Nonconservative Discontinuous Galerkin Discretization and Application to the Navier-Stokes-Korteweg System

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Outline

- The isothermal Navier-Stokes-Korteweg System as a model for a compressible flow with phase transition
- The Local Discontinuous Galerkin Method, a general Framework
  - First order conservative systems
  - Higher order derivatives
  - Nonconservative terms
- Well-balanced higher order DG-discretization of the Navier-Stokes-Korteweg system
- Identification of physical parameters and validation of the model

Isothermal Navier-Stokes-Korteweg Model

$$
\begin{aligned}
\rho_t + \nabla \cdot (\rho \mathbf{u}) &= 0 \\
(\rho \mathbf{u})_t + \nabla \cdot (\rho \mathbf{u}\mathbf{u}^T) + \nabla p(\rho) &= \nabla \cdot \tau + \nabla \cdot \mathbf{K}
\end{aligned}
$$

in $\Omega \times (0, T)$, $\varepsilon, \lambda > 0$

$$
\begin{aligned}
\tau &= \varepsilon \left(\nabla \mathbf{u} + \nabla \mathbf{u}^T \right) - \frac{2}{3} \varepsilon (\nabla \cdot \mathbf{u}) \mathbf{I} \\
\mathbf{K} &= \lambda \left[\left(\rho \Delta \rho + \frac{1}{2} |\nabla \rho|^2 \right) \mathbf{I} - \nabla \rho \nabla \rho^T \right]
\end{aligned}
$$

Initial data: $\rho(\cdot, 0) = \rho_0, \ \mathbf{u}(\cdot, 0) = \mathbf{u}_0$ in Ω

Bnd. cond.: $\nabla \rho \cdot \mathbf{n} = 0, \ \mathbf{u} = \mathbf{0}$ on $\partial\Omega \times (0, T)$

Isothermal Navier-Stokes-Korteweg Model

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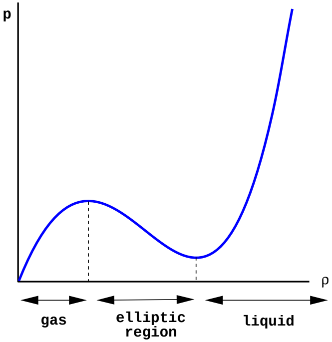
Van der Waals eq. of state

$R, a, b > 0$,

θ_{ref}: reference temperature below the critical temperature,

$p(\rho) = R\frac{\rho\theta_{ref}}{b-\rho} - a\rho^2$.



Isothermal Navier-Stokes-Korteweg Model

$$\begin{aligned} \rho_t + \nabla \cdot (\rho \mathbf{u}) &= 0 \\ (\rho \mathbf{u})_t + \nabla \cdot (\rho \mathbf{u}\mathbf{u}^T) + \nabla p(\rho) &= \nabla \cdot \tau + \nabla \cdot \mathbf{K} \end{aligned}$$

Equivalent nonconservative form:

$$\begin{aligned} \rho_t + \nabla \cdot (\rho \mathbf{u}) &= 0 \\ (\rho \mathbf{u})_t + \nabla \cdot (\rho \mathbf{u}\mathbf{u}^T) + \rho \nabla \kappa(\rho, \Delta\rho) &= \nabla \cdot \tau \end{aligned}$$

$$\kappa = \mu(\rho) - \lambda \Delta \rho, \qquad \mu(\rho) = \int_0^\rho \frac{p'(s)}{s} ds$$

Discontinuous Galerkin Method

First order conservative systems (Cockburn, Shu)

$$\begin{aligned} \mathbf{u}_t + \mathcal{L}[\mathbf{u}] &= \mathbf{0} \quad \text{in } \Omega \subset \mathbb{R}^n,\ t \in (0, \infty), \\ \mathcal{L}[\mathbf{u}](x) &= \sum_{i=1}^{n} \frac{\partial}{\partial x_i} \mathbf{f}_i(\mathbf{u}(\mathbf{x})), \end{aligned}$$

with initial condition and suitable boundary conditions, $\mathbf{u}(\mathbf{x}, t) \in \mathbb{R}^d$.

Discretization

Space: $\mathbf{u}_h(\cdot, t) \in V_h^d = \left\{\varphi : \Omega \to \mathbb{R} \mid \varphi|_{\Delta_j} \in \mathbb{P}_k,\ \Delta_j \in \mathcal{T}_h\right\}^d$,
$\mathcal{T}_h$ mesh, partition of Ω.

Time: explicit / implicit Runge-Kutta methods.

Discontinuous Galerkin Method

Nonconservative products (Dal Maso, LeFloch, Murat)

Definition of the expression $\sum_{i=1}^{n} f_i(u) \cdot \frac{\partial}{\partial x_i} v$ as a measure μ for discontinuous functions $u, v \in V_h^d$.

$$
\begin{aligned}
\mu(\Omega) &= \int_{\Omega} d \left[\sum_{i=1}^{n} f_i(u) \cdot \frac{\partial}{\partial x_i} v \right]_{\phi} (x) \\
&= \sum_j \int_{\Delta_j} \sum_{i=1}^{n} f_i(u(x)) \cdot \frac{\partial}{\partial x_i} v(x)\, dx \\
&\quad + \sum_j \int_{\partial\Delta_j \setminus \partial\Omega} \left\{ \sum_{i=1}^{n} n_i f_i(u) \right\} \cdot [v]\, d\sigma(x).
\end{aligned}
$$

$\{\cdot\}$ average in some sense, $[v] = (v^+ - v^-)$ jump.

Discontinuous Galerkin Method

First order conservative systems (Cockburn, Shu)

$$\begin{aligned} \mathbf{u}_t + \mathcal{L}[\mathbf{u}] &= \mathbf{0} \quad \text{in } \Omega \subset \mathbb{R}^n,\ t \in (0,\infty), \\ \mathcal{L}[\mathbf{u}](x) &= \sum_{i=1}^{n} \frac{\partial}{\partial x_i} \mathbf{f}_i(\mathbf{u}(\mathbf{x})), \end{aligned}$$

Idea: For $\mathbf{u}_h \in V_h^d$ construct a *discrete differential* operator $\mathcal{L}_h : V_h^d \to V_h^d$ by (L^2-)projecting $\mathcal{L}[u]$ to V_h^d in some sense.

For smooth functions $\mathbf{u}, \varphi$ we have by partial integration

$$\begin{aligned} (\mathcal{L}[\mathbf{u}], \varphi)_\Omega &= \int_{\partial\Omega} \sum_{i=1}^{n} n_i \mathbf{f}_i(\mathbf{u}(\mathbf{x})) \cdot \varphi(\mathbf{x})\, d\sigma(\mathbf{x}) \\ &\quad - \int_{\Omega} \sum_{i=1}^{n} \mathbf{f}_i(\mathbf{u}(\mathbf{x})) \cdot \frac{\partial}{\partial x_i} \varphi(\mathbf{x})\, d\mathbf{x}, \end{aligned}$$

Discontinuous Galerkin Method

First order conservative systems (Cockburn, Shu)

$$\begin{aligned} \mathbf{u}_t + \mathcal{L}[\mathbf{u}] &= \mathbf{0} \quad \text{in } \Omega \subset \mathbb{R}^n,\ t \in (0,\infty), \\ \mathcal{L}[\mathbf{u}](x) &= \sum_{i=1}^{n} \frac{\partial}{\partial x_i} \mathbf{f}_i(\mathbf{u}(\mathbf{x})), \end{aligned}$$

For $\mathbf{u}_h \in V_h^d$ define $\mathcal{L}_h : V_h^d \to V_h^d$ by: $\quad \forall \varphi \in V_h^d$

$$\begin{aligned} (\mathcal{L}_h[\mathbf{u}_h], \varphi)_\Omega &= \int_{\partial\Omega} \sum_{i=1}^{n} n_i \mathbf{f}_i(\mathbf{u}_h(\mathbf{x})) \cdot \varphi(\mathbf{x})\ d\sigma(\mathbf{x}) \\ &\quad - \sum_j \int_{\Delta_j} \sum_{i=1}^{n} \mathbf{f}_i(\mathbf{u}_h(\mathbf{x})) \cdot \frac{\partial}{\partial x_i} \varphi(\mathbf{x})\ d\mathbf{x} \\ &\quad - \sum_j \int_{\partial\Delta_j \setminus \partial\Omega} \mathbf{g}(\mathbf{u}_h|_{\Delta_j}, \mathbf{u}_h|_{\Delta_{j'}}, \mathbf{n}) \cdot [\varphi]\ d\sigma(\mathbf{x}) \end{aligned}$$

Discontinuous Galerkin Method

First order conservative systems (Cockburn, Shu)

$$\begin{aligned} \mathbf{u}_t + \mathcal{L}[\mathbf{u}] &= \mathbf{0} \quad \text{in } \Omega \subset \mathbb{R}^n,\ t \in (0,\infty), \\ \mathcal{L}[\mathbf{u}](x) &= \sum_{i=1}^{n} \frac{\partial}{\partial x_i} \mathbf{f}_i(\mathbf{u}(\mathbf{x})), \end{aligned}$$

Semi-discrete formulation:

$$\left(\frac{\partial}{\partial t} \mathbf{u}_h(\cdot,t), \varphi \right)_\Omega + \left(\mathcal{L}_h[\mathbf{u}(\cdot,t)], \varphi \right)_\Omega = 0 \quad \forall \varphi \in V_h^d,\ t \in (0,\infty).$$

Initial values have to be projected to V_h^d.

Discontinuous Galerkin Method

Higher order derivatives (Bassi, Rebay, C., S.)

$$\mathbf{u}_t + \mathcal{L}^m[\mathbf{u}] = \mathbf{0} \quad \text{in } \Omega \subset \mathbb{R}^n,\ t \in (0, \infty),$$

where $\mathcal{L}^m$ is a differential operator of order m in divergence form.

Idea: express $\mathcal{L}^m$ as a combination of m first order (conservative) differential operators $\mathcal{L}^1_i$. Treat them as in the previous section.

$$\begin{aligned}
\mathbf{u}^0 &= \mathbf{u}, \\
\mathbf{u}^1 &= \mathcal{L}^1_1[(\mathbf{u}^0)], \\
\mathbf{u}^2 &= \mathcal{L}^1_2[(\mathbf{u}^0, \mathbf{u}^1)], \\
&\vdots \\
\mathcal{L}^m[\mathbf{u}] &= \mathcal{L}^1_m[(\mathbf{u}^0, \mathbf{u}^1, \ldots, \mathbf{u}^{m-1})].
\end{aligned}$$

Discontinuous Galerkin Method

Higher order derivatives (Bassi, Rebay, C., S.)

$$\mathbf{u}_t + \mathcal{L}^m[\mathbf{u}] \;=\; \mathbf{0} \quad \text{in } \Omega \subset \mathbb{R}^n,\; t \in (0,\infty),$$

where $\mathcal{L}^m$ is a differential operator of order m in divergence form.

Example:

$$\begin{aligned}
\mathcal{L}^2[u] &= -\nabla \cdot (\mu(u)\nabla u) \\
\mathcal{L}^1_1[u] &= \nabla u \\
\mathcal{L}^1_2[u,\mathbf{v}] &= \nabla \cdot (\mu(u)\mathbf{v}) \\
\mathcal{L}^2[u] &= \mathcal{L}^1_2[u, \mathcal{L}^1_1[u]]
\end{aligned}$$

Discontinuous Galerkin Method

Non-conservative systems (Hulsen)
Consider the non-conservative differential operator

$$\mathcal{L}[\mathbf{u}](x) = \sum_{i=1}^{n} \mathbf{A}_i(\mathbf{u}(\mathbf{x}))\, \frac{\partial}{\partial x_i}\mathbf{u}(\mathbf{x})$$

Idea: Construct a discrete operator $\mathcal{L}_h : V_h^d \to V_h^d$

For smooth functions we have

$$(\mathcal{L}[\mathbf{u}], \varphi)_\Omega = \int_\Omega \sum_{i=1}^{n} \varphi(x)^T \mathbf{A}_i(\mathbf{u}(\mathbf{x}))\, \frac{\partial}{\partial x_i}\mathbf{u}(\mathbf{x})\, d\mathbf{x}$$

Non-conservative systems (Hulsen)
Consider the non-conservative differential operator

$$\mathcal{L}[\mathbf{u}](x) = \sum_{i=1}^{n} \mathbf{A}_i(\mathbf{u}(\mathbf{x}))\, \frac{\partial}{\partial x_i}\mathbf{u}(\mathbf{x})$$

For $\mathbf{u}_h \in V_h^d$ define $\mathcal{L}_h[\mathbf{u}_h] \in V_h^d$ such that for all $\varphi \in V_h^d$ we have

$$\begin{aligned}(\mathcal{L}_h[\mathbf{u}_h], \varphi)_\Omega \;&=\; \sum_j \int_{\Delta_j} \sum_{i=1}^{n} \varphi(x)^T \mathbf{A}_i(\mathbf{u}_h(\mathbf{x}))\, \frac{\partial}{\partial x_i}\mathbf{u}_h(\mathbf{x})\; d\mathbf{x} \\ &+ \sum_j \int_{\partial\Delta_j \setminus \partial\Omega} \left\{ \sum_{i=1}^{n} n_i \varphi^T \mathbf{A}_i(\mathbf{u}_h) \right\} [\mathbf{u}_h]\; d\sigma\end{aligned}$$

NSK Discontinuous Galerkin Discretization

1d NSK system (non-conservative form)

$$\begin{aligned} \rho_t + (\rho u)_x &= 0, \\ (\rho u)_t + (\rho u^2)_x + \rho \kappa_x &= \varepsilon u_{xx}, \\ \kappa &= \mu(\rho) - \lambda \rho_{xx}. \end{aligned}$$

1st step

$$\begin{pmatrix} \rho_x \\ u_x \end{pmatrix} = \mathcal{L}_1^1[\rho, \rho u],$$

$$\mathbf{f}(\rho, \rho u) = \begin{pmatrix} \rho \\ \frac{\rho u}{\rho} \end{pmatrix} \quad \mathbf{g}(\rho^-, \rho u^-, \rho^+, \rho u^+, n) = n \begin{pmatrix} \{\rho\} \\ \left\{ \frac{\rho u}{\rho} \right\} \end{pmatrix}$$

$$\{\varphi\} = \frac{1}{2}(\rho^+ + \rho^-), \quad [\varphi] = (\varphi^+ - \varphi^-)$$

NSK Discontinuous Galerkin Discretization

1d NSK system (non-conservative form)

$$\begin{aligned} \rho_t + (\rho u)_x &= 0, \\ (\rho u)_t + (\rho u^2)_x + \rho \kappa_x &= \varepsilon u_{xx}, \\ \kappa &= \mu(\rho) - \lambda \rho_{xx}. \end{aligned}$$

2nd step

$$\kappa = \mathcal{L}_2^1[\rho, \rho_x] = \mu(\rho) - (\lambda \rho_x)_x$$

- treatment of $(\lambda \rho_x)_x$ as in step 1
- treatment of $\mu(\rho)$ as a source term

NSK Discontinuous Galerkin Discretization

1d NSK system (non-conservative form)

$$\begin{aligned} \rho_t + (\rho u)_x &= 0, \\ (\rho u)_t + (\rho u^2)_x + \rho\kappa_x &= \varepsilon u_{xx}, \\ \kappa &= \mu(\rho) - \lambda\rho_{xx}. \end{aligned}$$

3rd step

$$\mathcal{L}_3^1[\rho, \rho u, u_x, \kappa] = \begin{pmatrix} \rho u \\ \rho u^2 - \varepsilon u_x \end{pmatrix}_x + \begin{pmatrix} 0 \\ \rho\kappa_x \end{pmatrix}$$

$$\mathbf{g}(\rho^\pm, \rho u^\pm, u_x^\pm, \kappa^\pm, n) = \begin{pmatrix} \{\rho u\}n - \alpha[\kappa] \\ \{\rho u^2 - \varepsilon u_x\}n - \alpha[\rho u] + \{\rho\}[\kappa]n \end{pmatrix}$$

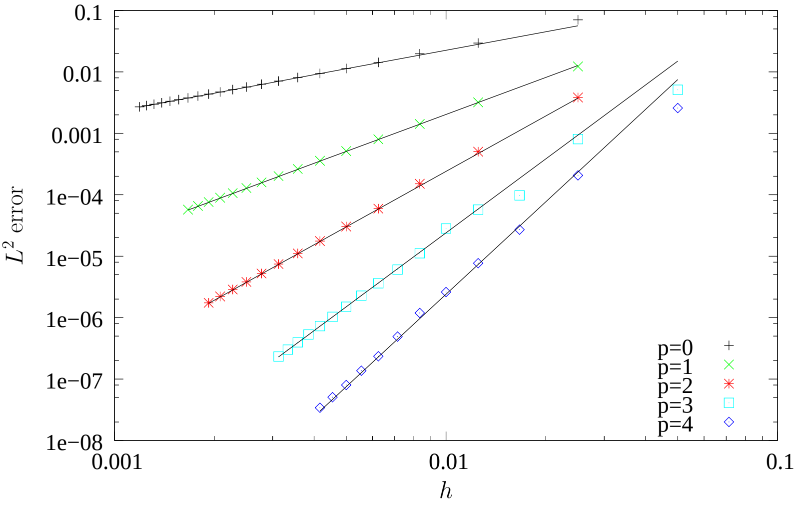
$\alpha[]$: *numerical viscosity* similar to Lax-Friedrichs flux.

NSK Discontinuous Galerkin Discretization

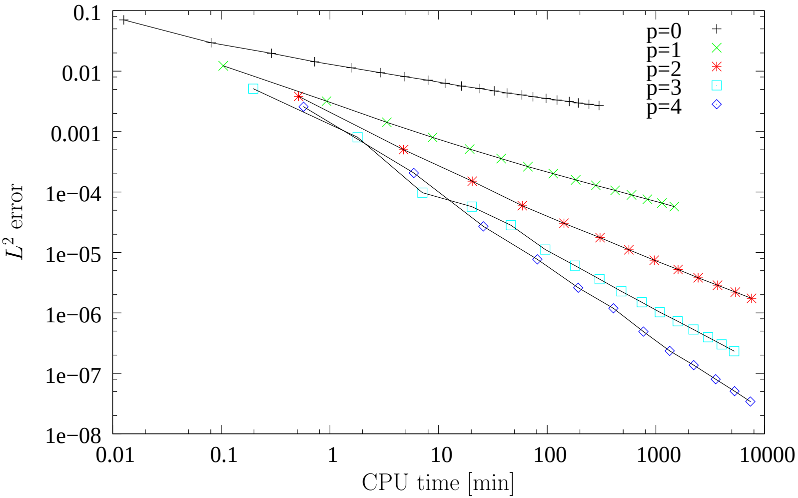
- The higher order schemes are well balanced
- Total physical energy decreases monotonically with time for smooth solutions of NSK. Numerical experiments indicate that the discrete total energy decreases (mostly) monotonically
- Test case traveling wave solution in 1d, 2d, 3d,
  test case static bubble 2d, 3d,
  triangular / tetrahedral mesh:

  k-th order scheme => k-th order convergence
  k=1,2,3,4,5
- Higher order schemes are more efficient schemes

NSK Discontinuous Galerkin Discretization



NSK Discontinuous Galerkin Discretization

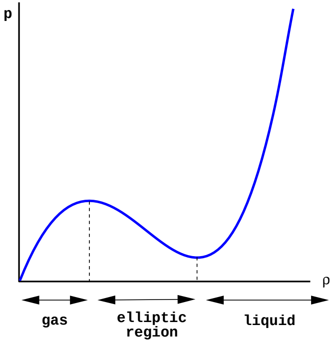


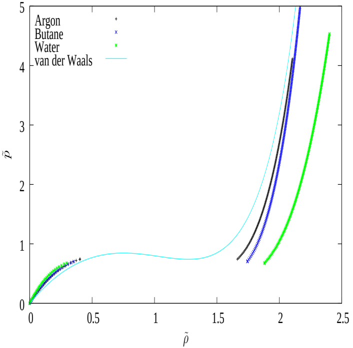
Numerical Experiment: Bubble Ensemble

- fourth order Discontinuous Galerkin scheme
- second order implicit Runge-Kutta method
- adaptive refined nonconform triangular mesh
- parallel (MPI), 16 Processors
- load-balanced (ParMETIS)

movie: Bubble Ensemble.avi

Temperature Range





Left figure: $\theta_{ref} = 0.85 \cdot \theta_{crit}$, right figure: $\theta_{ref} = 0.95 \cdot \theta_{crit}$.

Elliptic region must not be too large, i.e., $\theta_{ref} > 0.7 \cdot \theta_{crit}$.

Water for example $\theta_{ref} > 180$ degree Celsius.

Physical Parameters

Viscosity

The viscosity parameter ε is fixed to some constant between the viscosity in the liquid and the vapour phase.

Capillarity

The capillarity parameter λ is related (at least at static equilibrium) to surface tension (Kraus, Dreyer) by the formula

$$\sigma(\theta_{ref}) = c_0(\theta_{ref})\sqrt{\lambda}.$$

- interface width also proportional to $\sqrt{\lambda}$
- correct surface tension implies interface width $\approx 1nm$
- maximal diameter of computational domain $\approx 1\mu m$

Numerical Experiment: Oscillating Bubble

movie: Oscillating Bubble.avi

- Almost no compression in the vapour phase
- All mass is transferred over the interface
- No free parameter in the model to control this behaviour

Summary

Numerics:

- Efficient Discontinuous Galerkin Schemes in 1d/2d/3d (adaptive, parallel, load-balanced)
- Higher order time integration by means of implicit, explicit, semi-implicit Runge-Kutta methods

Model:

- Applicable only in the *high* temperature regime $(> 0.7 \cdot \theta_{crit})$
- Applicable only to very small domains (micro meter regime)
- No control on the mass transfer over the interface