A posteriori analysis of a discontinuous Galerkin scheme for a diffuse interface model

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Outline

1. Van-der-Waals fluid model
2. Relative entropy stability framework
   - convex energy
   - non-convex energy
3. Semi-discrete dG scheme
4. Reconstruction and error estimate

Van-der-Waals fluid model

One space dimension; describing fluid flows undergoing liquid-vapor phase transition:

$$\begin{aligned} u_t - v_x &= 0 \\ v_t - W'(u)_x &= \mu v_{xx} - \gamma u_{xxx} \end{aligned} \tag{vdW}$$

- u specific volume, v velocity
- W non-convex energy density $\Rightarrow$ (vdW) is hyperbolic-elliptic
- $W \in C^3(\mathbb{R}, [0, \infty))$
- $\gamma > 0$ capillarity parameter, $\mu \geq 0$ viscosity.

We consider the problem on the flat circle, denoted S^1.

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Associated energy balance

$$\Big(W(u)+\frac{\gamma}{2}(u_x)^2+\frac{1}{2}v^2\Big)_t-\Big(vW'(u)-\gamma v u_{xx}+\gamma v_x u_x+\mu v v_x\Big)_x+\mu(v_x)^2 = 0.$$

Recall: Standard relative entropy (W strictly convex)

Consider the non-regularized, hyperbolic problem

$$\begin{aligned} u_t - v_x &= 0 \\ v_t - W'(u)_x &= 0 \end{aligned}$$

with W strictly convex.
Solutions (u, v), $(\tilde{u}, \tilde{v})$ can be compared by their relative entropy

$$\int_{S^1} W(\tilde{u}) - W(u) - W'(u)(\tilde{u} - u) + \frac{1}{2}(\tilde{v} - v)^2 \,\mathrm{d}\, x,$$

which is equivalent to

$$\|\tilde{u} - u\|^2_{L^2(S^1)} + \|\tilde{v} - v\|^2_{L^2(S^1)}.$$

Recall: Standard relative entropy (W strictly convex)

The relative entropy satisfies

$$
\begin{aligned}
&\frac{\mathrm{d}}{\mathrm{d}\,t}\int_{S^1} W(\tilde{u}) - W(u) - W'(u)(\tilde{u}-u) + \frac{1}{2}(\tilde{v}-v)^2 \,\mathrm{d}\,x \\
&- \int_{S^1} \Big(\tilde{v}\,W'(\tilde{u}) - vW'(u) - W'(u)(\tilde{v}-v) - v(W'(\tilde{u}) - W'(u))\Big)_x \,\mathrm{d}\,x \\
&\leq \int_{S^1} v_x\big(W'(\tilde{u}) - W'(u) - W''(u)(\tilde{u}-u)\big)\,\mathrm{d}\,x.
\end{aligned}
$$

Standard relative entropy argument (W strictly convex)

For $|W'''|$ bounded and v Lipschitz this implies

$$\begin{aligned}
&\frac{\mathrm{d}}{\mathrm{d}\,t}\int_{S^1} W(\tilde{u}) - W(u) - W'(u)(\tilde{u}-u) + \frac{1}{2}(\tilde{v}-v)^2 \,\mathrm{d}\,x \\
&\leq C\big(\|\tilde{u}-u\|^2_{L^2(S^1)} + \|\tilde{v}-v\|^2_{L^2(S^1)}\big) \\
&\leq C\int_{S^1} W(\tilde{u}) - W(u) - W'(u)(\tilde{u}-u) + \frac{1}{2}(\tilde{v}-v)^2 \,\mathrm{d}\,x.
\end{aligned}$$

Therefore, by Gronwall's Lemma, the relative entropy grows at most exponentially and, therefore, for $t > s$

$$\begin{aligned}
&\|\tilde{u}(t,\cdot) - u(t,\cdot)\|_{L^2} + \|\tilde{v}(t,\cdot) - v(t,\cdot)\|_{L^2} \\
&\qquad \leq e^{C(t-s)}\Big(\|\tilde{u}(s,\cdot) - u(s,\cdot)\|_{L^2} + \|\tilde{v}(s,\cdot) - v(s,\cdot)\|_{L^2}\Big).
\end{aligned}$$

Back to the multi-phase case, i.e., W not convex

Regularized model:

$$\begin{aligned} u_t - v_x &= 0 \\ v_t - W'(u)_x &= \mu v_{xx} - \gamma u_{xxx}. \end{aligned}$$

For different (u, v) $(\tilde{u}, \tilde{v})$ their relative entropy is given by

$$\int_{S^1} W(\tilde{u}) - W(u) - W'(u)(\tilde{u} - u) + \frac{1}{2}(\tilde{v} - v)^2 + \frac{\gamma}{2}(\tilde{u}_x - u_x)^2 \,\mathrm{d}\, x,$$

which is not convex, as W is not convex and γ is small.
On S^1 there are no boundary terms, and we obtain

$$\begin{aligned} &\frac{\mathrm{d}}{\mathrm{d}\, t} \int_{S^1} W(\tilde{u}) - W(u) - W'(u)(\tilde{u} - u) + \frac{1}{2}(\tilde{v} - v)^2 + \frac{\gamma}{2}(\tilde{u}_x - u_x)^2 \,\mathrm{d}\, x \\ &\leq \int_{S^1} v_x (W'(\tilde{u}) - W'(u) - W''(u)(\tilde{u} - u)) - \mu (v_x - \tilde{v}_x)^2 \,\mathrm{d}\, x. \end{aligned}$$

Estimating the partial relative entropy rate

Idea: Remove the W terms from the relative entropy. Indeed

$$
\begin{aligned}
&\partial_t\Big(W(\tilde u) - W(u) - W'(u)(\tilde u - u)\Big)\\
=&W'(\tilde u)\tilde u_t - W'(u)u_t - W''(u)u_t(\tilde u - u) - W'(u)\tilde u_t + W'(u)u_t\\
=&\tilde v_x W'(\tilde u) - \tilde v_x W'(u) - v_x W''(u)(\tilde u - u).
\end{aligned}
$$

Thus, we can shift the W terms to the right hand side and find

$$
\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}\,t}\int_{S^1} \frac{1}{2}(\tilde v - v)^2 + \frac{\gamma}{2}(\tilde u_x - u_x)^2 \,\mathrm{d}\,x&\\
\le \int_{S^1} (v - \tilde v)_x (W'(\tilde u) - W'(u)) - \mu(v_x - \tilde v_x)^2 \,\mathrm{d}\,x&.
\end{aligned}
$$

Continuous dependence on initial data

Lemma (JG '13)

For $\mu > 0$ *let* $u_0, \tilde{u}_0 \in H^3(S^1)$, $v_0, \tilde{v}_0 \in H^2(S^1)$ *be given with* $\int_{S^1} (u_0 - \tilde{u}_0)\,\mathrm{d}x = 0$.
Then, for any $T > 0$*, it exists a constant* $C = C(u_0, v_0, \gamma, \mu, T)$ *such that*

$$\|v(t,\cdot) - \tilde{v}(t,\cdot)\|_{L^2(S^1)} + |u(t,\cdot) - \tilde{u}(t,\cdot)|_{H^1(S^1)} \leq C\Big(\|v_0 - \tilde{v}_0\|_{L^2(S^1)} + |u_0 - \tilde{u}_0|_{H^1(S^1)}\Big)$$

for all $t \leq T$.

Sketch of the proof: For any $T > 0$ there exist strong solutions

$$u, \tilde{u} \in C^1((0,T), L^2(S^1)) \cap C^0((0,T), H^3(S^1))$$
$$v, \tilde{v} \in C^1((0,T), L^2(S^1)) \cap C^0((0,T), H^2(S^1)).$$

Sketch of the proof

Due to the energy inequality and the continuous embedding $H^1(S^1) \to C^0(S^1)$, we find that $\|u\|_{L^\infty}, \|\tilde{u}\|_{L^\infty} < \infty$.
The partial relative entropy calculation leads to

$$\frac{\mathrm{d}}{\mathrm{d}\,t} \int_{S^1} \frac{1}{2}(\tilde{v} - v)^2 + \frac{\gamma}{2}(\tilde{u}_x - u_x)^2 \,\mathrm{d}\,x \\ = \int_{S^1} (\tilde{v} - v)_x (W'(u) - W'(\tilde{u})) - \mu(v_x - \tilde{v}_x)^2 \,\mathrm{d}\,x.$$

Such that by Young's and Poincaré's inequality

$$\frac{\mathrm{d}}{\mathrm{d}\,t} \int_{S^1} \frac{1}{2}(\tilde{v} - v)^2 + \frac{\gamma}{2}(\tilde{u}_x - u_x)^2 \,\mathrm{d}\,x \leq C \int_{S^1} \frac{\gamma}{2}(\tilde{u}_x - u_x)^2 \,\mathrm{d}\,x.$$

Gronwall's Lemma concludes the proof.

Continuous dependence on initial data for $\mu = 0$

Lemma (JG '13)

For $\mu = 0$ let solutions

$$u, \tilde{u} \in C^1((0,T), L^2(S^1)) \cap C^0((0,T), H^3(S^1))$$
$$v, \tilde{v} \in C^1((0,T), L^2(S^1)) \cap C^0((0,T), H^1(S^1))$$

corresponding to initial data (u_0, v_0) and $(\tilde{u}_0, \tilde{v}_0)$ be given with $\int_{S^1} (u_0 - \tilde{u}_0)\, \mathrm{d}x = 0$. Let $|W''|$ be bounded.
Then it exists a constant $C = C(u_0, v_0, \gamma, T)$ such that

$$\|v(t,\cdot) - \tilde{v}(t,\cdot)\|_{L^2(S^1)} + |u(t,\cdot) - \tilde{u}(t,\cdot)|_{H^1(S^1)} \leq C\Big(\|v_0 - \tilde{v}_0\|_{L^2(S^1)} + |u_0 - \tilde{u}_0|_{H^1(S^1)}\Big)$$

for all $t \leq T$.

Sketch of the proof

The partial relative entropy calculation leads to

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}\,t}\int_{S^1}\frac{1}{2}(\tilde{v}-v)^2+\frac{\gamma}{2}(\tilde{u}_x-u_x)^2\,\mathrm{d}\,x \\ &= \int_{S^1}(\tilde{v}-v)_x(W'(u)-W'(\tilde{u}))\,\mathrm{d}\,x \\ &\leq \int_{S^1}(\tilde{v}-v)^2+((W'(u)-W'(\tilde{u}))_x)^2\,\mathrm{d}\,x \\ &\leq C\int_{S^1}\frac{1}{2}(\tilde{v}-v)^2+\frac{\gamma}{2}(\tilde{u}_x-u_x)^2\,\mathrm{d}\,x\end{aligned}$$

using Young's and Poincaré's inequality.
Applying Gronwall's Lemma concludes the proof.

Semi-discrete dG scheme (from now on $\mu = 0$)

Decompose $[0, 1]$ into $0 = x_0 < x_1 < \cdots < x_N = 1$. Identify 0 and 1.
$\mathbb{V}_q :=$ space of (discontinuous) piece-wise polynomials of degree $\leq q$,
$\mathbb{V}_q^c := \mathbb{V}_q \cap C^0(S^1)$.

Find $u_h, v_h \in C^1((0, T), \mathbb{V}_q)$, $\tau_h \in C^0([0, T], \mathbb{V}_q)$ such that

$$
\begin{aligned}
0 &= \int_{S^1} \partial_t u_h \Phi - G[u_h]\Phi \,\mathrm{d}\, x \quad \forall \Phi \in \mathbb{V}_q \\
0 &= \int_{S^1} \partial_t v_h \Psi - G[\tau_h]\Psi \,\mathrm{d}\, x \quad \forall \Psi \in \mathbb{V}_q \\
0 &= \int_{S^1} \tau_h Z - W'(u_h) Z \,\mathrm{d}\, x + \gamma a_h(u_h, Z) \quad \forall Z \in \mathbb{V}_q,
\end{aligned}
$$

where a_h is an interior penalty discretisation of the Laplacian and G denotes a discrete gradient operator.

Discretisations

For $g_h \in \mathbb{V}_q$ we define $G[g_h] \in \mathbb{V}_q$ by

$$\int_{S^1} G[g_h]\Phi \, \mathrm{d}x = \sum_{i=0}^{N-1} \left(\int_{x_i}^{x_{i+1}} (g_h)_x \Phi \, \mathrm{d}x - [\![g_h]\!]_{x_i} \{\!\{ \Phi \}\!\}_{x_i} \right)$$

for all $\Phi \in \mathbb{V}_q$.

For $f_h, g_h \in \mathbb{V}_q$ we define

$$a_h(f_h, g_h) := \sum_{i=0}^{N-1} \Bigg(\int_{x_i}^{x_{i+1}} (f_h)_x (g_h)_x \, \mathrm{d}x - [\![f_h]\!]_{x_i} \{\!\{ (g_h)_x \}\!\}_{x_i} - [\![g_h]\!]_{x_i} \{\!\{ (f_h)_x \}\!\}_{x_i} + \frac{\sigma}{h} [\![f_h]\!]_{x_i} [\![g_h]\!]_{x_i} \Bigg),$$

for some $\sigma \gg 1$, such that $a_h : \mathbb{V}_q \times \mathbb{V}_q \to \mathbb{R}$ is coercive.

Reconstruction 1

$\hat{\tau} \in \mathbb{V}_{q+1}$ is defined by

$$0 = \int_{S^1} (\hat{\tau}_x - G[\tau_h])\Psi \,\mathrm{d}\, x \quad \forall \Psi \in \mathbb{V}_q \quad \text{and}$$

$$\hat{\tau}(x_n^-) = \frac{\tau_h(x_n^-) + \tau_h(x_n^+)}{2} \quad \forall n \in \{0, \ldots, N-1\}.$$

It can be shown that

- $\hat{\tau}$ is continuous.
- $\|\hat{\tau} - \tau_h\|^2_{L^2(S^1)} \leq \sum_{i=0}^{N-1} (x_{i+1} - x_i)\Big([\![\tau_h]\!]^2_{x_i} + [\![\tau_h]\!]^2_{x_{i+1}} \Big).$

Reconstruction 2

$\tilde{u} \in H^3(S^1)$ is defined by

$$0 = \gamma \partial_{xx} \tilde{u} - P^c_{q+1}(W'(u_h)) + \hat{\tau},$$

where $P^c_{q+1} : L^2(S^1) \to \mathbb{V}^c_{q+1}$ is the L^2-projection, and

$$\int_{S^1} (u - \tilde{u}) \, \mathrm{d}x = 0.$$

Using elliptic regularity and a posteriori control of elliptic reconstructions we have

$$\begin{aligned} \|\tilde{u} - u_h\|_{dG} := \Big(\sum |\tilde{u} - u_h|^2_{H^1((x_i, x_{i+1}))} + \sum |\, [\![\tilde{u} - u_h]\!]_{x_i} |^2 \Big)^{\frac{1}{2}} \\ \leq C \| P^c_{q+1}(W'(u_h)) - W'(u_h) \|_{H^{-1}(S^1)} \\ + C \|\hat{\tau} - \tau_h\|_{H^{-1}(S^1)} + H[u_h, W'(u_h), \tau_h], \end{aligned}$$

where $H[u_h, W'(u_h), \tau_h]$ is an explicitly computable estimator, expected to be of order h^q.

Reconstruction 2 cont'd

$$\|P^c_{q+1}(W'(u_h)) - W'(u_h)\|_{H^{-1}(S^1)} \leq C\sqrt{\sum_i (x_{i+1} - x_i) |\llbracket u_h \rrbracket|^2} \\ + C \sup_i (x_{i+1} - x_i)^{q+1} |W'(u_h)|_{H^1((x_i, x_{i+1}))}.$$

According to arguments provided by Nochetto and Makridakis '06 terms of the structure

$$\sqrt{\sum_i (x_{i+1} - x_i) |\llbracket \cdot_h \rrbracket|^2}$$

are expected to be of optimal order.

Reconstruction 3

$\hat{v} \in \mathbb{V}_{q+1}$ is defined by

$$0 = \int_{S^1} (\hat{v}_x - G[v_h])\Psi \,\mathrm{d}\, x \;\; \forall \Psi \in \mathbb{V}_q \quad \text{and} \quad \hat{v}(x_n^-) = \frac{v_h(x_n^-) + v_h(x_n^+)}{2} \; \forall n.$$

$\tilde{v} \in H^2(S^1)$ is defined by

$$0 = \partial_{xx}\tilde{v} - \partial_{xt}\tilde{u} \quad \text{and} \quad \int_{S^1} \tilde{v} - v_h \,\mathrm{d}x = 0.$$

$\hat{v}$ is continuous and

$$\|\hat{v} - v_h\|^2_{L^2(S^1)} \leq \sum_{i=0}^{N-1} (x_{i+1} - x_i)\Big([\![v_h]\!]^2_{x_i} + [\![v_h]\!]^2_{x_{i+1}} \Big),$$

while

$$\|\tilde{v} - \hat{v}\|_{L^2(S^1)} \leq \|\partial_t \tilde{u} - \partial_t u_h\|_{dG}.$$

Perturbed equation

By definition the reconstructions satisfy (point-wise a.e.)

$$\tilde{u}_t - \tilde{v}_x = 0$$
$$(v_h)_t - \hat{\tau}_x = 0$$

which implies, by definition of $\tilde{u}$,

$$(v_h)_t - (P^c_{q+1}(W'(u_h)))_x + \gamma \tilde{u}_{xxx} = 0.$$

Thus,

$$\tilde{u}_t - \tilde{v}_x = 0$$
$$\tilde{v}_t - W'(\tilde{u})_x = -\gamma \tilde{u}_{xxx} + E,$$

where the residual E is given by

$$E := \partial_t(\tilde{v} - v_h) + \partial_x(P^c_{q+1}(W'(u_h)) - W'(\tilde{u})).$$

By the estimates above, E is bounded explicitly in terms of u_h, v_h, τ_h.

Partial relative entropy

Then, the partial relative entropy calculation implies

$$\frac{\mathrm{d}}{\mathrm{d}\,t}\int_{S^1}\frac{1}{2}(\tilde{v}-v)^2+\frac{\gamma}{2}(\tilde{u}_x-u_x)^2\,\mathrm{d}\,x$$
$$=\int_{S^1}(v-\tilde{v})(W'(\tilde{u})-W'(u))_x\,\mathrm{d}\,x+\int_{S^1}(v-\tilde{v})E\,\mathrm{d}\,x.$$

We infer

$$\frac{\mathrm{d}}{\mathrm{d}\,t}\int_{S^1}\frac{1}{2}(\tilde{v}-v)^2+\frac{\gamma}{2}(\tilde{u}_x-u_x)^2\,\mathrm{d}\,x$$
$$\leq C\int_{S^1}\frac{1}{2}(\tilde{v}-v)^2+\frac{\gamma}{2}(\tilde{u}_x-u_x)^2\,\mathrm{d}\,x+\int_{S^1}E^2\,\mathrm{d}\,x.$$

Error estimate

Applying Gronwall's Lemma and triangle inequality gives

Theorem (JG, Makridakis, Pryer '14)

Let (u_h, v_h) *denote the solution of the semi-discrete dG scheme. Let* (u, v) *be a weak solution of* (vdW) *with*

$$u \in C^1((0,T), L^2(S^1)) \cap C^0([0,T], H^3(S^1))$$
$$v \in C^1((0,T), L^2(S^1)) \cap C^0([0,T], H^1(S^1))$$

Then, there is C>0 such that,

$$\|v_h(t,\cdot) - v(t,\cdot)\|^2_{L^2(S^1)} + |u_h(t,\cdot) - u(t,\cdot)|^2_{dG} \leq C\big(E_1 + E_2 + E_3\big),$$

where
$$E_1 := \Big(\|\tilde{v}(0,\cdot) - v_0\|^2_{L^2(S^1)} + |\tilde{u}(0,\cdot) - u_0|^2_{H^1(S^1)}\Big)\exp(Ct)$$
$$E_2 := \int_0^t \int_{S^1} E^2 \,\mathrm{d}x\,\mathrm{d}t \cdot \exp(Ct)$$
$$E_3 := \|\tilde{v}(t,\cdot) - v_h(t,\cdot)\|^2_{L^2(S^1)} + |\tilde{u}(t,\cdot) - u_h(t,\cdot)|^2_{dG}.$$

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Note that E_1, E_2, E_3 *can be explicitly bounded in terms of* u_h, v_h, τ_h.

Summary and outlook

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- New stability framework for regularized hyperbolic-elliptic problems.
- Derived an a posteriori error estimate.
- Estimate depends sensitively on γ, blows up for $\gamma \to 0$.
- Stability framework can also be used for model convergence.

Outlook

- Numerical experiments.
- Extension to fully discrete scheme.
- Extension to several space dimensions.
- Including viscosity.

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Thank you for your attention!