# Geometric variational finite element discretization of compressible fluids

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# Motivation

- Main motivation: derivation of geometrically consistent numerical schemes for Geophysical Fluid Dynamics.

- Atmospheric and oceanic circulation: start with the compressible Euler equations

$$\begin{cases} \partial_t u + u \cdot \nabla u + \operatorname{curl} R \times u + \dfrac{1}{\rho} \nabla p = -\nabla \phi, \\ \partial_t \rho + \operatorname{div}(\rho u) = 0, \qquad \partial_t s + \operatorname{div}(s u) = 0. \end{cases}$$

$\rightsquigarrow$ various approximations: pseudo-incompressible, anelastic, Boussinesq, shallow water, quasigeostrophic, ...

**Properties**:

- All these models (in the conservative case) admit a Hamiltonian formulation (Poisson bracket) and a Lagrangian formulation (variational principles)
- These approximations can be made at the level of the Lagrangian, i.e. the approximate equations can be derived geometrically from an approximate Lagrangian.
- All conservation laws have a geometric explanation. Main examples: Kelvin circulation theorem, conservation of potential vorticity
- Large scale dynamics: global behavior is more important than local high accuracy.

**Goal**: Develop an integrator that respects as much as possible these properties. One systematic way:

**GEOMETRIC VARIATIONAL DISCRETIZATION**.

**PLAN**:

**1.** Geometric variational formulation of hydrodynamics

**2.** Discrete Lie group setting

**3.** Finite element variational integrator

**4.** Compressible fluids

**5.** Incompressible fluid with variable density

**6.** Some proofs

**7.** Connection with older approaches

# 1. Geometric variational formulation of hydrodynamics

- Early variational principles: at least since Herivel [1955], Serrin [1959], Newcomb [1962], Lin [1963], Seliger and Whitham [1968], Bretherton [1970]

- As mechanical systems on Lie groups: Arnold [1965], Marsden, Weinstein [1983], Marsden, Ratiu, Weinstein [1984], Holm, Marsden, Ratiu [1998]

**1.1 Lagrangian description of hydrodynamics**:

Fluid dynamics in a compact manifold $\Omega$ with boundary.
Lagrangian motion $X \in \Omega \mapsto x = \varphi(t, X) \in \Omega$

- Configuration Lie group: $G = \mathrm{Diff}(\Omega)$, compressible fluids;
  $G = \mathrm{Diff}_{\mathrm{vol}}(\Omega)$, incompressible fluids

- Lagrangian: $L : TG \to \mathbb{R}$,

$$L(\varphi, \dot{\varphi}) = \int_\Omega \frac{1}{2} \varrho_0 |\dot{\varphi}|^2 \mathrm{d}X - \int_\Omega E(\varphi, \nabla\varphi, \varrho_0, S_0) \mathrm{d}X$$

Depends on reference fields $\varrho_0(X)$, $S_0(X)$.

- Hamilton's principle: critical action principle for the flow $x = \varphi(t, X)$:

$$\delta \int_0^T L(\varphi, \dot{\varphi}) dt = 0, \quad \delta\varphi \text{ arbitrary variations} \longrightarrow \text{Fluid equations in Lagr. variables.}$$

## 1.2 Eulerian (spatial) description of hydrodynamics

Invariance of $L$ with respect to diffeomorphisms that preserve $\varrho_0$ and $S_0$

- Eulerian fields:

$$u := \dot{\varphi} \circ \varphi^{-1} \qquad \text{Eulerian velocity}$$

$$\rho := (\varrho_0 \circ \varphi^{-1}) |\det D\varphi^{-1}| \qquad \text{Eulerian mass density}$$

$$s := (S_0 \circ \varphi^{-1}) |\det D\varphi^{-1}| \qquad \text{Eulerian entropy density}$$

- Lagrangian in Eulerian description:

$$\ell(u, \rho, s) = \int_\Omega \left[ \frac{1}{2} \rho |u|^2 - \epsilon(\rho, s) \right] \mathrm{d}x$$

- Hamilton's principle in Eulerian form (Euler-Poincaré):

$$\delta \int_0^T \ell(u, \rho, s) dt = 0, \quad \delta u = \partial_t \zeta + [u, \zeta], \quad \delta \rho = -\operatorname{div}(\rho \zeta), \quad \delta s = -\operatorname{div}(s \zeta).$$

- Equations of motion:

$$\begin{cases} \partial_t \dfrac{\delta \ell}{\delta u} + \mathcal{L}_u \dfrac{\delta \ell}{\delta u} = \rho \nabla \dfrac{\delta \ell}{\delta \rho} + s \nabla \dfrac{\delta \ell}{\delta s} \\ \partial_t \rho + \operatorname{div}(\rho u) = 0, \quad \partial_t s + \operatorname{div}(s u) = 0. \end{cases}$$

## 1.3 Abstract Lie group geometric formulation

Poisson structure (Lie-Poisson): Marsden, Ratiu, Weinstein [1984]
Variational structure (Euler-Poincaré): Holm, Marsden, Ratiu [1998]

$G$ Lie group (configuration space);
$V$ vector space (advected quantities);
$G \times V \to V$, $(g, a) \mapsto a \cdot g$ right representation;

Lagrangian: $L_{a_0} : TG \to \mathbb{R}$, $a_0 \in V$, with $L(gh, \dot{g}h, a_0 \cdot h) = L(g, \dot{g}, a_0)$ for all $h \in G$;

Reduced Lagrangian: $\ell : \mathfrak{g} \times V \to \mathbb{R}$, $\ell(u, a) = \ell(\dot{g}g^{-1}, a_0 \cdot g^{-1}) = L(g, \dot{g}, a_0)$.

Given $g(t) \in G$, define $u(t) = \dot{g}(t)g(t)^{-1} \in \mathfrak{g}$, $a(t) = a_0 \cdot g(t)^{-1} \in V$;

$$\delta \int_0^T L(g, \dot{g})\mathrm{d}t = 0 \iff \text{Euler-Lagrange equations}$$

$$\iff \delta \int_0^T \ell(u, a)\mathrm{d}t = 0, \quad \delta u = \partial_t v + [v, u], \quad \delta a + a \cdot v = 0$$

$$\iff \frac{d}{dt}\frac{\delta \ell}{\delta u} + \mathrm{ad}_u^* \frac{\delta \ell}{\delta u} = \frac{\delta \ell}{\delta a} \diamond a$$

An essential modelling tool in fluid mechanics, with lots of extensions:

– free boundary;

– GFD;

– liquid crystals;

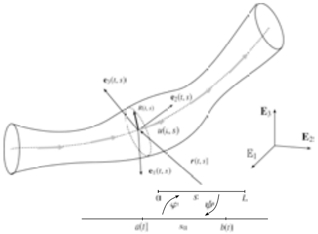
– superfluids;

– fluid-structure interaction;

– thermodynamics;

– stochastic;

– .....



e.g.: Holm [2002], FGB, Ratiu [2009], FGB, Marsden, Ratiu [2012], FGB, Ratiu, Tronci [2013], Holm [2015,....], FGB, Yoshimura [2017,....], FGB, Putkaradze [2014,....], ....

**Goal**: carry out the numerical discretization in a geometry preserving way by respecting the geometric variational formulation.

**Main idea**:
- "replace" this group by a finite dimensional Lie group approximation
- apply the variational principles on this finite dimensional Lie group
- temporal discretization in a structure preserving way

– Original idea & incompressible ideal case:
Pavlov, Mullen, Tong, Kanso, Marsden, Desbrun [2010]

– Several developments (motivated by GFD):
Rotating Boussinesq GFD equations: Desbrun, Gawlik, FGB, Zeitlin [2014]
Various generalizations of discrete group: Liu, Mason, Hodgson, Tong, Desbrun [2015]
Finite elements for incompressible: Natale and Cotter [2018]
Anelastic and pseudo-incompressible GFD & unstructured grids: Bauer and FGB [2017]
Compressible fluids & rotating shallow water: Bauer and FGB [2018]
On the sphere: Brecht, Bauer, Bihlo, FGB, MacLachlan [2019]

# 2. Discrete Lie group setting

## 2.1 Discrete diffeomorphism groups

- $\mathcal{T}_h$ triangulation of $\Omega$, maximum element diameter $h$.
- Assume $\mathcal{T}_h$ belongs to a shape-regular, quasi-uniform family $\{\mathcal{T}_h\}$:

$$\max_{K\in\mathcal{T}_h} \frac{h_K}{\rho_K} \leq C_1, \text{ and } \max_{K\in\mathcal{T}_h} \frac{h}{h_K} \leq C_2,$$

  $h_K$ and $\rho_K$ diameter and inradius of a simplex $K$.
- Discrete functions: finite element space $V_h \subset L^2(\Omega)$ associated to $\mathcal{T}_h$
- Finite dimensional version of $\mathrm{Diff}(\Omega)$: chosen as

$$G_h = \{q \in GL(V_h) \mid q\mathbf{1} = \mathbf{1}\},$$

  $\mathbf{1}$ discrete representative of constant function 1.
- Lie algebra

$$\mathfrak{g}_h = \{A \in L(V_h, V_h) \mid A\mathbf{1} = 0\}$$

  $\rightsquigarrow$ potential candidates to be discrete vector fields;
  $\rightsquigarrow$ As linear maps these discrete vector fields act as discrete derivations on $V_h$;
  $\rightsquigarrow$ Natural to choose them as discrete distributional directional derivatives.

## 2.2 Outline

- Discrete distributional directional derivatives form a subspace of the Lie algebra $\mathfrak{g}_h$.

- This space is isomorphic to a well-known finite element space!! Raviart-Thomas space (main result)

- This space is NOT a Lie subalgebra of $\mathfrak{g}_h$

## 2.3 Discrete distributional derivative

$H(\text{div}, \Omega) = \{u \in L^2(\Omega)^n \mid \text{div}\, u \in L^2(\Omega)\}$.
$H_0(\text{div}, \Omega) = \{u \in H(\text{div}, \Omega) \mid u \cdot n = 0 \text{ on } \partial\Omega\}$.

### Definition

Given $u \in H(\text{div}, \Omega)$, the **distributional derivative in the direction** $u$ is $\nabla_u^{\text{dist}} : L^2(\Omega) \to C_0^\infty(\Omega)'$ defined by

$$\int_\Omega (\nabla_u^{\text{dist}} f) g \,\mathrm{d}x = -\int_\Omega f \,\text{div}(gu) \,\mathrm{d}x, \ \forall g \in C_0^\infty(\Omega).$$

$r \geq 0$ integer, $\mathcal{T}_h$ triangulation of $\Omega$

$$V_h^r = \{f \in L^2(\Omega) \mid f|_K \in P_r(K), \ \forall K \in \mathcal{T}_h\}.$$

### Definition

Given $A \in \mathfrak{gl}(V_h^r)$ and $u \in H_0(\text{div}, \Omega) \cap L^p(\Omega)^n$, $p > 2$, we say that $A$ **approximates** $-u$ **in** $V_h^r$ if whenever $f \in L^2(\Omega)$ and $f_h \in V_h^r$ is a sequence satisfying $\|f - f_h\|_{L^2(\Omega)} \to 0$, we have

$$\langle A f_h - \nabla_u^{\text{dist}} f, g \rangle \to 0, \quad \forall g \in C_0^\infty(\Omega).$$

$A$ is a consistent approximation of $\nabla_u^{\text{dist}}$ in $V_h^r$.

## Proposition (Gawlik and FGB)

Given $u \in H_0(\mathrm{div}, \Omega) \cap L^p(\Omega)^n$, $p > 2$, and $r \geq 0$ an integer, a consistent approximation of $\nabla_u^{\mathrm{dist}}$ in $V_h^r$ is $A_u \in \mathfrak{gl}(V_h^r)$ given by

$$\langle A_u f, g\rangle := \sum_{K \in \mathcal{T}_h} \int_K (\nabla_u f) g \,\mathrm{d}x - \sum_{e \in \mathcal{E}_h^0} \int_e u \cdot [\![f]\!]\{g\} \,\mathrm{d}s.$$

Considered in Natale, Cotter [2018] for the ideal fluid.

## Proposition

For all $u \in H_0(\mathrm{div}, \Omega) \cap L^p(\Omega)^n$, $p > 2$:

$$A_u \mathbf{1} = 0 \quad \text{and} \quad \langle A_u f, g\rangle + \langle f, A_u g\rangle + \langle f, (\mathrm{div}\, u) g\rangle = 0$$

$\rightsquigarrow$ well-defined linear map

$$\mathsf{A} : H_0(\mathrm{div}, \Omega) \cap L^p(\Omega)^n \to \mathfrak{g}_h^r \subset L(V_h^r, V_h^r), \qquad u \mapsto \mathsf{A}(u) = A_u$$

$\mathfrak{g}_h^r = \{A \in L(V_h^r, V_h^r) \mid A\mathbf{1} = 0\}$ Lie algebra of $G_h^r$.

## 2.4 Relation with Raviart-Thomas finite element spaces

### Definition

For $r \geq 0$, define $S_h^r \subset \mathfrak{g}_h^r$ as

$$S_h^r := \operatorname{Im} \mathrm{A} = \{A_u \in L(V_h^r, V_h^r) \mid u \in H_0(\operatorname{div}, \Omega)\}.$$

### Theorem (Gawlik and FGB)

The space $S_h^r \subset \mathfrak{g}_h^r$, $r \geq 0$, is isomorphic to the Raviart-Thomas space of order $2r$

$$RT_{2r}(\mathcal{T}_h) = \left\{u \in H_0(\operatorname{div}, \Omega) \mid u|_K \in (P_{2r}(K))^n + xP_{2r}(K), \forall K \in \mathcal{T}_h\right\}.$$

An isomorphism is given by $u \in RT_{2r}(\mathcal{T}_h) \mapsto A_u \in S_h^r$.

- Lie algebra elements in $S_h^r \subset \mathfrak{g}_h^r$ correspond to discrete vector fields;
- $S_h^r$ is NOT a Lie subalgebra of $\mathfrak{g}_h^r$.

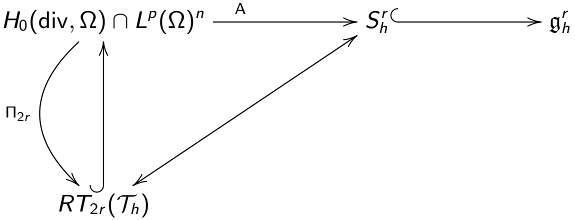
Proof: Later!

## Proposition

The kernel of A : $H_0(\mathrm{div},\Omega)\cap L^p(\Omega)^n \mapsto \mathfrak{g}_h^r$, $u\mapsto \mathrm{A}(u)=A_u$ is

$$\ker \mathrm{A} = \{u\in H_0(\mathrm{div},\Omega)\cap L^p(\Omega)^n \mid \Pi_{2r}(u)=0\} = \ker \Pi_{2r},$$

$\Pi_{2r} : H_0(\mathrm{div},\Omega)\cap L^p(\Omega)^n \to RT_{2r}(\mathcal{T}_h)$ global interpolation operator.




$u\in H_0(\mathrm{div},\Omega)$, $\exists!\ \bar{u}\in RT_{2r}(\mathcal{T}_h)$ s.t. $A_u = A_{\bar{u}}$

## 2.5 The Lie algebra-to-vector fields map

- Construct a method valid for a large class of Lagrangians
  $\rightsquigarrow$ Lie algebra-to-vector fields map
- Use of Lagrange-d'Alembert principle of nonholonomic mechanics (e.g. Bloch [2003])
  $\rightsquigarrow$ Lie algebra-to-vector fields map at least defined on $S_h^r + [S_h^r, S_h^r]$

(cannot use $A_u \mapsto u$!!)

**Definition**

For $r \geq 0$ define **Lie algebra-to-vector field map** $\widehat{\ } : L(V_h^r, V_h^r) \to [V_h^r]^n$

$$\widehat{A} := \sum_{k=1}^{n} A(I_h^r(x^k))e_k,$$

$I_h^r : L^2(\Omega) \to V_h^r$ : $L^2$-orthogonal projector onto $V_h^r$.

## Proposition

$u \in H_0(\mathrm{div}, \Omega) \cap L^p(\Omega)$:

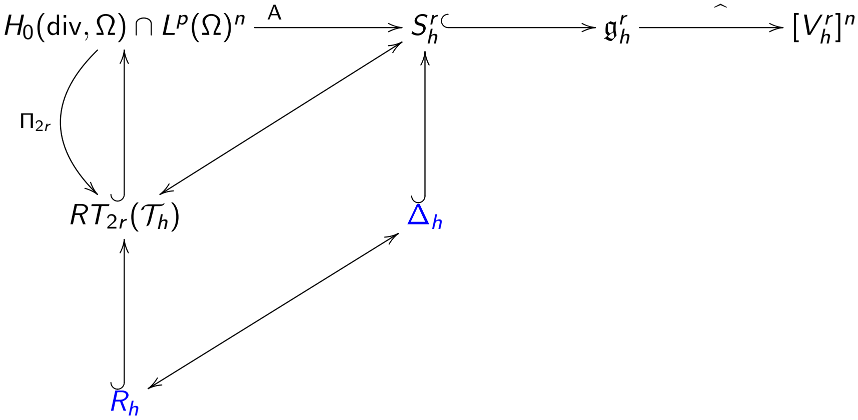
- If $r \geq 1$:

$$(\widehat{A_u})^k = I_h^r(u^k), \quad k = 1, ..., n.$$

- If $r = 0$:

$$\widehat{A_u}|_K = \frac{1}{2|K|} \sum_{e \in K} \int_e u \cdot n_{e_-} (b_{e_+} - b_{e_-}) \mathrm{d}s$$

$n_{e_-}$ normal vector field pointing from $K_-$ to $K_+$;
$b_{e_\pm}$ barycenters of $K_\pm$.




Not yet complete....

# 3. Finite element variational integrator

## 3.1 Semidiscrete Euler-Poincaré-d'Alembert equations

Given $\ell(u, \rho)$:

- Discrete Lagrangian $\ell_d : \mathfrak{g}_h^r \times V_h^r \to \mathbb{R}$

$$\ell_d(A, D) := \ell(\widehat{A}, D)$$

- Action on discrete densities

$$g \in G_h^r : \qquad \langle D \cdot g, E \rangle = \langle D, gE \rangle, \quad \forall E \in V_h^r.$$

$$B \in \mathfrak{g}_h^r : \qquad \langle D \cdot B, E \rangle = \langle D, BE \rangle, \quad \forall E \in V_h^r.$$

- Nonholonomic constraint

$$\Delta_h \subset S_h^r \subset \mathfrak{g}_h^r$$

- Euler-Poincaré-d'Alembert variational principle

Duality pairing $\langle\!\langle K, A\rangle\!\rangle$, $K \in (\mathfrak{g}^r_h)^*$, $A \in \mathfrak{g}^r_h$.

Given $g(t) \in G^r_h$ define $A(t) = \dot{g}(t)g(t)^{-1}$ and $D(t) = D_0 \cdot g(t)^{-1}$

The following are equivalent for $A(t) \in \Delta_h$ and $D(t) \in V^r_h$:

**(i)**

$$\delta \int_0^T \ell_d(A, D)\mathrm{d}t = 0, \qquad \delta A = \partial_t B + [B, A] \quad \text{and} \quad \delta D = -D \cdot B,$$

for all $B(t) \in \Delta_h$ with $B(0) = B(T) = 0$.

**(ii)**

$$\left\langle\!\!\left\langle \partial_t \frac{\delta \ell_d}{\delta A}, B \right\rangle\!\!\right\rangle + \left\langle\!\!\left\langle \frac{\delta \ell_d}{\delta A}, [A, B] \right\rangle\!\!\right\rangle + \left\langle \frac{\delta \ell_d}{\delta D}, D \cdot B \right\rangle = 0, \quad \forall t \in (0, T), \quad \forall\, B \in \Delta_h.$$

$$\text{equivalently} \quad : \partial_t \frac{\delta \ell_d}{\delta A} + \mathrm{ad}^*_A \frac{\delta \ell_d}{\delta A} - \frac{\delta \ell_d}{\delta D} \diamond D \in \Delta_h^\circ, \quad \forall t \in (0, T)$$

Differential equation for $D(t)$:

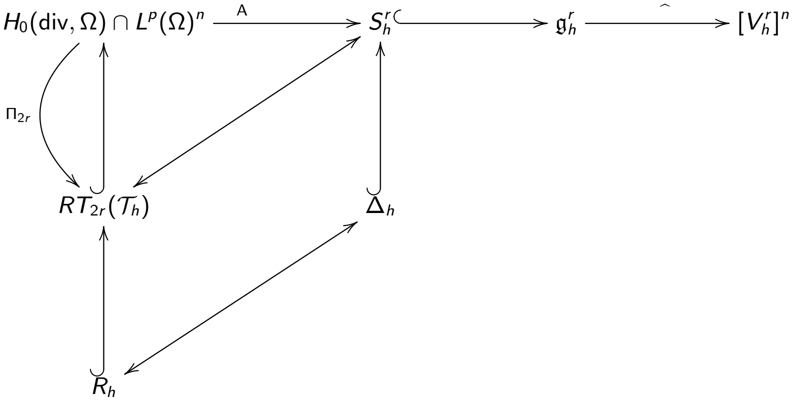
$$\langle \partial_t D, E \rangle + \langle D, AE \rangle = 0, \quad \forall t \in (0, T), \quad \forall\, E \in V^r_h.$$

- Choice of $\Delta_h$

$\Delta_h \subset S_h^r$ such that

$$A \in \Delta_h \to \frac{\delta \ell_d}{\delta A}(A, D) \in (\mathfrak{g}_h^r)^* / \Delta_h^\circ$$

is a diffeomorphism for all $D \in V_h^r$ strictly positive.



# 4. Compressible fluids

Focus on the barotropic fluid for simplicity

$$\ell(u,\rho) = \int_\Omega \left[\frac{1}{2}\rho|u|^2 - \rho e(\rho)\right]\mathrm{d}x$$

All results below can be naturally extended to more general Lagrangians, such as the class of rotating stratified fully compressible fluids (Gawlik and FGB [2020])

$$\ell(u,\rho,s) = \int_\Omega \left[\frac{1}{2}\rho|u|^2 + \rho R\cdot u - \epsilon(\rho,s) - \rho\phi\right]\mathrm{d}x$$

## 4.1 Discrete Lagrangian

$$\ell_d(A,D) := \ell(\widehat{A},D) = \int_\Omega \left[\frac{1}{2}D|\widehat{A}|^2 - De(D)\right]\mathrm{d}x.$$

$$\frac{\delta \ell_d}{\delta A} = I_h^r(D\widehat{A})^\flat, \quad \frac{\delta \ell_d}{\delta D} = I_h^r\Big(\frac{1}{2}|\widehat{A}|^2 - e(D) - D\frac{\partial e}{\partial D}\Big).$$

## 4.2 Choice of $\Delta_h$ ($R_h$)

**Lemma**

$$\ker\left(A \in \Delta_h \to I_h^r(D\widehat{A})^\flat \in (\mathfrak{g}_h^r)^*/\Delta_h^\circ\right) = \{0\} \iff R_h \subset BDM_r(\mathcal{T}_h)$$

**Proof.**

$$\begin{aligned}
\ker &= \left\{A_u \in \Delta_h \mid I_h^r(D\widehat{A})^\flat \in \Delta_h^\circ\right\} \\
&= \left\{A_u \in \Delta_h \mid \langle I_h^r(DI_h^r(u)), I_h^r(v)\rangle = 0,\ \forall v \in R_h\right\} \\
&= \left\{A_u \in \Delta_h \mid \langle DI_h^r(u), I_h^r(v)\rangle = 0,\ \forall v \in R_h\right\}.
\end{aligned}$$

By main theorem: $u \in R_h \subset RT_{2r}(\mathcal{T}_h) \leftrightarrow A_u \in \Delta_h \subset \mathfrak{g}_h^r$ isomorphism

$$\ker = \{u \in R_h \mid \langle DI_h^r(u), I_h^r(v)\rangle = 0,\ \forall v \in R_h\}.$$

This space is zero if and only if $R_h \subset BDM_r(\mathcal{T}_h)$. ■

## 4.3 Geometric variational element scheme for compressible fluids

- Equations of motion

$$\begin{cases} \langle \partial_t(D\widehat{A}), \widehat{B}\rangle + \langle D\widehat{A}, \widehat{[A,B]}\rangle + \langle I_h^r(\frac{1}{2}|\widehat{A}|^2 - e(D) - D\frac{\partial e}{\partial D}), D\cdot B\rangle = 0, \quad \forall B \in \Delta_h \\ \langle \partial_t D, E\rangle + \langle D, AE\rangle = 0, \quad \forall E \in V_h^r. \end{cases}$$

- Equivalently, in terms of $\rho_h = D$, $u_h = -\widehat{A}$, $\sigma_h = E$, and $v_h = -\widehat{B}$:
Seek $u_h \in R_h$ and $\rho_h \in V_h^r$ such that

$$\begin{cases} \langle \partial_t(\rho_h u_h), v_h\rangle + a_h(w_h, u_h, v_h) - b_h(v_h, f_h, \rho_h) = 0, \quad \forall v_h \in R_h \\ \langle \partial_t \rho_h, \sigma_h\rangle - b_h(u_h, \sigma_h, \rho_h) = 0, \quad \forall \sigma_h \in V_h^r, \end{cases}$$

- $w_h = I_h^r(\rho_h u_h)$, $f_h = I_h^r\left(\frac{1}{2}|u_h|^2 - e(\rho_h) - \rho_h\frac{\partial e}{\partial \rho_h}\right)$, and

- $$a_h(w,u,v) = \sum_{K\in\mathcal{T}_h}\int_K w\cdot(v\cdot\nabla u - u\cdot\nabla v)\,dx + \sum_{e\in\mathcal{E}_h^0}\int_e (v\cdot n[u] - u\cdot n[v])\cdot\{w\}\mathrm{d}s$$

- $$b_h(w,f,g) = \sum_{K\in\mathcal{T}_h}\int_K (w\cdot\nabla f)g\,dx - \sum_{e\in\mathcal{E}_h^0} w\cdot[[f]]\{g\}\mathrm{d}s.$$

## 4.4 Temporal discretization

OPTION 1: variational discretization

OPTION 2: energy preserving discretization

$$\left\langle\!\!\left\langle \frac{1}{\Delta t}\left(\frac{\delta \ell_d}{\delta A_k} - \frac{\delta \ell_d}{\delta A_{k-1}}\right), B_k \right\rangle\!\!\right\rangle + \frac{1}{2}\left\langle\!\!\left\langle \frac{\delta \ell_d}{\delta A_{k-1}} + \frac{\delta \ell_d}{\delta A_k}, [A_{k-1/2}, B_k] \right\rangle\!\!\right\rangle + \langle F_{k-1/2}, D_{k-1/2} \cdot B_k \rangle = 0, \quad \forall\, B_k \in \Delta_h,$$

$$\left\langle \frac{D_k - D_{k-1}}{\Delta t}, E_k \right\rangle + \langle D_{k-1/2} \cdot A_{k-1/2}, E_k \rangle = 0, \quad \forall E_k \in V_h^r.$$

where

$$F_{k-1/2} = \frac{1}{2} \widehat{A_{k-1}} \cdot \widehat{A_k} - f(D_{k-1}, D_k), \qquad f(x,y) = \frac{ye(y) - xe(x)}{y - x}$$

(reminiscent of a discrete gradient method Hairer, Lubich, Wanner [2006])

## 4.5 Convergences

Rotating shallow water, $\Omega = (-1,1) \times (-1,1)$;
$u(x,y,0) = (0,0)$, $\rho(x,y,0) = 2 + \sin(\pi x/2)\sin(\pi y/2)$;
$\mathcal{T}_h$, uniform, $R_h = RT_r(\mathcal{T}_h)$, $V_h^r$, $r = 0,1,2$.

- $L^2$-errors in $u$ and $\rho$ at $T = 0.5$ by comparing with an "exact solution" obtained with $h = 2^{-5}$, $r = 2$. ($\Delta t = 0.00625$, $h = 2^{-j}$, $j = 0,1,2,3$)

| $r$ | $h^{-1}$ | $\lVert u_h - u\rVert_{L^2(\Omega)}$ | Rate | $\lVert \rho_h - \rho\rVert_{L^2(\Omega)}$ | Rate |
|---|---|---|---|---|---|
| 0 | 1 | $3.58 \cdot 10^{-1}$ | | $2.10 \cdot 10^{-1}$ | |
| | 2 | $1.84 \cdot 10^{-1}$ | 0.96 | $1.17 \cdot 10^{-1}$ | 0.85 |
| | 4 | $9.31 \cdot 10^{-2}$ | 0.99 | $5.58 \cdot 10^{-2}$ | 1.06 |
| | 8 | $4.64 \cdot 10^{-2}$ | 1.00 | $2.74 \cdot 10^{-2}$ | 1.03 |
| 1 | 1 | $1.43 \cdot 10^{-1}$ | | $1.00 \cdot 10^{-1}$ | |
| | 2 | $4.36 \cdot 10^{-2}$ | 1.71 | $2.43 \cdot 10^{-2}$ | 2.05 |
| | 4 | $1.37 \cdot 10^{-2}$ | 1.68 | $6.85 \cdot 10^{-3}$ | 1.83 |
| | 8 | $4.40 \cdot 10^{-3}$ | 1.63 | $1.74 \cdot 10^{-3}$ | 1.97 |
| 2 | 1 | $2.78 \cdot 10^{-2}$ | | $1.83 \cdot 10^{-2}$ | |
| | 2 | $7.80 \cdot 10^{-3}$ | 1.83 | $4.61 \cdot 10^{-3}$ | 1.99 |
| | 4 | $1.81 \cdot 10^{-3}$ | 2.11 | $6.35 \cdot 10^{-4}$ | 2.86 |
| | 8 | $4.50 \cdot 10^{-4}$ | 2.00 | $1.15 \cdot 10^{-4}$ | 2.46 |

- Convergence wrt $\Delta t$ of $L^2$-errors in $u$ and $\rho$ at $T = 0.5$ ($h = 2^{-4}$, $r = 2$)

| $\Delta t^{-1}$ | $\lVert u_h - u\rVert_{L^2(\Omega)}$ | Rate | $\lVert \rho_h - \rho\rVert_{L^2(\Omega)}$ | Rate |
|---|---|---|---|---|
| 2 | $4.93 \cdot 10^{-2}$ | | $9.95 \cdot 10^{-2}$ | |
| 4 | $1.68 \cdot 10^{-2}$ | 1.55 | $3.12 \cdot 10^{-2}$ | 1.67 |
| 8 | $5.03 \cdot 10^{-3}$ | 1.74 | $8.92 \cdot 10^{-3}$ | 1.81 |
| 16 | $1.44 \cdot 10^{-3}$ | 1.80 | $2.43 \cdot 10^{-3}$ | 1.88 |

## 4.6 Rayleigh-Taylor instability

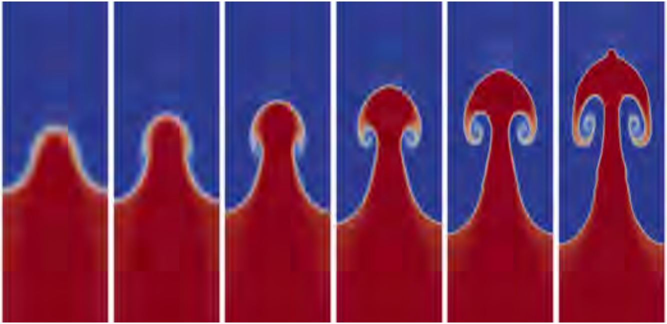
$$\ell(u,\rho,s)=\int_\Omega\left[\frac{1}{2}\rho|u|^2-\rho e(\rho,\eta)-\rho\phi\right]\mathrm{d}x,\qquad e(\rho,\eta)=Ke^{\eta/C_v}\rho^{\gamma-1}$$

where $\gamma=5/3$, $K=C_v=1$, $\phi=-y$

$\Omega=(0,1/4)\times(0,1)$, $R_h=RT_0(\mathcal{T}_h)$ and $V_h^1$ on uniform $\mathcal{T}_h$, $h=2^{-8}$, with upwinding (later), $\Delta t=0.01$.

$$\rho(x,y,0)=1.5-0.5\tanh\left(\frac{y-0.5}{0.02}\right)$$

Contours of the mass density at $t = 1.0, 1.2, 1.4, 1.6, 1.8, 2.0$ in the Rayleigh-Taylor instability simulation with the energy-preserving time discretization



Energy preserved exactly up to roundoff errors.

## 5.1 Equations and variational principle

- Lagrangian version (Hamilton's principle): seek $\varphi : [0, T] \to \mathrm{Diff}_{\mathrm{vol}}(\Omega)$ such that

$$\delta \int_0^T L(\varphi, \dot{\varphi}) \mathrm{d}t = 0, \qquad L(\varphi, \dot{\varphi}) = \int_\Omega \frac{1}{2} \varrho_0 |\dot{\varphi}|^2 \mathrm{d}X$$

for all $\delta\varphi$ vanishing at the endpoints.

- Eulerian version (Euler-Poincaré)

$$\delta \int_0^T \ell(u, \rho) \mathrm{d}t = 0, \qquad \ell(u, \rho) = \int_\Omega \frac{1}{2} \rho |u|^2 \mathrm{d}x$$

for all variations $\delta u$, $\delta\rho$ of the form

$$\delta u = \partial_t \zeta + [u, \zeta], \qquad \delta\rho = -\operatorname{div}(\rho\zeta)$$

- Incompressible fluids with variable density

$$\begin{cases} \rho(\partial_t u + u \cdot \nabla u) = -\nabla p, \\ \partial_t \rho + \operatorname{div}(\rho u) = 0, \qquad \operatorname{div} u = 0. \end{cases}$$

## 5.2 Discrete setting

$$G_h^r = \{q \in GL(V_h^r) \mid q\mathbf{1} = \mathbf{1},\ \langle qf, qg\rangle = \langle f, g\rangle\},$$

$$\mathfrak{g}_h^r = \{A \in L(V_h^r, V_h^r) \mid A\mathbf{1} = 0,\ \langle Af, g\rangle + \langle f, Ag\rangle = 0,\ \forall\, f, g \in V_h^r\}$$

$R_h = \{u \in BDM_r(\mathcal{T}_h), \operatorname{div} u = 0\} \rightsquigarrow \Delta_h \subset \mathfrak{g}_h^r$

$$\ell_d(A, D) := \ell(\widehat{A}, D) = \int_\Omega \frac{1}{2} D|\widehat{A}|^2 \mathrm{d}x.$$

$$\frac{\delta \ell_d}{\delta A} = I_h^r(D\widehat{A})^\flat, \quad \frac{\delta \ell_d}{\delta D} = I_h^r\Big(\frac{1}{2}|\widehat{A}|^2\Big).$$

## 5.3 Geometric variational element scheme for incompressible fluids with variable density

- Equations of motion

$$\begin{cases} \left\langle \partial_t(D\widehat{A}), \widehat{B} \right\rangle + \left\langle D\widehat{A}, \widehat{[A, B]} \right\rangle + \left\langle I_h^r\left(\frac{1}{2}|\widehat{A}|^2\right), D \cdot B \right\rangle = 0, \quad \forall B \in \Delta_h \\ \left\langle \partial_t D, E \right\rangle + \left\langle D, AE \right\rangle = 0, \quad \forall E \in V_h^r. \end{cases}$$

- Equivalently, in terms of $\rho_h = D$, $u_h = -\widehat{A}$, $\sigma_h = E$, and $v_h = -\widehat{B}$:
  Seek $u_h \in BDM_r(\mathcal{T}_h)$, $\rho_h \in V_h^r$, $p_h \in V_h^{r-1} \cap L^2_{\int=0}(\Omega)$ such that

$$\begin{cases} \left\langle \partial_t(\rho_h u_h), v_h \right\rangle + a_h(w_h, u_h, v_h) - b_h(v_h, f_h, \rho_h) = \left\langle p_h, \operatorname{div} v_h \right\rangle, \quad \forall v_h \in BDM_r(\mathcal{T}_h) \\ \left\langle \partial_t \rho_h, \sigma_h \right\rangle - b_h(u_h, \sigma_h, \rho_h) = 0, \quad \forall \sigma_h \in V_h^r, \\ \left\langle \operatorname{div} u_h, q \right\rangle = 0, \quad \forall q_h \in V_h^{r-1} \cap L^2_{\int=0}(\Omega) \end{cases}$$

with $w_h = I_h^r(\rho_h u_h)$, $f_h = I_h^r\left(\frac{1}{2}|u_h|^2\right)$.

## 5.4 Spatial discretization

**Proposition (Gawlik & FGB)**

The semidiscrete solution satisfies

$$\frac{d}{dt}\int_\Omega \rho_h \mathrm{d}x = 0$$

$$\frac{d}{dt}\int_\Omega \rho_h^2 \mathrm{d}x = 0$$

$$\frac{d}{dt}\int_\Omega \rho_h |u_h|^2 \mathrm{d}x = 0$$

$$\operatorname{div} u_h = 0$$

**Proof.** Use $a(w,u,v) = -a(w,v,u)$ and $b(u,f,g) = -b(u,g,f)$

$u_h \in BDM_r(\mathcal{T}_h) \rightsquigarrow \operatorname{div} u_h \in V_h^{r-1}$
$\int_\Omega \operatorname{div} u_h \mathrm{d}x = \int_{\partial\Omega} u_h \cdot n \mathrm{d}s = 0 \rightsquigarrow \operatorname{div} u_h \in V_h^{r-1} \cap L^2_{\int=0}(\Omega)$
So $\operatorname{div} u_h = 0$ by last equation.

## 5.5 Temporal discretization

Seek $u_k \in BDM_r(\mathcal{T}_h)$, $\rho_k \in V_h^r$, $p_k \in V_h^{r-1} \cap L^2_{\int=0}(\Omega)$ such that

$$\begin{cases} \langle \dfrac{\rho_{k+1} u_{k+1} - \rho_k u_k}{\Delta t}, v\rangle + a_h\Big(\dfrac{\rho_k u_k + \rho_{k+1} u_{k+1}}{\Delta t}, \dfrac{u_k + u_{k+1}}{2}, v\Big) \\ \qquad\qquad -b_h\Big(v, I_h(\dfrac{1}{2} u_k \cdot u_{k+1}), \dfrac{\rho_k + \rho_{k+1}}{2}\Big) = \langle p_{k+1}, \operatorname{div} v\rangle\,, \quad \forall v \in BDM_r(\mathcal{T}_h) \\ \langle \dfrac{\rho_{k+1} - \rho_k}{\Delta t}, \sigma\rangle - b_h\Big(\dfrac{u_k + u_{k+1}}{2}, \sigma, \dfrac{\rho_k + \rho_{k+1}}{2}\Big) = 0, \quad \forall \sigma_h \in V_h^r, \\ \langle \operatorname{div} u_{k+1}, q\rangle = 0, \quad \forall q \in V_h^{r-1} \cap L^2_{\int=0}(\Omega) \end{cases}$$

## Proposition (Gawlik & FGB)

The fully discrete solution of incompressible fluid with variable density satisfies

$$\int_\Omega \rho_{k+1} \mathrm{d}x = \int_\Omega \rho_k \mathrm{d}x$$

$$\int_\Omega \rho_{k+1}^2 \mathrm{d}x = \int_\Omega \rho_k^2 \mathrm{d}x$$

$$\int_\Omega \frac{1}{2}\rho_{k+1}|u_{k+1}|^2 \mathrm{d}x = \int_\Omega \frac{1}{2}\rho_k|u_k|^2 \mathrm{d}x$$

$$\operatorname{div} u_k = 0$$

## 5.6 Previous works

For ideal fluid ($\rho = 1$):

recovers Guzman, Shu, Sequeria [2016] and Natale, Cotter [2018].

For incompressible fluid with variable density:

Closest work is Guermond and Quartepelle [2000]

Their spatial discretization preserves

$$\int_\Omega \rho_h \mathrm{d}x, \qquad \int_\Omega \rho_h^2 \mathrm{d}x, \qquad \int_\Omega \rho_h |u_h|^2 \mathrm{d}x$$

but incompressibility constraint is only satisfied in a weak sense.

Temporal discretization does not preserve

$$\int_\Omega \rho_k^2 \mathrm{d}x \quad \text{and} \quad \int_\Omega \rho_k |u_k|^2 \mathrm{d}x$$

## 5.7 Rayleigh-Taylor instability

$\Omega = (-1/2, 1/2) \times (-2, 2)$ with initial conditions

$$u(x, y, 0) = (0, 0),$$
$$\rho(x, y, 0) = 2 + \tanh\left(\frac{y + 0.1\cos(2\pi x)}{0.1}\right).$$

add a gravitational forcing term $\langle (0, -g)\rho_{k+1/2}, v\rangle$, $g = 10$

Finite element spaces $u_k \in R_h = RT_0(\mathcal{T}_h)$, $\rho_k \in DG_1(\mathcal{T}_h)$, and $p_k \in DG_0(\mathcal{T}_h) \cap L^2_{\int=0}(\Omega)$ on uniform $\mathcal{T}_h$, $h = 2^{-j}$, $j = 4, 5, 6$, $\Delta t = 0.01$, with upwind.

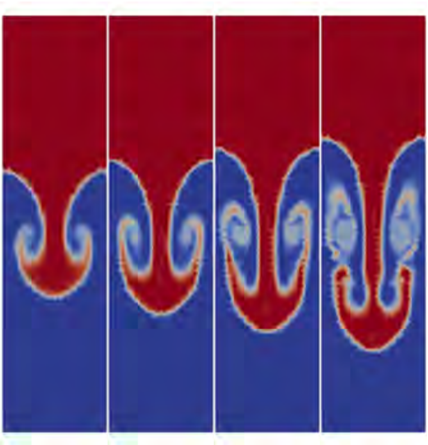


Figure: Density contours at $t = 0.8, 0.95, 1.1, 1.25$ in the Rayleigh-Taylor instability simulation with $h = 2^{-4}$.

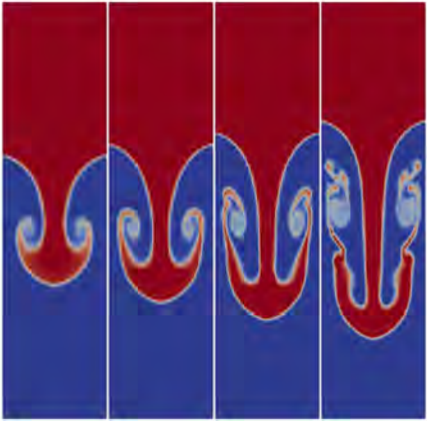


Figure: Density contours at $t = 0.8, 0.95, 1.1, 1.25$ in the Rayleigh-Taylor instability simulation with $h = 2^{-5}$.

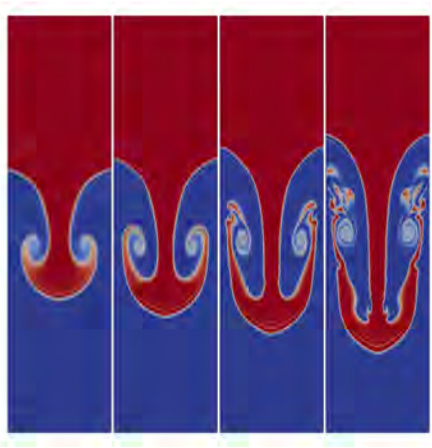


Figure: Density contours at $t = 0.8, 0.95, 1.1, 1.25$ in the Rayleigh-Taylor instability simulation with $h = 2^{-6}$.

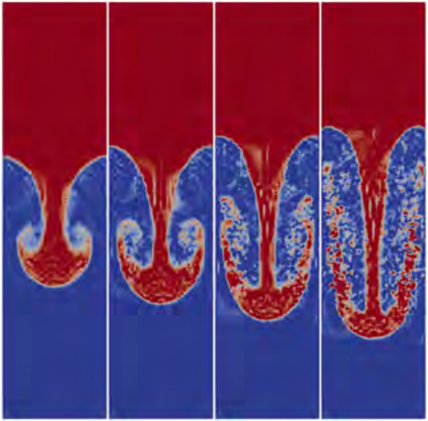


Figure: Density contours at $t = 0.8, 0.95, 1.1, 1.25$ in the Rayleigh-Taylor instability simulation with $h = 2^{-5}$ and no upwinding.

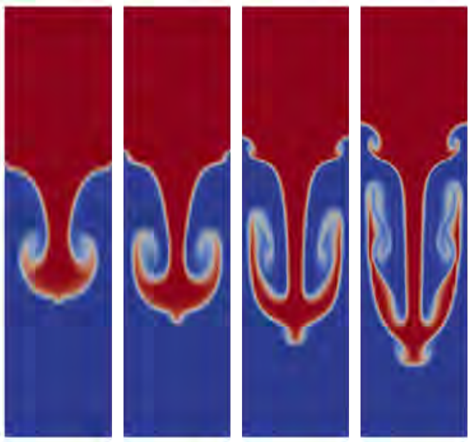


Figure: Density contours at $t = 0.8, 0.95, 1.1, 1.25$ in the Rayleigh-Taylor instability simulation, obtained using Guermond and Quartapelle [2000] with $h = 2^{-5}$, $\Delta t = 0.01$.

The two methods under comparison produce qualitatively similar results for $t < 1$, and begin to deviate somewhat as $t$ increases.

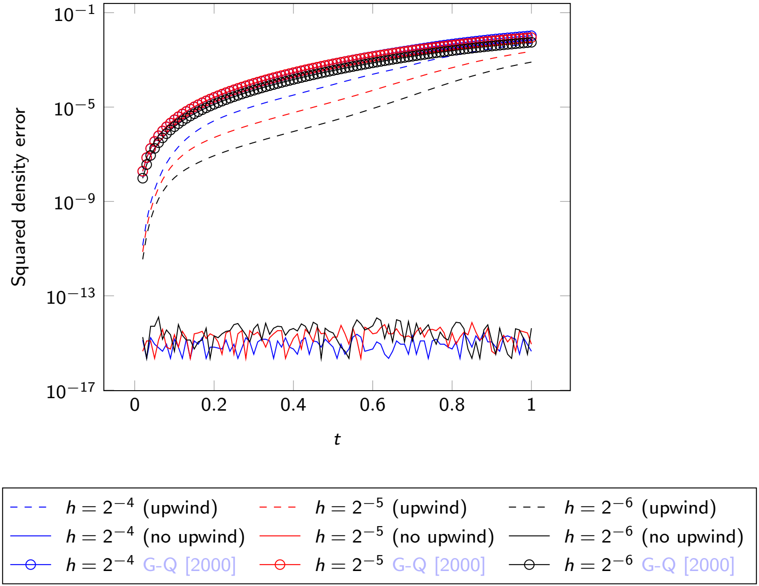



Figure: Squared density errors $|1 - F(t)/F(0)|$, $F(t) = \int_\Omega \rho_h(t)^2 \, dx$, in the RTI.

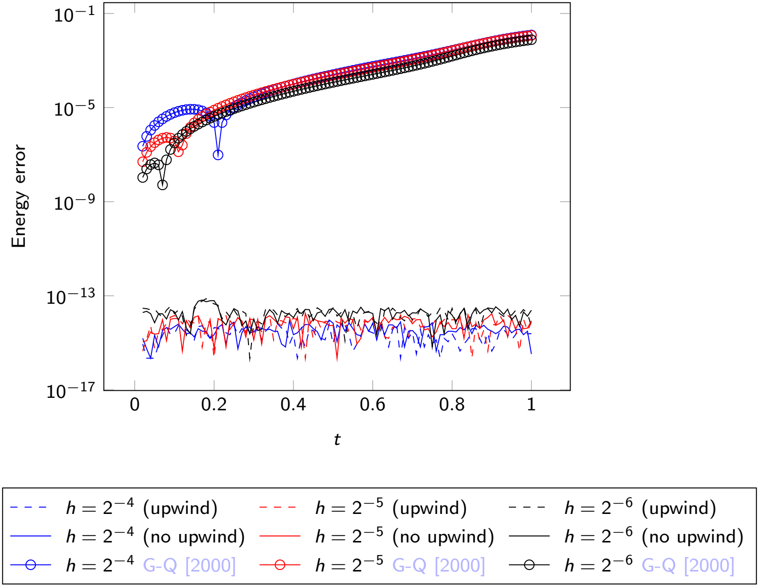



Figure: Energy errors $|1 - E(t)/E(0)|$, $E(t) = \int_\Omega \left(\frac{1}{2}\rho_h(t)u_h(t) \cdot u_h(t) + \rho_h(t)gy\right)\, dx$, in RTI. (The curves labelled G-Q [2000] appear nonsmooth because the sign of $1 - E(t)/E(0)$ changes from negative to positive near $t = 0$.)

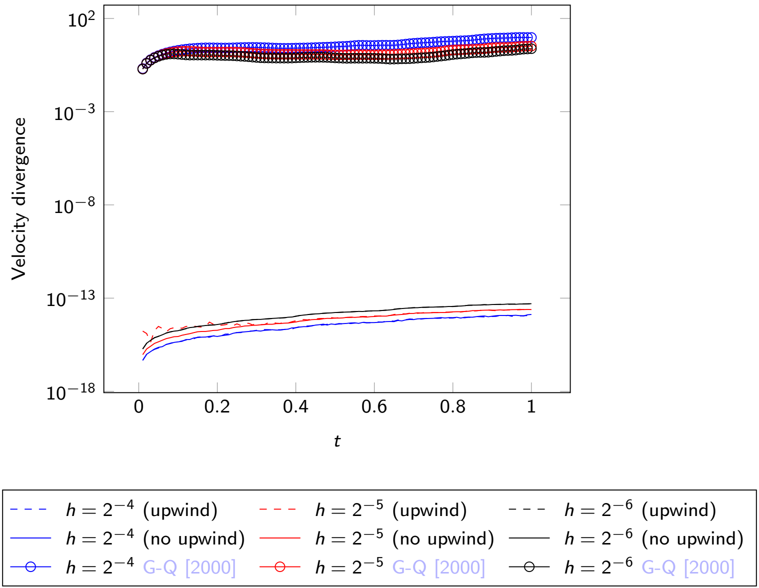



Figure: $L^2$-norm of the divergence of the velocity field in the Rayleigh-Taylor instability simulation.

# 6. Proof of the theorem

**Theorem (Gawlik and FGB)**

The space $S_h^r$ of discrete distributional derivatives on $V_h^r$ is isomorphic to $RT_{2r}(\mathcal{T}_h)$:

$$u \in RT_{2r}(\mathcal{T}_h) \longleftrightarrow A_u \in S_h^r$$

Recall:

- $S_h^r = \{A_u \mid u \in \mathrm{H}\}, \qquad \mathrm{H} := H_0(\mathrm{div}, \Omega) \cap L^p(\Omega)^n$
- $\langle A_u f, g\rangle := \sum_{K \in \mathcal{T}_h} \int_K (\nabla_u f) g \, \mathrm{d}x - \sum_{e \in \mathcal{E}_h^0} \int_e u \cdot [\![f]\!]\{g\} \, \mathrm{d}s$
- $RT_{2r}(\mathcal{T}_h) = \left\{u \in H_0(\mathrm{div}, \Omega) \mid u|_K \in (P_{2r}(K))^n + xP_{2r}(K), \forall K \in \mathcal{T}_h\right\}$
- Basis of the dual (Brezzi, Fortin [1991])

$$u \mapsto \int_e (u \cdot n) p \, \mathrm{d}s, \quad p \in P_{2r}(e), \, e \in \mathcal{E}_h^0,$$

$$u \mapsto \int_K u \cdot p \, \mathrm{d}x \quad p \in P_{2r-1}(K)^n, \, K \in \mathcal{T}_h.$$

- STEP 1: Working with $\mathsf{A}^*$:

Linear map:

$$\mathsf{A} : \mathsf{H} \to \mathfrak{gl}(V_h^r), \qquad u \mapsto \mathsf{A}(u) = A_u$$

Dual map

$$\mathsf{A}^* : \mathfrak{gl}(V_h^r)^* \to \mathsf{H}^*$$

We have

$$\dim(\operatorname{Im}\mathsf{A}) = \dim(\operatorname{Im}\mathsf{A}^*)$$

$$\operatorname{Im}\mathsf{A}^* = \left\{ \sum_{i=1}^{N} c_i \mathsf{A}^*(f_i \otimes g_i) \in \mathsf{H}^* \;\middle|\; N \in \mathbb{N},\ f_i, g_i \in V_h^r,\ c_i \in \mathbb{R},\ i = 1, 2, \ldots, N \right\},$$

$\mathsf{A}^*(f \otimes g)(u) = \langle f, A_u g \rangle$

- STEP 2: $\operatorname{Im} A^*$ is spanned by the functionals

$$u \mapsto \int_e (u \cdot n) pq \, \mathrm{d}s, \quad p, q \in P_r(e),\ e \in \mathcal{E}_h^0,$$

$$u \mapsto \int_K (u \cdot \nabla q) p \, \mathrm{d}x \quad p, q \in P_r(K),\ K \in \mathcal{T}_h.$$

Given $e = K_1 \cap K_2$ choose

$$f|_{K_1} = p \in P_r(K_1),\ f|_{\Omega \setminus K_1} = 0 \quad \text{and} \quad g|_{K_2} = -2q \in P_r(K_2),\ g|_{\Omega \setminus K_2} = 0$$

$$\rightsquigarrow \quad \langle f, A_u g \rangle = \int_e (u \cdot n) pq \, \mathrm{d}s$$

Given $K$ choose

$$f|_K = p \in P_r(K),\ f|_{\Omega \setminus K} = 0 \quad \text{and} \quad g|_K = q \in P_r(K),\ g|_{\Omega \setminus K} = 0$$

$$\rightsquigarrow \quad \langle f, A_u g \rangle = \int_K (u \cdot \nabla q) p \, \mathrm{d}x - \frac{1}{2} \int_{\partial K} (u \cdot n) pq \, \mathrm{d}s.$$

Appropriate linear combinations yields the desired functionals.

- STEP 3: Im $A^*$ is spanned by the functionals

$$u \mapsto \int_e (u \cdot n) p \, \mathrm{d}s, \quad p \in P_{2r}(e), \, e \in \mathcal{E}_h^0,$$

$$u \mapsto \int_K u \cdot p \, \mathrm{d}x \quad p \in P_{2r-1}(K)^n, \, K \in \mathcal{T}_h.$$

First functional: follows from

$$\left\{ \sum_{i=1}^N p_i q_i \mid N \in \mathbb{N}, \, p_i, q_i \in P_r(K), \, i = 1, 2, \ldots, N \right\} = P_{2r}(K).$$

Trivial

Second functional: follows from

$$\left\{ \sum_{i=1}^N p_i \nabla q_i \mid N \in \mathbb{N}, \, p_i, q_i \in P_r(K), \, i = 1, 2, \ldots, N \right\} = P_{2r-1}(K)^n, n = 2, 3.$$

By induction.

# 7. Connections with older approaches

In the lowest-order setting ($r = 0$), $V_h^0 = \mathbb{R}^N$.

- $\mathfrak{g}_h^0 = \left\{ A \in \mathbb{R}^{N\times N} \;\middle|\; \sum_{j=1}^N A_{ij} = 0 \right\}$
- the components of $A = A_u$ relative to the basis $\{1_{K_i}\}_i \subset V_h$ are

$$
\begin{aligned}
A_{ij} &= -\frac{1}{2|K_i|} \int_{K_i \cap K_j} u \cdot n \,\mathrm{d}s, \quad j \in N(i), \\
A_{ii} &= \frac{1}{2|K_i|} \int_{K_i} \operatorname{div} u \,\mathrm{d}x,
\end{aligned}
\tag{1}
$$

  and $A_{ij} = 0$ for all other $j$.
- hence the nonholonomic constraint is

$$S_h^0 = \operatorname{Im} \mathrm{A} = \left\{ A \in \mathfrak{g}_h^0 \mid A_{ij} = 0,\ \forall j \notin N(i) \cup \{i\},\ \ A^{\mathsf{T}} \Theta + \Theta A \text{ is diagonal} \right\}$$

See Bauer, FGB [2018].

# 8. Conclusion

- Used the geometric formulation of hydrodynamics to design structure preserving spatial and temporal discretization of fluid flow valid in 2D and 3D.
- We connected with finite elements, one of the largest class of discretization methods for fluids.
- All the steps are guided by geometry (including choice of finite element space).
- Interesting connection with nonholonomic mechanics.
- The geometric approach yields new schemes via a constructive approach and more conservation properties.
- This geometric framework allows for several natural extensions to other fluid models - under investigation.

| Continous diffeomorphism | Discrete diffeomorphisms |
|---|---|
| $\mathrm{Diff}(\Omega) \ni \varphi$ | $G_h^r \ni g$ |
| **Lie algebra** | **Discrete diffeomorphisms** |
| $\mathfrak{X}(\Omega) \ni u$ | $\mathfrak{g}_h^r \ni A$ |
| **Group action on functions** | **Group action on discrete functions** |
| $f \mapsto f \circ \varphi$ | $f \mapsto g^{-1} f$ |
| **Lie algebra action on functions** | **Lie algebra action on discrete functions** |
| $f \mapsto \nabla_u f$ | $f \mapsto -Af$ |
| **Group action on densities** | **Group action on discrete densities** |
| $\rho \mapsto (\rho \circ \varphi) J\varphi$ | $D \mapsto g^{-1} \cdot D$ |
| **Lie algebra action on densities** | **Lie algebra action on discrete densities** |
| $\rho \mapsto \mathrm{div}(\rho u)$ | $D \mapsto -A \cdot D$ |
| **Hamilton's principle** | **Lagrange-d'Alembert principle** |
| $\delta \int_0^T L_{\rho_0}(\varphi, \dot{\varphi}) \mathrm{d}t = 0$,<br>for arbitrary variations $\delta\varphi$ | $\delta \int_0^T L_{D_0}(g, \dot{g}) dt = 0$, $\dot{g}g^{-1} \in \Delta_h$,<br>for variations $\delta g g^{-1} \in \Delta_h$ |
| **Eulerian velocity and density** | **Eulerian discrete velocity and discrete density** |
| $u = \dot{\varphi} \circ \varphi^{-1}$, $\rho = (\rho_0 \circ \varphi^{-1}) J\varphi^{-1}$ | $A = \dot{g}g^{-1}$, $D = g \cdot D_0$ |
| **Euler-Poincaré principle** | **Euler-Poincaré-d'Alembert principle** |
| $\delta \int_0^T \ell(u, \rho) \mathrm{d}t = 0$, $\delta u = \partial_t \zeta + [\zeta, u]$,<br>$\delta\rho = -\mathrm{div}(\rho\zeta)$ | $\delta \int_0^T \ell(A, D) \mathrm{d}t = 0$, $\quad \delta A = \partial_t B + [B, A]$,<br>$\delta D = B \cdot D$, $\quad A, B \in \Delta_h$ |
| **Compressible Euler equations** | **Discrete compressible Euler equations** |
| $\partial_t \frac{\delta \ell}{\delta u} + \mathcal{L}_u \frac{\delta \ell}{\delta u} = \rho \nabla \frac{\delta \ell}{\delta \rho}$<br>$\partial_t \rho + \mathrm{div}(\rho u) = 0$ | $\partial_t \frac{\delta \ell_d}{\delta A} + \mathrm{ad}_A^* \frac{\delta \ell_d}{\delta A} - \frac{\delta \ell_d}{\delta D} \diamond D \in \Delta_h^\circ$<br>$\partial_t D - A \cdot D = 0$ |

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# THANK YOU!