

Second-Order Invariant Domain Preserving Approximation Of The Compressible Navier–Stokes 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](#) (co-PI, Dept. Math., TAMU, TX)

[Ignacio Tomas](#) (Sandia National Laboratories, NM)

Support:



Lawrence Livermore
National Laboratory



Outline



Background and
objectives

- 1 Background for the this work
- 2 Compressible Navier-Stokes
- 3 Numerical illustrations



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

Some results established so far

- 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)**
 - MPI
 - Multithreading
 - SIMD vectorisation
- Invariant domain preserving approximation of Euler equation with tabulated equation of state. **Clayton, G, Popov (2021)**.
- **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)**
- Beyond SSP ... explicit and IMEX ... (in preparation).
- Invariant domain preserving approximation for mixed approximation.



Current work: extreme scalability

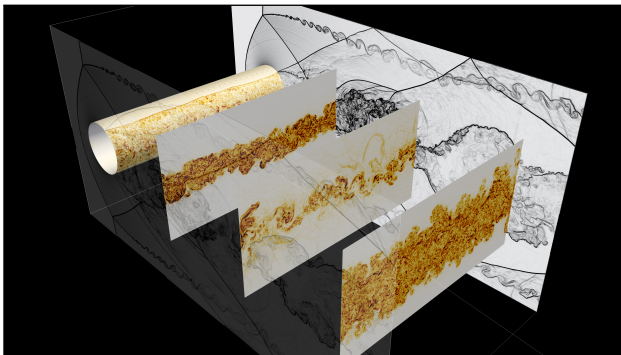


Figure: Continuous Q_1 elements, 1.817B grid points, Maier, Kronbichler (2021)



Outline



Compressible
Navier-Stokes

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Objectives

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

$$\partial_t \rho + \nabla \cdot (\mathbf{v} \rho) = 0,$$

$$\partial_t \mathbf{m} + \nabla \cdot (\mathbf{v} \otimes \mathbf{m} + \rho(\mathbf{u})\mathbb{I} - \mathfrak{s}(\mathbf{v})) = \mathbf{f},$$

$$\partial_t E + \nabla \cdot (\mathbf{v}(E + \rho(\mathbf{u})) - \mathfrak{s}(\mathbf{v})\mathbf{v} + \mathbf{k}(\mathbf{u})) = \mathbf{f} \cdot \mathbf{v}.$$

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

$$\mathfrak{s}(\mathbf{v}) = 2\mu \mathfrak{e}(\mathbf{v}) + (\lambda - \frac{2}{3}\mu) \nabla \cdot \mathbf{v} \mathbb{I}, \quad \mathfrak{e}(\mathbf{v}) = \frac{1}{2} (\nabla \mathbf{v} + (\nabla \mathbf{v})^T),$$

$$\mathbf{k}(\mathbf{u}) = -c_v^{-1} \kappa \nabla e,$$

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



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Objectives

- Two invariant domains can be identified:

$$\mathcal{A} := \{\mathbf{u} \mid \rho > 0, e(\mathbf{u}) > 0, s(\mathbf{u}) > s_{\min}\},$$

$$\mathcal{B} := \{\mathbf{u} \mid \rho > 0, e(\mathbf{u}) > 0\},$$

For Euler

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 (ρ, \mathbf{v}, e) (primitive variables).
 - Some advocate “entropy variable” and “entropy stability”. Why?
- How to do the explicit-implicit time stepping?
 - Most “IMEX” methods cannot make the difference between conserved and primitive variables.
 - Very few **mathematically precise/correct** results on the topic: **Zhang & Shu (2017)** with $\Delta t \leq ch^2$.



Our solution

Our solution (an overview)

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

$$\partial_t \rho + \nabla \cdot (\mathbf{v} \rho) = 0,$$

$$\partial_t \mathbf{m} + \nabla \cdot (\mathbf{v} \otimes \mathbf{m} + \rho(\mathbf{u}) \mathbb{I}) = \mathbf{0},$$

$$\partial_t E + \nabla \cdot (\mathbf{v}(E + \rho(\mathbf{u}))) = 0,$$

$$\mathbf{v} \cdot \mathbf{n}|_{\partial D} = 0, \quad \text{or other admissible BC.}$$

- Parabolic operator

$$\partial_t \rho = 0,$$

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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?



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 (**entropy viscosity commutator**).
- (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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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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(I) Hyperbolic step; GMS-GV scheme

- Set

$$\mathbf{c}_{ij} := \int_D \varphi_i \nabla \varphi_j \, dx, \quad \mathbf{n}_{ij} := \frac{\mathbf{c}_{ij}}{\|\mathbf{c}_{ij}\|_{\ell^2}},$$

$$m_i := \int_D \varphi_i \, dx.$$

(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 $\mathbf{U}_i^{\mathbf{L}, n+1}$

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

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



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SKIP BORING DETAILS



(I) 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 $1 - 4\Delta t \frac{\sum_{j \in \mathcal{I}(i) \setminus \{i\}} d_{ij}^{L,n}}{m_i} \geq 0$.
- Let $\mathcal{B} \subset \mathcal{A}$ be a convex invariant set
- Then

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

- This is the generalization of the maximum principle for any discretization (any mesh), in any space dimension, for any hyperbolic system.
- GMS-GV is a bulletproof scheme. GMS-GV cannot fail.



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(II) High-order viscosity: be careful

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, $d_{ij}^{H,n} = 0$ may seem to be a good idea (if your world is linear), but it is always a bad idea.
- Using linear stabilization may seem to be a good idea (if your world is linear), but it is not robust w.r.t. entropy inequalities.



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(II) High-order viscosity: Commutator-based entropy viscosities

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- Consider an entropy pair $(\eta(\mathbf{v}), \mathbf{F}(\mathbf{v}))$.
- Key idea: measure smoothness of an entropy using the [chain rule](#).

$$\nabla \cdot (\mathbf{F}(\mathbf{u})) = (\nabla \eta(\mathbf{u}))^\top \nabla \cdot (\mathbf{f}(\mathbf{u}))$$

- Commutator-based [entropy viscosity](#) is defined by setting

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(III) Convex limiting: Strategy

Strategy

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

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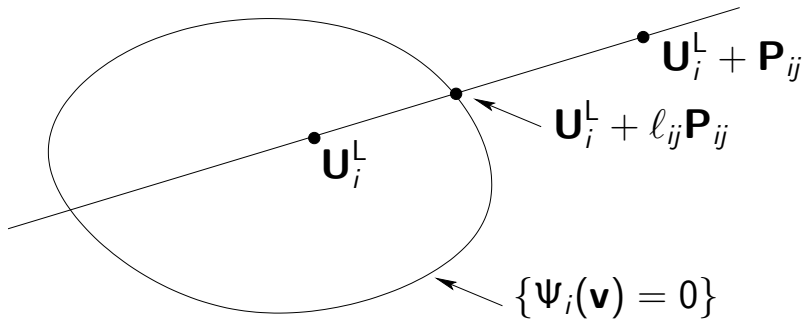


Overview of solution strategy

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(III) Limiting strategy



Summary of the hyperbolic step

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

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Parabolic step

$$\begin{aligned}\partial_t \rho &= 0, \\ \partial_t \mathbf{m} - \nabla \cdot (\mathbb{s}(\mathbf{v})) &= \mathbf{f}, \\ \partial_t E + \nabla \cdot (\mathbf{k}(\mathbf{u}) - \mathbb{s}(\mathbf{v})\mathbf{v}) &= \mathbf{f} \cdot \mathbf{v}, \\ \mathbf{v}|_{\partial D} &= \mathbf{0}, \quad \mathbf{k}(\mathbf{u}) \cdot \mathbf{n}|_{\partial D} = 0.\end{aligned}$$

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Parabolic step: density update

- Density update

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



Parabolic step: velocity update

- Introduce bilinear form associated with viscous dissipation,

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

- 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

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Parabolic step: internal energy update

- Bilinear form associated with the thermal diffusion

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

- 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:

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Caution

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Parabolic step: internal energy update

Solution

- Use backward Euler for **low-order** internal energy $e_i^{L,n+1}$.
- And use FCT to limit.

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Parabolic step: internal energy update (limiting from below)

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 :

$$\begin{aligned} \varrho_i^{n+1} &= \varrho_i^n > 0, & \forall i \in \mathcal{V}, \\ \min_{j \in \mathcal{V}} e_j^{n+1} &\geq \min_{j \in \mathcal{V}} e_j^n > 0, \\ \sum_{i \in \mathcal{V}} m_i E_i^{n+1} &= \sum_{i \in \mathcal{V}} m_i E_i^n + \sum_{i \in \mathcal{V}} \Delta t m_i \mathbf{F}_i^{n+\frac{1}{2}} \cdot \mathbf{V}_i^{n+\frac{1}{2}}. \end{aligned}$$



Full algorithm

- Let $S_{1h}(t + \Delta t, t) : \mathbf{P}(\mathcal{T}_h) \rightarrow \mathbf{P}(\mathcal{T}_h)$ denote the nonlinear update for the hyperbolic substep from t to $t + \Delta t$.
- Let $S_{2h}(t + \Delta t, t) : \mathbf{P}(\mathcal{T}_h) \times \mathbf{P}(\mathcal{T}_h) \rightarrow \mathbf{P}(\mathcal{T}_h)$ 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:

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

- Or

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

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

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

- Or

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

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

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Full algorithm

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Main result

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

- Let $\mathbf{P}(\mathcal{T}_h)$ be a discrete space as 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

- 1 Background for the this work
- 2 Compressible Navier-Stokes
- 3 **Numerical illustrations**



1D convergence tests

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

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

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

l	$\delta_1(t)$	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, $t = 3$, $\text{CFL} \in \{0.4, 0.9\}$.

CFL	I	$\delta_1(t)$	rate	$\delta_2(t)$	rate	$\delta_\infty(t)$	rate
0.4	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
	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
0.9	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
	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)**).

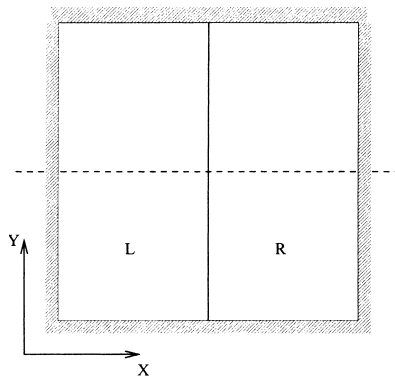


Figure: Description of the problem

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

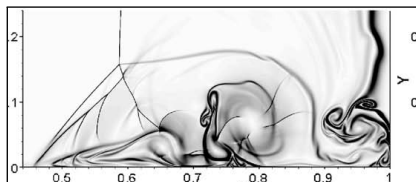


2D benchmark

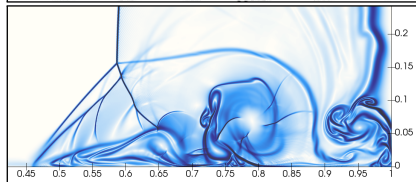
SKIP BORING DETAILS



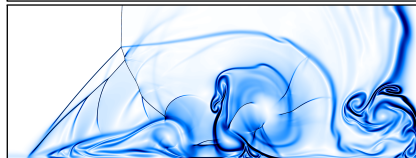
2D benchmark



Uniform Cartesian mesh
 4000×2000 (OSMP7).



Nonuniform Delaunay triangulation
 \mathbb{P}_1 FE, (0.86M grid points)

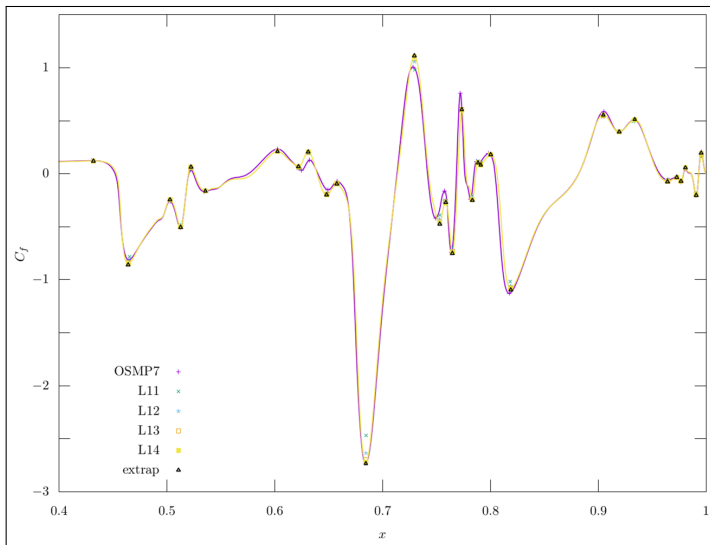


Non uniform quadrangular mesh
 \mathbb{Q}_1 FE (128M grid points)

Figure: Comparison with Daru&Tenaud (2009). Density at $t = 1$ for $\mu \in \{10^{-3}\}$.



2D benchmark

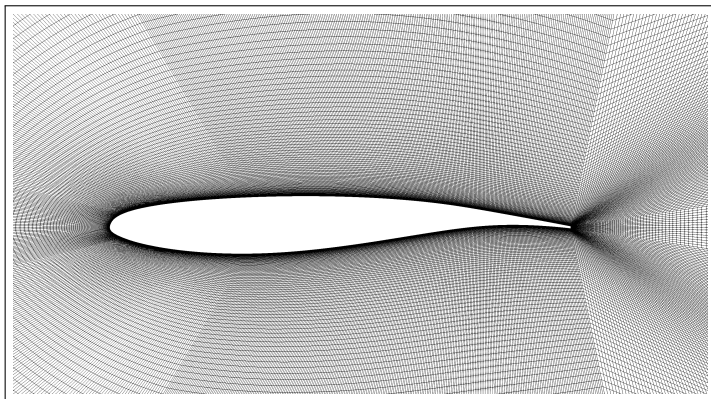


Skin friction coefficient at time $t = 1.00$. The continuous lines are for the finest level and the OSMP7 scheme as reported in **Daru&Tenaud (2009)**.



AOT15a airfoil

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

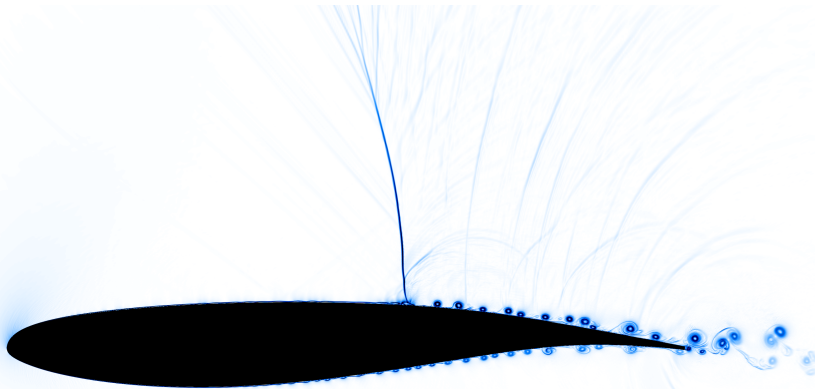


Onera OAT15a airfoil with graded mesh used in our computations. Actual hexahedral 3D mesh is created by extruding the quadrilateral 2D mesh in the z-direction.



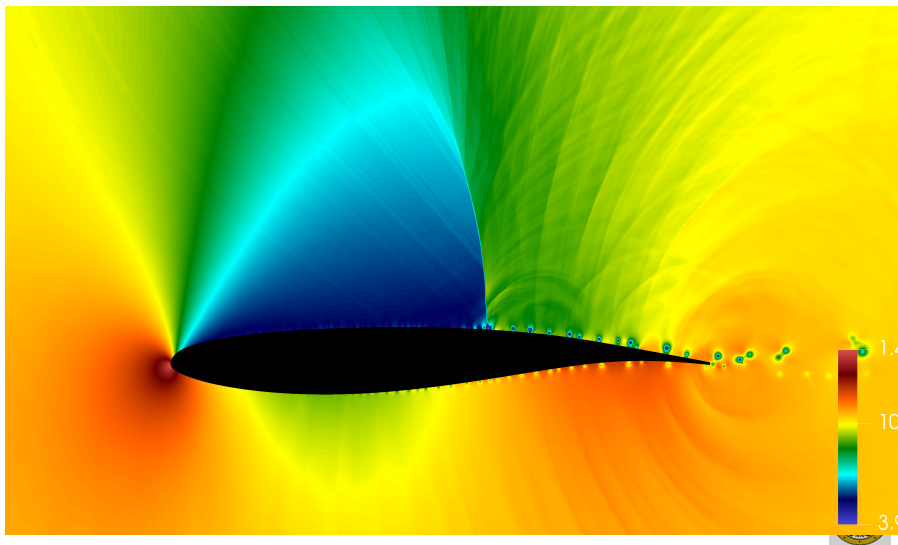
2D results

Airfoil OAT15a at $Re=3\,000\,000$, 2D, schlieren plot:



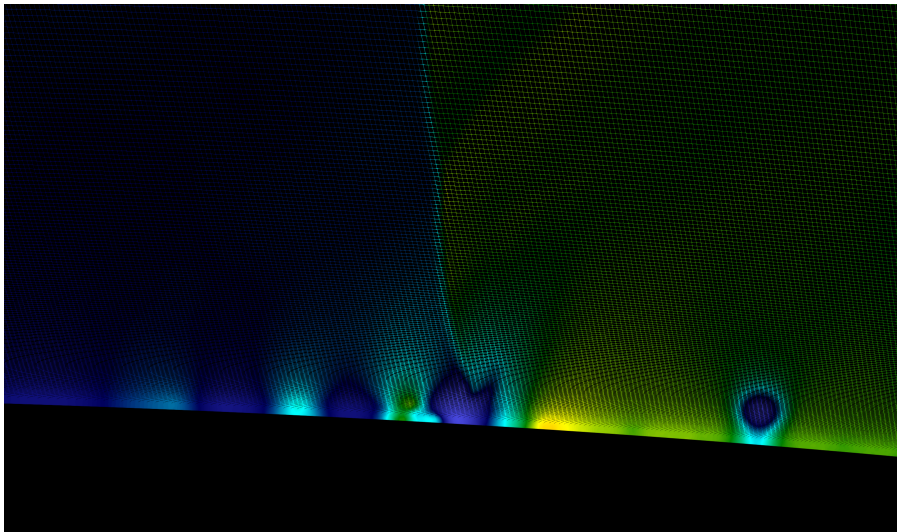
2D results

Airfoil OAT15a at $Re=3\,000\,000$, 2D, pressure:



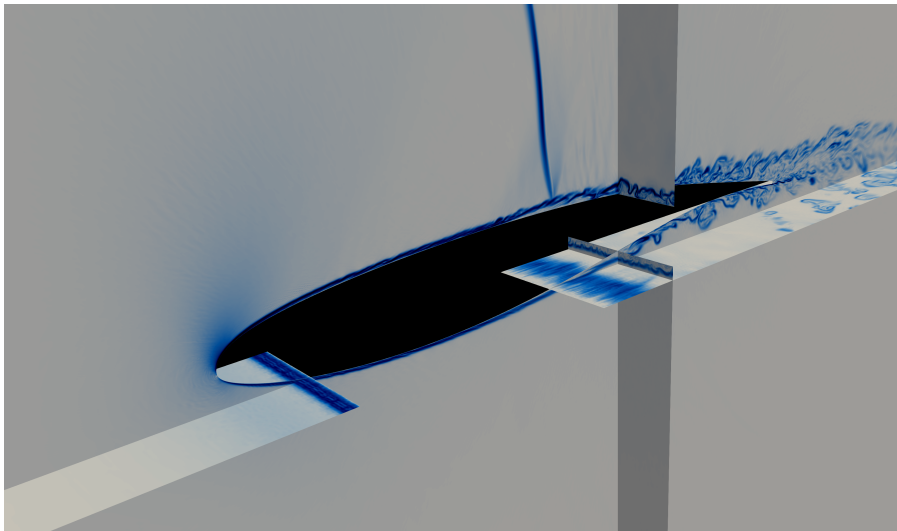
2D results

Airfoil OAT15a at $Re=3\,000\,000$, 2D, mesh resolution:



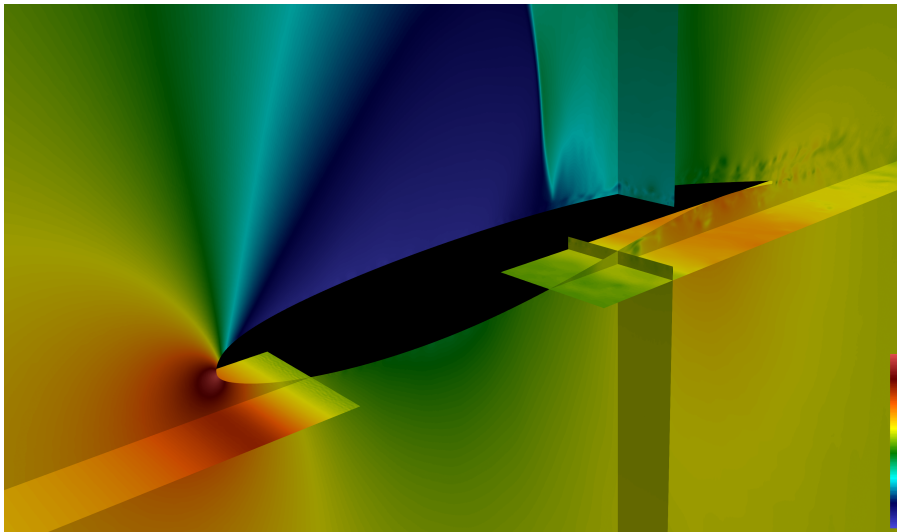
3D results

Airfoil OAT15a at $Re=3\,000\,000$, 3D, schlieren:



3D results

Airfoil OAT15a at $Re=3\,000\,000$, 3D, pressure



3D results

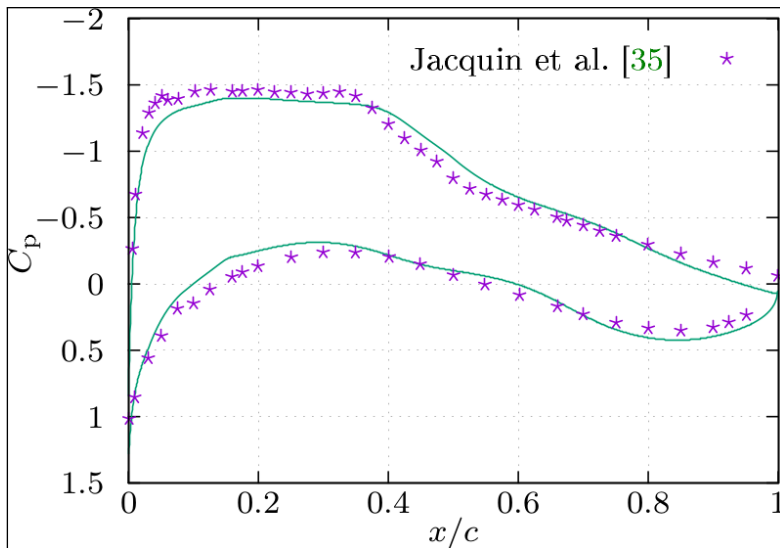


Figure: time- and z-averaged pressure coefficient. Comparison with experiments.



Strong scaling tests

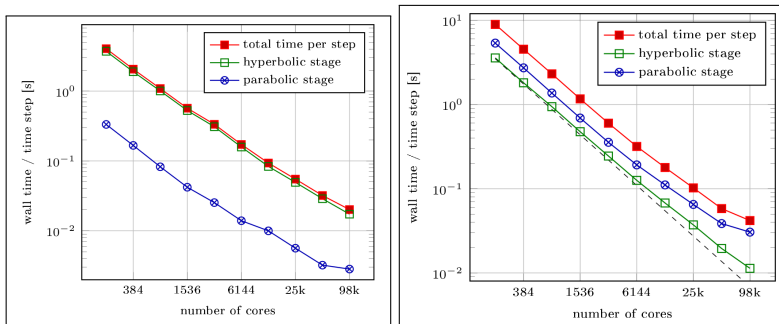


Figure: Scaling analysis broken down to show the contributions of the hyperbolic and parabolic parts. Left: 3D Onera OAT15a airfoil, with 34.5 million grid points. Right: 2D shocktube with 134 million grid points.



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 (Ryujin) of our shallow water code.
- 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.

