A simple robust and accurate a posteriori subcell finite volume limiter for the discontinuous Galerkin method

Michael Dumbser

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Starting Point: Very General Form of the Governing PDE

We want to construct numerical schemes for very general hyperbolic-parabolic systems of nonlinear time-dependent partial differential equations in multiple space dimensions of the following general form:

\[
\frac{\partial Q}{\partial t} + \nabla \cdot F(Q, \nabla Q) + B(Q) \cdot \nabla Q = S(Q) \quad \text{(PDE)}
\]

The nonlinear flux tensor \( F \) can also depend on the gradient of \( Q \), to take into account parabolic terms, such as viscous effects. The third term is a non-conservative term that is important in many multi-fluid, multi-phase and shallow water models. The source term on the right hand side may also be stiff.

Many of the mathematical models relevant for science and engineering can be cast in the form of eqn. (PDE).

Main difficulty: solutions of (PDE) can contain smooth features and discontinuities at the same time.
The Discontinuous Galerkin Finite Element Method

Consider only a system of conservation laws of the form

$$\frac{\partial Q}{\partial t} + \nabla \cdot F(Q) = 0$$  \hspace{1cm} (SCL)

The discrete solution at time $t^n$ is represented by piecewise polynomials of degree $N$ over spatial control volumes $T_i$ as

$$u_h(x, t^n) = \sum_l \Phi_l(x) \hat{u}_l^n, \quad x \in T_i$$  \hspace{1cm} (DS)

Multiplication of (SCL) with a test function $\phi_k$ from the space of piecewise polynomials of degree $N$ and integration over a control volume $T_i$ yields after integration by parts:

$$\int_{T_i} \phi_k \frac{\partial Q}{\partial t} \, dx + \int_{\partial T_i} \phi_k F(Q) \cdot n \, dS - \int_{T_i} \nabla \phi_k F(Q) \, dx = 0.$$
The Discontinuous Galerkin Finite Element Method

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$$u_h(x, t^n) = \sum_l \Phi_l(x) \hat{u}_l^n, \quad x \in T_i$$ \hspace{1cm} (DS)$$

Introducing the discrete solution (DS) and a numerical flux $G$ (Riemann solver):

$$\int_{T_i} \phi_k \frac{\partial u_h}{\partial t} \, dx + \int_{\partial T_i} \phi_k G(u_h^-, u_h^+) \cdot n \, ds - \int_{T_i} \nabla \phi_k F(u_h) \, dx = 0.$$

Note the similarity with high order finite volume schemes:

$$\int_{T_i} \frac{\partial u_h}{\partial t} \, dx + \int_{\partial T_i} G(w_h^-, w_h^+) \cdot n \, ds = 0.$$

For the first order case, both methods are identical.
General $P_N^P_M$ Schemes on Unstructured Meshes

1. **Unification** of discontinuous Galerkin (DG) and high order finite volume (FV) schemes: **reconstruction** of piecewise polynomials $w_h$ of degree $M$ from piecewise polynomials $u_h$ of degree $N$ using $L^2$-projection on a stencil $S_i$:

$$u_h(\vec{x}, t^n) = \sum_l \Phi_l(\vec{x}) \hat{u}_l^n \quad w_h(\vec{x}, t^n) = \sum_l \Psi_l(\vec{x}) \hat{w}_l^n$$

Stencil definition: 

$$S_i = \bigcup_{k=1}^{n_e} T_j(k)$$

**Reconstruction equations** ($L^2$-projection):

$$[\Phi_k, w_h]_{I_j}^{t^n} = [\Phi_k, u_h]_{I_j}^{t^n} \quad \forall T_j \in S_i.$$

The reconstruction equations are solved using constrained LSQ. For FV, shock capturing is obtained via a **nonlinear** WENO reconstruction.
General $P_N P_M$ Schemes on Unstructured Meshes

1. Reconstruction of piecewise polynomials $w_h$ of degree $M$ from piecewise polynomials $u_h$ of degree $N$ using $L2$-projection on a stencil $S_i$:

\[
\begin{align*}
\mathcal{O}(1) & : P_0 P_0 \\
\mathcal{O}(2) & : P_0 P_1, P_1 P_1 \\
\mathcal{O}(3) & : P_0 P_2, P_1 P_2, P_2 P_2 \\
\mathcal{O}(4) & : P_0 P_3, P_1 P_3, P_2 P_3, P_3 P_3 \\
& \vdots \\
\mathcal{O}(M+1) & : P_0 P_M, \ldots, P_N P_M, \ldots, P_M P_M
\end{align*}
\]
General $P_NP_M$ Schemes on Unstructured Meshes

2. Local **predictor** that computes a solution *in the small* of the local Cauchy-Problem for (PDE) with initial data $w_h$. This allows the construction of **high order one-step** schemes in time.

- Cauchy-Kovalewski procedure, based on Taylor series and successive differentiation of the governing PDE (**strong** form of the PDE), see MUSCL, ENO, original ADER. **Not** able to treat stiff sources, **not** applicable to general PDE for higher than second order schemes.

- **Element-local** space-time discontinuous Galerkin predictor (**weak** form of the PDE in space-time). Applicable to general PDE with **stiff** source terms.
Local Space-Time DG Predictor Method

PDE transformed to the space-time reference element

$$\frac{\partial}{\partial \tau} Q + \nabla \xi \cdot F^*(Q, \nabla Q) = S^* - B^*(Q) \cdot \nabla Q := P^*(Q, \nabla Q)$$

Multiplication with a piecewise polynomial **space-time test function** $\theta_k(x,t)$ of degree $M$ and integration in space and time yields

$$\left\langle \theta_k, \frac{\partial}{\partial \tau} q_h \right\rangle + \left\langle \theta_k, \nabla \xi \cdot F^*(q_h, \nabla q_h) \right\rangle = \left\langle \theta_k, P^*(q_h, \nabla q_h) \right\rangle$$

Element-local space-time ansatz

$$q_h = q_h(\xi, \tau) = \sum_l \theta_l(\xi, \tau) \hat{q}_l := \theta \hat{q}_l$$

$$\nabla_\xi q_h = \nabla_\xi q_h(\xi, \tau) = \sum_l \theta_l(\xi, \tau) \hat{q}_l' := \theta \hat{q}_l'$$

Integration by parts in time only

$$[\theta_k, q_h]^1 - [\theta_k w_h]^0 - \left\langle \frac{\partial}{\partial \tau} \theta_k, q_h \right\rangle + \left\langle \theta_k, \nabla \xi \cdot F^*(q_h, \nabla q_h) \right\rangle = \left\langle \theta_k, P^*(q_h, \nabla q_h) \right\rangle.$$
Local Space-Time DG Predictor Method

Inserting the polynomial ansatz yields

\[
\left( [\theta_k, \theta_l]^1 - \left\langle \frac{\partial}{\partial \tau} \theta_k, \theta_l \right\rangle \right) \hat{q}_l^{i+1} = [\theta_k, \psi_m]^0 \hat{w}_m^n + \left\langle \theta_k, \theta_l \right\rangle \hat{P}_l^i - \left\langle \theta_k, \nabla \xi \theta_l \right\rangle \cdot \hat{F}_l^i
\]

Or, in more compact matrix-vector notation, we get the following nonlinear but element-local equation system:

\[
K_1 \hat{q}_l = F_0 \hat{w}_m^n + M \hat{P}_l - K_\xi \cdot \hat{F}_l
\]

For its solution, we use the following fixed-point iteration scheme:

\[
K_1 \hat{q}_l^{i+1} = F_0 \hat{w}_m^n + M \hat{P}_l^i - K_\xi \cdot \hat{F}_l^i \quad \text{(FP)}
\]

In the stiff case (e.g. resistive RMHD), the source term \( S \) is taken locally implicit in (FP).
General $P_NP_M$ Schemes on Unstructured Meshes

3. Explicit corrector scheme

Multiply eqn. (PDE) with spatial test functions $\phi_k$ (piecewise polynomials of degree $N$) and integrate in space and time:

$$\left\langle \Phi_k, \frac{\partial}{\partial t} Q \right\rangle_{T_i} + \left\langle \Phi_k, \nabla \cdot F(Q, \nabla Q) + B(Q) \cdot \nabla Q \right\rangle_{T_i} = \left\langle \Phi_k, S(Q) \right\rangle_{T_i}$$

Integration by parts in time yields then the fully-discrete $P_NP_M$ scheme

$$[\Phi_k, u_h^{n+1}]_{T_i}^{t_{n+1}} - [\Phi_k, u_h^{n}]_{T_i}^{t_n} + \left\langle \Phi_k, \nabla F(q_h, \nabla q_h) + B(q_h) \cdot \nabla q_h \right\rangle_{T_i \setminus \partial T_i} \bigg|_{t_n}^{t_{n+1}}$$

$$+ \left\{ \Phi_k, \mathcal{D}_{i+\frac{1}{2}}^{-} (q_h^{-}, \nabla q_h^{-}, q_h^{+}, \nabla q_h^{+}) \cdot \vec{n} \right\}_{\partial T_i} = \left\langle \Phi_k, S(q_h) \right\rangle_{T_i},$$

with a path-conservative jump term [Toumi 1992, Parés 2006, Castro et al. 2006], formally consistent with the theory of [Dal Maso, Le Floch and Murat, 1995]. If the PDE is conservative ($B(Q)=0$), then the method reduces to a classical fully conservative scheme.
Summary of the Algorithm

(1) Use the $P_N P_M$ reconstruction operator at the current time $t^n$ to reconstruct the polynomials $w_h$ of degree $M$ from the polynomials $u_h$ of degree $N$ that are stored and evolved in each cell.

$$w_h^n = R_h (u_h^n)$$

(2) Use the local space-time DG predictor method to obtain for each cell a space-time predictor polynomial of degree $M$, valid in the time interval $[t^n, t^{n+1}]$.

$$q_h = E_h (w_h^n)$$

(3) Use the globally explicit one-step $P_N P_M$ corrector scheme to evolve the piecewise polynomial data $u_h$ of degree $N$ from time $t^n$ to time $t^{n+1}$.

$$u_h^{n+1} = u_h^n + P_N^M (q_h, \nabla q_h)$$

**Special cases:**

- $N = 0$: classical high order finite volume scheme
- $N = M$: usual DG finite element scheme
Some Results of Unlimited PNPM Schemes

To verify the order of accuracy, we use the resistive relativistic MHD (RRMHD) equations. In the stiff case \((\sigma \rightarrow \infty)\) the system tends to the ideal relativistic MHD (RMHD) equations, for which exact solutions are known [Del Zanna et al. 2007].

**Governing PDE System**

\[
\begin{align*}
\partial_t D + \partial_i (D v^i) &= 0, \\
\partial_t S_j + \partial_j Z_j &= 0, \\
\partial_t \tau + \partial_i S^i &= 0, \\
\partial_t E^i - \epsilon^{ijk} \partial_j B_k + \partial_t \Psi &= -f^i, \\
\partial_t B^i + \epsilon^{ijk} \partial_j E_k + \partial_t \Phi &= 0, \\
\partial_t \Psi + \partial_i E^i &= \rho_e - \kappa \Psi, \\
\partial_t \Phi + \partial_i B^i &= -\kappa \Phi, \\
\partial_t \rho_e + \partial_j f^j &= 0,
\end{align*}
\]

**Conserved quantities**

\[
\begin{align*}
D &= \rho \Gamma, \\
S^i &= \omega \Gamma^2 v^i + \epsilon^{ijk} F_j B_k, \\
\tau &= \omega \Gamma^2 - p + \frac{1}{2} (E^2 + B^2),
\end{align*}
\]

**Variables used in the fluxes**

\[
Z^i_j = \omega \Gamma^2 v^i v_j - E^i E_j - B^i B_j + \left[ p + \frac{1}{2} (E^2 + B^2) \right] \delta^i_j
\]

\[
p = (\gamma - 1) \rho \epsilon = \gamma_1 (\epsilon - \rho)
\]

**Ohm’s law (stiff source term)**

\[
\vec{J} = \rho_e \vec{v} + \sigma I \bar{E} + \vec{v} \times \vec{B} - (\bar{E} \cdot \vec{v}) \vec{v}
\]
### Some Results of Unlimited PNPM Schemes

**Table 1**  
Large amplitude Alfvén wave. Convergence study of $P_nP_M$ schemes from third to fifth order of accuracy. $\sigma = 10^7$, apart from the $P_1P_4$ scheme where $\sigma = 10^8$. Errors are computed for variable $B_y$.

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<th>$P_0P_2$</th>
<th>$P_1P_2$</th>
<th>$P_2P_2$</th>
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**Table 2**  
Large amplitude Alfvén wave. Verification of the order of accuracy for a variable affected by the stiff source term. We use the quantity $E_y$ and some selected $P_nP_M$ schemes.

<table>
<thead>
<tr>
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<th>$P_0P_3$</th>
<th>$P_1P_4$</th>
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</table>
Some Results of Unlimited PNPM Schemes

Compressible MHD turbulence (viscous & resistive MHD - VRMHD)  

CFD & Aeroacoustics (compressible Navier-Stokes)
Some Results of Unlimited PNPM Schemes

Seismic wave propagation in complex heterogeneous media, poroelasticity (linear elasticity, anisotropy, attenuation, stiff sources)
Objectives

(1) Design a **new limiter** for the discontinuous Galerkin finite element method \((N=M)\) for nonlinear PDE that is **simple, robust** and **accurate**

(2a) The new limiter **must not destroy** the subcell resolution capability of the DG scheme, neither at discontinuities, nor in smooth regions, where it might have been erroneously activated, or, equivalently

(2b) The limiter must act on a characteristic **length scale** of \(h/(N+1)\) and **not** on the length scale \(h\) of the main grid, i.e. accuracy improves with \(N\) **even at shocks**

(3) The DG limiter should **not** contain **problem-dependent parameters**, like, e.g., the well-known parameter \(M\) of the classical TVB limiter of Cockburn and Shu.

(4) The new limiter should work well for **very high** polynomial degrees, say \(N=9\).

(5) Ideally, the final DG scheme should become **as robust** as a traditional **second order TVD finite volume scheme**, but **more accurate** on a given computational mesh of characteristic mesh size \(h\)
A new *a posteriori* limiter of DG-FEM methods

- Conventional DG limiters use either artificial viscosity, which needs parameters to be tuned, or nonlinear FV-type reconstruction/limiters (TVB, WENO, HWENO), which *usually destroy* the subcell resolution properties.

- Our new approach extends the successful *a posteriori* MOOD method of Loubère et al., developed in the FV context, also to the DG-FEM framework.

- As very simple *a posteriori* detection criteria, we only use
  - A relaxed discrete maximum principle (DMP) in the sense of polynomials
  - *Positivity* of the solution and absence of floating point errors (*NaN*)

- If one of these criteria is violated after a time step, the scheme *goes back* to the old time step and *recomputes* the solution in the troubled cells, using a more robust ADER-WENO or TVD FV scheme on a *fine subgrid* composed of $2N+1$ subcells per space dimension
A new a posteriori limiter of DG-FEM methods

- Classical DG limiters, like WENO/HWENO/slope/moment limiters are based on **nonlinear data post-processing**, while the new DG limiter **recomputes** the discrete solution with a more robust scheme, starting again from a **valid solution** available at the old time level.

- Alternative description: dynamic, element-local **checkpointing** and **restarting** of the solver with a more robust scheme on a finer grid.

- This enables the limiter even to **cure** floating point errors (**NaN** values appearing after division by zero or after taking roots of negative numbers).

- The new method is by construction **positivity preserving**, **iff** the underlying finite volume scheme on the subgrid preserves positivity.

- **Local limiter** (in contrast to WENO limiters for DG), since it requires only information from the cell and its direct neighborhood.

- As **accurate** as a high order **unlimited DG scheme** in smooth flow regions, but at the same time as **robust** as a **second order TVD scheme** at shocks or other discontinuities, but also at strong rarefactions.
If a classical nonlinear reconstruction-based DG limiter is activated erroneously, there may be important physical information that is lost forever!
A new a posteriori limiter of DG-FEM methods

DG polynomials of degree $N=8$ (left) and equivalent data representation on $2N+1=17$ subcells (right). Arrows indicate projection (red) and reconstruction (blue).

We use $2N+1$ subcells to match the DG time step ($\text{CFL}<1/(2N+1)$) on the coarse grid with the FV time step ($\text{CFL}<1$) on the fine subgrid.

$$\mathcal{R} \circ \mathcal{P} = \mathcal{I}$$
A new \textit{a posteriori} limiter of DG-FEM methods

Projection from the DG polynomials to the subcell averages

\[ v^n_{i,j} = \frac{1}{|S_{i,j}|} \int_{S_{i,j}} u_h(x, t^n) \, dx = \frac{1}{|S_{i,j}|} \int_{S_{i,j}} \phi_l(x) \, dx \hat{u}^n_l, \quad \forall S_{i,j} \in S_i. \]

Reconstruction of DG polynomials from the subcell averages

\[ \int_{S_{i,j}} u_h(x, t^n) \, dx = \int_{S_{i,j}} v_h(x, t^n) \, dx, \quad \forall S_{i,j} \in S_i. \]

\[ \int_{T_i} u_h(x, t^n) \, dx = \int_{T_i} v_h(x, t^n) \, dx. \quad \text{Linear constraint: conservation} \]

Overdetermined system, solved by a constrained LSQ algorithm.
Relaxed DMP in the sense of polynomials

\[
\min_{y \in \mathcal{V}_i} (u_h(y, t^n)) - \delta \leq u_h^*(x, t^{n+1}) \leq \max_{y \in \mathcal{V}_i} (u_h(y, t^n)) + \delta.
\]
Summary of the ADER-DG-MOOD scheme

Verification of the DMP and the positivity on the candidate solution \( u_h^*(x, t^{n+1}) \):

\[
\min_{y \in \mathcal{V}_i} (v_h(y, t^n)) - \delta \leq v_h^*(x, t^{n+1}) \leq \max_{y \in \mathcal{V}_i} (v_h(y, t^n)) + \delta, \quad \forall x \in T_i,
\]

\[
\pi_k(u_h^*(x, t^{n+1})) > 0, \quad \forall x \in T_i, \quad \forall k,
\]

If a cell does not satisfy both criteria, flag it as troubled cell, \( \beta_i^{n+1} = 1 \), discard the DG solution and recompute it with a more robust third order ADER-WENO or an even more robust second order TVD finite volume scheme on the fine subgrid:

\[
v_h(x, t^{n+1}) = A(v_h(x, t^n))
\]

\[
v_h(x, t^n) = \begin{cases} 
    \mathcal{P}(u_h(x, t^n)) & \text{if } \beta_j^n = 0, \\
    A(v_h(x, t^{n-1})) & \text{if } \beta_j^n = 1.
\end{cases} \quad x \in T_j \quad \forall T_j \in \mathcal{V}_i.
\]

Finally, reconstruct the DG polynomial from the subcell averages:

\[
u_h(x, t^{n+1}) = R(v_h(x, t^{n+1})) \quad \text{or} \quad u_h(x, t^{n+1}) = R(A(v_h(x, t^n)))
\]
### Numerical Convergence Results P2-P9 (2D Euler)

<table>
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<th>$N_x$</th>
<th>$L^1$ error</th>
<th>$L^2$ error</th>
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ADER-DG-MOOD Results

Sod shock tube,
20x5 elements (N=9)

Limited cells (red),
Unlimited cells (blue)
ADER-DG-MOOD Results

Lax shock tube,
20x5 elements (N=9)

Limited cells (red),
Unlimited cells (blue)
A posteriori subcell finite volume limiting of the Discontinuous Galerkin method

ADER-DG-MOOD Results

Shock-density interaction problem of Shu & Osher
40x5 cells (N=9). Unlimited cells (blue) and limited cells (red)
Double Mach Reflection Problem

300x100 cells (N=2, 5, 9). Unlimited cells (blue) and limited cells (red)
A posteriori subcell finite volume limiting of the Discontinuous Galerkin method

3D Spherical Explosion Problem

100³ cells (N=9), corresponding to 10 billion space-time degrees of freedom per time step. Unlimited cells (blue) and limited cells (red)
Extension to high order AMR: Grid and Data Structure

One refinement level & virtual cells

Two refinement levels & virtual cells
AMR with Time-Accurate Local Time Stepping (LTS)

Within our high order ADER one-step predictor-corrector approach, LTS is almost trivial:
Double Mach Reflection Problem (FV)
MHD Orszag-Tang Vortex (FV)

Memory and CPU time comparison of the third order ADER-WENO AMR method and ADER-WENO on a uniform fine grid for the Orszag–Tang problem. Memory consumption is measured in maximum number of elements and CPU time is normalized with respect to the simulation on the fine uniform mesh.

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MHD Rotor Problem (FV)

Memory and CPU time comparison of the third order ADER-WENO AMR method and ADER-WENO on a uniform fine grid for the MHD rotor problem. Memory consumption is measured in maximum number of elements and CPU time is normalized with respect to the total wallclock time on the uniform mesh.

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Coupling of *a posteriori* subcell limiters for DG with AMR

ADER-DG (N=9) with AMR & LTS. Unlimited cells (blue) and limited cells (red)
Coupling of AMR with a posteriori subcell limiters for DG

ADER-DG (N=9) with a posteriori ADER-WENO subcell limiter, space-time adaptive mesh refinement (AMR) and LTS yields an unprecedented resolution of shocks and contact waves.
Coupling of AMR with a posteriori subcell limiters for DG

Double Mach reflection problem using ADER-DG (N=9) with a posteriori ADER-WENO subcell limiter, space-time adaptive mesh refinement (AMR) & LTS
RMHD blast wave problem

ADER-DG (N=3) with a posteriori TVD subcell limiter.
Natural Extension to Unstructured Meshes

Subgrid for $N=1$ to $N=6$ in 2D
Natural Extension to Unstructured Meshes

Subgrid for N=1 to N=5 in 3D
Natural Extension to Unstructured Meshes

Circular explosion problem in 2D ($N=5$)
Natural Extension to Unstructured Meshes

Spherical explosion problem in 3D ($N=3$)
A posteriori subcell finite volume limiting of the Discontinuous Galerkin method

Natural Extension to Unstructured Meshes

Mach 3 flow over a sphere (N=3)
First Order Hyperbolic Formulation of Continuum Mechanics

\[
\frac{\partial \rho}{\partial t} + \frac{\partial \rho \nu_k}{\partial x_k} = 0, \quad (1a)
\]

\[
\frac{\partial \rho \nu_i}{\partial t} + \frac{\partial \left( \rho \nu_i \nu_k + p \delta_{ik} - \sigma_{ik} \right)}{\partial x_k} = 0, \quad (1b)
\]

\[
\frac{\partial A_{ik}}{\partial t} + \frac{\partial A_{im} \nu_m}{\partial x_k} + \nu_j \left( \frac{\partial A_{ik}}{\partial x_j} - \frac{\partial A_{ij}}{\partial x_k} \right) = - \frac{\psi_{ik}}{\theta_1(\tau_1)}, \quad (1c)
\]

\[
\frac{\partial \rho J_i}{\partial t} + \frac{\partial \left( \rho J_i \nu_k + T \delta_{ik} \right)}{\partial x_k} = - \frac{\rho H_i}{\theta_2(\tau_2)}, \quad (1d)
\]

\[
\frac{\partial \rho S}{\partial t} + \frac{\partial \left( \rho s \nu_k + H_k \right)}{\partial x_k} = \frac{\rho}{\theta_1(\tau_1) T} \psi_{ik} \psi_{ik} + \frac{\rho}{\theta_2(\tau_2) T} H_i H_i \geq 0, \quad (1e)
\]

\[
\frac{\partial \rho E}{\partial t} + \frac{\partial \left( v_k \rho E + \nu_i \left( p \delta_{ik} - \sigma_{ik} \right) + q_k \right)}{\partial x_k} = 0, \quad (2)
\]

First Order Hyperbolic Formulation of Continuum Mechanics

**Overdetermined PDE system**, which is consistent if and only if the total energy $E$ is a **potential** that depends on the other state variables:

$$E = E(\rho, s, \mathbf{v}, A, \mathbf{J})$$

All the other fluxes (pressure, viscous stress tensor) and the dissipative source term are then a direct **consequence** of the choice of $E$:

**Pressure:**

$$p = \rho^2 E_\rho$$

**Temperature:**

$$T = E_s$$

**Stress tensor:**

$$[\sigma_{ik}] = \sigma = -[\rho A_{mi} E_{Amk}]$$

**Heat flux vector:**

$$[q_k] = \mathbf{q} = [E_s E_{Jk}]$$

**Strain relaxation:**

$$[\psi_{ik}] = \psi = [E_{Ai_k}] \quad \sigma = -\rho A^T \psi$$

**Heat flux relaxation:**

$$[H_i] = \mathbf{H} = [E_{Ji}] \quad \mathbf{q} = T \mathbf{H}$$

Furthermore, some positive functions of the relaxation times $\tau_1$ and $\tau_2$:

$$\theta_1 = \theta_1(\tau_1) > 0 \quad \theta_2 = \theta_2(\tau_2) > 0$$
First Order Hyperbolic Formulation of Continuum Mechanics

Choice of the total energy potential:

\[ E(\rho, s, v, A, J) = E_1(\rho, s) + E_2(A, J) + E_3(v). \]

Classical equation of state, e.g. ideal gas EOS (micro-scale):

\[ E_1(\rho, s) = \frac{c_0^2}{\gamma(\gamma - 1)}, \quad c_0^2 = \gamma \rho^{\gamma-1} c_s^2/c_v \]

Classical kinetic energy (macro-scale):

\[ E_3(v) = \frac{1}{2} v_i v_i \]

Energy stored in the meso-scale, due to deformations and heat-flux:

\[ E_2(A, J) = \frac{c_s^2}{4} G_{ij}^{TF} G_{ij}^{TF} + \frac{\alpha^2}{2} J_i J_i \]

\[ [G_{ij}^{TF}] = \text{dev}(G) = G - \frac{1}{3} \text{tr}(G) I, \quad \text{and} \quad G = A^T A. \]
First Order Hyperbolic Formulation of Continuum Mechanics

Stress tensor:

\[ \sigma = -\rho A^T \psi = -\rho A^T E_A = -\rho c_s^2 G \text{dev}(G) \]

\[ E_A = c_s^2 A \text{dev}(G) \]

Strain relaxation source term:

\[ -\frac{\psi}{\theta_1(\tau_1)} = -\frac{E_A}{\theta_1(\tau_1)} = -\frac{3}{\tau_1} |A|^{\frac{5}{3}} A \text{dev}(G) \]

with

\[ \theta_1(\tau_1) = \tau_1 c_s^2 / 3 |A|^{-\frac{5}{3}} \]

Heat flux vector:

\[ q = T \mathbf{H} = E_s E_J = \alpha^2 T \mathbf{J} \]

\[ E_J = \alpha^2 \mathbf{J} \]

Thermal impulse relaxation source term:

\[ -\frac{\rho \mathbf{H}}{\theta_2(\tau_2)} = -\frac{\rho E_J}{\theta_2(\tau_2)} = -\frac{T}{T_0} \frac{\rho_0}{\rho} \frac{\rho J}{\tau_2} \]

\[ \theta_2 = \tau_2 \alpha^2 \frac{\rho}{\rho_0} \frac{T_0}{T} \]
First Order Hyperbolic Formulation of Continuum Mechanics

Compatibility condition:

\[
\begin{align*}
(E - V E_V - s E_s - v_i E_v_i - J_i E_{J_i}) \cdot (1a) + (\rho E)_{\rho v_i} \cdot (1b) + \\
+ (\rho E)_{A_{ik}} \cdot (1c) + (\rho E)_{\rho J_i} \cdot (1d) + (\rho E)_{\rho s} \cdot (1e) \equiv (2)
\end{align*}
\]

The dissipative mechanisms on the right hand side of the GPR model are chosen such that total energy is conserved (first law of thermodynamics) and that entropy production is non-negative (second law of thermodynamics).

Use of the thermodynamic dual variables (factors above)

\[
r = E - V E_V - s E_s - v_i E_v_i - J_i E_{J_i}, \quad v_i = (\rho E)_{\rho v_i}, \]

\[
\alpha_{ik} = (\rho E)_{A_{ik}}, \quad \Theta_i = (\rho E)_{\rho J_i}, \quad \sigma = (\rho E)_{\rho s}
\]

and the Legendre transform of the potential \( E \) lead to the new potential

\[
L(r, v_i, \alpha_{ik}, \Theta_i, \sigma) = r \rho + v_i \rho v_i + \alpha_{ik} A_{ik} + \Theta_i \rho J_i + \sigma \rho s - \rho E
\]
First Order Hyperbolic Formulation of Continuum Mechanics

and to the following PDE system (only LHS shown here), which is also directly connected to a variational formulation (minimization of a Lagrangian):

\[
\frac{\partial L_r}{\partial t} + \frac{\partial (v_k L)_r}{\partial x_k} = 0,
\]

\[
\frac{\partial L_{v_i}}{\partial t} + \frac{\partial (v_k L)_{v_i}}{\partial x_k} + L_{\alpha i m} \frac{\partial \alpha_{km}}{\partial x_k} - L_{\alpha m k} \frac{\partial \alpha_{mk}}{\partial x_i} = 0,
\]

\[
\frac{\partial L_{\alpha il}}{\partial t} + \frac{\partial (v_k L)_{\alpha il}}{\partial x_k} + L_{\alpha i ml} \frac{\partial \gamma_{ml}}{\partial x_i} - L_{\alpha il m} \frac{\partial \gamma_{ml}}{\partial x_k} = 0,
\]

\[
\frac{\partial L_{\Theta i}}{\partial t} + \frac{\partial (v_k L)_{\Theta i}}{\partial x_k} + \frac{\partial \sigma \delta_{ik}}{\partial x_k} = 0,
\]

\[
\frac{\partial L_{\Theta r}}{\partial t} + \frac{\partial (v_k L)_{\Theta r}}{\partial x_k} + \frac{\partial \Theta_{kr}}{\partial x_k} = 0,
\]

The above system is symmetric. It is hyperbolic, iff the potential \( L \) is convex.

\[
\mathcal{M}(P) \frac{\partial P}{\partial t} + \mathcal{H}_k(P) \frac{\partial P}{\partial x_k} = 0 \quad \mathcal{M}^T = \mathcal{M} \quad \mathcal{H}_k^T = \mathcal{H}_k
\]
First Order Hyperbolic Formulation of Continuum Mechanics

Asymptotic (stiff) relaxation limit of the stress tensor:

\[
\dot{G} = \frac{\partial G}{\partial t} + \mathbf{v} \cdot \nabla G
\]

\[
\dot{G} = - \left( G \nabla \mathbf{v} + \nabla \mathbf{v}^T G \right) + \frac{2}{\rho \theta_1} \sigma,
\]

Chapman-Enskog expansion of \( G \)...

\[
G = G_0 + \tau_1 G_1 + \tau^2_1 G_2 + ...
\]

... and some calculations ...

\[
\frac{d}{dt}(G_0 + \tau_1 G_1 + ...) = - \left( (G_0 + \tau_1 G_1 + ...) \nabla \mathbf{v} + \nabla \mathbf{v}^T (G_0 + \tau_1 G_1 + ...) \right) - \frac{6}{\tau_1} |G_0 + \tau_1 G_1 + ...|^{\frac{5}{6}} (G_0 + \tau_1 G_1 + ...) \text{dev}(G_0 + \tau_1 G_1 + ...),
\]
First Order Hyperbolic Formulation of Continuum Mechanics

\[ \tau_1^{-1} \left( \frac{6|G_0|^{\frac{5}{3}} G_0 \text{dev}(G_0)}{0} \right) + \tau_1^0 \left( \frac{dG_0}{dt} + \ldots \right) + \ldots = 0. \]

... yield the important results:

\[ \text{dev}(G_0) = 0, \quad \Rightarrow \quad G_0 - \frac{1}{3} \text{tr}(G_0) I = 0, \quad \Rightarrow \quad G_0 = \frac{1}{3} \text{tr}(G_0) I. \]

Retaining only up to first order terms, we get:

\[ G = g I + \tau_1 G_1 = A^T A, \quad g := \frac{1}{3} \text{tr}(G_0) \]

\[ |G| = g^3 = |A|^2, \quad \Rightarrow \quad g = \frac{1}{3} \text{tr}(G_0) = \frac{1}{3} \text{tr}(G_0) = \left( \frac{\rho}{\rho_0} \right)^{\frac{2}{3}}. \]

\[ \sigma = -\tau_1 \rho_0 c_s^2 g^{\frac{5}{2}} \text{dev}(G_1). \]
First Order Hyperbolic Formulation of Continuum Mechanics

For the evolution equation of \( \text{dev}(G) \), we get:

\[
\frac{d}{dt} \text{dev}(G) + G \nabla v + \nabla v^T G - \frac{1}{3} \text{tr}(G \nabla v + \nabla v^T G) I = -\frac{6}{\tau_1} |G|^{5/6} \text{dev}(G_{\text{dev}}(G)).
\]

Retaining only the leading terms leads to

\[
G_0 \nabla v + \nabla v^T G_0 - \frac{2}{3} \text{tr}(G_0 \nabla v) I = -6 |G_0|^{7/6} \text{dev}(G_1).
\]

Recall that \( G_0 = \rho I \), hence

\[
g \left( \nabla v + \nabla v^T - \frac{2}{3} \text{tr}(\nabla v) I \right) = -6 \rho^{7/2} \text{dev}(G_1).
\]

In the stiff limit, the classical Navier-Stokes stress tensor is recovered:

\[
\sigma = \frac{1}{6} \tau_1 \rho_0 c_s^2 \left( \nabla v + \nabla v^T - \frac{2}{3} \text{tr}(\nabla v) I \right) := \mu \left( \nabla v + \nabla v^T - \frac{2}{3} (\nabla \cdot v) I \right),
\]
First Order Hyperbolic Formulation of Continuum Mechanics

Note that the Navier-Stokes stress tensor is a direct consequence of the choice of a quadratic energy potential in terms of \( \text{dev}(G) \). We never have put the Navier-Stokes stress tensor explicitly into the model!

Similar calculations for the heat flux lead to the classical Fourier law:

\[
\frac{\partial \rho J}{\partial t} + \nabla \cdot (\rho J \otimes u) + \nabla T = -\frac{1}{\tau_2} \frac{T}{T_0} \rho_0 \rho J.
\]

\[
J = J_0 + \tau_2 J_1 + \tau_2^2 J_2 + ..., 
\]

\[
\tau_2^{-1} \left( \frac{T}{T_0} \frac{\rho_0}{\rho} J_0 \right) + \tau_2^0 \left( \frac{\partial \rho J_0}{\partial t} + \nabla \cdot (\rho J_0 \otimes u) + \nabla T + \frac{T}{T_0} \frac{\rho_0}{\rho} \rho J_1 \right) + ... = 0,
\]

\[
J_0 = 0.
\]

\[
J = -\tau_2 \frac{T_0}{\rho_0} \frac{\nabla T}{T}.
\]

\[
q = \alpha^2 T J = -\alpha^2 \tau_2 \frac{T_0}{\rho_0} \nabla T := -\kappa \nabla T
\]
First Order Hyperbolic Formulation of Continuum Mechanics

Or, since 2016 is the Leibniz year, to say it with the words of Gottfried Wilhelm Leibniz (1646-1716)

omnibus ex nihilo ducendis sufficit unum

in order to derive everything from nothing, one is enough

(for the GPR model, the one is the potential)
First Order Hyperbolic Formulation of Continuum Mechanics

The relaxation time $\tau_1$ and the shear wave speed $c_s$ of the GPR model can be obtained *experimentally via ultra sound measurements* of the phase velocity of longitudinal pressure waves, which is *different* for low and high frequencies. This effect is well known in the research field of ultra-sound. It is *not predicted* by the classical Navier-Stokes equations of fluid mechanics, but by the GPR model!

$$\lambda_{5,6} = \pm \sqrt{c_0^2 + \frac{4}{3} c_s^2}$$

**Fig. 1.** Phase velocity of the longitudinal wave (left) and shear wave (right) versus log($\omega$) propagating in a viscous gas with parameters $\rho = 1.177$ kg/m$^3$, $\gamma = 1.4$, $c_v = 718$ J/(kgK), $s = 8100$, $c_0 = 344.3$ m/s, $c_s = 50$ m/s, $\mu = 1.846 \cdot 10^{-5}$ Pa s, $\tau_1 = 3.76 \cdot 10^{-8}$ s.
A posteriori subcell finite volume limiting of the Discontinuous Galerkin method

Blasius Boundary Layer + Poiseille Flow
Lid-Driven Cavity Flow at Re=100
Double Shear-Layer

GPR model

Navier-Stokes
Double Shear-Layer

distortion tensor A
Compressible Mixing Layer

Navier-Stokes

GPR model
3D Taylor-Green Vortex
3D Taylor-Green Vortex
3D Taylor-Green Vortex
Viscous heat-conducting shock
Lamb’s problem from solid mechanics (simply let $\tau_1 \rightarrow \infty$)
Conclusions I

• New, simple robust and accurate *a posteriori* subcell finite volume limiter for the discontinuous Galerkin finite element method available for uniform and space-time adaptive (AMR) Cartesian grids as well as for general triangular and tetrahedral unstructured meshes

• The *a posteriori* MOOD framework of Loubère, Clain and Diot has been found to be an ideal framework to devise a simple and robust limiter for DG schemes

• Why *a posteriori*: It is much simpler to **observe** (and cure) the occurrence of a troubled cell rather than to **predict** (and avoid) its occurrence from given data.

• Element-local **checkpointing** and solver **restarting** is even able to **cure** floating point errors (**NaN**, e.g. after division by zero)

• Tested on a large set of different hyperbolic PDE systems

• Application to the thermodynamically consistent **hyperbolic** model of continuum mechanics of Godunov, Peshkov and Romenski (GPR), where all processes have **finite speeds**, including **dissipative** ones
Conclusions II

Wavespeeds are finite, hence the world is hyperbolic.
Outlook

• Extension of the new DG limiter to **moving unstructured** meshes (ALE)

• Extension of the method to an extended GPR model that also includes **electro-magnetic** wave propagation (Maxwell eqn.), reducing to the viscous & resistive MHD equations in the stiff limit, but which also includes **electrodynamics** in **moving dielectric solids**.

• Thanks to the presence of **finite wave speeds** for all physical effects in the GPR model (including dissipative effects):

  Extension of the GPR model to the special & general **relativistic case**. This model would then include **classical Newtonian continuum mechanics** as well as **relativistic continuum mechanics** and **electrodynamics** and the description of the resulting gravitational waves in one single **hyperbolic** PDE system.
References


