On energy-stable schemes for two Vesicle Membrane phase-field models

Francisco Guillén-González (Universidad de Sevilla) guillen@us.es
Joint work with: **Giordano Tierra** (University of Notre Dame, USA).

Depto. EDAN and IMUS. Universidad de Sevilla

SciCADE2013, Valladolid16-20 September 2013

A diffuse interface model

- Hydrodynamic system modeling the deformation of vesicle membranes in incompressible viscous fluids.
- The system consists of the Navier-Stokes equations coupled with a fourth order phase-field equation.

Sharp interface equilibrium model

- The equilibrium configurations of vesicle membranes can be characterized by the **Helfrich** bending elasticity energy of the surface [W. Helfrich 73, Elastic properties of lipid bilayers: theory and possible experiments]
  such that they are minimizers of the bending energy under possible constraints like prescribed surface area (incompressibility of the membrane) and bulk volume (the change in volume is normally a much slower process in comparison with the shape change).
- Let Γ be a smooth, surface representing the membrane of the vesicle. The most simplified form of the interfacial energy is

$$E_{elastic} = \int_\Gamma \frac{k}{2}(H - H_0)^2 ds$$

  where H is the mean curvature of Γ, k is the bending rigidity and H_0 is the spontaneous curvature that describes certain physical/chemical difference between the inside and the outside of the membrane.
- For the simplicity, we assume that k is a positive constant and $H_0 = 0$.

Diffuse interface model

- ϕ takes the value 1 inside of the vesicle membrane and -1 outside.
- The phase-field approximation of the Helfrich bending elasticity energy is given by a modified **Willmore Bending energy**:

$$E_\varepsilon(\phi) = \frac{1}{2\varepsilon}\int_\Omega \left(-\varepsilon\Delta\phi + \frac{1}{\varepsilon}f(\phi)\right)^2 dx \quad \text{with} \quad f(\phi) = (\phi^2 - 1)\phi$$

  $\varepsilon > 0$ is a small positive parameter (compared to the vesicle size) that characterizes the transition layer of the phase function.
  [Du, Liu, Wang 04], [Wang 08]
- Convergence of the phase-field model to the original sharp interface model as the transition width of the diffuse interface $\varepsilon \to 0$
  [Du, Liu, Ryham, Wang 05], [Wang 08]
- Diffuse interface models simplify numerical approximations because it suffices to consider a fixed computational grid rather than tracking the position of the interface

Dynamics model

Model: Interaction of a vesicle membrane with the fluid field, which describes the evolution of vesicles immersed in an incompressible, Newtonian fluid.
PDE system (Navier-Stokes + Allen-Cahn): For $\nu, \lambda, \gamma > 0$ (constants):

$$\begin{cases} \partial_t \boldsymbol{u} + (\boldsymbol{u} \cdot \nabla)\boldsymbol{u} - \nu \Delta \boldsymbol{u} + \nabla p - \lambda \left(\frac{\delta E_\varepsilon}{\delta \phi} \right) \nabla \phi = 0, \\ \nabla \cdot \boldsymbol{u} = 0, \\ \partial_t \phi + \boldsymbol{u} \cdot \nabla \phi = -\gamma \left(\frac{\delta E_\varepsilon}{\delta \phi} \right). \end{cases}$$

System can be obtained via an energetic variation approach [Yue, Feng, Liu, Shen 04], [Hyon, Kwak, Liu 10]
Energy law (Lyapunov functional): Calling $E_{tot}(\boldsymbol{u}, \phi) = E_{kin}(\boldsymbol{u}) + \lambda\, E_\varepsilon(\phi)$:

$$\frac{d}{dt} E_{tot}(\boldsymbol{u}, \phi) + \nu \|\nabla \boldsymbol{u}\|^2_{L^2(\Omega)} + \lambda\gamma \left\| \frac{\delta E_\varepsilon}{\delta \phi} \right\|^2_{L^2(\Omega)} = 0.$$

For simplicity, we take $\nu, \lambda, \gamma = 1$

Two global constraints of conservation for the vesicle volume and surface area:

$$A(\phi) = \int_\Omega \phi \, dx \quad \text{and} \quad B(\phi) = \int_\Omega \left(\frac{\varepsilon}{2} |\nabla \phi|^2 + \frac{1}{\varepsilon} F(\phi) \right) dx,$$

where $F(\phi) = \frac{1}{4}(\phi^2 - 1)^2$ (Note that $f(\phi) = F'(\phi)$)
Introducing the auxiliary variable

$$\omega = -\varepsilon \Delta \phi + \frac{1}{\varepsilon} f(\phi),$$

then

$$E_\varepsilon(\phi) = E_\varepsilon(\omega) = \frac{1}{2\varepsilon} \int_\Omega \omega^2 dx$$

Some variational computations gives:

$$\frac{\delta A}{\delta \phi} = 1, \quad \frac{\delta B}{\delta \phi} = \omega$$

and

$$\frac{\delta E_\varepsilon}{\delta \phi} = -\Delta \omega + \frac{1}{\varepsilon^2} \omega f'(\phi)$$

Lagrange multiplier problem

Idea: Modify the generic model to enforce the two physical constraints by Lagrange multipliers ($\lambda_1(t), \lambda_2(t)$) and introduce an extra unknown z:

$$\begin{cases} \partial_t \boldsymbol{u} - \Delta \boldsymbol{u} + (\boldsymbol{u} \cdot \nabla)\boldsymbol{u} + \nabla p - z \nabla \phi = 0, \\ \nabla \cdot \boldsymbol{u} = 0, \\ \partial_t \phi + \boldsymbol{u} \cdot \nabla \phi + z = 0, \\ A(\phi) = \alpha \ (= A(\phi_0)), \quad B(\phi) = \beta \ (= B(\phi_0)), \\ + \ I.C. \ \text{ and } \ B.C. \end{cases}$$

where

$$z = \frac{\delta E_\varepsilon}{\delta \phi} + \lambda_1(t) \frac{\delta A}{\delta \phi} + \lambda_2(t) \frac{\delta B}{\delta \phi} = -\Delta \omega + \frac{1}{\varepsilon^2} \omega f'(\phi) + \lambda_1(t) + \lambda_2(t)\, \omega,$$

Reformulation of the model (I): time derivatives

Taking the time derivative of the ω-equation:

$$\begin{cases} \partial_t \omega = -\varepsilon \Delta \partial_t \phi + \dfrac{1}{\varepsilon} f'(\phi) \partial_t \phi, \quad t \in (0, T), \\ \omega|_{t=0} = \omega_0 := -\varepsilon \Delta \phi_0 + \dfrac{1}{\varepsilon} f(\phi_0) \end{cases}$$

Taking the time derivative of the two constraints:

$$\begin{cases} \displaystyle\int_\Omega \partial_t \phi = 0, \quad \int_\Omega \omega\, \partial_t \phi = 0, \quad t \in (0, T), \\ A(\phi_0) = \alpha, \quad B(\phi_0) = \beta \end{cases}$$

Reformulation of the model (II): dissipation of free energy

Then

$$
\begin{cases}
\partial_t \boldsymbol{u} - \Delta \boldsymbol{u} + (\boldsymbol{u}\cdot\nabla)\boldsymbol{u} + \nabla p - z\nabla\phi = 0, & \boldsymbol{u} \\
\nabla\cdot\boldsymbol{u} = 0, & p \\
\partial_t\phi + \boldsymbol{u}\cdot\nabla\phi + z = 0, & z \\
-\Delta\omega + \frac{1}{\varepsilon^2}\omega\, f'(\phi) + \lambda_1(t) + \lambda_2(t)\,\omega - z = 0, & \partial_t\phi \\
\frac{1}{\varepsilon}\partial_t\omega = -\Delta\partial_t\phi + \frac{1}{\varepsilon^2} f'(\phi)\partial_t\phi, & \omega \\
\int_\Omega \partial_t\phi = 0, \quad \int_\Omega \omega\,\partial_t\phi = 0, & \\
+\ I.C. \ \text{and} \ B.C. &
\end{cases}
$$

Modified Energy Law:

$$\frac{d}{dt}E_{tot}(\boldsymbol{u},\omega) + \|\nabla\boldsymbol{u}\|_{L^2}^2 + \|z\|_{L^2}^2 = 0,$$

with $E_{tot}(\boldsymbol{u},\omega) = E_{kin}(\boldsymbol{u}) + E_\varepsilon(\omega)$.

First order, linear and unconditionally energy-stable scheme.

Given $\boldsymbol{u}^n, \phi^n, \omega^n$, find $\boldsymbol{u}^{n+1}, p^{n+1}, \phi^{n+1}, \omega^{n+1}, \lambda_1^{n+1}, \lambda_2^{n+1}$ s.t.

$$
\left\{
\begin{array}{ll}
\left(\delta_t \boldsymbol{u}^{n+1}, \bar{\boldsymbol{u}}\right) + c(\boldsymbol{u}^n, \boldsymbol{u}^{n+1}, \bar{\boldsymbol{u}}) + (\nabla \boldsymbol{u}^{n+1}, \nabla \bar{\boldsymbol{u}}) & \\
-(p^{n+1}, \nabla \cdot \bar{\boldsymbol{u}}) - \left(z^{n+1} \nabla \phi^n, \bar{\boldsymbol{u}}\right) = 0, & \boldsymbol{u}^{n+1} \\
(\nabla \cdot \boldsymbol{u}^{n+1}, \bar{p}) = 0, & p^{n+1} \\
\left(\delta_t \phi^{n+1}, \bar{z}\right) + (\boldsymbol{u}^{n+1} \cdot \nabla \phi^n, \bar{z}) + (z^{n+1}, \bar{z}) = 0, & z^{n+1} \\
(\nabla \omega^{n+1}, \nabla \bar{\phi}) + \dfrac{1}{\varepsilon^2}(f'(\phi^n)\omega^{n+1}, \bar{\phi}) + \lambda_1^{n+1}(1, \bar{\phi}) + \lambda_2^{n+1}(\omega^n, \bar{\phi}) & \\
-(z^{n+1}, \bar{\phi}) = 0, & \delta_t \phi^{n+1} \\
\dfrac{1}{\varepsilon}\left(\delta_t \omega^{n+1}, \bar{\omega}\right) - \left(\nabla \delta_t \phi^{n+1}, \nabla \bar{\omega}\right) - \dfrac{1}{\varepsilon^2}\left(f'(\phi^n)\delta_t \phi^{n+1}, \bar{\omega}\right) = 0, & \omega^{n+1} \\
\displaystyle\int_\Omega \delta_t \phi^{n+1} = 0 \quad \text{and} \quad \int_\Omega \omega^n \delta_t \phi^{n+1} = 0. &
\end{array}
\right.
$$

Unconditional energy-stability,

$$\delta_t E_{tot}(\boldsymbol{u}^{n+1}, \omega^{n+1}) + \|\nabla \boldsymbol{u}^{n+1}\|_{L^2}^2 + \|z^{n+1}\|_{L^2}^2 + ND^{n+1} = 0,$$

where

$$ND^{n+1} = \frac{k}{2}\|\delta_t \boldsymbol{u}^{n+1}\|_{L^2}^2 + \frac{k}{2\varepsilon}\|\delta_t \omega^{n+1}\|_{L^2}^2 \geq 0$$

Moreover, this scheme is well-defined.

Vesicle membranes. Penalized problem.

Adding two penalty terms to the elastic bending energy $E_\varepsilon(\phi)$ to approximate the volume and surface area constraints.

The modified energy reads

$$\widehat{E}_{\varepsilon,\eta}(\omega,\phi) = E_\varepsilon(\omega) + \frac{1}{2\eta}[A(\phi)-\alpha]^2 + \frac{1}{2\eta}[B(\phi)-\beta]^2$$

where $\eta > 0$ is a penalization parameter.

Consider the new unknown

$$\widehat{z} = \frac{\delta \widehat{E}_{\varepsilon,\eta}(\omega(\phi),\phi)}{\delta\phi} = -\Delta\omega + \frac{1}{\varepsilon^2} f'(\phi)\omega + \frac{1}{\eta}(A(\phi)-\alpha) + \frac{1}{\eta}(B(\phi)-\beta)\omega,$$

we get the following reformulation:

$$\begin{cases} \partial_t \boldsymbol{u} + \boldsymbol{u}\cdot\nabla\boldsymbol{u} + \nabla p - \Delta\boldsymbol{u} - \widehat{z}\,\nabla\phi = 0, & \boldsymbol{u} \\ \nabla\cdot\boldsymbol{u} = 0, & p \\ \partial_t\phi + \boldsymbol{u}\cdot\nabla\phi + \widehat{z} = 0, & \widehat{z} \\ -\Delta\omega + \dfrac{1}{\varepsilon^2} f'(\phi)\omega + \dfrac{1}{\eta}(A(\phi)-\alpha) + \dfrac{1}{\eta}(B(\phi)-\beta)\omega - \widehat{z} = 0, & \partial_t\phi \\ \dfrac{1}{\varepsilon}\partial_t\omega - \Delta\partial_t\phi + \dfrac{1}{\varepsilon^2} f'(\phi)\partial_t\phi = 0. & \omega \end{cases}$$

Energy Law:

$$\frac{d}{dt}\widehat{E}_{tot}(\boldsymbol{u},\omega) + \|\nabla u\|^2_{L^2} + \|\widehat{z}\|^2_{L^2} = 0,$$

where $\widehat{E}_{tot}(\boldsymbol{u},\omega,\phi) = E_{kin}(\boldsymbol{u}) + \widehat{E}_{\varepsilon,\eta}(\omega,\phi)$.

RK: Since the expression of ω in function of ϕ has been derivate in time, in order to get this energy law, this expression must be written explicitly in the term

$$(B(\phi)-\beta)\omega = (B(\phi)-\beta)(-\varepsilon\Delta\phi + \frac{1}{\varepsilon} f(\phi))$$

First order, nonlinear and unconditionally energy-stable scheme.

$$\left\{\begin{array}{ll}\left(\delta_t \boldsymbol{u}^{n+1}, \bar{u}\right) + c(\boldsymbol{u}^n, \boldsymbol{u}^{n+1}, \bar{\boldsymbol{u}}) + (\nabla \boldsymbol{u}^{n+1}, \nabla \bar{\boldsymbol{u}}) & \\ -(p^{n+1}, \nabla \cdot \bar{\boldsymbol{u}}) - \left(\nabla \phi^n \widehat{z}^{n+1}, \bar{\boldsymbol{u}}\right) = 0, & \boldsymbol{u}^{n+1} \\ (\nabla \cdot \boldsymbol{u}^{n+1}, \bar{p}) = 0, & p^{n+1} \\ \left(\delta_t \phi^{n+1}, \bar{z}\right) + (\boldsymbol{u}^{n+1} \cdot \nabla \phi^n, \bar{z}) + (\widehat{z}^{n+1}, \bar{z}) = 0, & \widehat{z}^{n+1} \\ (\nabla \omega^{n+1}, \nabla \bar{\phi}) + \dfrac{1}{\varepsilon^2}(f'(\phi^n)\omega^{n+1}, \bar{\phi}) + \dfrac{1}{\eta}(A(\phi^{n+1}) - \alpha)(1, \bar{\phi}) & \\ +\dfrac{1}{\eta}\left(B(\phi^{n+1}) - \beta\right)\left[\varepsilon(\nabla \phi^{n+1}, \nabla \bar{\phi}) + \dfrac{1}{\varepsilon}(f^k(\phi^{n+1}, \phi^n), \bar{\phi})\right] - (\widehat{z}^{n+1}, \bar{\phi}) = 0, & \delta_t \phi^{n+1} \\ \dfrac{1}{\varepsilon}(\delta_t \omega^{n+1}, \bar{\omega}) - \left(\nabla \delta_t \phi^{n+1}, \nabla \bar{\omega}\right) - \dfrac{1}{\varepsilon^2}\left(f'(\phi^n)\delta_t \phi^{n+1}, \bar{\omega}\right) = 0. & \omega^{n+1}\end{array}\right.$$

where $f^k(\phi^{n+1}, \phi^n)$ will be an adequate approx. of $f(\phi(t_{n+1}))$.

Energy-stability.

Discrete Energy Law:

$$\delta_t \widehat{E}_{tot}(\boldsymbol{u}^{n+1}, \omega^{n+1}, \phi^{n+1}) + \|\nabla \boldsymbol{u}^{n+1}\|_{L^2}^2 + \|\widehat{z}^{n+1}\|_{L^2}^2 + \widehat{ND}^{n+1} = 0$$

where $\widehat{ND}^{n+1}$ is the numerical residual:

$$\widehat{ND}^{n+1} = \frac{k}{2}\|\delta_t \boldsymbol{u}^{n+1}\|_{L^2}^2 + \frac{k}{2\varepsilon}\|\delta_t \omega^{n+1}\|_{L^2}^2 + \frac{k}{2\eta}(\delta_t A(\phi^{n+1}))^2$$

$$+\frac{k}{2\eta}(\delta_t B(\phi^{n+1}))^2 - \frac{1}{\eta}(B(\phi^{n+1}) - \beta)(ND_{philic}^{n+1} + ND_{phobic}^{n+1})$$

with

$$ND_{philic}^{n+1} = k\frac{\varepsilon}{2\eta}\|\delta_t \nabla \phi^{n+1}\|_{L^2}^2$$

$$ND_{phobic}^{n+1} = \int_\Omega f^k(\phi^{n+1}, \phi^n)\delta_t \phi^{n+1} - \delta_t \int_\Omega F(\phi^{n+1}).$$

Since $B(\phi^{n+1}) - \beta$ has no sign, the scheme is unconditional energy-stable if

$$ND^{n+1}_{philic} = 0 \quad \text{and} \quad ND^{n+1}_{phobic} = 0$$

It can be reached by using the mid-point approximation. That is, to change

$$\left[\varepsilon(\nabla\phi^{n+1}, \nabla\bar{\phi}) + \frac{1}{\varepsilon}(f^k(\phi^{n+1}, \phi^n), \bar{\phi})\right]$$

by

$$\left[\varepsilon(\nabla\left(\frac{\phi^{n+1} + \phi^n}{2}\right), \nabla\bar{\phi}) + \frac{1}{\varepsilon}(\frac{F(\phi^{n+1}) - F(\phi^n)}{\phi^{n+1} - \phi^n}, \bar{\phi})\right].$$

$2D$ Numerical simulations. A celular membrane through a strangulation zone

- Penalized problem
- Parameters: $\nu = 1{,}0$, $\lambda = 0{,}01$, $\gamma = 0{,}01$, $\varepsilon = 0{,}01$, $\eta = 10000$.
- Splitting fluid/phase-field and linearized scheme (taking $A(\phi)$, $B(\phi)$ in ϕ^n
- Potencial approximacion **OD2** [F-GG& G.Tierra 12]
- Initial Condition $\boldsymbol{u} = 0$
- Time step $\Delta t = 0{,}00001$
- Continuous Finite element approx.: velocity $P1b$ and others $P1$

View I

Conclusions and Future work.

Conclusions

1. Two models and two energy-stable first-order fully discrete schemes.
2. Lagrange multipliers model let us to define linear stable schemes

Future work

1. Splitting in time stable schemes
2. Second order stable schemes
3. Introduce a well-defined and convergent iterative scheme convergent towards the nonlinear scheme
4. Numerical simulations