An introduction to generalized gradient flows and application to complex porous media flows

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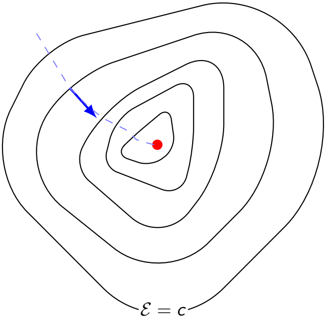
What is a gradient flow ?

Gradient flow

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{u}(t) = -\nabla_{\mathbf{u}}\mathcal{E}(\mathbf{u}(t))$$



System without inertia

Energy (entropy) dissipation

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{E}(\mathbf{u}) = \langle \frac{\mathrm{d}}{\mathrm{d}t}\mathbf{u}, \boldsymbol{\nabla}_{\mathbf{u}}\mathcal{E}(\mathbf{u})\rangle = -\frac{1}{2}\left|\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{u}\right|^2 - \frac{1}{2}\left|\boldsymbol{\nabla}_{\mathbf{u}}\mathcal{E}(\mathbf{u})\right|^2 \le 0.$$

Long time behavior

- Stable stationary solutions are local minima of $\mathcal{E}$
- Convergence towards a steady state as $t \to +\infty$ (Lasalle invariance principle)

Let us generalize a little bit

If $\mathbf{u}(t) \in H$ and $\mathcal{E} : H \to \mathbb{R}$, then

- $\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{u} \in H$
- $D\mathcal{E}(\mathbf{u}) \in H'$

▶ Riesz theorem:

$$G : \begin{cases} H' & \to & H \\ D\mathcal{E}(\mathbf{u}) & \to & \boldsymbol{\nabla}_{\mathbf{u}}\mathcal{E}(\mathbf{u}) \end{cases}$$

Let us generalize a little bit

If $\mathbf{u}(t) \in \mathcal{M}$ and $\mathcal{E} : \mathcal{M} \to \mathbb{R}$, then

- $\dfrac{\mathrm{d}}{\mathrm{d}t}\mathbf{u} \in T_{\mathbf{u}}\mathcal{M}$
- $D\mathcal{E}(\mathbf{u}) \in T_{\mathbf{u}}\mathcal{M}^*$

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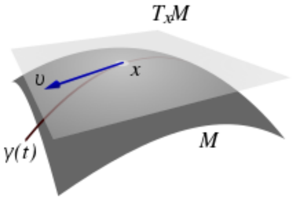
$$G(\mathbf{u}) : \begin{cases} T_{\mathbf{u}}\mathcal{M}^* & \to & T_{\mathbf{u}}\mathcal{M} \\ D\mathcal{E}(\mathbf{u}) & \to & \boldsymbol{\nabla}_{\mathbf{u}}\mathcal{E}(\mathbf{u}) \end{cases}$$



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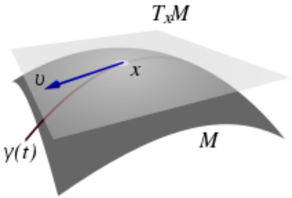

One readily checks that $G(\mathbf{u}) > 0$ and $G(\mathbf{u})^T = G(\mathbf{u})$

$$\Psi(\mathbf{u}, \boldsymbol{\xi}) = \frac{1}{2} G(\mathbf{u})^{-1} \boldsymbol{\xi} \cdot \boldsymbol{\xi} \quad \Longrightarrow \quad D\mathcal{E}(\mathbf{u}) = \nabla_{\boldsymbol{\xi}} \Psi(\mathbf{u}, \nabla_{\mathbf{u}}\mathcal{E}(\mathbf{u}))$$

Generalized gradient flow

$$\nabla_{\boldsymbol{\xi}} \Psi(\mathbf{u}, \partial_t \mathbf{u}) + D\mathcal{E}(\mathbf{u}) = 0 \quad \Leftrightarrow \quad \partial_t \mathbf{u} \in \mathrm{argmin}_{\boldsymbol{\xi}} \left(\Psi(\mathbf{u}, \boldsymbol{\xi}) + D\mathcal{E}(\mathbf{u}) \cdot \boldsymbol{\xi} \right)$$

The recipe of generalized gradient flow

[Mielke '11, Peletier '14]

(i) The state space $\mathcal{M}$ containing the state variable $\mathbf{u}$

(ii) An energy $\mathcal{E} : \mathcal{M} \to \mathbb{R} \cup \{+\infty\}$ (possibly non-smooth and singular)
The subdifferential $\partial\mathcal{E}(\mathbf{u})$ of $\mathcal{E}$ at $\mathbf{u}$ is possibly multivalued

(iii) A convex dissipation potential $\bigcup_{\mathbf{u}\in\mathcal{M}}\{\mathbf{u}\} \times T_{\mathbf{u}}\mathcal{M} \to \mathbb{R}_+$ with $\Psi(\mathbf{u}, \mathbf{0}) = 0$

(iv) Steepest descent condition:

$$\partial_t \mathbf{u} \in \underset{\boldsymbol{\xi}\in T_{\mathbf{u}}\mathcal{M}}{\operatorname{argmin}} \left[\Psi(\mathbf{u}, \boldsymbol{\xi}) + \sup_{\boldsymbol{\mu}\in\partial\mathcal{E}(\mathbf{u})} \boldsymbol{\mu}\cdot\boldsymbol{\xi} \right]$$

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RMK: Often, it is suitable to describe the dual dissipation potential

$$\boldsymbol{\nu} \mapsto \Psi^*(\mathbf{u}, \boldsymbol{\nu}) = \sup_{\boldsymbol{\xi}} \left[\boldsymbol{\xi}\cdot\boldsymbol{\nu} - \Psi(\mathbf{u}, \boldsymbol{\xi}) \right]$$

Duality and Onsager reciprocal relation

- The time variations $\partial_t \mathbf{u} \in T_{\mathbf{u}}\mathcal{M}$ and potentials $\boldsymbol{\mu} \in T_{\mathbf{u}}\mathcal{M}^*$ are in duality

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{E}(\mathbf{u}) = \langle \partial_t \mathbf{u}\ ,\ \boldsymbol{\mu} \rangle = -\Psi(\mathbf{u}, \partial_t \mathbf{u}) - \Psi^*(\mathbf{u}, -\boldsymbol{\mu}) \leq 0, \qquad \boldsymbol{\mu} \in \partial\mathcal{E}(\mathbf{u})$$

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- For balance laws, time variations can be deduced from fluxes

$$\boldsymbol{\xi} + \boldsymbol{\nabla}_x \cdot \boldsymbol{F} = 0, \qquad \boldsymbol{\xi} \in T_{\mathbf{u}}\mathcal{M}, \ x \in \Omega,$$

then dissipation potential

$$\Psi(\mathbf{u}, \boldsymbol{\xi}) = \inf_{\boldsymbol{F}} \int_\Omega \psi(\mathbf{u}, \boldsymbol{F})\mathrm{d}x, \quad \text{e.g. } \psi(\mathbf{u}, \boldsymbol{F}) = \frac{1}{2}\mathbb{A}(\mathbf{u})\boldsymbol{F} \cdot \boldsymbol{F}, \quad \mathbb{A}(\mathbf{u}) \in \mathcal{S}_n^{++}$$

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- For conservation laws

$$\partial_t \mathbf{u} + \boldsymbol{\nabla}_x \cdot \boldsymbol{J} = 0,$$

the 'gradient flow' flux is the one that fulfills Onsager's reciprocal

$$\boldsymbol{J} \in \partial\psi^*(\mathbf{u}, -\boldsymbol{\nabla}_x\boldsymbol{\mu}) = -\mathbb{A}(\mathbf{u})^{-1}\boldsymbol{\nabla}_x\boldsymbol{\mu}, \qquad \boldsymbol{\mu} \in \partial\mathcal{E}(\mathbf{u})$$

Example 1: immiscible incompressible two-phase flows

[C.-Gallouët-Monsaingeon '15 '17]

- *State space:*

$$\mathcal{M} = \left\{ \boldsymbol{s} = (s_o, s_w) : \Omega \to \mathbb{R}^2_+ \,\middle|\, s_o + s_w = 1 \text{ and } \int_\Omega \phi s_\alpha = \int_\Omega \phi s_\alpha^{\text{ini}} \right\}$$

$$T_{\boldsymbol{s}}\mathcal{M} \simeq \left\{ \boldsymbol{\xi} = (\xi_o, \xi_w) : \Omega \to \mathbb{R}^2 \,\middle|\, \xi_o + \xi_w = 0 \text{ and } \int_\Omega \phi \xi_\alpha = 0 \right\}$$

- *Energy functional:*

$$\mathcal{E}(\boldsymbol{s}) = \int_\Omega \phi \left[\Pi(s_o) + \sum_\alpha s_\alpha \rho_\alpha g z \right], \qquad \Pi'(s_o) = p_c(s_o)$$

$$\partial\mathcal{E}(\boldsymbol{s}) = \left\{ \mathbf{h} = (h_o, h_w) = (p_o + \rho_o g z, p_w + \rho_w g z) \,\middle|\, p_o - p_w = p_c(s_o) \right\}$$

Example 1: immiscible incompressible two-phase flows

[C.-Gallouët-Monsaingeon '15 '17]

- *Dissipation potential:* $\phi\boldsymbol{\xi} + \boldsymbol{\nabla}\cdot\boldsymbol{F} = \mathbf{0}$ with $\Psi(\boldsymbol{s},\boldsymbol{\xi}) = \inf_{\boldsymbol{F}} \int_\Omega \psi(\boldsymbol{s},\boldsymbol{F})$,

$$\psi(\boldsymbol{s},\boldsymbol{F}) = \sum_\alpha \frac{\mu_\alpha}{2k_\alpha(s_\alpha)}\mathbb{K}^{-1}F_\alpha\cdot F_\alpha$$

- *Steepest descent condition:*

$$\boldsymbol{J} = (J_o, J_w) \in \underset{\boldsymbol{F}}{\operatorname{argmin}}\left[\Psi(\boldsymbol{s},\boldsymbol{F}) + \sup_{\mathbf{h}\in\partial\mathcal{E}(\mathbf{u})}\sum_\alpha \boldsymbol{\nabla} h_\alpha\cdot F_\alpha\right]$$

We recover the Darcy Muskat law:

$$J_\alpha = -\frac{k_\alpha(s_\alpha)}{\mu_\alpha}\mathbb{K}\boldsymbol{\nabla}(p_\alpha + \rho_\alpha g z)$$

Example 2: linear poromechanics

[Both-Kumar-Nordbotten-Radu '19]

- *State space:*

$$H = \{(\mathbf{u}, \theta) : \Omega \to \mathbb{R}^d \times \mathbb{R}\}, \qquad TH = \{(\boldsymbol{v}, \xi) : \Omega \to \mathbb{R}^d \times \mathbb{R}\}$$

  - $\mathbf{u}$: porous matrix displacement,
  - θ: rescaled mass perturbation (dimensionless)

- *Energy:* elastic energy of the matrix + fluid

$$\mathcal{E}(\mathbf{u}, \theta) = \int_\Omega \left[\frac{1}{2}\mathbb{C}\epsilon(\mathbf{u}) : \epsilon(\mathbf{u}) + \frac{M}{2}\|\theta - \alpha \boldsymbol{\nabla} \cdot \mathbf{u}\|^2\right]$$

$$D\mathcal{E}(\mathbf{u}, \theta) \cdot (\boldsymbol{v}, \xi) = \int_\Omega [\mathbb{C}\epsilon(\mathbf{u}) : \epsilon(\boldsymbol{v}) + M(\theta - \alpha \boldsymbol{\nabla} \cdot \mathbf{u})(\xi - \alpha \boldsymbol{\nabla} \cdot \boldsymbol{v})]$$

Example 2: linear poromechanics

[Both-Kumar-Nordbotten-Radu '19]

- *Dissipation potential*: $\xi + \nabla \cdot \boldsymbol{F} = 0$, and dissipation only in the fluid part

$$\Psi(\boldsymbol{v}, \xi) = \inf_{\xi + \nabla \cdot \boldsymbol{F} = 0} \frac{1}{2} \int_\Omega \mathbb{K}^{-1} \boldsymbol{F} \cdot \boldsymbol{F}$$

- *Steepest descent condition:* find $\boldsymbol{J}$ such that $\partial_t \theta + \nabla \cdot \boldsymbol{J} = 0$ and

$$(\partial_t \mathbf{u}, \boldsymbol{J}) \in \operatorname{argmin} \left[\frac{1}{2} \int_\Omega \mathbb{K}^{-1} \boldsymbol{F} \cdot \boldsymbol{F} - D\mathcal{E}(\mathbf{u}, \theta)(\boldsymbol{v}, \nabla \cdot \boldsymbol{F}) \right]$$

Resulting system: Biot's model for poromechanics

$$\begin{cases} \partial_t \theta + \nabla \cdot \boldsymbol{J} = 0 \\ \boldsymbol{J} = -M\mathbb{K} \nabla (\theta - \alpha \nabla \cdot \mathbf{u}) \\ \int_\Omega \left[\mathbb{C}\epsilon(\mathbf{u}) : \epsilon(\boldsymbol{v}) + \mathbb{K}^{-1} \boldsymbol{J} \cdot \boldsymbol{v} \right] = 0, \quad \forall \boldsymbol{v} \end{cases}$$

Example 3: Chemistry

[Mielke '11]

R chemical reactions

$$\alpha_1^r X_1 + \cdots + \alpha_N^r X_N \underset{k_b^r}{\overset{k_f^r}{\rightleftharpoons}} \beta_1^r X_1 + \cdots + \beta_N^r X_N, \qquad 1 \leq r \leq R$$

with mass action law and detailed balance

$$\kappa^r := k_f^r \left(\boldsymbol{c}^{\mathrm{eq}}\right)^{\boldsymbol{\alpha}^r} = k_b^r \left(\boldsymbol{c}^{\mathrm{eq}}\right)^{\boldsymbol{\beta}^r}$$

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- *State space:*

$$\mathcal{M} = \{\boldsymbol{c} = (c_1, \ldots, c_N) \in \mathbb{R}^N_{>0}\}, \qquad T_{\boldsymbol{c}}\mathcal{M} = \{\boldsymbol{\mu} \in \mathbb{R}^N\}$$

- *Energy:*

$$\mathcal{E}(\boldsymbol{c}) = \sum_{i=1}^N c_i \log \frac{c_i}{c_i^{\mathrm{eq}}}, \qquad \boldsymbol{\mu} = \left(\log \frac{c_i}{c_i^{\mathrm{eq}}}\right)_i$$

Example 3: Chemistry

[Mielke '11]

- *Dissipation potential:* rather define the dual dissipation potential

$$\Psi^*(\boldsymbol{c}, \boldsymbol{\nu}) = \sum_{r=1}^{R} \frac{\kappa^r}{2} \Lambda \left(\frac{\boldsymbol{c}^{\boldsymbol{\alpha}^r}}{(\boldsymbol{c}^{\mathrm{eq}})^{\boldsymbol{\alpha}^r}}, \frac{\boldsymbol{c}^{\boldsymbol{\beta}^r}}{(\boldsymbol{c}^{\mathrm{eq}})^{\boldsymbol{\beta}^r}} \right) (\boldsymbol{\nu} \cdot (\boldsymbol{\alpha}^r - \boldsymbol{\beta}^r))^2$$

where $\Lambda(s, t) = \frac{s-t}{\log(s)-\log(t)}$ is the logarithmic mean.

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where $\Lambda(s,t) = \frac{s-t}{\log(s)-\log(t)}$ is the logarithmic mean.

- *Steepest descent condition:*

$$\partial_t \boldsymbol{c} \in \underset{\boldsymbol{\xi}}{\operatorname{argmin}} \left[\Psi(\boldsymbol{c},\boldsymbol{\xi}) + \boldsymbol{\mu}\cdot\boldsymbol{\xi}\right] \quad \Leftrightarrow \quad \partial_{\boldsymbol{\xi}} \Psi(\boldsymbol{c}, \partial_t \boldsymbol{c}) + \boldsymbol{\mu} = \mathbf{0}$$

$$\Leftrightarrow \quad \partial_t \boldsymbol{c} = \partial_{\boldsymbol{\xi}} \Psi^*(\boldsymbol{c}, -\boldsymbol{\mu}) = \sum_{i=1}^{R} \left(k_b^r \boldsymbol{c}^{\boldsymbol{\beta}^r} - k_f^r \boldsymbol{c}^{\boldsymbol{\alpha}^r}\right)(\boldsymbol{\alpha}^r - \boldsymbol{\beta}^r)$$

Example 4: multicomponent diffusion (Stefan-Maxwell)

[Bothe '11], [Jüngel-Stelzer '13], [C.-Ehrlacher-Monasse '20]

▷ Multicomponent fluid:

- $\boldsymbol{c} = (c_1, \ldots, c_N)$ concentrations with $\langle \boldsymbol{c}, \mathbf{1} \rangle = \sum_i c_i = 1$.
- $\mathfrak{J} = (\boldsymbol{J}_1, \ldots, \boldsymbol{J}_N)$ fluxes, with

$$\partial_t c_i + \nabla \cdot \boldsymbol{J}_i = 0$$

▷ Stefan-Maxwell relation:

$$\mathbb{A}(\boldsymbol{c})\mathfrak{J} + \nabla \boldsymbol{c} = \mathbf{0}, \qquad \langle \mathfrak{J}, \mathbf{1} \rangle = \sum_i \boldsymbol{J}_i = \mathbf{0}.$$

with $\mathbb{A}(\boldsymbol{c}) = (A_{i,j}(\boldsymbol{c}))$ not invertible given by

$$A_{i,j}(\boldsymbol{c}) = \begin{cases} \sum_{k \neq i} \frac{c_k}{d_{i,k}} & \text{if } i = j \\ -\frac{c_i}{d_{i,j}} & \text{if } i \neq j \end{cases}$$

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$$\partial_t c_i + \boldsymbol{\nabla} \cdot \boldsymbol{J}_i = 0$$

▷ Stefan-Maxwell relation:

$$\mathbb{B}(\boldsymbol{c})\mathfrak{J} + \boldsymbol{\nabla} \log(\boldsymbol{c}) = \mathbf{0}, \qquad \langle \mathfrak{J}, \mathbf{1} \rangle = \sum_i \boldsymbol{J}_i = \mathbf{0}.$$

with $\mathbb{B}(\boldsymbol{c}) = (B_{i,j}(\boldsymbol{c}))$ not invertible but symmetric positive semi-definite given by

$$B_{i,j}(\boldsymbol{c}) = \begin{cases} \sum_{k \neq i} \frac{c_k}{c_i d_{i,k}} & \text{if } i = j \\ -\frac{1}{d_{i,j}} & \text{if } i \neq j \end{cases}$$

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$$\mathcal{M} = \{\boldsymbol{c} \in \mathbb{R}^N_{>0} \mid \langle \boldsymbol{c}, \mathbf{1} \rangle = 1\}, \qquad TH = \{\boldsymbol{\mu} \in \mathbb{R}^N \mid \langle \boldsymbol{\mu}, \mathbf{1} \rangle = 0\}.$$

- *Energy:*

$$\mathcal{E}(\boldsymbol{c}) = \sum_{i=1}^{N} c_i \log(c_i), \qquad \boldsymbol{\mu} = (\log(c_i))_i$$

- *Dissipation potential:*

$$\Psi(\boldsymbol{c}, \boldsymbol{J}) = \frac{1}{2}\mathbb{B}(\boldsymbol{c})\boldsymbol{J} \cdot \boldsymbol{J} + \chi(\boldsymbol{J}), \qquad \chi(\boldsymbol{J}) = \begin{cases} 0 & \text{if } \langle \boldsymbol{J}, \mathbf{1} \rangle = 0, \\ +\infty & \text{otherwise.} \end{cases}$$

Why such a machinery?

A framework for the derivation of stable coupled models

- Multiphase-multicomponent flows in porous media [Smaï '20]
- Bulk/surface (or fracture) interaction [Glitzky-Mielke '13]
- Problems on moving domains (ongoing)

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An inspiration to design numerical methods

- Variational (optimization based) schemes [Li-Lu-Wang '20], [C.-Gallouët-Todeschi '20], [Van Brunt-Farell-Monroe '20], ...
- More generally, it helps to design stable numerical schemes

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A guide to build numerical solvers

- Optimization based solvers for variational schemes [Both-Kumar-Nordbotten-Radu'19], [Li-Lu-Wang '20]
- Primal $\boldsymbol{c} \in \mathcal{M}$ and dual $\boldsymbol{\mu} \in T_{\mathbf{u}}\mathcal{M}^*$ variables
  variable switch based strategies (Sabrina's talk)