General weak formulation for gradient flows

STEP
1

Definition: A **gradient structure** is a triple $(\mathcal{Q}, \mathcal{E}, \mathbb{K})$ of a state (function) space $\mathcal{Q}$, an energy functional $\mathcal{E} : \mathcal{Q} \to \mathbb{R}$ and a symmetric positive Onsager operator $\mathbb{K}(q) : \mathcal{Q}^* \to \mathcal{Q}$, *i.e.*, $\mathbb{K}(q) = \mathbb{K}^*(q) \geq 0$), such that the *gradient flow dynamics* for $q : [0,T] \to \mathcal{Q}$ is given by the evolution

$$\partial_t q = -\,\mathbb{K}(q)\mathrm{D}\mathcal{E}(q).$$

By construction we have

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{E}(q(t)) = \langle \mathrm{D}\mathcal{E}(q), \partial_t q\rangle = -\,\langle \mathrm{D}\mathcal{E}(q), \mathbb{K}(q)\mathrm{D}\mathcal{E}(q)\rangle \overset{\mathbb{K}\geq 0}{\leq} 0.$$

STEP
2

Definition: An **extended gradient structure** is a *gradient structure* and a pair $(\mathcal{U}, \mathbb{M})$ of a function space $\mathcal{U}$ and operator $\mathbb{M} : \mathcal{Q} \to \mathcal{U}^*$ that satisfies

$$\mathbb{M}\partial_t q = -\,\mathbb{M}\mathbb{K}(q)\mathbb{M}^*\eta$$
$$\mathbb{M}^*\eta = \mathrm{D}\mathcal{E}(q)$$

which is trivially equivalent to the gradient structure for invertible $\mathbb{M}$. Otherwise we have introduced a new operator $\hat{\mathbb{K}}(q) = \mathbb{M}\mathbb{K}(q)\mathbb{M}^* : \mathcal{U} \to \mathcal{U}^*$, which servers as a basis for a saddle point problem.

STEP
3

Definition: The **weak formulation of the extended gradient structure** is given by a positive symmetric bilinear form $a_q(\eta,\xi) = \langle \mathbb{M}^*\eta, \mathbb{K}(q)\mathbb{M}^*\xi\rangle_{\mathcal{Q}} = \langle \hat{\mathbb{K}}(q)\eta, \xi\rangle_{\mathcal{U}}$ and a bilinear form $b(v,\xi) = \langle \mathbb{M}^*\eta, v\rangle_{\mathcal{Q}}$ such that the gradient flow dynamics satisfies: For $q : [0,T] \to \mathcal{Q}$ at each time there exists an $\eta \in \mathcal{U}$

$$\begin{aligned} a_q(\eta,\xi) + b(\partial_t q, \xi) &= 0 \\ b(v,\eta) &= \langle \mathrm{D}\mathcal{E}(q), v\rangle_{\mathcal{Q}} \end{aligned} \qquad \text{for all } (\xi, v) \in \mathcal{U}\times\mathcal{Q}$$

H. Abels, H. Garcke & G. Grün (2012). Thermodynamically consistent, frame indifferent diffuse interface models … Math Models Methods Appl Sci
A. Mielke (2003). Energetic formulation of multiplicative elasto-plasticity using dissipation distances. *Contin. Mech. Thermodyn.*
A. Glitzky & A. Mielke (2013). A gradient structure for systems coupling reaction–diffusion effects in bulk and interfaces. ZAMP

Examples for weak extended gradient structure

Cahn-Hilliard: $\mathscr{E}(\varphi) = \int_\Omega \frac{\varepsilon}{2}|\nabla\varphi|^2 + \varepsilon^{-1}W(\varphi)\,\mathrm{d}x$ where $W(\varphi) = \frac{1}{2}(1-\varphi^2)^2$

$$a_\varphi(\eta,\xi) = \int_\Omega m(\varphi)\nabla\eta\cdot\nabla\xi\,\mathrm{d}x \qquad b(v,\xi) = \int_\Omega v\xi\,\mathrm{d}x$$

Colab: **Cell 5**

Diffusion: $\mathscr{E}(\varphi) = \int_\Omega \varphi(\log\varphi - 1)\,\mathrm{d}x$

$$a_\varphi(\eta,\xi) = \int_\Omega \mu\varphi\nabla\eta\cdot\nabla\xi\,\mathrm{d}x \qquad b(v,\xi) = \int_\Omega v\xi\,\mathrm{d}x$$

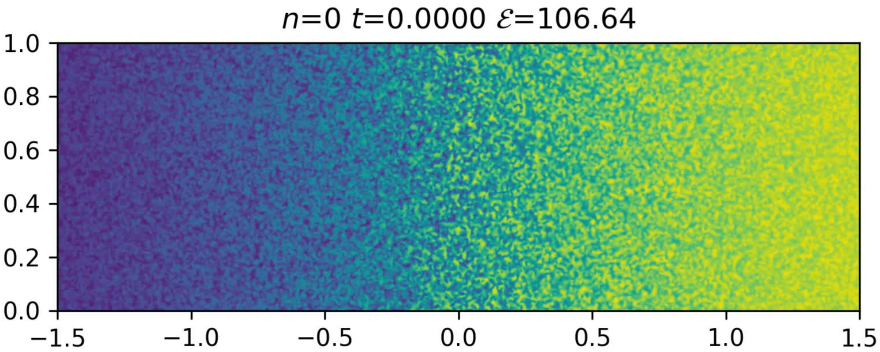
Colab: **Cell 6**

Nontrivial example: $\mathscr{Q} = H^1(\Omega), \mathscr{U} = H^1(\Omega)\times L^2(\partial\Omega)$ $\qquad \mathscr{E}(q) = \int_\Omega E(q,\nabla q)\,\mathrm{d}x$

$$a_q(\eta,\xi) = \int_\Omega \nabla\eta_1\cdot\nabla\xi_1\,\mathrm{d}x + \int_{\partial\Omega}\eta_2\xi_2\,\mathrm{d}s \qquad b(v,\xi) = \int_\Omega v\xi_1\,\mathrm{d}x + \int_{\partial\Omega} v\xi_2\,\mathrm{d}s$$

FEniCS Example 1: Cahn-Hilliard

$$\mathcal{E}(\varphi) = \int_\Omega \frac{\varepsilon}{2}|\nabla\varphi|^2 + \varepsilon^{-1}W(\varphi)\,\mathrm{d}x \qquad W(\varphi) = \tfrac{1}{2}(1-\varphi^2)^2 \qquad a_\varphi(\eta,\xi) = \int_\Omega m(\varphi)\nabla\eta\cdot\nabla\xi\,\mathrm{d}x \qquad b(v,\xi) = \int_\Omega v\xi\,\mathrm{d}x$$




```
FE   = FiniteElement("P", mesh.ufl_cell(), 1)   # scalar element
UxQ  = FunctionSpace(mesh,MixedElement([FE,FE]))# mixed space

# single time step
def evolve(old_q_ext, tau):
    q_ext,v_ext     = Function(UxQ),TestFunction(UxQ)
    eta,phi         = split(q_ext)
    xi,v            = split(v_ext)
    old_eta,old_phi = split(old_q_ext)

    E   = eps/2*inner(grad(phi),grad(phi))*dx + 1/(2*eps)*(1-phi**2)**2*dx
    Res  = tau*inner(grad(eta),grad(xi))*dx + xi*(phi-old_phi)*dx
    Res += eta*v*dx - derivative(E, q_ext, v_ext)

    q_ext.assign(old_q_ext)
    solve(Res==0, q_ext )
    E = assemble(E)
    return q_ext,E
```

$$a_\varphi(\eta,\xi) + b(\partial_t\varphi,\xi) = 0$$

$$b(v,\eta) = \langle \mathrm{D}\mathcal{E}(\varphi), v\rangle$$

with $\partial_t\varphi \approx \tau^{-1}(\varphi - \varphi^{n-1})$

Entire implementation < 50 lines of Python / FEniCS.

Colab: **Cell 5**

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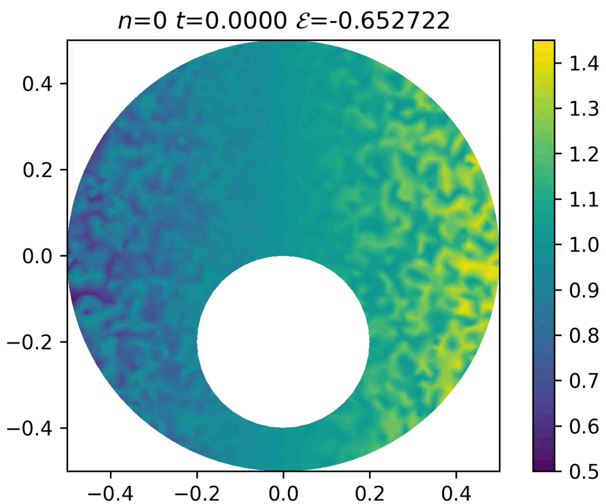
FEniCS Example 2: Diffusion

$$\mathscr{E}(\varphi) = \int_\Omega \varphi(\log\varphi - 1)\,\mathrm{d}x \qquad a_\varphi(\eta,\xi) = \int_\Omega \mu\varphi\nabla\eta\cdot\nabla\xi\,\mathrm{d}x \qquad b(v,\xi) = \int_\Omega v\xi\,\mathrm{d}x$$



$$a_\varphi(\eta,\xi) + b(\partial_t\varphi,\xi) = 0$$

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def evolve(old_q_ext, tau):
    q_ext,v_ext     = Function(UxQ),TestFunction(UxQ)
    eta,phi         = split(q_ext)
    xi,v            = split(v_ext)
    old_eta,old_phi = split(old_q_ext)

    E   = phi*(ln(phi)-1)*dx
    Res  = tau*old_phi*inner(grad(eta),grad(xi))*dx + xi*(phi-old_phi)*dx
    Res += eta*v*dx - derivative(E, q_ext, v_ext)

    q_ext.assign(old_q_ext)
    parameters["form_compiler"]["quadrature_degree"] = 3
    solve(Res==0, q_ext )
    E = assemble(E)
    return q_ext,E
```

Colab: **Cell 6**

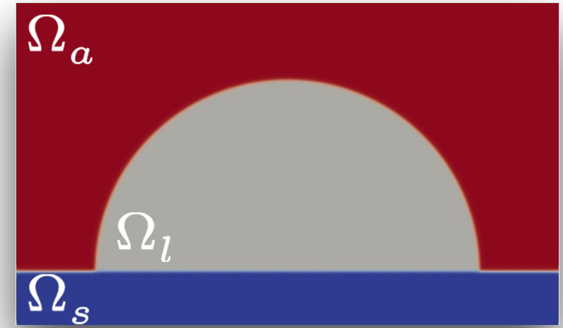
Three Phase system (*solid*-liquid-air)

Model

state $q = (u, \varphi) = (u, \varphi_1, \varphi_2)$

with displacement $u : \Omega \to \mathbb{R}^2$

and phase fields $\varphi_i : \Omega \to \mathbb{R}$



$$\varphi_1 = \begin{cases} +1 \text{ in } \Omega_s \\ -1 \text{ else} \end{cases} \qquad \varphi_2 = \begin{cases} +1 \text{ in } \Omega_l \\ -1 \text{ else} \end{cases} \qquad \varphi_3 = 1 - \varphi_1 - \varphi_2 = \begin{cases} +1 \text{ in } \Omega_a \\ -1 \text{ else} \end{cases}$$

free energy $\mathscr{E}(u, \varphi) = \int_\Omega W_{\mathrm{el}}(\mathbb{I} + \nabla u, \varphi) + W_{\mathrm{pf}}(\mathbb{I} + \nabla u, \varphi, \nabla \varphi) \mathrm{d}X$

$$W_{\mathrm{el}}(F, \varphi) = \frac{\boxed{G(\varphi)}}{2} \mathrm{Tr}(F^T F - I)$$

Neo-Hookean elasticity (elastic modulus $G(\varphi)$)

$$W_{\mathrm{pf}}(F, \varphi_i, \nabla \varphi_i) = \sum_i \gamma_i \left[\frac{1}{2\varepsilon} \left(\varphi_i^2 - 1 \right)^2 + \frac{\varepsilon}{2} \boxed{| F^{-T} \nabla \varphi_i |^2} \right]$$

Double well potential with gradient term (surface tension γ_i, interface width $\varepsilon > 0$)

Lagrangian $\mathscr{L}(u, \varphi, \lambda) = \mathscr{E}(u, \varphi) + \int_\Omega \lambda(\det(\mathbb{I} + \nabla u) - 1) \mathrm{d}X$

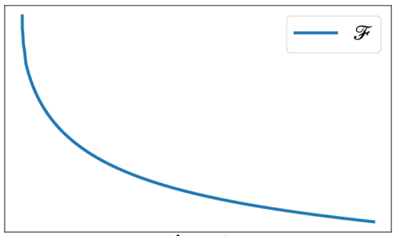
- Coupling via shear modulus $G(\varphi)$
- Coupling interface energy and diffusion/phase transition

Coupled nonlinear elasticity and phase fields

Recall the saddle point structure

$$\begin{aligned} a(\eta, \xi) + b(\partial_t q, \xi) &= 0 \\ b(v, \eta) &= \langle \mathrm{D}\mathscr{L}(q, \lambda), v \rangle \end{aligned}$$

with $q = (u, (\varphi_1, \varphi_2)), w = (w_u, w_\varphi)$ for $w \in \{\eta, \xi, v\}$



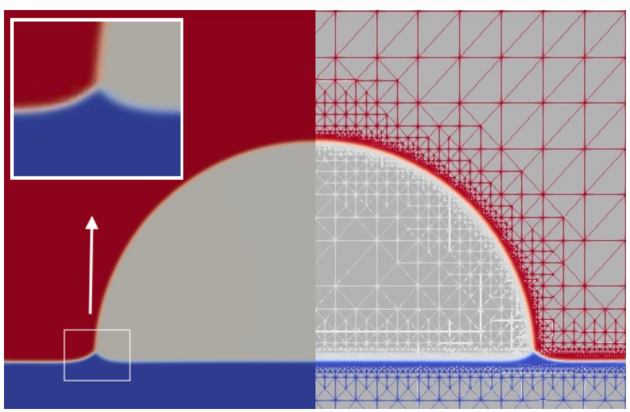
time t

Weak formulation

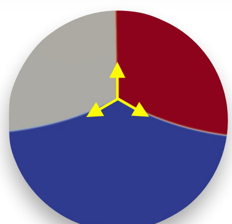
$$\begin{aligned} (M_{\mathrm{D}} \eta_u, \xi_u)_{L^2} + (\dot{u}, \xi_u)_{L^2} &= 0 \\ (m_{\mathrm{CH}} F^{-T} \nabla \eta_\varphi, F^{-T} \nabla \xi_\varphi)_{L^2} + (\dot{\varphi}, \xi_\varphi)_{L^2} &= 0 \\ (\eta_u, v_u)_{L^2} &= \langle \mathrm{D}_u \mathscr{L}(u, \varphi, \lambda), v_u \rangle \\ (\eta_\varphi, v_\varphi)_{L^2} &= \langle \mathrm{D}_\varphi \mathscr{L}(u, \varphi, \lambda), v_\varphi \rangle \\ 0 &= \langle \mathrm{D}_\lambda \mathscr{L}(u, \varphi, \lambda), v_\lambda \rangle \end{aligned}$$

- Darcy/Stokes dissipation M_{D}, Cahn Hilliard mobility m_{CH}
- Incremental minimization scheme
- Sharp-interface limit $\varepsilon \to 0$

Adaptive mesh refinement



Particular interest: three phase contact line



Neumann triangle

Different droplet shapes

Visualization and post-processing… ParaView

(open-source, multi-platform data analysis and visualization application)