Second-Order Invariant Domain Preserving Approximation Of The Compressible Navier–Stokes Equations

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for Hyperbolic Equations
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Collaborators and acknowledgments

This work done in collaboration with:
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Matthias Maier (Dept. Math., TAMU, TX)
Bojan Popov (Dept. Math., TAMU, TX)
Ignacio Tomas (Sandia National Laboratories, NM)

Support:

AFOSR AIR FORCE OFFICE OF SCIENTIFIC RESEARCH
ARL
Lawrence Livermore National Laboratory
NSF

Outline

Background and objectives

Long term objectives of the research program

Objectives

Develop numerical techniques for solving nonlinear conservation equations (PDEs with dominant hyperbolic features) with the following guaranteed/certified properties:

- Be invariant domain preserving.
- Be asymptotic preserving (or well-balanced).
- Be (somewhat) discretization agnostic.
- Satisfy some entropy inequalities.

Key challenge: The above properties must be guaranteed/certified.

Why?

Numerical methods with certified properties

- are robust.
- can be used in confidence with very little know-how from the user.
- do not involve numerical parameter "to learn."

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Fields of applications

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- Compressible Euler equations (transonic to hypersonic)
- Euler-Poisson equations
- Compressible Navier-Stokes
- Gray radiation hydrodynamics
- Ideal magnetohydrodynamics
- Radiation transport
- Multi-material fluid flows
- Shallow water equations

Results established so far

Results established so far (since 2014)

- Visous regularization of Euler equations is compatible with every generalized entropy only if viscosity is equally applied on all the conserved variables. **Guermond, Popov (2014)**.
- Universal, discretization agnostic, invariant domain preserving technique, (First-order accurate in space). **Guermond, Popov (2016) (2017)**.
- Discretization agnostic limiting technique called convex limiting. Bounds using thermodynamic-based quasiconvave functionals are imposed locally. **Guermond, Nazarov, Popov, Tomas, (2018) (2019)**.
- Extension to ALE discretizations. **Guermond, Popov, Saavedra (2017) (2019) (2020)**.
- Various extensions to Serre & Saint-Venant equations, **Azerad, Farthing, Guermond, Kees, Quesada, Tovar, Popov (2017) (2018) (2019)**.
- Asymptotic and invariant domain preserving approximation of radiation transport. (First-order in streaming regime, second-order in diffusion regime). **Guermond, Popov, Ragusa (2020)**
- Robustness is guaranteed for all the above methods up to second-order accuracy.

Current work

Current work

- Demonstration of extreme scalability of the proposed algorithms for the compressible Euler equations and other hyperbolic systems using the deal.ii library, **Maier, Kronbichler (2021)**

Current work: extreme scalability

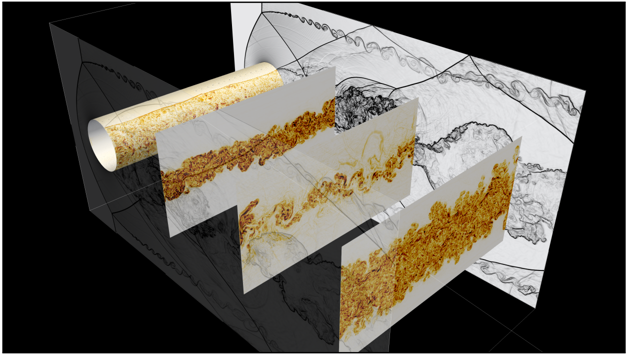

Figure: Continuous $\mathbb{Q}_1$ elements, 1.817B grid points, **Maier, Kronbichler (2021)**

Current work

Current work

- Topic of the today: extension to compressible Navier-Stokes using semi-implicit time stepping
  - Second-order accurate technique that is guaranteed to be invariant domain preserving technique under hyperbolic CFL. **G, Maier, Popov Tomas (2021)**

Outline

Compressible Navier-Stokes

Objectives

- Conservation equation for $\mathbf{u} = (\rho, \mathbf{m}, E)$:

$$\begin{aligned} &\partial_t \rho + \nabla\cdot(\mathbf{v}\rho) = 0, \\ &\partial_t \mathbf{m} + \nabla\cdot(\mathbf{v} \otimes \mathbf{m} + p(\mathbf{u})\mathbb{I} - \mathbb{s}(\mathbf{v})) = \mathbf{f}, \\ &\partial_t E + \nabla\cdot(\mathbf{v}(E + p(\mathbf{u})) - \mathbb{s}(\mathbf{v})\mathbf{v} + \mathbf{k}(\mathbf{u})) = \mathbf{f}\cdot\mathbf{v}. \end{aligned}$$

- + BC and Initial data.
- Fluid is Newtonian and heat-flux follows Fourier's law:

$$\begin{aligned} &\mathbb{s}(\mathbf{v}) = 2\mu\mathbb{e}(\mathbf{v}) + (\lambda - \tfrac{2}{3}\mu)\nabla\cdot\mathbf{v}\mathbb{I}, \qquad \mathbb{e}(\mathbf{v}) = \tfrac{1}{2}(\nabla\mathbf{v} + (\nabla\mathbf{v})^{\mathsf{T}}), \\ &\mathbf{k}(\mathbf{u}) = -c_v^{-1}\kappa\nabla e, \end{aligned}$$

with $\mu > 0$, $\lambda \geq 0$, and $\kappa > 0$.

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Objectives

- Two invariant domains can be identified:

$$\mathcal{A} := \{\mathbf{u} \mid \rho > 0,\ e(\mathbf{u}) > 0,\ s(\mathbf{u}) > s_{\text{min}}\}, \qquad \text{For Euler}$$
$$\mathcal{B} := \{\mathbf{u} \mid \rho > 0,\ e(\mathbf{u}) > 0\}, \qquad \text{For NS}$$

Difficulties: conflicting invariant sets and conflicting variables

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- Which invariant domain to preserve?
  - Minimum entropy principle is true for Euler.
  - Minimum entropy principle is false for NS.
- Which variable should be used?
  - "Right variable" for Euler is $\mathbf{u} = (\rho, \mathbf{m}, E)$ (conserved variables).
  - "Right variable" for NS is $(\rho, \mathbf{v}, e)$ (primitive variables).
  - Some advocate "entropy variable" and "entropy stability". (Seems very popular. Why? Pied Piper effect?)
- How to do the explicit-implicit time stepping?
  - The so-called "IMEX" literature is a desert on this topic.
  - One of the very few mathematically correct result we know: **Zhang & Shu (2017)**; but $\Delta t \leq ch^2$.

Our solution

Our solution (an overview)

- Use operator splitting to separate hyperbolic part and parabolic part.
- Hyperbolic operator

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- But how can it be done properly?

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Our solution

Our solution (an overview)

- Combine the explicit and implicit part using Strang's splitting in some clever way.
- The devil is in the details. Just "invoking" Strang's splitting is wishful thinking.

Our solution

Our solution for the hyperbolic part (an overview)

- Use conserved variables for the hyperbolic part.
- Make the hyperbolic part explicit.
- Invoke the "invariant-domain" technology with "convex limiting" for the explicit hyperbolic part.

Our solution

Our solution for the parabolic part (an overview)

- Use primitive variables for the parabolic part.
- Make the viscous terms implicit (in some clever way).
- Make the implicit algorithm "invariant-domain" preserving up to second-order in time.

Comments about IMEX vs. Strang

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- We are not aware (yet?) of the existence of any second-order IMEX technique that is invariant domain preserving for the NS equations and that is not somewhat equivalent to Strang splitting or a variation thereof.
- There is a very fundamental difficulty here: How to go beyond second-order and guarantee some "invariant-domain" preserving properties?

Brief description of the method

- Sequence of shape-regular meshes $(\mathcal{T}_h)_{h>0}$.
- Scalar-valued finite element space $P(\mathcal{T}_h)$ with basis functions $\{\varphi_i\}_{i\in\mathcal{V}}$. (Assume $P(\mathcal{T}_h) \subset C^0(\overline{D};\mathbb{R})$ for simplicity.)
- Vector-valued approximation space $\mathbf{P}(\mathcal{T}_h) := (P(\mathcal{T}_h))^{d+2}$. ($\Leftarrow$ current weakness)

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Hyperbolic step

- The hyperbolic step consists of solving

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Overview of solution strategy

Three step strategy

(i) Construct low-order invariant domain preserving method (GMS-GV).

(ii) Construct a high-order scheme that may not be invariant domain preserving.

(iii) Apply convex limiting with correct bounds inferred from low-order solution to get a high-order method that is invariant domain preserving.

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Hyperbolic step; GMS-GV scheme

- Set

$$\mathbf{c}_{ij} := \int_D \varphi_i \nabla \varphi_j \,\mathrm{d}x, \quad \mathbf{n}_{ij} := \frac{\mathbf{c}_{ij}}{\|\mathbf{c}_{ij}\|_{\ell^2}},$$
$$m_i := \int_D \varphi_i \,\mathrm{d}x.$$

(these are the only mesh-dependent coefficients of the method!)

- Let Δt be some time step.
- Let $\mathbf{u}_h(\cdot, t^n)$ approximated by $\sum_{i\in\mathcal{V}} \mathbf{U}_i^n \varphi_i$, $\mathbf{U}_i^n \in \mathbf{P}(\mathcal{T}_h) \cap \mathcal{A}$ (some current admissible state).
- Compute low-order update $\mathbf{U}_i^{\mathrm{L},n+1}$

$$\frac{m_i}{\Delta t}(\mathbf{U}_i^{\mathrm{L},n+1} - \mathbf{U}_i^n) + \sum_{j\in\mathcal{I}(i)} \mathbb{f}(\mathbf{U}_j^n)\mathbf{c}_{ij} - \sum_{j\in\mathcal{I}(i)\setminus\{i\}} d_{ij}^{\mathrm{L},n}(\mathbf{U}_j^n - \mathbf{U}_i^n) = \mathbf{0}.$$

- $d_{ij}^{\mathrm{L},n}$ low-order graph viscosity.

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GMS-GV scheme

Key ideas (Lax, Perthame, Tadmor, Shu, etc.)

- Let $i \in \mathcal{V}$, $j \in \mathcal{I}(i)$.
- Define unit vector $\mathbf{n}_{ij} := \frac{\mathbf{c}_{ij}}{\|\mathbf{c}_{ij}\|_{\ell^2}}$
- Consider sates $\mathbf{U}_i^n$ and $\mathbf{U}_j^n$.
- Consider 1D Riemann problem

$$\partial_t \mathbf{u} + \partial_x(\mathbb{f}(\mathbf{u})\mathbf{n}_{ij}) = 0, \quad (x,t) \in \mathbb{R}\times\mathbb{R}_+, \qquad \mathbf{u}(x,0) = \begin{cases} \mathbf{U}_i^n, & \text{if } x < 0 \\ \mathbf{U}_j, & \text{if } x > 0, \end{cases}$$

- Recall that $\mathbb{f}'(\mathbf{u})\mathbf{n}_{ij}$ is diagonalizable with real eigenvalues.

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$$\partial_t \mathbf{u} + \partial_x(\mathbb{f}(\mathbf{u})\mathbf{n}_{ij}) = 0, \quad (x,t) \in \mathbb{R}\times\mathbb{R}_+, \qquad \mathbf{u}(x,0) = \begin{cases} \mathbf{U}_i^n, & \text{if } x < 0 \\ \mathbf{U}_j, & \text{if } x > 0, \end{cases}$$

- Recall that $\mathbb{f}'(\mathbf{u})\mathbf{n}_{ij}$ is diagonalizable with real eigenvalues.

GMS-GV scheme

Key ideas (Lax, Perthame, Tadmor, Shu, etc.)

- Let $i \in \mathcal{V}$, $j \in \mathcal{I}(i)$.
- Define unit vector $\mathbf{n}_{ij} := \frac{\mathbf{c}_{ij}}{\|\mathbf{c}_{ij}\|_{\ell^2}}$
- Consider sates $\mathbf{U}_i^n$ and $\mathbf{U}_j^n$.
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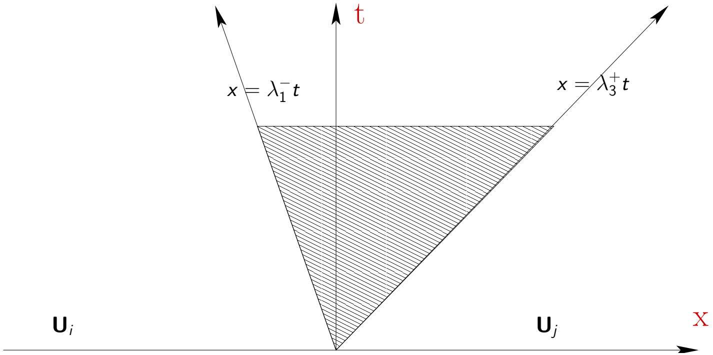

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- Introduce $\lambda_{\max}(\mathbf{n}_{ij}, \mathbf{U}_i^n, \mathbf{U}_j^n)$, an upper bound on maximum wave speed.

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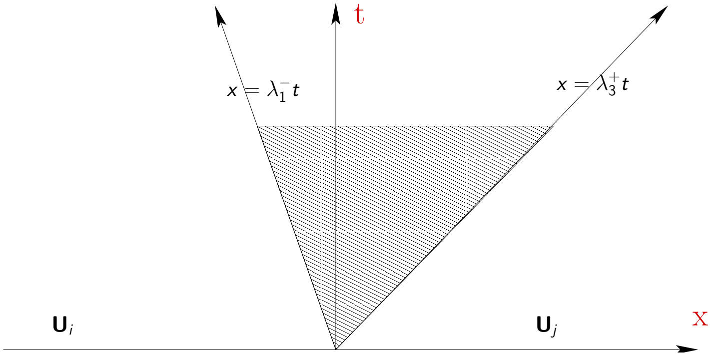

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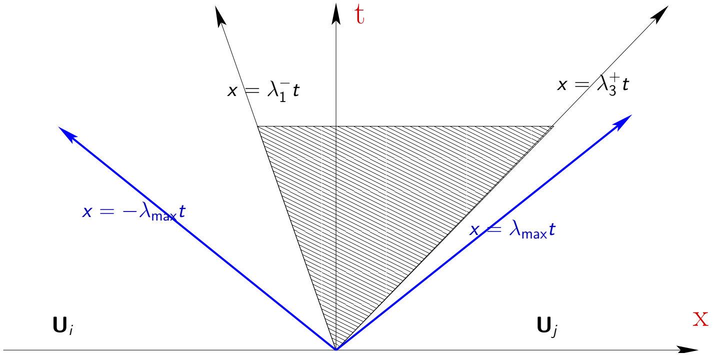

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$$d_{ij}^{\mathrm{L},n} := \max(\lambda_{\max}(\mathbf{n}_{ij}, \mathbf{U}_i^n, \mathbf{U}_j^n)\|\mathbf{c}_{ij}\|_{\ell^2}, \lambda_{\max}(\mathbf{n}_{ji}, \mathbf{U}_j^n, \mathbf{U}_i^n)\|\mathbf{c}_{ji}\|_{\ell^2}).$$

- Introduce auxiliary states ("bar states")

$$\overline{\mathbf{U}}_{ij}^n := \frac{1}{2}(\mathbf{U}_i^n + \mathbf{U}_j^n) - (\mathbb{f}(\mathbf{U}_j^n) - \mathbb{f}(\mathbf{U}_i^n))\frac{\mathbf{c}_{ij}}{2d_{ij}^{\mathrm{L},n}}.$$

Lemma (Invariance of the auxiliary states, JLG+BP (2016-2018))

Let $\mathcal{B} \subset \mathcal{A}$ be any convex invariant set. Then

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GMS-GV scheme

Key observation

- Convex combination

$$\mathbf{U}_i^{\mathsf{L},n+1} = \left(1 - 2\Delta t \frac{\sum_{j\in\mathcal{I}(i)\setminus\{i\}} d_{ij}^{\mathsf{L},n}}{m_i}\right)\mathbf{U}_i^n + \sum_{j\in\mathcal{I}(i)\setminus\{i\}} \frac{2\Delta t d_{ij}^{\mathsf{L},n}}{m_i}\overline{\mathbf{U}}_{ij}^n.$$

GMS-GV scheme

Theorem (GMS-GV, Local invariance, JLG+BP (2016-2018))

- *Let* $n \geq 0$ *and let* $i \in \mathcal{V}$.
- *Assume that* Δt *is small enough so that* $1 - 4\Delta t \frac{\sum_{j \in \mathcal{I}(i)\setminus\{i\}} d_{ij}^{\mathrm{L},n}}{m_i} \geq 0$.
- *Let* $\mathcal{B} \subset \mathcal{A}$ *be a convex invariant set*
- *Then*

$$(\mathbf{U}_j^n \in \mathcal{B},\ \forall j \in \mathcal{I}(i)) \Longrightarrow (\mathbf{U}_i^{\mathrm{L},n+1} \in \mathcal{B}).$$

- This is the generalization of the maximum principle for any discretization (any mesh), in any space dimension, for any hyperbolic system.
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Key idea

Reduce the graph viscosity d_{ij}^{n} as much as possible to be as close as possible to the Galerkin solution (very accurate).

Be careful: do not be too greedy

- Using zero artificial viscosity, $d_{ij}^{\mathrm{H},n} = 0$ may seem to be a good idea (if your world is linear), but it is always a bad idea.
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$$\boxed{\nabla\cdot(\mathbf{F}(\mathbf{u})) = (\nabla\eta(\mathbf{u}))^{\mathsf{T}}\nabla\cdot(\mathbb{f}(\mathbf{u}))}$$

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$$R_i^n := \frac{\sum_{j\in\mathcal{I}(i)}(\mathbf{F}(\mathbf{U}_j^n) - (\eta'(\mathbf{U}_i^n))^{\mathsf{T}}\mathbb{f}(\mathbf{U}_j^n))\mathbf{c}_{ij}}{\|\sum_{j\in\mathcal{I}(i)}(\mathbf{F}(\mathbf{U}_j^n)\mathbf{c}_{ij}\| + \|\sum_{j\in\mathcal{I}(i)}(\eta'(\mathbf{U}_i^n))^{\mathsf{T}}\mathbb{f}(\mathbf{U}_j^n))\mathbf{c}_{ij}\|}$$

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Convex limiting: Strategy

Strategy

- Let $\Psi : \mathcal{B} \to \mathbb{R}$ be a quasiconcave functional (ex: density, internal energy, entropy, . . .).
- Assume low-order update satisfies $\Psi(\mathbf{U}_i^{\mathrm{L},n+1}) \geq 0$.
- We want to "limit" the high-order update $\mathbf{U}_i^{\mathrm{H},n+1} \to \mathbf{U}_i^{n+1}$ so that

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Lemma (Fundamental bounds on the GMS-GV scheme, JLG+BP+IT (2018))

- *Let $\mathcal{B} \subset \mathcal{A} \subset \mathbb{R}^m$ be any convex set.*
- *Let $\Psi : \mathcal{B} \to \mathbb{R}$ be any quasiconcave functional.*
- *Let $n \geq 0$, $i \in \mathcal{V}$. Assume that $1 - 2dt \frac{\sum_{j\in\mathcal{I}(i)} d_{ij}^{\mathrm{L},n}}{m_i} \geq 0$.*
- *Let $\{\overline{\mathbf{U}}_{ij}^n\}_{j\in\mathcal{I}(i)}$ be the auxiliary states. Define the following quantity:*

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Convex limiting: Abstract framework

Abstract framework

- Invariant domain preserving low-order solution (GMS-GV):

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$$\mathbf{U}_i^{\mathrm{H},n+1} = \mathbf{U}_i^{\mathrm{L},n+1} + \sum_{j\in\mathcal{I}(i)\setminus\{i\}} \mathbf{A}_{ij}^n, \qquad \mathbf{A}_{ij}^n = \frac{\Delta t}{m_i}(\mathbf{F}_{ij}^{\mathrm{H},n} - \mathbf{F}_{ji}^{\mathrm{L},n}).$$

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Limiter set in not empty because $\ell_{ij} = 0$ is an admissible limiter.

The above program is meaningful!

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$$\frac{m_i}{\Delta t}(\mathbf{U}_i^{\mathrm{H},n+1} - \mathbf{U}_i^n) + \sum_{j\in\mathcal{I}(i)} \mathbf{F}_{ij}^{\mathrm{H},n} = \mathbf{0}, \qquad \mathbf{F}_{ij}^{\mathrm{H},n} = -\mathbf{F}_{ji}^{\mathrm{H},n}.$$

- Difference,

$$\mathbf{U}_i^{\mathrm{H},n+1} = \mathbf{U}_i^{\mathrm{L},n+1} + \sum_{j\in\mathcal{I}(i)\backslash\{i\}} \mathbf{A}_{ij}^n, \qquad \mathbf{A}_{ij}^n = \frac{\Delta t}{m_i}(\mathbf{F}_{ij}^{\mathrm{H},n} - \mathbf{F}_{ji}^{\mathrm{L},n}).$$

Lemma (Limiter set not empty)

Limiter set in not empty because $\ell_{ij} = 0$ is an admissible limiter.

The above program is meaningful!

Convex limiting: Abstract framework

Abstract framework

- Invariant domain preserving low-order solution (GMS-GV):

$$\frac{m_i}{\Delta t}(\mathbf{U}_i^{\mathrm{L},n+1} - \mathbf{U}_i^n) + \sum_{j\in\mathcal{I}(i)} \mathbf{F}_{ij}^{\mathrm{L},n} = \mathbf{0}, \qquad \mathbf{F}_{ij}^{\mathrm{L},n} = -\mathbf{F}_{ji}^{\mathrm{L},n}.$$

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- Difference, compute limiter $\ell_{ij} = \ell_{ji} \in [0,1]$ as large as possible s.t.:

$$\Psi_i(\mathbf{U}_i^{\mathrm{L},n+1} + \sum_{j\in\mathcal{I}(i)\backslash\{i\}} \ell_{ij}\mathbf{A}_{ij}^n) \geq 0, \qquad \mathbf{A}_{ij}^n = \frac{\Delta t}{m_i}(\mathbf{F}_{ij}^{\mathrm{H},n} - \mathbf{F}_{ji}^{\mathrm{L},n}).$$

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Convex limiting: Abstract framework

Strategy

Divide and conquer: Take care of each pair (i, j) separately.

Lemma

- *Let* $\{\lambda_j\}_{j\in\mathcal{I}(i)\setminus\{i\}}$ *be any set of strictly positive convex coefficients.*
- *Let* $\mathbf{P}_{ij}^n := \frac{1}{\lambda_j}\mathbf{A}_{ij}^n$.
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- *Let* $\Psi_i : \mathcal{B} \to \mathbb{R}$ *be a quasiconcave function.*
- *Compute largest limiting parameters* $\ell_{ij} \in [0, 1]$ *such that* $\Psi_i^l(\mathbf{U}_i^{\mathrm{L},n+1} + \ell_{ij}\mathbf{P}_{ij}^n) \geq 0$, *for all* $j \in \mathcal{I}(i)\setminus\{i\}$.

Then the following inequality holds true (owing to quasiconcavity):

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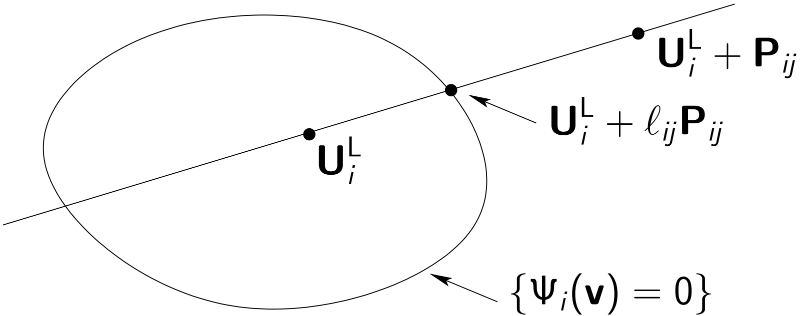
Limiting strategy



Hyperbolic step

- Let $S_{1h}(t_n + \Delta t, t_n) : \mathbf{P}(\mathcal{T}_h) \to \mathbf{P}(\mathcal{T}_h)$ denote the nonlinear update for the hyperbolic problem described in Guermond, Nazarov, Popov, Tomas, (2018) (2019).

Theorem (GNPT (2018) (2019))

S_{1h} is locally invariant domain preserving if CFL ≤ 1.

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S_{1h} is locally invariant domain preserving if CFL ≤ 1.

Parabolic step

$$\partial_t \rho = 0,$$
$$\partial_t \mathbf{m} - \nabla\cdot(\mathbb{s}(\mathbf{v})) = \mathbf{f},$$
$$\partial_t E + \nabla\cdot(\mathbf{k}(\mathbf{u}) - \mathbb{s}(\mathbf{v})\mathbf{v}) = \mathbf{f}\cdot\mathbf{v},$$
$$\mathbf{v}_{|\Gamma} = \mathbf{0}, \qquad \mathbf{k}(\mathbf{u})\cdot\mathbf{n}_{|\Gamma} = 0.$$

- Let Δt be some time step.
- Let $\mathbf{u}_h^n \in \mathbf{P}(\mathcal{T}_h) \cap \mathcal{B}$ (some current admissible state).

Parabolic step

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Parabolic step: density update

- Density update

$$\varrho_i^{n+1} := \varrho_i^n, \qquad \forall i \in \mathcal{V}.$$

Parabolic step: velocity update

- Introduce bilinear form associated with viscous dissipation,

$$a(\mathbf{v},\mathbf{w}) := \int_D \mathbb{s}(\mathbf{v}){:}\mathbb{e}(\mathbf{w})\,\mathrm{d}x, \qquad \mathbf{v},\mathbf{w} \in \mathbf{H}_0^1(D) := H_0^1(D;\mathbb{R}^d).$$

- Let $\{\mathbf{e}_k\}_{k\in\{1:d\}}$ be the canonical Cartesian basis of $\mathbb{R}^d$. For any $i \in \mathcal{V}$ and $j \in \mathcal{I}(i)$ define $d\times d$ matrix $\mathbb{B}_{ij} \in \mathbb{R}^{d\times d}$ by setting

$$(\mathbb{B}_{ij})_{kl} := a(\varphi_j\mathbf{e}_l, \varphi_i\mathbf{e}_k) := \int_D \mathbb{s}(\varphi_j\mathbf{e}_l){:}\nabla s(\varphi_i\mathbf{e}_k)\,\mathrm{d}x, \qquad \forall k,l \in \{1{:}d\}.$$

- Let $\mathbf{f}_h^{n+\frac{1}{2}} := \sum_{j\in\mathcal{V}} \mathbf{F}_j^{n+\frac{1}{2}}\varphi_j \in \mathbf{P}(\mathcal{T}_h)$ approximate $\mathbf{f}(t_n + \frac{1}{2}\Delta t)$. Use Crank-Nicolson to compute $\mathbf{u}_h^{n+1}$: solve for $\mathbf{V}^{n+\frac{1}{2}}$ s.t.

$$\begin{cases} \varrho_i^n m_i \mathbf{V}^{n+\frac{1}{2}} + \frac{1}{2}\Delta t \sum_{j\in\mathcal{I}(i)} \mathbb{B}_{ij}\mathbf{V}^{n+\frac{1}{2}} = m_i\mathbf{M}_i^n + \frac{1}{2}\Delta t\, m_i \mathbf{F}_i^{n+\frac{1}{2}}, & \forall i \in \mathcal{V}^\circ \\ \mathbf{V}_i^{n+\frac{1}{2}} = \mathbf{0}, & \forall i \in \mathcal{V}^\partial, \end{cases}$$

- And set

$$\mathbf{V}_i^{n+1} := 2\mathbf{V}^{n+\frac{1}{2}} - \mathbf{V}_i^n, \qquad \mathbf{M}_i^{n+1} := \varrho_i^{n+1}\mathbf{V}_i^{n+1}, \qquad \forall i \in \mathcal{V}.$$

Parabolic step: velocity update

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- Let $\mathbf{f}_h^{n+\frac12} := \sum_{j\in\mathcal{V}} \mathbf{F}_j^{n+\frac12}\varphi_j \in \mathbf{P}(\mathcal{T}_h)$ approximate $\mathbf{f}(t_n+\frac12\Delta t)$. Use Crank-Nicolson to compute $\mathbf{u}_h^{n+1}$: solve for $\mathbf{V}^{n+\frac12}$ s.t.

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Parabolic step: internal energy update

- Bilinear form associated with the thermal diffusion

$$b(e,w) := c_v^{-1}\kappa \int_D \nabla e\cdot\nabla w \,\mathrm{d}x, \qquad \forall e,w \in H^1(D).$$

- For any $i \in \mathcal{V}$ and $j \in \mathcal{I}(i)$ we set

$$\beta_{ij} := b(\varphi_j, \varphi_i).$$

- We further assume that the acute angle condition holds:

$$\beta_{ij} \leq 0, \quad \forall i \neq j \in \mathcal{V}.$$

Parabolic step: internal energy update

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Parabolic step: internal energy update (high-order update)

- Introduce $\mathbf{v}_h^{n+\frac{1}{2}} := \sum_{i\in\mathcal{V}} \mathbf{V}_i^{n+\frac{1}{2}} \varphi_i$ and define

$$\mathrm{K}_i^{n+\frac{1}{2}} := \frac{1}{m_i} \int_D \mathbb{s}(\mathbf{v}^{n+\frac{1}{2}}) : \mathbb{e}(\mathbf{v}^{n+\frac{1}{2}}) \varphi_i \, \mathrm{d}x, \qquad \forall i \in \mathcal{V}.$$

- Then update internal energy $\mathrm{e}_i^{\mathrm{H},n+\frac{1}{2}}$

$$m_i \varrho_i^n (\mathrm{e}_i^{\mathrm{H},n+\frac{1}{2}} - \mathrm{e}_i^n) + \tfrac{1}{2}\Delta t \sum_{j\in\mathcal{I}(i)} \beta_{ij} \mathrm{e}_i^{\mathrm{H},n+\frac{1}{2}} = \tfrac{1}{2}\Delta t m_i \mathrm{K}_i^{n+\frac{1}{2}}, \qquad \forall i \in \mathcal{V}.$$

- Update internal energy $\mathrm{e}_i^{\mathrm{H},n+1}$

$$\mathrm{e}_i^{\mathrm{H},n+1} = 2\mathrm{e}_i^{\mathrm{H},n+\frac{1}{2}} - \mathrm{e}_i^n, \qquad \forall i \in \mathcal{V}.$$

Caution

No guarantee of positivity of the internal energy here.

Parabolic step: internal energy update (high-order update)

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$$\mathsf{K}_i^{n+\frac{1}{2}} := \frac{1}{m_i}\int_D \mathbb{s}(\mathbf{v}^{n+\frac{1}{2}}):\mathbb{e}(\mathbf{v}^{n+\frac{1}{2}})\varphi_i \,\mathrm{d}x, \qquad \forall i \in \mathcal{V}.$$

- Then update internal energy $\mathsf{e}_i^{\mathrm{H},n+\frac{1}{2}}$

$$m_i\varrho_i^n(\mathsf{e}_i^{\mathrm{H},n+\frac{1}{2}} - \mathsf{e}_i^n) + \tfrac{1}{2}\Delta t \sum_{j\in\mathcal{I}(i)} \beta_{ij}\mathsf{e}_i^{\mathrm{H},n+\frac{1}{2}} = \tfrac{1}{2}\Delta t m_i \mathsf{K}_i^{n+\frac{1}{2}}, \qquad \forall i \in \mathcal{V}.$$

- Update internal energy $\mathsf{e}_i^{\mathrm{H},n+1}$

$$\mathsf{e}_i^{\mathrm{H},n+1} = 2\mathsf{e}_i^{\mathrm{H},n+\frac{1}{2}} - \mathsf{e}_i^n, \qquad \forall i \in \mathcal{V}.$$

Caution

No guarantee of positivity of the internal energy here.

Parabolic step: internal energy update (high-order update)

- Introduce $\mathbf{v}_h^{n+\frac{1}{2}} := \sum_{i\in\mathcal{V}} \mathbf{V}_i^{n+\frac{1}{2}}\varphi_i$ and define

$$\mathrm{K}_i^{n+\frac{1}{2}} := \frac{1}{m_i}\int_D \mathbb{s}(\mathbf{v}^{n+\frac{1}{2}}){:}\mathbb{e}(\mathbf{v}^{n+\frac{1}{2}})\varphi_i \,\mathrm{d}x, \qquad \forall i\in\mathcal{V}.$$

- Then update internal energy $\mathrm{e}_i^{\mathrm{H},n+\frac{1}{2}}$

$$m_i\varrho_i^n(\mathrm{e}_i^{\mathrm{H},n+\frac{1}{2}} - \mathrm{e}_i^n) + \tfrac{1}{2}\Delta t \sum_{j\in\mathcal{I}(i)} \beta_{ij}\mathrm{e}_i^{\mathrm{H},n+\frac{1}{2}} = \tfrac{1}{2}\Delta t m_i \mathrm{K}_i^{n+\frac{1}{2}}, \qquad \forall i\in\mathcal{V}.$$

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No guarantee of positivity of the internal energy here.

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- Introduce $\mathbf{v}_h^{n+\frac{1}{2}} := \sum_{i\in\mathcal{V}} \mathbf{V}_i^{n+\frac{1}{2}} \varphi_i$ and define

$$\mathsf{K}_i^{n+\frac{1}{2}} := \frac{1}{m_i}\int_D \mathbb{s}(\mathbf{v}^{n+\frac{1}{2}}):\mathbb{e}(\mathbf{v}^{n+\frac{1}{2}})\varphi_i \,\mathrm{d}x, \qquad \forall i \in \mathcal{V}.$$

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$$m_i \varrho_i^n (\mathsf{e}_i^{\mathrm{H},n+\frac{1}{2}} - \mathsf{e}_i^n) + \tfrac{1}{2}\Delta t \sum_{j\in\mathcal{I}(i)} \beta_{ij} \mathsf{e}_i^{\mathrm{H},n+\frac{1}{2}} = \tfrac{1}{2}\Delta t m_i \mathsf{K}_i^{n+\frac{1}{2}}, \qquad \forall i \in \mathcal{V}.$$

- Update internal energy $\mathsf{e}_i^{\mathrm{H},n+1}$

$$\mathsf{e}_i^{\mathrm{H},n+1} = 2\mathsf{e}_i^{\mathrm{H},n+\frac{1}{2}} - \mathsf{e}_i^n, \qquad \forall i \in \mathcal{V}.$$

Caution

No guarantee of positivity of the internal energy here.

Parabolic step: internal energy update (low-order update)

- Use backward Euler for low-order internal energy $e_i^{L,n+1}$.
- Update low-order internal energy $e_i^{L,n+1}$

$$m_i \varrho_i^n (e_i^{L,n+1} - e_i^n) + \Delta t \sum_{j \in \mathcal{I}(i)} \beta_{ij} e_j^{L,n+1} = \Delta t m_i K_i^{n+\frac{1}{2}}, \qquad \forall i \in \mathcal{V}.$$

Lemma (Minimum principle)

Let $\mathbf{U}^n$ be an admissible state. Then for all $\Delta t > 0$:

$$\min_{j \in \mathcal{V}} e_j^{L,n+1} \geq \min_{j \in \mathcal{V}} (e_j^n + \frac{\Delta t}{\varrho_j^n} K_j^{n+\frac{1}{2}}) \geq \min_{j \in \mathcal{V}} e_j^n \geq 0.$$

Parabolic step: internal energy update (low-order update)

- Use backward Euler for low-order internal energy $\mathsf{e}_i^{\mathsf{L},n+1}$.
- Update low-order internal energy $\mathsf{e}_i^{\mathsf{L},n+1}$

$$m_i \varrho_i^n (\mathsf{e}_i^{\mathsf{L},n+1} - \mathsf{e}_i^n) + \Delta t \sum_{j \in \mathcal{I}(i)} \beta_{ij} \mathsf{e}_j^{\mathsf{L},n+1} = \Delta t m_i \mathsf{K}_i^{n+\frac{1}{2}}, \qquad \forall i \in \mathcal{V}.$$

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Parabolic step: internal energy update (limiting from below)

- Limit $\mathrm{e}_j^{\mathrm{H},n+1}$ to ensure positivity.
- Observe

$$m_i \varrho_i^n(\mathrm{e}_i^{\mathrm{H},n+1} - \mathrm{e}_i^{\mathrm{L},n+1}) = \sum_{j\in\mathcal{I}(i)\setminus\{i\}} A_{ij},$$

  where $A_{ij} := -\frac{1}{2}\Delta t \beta_{ij}(\mathrm{e}_j^{\mathrm{H},n+1} - \mathrm{e}_i^{\mathrm{H},n+1} + \mathrm{e}_j^n - \mathrm{e}_i^n - 2\mathrm{e}_j^{\mathrm{L},n+1} + 2\mathrm{e}_i^{\mathrm{L},n+1})$,
- The high-order update of the internal energy is now defined by using FCT limiting to enforce $\mathrm{e}_i^{n+1} \geq \min_{j\in\mathcal{V}} \mathrm{e}_j^n$.

$$m_i \varrho_i^n(\mathrm{e}_i^{n+1} - \mathrm{e}_i^{\mathrm{L},n+1}) = \sum_{j\in\mathcal{I}(i)\setminus\{i\}} \ell_{ij} A_{ij}, \qquad \ell_{ij} := \begin{cases} \min(\ell_i^+, \ell_j^-), & \text{if } A_{ij} \geq 0, \\ \min(\ell_i^-, \ell_j^+), & \text{if } A_{ij} < 0. \end{cases}$$

Parabolic step: internal energy update (limiting from below)

- Limit $\mathsf{e}_j^{\mathrm{H},n+1}$ to ensure positivity.
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$$m_i \varrho_i^n (\mathsf{e}_i^{\mathrm{H},n+1} - \mathsf{e}_i^{\mathrm{L},n+1}) = \sum_{j\in\mathcal{I}(i)\setminus\{i\}} A_{ij},$$

where $A_{ij} := -\frac{1}{2}\Delta t \beta_{ij} (\mathsf{e}_j^{\mathrm{H},n+1} - \mathsf{e}_i^{\mathrm{H},n+1} + \mathsf{e}_j^n - \mathsf{e}_i^n - 2\mathsf{e}_j^{\mathrm{L},n+1} + 2\mathsf{e}_i^{\mathrm{L},n+1})$,

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Parabolic step: internal energy update (limiting from below)

- Limit $e_j^{H,n+1}$ to ensure positivity.
- Observe

$$m_i \varrho_i^n (e_i^{H,n+1} - e_i^{L,n+1}) = \sum_{j \in \mathcal{I}(i)\setminus\{i\}} A_{ij},$$

where $A_{ij} := -\frac{1}{2}\Delta t \beta_{ij}(e_j^{H,n+1} - e_i^{H,n+1} + e_j^n - e_i^n - 2e_j^{L,n+1} + 2e_i^{L,n+1}),$

- The high-order update of the internal energy is now defined by using FCT limiting to enforce $e_i^{n+1} \geq \min_{j\in\mathcal{V}} e_j^n$.

$$m_i \varrho_i^n (e_i^{n+1} - e_i^{L,n+1}) = \sum_{j \in \mathcal{I}(i)\setminus\{i\}} \ell_{ij} A_{ij}, \qquad \ell_{ij} := \begin{cases} \min(\ell_i^+, \ell_j^-), & \text{if } A_{ij} \geq 0, \\ \min(\ell_i^-, \ell_j^+), & \text{if } A_{ij} < 0. \end{cases}$$

Parabolic step: internal energy update (limiting from below)

- Update total energy,

$$E_i^{n+1} = \varrho_i^{n+1} \mathrm{e}_i^{n+1} + \tfrac{1}{2}\varrho_i^n \|\mathbf{V}_i^{n+1}\|_{\ell^2}^2, \qquad \forall i \in \mathcal{V}.$$

- The main result is the following.

Theorem (Positivity and conservation)

Let $\mathbf{U}^n$ be an admissible state. Let $\mathbf{U}^{n+1}$ be the parabolic update. Then, $\mathbf{U}^{n+1}$ is an admissible state, i.e., $\mathbf{U}_i^{n+1} \in \mathcal{B}$ for all $i \in \mathcal{V}$ and all Δt, and the following holds for all $i \in \mathcal{V}$ and all Δt:

$$\varrho_i^{n+1} = \varrho_i^n > 0, \qquad \forall i \in \mathcal{V},$$

$$\min_{j\in\mathcal{V}} \mathrm{e}_j^{n+1} \geq \min_{j\in\mathcal{V}} \mathrm{e}_j^n > 0,$$

$$\sum_{i\in\mathcal{V}} m_i \mathrm{E}_i^{n+1} = \sum_{i\in\mathcal{V}} m_i \mathrm{E}_i^n + \sum_{i\in\mathcal{V}} \Delta t\, m_i \mathbf{F}_i^{n+\frac{1}{2}} \cdot \mathbf{V}_i^{n+\frac{1}{2}}.$$

Parabolic step: internal energy update (limiting from below)

- Update total energy,

$$E_i^{n+1} = \varrho_i^{n+1}\mathsf{e}_i^{n+1} + \tfrac{1}{2}\varrho_i^n\|\mathbf{V}_i^{n+1}\|_{\ell^2}^2, \qquad \forall i \in \mathcal{V}.$$

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Full algorithm

- Let $S_{1h}(t+\Delta t, t) : \mathbf{P}(\mathcal{T}_h) \to \mathbf{P}(\mathcal{T}_h)$ denote the nonlinear update for the hyperbolic substep from t to $t+\Delta t$.
- Let $S_{2h}(t+\Delta t, t) : \mathbf{P}(\mathcal{T}_h) \times \mathbf{P}(\mathcal{T}_h) \to \mathbf{P}(\mathcal{T}_h)$ be the nonlinear update for the parabolic substep from t to $t+\Delta t$.
- The update $\mathbf{u}_h^{n+1} \in \mathbf{P}(\mathcal{T}_h)$ is computed as follows:

$$\mathbf{u}_h^{n+1} = S_{1h}(t_n+\Delta t, t_n+\tfrac{1}{2}\Delta t) \circ S_{2h}(t_n+\Delta t, t_n) \circ (S_{1h}(t_n+\tfrac{1}{2}\Delta t, t_n)(\mathbf{u}_h^n), \mathbf{f}_h^{n+\frac{1}{2}}).$$

- Or

$$\begin{aligned}
\mathbf{w}_h^1 &:= S_{1h}(t_n+\tfrac{1}{2}\Delta t, t_n)(\mathbf{u}_h^n),\\
\mathbf{w}_h^2 &:= S_{2h}(t_n+\Delta t, t_n)(\mathbf{w}_h^1, \mathbf{f}_h^{n+\frac{1}{2}}),\\
\mathbf{u}_h^{n+1} &:= S_{1h}(t_n+\Delta t, t_n+\tfrac{1}{2}\Delta t)(\mathbf{w}_h^2).
\end{aligned}$$

Full algorithm

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$$\mathbf{w}_h^1 := S_{1h}(t_n+\tfrac{1}{2}\Delta t, t_n)(\mathbf{u}_h^n),$$
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$$\mathbf{u}_h^{n+1} := S_{1h}(t_n + \Delta t, t_n + \tfrac{1}{2}\Delta t)(\mathbf{w}_h^2).$$

Full algorithm

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- Or

$$\begin{aligned}
\mathbf{w}_h^1 &:= S_{1h}(t_n+\tfrac{1}{2}\Delta t, t_n)(\mathbf{u}_h^n), \\
\mathbf{w}_h^2 &:= S_{2h}(t_n+\Delta t, t_n)(\mathbf{w}_h^1, \mathbf{f}_h^{n+\frac{1}{2}}), \\
\mathbf{u}_h^{n+1} &:= S_{1h}(t_n+\Delta t, t_n+\tfrac{1}{2}\Delta t)(\mathbf{w}_h^2).
\end{aligned}$$

Main result

Theorem (JLG+BP+MM+IT (2020))

- *Let* $\mathbf{P}(\mathcal{T}_h)$ *be a discrete space a described in* **Guermond-Popov-Tomas (2019)**.
- *Let* $\mathbf{u}_h^n \in \mathbf{P}(\mathcal{T}_h)$ *and* $\mathbf{u}_h^n(\mathbf{x}) \in \mathcal{B}$ *for all* $\mathbf{x}$.
- *Let* $\Delta t \leq \Delta t_0(\mathbf{u}^h)$, *where* $\Delta t_0(\mathbf{u}^h)$ *is the largest hyperbolic time step that makes the algorithm in* **Guermond-Popov-Tomas (2019)** *invariant-domain preserving for the Euler problem.*
- *Let* $\mathbf{u}_h^{n+1} \in \mathbf{P}(\mathcal{T}_h)$ *be computed as above (previous slide).*
- *Then* $\mathbf{u}_h^{n+1}(\mathbf{x}) \in \mathcal{B}$ *for all* $\mathbf{x}$.
- *The algorithm is conservative (global mass and total energy conserved).*

Outline

Numerical illustration

1D convergence tests

- 1D convergence tests. Viscous shockwave. Exact solution by **Becker (1922)**.
- Truncated domain $D = (-1, 1.5)$.
- Consolidated error indicator, $q \in \{1, 2\infty\}$:

$$\delta_q(t) := \frac{\|\rho_h(t) - \rho(t)\|_{L^q(D)}}{\|\rho(t)\|_{L^q(D)}} + \frac{\|\mathbf{m}_h(t) - \mathbf{m}(t)\|_{\mathbf{L}^q(D)}}{\|\mathbf{m}(t)\|_{\mathbf{L}^q(D)}} + \frac{\|E_h(t) - E(t)\|_{L^q(D)}}{\|E(t)\|_{L^q(D)}}.$$

Table: 1D Viscous shockwave (exact solution by Becker (1922)), $\mathbb{P}_1$ meshes. Convergence tests, $t = 3$, CFL $= 0.4$.

I	$\delta_1(t)$	rate	$\delta_2(t)$	rate	$\delta_\infty(t)$	rate
50	5.85E-02	–	3.11E-01	–	8.28E-03	–
100	2.50E-02	1.23	1.91E-01	0.71	2.82E-03	1.55
200	4.83E-03	2.37	3.27E-02	2.54	5.13E-04	2.46
400	1.07E-03	2.17	9.79E-03	1.74	9.32E-05	2.46
800	2.52E-04	2.09	2.29E-03	2.10	2.02E-05	2.21
1600	6.20E-05	2.02	5.76E-04	1.99	4.89E-06	2.05
3200	1.55E-05	2.00	1.46E-04	1.98	1.23E-06	1.99

2D convergence tests

- 1D Viscous shockwave computed in 2D. Exact solution by **Becker (1922)**.
- Truncated domain: $D = (-0.5, 1) \times (0, 1)$.
- Same consolidated error indicator, $q \in \{1, 2\infty\}$ as in 1D.

Table: 2D Viscous schockwave, $\mathbb{P}_1$ nonuniform Delaunay meshes, $t = 3$, CFL $\in \{0.4, 0.9\}$.

CFL	I	$\delta_1(t)$	rate	$\delta_2(t)$	rate	$\delta_\infty(t)$	rate
	4458	8.99E-03	–	1.49E-02	–	1.20E-01	–
	17589	1.35E-03	2.76	3.04E-03	2.31	3.23E-02	1.91
0.4	34886	5.19E-04	2.80	1.47E-03	2.13	1.44E-02	2.36
	69781	2.45E-04	2.17	7.20E-04	2.05	7.93E-03	1.72
	139127	1.04E-04	2.47	3.71E-04	1.93	3.27E-03	2.56
	4458	6.99E-03	–	2.03E-02	–	1.58E-01	–
	17589	9.51E-04	2.91	3.39E-03	2.61	3.61E-02	2.15
0.9	34886	3.98E-04	2.54	1.60E-03	2.20	1.55E-02	2.47
	69781	1.79E-04	2.30	7.54E-04	2.17	8.23E-03	1.83
	139127	8.17E-05	2.28	3.67E-04	2.09	3.28E-03	2.67

2D benchmark

- Shock/viscous boundary layer interaction (**Daru&Tenaud (2000, 2009)**).

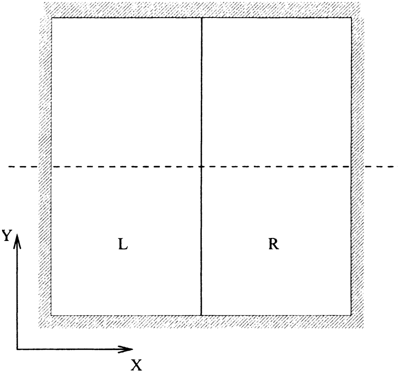
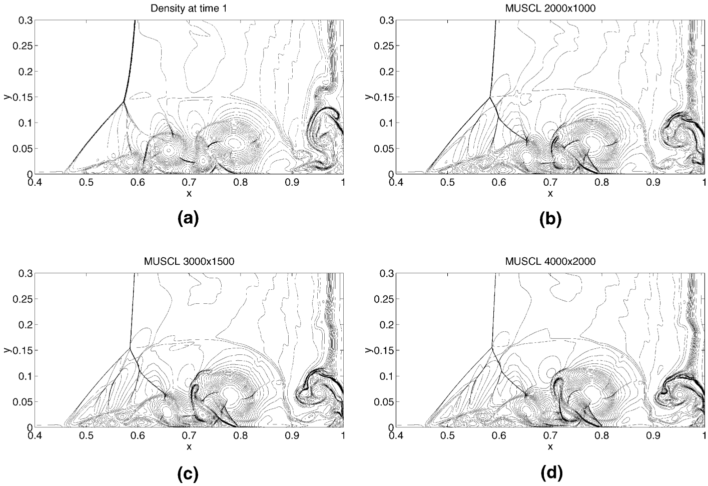


Figure: Description of the problem

- "Standard methods" are known to give "various answers" depending on the method (**Daru&Tenaud (2000)**, **Sjogreen&Yee (2003)**)

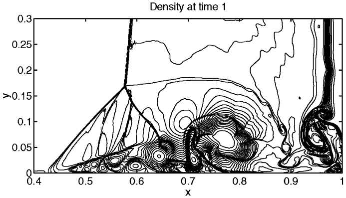
2D benchmark

- Sample from **Sjogreen&Yee (2003)**

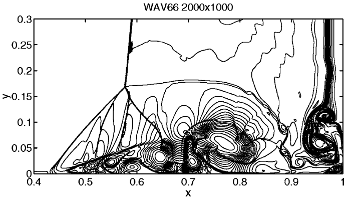


2D benchmark

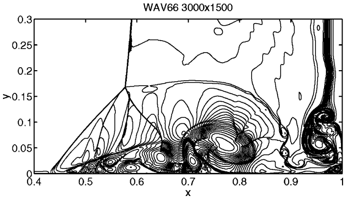
- Sample from **Sjogreen&Yee (2003)**



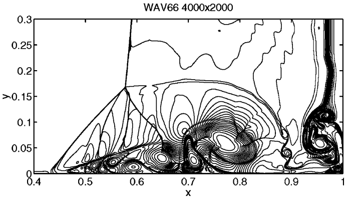
(a)



(b)



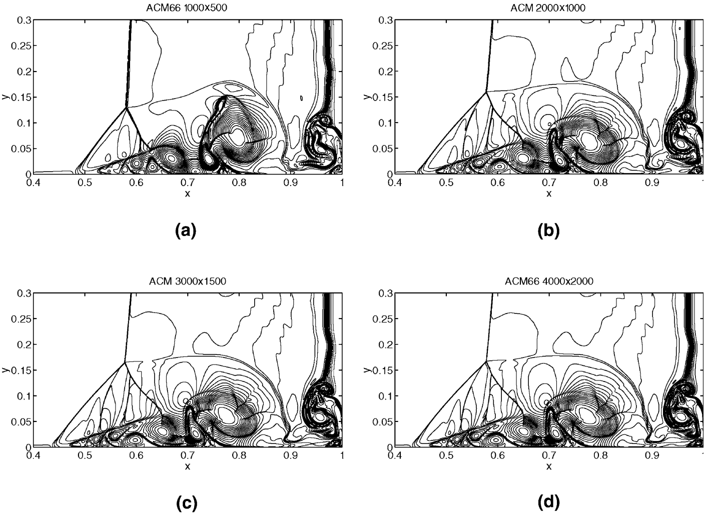
(c)



(d)

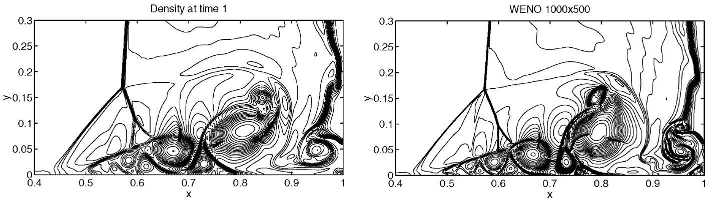
2D benchmark

- Sample from **Sjogreen&Yee (2003)**



2D benchmark

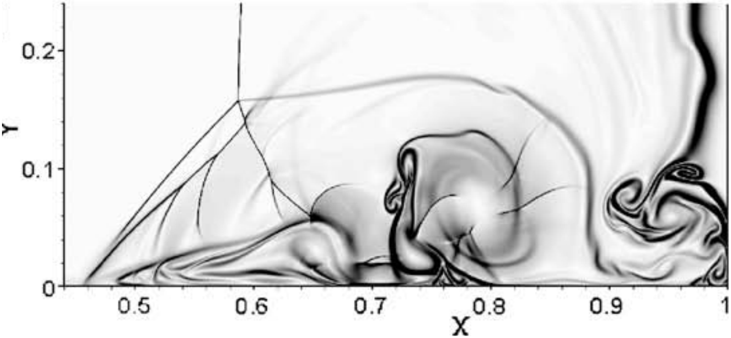
- Sample from **Sjogreen&Yee (2003)**



(a) **(b)**

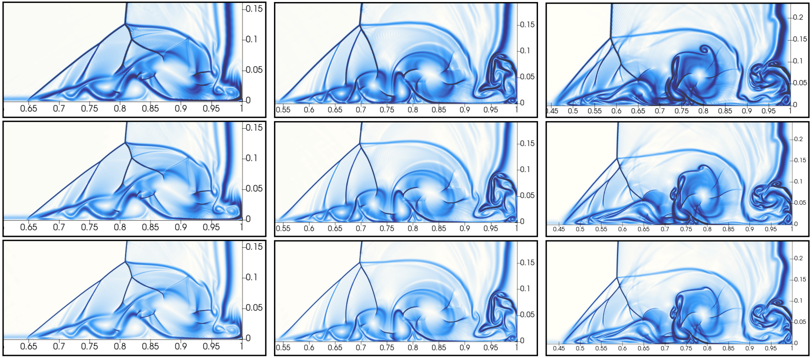
2D benchmark

- Sample from **Daru&Tenaud (2009)**



4000×2000 (OSMP7)

2D benchmark using present method



$t = 0.6$ $t = 0.8$ $t = 1$

Figure: 2D shocktube test. Density at $t \in \{0.6, 0.8, 1\}$ with $\mu = 10^{-3}$. Meshes with increasing refinement level: Mesh 1, 359388 grid point; Mesh 2, 684996 grid point; Mesh 3, 859765 grid points.

2D benchmark

- Comparison with **Daru&Tenaud (2009)**

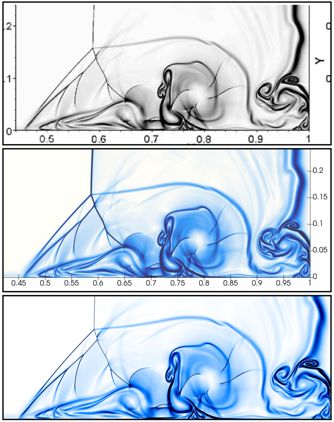


Figure: 2D shocktube test, Density at $t = 1$ for $\mu \in \{10^{-3}\}$. Top: 4000×2000 (OSMP7). Center: Delaunay triangulation $\mathbb{P}_1$ FE, (0.86M grid points). Bottom $\mathbb{Q}_1$ FE (128M grid points).

2D benchmark using present method. Decreasing μ

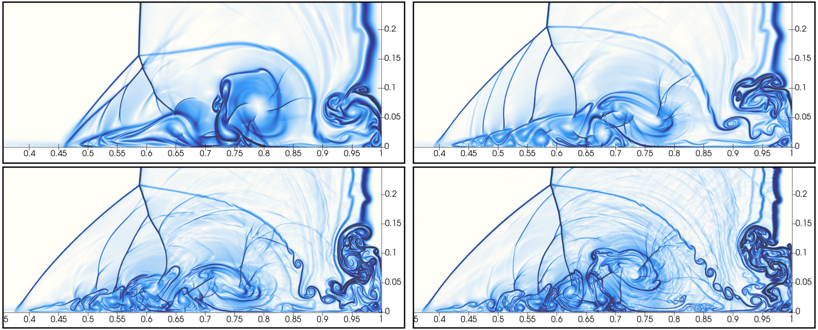


Figure: 2D shocktube test, mesh 4. Density at $t = 1$ for $\mu \in \{10^{-3}, 5\times10^{-4}, 2\times10^{-4}, 10^{-4}\}$.

AOT15a airfoil

- AOTa15 airfoil at Mach 0.73, Reynolds 3×10^6, angle 3.5^o.
- Grid heavily graded with a minimal resolution in the viscous sublayer of 2.1 micrometer vertical to 60 micrometer horizontal (anistropy 30:1).

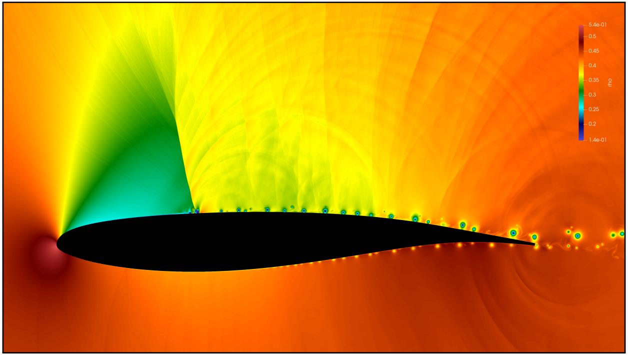


Figure: Continuous $\mathbb{Q}_1$ elements, 8.5M grid points. Density. (M. Maier, deal.ii)

AOT15a airfoil

- AOTa15 airfoil at Mach 0.73, Reynolds 3×10^6, angle 3.5^o.
- Grid heavily graded with a minimal resolution in the viscous sublayer of 2.1 micrometer vertical to 60 micrometer horizontal (anistropy 30:1).

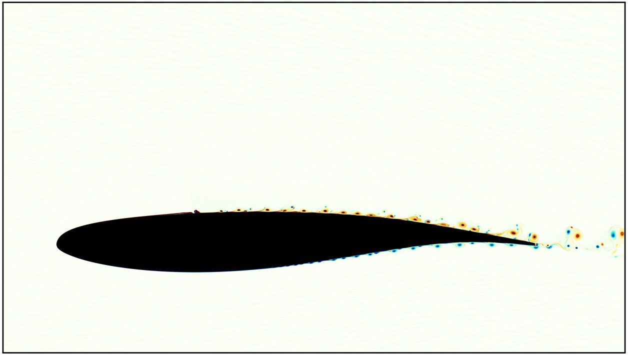


Figure: Continuous $\mathbb{Q}_1$ elements, 8.5M grid points. Vorticity. (M. Maier, deal.ii)

AOT15a airfoil

- AOTa15 airfoil at Mach 0.73, Reynolds 3×10^6, angle 3.5^o.
- Grid heavily graded with a minimal resolution in the viscous sublayer of 2.1 micrometer vertical to 60 micrometer horizontal (anistropy 30:1).

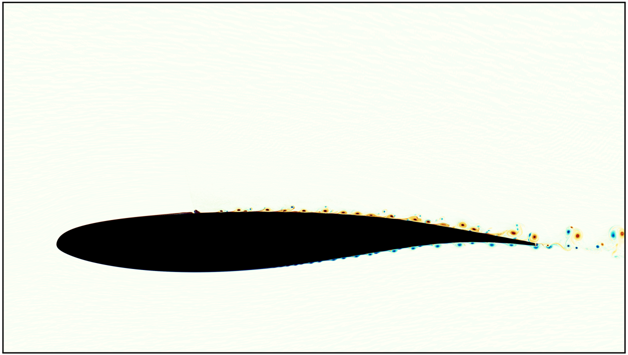


Figure: Continuous $\mathbb{Q}_1$ elements, 8.5M grid points. Vorticity close to trailing edge. (M. Maier, deal.ii)

AOT15a airfoil

- AOTa15 airfoil at Mach 0.73, Reynolds 3×10^6, angle 3.5^o.
- Grid heavily graded with a minimal resolution in the viscous sublayer of 2.1 micrometer vertical to 60 micrometer horizontal (anistropy 30:1).

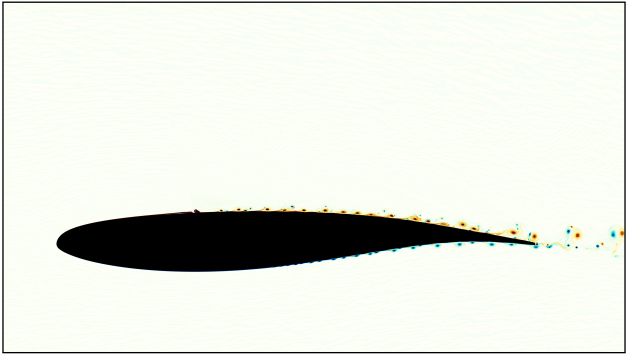


Figure: Continuous $\mathbb{Q}_1$ elements, 8.5M grid points. Buffeting phenomenon. (M. Maier, deal.ii)

jump to next

Current work

Collaborative team: J.-L. Guermond, M. Kronbichler, M. Maier, M. Nazarov, B. Popov, L. Saavedra, M. Sheridan, I. Tomas, E. Tovar.

- Implementation in Deal.II (M. Maier and M. Kronblischer); quantitative comparisons with benchmarks; 3D simulation of transonic wing.
- Extension beyond second-order. Current " one-size fits all IMEX" technology is inadequate.
- Gray radiation hydrodynamics.
- Euler-Poisson.
- Third- and fourth-order in space with guaranteed properties and reasonable low-order stencil.