Generalized Gradient Structures for Semi-discrete TPFA Finite Volume Methods

FVOT Workshop
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Gradient Structures

Aggregation-Diffusion

$$\mathscr{F}'(\rho)(x) = V(x) + \int W(x-y)\,\rho(dy)$$

Cont. Eqn. $$\partial_t \rho + \mathbf{div}\, J = 0$$

Kin. Rel. $$J = -\,\varepsilon \nabla \rho - \rho \nabla \mathscr{F}'(\rho) = -\,\rho \nabla \mathscr{E}_\varepsilon'(\rho)$$

Driving Energy $$\mathscr{E}_\varepsilon(\rho) = \varepsilon \int \phi(\rho(x))\,dx + \mathscr{F}(\rho)$$

Gradient Structures

Aggregation-Diffusion

$$\mathcal{E}_\varepsilon(\rho) = \varepsilon \int \phi(\rho(x))\, dx + \mathcal{F}(\rho)$$

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Kin. Rel. $J = -\varepsilon \nabla \rho - \rho \nabla \mathcal{F}'(\rho) = -\rho \nabla \mathcal{E}'_\varepsilon(\rho)$

Force-Flux $= \partial_2 \mathcal{R}^*(\rho, -\nabla \mathcal{E}'_\varepsilon(\rho))$

2-Wasserstein Action

(dual) Diss. Pot. $\mathcal{R}^*(\rho, \xi) = \dfrac{1}{2} \displaystyle\int |\xi|^2 d\rho$ $\qquad \mathcal{R}(\rho, J) = \dfrac{1}{2} \displaystyle\int \left| \frac{dJ}{d\rho} \right|^2 d\rho$

Legendre Duality

$$\mathcal{R}(\rho, J) + \mathcal{R}^*(\rho, -\nabla \mathcal{E}'_\varepsilon(\rho)) = \langle J, -\nabla \mathcal{E}'_\varepsilon(\rho) \rangle$$

$$\int |-\nabla \mathcal{E}'_\varepsilon(\rho)|^2 d\rho = -\frac{d}{dt} \mathcal{E}_\varepsilon(\rho)$$ **Chain rule**

Gradient Structures

Aggregation-Diffusion

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Legendre Duality

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Energy-dissipation balance

$$0 \le \underbrace{\int_s^t \mathscr{R}(\rho, J) + \overbrace{\mathscr{R}^*(\rho, -\nabla \mathscr{E}'_\varepsilon(\rho))}^{\text{Fisher information}}\,dr + \mathscr{E}_\varepsilon(\rho_t) - \mathscr{E}_\varepsilon(\rho_s)}_{\mathscr{L}([s,t];(\rho,J))} = 0$$

Gradient Structures

Aggregation-Diffusion

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Gradient Flow A density-flux pair (ρ, J) is an $(\mathscr{R}^*, \mathscr{E})$-gradient flow if

- (ρ, J) satisfies **Cont. Eqn.** and
- **Energy-dissipation balance**

Otto-Wasserstein Gradient Flow

$$\mathscr{L}([s,t];(\rho, J)) = 0 \qquad \forall [s,t] \subset [0,T]$$

Finite Volume Methods

$$\partial_t \rho + \textbf{div}\, J = 0$$

Discrete continuity equation

p is the law of a random walk with net jump intensities J

Setting $\mathsf{p}_K = \rho(K),\, K \in \mathcal{T}$

Cont. Eqn. $$\partial_t \mathsf{p} + \overline{\textbf{div}}\, \mathsf{J} = 0, \qquad \overline{\textbf{div}}\, \mathsf{J}(K) = \sum_{L \sim K} \mathsf{J}_{KL}$$

Discrete structures

Vertex function $\varphi \in B(\mathcal{T})$

Edge function $\mathsf{j} \in B(\mathcal{T} \times \mathcal{T})$

Discrete **Gradient** $\overline{\nabla} : B(\mathcal{T}) \to B(\mathcal{T} \times \mathcal{T}); \quad \overline{\nabla}\varphi\,(K, L) = \varphi(L) - \varphi(K)$

Discrete **Divergence** $\overline{\nabla} \odot : B(\mathcal{T} \times \mathcal{T}) \to B(\mathcal{T}); \quad \overline{\nabla} \odot \mathsf{j} = \sum_L \left(\mathsf{j}_{KL} - \mathsf{j}_{LK}\right)$

$$\sum_{K,L} \overline{\nabla}\varphi(K, L)\, \mathsf{j}_{KL} = -\sum_K \varphi(K)\, \overline{\nabla} \odot \mathsf{j}\,(K) = -\langle \varphi, \overline{\textbf{div}}\, \mathsf{J} \rangle, \qquad \mathsf{J} = \mathsf{j} - s_\# \mathsf{j}$$

Finite Volume Methods

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$$\overline{\mathbf{div}}\, \mathsf{J}(K) = \sum_{L \sim K} \mathsf{J}_{KL}$$

Examples:

Upwind $\mathsf{J}_{KL} = \tau_{KL}\left(\xi_{KL}^{+}\, \mathsf{u}_K - \xi_{KL}^{-}\, \mathsf{u}_L\right)$

$$\mathsf{u}_K = \frac{\rho_K}{|K|}$$

B-schemes $\mathsf{J}_{KL} = \varepsilon\tau_{KL}\left(\mathfrak{b}(\xi_{KL}/\varepsilon)\, \mathsf{u}_K - \mathfrak{b}(-\xi_{KL}/\varepsilon)\, \mathsf{u}_L\right)$

SG $\mathfrak{b}(r) = r/(e^r - 1)$

SQRA $\mathfrak{b}(r) = e^{-r/2}$

Question: **Is there a (generalized) gradient structure** $(\mathsf{R}^*, \mathsf{E})$ **such that**

Force-Flux $\mathsf{J} = \partial_2 \mathsf{R}^*(\mathsf{p}, -\overline{\nabla}\mathsf{E}'(\mathsf{p}))$ **?** **Yes!** **Many!**

Good(?) Gradient Structures

$$\mathsf{J} = \partial_2 \mathsf{R}^*(\mathsf{p}, -\overline{\nabla}\mathsf{E}'(\mathsf{p}))$$

Driving Energy

$$\mathsf{E}_\varepsilon(\mathsf{p}) = \varepsilon \sum_K |K|\, \phi(\mathsf{u}_K) + \mathsf{F}(\mathsf{p})$$

(dual) Diss. Pot.

$$\mathsf{R}^*_\varepsilon(\mathsf{p}, \xi) = \frac{1}{2} \sum_{K,L} \vartheta^{\varepsilon,\mathsf{p}}_{KL}\, \Psi^*_\varepsilon(\xi_{KL})\, \mathfrak{m}(\mathsf{p}_K, \mathsf{p}_L)$$

Examples:

Maas-Mielke $\Psi^*_\varepsilon(\xi) = \xi^2, \quad \mathfrak{m} = \mathfrak{m}_{log}$ — R_ε **metric**

Cosh $\Psi^*_\varepsilon(\xi) = 4\varepsilon^2\big(\cosh(\xi/(2\varepsilon)) - 1\big), \quad \mathfrak{m} = \mathfrak{m}_{geo}$ — R_ε **non-metric**

SG-Cosh

$$\vartheta^{\varepsilon,\mathsf{p}}_{KL} = 2\tau_{KL} \frac{(\mathsf{Q}^\mathsf{p}_L - \mathsf{Q}^\mathsf{p}_K)/\varepsilon}{\exp(\mathsf{Q}^\mathsf{p}_L/\varepsilon) - \exp(\mathsf{Q}^\mathsf{p}_K/\varepsilon)}, \qquad \mathsf{Q}^\mathsf{p}_K = \mathsf{F}'(\mathsf{p})(K)$$

Force-Flux

$$\partial_2 \mathsf{R}^*_\varepsilon(\mathsf{p}, -\overline{\nabla}\mathsf{E}'_\varepsilon(\mathsf{p}))(K, L) = \varepsilon\tau_{KL}\mathfrak{b}((\mathsf{Q}^\mathsf{p}_L - \mathsf{Q}^\mathsf{p}_K)/\varepsilon)\, \mathsf{u}_K = \mathsf{J}_{KL}$$

Question: Are they good?

Good(?) Gradient Structures

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Question: Are they good? **No**

Desirable properties of R^*

- ***Tilt invariant*, i.e., independent of F**
- **Stable under $\varepsilon \to 0$ limit.**

Properties of continuous dissipation potentials

Good(?) Gradient Structures

$\mathsf{J} = \partial_2 \mathsf{R}^*(\mathsf{p}, -\overline{\nabla}\mathsf{E}'(\mathsf{p}))$

Driving Energy

$$\mathsf{E}_\varepsilon(\mathsf{p}) = \varepsilon \sum_K |K| \phi(\mathsf{u}_K) + \mathsf{F}(\mathsf{p})$$

(dual) Diss. Pot.

$$\mathsf{R}^*_\varepsilon(\mathsf{p}, \xi) = \sum_{K,L} \tau_{KL}\, \alpha^*_\varepsilon\big(\mathsf{u}_K, \mathsf{u}_L, \xi_{KL}\big)$$

Question: **Are they good?** **No**

Desirable properties of R^*

- ***Tilt invariant*, i.e., independent of** F
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Properties of continuous dissipation potentials

Idea: **Use Kin. Rel. to derive** α^*_ε

Good(?) Gradient Structures

$$\mathsf{J} = \partial_2 \mathsf{R}^*(\mathsf{p}, -\overline{\nabla}\mathsf{E}'(\mathsf{p}))$$

Driving Energy

$$\mathsf{E}_\varepsilon(\mathsf{p}) = \varepsilon \sum_K |K|\,\phi(\mathsf{u}_K) + \mathsf{F}(\mathsf{p})$$

(dual) Diss. Pot.

$$\mathsf{R}^*_\varepsilon(\mathsf{p}, \xi) = \sum_{K,L} \tau_{KL}\, \alpha^*_\varepsilon\big(\mathsf{u}_K, \mathsf{u}_L, \xi_{KL}\big)$$

Idea: **Use Kin. Rel. to derive** α^*_ε

Force

$$\xi_{KL} = -\overline{\nabla}\mathsf{E}'(\mathsf{p})(K, L) = -\varepsilon \log \frac{\mathsf{u}_L}{\mathsf{u}_K} - \big(\mathsf{Q}^\mathsf{p}_L - \mathsf{Q}^\mathsf{p}_K\big), \qquad \mathsf{Q}^\mathsf{p}_K = \mathsf{F}'(\mathsf{p})(K)$$

Kin. Rel.

$$\mathsf{J}_{KL} = \varepsilon\tau_{KL}\Big(\mathfrak{b}((\mathsf{Q}^\mathsf{p}_L - \mathsf{Q}^\mathsf{p}_K)/\varepsilon)\,\mathsf{u}_K - \mathfrak{b}(-(\mathsf{Q}^\mathsf{p}_L - \mathsf{Q}^\mathsf{p}_K)/\varepsilon)\,\mathsf{u}_L\Big)$$

$$= \varepsilon\tau_{KL}\sinh(\xi_{KL}/(2\varepsilon))\,\mathfrak{m}_{HL}\big(\mathsf{u}_K e^{-\xi_{KL}/(2\varepsilon)}, \mathsf{u}_L e^{\xi_{KL}/(2\varepsilon)}\big)$$

$$= \tau_{KL}\,\partial_\xi\,\alpha^*_\varepsilon\,(\mathsf{u}_K, \mathsf{u}_L, \xi_{KL})$$

$$\alpha^*_\varepsilon\,(a, b, \xi) = 2\varepsilon^2 \int_0^{\xi/(2\varepsilon)} \sinh(r)\,\mathfrak{m}_{HL}(ae^{-r}, be^{r})\,dr$$

Good Gradient Structure

$\mathsf{J} = \partial_2 \mathsf{R}^*(\mathsf{p}, -\overline{\nabla}\mathsf{E}'(\mathsf{p}))$

(dual) Diss. Pot. $$\mathsf{R}^*_\varepsilon(\mathsf{p}, \xi) = \sum_{K,L} \tau_{KL}\, \alpha^*_\varepsilon\big(\mathsf{u}_K, \mathsf{u}_L, \xi_{KL}\big)$$ **Independent of F!**

$$\alpha^*_\varepsilon(a, b, \xi) = 2\varepsilon^2 \int_0^{\xi/(2\varepsilon)} \sinh(r)\, \mathfrak{m}_{HL}(ae^{-r}, be^{r})\, dr$$

Properties of α^*_ε

- Superlinear at infinity and convex in ξ,
  positively 1-homogeneous and jointly concave in (a, b)
  $\rightsquigarrow$ **Dynamical-Variational Transport Cost**
- $$\alpha^*_\varepsilon(a, b, \xi) \longrightarrow \frac{1}{4}\big(a\,|\xi^+|^2 + b\,|\xi^-|^2\big) \quad \text{as} \quad \varepsilon \to 0$$ **Stable under $\varepsilon \to 0$**
  $$=: \alpha^*_0(a, b, \xi)$$ **Upwind**
- $$\alpha^*_\varepsilon(a, b, -\varepsilon \log(a/b) - q) \longrightarrow \alpha^*_0(a, b, q)$$ **Fisher information** $\mathsf{R}^*_\varepsilon(\mathsf{p}, -\overline{\nabla}\mathsf{E}'_\varepsilon(\mathsf{p}))$
- and more...

Good Gradient Structure

$$\mathsf{J} = \partial_2 \mathsf{R}^*(\mathsf{p}, -\overline{\nabla}\mathsf{E}'(\mathsf{p}))$$

Driving Energy

$$\mathsf{E}_\varepsilon(\mathsf{p}) = \varepsilon \sum_K |K| \phi(\mathsf{u}_K) + \mathsf{F}(\mathsf{p})$$

(dual) Diss. Pot.

$$\mathsf{R}^*_\varepsilon(\mathsf{p}, \xi) = \sum_{K,L} \tau_{KL}\, \alpha^*_\varepsilon\left(\mathsf{u}_K, \mathsf{u}_L, \xi_{KL}\right)$$

SG

$$\mathsf{J}_{KL} = \tau_{KL}\, \partial_\xi\, \alpha^*_\varepsilon\, (\mathsf{u}_K, \mathsf{u}_L, \xi_{KL})$$

Legendre Duality

$$\alpha_\varepsilon\left(\mathsf{u}_K, \mathsf{u}_L, \frac{\mathsf{J}_{KL}}{\tau_{KL}}\right) + \alpha^*_\varepsilon\, (\mathsf{u}_K, \mathsf{u}_L, \xi_{KL}) = \frac{\mathsf{J}_{KL}}{\tau_{KL}}\, \xi_{KL}$$

Gradient Flow A density-flux pair (p, J) is an $(\mathsf{R}^*_\varepsilon, \mathsf{E}_\varepsilon)$-gradient flow if

- (p, J) satisfies **Cont. Eqn.** $\partial_t \mathsf{p} + \overline{\mathbf{div}}\, \mathsf{J} = 0$, and
- **Energy-dissipation balance**

$$0 \leq \int_s^t \mathsf{R}_\varepsilon(\mathsf{p}, \mathsf{J}) + \mathsf{R}^*_\varepsilon(\mathsf{p}, -\overline{\nabla}\mathsf{E}'_\varepsilon(\mathsf{p}))\, dr + \mathsf{E}_\varepsilon(\mathsf{p}_t) - \mathsf{E}_\varepsilon(\mathsf{p}_s) = 0$$

Good Gradient Structure

$$J = \partial_2 R^*(p, -\overline{\nabla} E'(p))$$

Driving Energy

$$E_\varepsilon(p) = \varepsilon \sum_K |K| \phi(u_K) + F(p) \longrightarrow F(p)$$

(dual) Diss. Pot.

$$R^*_\varepsilon(p, \xi) = \sum_{K,L} \tau_{KL}\, \alpha^*_\varepsilon\big(u_K, u_L, \xi_{KL}\big) \longrightarrow \sum_{K,L} \tau_{KL}\, \alpha^*_0\big(u_K, u_L, \xi_{KL}\big)$$

Gradient Flow A density-flux pair (p, J) is an $(R^*_\varepsilon, E_\varepsilon)$-gradient flow if

- (p, J) satisfies **Cont. Eqn.** $\partial_t p + \overline{\mathbf{div}}\, J = 0$, and
- **Energy-dissipation balance**

$$0 \leq \int_s^t R_\varepsilon(p, J) + R^*_\varepsilon(p, -\overline{\nabla} E'_\varepsilon(p))\, dr + E_\varepsilon(p_t) - E_\varepsilon(p_s) = 0$$

Result: **For each $\varepsilon > 0$, $(R^*_\varepsilon, E_\varepsilon)$-gradient flow density-flux pair $(p^\varepsilon, J^\varepsilon)$ exist**

Question: **Gradient structure for $\varepsilon = 0$?**

From SG to Upwind

$$\partial_t \mathsf{p} + \overline{\mathbf{div}}\, \mathsf{J} = 0$$

Let $(\mathsf{p}^\varepsilon, \mathsf{J}^\varepsilon)$ be an $(\mathsf{R}^*_\varepsilon, \mathsf{E}_\varepsilon)$-gradient flow

$$0 \le \int_s^t \mathsf{R}_\varepsilon(\mathsf{p}^\varepsilon, \mathsf{J}^\varepsilon) + \mathsf{R}^*_\varepsilon(\mathsf{p}^\varepsilon, -\overline{\nabla}\mathsf{E}'_\varepsilon(\mathsf{p}^\varepsilon))\, dr + \mathsf{E}_\varepsilon(\mathsf{p}^\varepsilon_t) - \mathsf{E}_\varepsilon(\mathsf{p}^\varepsilon_s) = 0$$

Result: **There exists (p, J) satisfying Cont. Eqn. such that**

- **Compactness:** $\mathsf{p}^\varepsilon_t \rightharpoonup^* \mathsf{p}_t$ **in** $\mathscr{M}^+(\mathscr{T})$ **for every** $t \ge 0$

  $\mathsf{J}^\varepsilon_t \otimes dt \rightharpoonup^* \mathsf{J}_t \otimes dt$ **in** $\mathscr{M}^+([0,T] \times \mathscr{T} \times \mathscr{T})$

- **Liminf inequality:** $\frac{1}{2}\int_s^t \mathsf{R}_0(\mathsf{p}, 2\mathsf{J})\, dr \le \liminf_{\varepsilon\to 0} \int_s^t \mathsf{R}_\varepsilon(\mathsf{p}^\varepsilon, \mathsf{J}^\varepsilon)\, dr$

  $$\frac{1}{2}\int_s^t \mathsf{R}^*_0(\mathsf{p}, -\overline{\nabla}\mathsf{F}'(\mathsf{p}))\, dr \le \liminf_{\varepsilon\to 0} \int_s^t \mathsf{R}^*_\varepsilon(\mathsf{p}^\varepsilon, -\overline{\nabla}\mathsf{E}'_\varepsilon(\mathsf{p}^\varepsilon))\, dr$$

- **Energy convergence:** $\lim_{\varepsilon\to 0} \mathsf{E}_\varepsilon(\mathsf{p}^\varepsilon_t) = \mathsf{F}(\mathsf{p}_t)$ **for every** $t \ge 0$

From SG to Upwind

$$\partial_t \mathsf{p} + \overline{\mathbf{div}}\, \mathsf{J} = 0$$

Let $(\mathsf{p}^\varepsilon, \mathsf{J}^\varepsilon)$ **be an** $(\mathsf{R}^*_\varepsilon, \mathsf{E}_\varepsilon)$**-gradient flow**

$$\int_s^t \mathsf{R}_0(\mathsf{p}, 2\mathsf{J}) + \mathsf{R}^*_0(\mathsf{p}, -\overline{\nabla}\mathsf{F}'(\mathsf{p}))\, dr + 2\mathsf{F}(\mathsf{p}_t) - 2\mathsf{F}(\mathsf{p}_s) \le 0$$

Result: **There exists** (p, J) **satisfying Cont. Eqn. such that**

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- **Energy convergence:** $\lim_{\varepsilon \to 0} \mathsf{E}_\varepsilon(\mathsf{p}^\varepsilon_t) = \mathsf{F}(\mathsf{p}_t)$ **for every** $t \ge 0$

From SG to Upwind

$$\partial_t \mathsf{p} + \overline{\mathbf{div}}\, \mathsf{J} = 0$$

Let $(\mathsf{p}^\varepsilon, \mathsf{J}^\varepsilon)$ **be an** $(\mathsf{R}_\varepsilon^*, \mathsf{E}_\varepsilon)$**-gradient flow**

Chain rule $$0 \leq \int_s^t \mathsf{R}_0(\mathsf{p}, 2\mathsf{J}) + \mathsf{R}_0^*(\mathsf{p}, -\overline{\nabla}\mathsf{F}'(\mathsf{p}))\, dr + 2\mathsf{F}(\mathsf{p}_t) - 2\mathsf{F}(\mathsf{p}_s) \leq 0$$

Result: **There exists** (p, J) **satisfying Cont. Eqn. such that**

- **Compactness:** $\mathsf{p}_t^\varepsilon \rightharpoonup^* \mathsf{p}_t$ **in** $\mathscr{M}^+(\mathscr{T})$ **for every** $t \geq 0$

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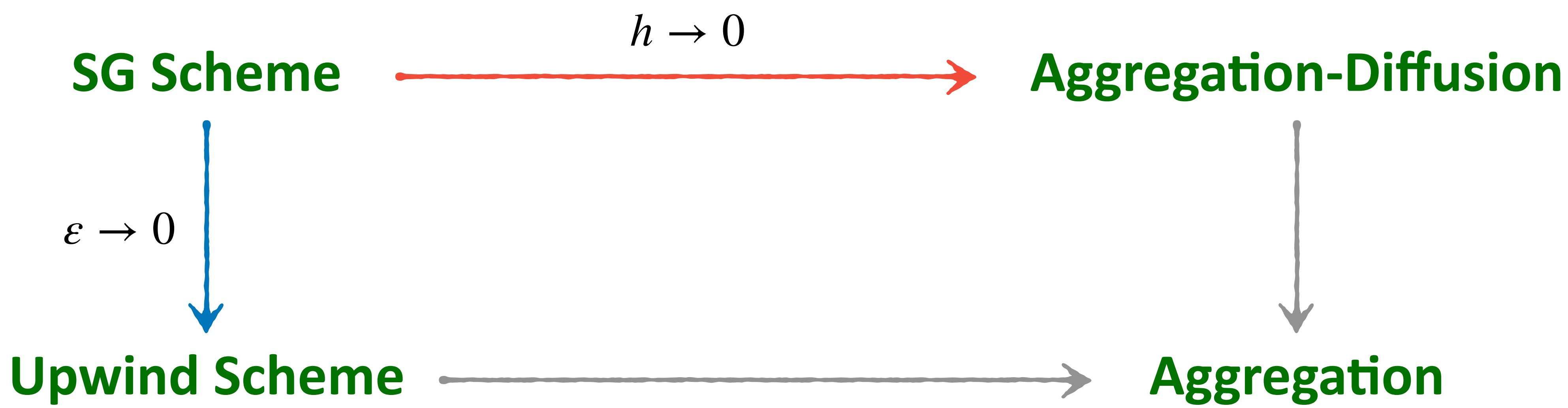
- **Liminf inequality:** $$\frac{1}{2}\int_s^t \mathsf{R}_0(\mathsf{p}, 2\mathsf{J})\, dr \leq \liminf_{\varepsilon \to 0} \int_s^t \mathsf{R}_\varepsilon(\mathsf{p}^\varepsilon, \mathsf{J}^\varepsilon)\, dr$$

  $$\frac{1}{2}\int_s^t \mathsf{R}_0^*(\mathsf{p}, -\overline{\nabla}\mathsf{F}'(\mathsf{p}))\, dr \leq \liminf_{\varepsilon \to 0} \int_s^t \mathsf{R}_\varepsilon^*(\mathsf{p}^\varepsilon, -\overline{\nabla}\mathsf{E}_\varepsilon'(\mathsf{p}^\varepsilon))\, dr$$

- **Energy convergence:** $\lim_{\varepsilon \to 0} \mathsf{E}_\varepsilon(\mathsf{p}_t^\varepsilon) = \mathsf{F}(\mathsf{p}_t)$ **for every** $t \geq 0$

Summary

- **Good** (generalized) Gradient Structure for **SG** and **Upwind**
- **SG** to **Upwind** limit via **Evolutionary Γ-convergence**



let the real show begin…