Simulation and control of multiphase flows governed by the Cahn-Hilliard Navier-Stokes system

FBP - T& A 2012: Focus Session *Numerical methods for fluidic interfaces*

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(joint work with Michael Hintermüller & Christian Kahle)

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Outline

- **Numerical scheme for the Cahn-Hilliard Navier-Stokes system (along the lines of Kay, Styles, Welford I&FB 10, 2008). Cahn-Hilliard part with double-obstacle (Blowey-Elliott) potential**

- **Moreau-Yosida relaxation of the CH variational inequality**

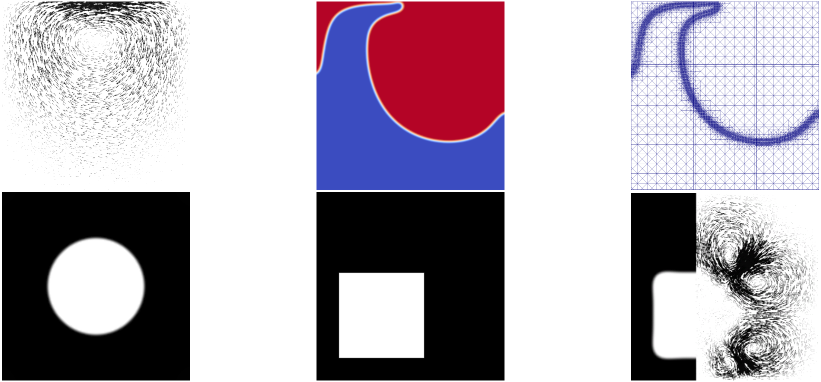
- **Adaption of the residual-based a posteriori concept proposed by Hintermüller, H., and Tber in OMS 2011 to CHNS**

- **Towards mpc control of multiphase flows (details in talk of Christian Kahle)**

Motivation: development of / complementation of

- **fully practical numerics for hydrodynamics of two-phase flows**
- **efficient, reliable, fully automatic adaptive concepts to resolve interface**
- **introduce control concepts**

Use of diffuse interface approach to cope e.g. with topology changes



Some literature

- **CHNS: Feng in SINUM 44, 2006**
- **CHNS: Kay, Styles, Welford in IFB 10, 2008**
- **CHNS: Aland, Voigt in J. Numer. Meth. Fluids, 2011**
- **2phase flow: Nguyen, Reusken J. Fourier Analysis & Applications 15, 2009; Reusken Springer Book, 2011, Tobiska et al (2007-2011)**
- **CH a posteriori: Banas, Nürnberg M2AN 43, 2009; Gräser, Kornhuber, Sack ENUMATH 2009; Hintermüller, H., Tber OMS, 2011**
- **CH numerical analysis: Blowey, Elliott; Barrett, Blowey; Copetti, Elliott; Gräser, Kornhuber; Barret, Blowey, Garcke, Blank, Butz, Garcke; ...**

Cahn-Hilliard-Navier-Stokes model

$$
\begin{aligned}
\partial_t \mathbf{u} - \frac{1}{Re}\Delta \mathbf{u} + \mathbf{u}\cdot\nabla\mathbf{u} + \nabla p + Kc\nabla w &= 0 && \text{in } \Omega_T = \Omega \times (0,T)\\
-\nabla\cdot\mathbf{u} &= 0 && \text{in } \Omega_T\\
c_t - \frac{1}{Pe}\Delta w + \nabla c\cdot\mathbf{u} &= 0 && \text{in } \Omega_T\\
-\gamma^2\Delta c + \Phi'(c) &= w && \text{in } \Omega_T\\
c(x,0) = c^0(x), \quad \mathbf{u}(x,0) &= \mathbf{u}^0(x) && \text{in } \Omega\\
\partial_\eta c = \partial_\eta w = 0, \mathbf{u} &= \mathbf{g} && \text{on } \partial\Omega\times(0,T)
\end{aligned}
$$

Re Reynolds number, Pe Peclét number, and K constant capillarity.
At the interface we use the double-obstacle potential according to Blowey and Elliott EJAM 1991.

$$
\Phi(c) = \begin{cases} \frac{1}{2}(1-c^2) & \text{if } c \in [-1,1] \\ \infty & \textit{else} \end{cases}
$$

Modeling (also with different densities) see e.g. Lowengrub, Truskinovsky Proc. R. Soc. London A (1998), Abels Habilitation thesis & Arch. Rational Mech. Anal. 194 (2009), Abels/Garcke/Grün (2010)

Semi-implicit time integration (along Kay, Styles & Welford)

$$
\begin{aligned}
(\mathbf{u},\mathbf{v}) + \frac{\tau}{Re}(\nabla\mathbf{u} : \nabla\mathbf{v}) + \tau B(\mathbf{u}_{old},\mathbf{u},\mathbf{v})& \\
-\tau(p,\nabla\cdot\mathbf{v}) + \tau K(c\nabla w,\mathbf{v}) = (\mathbf{u}_{old},\mathbf{v}) &\quad \forall\mathbf{v}\in\mathbf{H}_0^1(\Omega)\\
(-\nabla\cdot\mathbf{u},\chi) = 0 &\quad \forall\chi\in L^2(\Omega)\\
(c,v) + \frac{\tau}{Pe}(\nabla w,\nabla v) = \tau(c_{old},\mathbf{u}_{old}\cdot\nabla v) + (c_{old},v) &\quad \forall v\in H^1(\Omega)\\
\gamma^2(\nabla c,\nabla v-\nabla c) - (w,v-c) \geq (c_{old},v-c) &\quad \forall v\in\mathcal{K}
\end{aligned}
$$

Here, $\mathcal{K} := \{u\in H^1(\Omega); |u|\leq 1 \text{ a.e. in } \Omega\}$,
$B(\mathbf{u},\mathbf{v},\mathbf{w}) := \frac{1}{2}\int_\Omega(\mathbf{u}\cdot\nabla)\mathbf{v}\cdot\mathbf{w}\,dx - \frac{1}{2}\int_\Omega(\mathbf{u}\cdot\nabla)\mathbf{w}\cdot\mathbf{v}\,dx$, and

$$(\nabla\mathbf{v} : \nabla\mathbf{w}) := \int_\Omega \nabla\mathbf{v} : \nabla\mathbf{w}\,dx = \int_\Omega \sum_{i,j=1}^{n}(\nabla\mathbf{v})_{ij}(\nabla\mathbf{w})_{ij}\,dx$$

Space discretization on two different grids

Flow mesh with gridsize h, Taylor-Hood elements for the Navier–Stokes part:

$$
\begin{aligned}
(\mathbf{u}_h, \mathbf{v}) + \frac{\tau}{Re}(\nabla \mathbf{u}_h : \nabla \mathbf{v}) + \tau B(\mathbf{u}_{old}, \mathbf{u}_h, \mathbf{v}) \\
-\tau(p_h, \nabla \cdot \mathbf{v}) + \tau K(c_{\tilde{h}} \nabla w_{\tilde{h}}, \mathbf{v}) = (\mathbf{u}_{old}, \mathbf{v}) \forall \mathbf{v} \in \mathcal{V}_{\mathbf{h}}^{\mathbf{u}} \\
(\nabla \cdot \mathbf{u}_h, \chi) = 0 \forall \chi \in \mathcal{V}_h^p
\end{aligned}
$$

Concentration/potential mesh with gridsize $\tilde{h}$ for the order parameter $c_{\tilde{h}}$ and the chemical potential $w_{\tilde{h}}$:

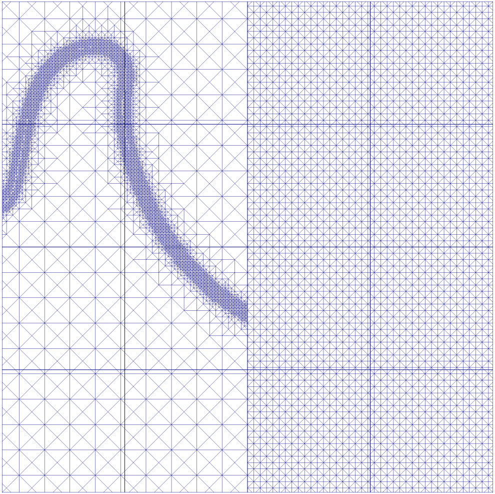
$$
(c_{\tilde{h}} - c_{old}, \phi)^{\tilde{h}} + \frac{\tau}{Pe}(\nabla w_{\tilde{h}}, \nabla \phi) - \tau(c_{old}, \mathbf{u}_{old} \cdot \nabla \phi) = 0 \forall \phi \in \mathcal{V}_{\tilde{h}}^{cw}
$$

$$
\gamma^2(\nabla c_{\tilde{h}}, \nabla v - \nabla c_{\tilde{h}}) - (w_{\tilde{h}}, v - c_{\tilde{h}}) \geq (c_{old}, v - c_{\tilde{h}}) \text{ for all } v \in \mathcal{V}_{\tilde{h}}^{cw} \text{ with } |v| \leq 1.
$$

$(\cdot, \cdot)^{\tilde{h}}$ denotes the lumped inner product.

Semi-implicit time integration sequentially couples CH to NS at every time step.

Concentration/potential mesh (left), flow mesh (right)



Relaxing the double obstacle potential using penalitzation

At every time step the CH part represents the Euler-Lagrange system of a PDE constrained minimization problem with control constraints (see e.g. Gräser, Kornhuber 2007; Blank, Butz, Garcke 2009);

$$\min_{c,w;|c|\leq 1,(w,1)=0} \underbrace{\frac{\gamma^2}{2}\|\nabla c\|^2 + \frac{\tau}{2Pe}\|\nabla w\|^2 - (c_{old}, w)}_{J(c,w)} \text{ s.t. } -\frac{\tau}{Pe}\Delta w = c_{old} - c - u_{old}\nabla c_{old}$$

Idea: Relax constraint $|v| \leq 1$ by penalization; i.e. replace $J(c, w)$ by

$$J_s(c, w) := J(c, w) + \frac{s}{2}\|\max(0, c-1)\|^2 + \frac{s}{2}\|\min(0, c+1)\|^2.$$

This with $\lambda_s(c_{\tilde{h}}) = s\max(0, c_{\tilde{h}} - 1) + s\min(0, c_{\tilde{h}} + 1)$ yields a nonlinear system to be solved at every time-step:

$$(c_{\tilde{h}} - c_{old}, \phi)^{\tilde{h}} + \frac{\tau}{Pe}(\nabla w_{\tilde{h}}, \nabla\phi) - \tau(c_{old}, \mathrm{u}_{old}\cdot\nabla\phi) = 0$$

$$\gamma^2(\nabla c_{\tilde{h}}, \nabla\phi) - (w_{\tilde{h}}, \phi)^{\tilde{h}} + (\lambda_s(c_{\tilde{h}}), \phi)^{\tilde{h}} - (c_{old}, \phi)^{\tilde{h}} = 0$$

Solution is performed using a semi-smooth Newton method. Performance mesh-independent (3-4 iterations to reach 1e-13)

Reliable error estimator

There exists a constant C depending only on the domain Ω and the smallest angle of the mesh $\mathcal{T}_h^{cw}$ such that

$$s^{-1}\|e_{\lambda_s}\|^2 + \frac{\tau}{Pe}\|\nabla e_w\|^2 + \gamma^2\|\nabla e_c\|^2 \leq C\eta_\Omega^2,$$

where

$$\eta_\Omega^2 = \left(\frac{\tau}{Pe}\right)^{-1} \sum_{T\in\mathcal{T}^{cw}} (\eta_T^{(1)})^2 + \gamma^{-2} \sum_{T\in\mathcal{T}^{cw}} (\eta_T^{(2)})^2 + \frac{\tau}{Pe} \sum_{E\in\mathcal{E}^{cw}} (\eta_E^{(1)})^2$$
$$+ \gamma^2 \sum_{E\in\mathcal{E}^{cw}} (\eta_E^{(2)})^2 + \gamma^{-2} \sum_{T\in\mathcal{T}^{cw}} (\eta_T^{(3)})^2.$$

With element indicators

$$\eta_T^{(1)} = h_T\|r_h^{(1)}\|_{0,T},\ \eta_T^{(2)} = h_T\|r_h^{(2)}\|_{0,T},\ \text{and } \eta_T^{(3)} = \|e_{\lambda_s^h}\|_{0,T} \text{ for all } T \in \mathcal{T}^{cw},$$

and edge indicators

$$\eta_E^{(1)} = h_E^{1/2}\|[\nabla w^h]_E \cdot \nu_E\|_{0,E},\ \eta_E^{(2)} = h_E^{1/2}\|[\nabla c^h]_E \cdot \nu_E\|_{0,E} \text{ for all } E \in \mathcal{E}^{cw}$$

the residuals are defined by (recall c^h, w^h discretized with $c(1)$ finite elements.

$$r_h^{(1)} := c^h - c_{old} + \tau \mathrm{div}(c_{old}\mathbf{u}_{old}),\ r_h^{(2)} := \pi_h(\lambda_s(c^h)) - w^h - c_{old},$$

Efficiency estimate

There exists a constant β depending on s^{-1}, γ, τ, Ω, and the smallest angle of the mesh $\mathcal{T}_h^{cw}$ such that

$$s^{-1}\|e_{\lambda_s}\|^2 + \frac{\tau}{Pe}\|\nabla e_w\|^2 + \gamma^2\|\nabla e_c\|^2 \geq$$
$$\beta\eta_\Omega^2 - \|e_{\lambda_s^h}\|^2 - \mathrm{osc}_h(r_h^{(1)},\Omega)^2 - \mathrm{osc}_h(r_h^{(2)},\Omega)^2.$$

Here

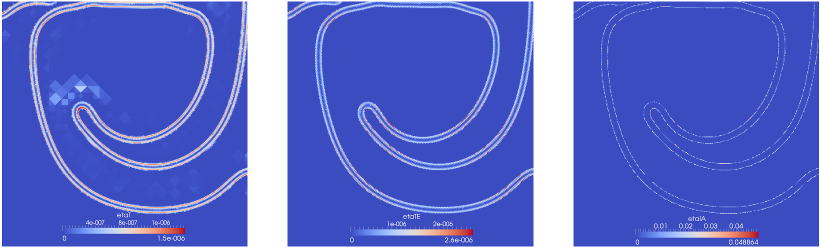
$$\mathrm{osc}_h(f,T) = \|h_T(f-\bar{f})\|_{0,T} \quad \text{for } T \in \mathcal{T}^{cw},$$
$$\mathrm{osc}_h(f,D) = \left(\sum_{T\in D}\mathrm{osc}_h(f,T)^2\right)^{1/2} \quad \text{for } D \subset \mathcal{T}^{cw}.$$

The Term $\|e_{\lambda_s^h}\|$ arises from the inexact evaluation of $\lambda_s(c^h)$ due to mass lumping techniques. If the lumping technique is replaced by an exact evaluation of $\lambda_s(c^h)$ yielding $\|e_{\lambda_s^h}\| = 0$ the estimator is both reliable and efficient.

Lid driven cavity

lid driven cavity

Contribution of error indicators η_T, η_{TE}, and η_{IA}

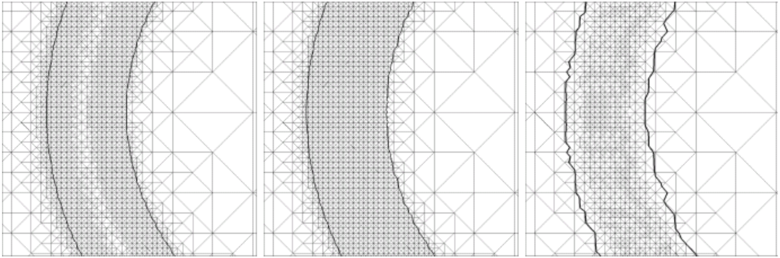


$$\eta_T := \left(\frac{\tau}{Pe}\right)^{-1} (\eta_T^{(1)})^2 + \gamma^{-2}(\eta_T^{(2)})^2,$$

$$\eta_{TE} := \sum_{E \in \mathcal{E}^{cw}(T)} \left(\frac{\tau}{Pe}(\eta_E^{(1)})^2 + \gamma^2(\eta_E^{(2)})^2\right), \text{ and}$$

$$\eta_{IA} := \gamma^{-2}(\eta_T^{(3)})^2.$$

Comparison with local meshes obtained by heuristic strategies



Left: our strategy, middle: mark if $|1 - |c|| > 0$, right: mark if $|\nabla c_{|_T}|$ large.

Towards model predictive control of multiphase flows (Talk Christian Kahle)

Given some initial state x_0, find a control law $\mathcal{B}u(t) = K(x(t))$ which steers the state $x(t)$ towards a given trajectory $\bar{x}$:

$$x(t) \stackrel{!}{\longrightarrow} \bar{x}(t) \quad t \to \infty$$

Mathematical model:

$$\begin{aligned} \dot{x}(t) + Ax(t) &= b(x,t) + \mathcal{B}u(t) \text{ state,} \\ y(t) &= \mathcal{C}x(t) \text{ observation,} \\ x(0) &= x_0 \end{aligned}$$

Here

- $\bar{x}$ desired stationary state, or
- $\bar{x}$ a reference trajectory obtained from open loop optimal control.

Instantaneous control of CHNS (more details in talk of Christian Kahle)

At each time instance t_k solve approximately the minimization problem

$$\min_{\mathbf{u}\in\mathbf{U}} J^k(c,\mathbf{u}) = \frac{1}{2}\int_\Omega (c - c_d^k)^2\,dx + \frac{\alpha}{2}\int_\Omega |\mathbf{u}|^2\,dx \qquad (P^k)$$

s.t.

$$\mathbf{y} - \frac{\tau}{Re}\Delta\mathbf{y} = \mathbf{u} + f \qquad (1)$$

$$c - \frac{\tau}{Pe}\Delta w = c_{old} - \tau\nabla c_{old}\mathbf{y} \qquad (2)$$

$$-\gamma^2\Delta c + \lambda_s(c) - w = c_{old} \qquad (3)$$

Here

$$f(c_{old}, w_{old}, \mathbf{y}_{old}) = \mathbf{y}_{old} - \tau c_{old}\nabla w_{old} - \tau(\mathbf{y}_{old}\nabla)\mathbf{y}_{old}$$

$$\lambda_s(c) = s(\max(0, c-1) + \min(0, c+1))$$

The gradient of J^k

The gradient of J^k is given by

$$\nabla J^k(\mathbf{u}_0^k) = \alpha \mathbf{u}_0^k + p_3$$

where p_3 stems from the solution to the adjoint system

$$-\gamma^2 \Delta p_2 + \lambda_s'(c) p_2 - \tau \nabla p_1 \cdot \mathbf{y} + p_1 = c - c_d \quad (4)$$

$$p_2 = -\frac{\tau}{Pe} \Delta p_1 \quad (5)$$

$$p_3 - \frac{\tau}{Re} \Delta p_3 = \tau c \nabla p_1. \quad (6)$$

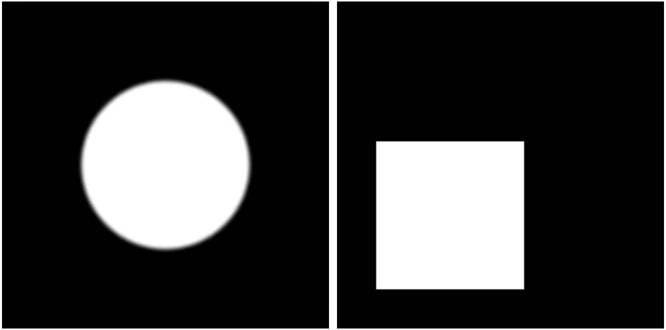
Instantaneous control

Idea: Perform only one gradient step to obtain an approximate solution to (P^k):

- **choose $\mathbf{u}_0^k, \rho > 0$**
- **set $\mathbf{u}^k = \mathbf{u}_0^k - \rho \tilde{\nabla} J^k(\mathbf{u}_0^k)$**
- **calculate the approximate solution c^k on time step k using $\mathbf{u}^k$**
- **go to next time step**

The Algorithm is well defined in the sense, that the systems (1)–(3) and (4)–(6) admit a unique solution.

Example: Circle2Square



Initial state (circle) and desired state (square)

Morphing: Circle2Square

Circle2Square

Circle2Square: snapshot of controlled states

Morphing: circle to 2 circles

One2Twobubbles

Morphing also offers other possibilities...

Hinze2Cow

which seem to work...

Thank you very much for your attention!

which seem to work...

Thank you very much for your attention!

Example: Cow2Elliot

Hinze2Cow

Example: Hinze2Elliot

Hinze2Cow