A priori error analysis of DG approximations of two-phase flows

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We are interested in compressible (isothermal) liquid-vapour flows described by diffuse interface models. Typical example: Navier-Stokes-Korteweg (NSK) system.

We focus on Discontinuous Galerkin (DG) (semi-)discretization.
Introduction

Isothermal Navier-Stokes-Korteweg model:

\[
\frac{\partial \rho}{\partial t} + \text{div}(\rho u) = 0
\]

\[
\frac{\partial}{\partial t} (\rho u) + \text{div}(\rho u \otimes u) = \lambda \nabla \text{div} u + \mu \text{div}(\nabla u + (\nabla u)^T)
\]

\[
- \nabla \left( p(\rho) - \frac{1}{2} \gamma |\nabla \rho|^2 - \gamma \rho \Delta \rho \right)
\]

\[
- \text{div}(\gamma \nabla \rho \otimes \nabla \rho).
\]

(NSK)

Associated energy functional:

\[
\int h(\rho) + \frac{\gamma}{2} |\nabla \rho|^2 + \frac{1}{2} \rho |u|^2 \, d\mathbf{x}
\]

with \( h \) and \( p \) related by Gibbs-Duhem equation: \( p(\rho) = \rho h'(\rho) - h(\rho) \).
Introduction

Many recent works on numerical methods for (NSK),

- (Semi-discrete) finite volume method [Jamet, Torres, Brackbill ’03]
- Explicit in time, local DG schemes [Diehl ’07]
- Implicit in time, continuous finite elements [Braack, Prohl ’13]
- Implicit in time, isogeometric finite elements [Liu, Gomez, Evans, Hughes, Landis ’13]
- Implicit in time, local DG [JG, Makridakis, Pryer ’14]
- Implicit in time, local DG [Tian, Xu, Kuerten, Van der Vegt ’14]
- Explicit in time, local DG method based on approximate model [Rohde, Neusser, Schleper ’15]

- ...

These works focus on stability/entropy dissipation of numerical methods and refinement at interface.
No a priori or a posteriori error analysis available.
Introduction

We consider one dimensional model problem (Lagrangian coordinates)

\[ \begin{align*}
  u_t - v_x &= 0 \\
  v_t - W'(u)_x &= \mu v_{xx} - \gamma u_{xxx}
\end{align*} \]  

(vdW)

with \( W \in C^\infty(\mathbb{R}, [0, \infty)) \) and \( \mu, \gamma > 0 \).

Unkowns: specific volume \( u \), velocity \( v \).

We have in mind the case that \( W \) has double well shape.

Goal:

Derive a priori error estimates without assuming convexity of \( W \).
Outline

1 Continuous Model and Stability

2 Semi-Discrete DG Scheme

3 A Priori Error Analysis

4 Numerical Experiments
Model Problem

We consider:

\[ u_t - v_x = 0 \]

\[ v_t - W'(u)_x = \mu v_{xx} - \gamma u_{xxx} \]  \hspace{1cm} (vdW)

with periodic boundary conditions.

For \( \mu = \gamma = 0 \) this would be the isothermal Euler equations in Lagrangian coordinates, which are hyperbolic if and only if \( W''(u) > 0 \).

Associated energy balance

\[ (W(u) + \frac{\gamma}{2}(u_x)^2 + \frac{1}{2}v^2)_t \]

\[ - (vW'(u) - \gamma vu_{xx} + \gamma v_x u_x + \mu vv_x)_x + \mu (v_x)^2 = 0. \]

We write \( \eta[u,v] := \int_{\Omega} W(u) + \frac{\gamma}{2}(u_x)^2 + \frac{1}{2}v^2 \, \text{d}x. \)
Relative Energy

Relative energy between functions \((u, v)\) and \((\tilde{u}, \tilde{v})\) is given by

\[
\eta[(u, v)| (\tilde{u}, \tilde{v})] := \eta[u, v] - \eta[\tilde{u}, \tilde{v}] - \int_{\mathbb{T}^1} \delta \eta[\tilde{u}, \tilde{v}] \left( \frac{u - \tilde{u}}{v - \tilde{v}} \right) \, dx,
\]

which for the energy at hand is:

\[
\eta[(u, v)| (\tilde{u}, \tilde{v})] = \int_{\mathbb{T}^1} W(u) - W(\tilde{u}) - W'(\tilde{u})(u - \tilde{u}) \]

\[
+ \frac{\gamma}{2} (u_x - \tilde{u}_x)^2 + \frac{1}{2} (v - \tilde{v})^2 \, dx.
\]

Reduced relative energy:

\[
\eta^R[(u, v)| (\tilde{u}, \tilde{v})] := \int_{\mathbb{T}^1} \frac{\gamma}{2} (u_x - \tilde{u}_x)^2 + \frac{1}{2} (v - \tilde{v})^2 \, dx.
\]
Estimate of Reduced Relative Energy Rate

Let \((u, v)\) be a strong solution to (vdW) and let \((\tilde{u}, \tilde{v})\) solve

\[
\begin{align*}
\dot{\tilde{u}}_t - \tilde{v}_x &= 0 \\
\dot{\tilde{v}}_t - W'(\tilde{u})_x &= \mu \tilde{v}_{xx} - \gamma \tilde{u}_{xxx} + R
\end{align*}
\]  

(\text{vdW-p})

for some \(R \in L^2([0, T] \times \mathbb{T}^1)\); then,

\[
\frac{d}{dt} \eta^R[(u,v)|(\tilde{u}, \tilde{v})] \leq \int_{\mathbb{T}^1} (v - \tilde{v})(W'(\tilde{u}) - W'(u))_x + (v - \tilde{v})R \, dx
\]

\[
\lesssim \eta^R[(u,v)|(\tilde{u}, \tilde{v})] + \|R\|_L^2.
\]

Lemma (JG; SIMA ’14)

Let \((u, v)\) be a strong solution to (vdW) and \((\tilde{u}, \tilde{v})\) a strong solution to (vdW-p) with \(\int u_0 - \tilde{u}_0 \, dx = 0\), then

\[
|\tilde{u}(t, \cdot) - u(t, \cdot)|_{H^1}^2 + \|\tilde{v}(t, \cdot) - v(t, \cdot)\|_{L^2}^2
\]

\[
\leq e^{Ct} \left( \|\tilde{u}_0 - u_0\|_{H^1}^2 + \|\tilde{v}_0 - v_0\|_{L^2}^2 + \int_0^t \|R\|_{L^2}^2 \right).
\]
Outline

1 Continuous Model and Stability

2 Semi-Discrete DG Scheme

3 A Priori Error Analysis

4 Numerical Experiments
Auxiliary Variables

Decompose $[0, 1]$ into $0 = x_0 < x_1 < \cdots < x_N = 1$. Identify $0$ and $1$. 

$\forall_p := \text{space of (discontinuous) piece-wise polynomials of degree } \leq p$. 

We introduce an auxiliary variable to avoid discretising the third order derivative directly:

\[
\begin{align*}
    u_t - v_x &= 0 \\
    v_t - \tau_x &= \mu v_{xx} \quad (\text{vdW}) \\
    \tau &= W'(u) - \gamma u_{xx}
\end{align*}
\]

Multiplying e.g. the first equation by a test function in $\phi = \forall_p$ and integrating by parts we obtain on each cell $K \in \mathcal{T}$

\[
\frac{d}{dt} \int_K u \phi \, dx = - \int_K v \phi_x \, dx + \int_{\partial K} n v \phi \, dx
\]

where $n \in \{\pm 1\}$ is a normal vector.
Auxiliary Variables

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\frac{d}{dt} \int_K u \phi \, d x = - \int_K v \phi_x \, d x + \int_{\partial K} n v \phi \, d x
$$

where $n \in \{\pm 1\}$ is a normal vector.
Auxiliary Variables

Decompose $[0, 1]$ into $0 = x_0 < x_1 < \cdots < x_N = 1$. Identify 0 and 1.

$\mathcal{V}_p := \text{space of (discontinuous) piece-wise polynomials of degree } \leq p.$

We introduce an auxiliary variable to avoid discretising the third order derivative directly:

$$u_t - v_x = 0$$
$$v_t - \tau_x = \mu v_{xx} \quad (\text{vdW})$$

$$\tau = W'(u) - \gamma u_{xx}$$

Multiplying e.g. the first equation by a test function in $\phi = \mathcal{V}_p$ and integrating by parts we obtain on each cell $K \in \mathcal{T}$

$$\frac{d}{dt} \int_K u \phi \, dx = - \int_K v \phi_x \, dx + \int_{\partial K} n v \phi \, dx$$

where $n \in \{\pm 1\}$ is a normal vector.
DG Discretization

If we do this on each cell using values from inside the cells on the boundaries, the problems on the cells are decoupled. By $u^\pm$ we denote traces of $u$ on the edges from the left and the right.

There is no preferred direction of transport of information. We choose

$$\frac{d}{dt} \int_K u \phi \, dx = - \int_K v \phi_x \, dx + \int_{\partial K} n v^+ \phi \, dx.$$ 

This is equivalent to

$$\frac{d}{dt} \int_K u \phi \, dx = \int_K v_x \phi \, dx + \int_{\partial K} n v \phi^- \, dx.$$ 

Summing over all $K \in \mathcal{T}$ we obtain

$$\frac{d}{dt} \int_{\mathcal{T}} u \phi \, dx = \int_{\mathcal{T}} v_x \phi \, dx + \int_{\mathcal{E}} [v] \phi^-$$

where $[v] := n^- v^- + n^+ v^+,$ and $\int_{\mathcal{T}} := \sum_{K \in \mathcal{T}} \int_K.$
Discrete Derivatives

For brevity we define discrete gradient operators: $G^+, G^- : \mathbb{V}_p \to \mathbb{V}_p$ by

$$\int_{\mathcal{T}^1} G^{\pm} (g_h) \Phi \, dx = \left( \int_{\mathcal{T}} (g_h)_x \Phi \, dx - \int_{\mathcal{E}} [g_h] \Phi^\pm \right) \quad \forall \Phi \in \mathbb{V}_p.$$

We also define an interior penalty discrete Laplacian:

$a_h : \mathbb{V}_p \times \mathbb{V}_p \to \mathbb{R}$

$$a_h(f_h, g_h) := \left( \int_{\mathcal{T}} (f_h)_x (g_h)_x \, dx - \int_{\mathcal{E}} [f_h] \{ (g_h)_x \} + [g_h] \{ (f_h)_x \} - \sigma h [f_h] [g_h] \right),$$

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

For brevity we define discrete gradient operators: $G^+, G^- : \mathbb{V}_p \to \mathbb{V}_p$ by

$$
\int_{\mathbb{T}^1} G^\pm (g_h) \Phi \, dx = \left( \int_{\mathcal{J}} (g_h)_x \Phi \, dx - \int_{\mathcal{E}} [g_h] \Phi^\pm \right) \quad \forall \Phi \in \mathbb{V}_p.
$$

We also define an interior penalty discrete Laplacian:

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$$
a_h(f_h, g_h) := \left( \int_{\mathcal{J}} (f_h)_x (g_h)_x \, dx \
- \int_{\mathcal{E}} [f_h] \{ (g_h)_x \} + [g_h] \{ (f_h)_x \} - \frac{\sigma}{h} [f_h] [g_h] \right),
$$

for some $\sigma \gg 1$, such that $a_h : \mathbb{V}_p \times \mathbb{V}_p \to \mathbb{R}$ is coercive.
Semi-Discrete Scheme

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

\[
0 = \int_{\mathbb{T}^1} \partial_t u_h \Phi - G^-(u_h) \Phi \, dx \quad \forall \Phi \in \mathbb{V}_p
\]

\[
0 = \int_{\mathbb{T}^1} \partial_t v_h \Psi - G^+(\tau_h) \Psi + \mu G^-(v_h) G^- (\Psi) \, dx \quad \forall \Psi \in \mathbb{V}_p \quad \text{(SDS)}
\]

\[
0 = \int_{\mathbb{T}^1} \tau_h Z - W'(u_h) Z \, dx - \gamma a_h(u_h, Z) \quad \forall Z \in \mathbb{V}_p.
\]

Solutions of (SDS) dissipate energy:

\[
\frac{d}{dt} \left( \int_{\mathbb{T}^1} W(u_h) + \frac{1}{2} (v_h)^2 \, dx + \frac{\gamma}{2} a_h(u_h, u_h) \right) = -\mu \int_{\mathbb{T}^1} (G^- [v_h])^2 \, dx \leq 0.
\]

A similar estimate holds, if (SDS) is discretized by a Crank-Nicolson type method in time.
Outline

1. Continuous Model and Stability
2. Semi-Discrete DG Scheme
3. A Priori Error Analysis
4. Numerical Experiments
Discrete Reduced Relative Energy Rate

Let \((u_h, v_h, \tau_h)\) be a solution of (SDS) and let \((\tilde{u}_h, \tilde{v}_h, \tilde{\tau}_h)\) be a solution of the following perturbed problem

\[
\int_{\mathbb{T}^1} \partial_t \tilde{u}_h \Phi - G^-(\tilde{v}_h) \Phi \, dx = 0 \quad \forall \, \Phi \in \mathcal{V}_p
\]

\[
\int_{\mathbb{T}^1} \partial_t \tilde{v}_h \Psi - G^+(\tilde{\tau}_h) \Psi + \mu G^-(\tilde{v}_h) G^-(\Psi) \, dx = \int_{\mathbb{T}^1} R_v \Psi \, dx \quad \forall \, \Psi \in \mathcal{V}_p
\]

\[
\int_{\mathbb{T}^1} \tilde{\tau}_h Z - W'(\tilde{u}_h) Z \, dx - \gamma a_h(\tilde{u}_h, Z) = \int_{\mathbb{T}^1} R_\tau Z \, dx \quad \forall \, Z \in \mathcal{V}_p,
\]

for some \(R_v, R_\tau\). Discrete version of relative energy:

\[
\eta^R_D[(u_h, v_h)|\tilde{u}_h, \tilde{v}_h)] := \int_{\mathbb{T}^1} \frac{1}{2} (v_h - \tilde{v}_h)^2 \, dx + \frac{\gamma}{2} a_h(u_h - \tilde{u}_h, u_h - \tilde{u}_h).
\]

Its rate satisfies

\[
\frac{d}{dt} \eta^R_D[(u_h, v_h)|\tilde{u}_h, \tilde{v}_h)] \lesssim \eta^R_D[(u_h, v_h)|\tilde{u}_h, \tilde{v}_h)] + \int_{\mathbb{T}^1} R_v^2 + \frac{1}{h^2} R_\tau^2 \, dx.
\]
Projections of the Exact Solution:

Strategy:

Insert projections of exact solution into (SDS) and bound residuals in terms of powers of $h$.

We denote $L_2$-orthogonal projection into $\mathbb{V}_p$ by $\mathcal{P}$.

We define $Q : C^1(\mathbb{T}^1) \to \mathbb{V}_p$ by

$$G^{-}[Q[w]] = \mathcal{P}[\partial_x w] \quad \text{and} \quad \int_{\mathbb{T}^1} Q[w] - w \, dx = 0.$$ 

Note: $G^{-}[Q[w]] = 0$ implies $Q[w]$ is constant.

For $\tau := W'(u) - \gamma u_{xx}$ we define $R[\tau] \in \mathbb{V}_p$ by

$$\int_{\mathbb{T}^1} R[\tau] \Psi \, dx = \int_{\mathbb{T}^1} W'(u) \Psi \, dx + \gamma a_h(\mathcal{P}[u], \Psi) \quad \forall \, \Psi \in \mathbb{V}_p.$$ 

Using $(\mathcal{P}[u], Q[v], R[\tau])$ as approximate solution of (SDS) we obtain:
A Priori Error Estimate

Theorem (JG, Pryer; BIT Num. Math. ’15)

Let $W \in C^{p+3}([0, \infty))$ and let the exact solution $(u, v)$ of (vdW) satisfy

\[ u \in C^1((0, T), H^{p+2}(T)) \cap C^0([0, T], C^{p+3}(T)) \cap C^0([0, T], C^{p+3}(T)), \]
\[ v \in C^1((0, T), C^{p+2}(T)) \cap C^0([0, T], C^{p+3}(T)) \cap C^0([0, T], C^{p+3}(T)). \]

Then, there exists $C > 0$ independent of $h$, so that

\[
\sup_{0 \leq t \leq T} \left( \| u_h(t, \cdot) - u(t, \cdot) \|_{dG} + \| v_h(t, \cdot) - v(t, \cdot) \|_{L_2(T)} \right) \leq C h^p.
\]

The constant $C$ scales like $\frac{1}{\sqrt{\gamma}} \exp \left( \frac{T}{2\gamma} \right)$. 

\[
\| u_h \|_{dG}^2 := \sum_{K \in \mathcal{T}} \| \partial_x u_h \|_{L_2(K)}^2 + \left\| \sqrt{h^{-1}_e} [u_h] \right\|_{L_2(\mathcal{E})}^2.
\]
Outline

1. Continuous Model and Stability
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4. Numerical Experiments
Numerical Experiment 1 – Comparison to Exact Solution

Double well and parameters:

\[ W(u) := \left(u^2 - 1\right)^2, \quad \gamma = \mu = 10^{-3}. \]

For the implementation we are using natural boundary conditions, that is

\[ \partial_x u_h = v_h = 0 \text{ on } [0,T) \times \partial(-1,1), \]

Then an approximate steady state solution is given by

\[ u(t, x) = \tanh\left(x \sqrt{\frac{2}{\gamma}}\right), \quad v(t, x) \equiv 0 \quad \forall t. \]

Temporal discretisation: 2nd order Crank-Nicolson.
Numerical Experiment 1 – Comparison to Exact Solution

$p=2$

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### Numerical Experiment 1 – Comparison to Exact Solution

$p=3$

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Numerical Experiment 2

\[ u_0 = \frac{\sin(50\pi x)}{100}, \quad v_0 = 0. \]

Temporal discretization: 2nd order Crank–Nicolson method.
\[ \gamma = 10^{-3}, \mu = 10^{-1}, W(u) = (u^2 - 1)^2 \]
Summary and Outlook

Summary:

- We presented a semi-discrete DG scheme for a model problem for compressible multi-phase flows.
- Stability of numerical method + projection $\implies$ a priori error estimate.
- The estimates are optimal in $h$, but blow up in the sharp interface limit $\gamma \to 0$.
- We can also prove an a posteriori error estimate by combining PDE stability and reconstruction.

Outlook:

- Extending the results to the (isothermal) Navier-Stokes-Korteweg model and two/three space dimensions.
- Extending the results to fully discrete schemes.
- Can we reduce the $\gamma$ dependence of the estimate (cf. results for Allen-Cahn equations)?