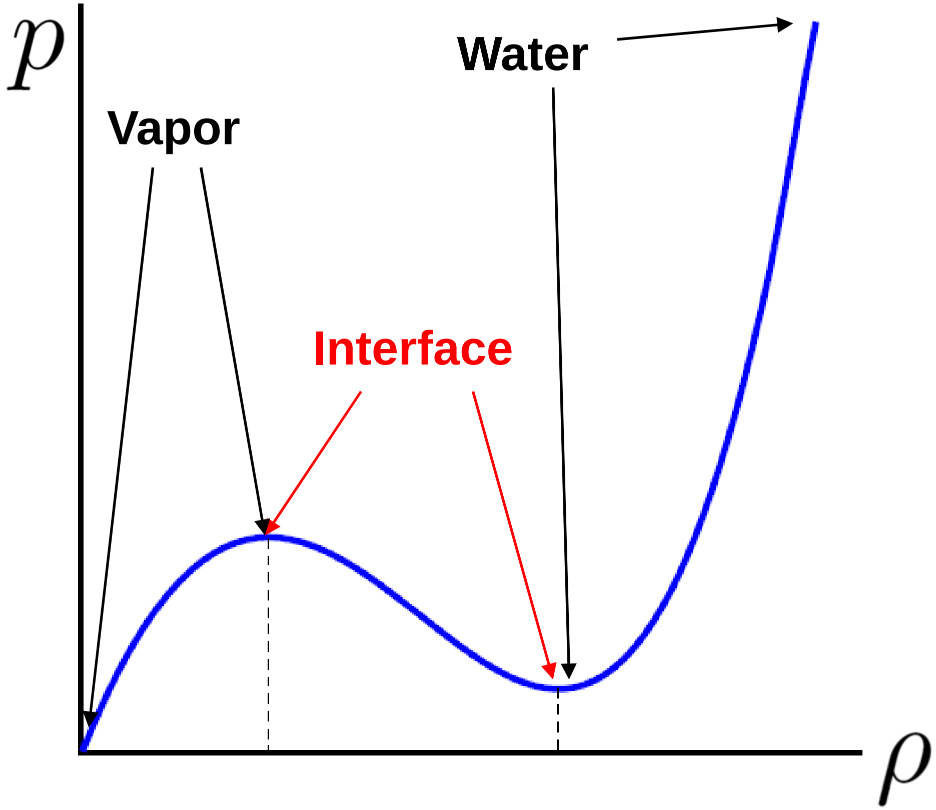
$$\frac{\partial \left(\rho u \right)}{\partial t} + \nabla \cdot \left(\rho u \otimes u \right) + \nabla p - \nabla \cdot \tau - \nabla . \varsigma = 0$$

$$\tau = \overline{\mu} \left(\nabla u + \nabla u^T \right) + \overline{\lambda} \nabla \cdot u \; I$$

$$\zeta = \lambda \left(\rho \Delta \rho + \frac{1}{2} \left| \nabla \rho \right|^2 \right) I - \lambda \nabla \rho \otimes \nabla \rho$$

Isothermal Navier-Stokes-Korteweg Equations

van der Waals equation, 1979



$$p(\rho) = Rb\frac{\rho\theta}{b-\rho} - a\rho^2$$

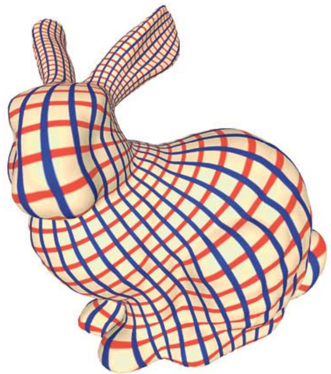
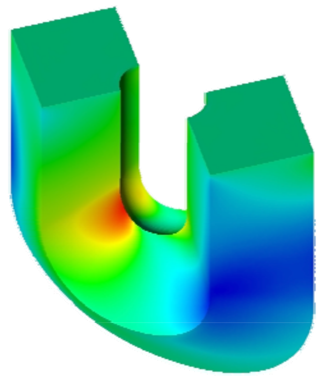
$\theta =$ temperature

Numerical methods for phase-field

- Spatial discretization
  - Spatial derivatives of *higher-order*
  - Need H^2*-conforming* elements or mixed methods
  - Mostly finite differences or spectral methods
  - Isogeometric analysis

Isogeometric Analysis

- Based on technologies (e.g., NURBS) from *computational geometry* used in:
  - Design
  - Animation
  - Graphic art
  - Visualization

- Includes standard FEA as a special case, but offers other possibilities:
  - Precise and efficient geometric modeling
  - Simplified mesh refinement
  - Superior approximation properties
  - *Smooth basis functions with compact support*
  - Ultimately, integration of design and analysis

Isothermal Navier-Stokes-Korteweg Equations

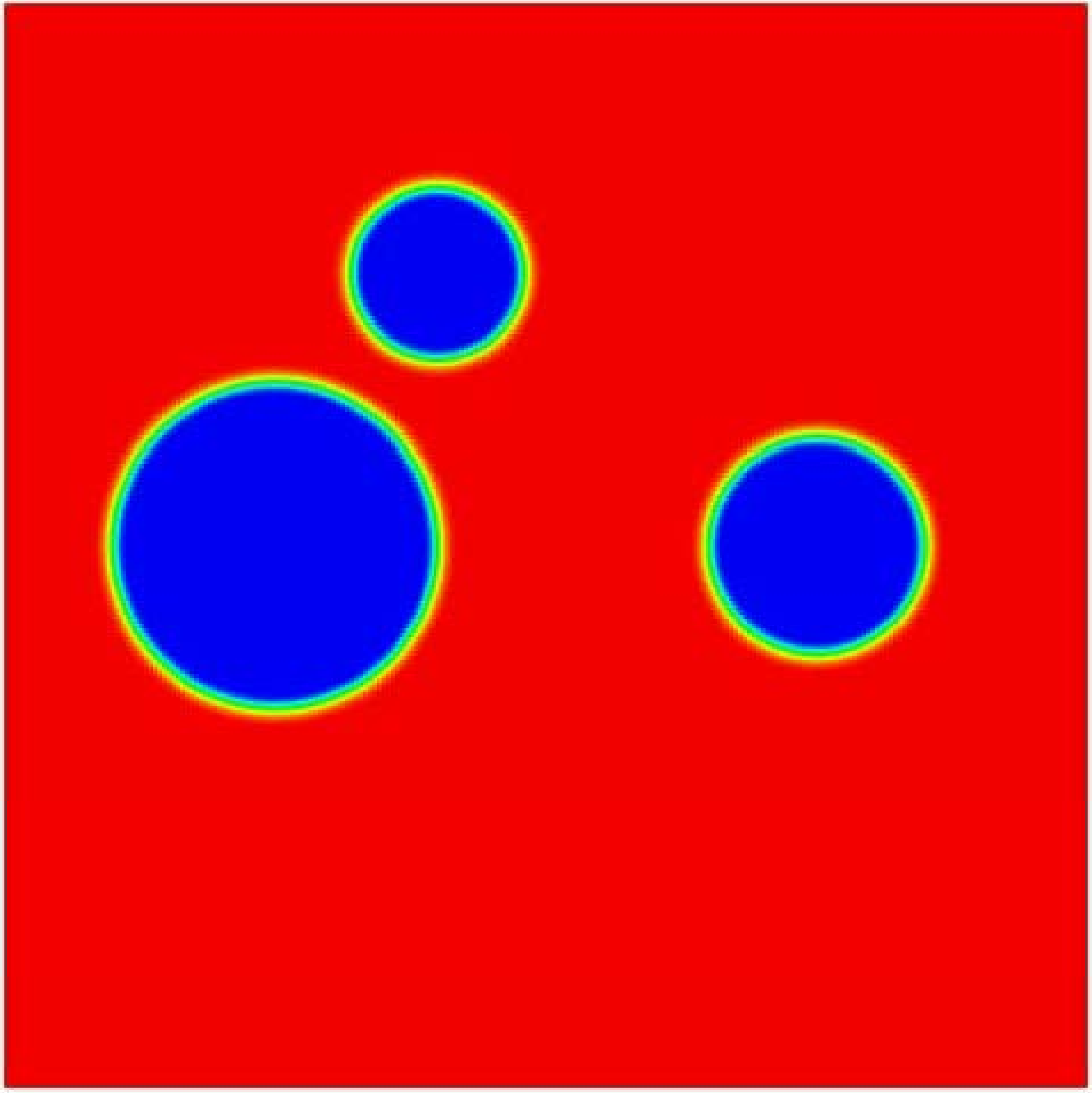
Variational Formulation

Find $U = \{\rho, u\} \in V$ such that $\forall W = \{q, w\} \in V$,

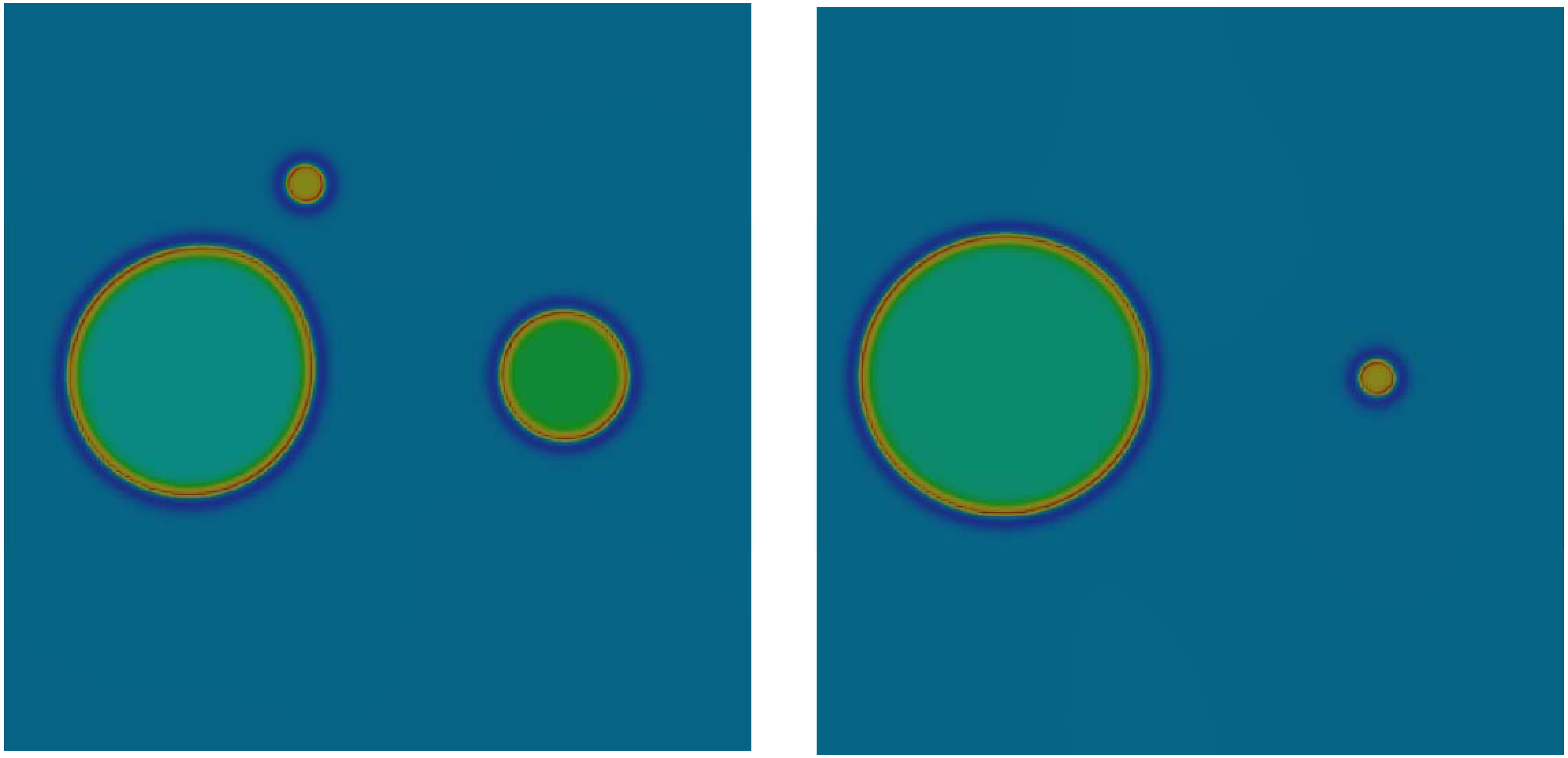
$B(W,U) = 0$ where

$$B(W,U) = \left(q, \frac{\partial \rho}{\partial t}\right)_\Omega + \left(w, u\frac{\partial \rho}{\partial t}\right)_\Omega + \left(w, \rho\frac{\partial u}{\partial t}\right)_\Omega$$
$$-\left(\nabla q, \rho u\right)_\Omega - \left(\nabla w, \rho u \otimes u\right)_\Omega - \left(\nabla \cdot w, p\right)_\Omega + \left(\nabla w, \tau\right)_\Omega$$
$$-\left(\nabla\nabla \cdot w, \lambda\rho\nabla\rho\right)_\Omega - \left(\nabla \cdot w, \lambda\nabla\rho \cdot \nabla\rho\right)_\Omega$$
$$-\left(w, \lambda\nabla\nabla\rho\nabla\rho\right)_\Omega - \left(\nabla w\nabla\rho, \lambda\nabla\rho\right)$$

Unstable equilibrium (256^2)

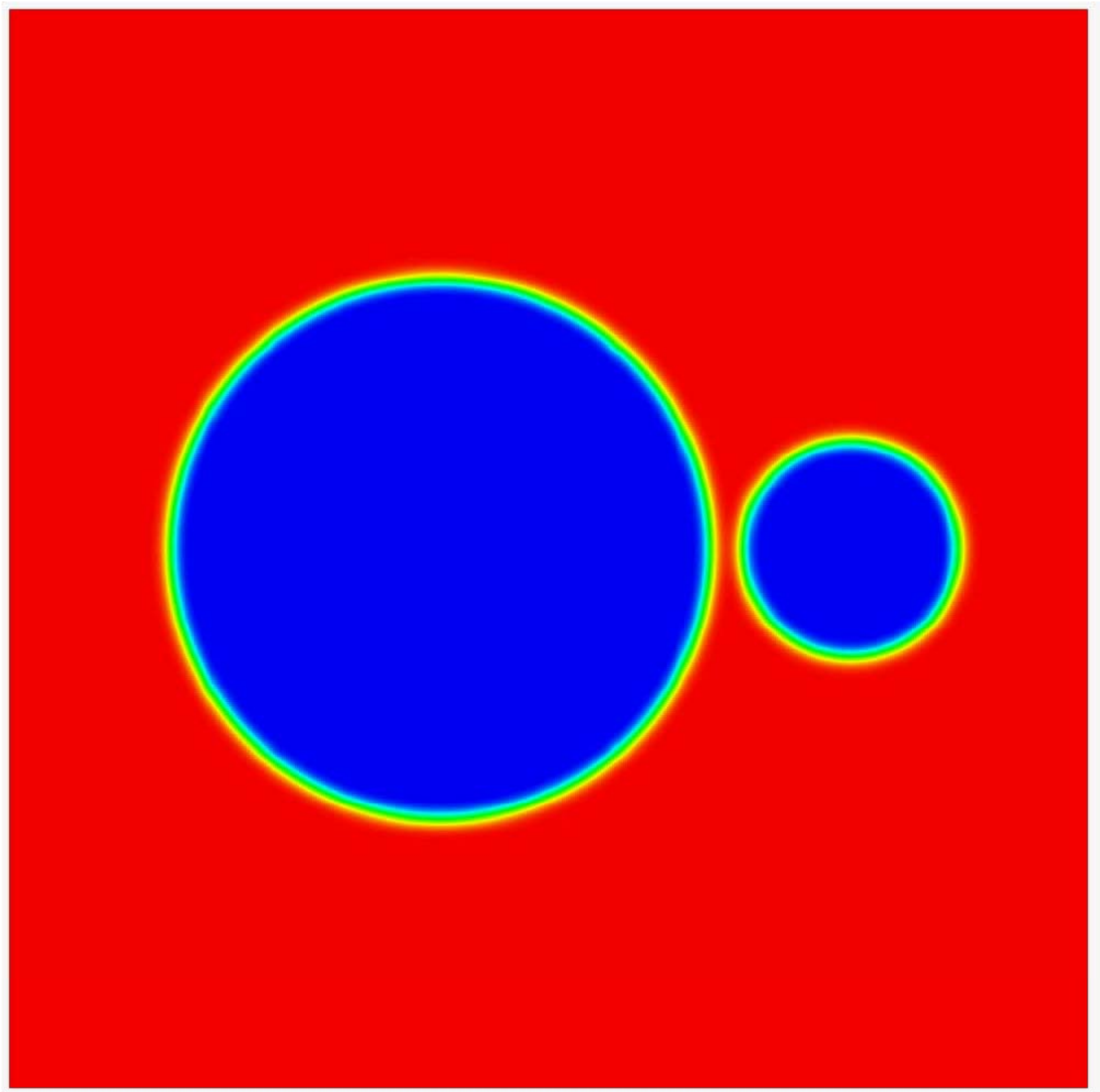


Unstable equilibrium (256^2)

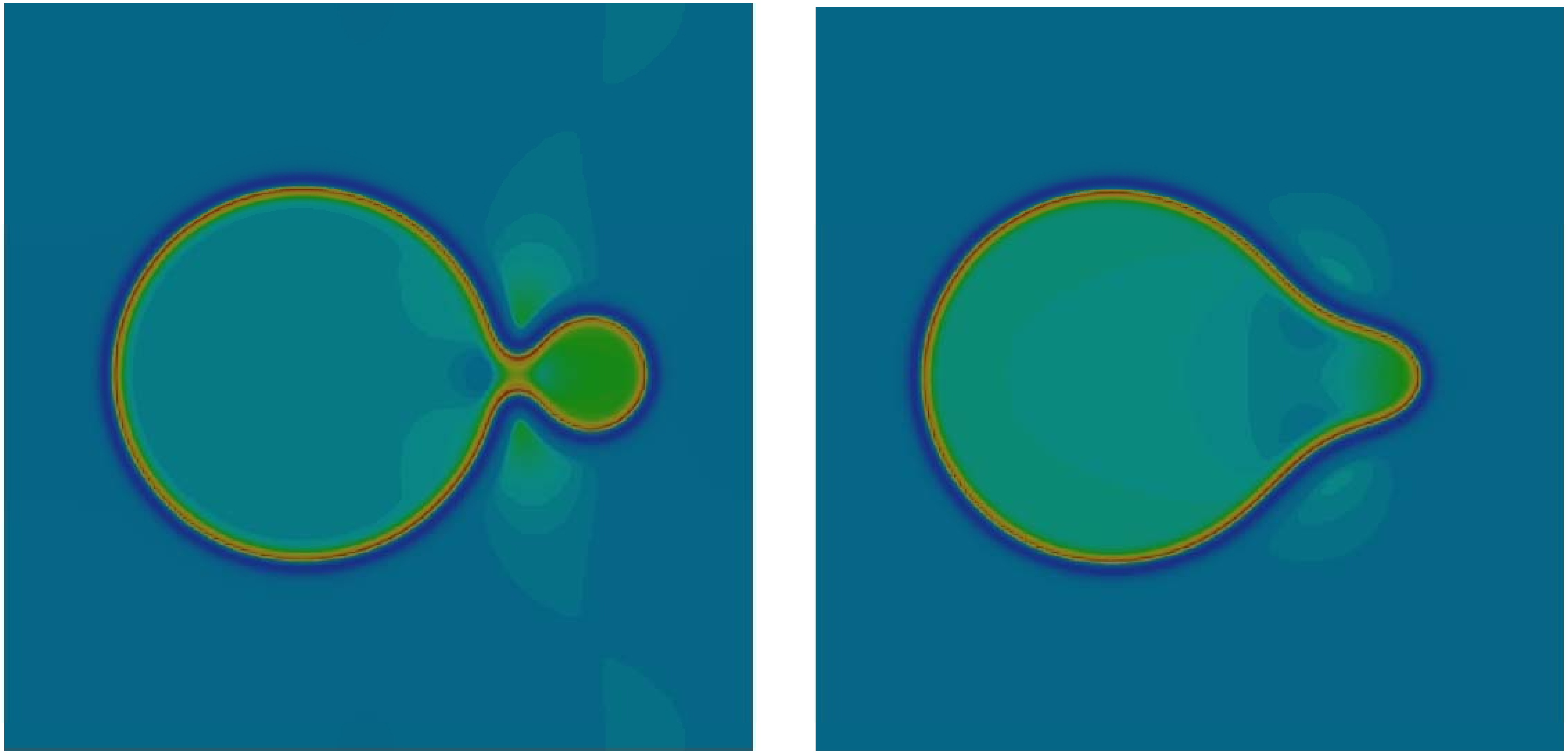


Pressure field

Coalescence (256^2)

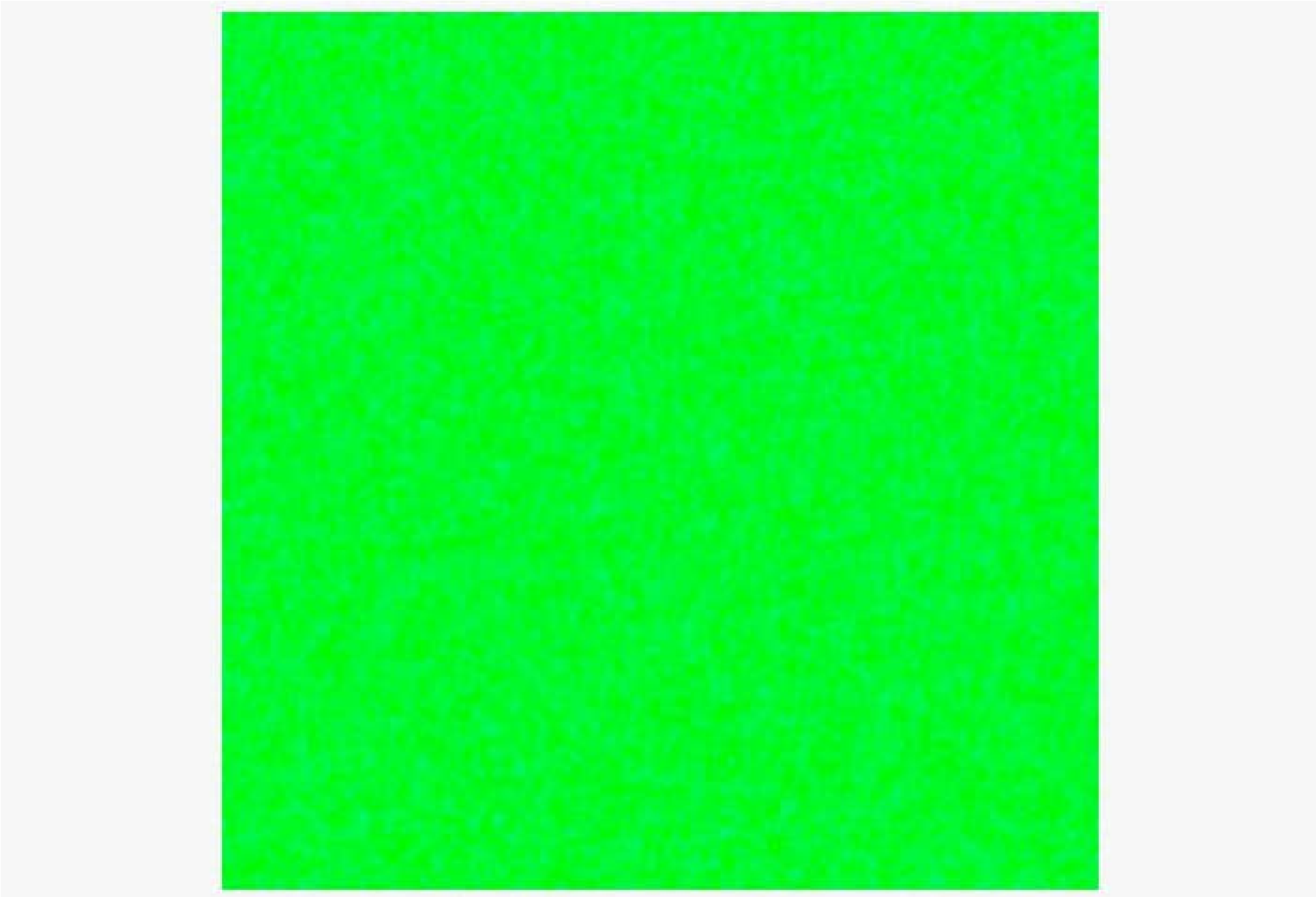


Coalescence (256^2)

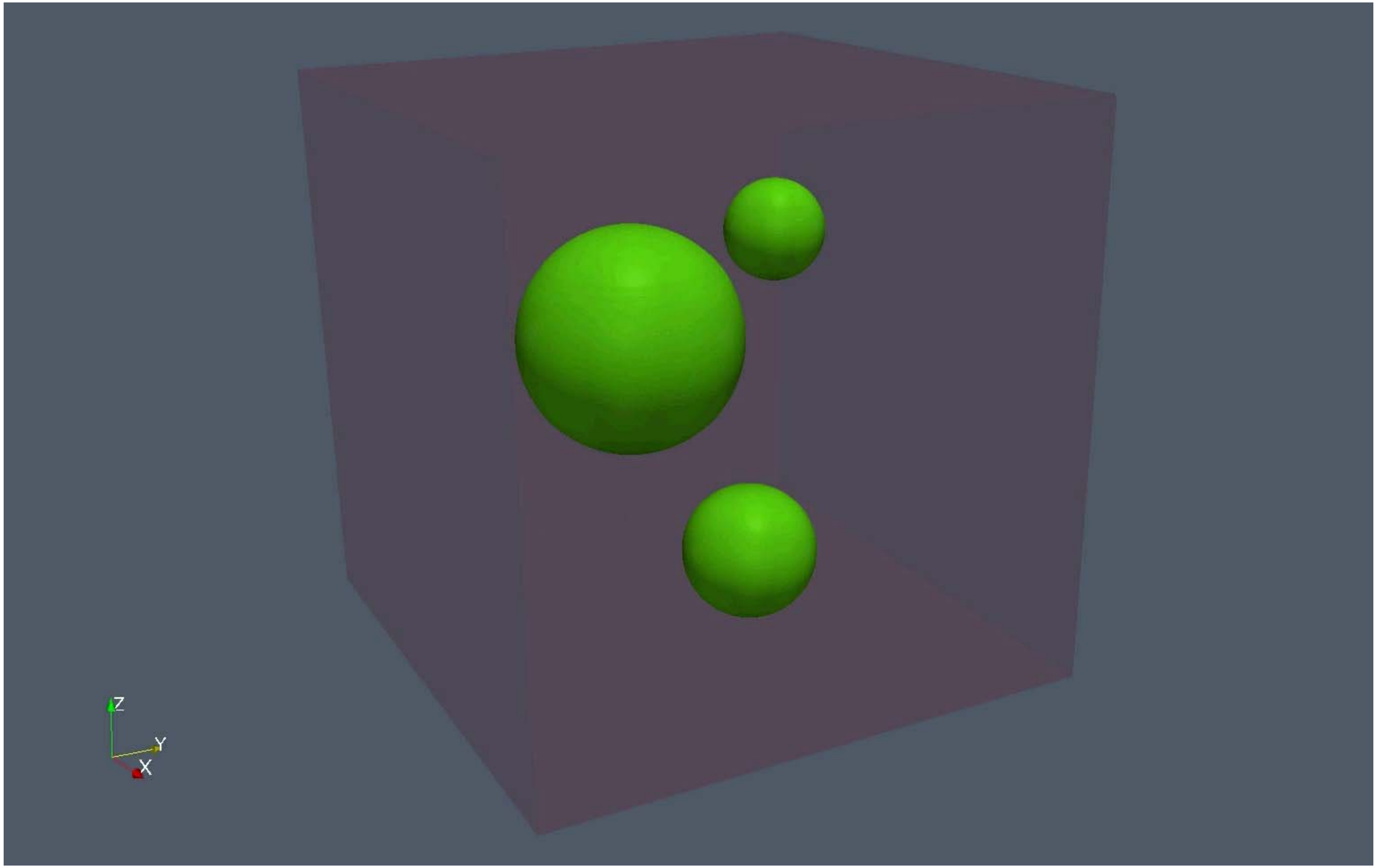


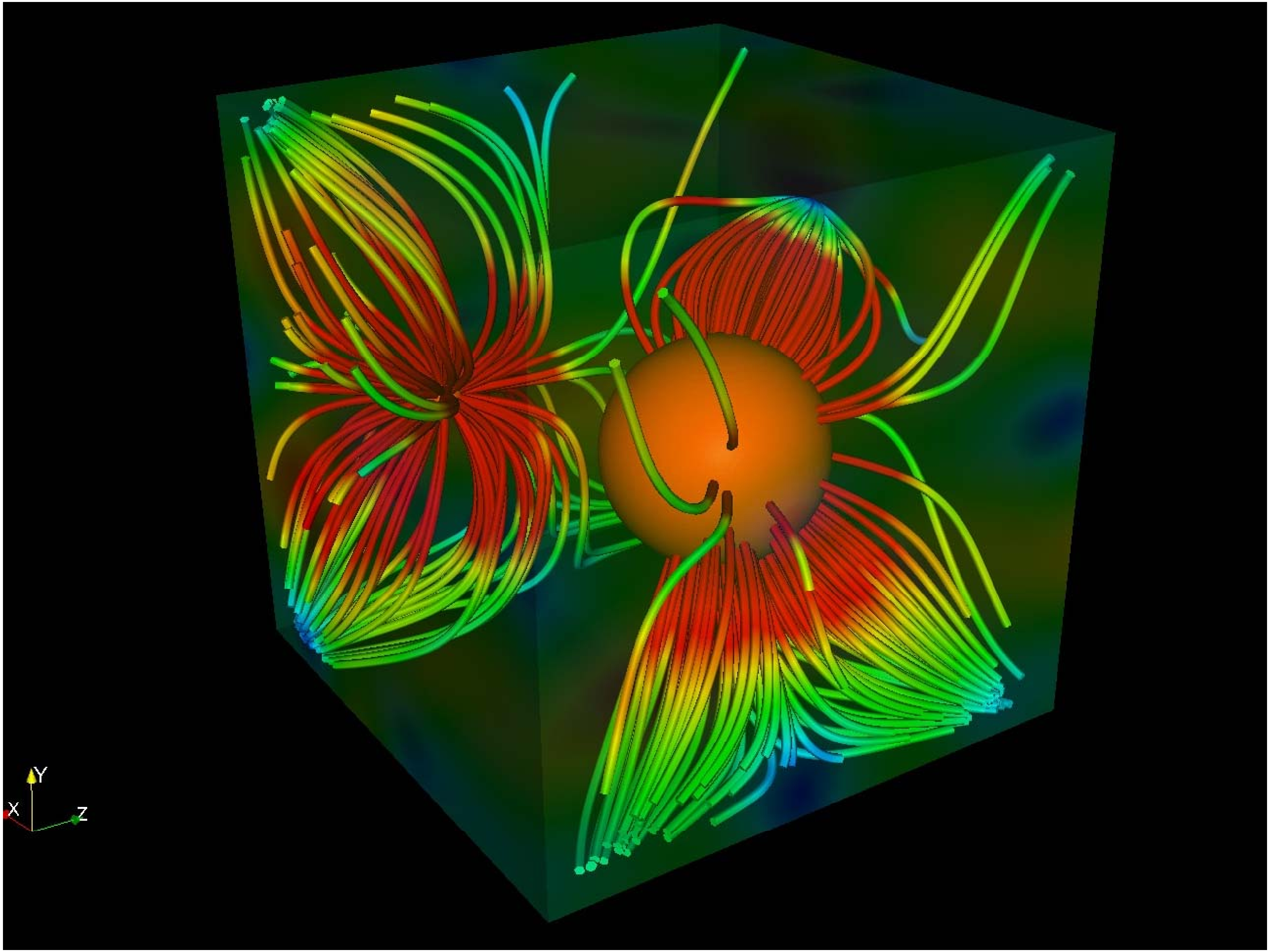
Pressure field

Spinodal decomposition (256^2)



Unstable equilibrium (128^3)





Y
X
Z

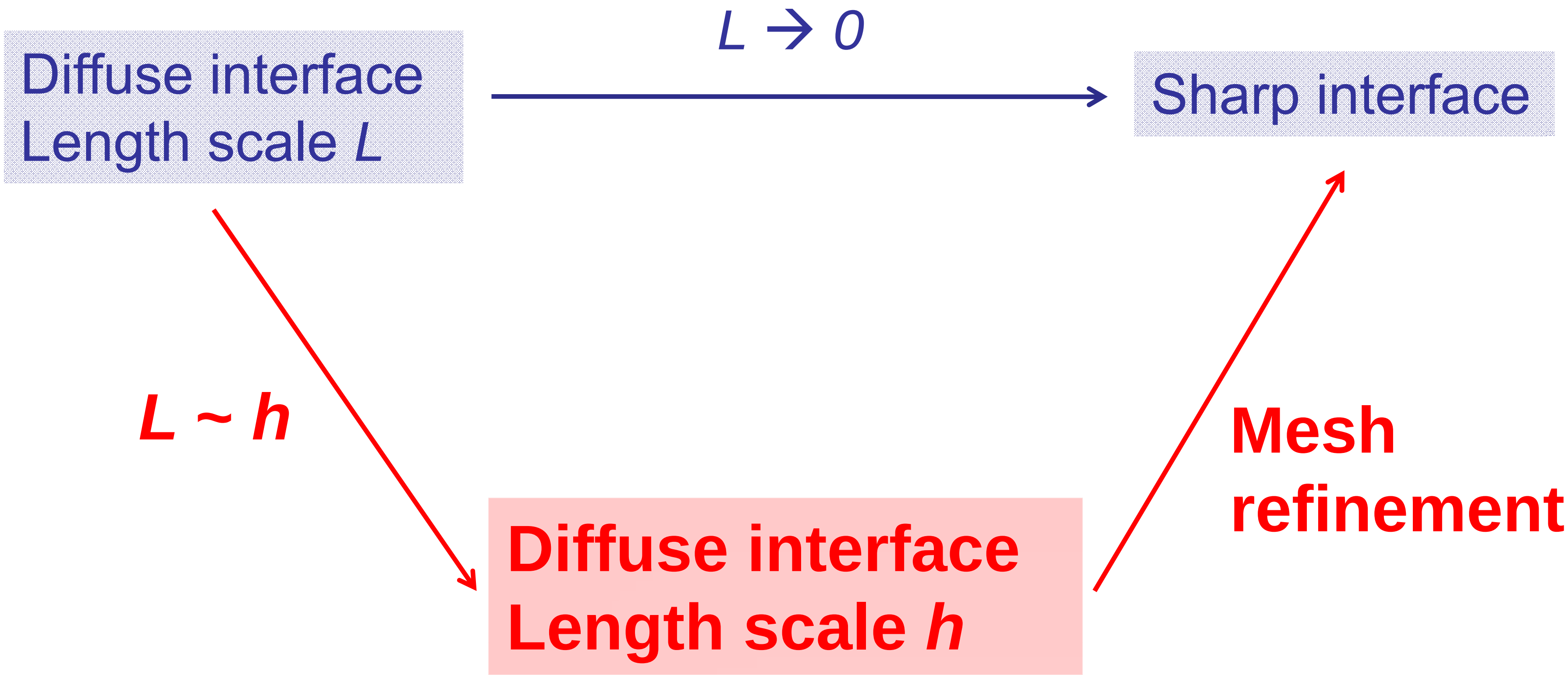
Refinement methodology

Diffuse interface
Length scale *L*

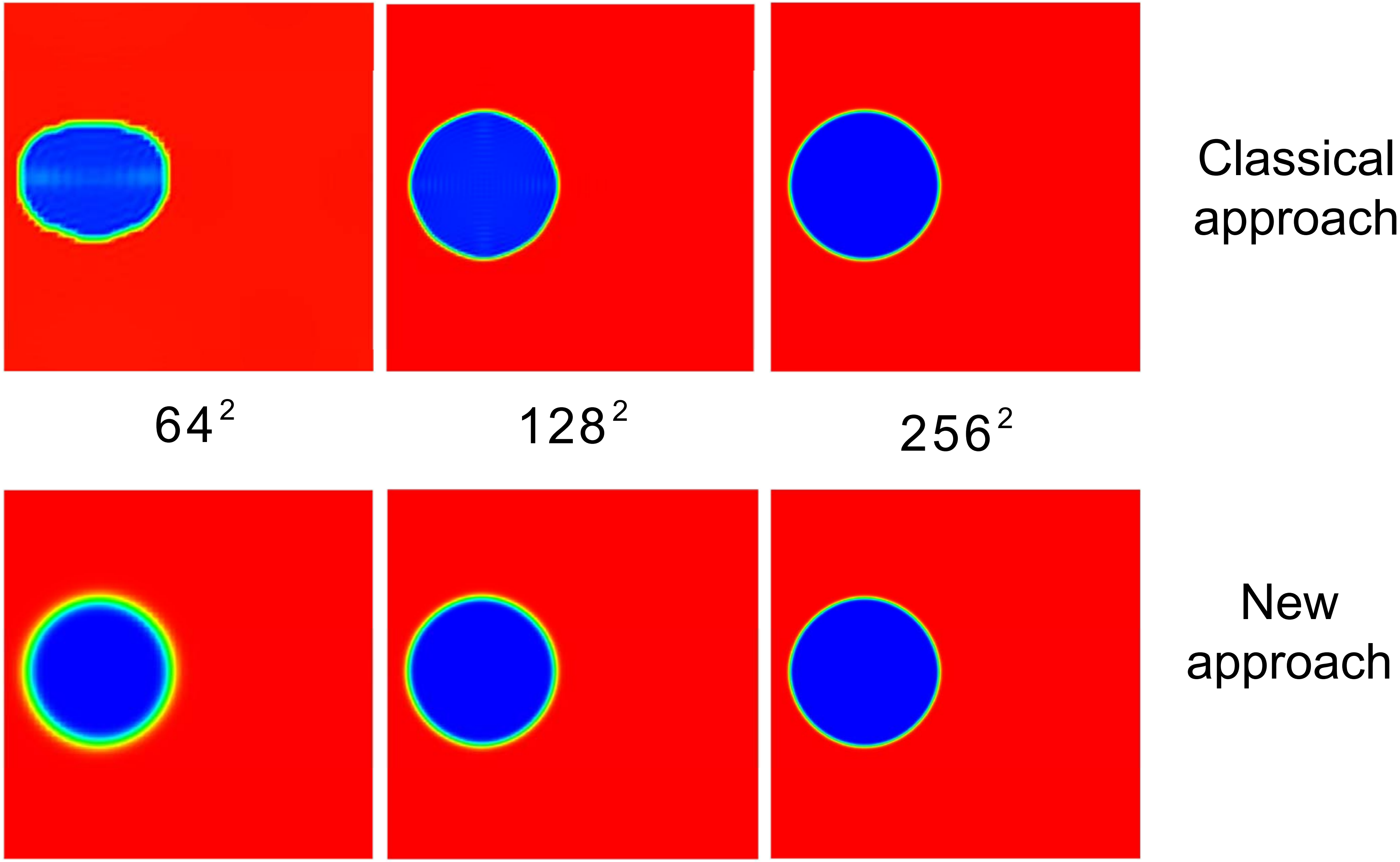
$L \rightarrow 0$

Sharp interface

Refinement methodology



Refinement methodology



Tumor growth simulation

Motivation:

- Second cause of death in the developed world
- It is believed that it will be the first in the 21st century

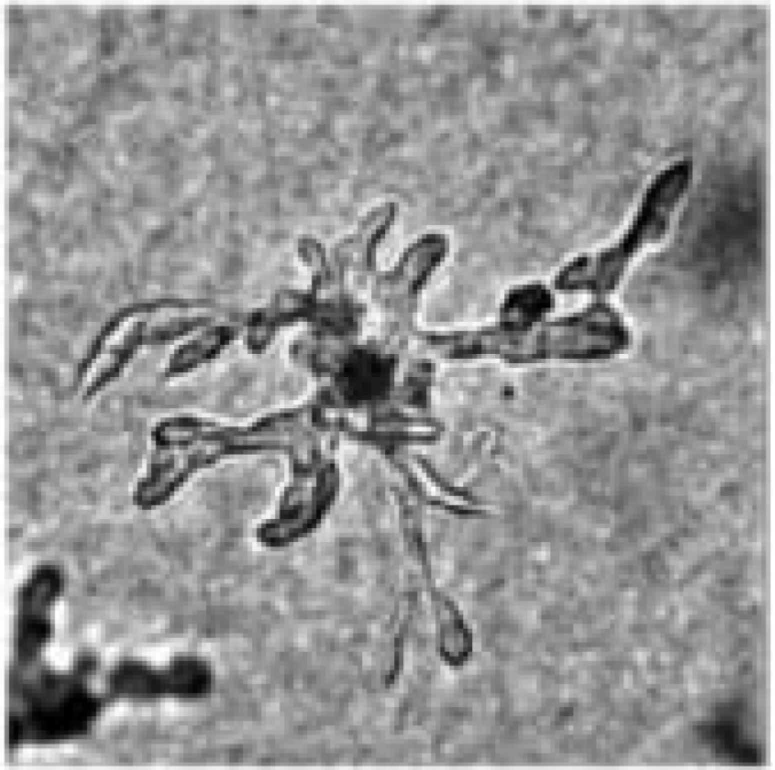
Potential:

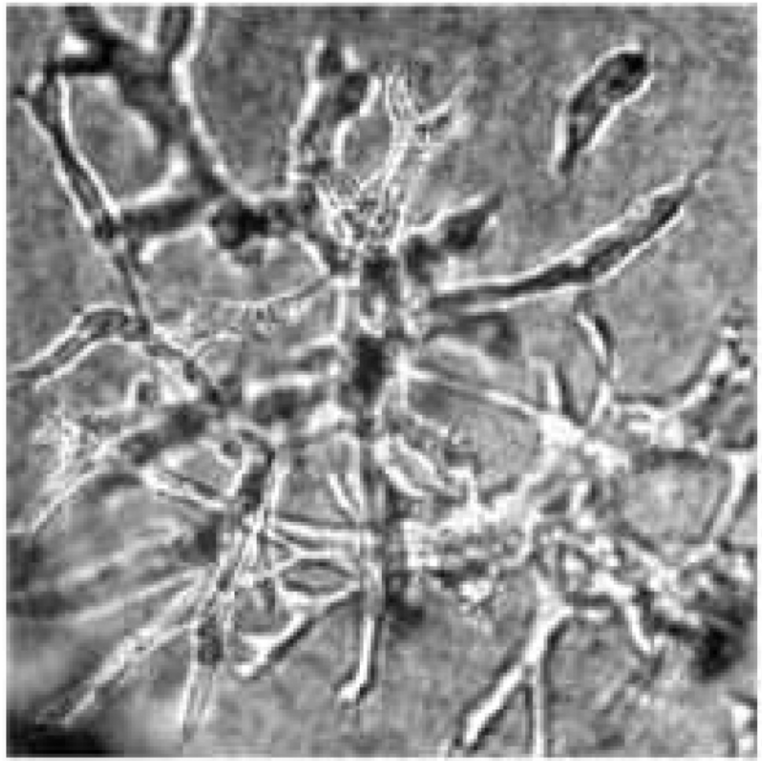
- Prediction of the tumor response for a given therapy
- Design of patient-specific therapies
- Paradigm shift: From *diagnosis* to *prediction*

Tumor growth simulation

- Several continuum theories of avascular tumor growth
- Based on Continuum Mechanics and Mixture Theory
- Nonlinear system of fourth-order PDE's
- V. Cristini *et ál, J. Math. Biol.* **58**:723-763, 2009

Fingered growth





Images obtained from an *in vitro* experiment (Pennacchetti et ál.)

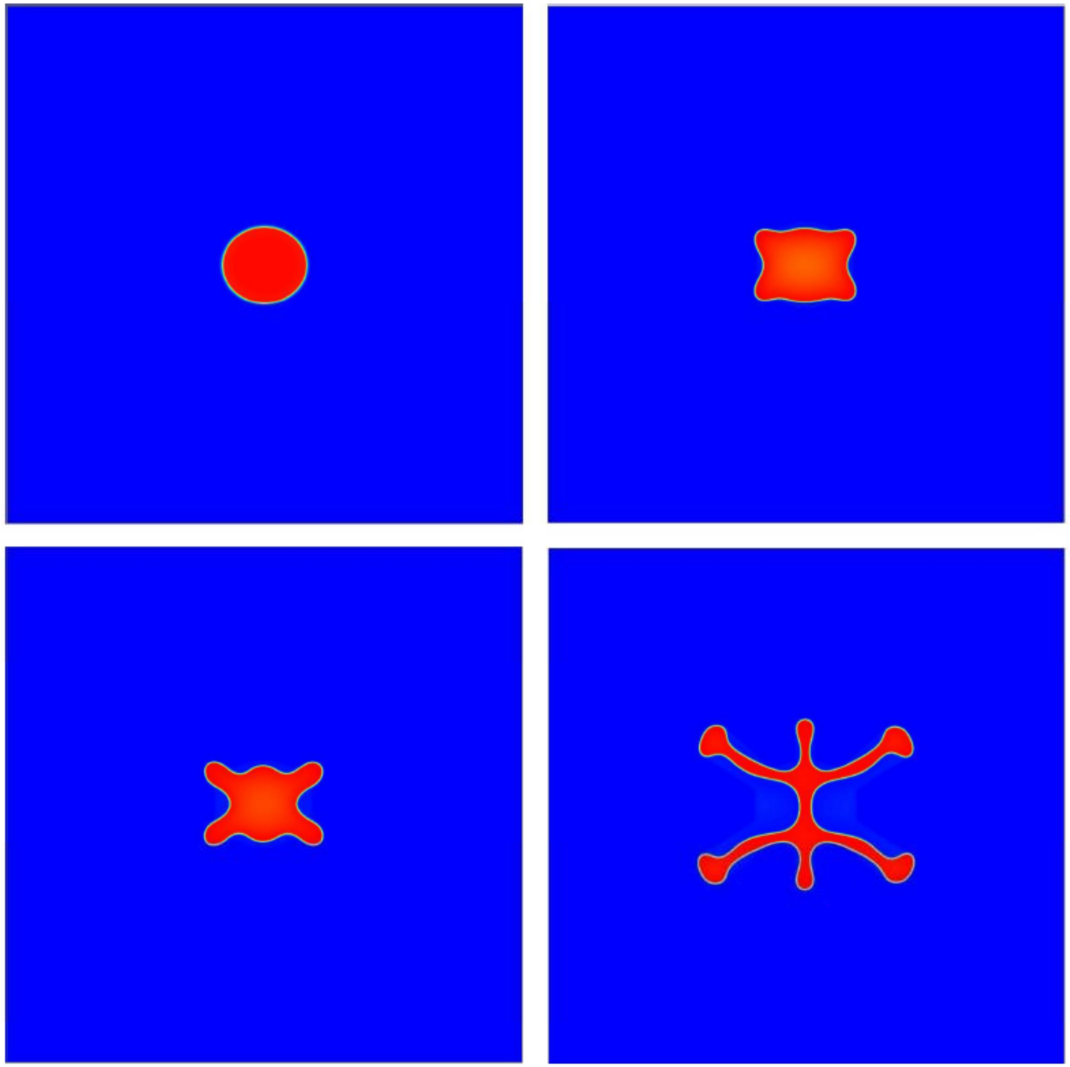
Continuum theories: V. Cristini *et ál.*

$$\frac{\partial \phi}{\partial t} = \nabla.\left(M\nabla\left(\mu - \varepsilon\chi\sigma - \varepsilon^2\Delta\phi\right)\right) + P\sigma\phi - A\phi$$

$$0 = \nabla.\left(D_\sigma(\phi)\nabla\sigma\right) - \sigma\phi$$

- Avascular growth
- Reproduces fingered growth
- Nonlinear system of fourth-order PDE's
- For 2D problems 2048^2 meshes are required

Continuum theories: V. Cristini *et ál.*



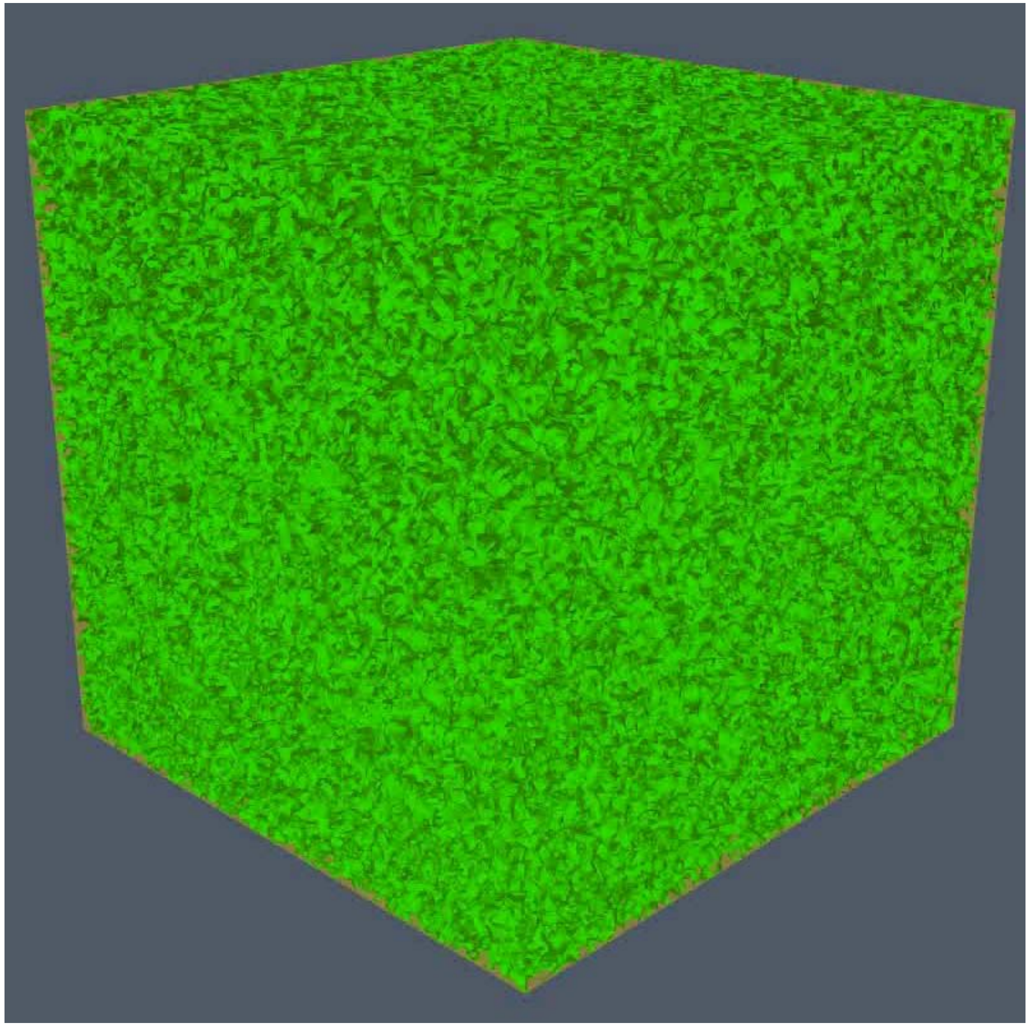
Simulation performed using Isogeometric Analysis (2048^2)

Provably Unconditionally Stable, Second-order Time-Accurate, Mixed Variational Methods for Phase-field Models

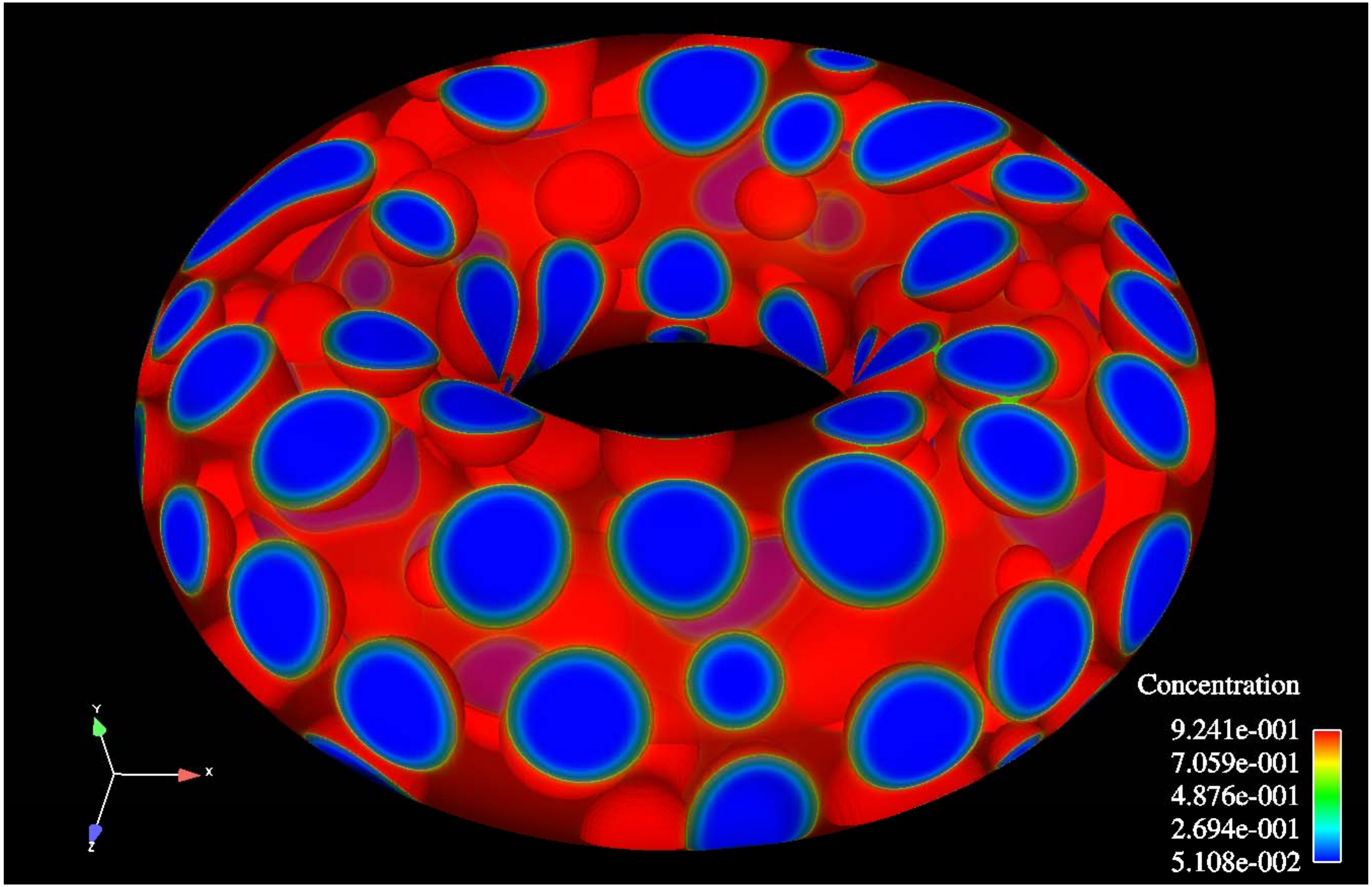
Cahn-Hilliard Equation (1957)

- Applications:
  - Phase segregation of binary alloys
  - Image processing
  - Planet formation
  - Growth of tumors
  - Etc.
- Spatial derivatives of order four

Phase segregation on a cube



Phase segregation on a torus



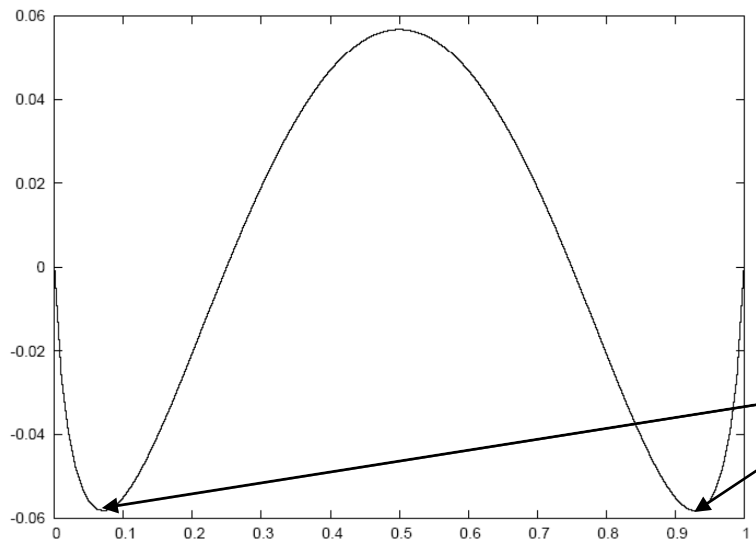
Ginzburg-Landau free-energy (1950)

$$E = \int_{\Omega} \left(\psi(c) + \frac{\lambda}{2} |\nabla c|^2 \right) \mathrm{d}x$$

Chemical energy

Surface energy

$$\psi(c) = NkT(c \log c + (1-c)\log(1-c)) + N\omega c(1-c)$$



Double well potential

Binodal points

Cahn-Hilliard Equation

Ginzburg-Landau free energy:

$$E = \int_{\Omega} \left(\psi(c) + \frac{\lambda}{2} |\nabla c|^2 \right) \mathrm{d}x$$

Conservation of mass:

$$\frac{\partial c}{\partial t} + \nabla \cdot J = 0$$

Dissipation of the free energy:

$$\frac{dE}{dt} \leq 0$$

Cahn-Hilliard Equation

Dynamics driven by variational derivative of energy:

$$J = -M_c \nabla \left(\frac{\delta E}{\delta c} \right), \qquad \frac{\delta E}{\delta c} = \mu_c - \lambda \Delta c, \qquad \mu_c = \psi'(c)$$

Cahn-Hilliard equation:

$$\frac{\partial c}{\partial t} = \nabla \cdot \left(M_c \nabla \left(\mu_c - \lambda \Delta c \right) \right),$$

$$M_c = Dc(1-c), \ \lambda \text{ const.}$$

Notion of Stability

Cahn-Hilliard equation:

$$\frac{\partial c}{\partial t} = \nabla \cdot \left(M_c \nabla \left(\mu_c - \lambda \Delta c \right) \right),$$

Ginzburg-Landau free energy:

$$E = \int_{\Omega} \left(\psi(c) + \frac{\lambda}{2} \left| \nabla c \right|^2 \right) \mathrm{d}x$$

Stability

$$\frac{dE}{dt} = -\int_{\Omega} \nabla \left(\frac{\delta E}{\delta c} \right) M_c \nabla \left(\frac{\delta E}{\delta c} \right) dx \;\Rightarrow\; \frac{dE}{dt} \le 0$$

Time integration of Cahn-Hilliard

- Explicit methods necessitate $\Delta t = O(\Delta x^4)$
- Standard implicit methods normally require $\Delta t = O(\Delta x^2)$
- *Unconditionally stable* methods are desired
- *Accuracy* can require Δt vary 10 orders of magnitude
- Time step *adaptivity* is absolutely necessary

Eyre’s Method (1997)

– Provably unconditionally *stable*

– *First-order* time accurate

– *State of the art* in computational phase-field

Eyre's Method (1997)

Cahn-Hilliard equation (Primal strong form):

$$\frac{\partial c}{\partial t} = \nabla \cdot \left(M_c \nabla \left(\mu_c - \lambda \Delta c \right) \right),$$

Cahn-Hilliard equation (Mixed strong form):

$$\frac{\partial c}{\partial t} = \nabla \cdot \left(M_c \nabla v \right)$$

$$v = \mu_c - \lambda \Delta c$$

Cahn-Hilliard equation (Mixed weak form):

$$\left(w, \frac{\partial c}{\partial t} \right) + \left(\nabla w, M_c \nabla v \right) = 0$$

$$(q, v) - (\nabla q, \lambda \nabla c) - (q, \mu_c) = 0$$

Eyre's Method (1997)

Semidiscrete formulation:

$$\left(w^h, \frac{\partial c^h}{\partial t}\right) + \left(\nabla w^h, M_c(c^h)\nabla v^h\right) = 0$$

$$\left(q^h, v^h\right) - \left(\nabla q^h, \lambda \nabla c^h\right) - \left(q^h, \mu_c(c^h)\right) = 0$$

Splitting of the chemical potential:

$$\mu_c(c^h) = \mu_D(c^h) + \mu_P(c^h)$$

$$\mu'_D(c) > 0; \;\; \mu'_P(c) < 0$$

Eyre's Method (1997)

$$\left(w^h, \frac{[\![c_n^h]\!]}{\Delta t} \right) + \left(\nabla w^h, M_c(c_{n+1}^h) \nabla v_{n+1}^h \right) = 0$$

$$\left(q^h, v_{n+1}^h \right) - \left(\nabla q^h, \lambda \nabla c_{n+1}^h \right) - \left(q^h, \mu_D(c_{n+1}^h) + \mu_P(c_n^h) \right) = 0$$

where

$$[\![c_n^h]\!] = c_{n+1}^h - c_n^h$$

- Provably *unconditionally stable*
- *First-order* time accurate

New Method

Semidiscrete formulation:

$$\left(w^h, \frac{\partial c^h}{\partial t}\right) + \left(\nabla w^h, M_c(c^h)\nabla v^h\right) = 0$$

$$\left(q^h, v^h - \mu_c(c^h)\right) - \left(\nabla q^h, \lambda \nabla c^h\right) = 0$$

Splitting of the chemical potential:

$$\mu_c(c^h) = \mu_1(c^h) + \mu_2(c^h)$$

$$\mu_1^{3)}(c) \geq 0; \;\; \mu_2^{3)}(c) \leq 0$$

New Method

$$\left(w^h, \frac{[\![c_n^h]\!]}{\Delta t_n}\right) + \left(\nabla w^h, M_c(c_{n+\alpha}^h)\nabla v_{n+1}^h\right) = 0$$

$$\left(q^h, v_{n+1}^h\right) - \left(\nabla q^h, \lambda \nabla c_{n+\alpha}^h\right) - \left(q^h, \frac{1}{2}\left(\mu_c(c_{n+1}^h) + \mu_c(c_n^h)\right)\right)$$

$$+\left(q^h, \frac{[\![c_n^h]\!]^2}{12}\left(\mu_1^{2)}(c_{n+1}^h) + \mu_2^{2)}(c_n^h)\right)\right) = 0$$

$$\alpha = \frac{1}{2} + \eta; \;\; \eta = \frac{1}{2}\tanh\left(\frac{\Delta t_n}{\delta}\right); \;\; \delta = C\frac{\lambda}{D} \equiv \text{intrinsic time scale}$$

- Provably *unconditionally stable*
- *Second-order* time accurate

Theorem

The *fully discrete* formulation of the new method

(1) Verifies mass conservation $\int c_n^h dx = \int c_0^h dx \ \forall n$

(2) Verifies the stability condition $E(c_{n+1}^h) \leq E(c_n^h) \ \forall n$

(3) Gives rise to a local truncation error bounded as

$$\left|\tau(t_n)\right| \leq K \Delta t_n^2 \ \ \forall t_n \in [0,T]$$

Proof (1)

(1) Verifies mass conservation $\int c_n^h dx = \int c_0^h dx \quad \forall n$

Take $w^h = 1$ in the weak form

Proof (2)

(2) Verifies the stability condition $E(c_{n+1}^h) \leq E(c_n^h)\ \forall n$

Take $w^h = v_{n+1}^h,\ q^h = [\![c_n^h]\!] / \Delta t_n$

Introduce the quadrature formulas

$$\int_a^b f(x)dx = \frac{b-a}{2}\big(f(a)+f(b)\big) - \frac{(b-a)^3}{12} f^{2)}(a) - \frac{(b-a)^4}{24} f^{3)}(\xi);\ \ \xi \in (a,b)$$

$$\int_a^b f(x)dx = \frac{b-a}{2}\big(f(a)+f(b)\big) - \frac{(b-a)^3}{12} f^{2)}(b) + \frac{(b-a)^4}{24} f^{3)}(\varsigma);\ \ \varsigma \in (a,b)$$

Proof (2) cont'd

(2) Verifies the stability condition $E(c_{n+1}^h) \leq E(c_n^h)\ \forall n$

Apply the quadrature formulas to the RHS of

$$\int_{c_n^h}^{c_{n+1}^h} \psi'_k(t)dt = \int_{c_n^h}^{c_{n+1}^h} \mu_k(t)dt$$

to get

$$\frac{[\![\psi_1(c_n^h)]\!]}{[\![c_n^h]\!]} + \frac{[\![c_n^h]\!]^3}{24}\mu_1^{3)}(c_{n+\xi}^h) = \frac{1}{2}\left(\mu_1(c_n^h) + \mu_1(c_{n+1}^h)\right) - \frac{[\![c_n^h]\!]^2}{12}\mu_1^{2)}(c_n^h);\ \xi \in (0,1)$$

$$\frac{[\![\psi_2(c_n^h)]\!]}{[\![c_n^h]\!]} - \frac{[\![c_n^h]\!]^3}{24}\mu_2^{3)}(c_{n+\xi}^h) = \frac{1}{2}\left(\mu_2(c_n^h) + \mu_2(c_{n+1}^h)\right) - \frac{[\![c_n^h]\!]^2}{12}\mu_2^{2)}(c_n^h);\ \zeta \in (0,1)$$

Proof (2) cont'd

(2) Verifies the stability condition $E(c_{n+1}^h) \leq E(c_n^h)\ \forall n$

Simple manipulation yields

$$\frac{[\![E(c^h)]\!]}{\Delta t_n} = -\left(\nabla v_{n+1}^h, M(c_{n+\alpha}^h)\nabla v_{n+1}^h\right)$$

$$-\left(\frac{[\![c_n^h]\!]^4}{24\Delta t_n}, \mu_1^{3)}(c_{n+\xi}^h) - \mu_2^{3)}(c_{n+\zeta}^h)\right)$$

$$-\left(\nabla[\![c_n^h]\!], \frac{\lambda\eta}{\Delta t_n}\nabla[\![c_n^h]\!]\right) \leq 0$$

Proof (3)

(3) Gives rise to a LTE bounded as $\left|\tau(t_n)\right| \leq K\Delta t_n^2$

We compare our method with the midpoint rule

$$\left(w^h, \frac{[\![c_n^h]\!]}{\Delta t_n}\right) + \left(\nabla w^h, M_c(c_{n+1/2}^h)\nabla v_{mid}^h\right) = 0$$

$$\left(q^h, v_{mid}^h\right) - \left(\nabla q^h, \lambda \nabla c_{n+1/2}^h\right) - \left(q^h, \mu_c(c_{n+1/2}^h)\right) = 0$$

Proof (3) cont'd

(3) Gives rise to a LTE bounded as $\left|\tau(t_n)\right| \leq K\Delta t_n^2$

The exact solution does not satisfy the discrete equations, giving rise to the local truncation error

$$\left(w^h, \frac{\left[\!\left[c^h(t_n) \right]\!\right]}{\Delta t_n}\right) + \left(\nabla w^h, M_c(c^h(t_{n+1/2}))\nabla \tilde{v}^h_{mid}\right) = \left(w^h, \tau_{mid}\right)$$

$$\left(q^h, \tilde{v}^h_{mid}\right) - \left(\nabla q^h, \lambda \nabla c^h(t_{n+1/2})\right) - \left(q^h, \mu_c(c^h(t_{n+1/2}))\right) = 0$$

Proof (3) cont'd

(3) Gives rise to a LTE bounded as $|\tau(t_n)| \leq K \Delta t_n^2$

We conclude that

$$\left(q^h, \tilde{v}^h\right) = \left(q^h, \tilde{v}^h_{mid}\right) + \mathrm{O}(\Delta t_n^2)$$

$$\left(w^h, \tau\right) = \left(w^h, \tau_{mid}\right) + \mathrm{O}(\Delta t_n^2)$$

Time-step adaptivity

Let C_n and V_n be the global vectors of dof

Given C_n, V_n and Δt_n

1: Compute C_{n+1}^{BE} using the BE method and Δt_n

2: Compute C_{n+1} using our method and Δt_n

3: Calculate $e_{n+1} = \left\| C_{n+1}^{BE} - C_{n+1} \right\| / \left\| C_{n+1} \right\|$

4: if $e_{n+1} > tol$ then

5: Recalculate the time step $\Delta t_n \leftarrow F(e_{n+1}, \Delta t_n)$

6: goto 1

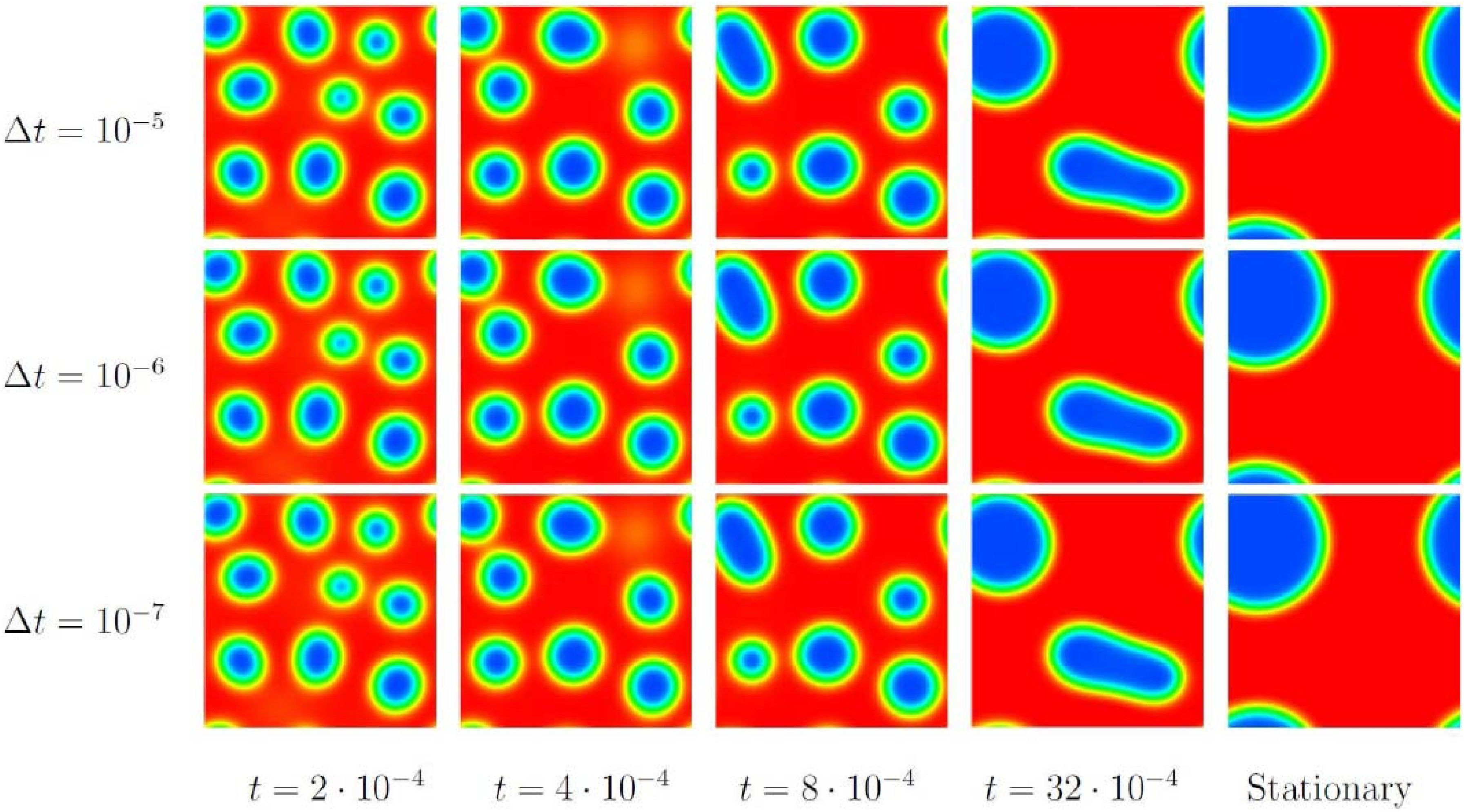
7: else

8: Update the time step $\Delta t_{n+1} = F(e_{n+1}, \Delta t_n)$

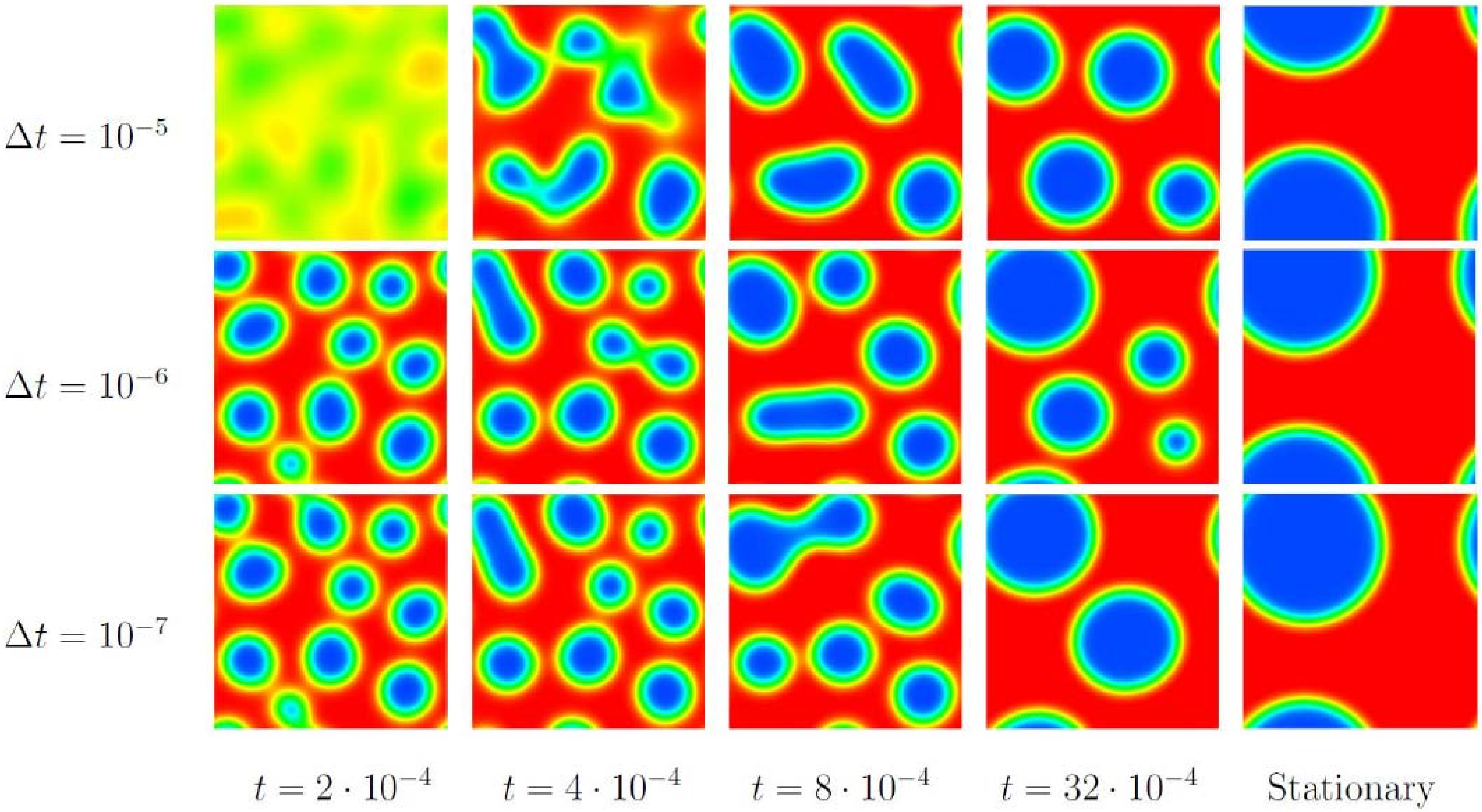
9: continue

10: end if

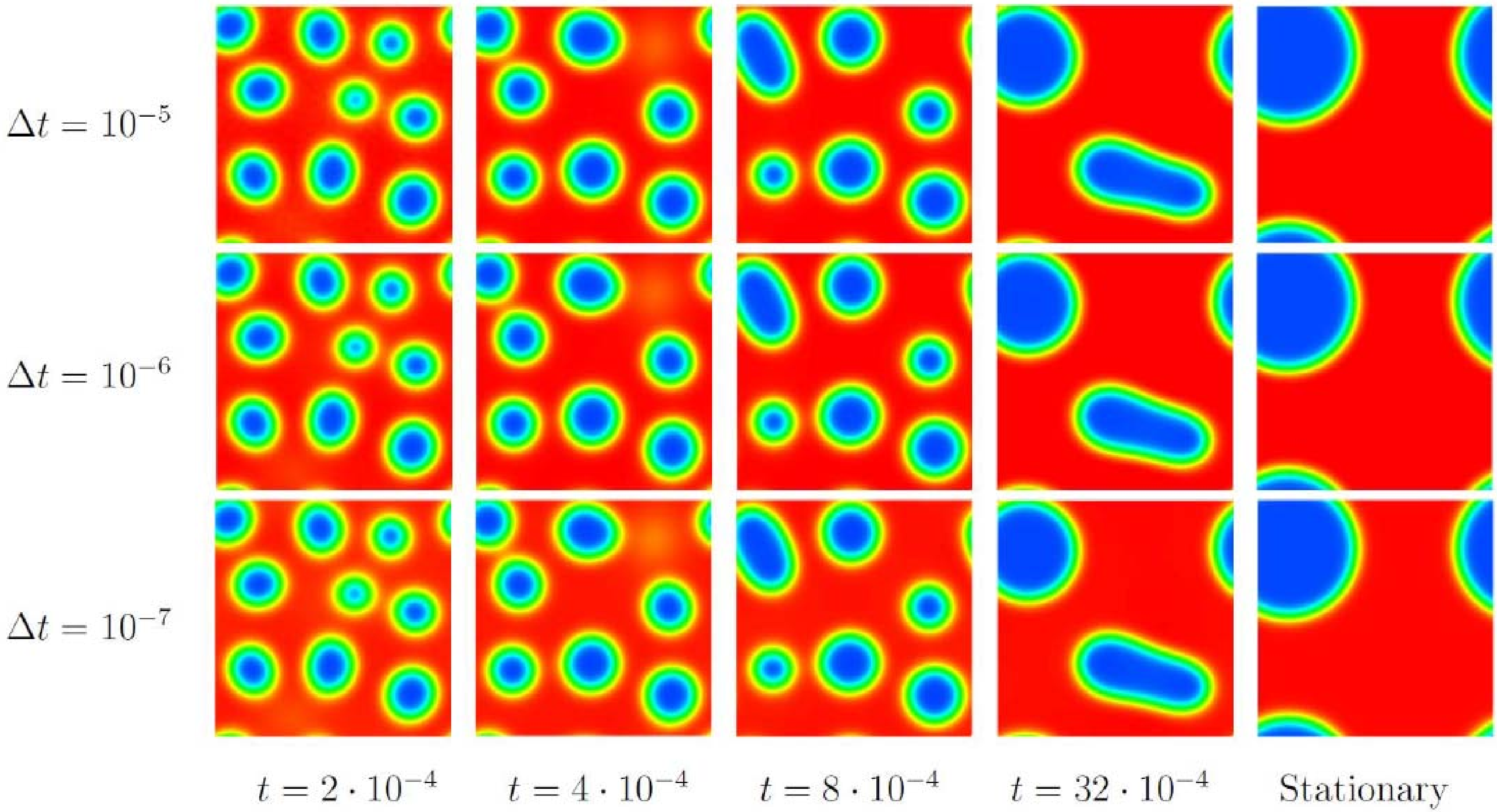
Example 1: Generalized-α



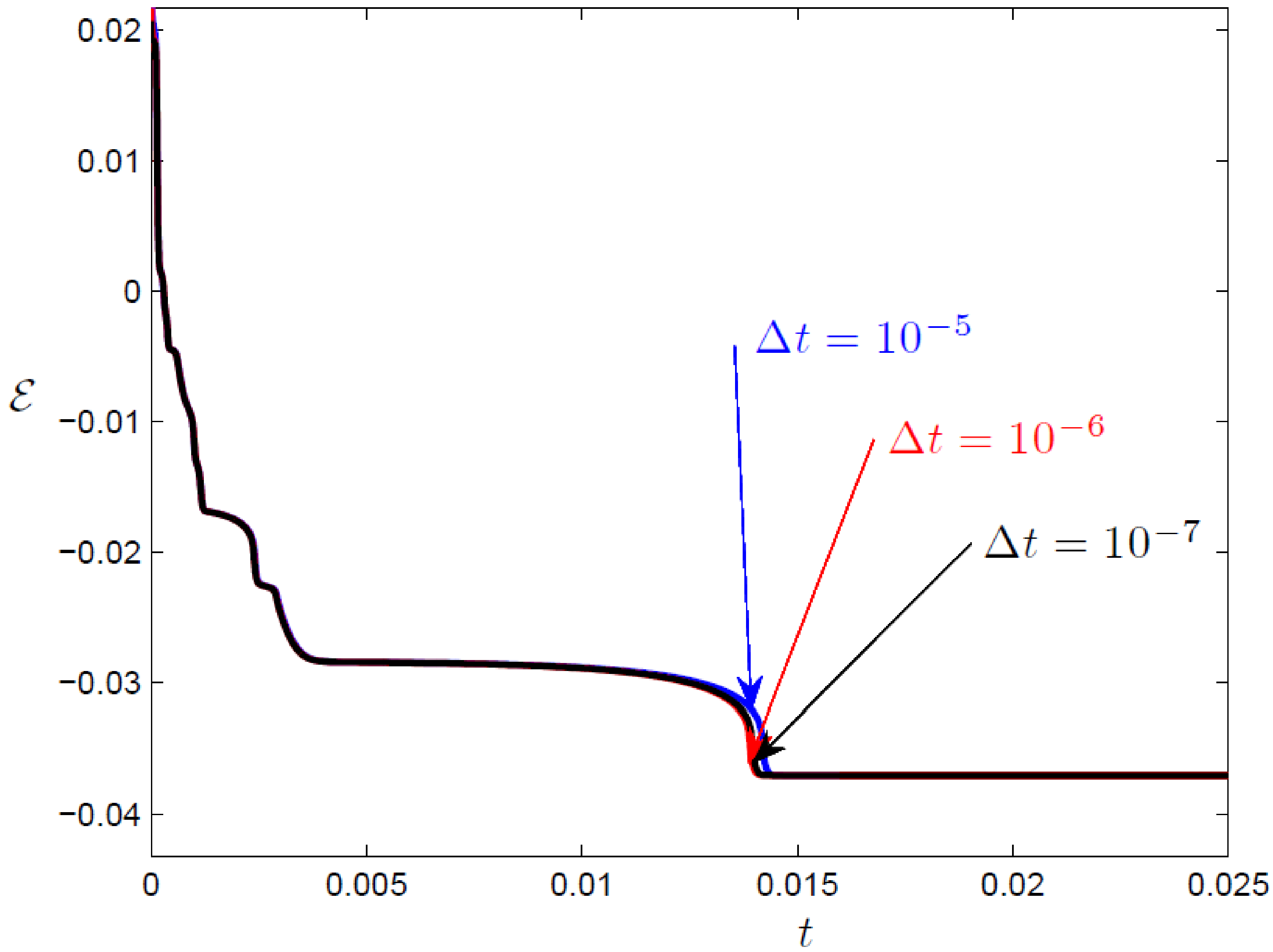
Example 1: Eyre's method



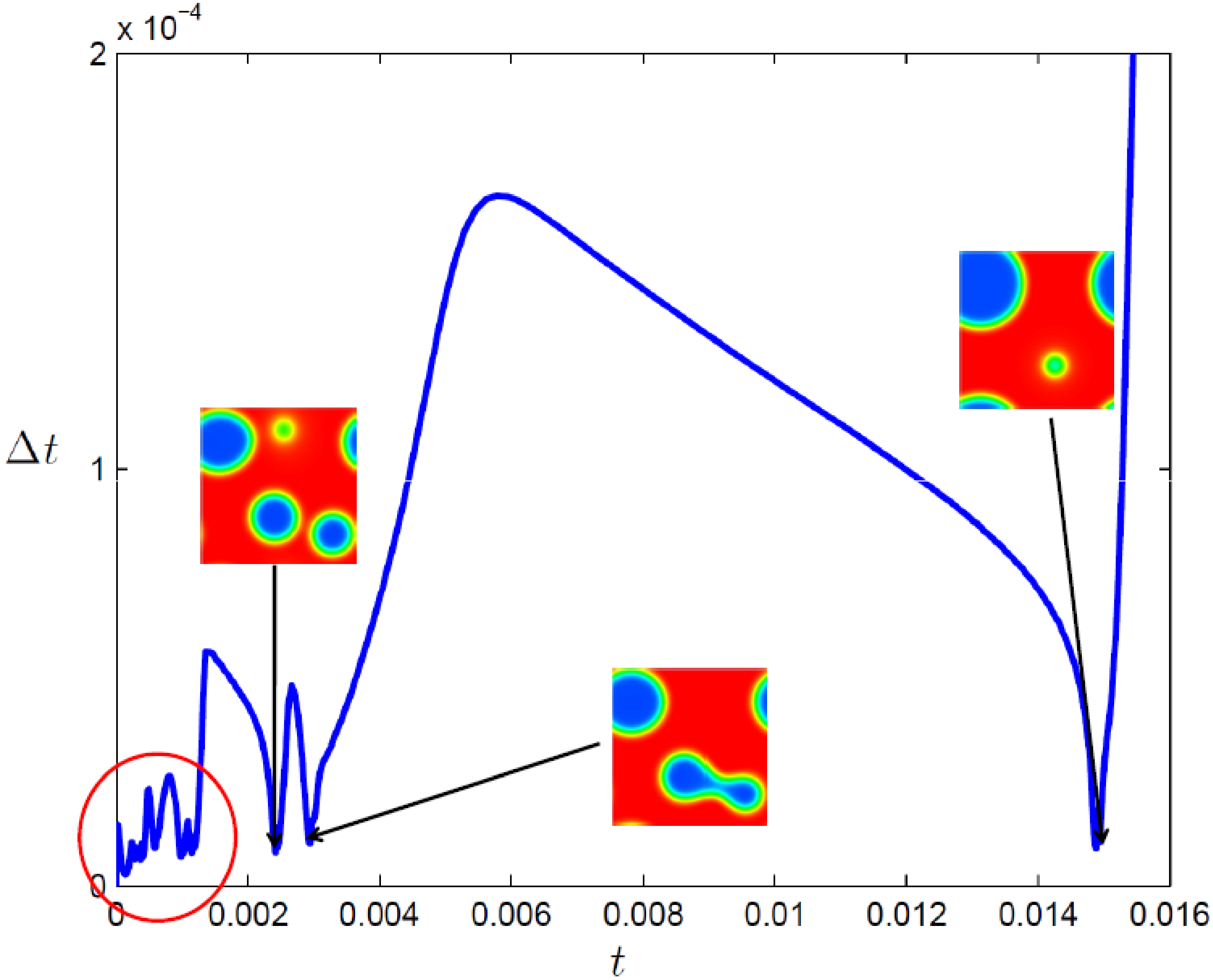
Example 1: New method



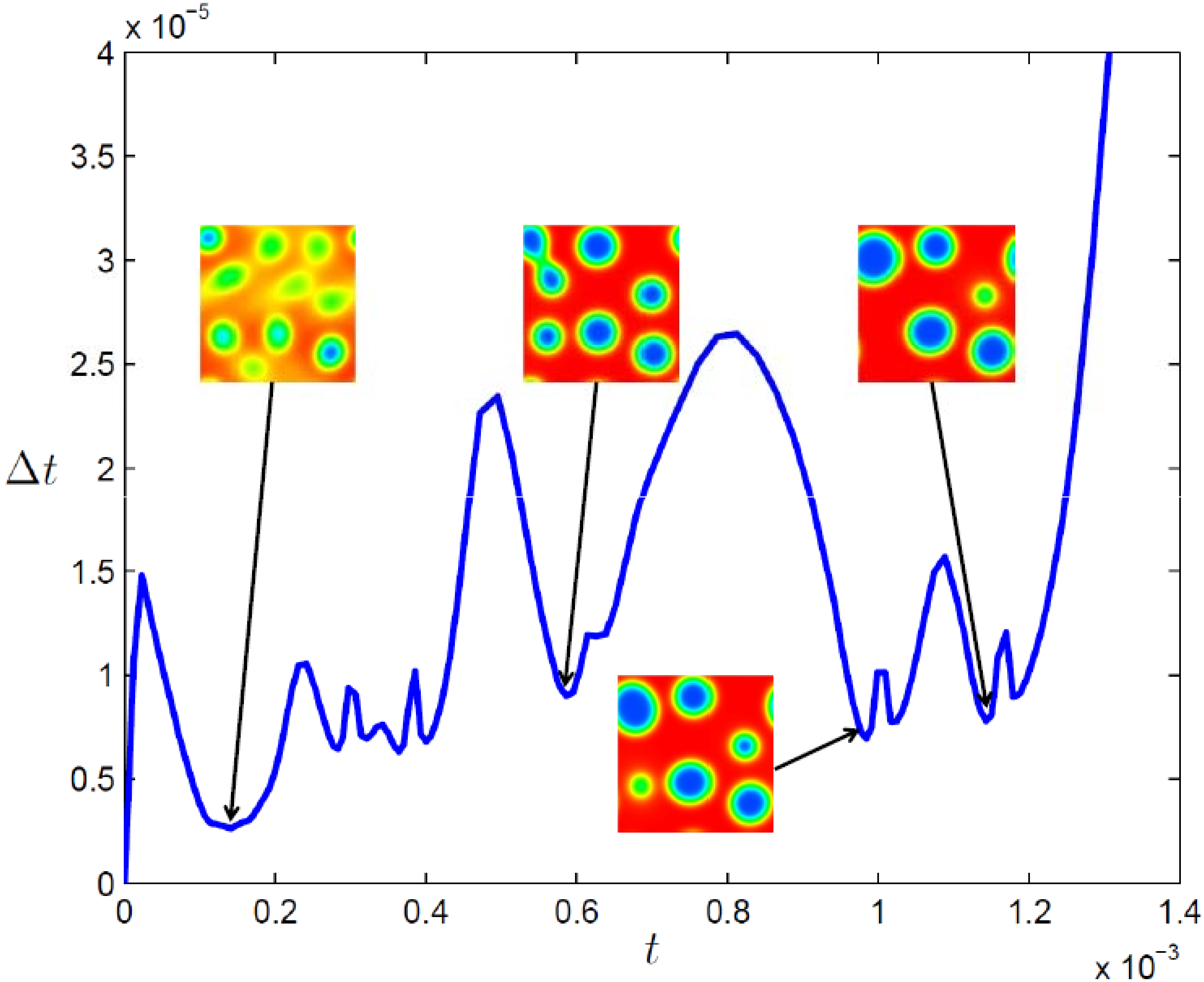
Example 1: New method



Repeat Example 1: Adaptivity



Repeat Example 1: Adaptivity



Conclusions

- Phase-field modeling is a powerful theory
- Potential for engineering problems
- Numerical solution is challenging
- Isogeometric analysis
- Adaptive time stepping
- Refinement methodology
- Provably unconditionally stable methods
- The efficient approximation of phase-field models may permit addressing problems intractable heretofore