

Geometric Variational Finite Element Discretizations for Fluids

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Abstract: We present an overview of finite element variational integrators for compressible and incompressible fluids with variable density. The numerical schemes are derived by discretizing, in a structure preserving way, the Lie group formulation of fluid dynamics on diffeomorphism groups and the associated variational principles. Given a triangulation on the fluid domain, the discrete group of diffeomorphisms is defined as a certain subgroup of the group of linear isomorphisms of a finite element space of functions. In this setting, discrete vector fields correspond to a certain subspace of the Lie algebra of this group. This subspace is shown to be isomorphic to a Raviart-Thomas finite element space. We illustrate the conservation properties of the scheme with the Rayleigh-Taylor instability test.

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1. INTRODUCTION

Numerical schemes that respect conservation laws and other geometric structures are of paramount importance in computational fluid dynamics, especially for problems relying on long time simulation. This is the case for geophysical fluid dynamics in the context of meteorological or climate prediction.

Schemes that preserve the geometric structures underlying the equations they discretize are known as geometric integrators, Hairer, Lubich, and Wanner (2006). One efficient way to derive geometric integrators is to exploit the variational formulation of the continuous equations and to mimic this formulation at the spatially and/or temporally discrete level. For instance, in classical mechanics, a time discretization of the Lagrangian variational formulation permits the derivation of numerical schemes, called variational integrators, that are symplectic, exhibit good energy behavior, and inherit a discrete version of Noether's theorem which guarantees the exact preservation of momenta arising from symmetries, see Marsden and West (2001).

Geometric variational integrators for fluid dynamics were first derived in Pavlov et al. (2010) for the Euler equations of a perfect fluid. It was suggested in Liu et al. (2015) that the variational discretization initiated in Pavlov et al. (2010) can be generalized by letting the discrete diffeomorphism group act on finite element spaces. Such an approach was developed in Natale and Cotter (2018) in the context of the ideal fluid and thus allowed for a higher order version of the method as well as an error estimate. For certain parameter choices, this high order method coincides with an $H(\text{div})$ -conforming finite element method studied in Guzman, Shu, and Sequeira (2016). The extension of the approach of Pavlov et al. (2010) to compressible

fluids has been carried out in Bauer and Gay-Balmaz (2019).

In this paper we present, following Gawlik and Gay-Balmaz (2020a,b), finite element variational discretizations for compressible and incompressible fluids with variable density, that extend these previous works.

2. VARIATIONAL FORMULATION FOR FLUIDS

In this section we recall the variational formulation of compressible fluids and incompressible fluids with variable density (also called nonhomogeneous incompressible fluids) in the Lagrangian and Eulerian formulations.

2.1 Lagrangian variational formulation

Solutions to the equations of compressible fluid flow in a bounded domain $\Omega \subset \mathbb{R}^n$ with smooth boundary can be formally regarded as curves $\varphi : [0, T] \rightarrow \text{Diff}(\Omega)$ that are critical for the Hamilton principle

$$\delta \int_0^T L(\varphi, \partial_t \varphi) dt = 0 \quad (1)$$

with respect to variations $\delta\varphi$ vanishing at the endpoints. Here $\text{Diff}(\Omega)$ is the group of diffeomorphisms of Ω and $\varphi(t) : \Omega \rightarrow \Omega$ is the map sending the position X of a fluid particle at time 0 to its position $x = \varphi(t, X)$ at time t . The function $L : T\text{Diff}(\Omega) \rightarrow \mathbb{R}$ in (1) is the Lagrangian given by the kinetic energy minus the potential energy. For a barotropic fluid it is given by

$$L(\varphi, \partial_t \varphi) = \int_{\Omega} \left[\frac{1}{2} \varrho_0 |\partial_t \varphi|^2 - \varrho_0 e(\varrho_0 / J\varphi) \right] dX, \quad (2)$$

where ϱ_0 is the mass density of the fluid in the reference configuration, $J\varphi$ is the determinant of the Jacobian of the

diffeomorphism φ , and e is the specific internal energy of the fluid.

2.2 Eulerian variational formulation

The Lagrangian (2) is invariant under the action of the subgroup $\text{Diff}(\Omega)_{\varrho_0} \subset \text{Diff}(\Omega)$ of diffeomorphisms that preserve ϱ_0 . As a consequence of this symmetry, one can write L in terms of the Eulerian velocity $u = \partial_t \varphi \circ \varphi^{-1}$ and mass density $\rho = (\varrho_0 \circ \varphi^{-1}) J \varphi^{-1}$ in the standard form

$$\ell(u, \rho) = \int_{\Omega} \left[\frac{1}{2} \rho |u|^2 - \rho e(\rho) \right] dx. \quad (3)$$

The Hamilton principle (1) induces the Euler-Poincaré variational principle

$$\delta \int_0^T \ell(u, \rho) dt = 0, \quad (4)$$

with respect to variations δu and $\delta \rho$ of the form

$$\delta u = \partial_t v + \mathcal{L}_u v, \quad \delta \rho = -\text{div}(\rho v), \quad (5)$$

with $v : [0, T] \rightarrow \mathfrak{X}(\Omega)$ and $v(0) = v(T) = 0$. Here $\mathfrak{X}(\Omega)$ denotes the Lie algebra of $\text{Diff}(\Omega)$, which consists of vector fields on Ω , with vanishing normal component on $\partial\Omega$. The conditions for criticality in (4) yield the balance of fluid momentum

$$\rho(\partial_t u + u \cdot \nabla u) = -\nabla p, \quad \text{with} \quad p = \rho^2 \frac{\partial e}{\partial \rho} \quad (6)$$

while $\rho = (\varrho_0 \circ \varphi^{-1}) J \varphi^{-1}$ yields the continuity equation

$$\partial_t \rho + \text{div}(\rho u) = 0.$$

2.3 Incompressible fluid with variable density

For the incompressible fluid, one considers the Hamilton principle (1) on the group

$$\text{Diff}_{\text{vol}}(\Omega) = \{\varphi \in \text{Diff}(\Omega) \mid J\varphi = 1\}$$

of volume preserving diffeomorphisms. The Lagrangian is given by the kinetic energy

$$L(\varphi, \partial_t \varphi) = \int_{\Omega} \frac{1}{2} \varrho_0 |\partial_t \varphi|^2 dX,$$

and is invariant under the action of the subgroup $\text{Diff}_{\text{vol}}(\Omega)_{\varrho_0} \subset \text{Diff}_{\text{vol}}(\Omega)$ of volume preserving diffeomorphisms that preserve ϱ_0 . Similarly as before, L can be written in terms of the Eulerian velocity $u = \partial_t \varphi \circ \varphi^{-1} \in \mathfrak{X}_{\text{vol}}(\Omega)$ and mass density $\rho = \varrho_0 \circ \varphi^{-1}$ in the standard form

$$\ell(u, \rho) = \int_{\Omega} \frac{1}{2} \rho |u|^2 dx. \quad (7)$$

Here $\mathfrak{X}_{\text{vol}}(\Omega)$ is the Lie algebra of $\text{Diff}_{\text{vol}}(\Omega)$, which consists of divergence free vector fields on Ω with vanishing normal component on $\partial\Omega$. The Euler-Poincaré variational principle (4)–(5), where now $v : [0, T] \rightarrow \mathfrak{X}_{\text{vol}}(\Omega)$, $v(0) = v(T) = 0$, yields the balance of fluid momentum

$$\rho(\partial_t u + u \cdot \nabla u) = -\nabla p, \quad \text{with} \quad \text{div} u = 0, \quad (8)$$

where the pressure p is found from the incompressibility condition.

3. SEMIDISCRETE VARIATIONAL FORMULATION

In this section we describe a semidiscrete setting appropriate for the derivation of a finite element variational integrator for compressible fluids, see Gawlik and Gay-Balmaz (2020b).

3.1 Discrete diffeomorphism groups

The starting point is the use of a finite dimensional Lie group approximation of $\text{Diff}(\Omega)$, given by

$$G_h = \{q \in GL(V_h) \mid q\mathbf{1} = \mathbf{1}\}, \quad (9)$$

for some finite element space $V_h \subset L^2(\Omega)$ associated to a triangulation \mathcal{T}_h of Ω , where $GL(V_h)$ is the group of invertible linear maps $V_h \rightarrow V_h$ and $\mathbf{1}$ is the constant function 1. The condition $q\mathbf{1} = \mathbf{1}$ encodes the fact that constant functions are preserved by the action of a diffeomorphism. Elements in the Lie algebra

$$\mathfrak{g}_h = \{A \in L(V_h, V_h) \mid A\mathbf{1} = 0\}, \quad (10)$$

with $L(V_h, V_h)$ the space of linear maps $V_h \rightarrow V_h$, are potential candidates to be discrete vector fields. As linear maps in \mathfrak{g}_h these discrete vector fields act as discrete derivations on V_h . It is thus natural to choose them as distributional directional derivatives.

3.2 Distributional directional derivative

We use the standard notation $H(\text{div}, \Omega) = \{u \in L^2(\Omega)^n \mid \text{div} u \in L^2(\Omega)\}$. For $r \geq 0$ an integer, we consider the subspace of $L^2(\Omega)$ given by

$$V_h^r = \{f \in L^2(\Omega) \mid f|_K \in P_r(K), \forall K \in \mathcal{T}_h\}, \quad (11)$$

where $P_r(K)$ denotes the space of polynomials of degree $\leq r$ on a simplex K . We denote by \mathcal{E}_h^0 the set of $(n-1)$ -simplices in \mathcal{T}_h not contained in $\partial\Omega$, and $H_0(\text{div}, \Omega) = \{u \in H(\text{div}, \Omega) \mid u \cdot n = 0 \text{ on } \partial\Omega\}$.

Definition 3.1. Given $u \in H(\text{div}, \Omega)$, the **distributional derivative in the direction u** is the linear map $\nabla_u^{\text{dist}} : L^2(\Omega) \rightarrow C_0^\infty(\Omega)'$ defined by

$$\int_{\Omega} (\nabla_u^{\text{dist}} f) g dx = - \int_{\Omega} f \text{div}(gu) dx, \quad \forall g \in C_0^\infty(\Omega), \quad (12)$$

with $C_0^\infty(\Omega)$ the space of smooth functions with compact support in the interior of Ω .

We give now a consistent approximation of the distributional derivative, which plays a fundamental role in our approach.

Proposition 3.1. Given $u \in H_0(\text{div}, \Omega) \cap L^p(\Omega)^n$, $p > 2$, and $r \geq 0$ an integer, a consistent approximation of ∇_u^{dist} in V_h^r is obtained by setting $A = A_u \in L(V_h^r, V_h^r)$ defined by

$$\begin{aligned} &\langle A_u f, g \rangle \\ &:= \sum_{K \in \mathcal{T}_h} \int_K (\nabla_u f) g dx - \sum_{e \in \mathcal{E}_h^0} \int_e u \cdot \llbracket f \rrbracket \{g\} ds, \end{aligned} \quad (13)$$

$\forall f, g \in V_h^r$, where $\llbracket f \rrbracket := f_1 n_1 + f_2 n_2$ and $\{g\} := \frac{1}{2}(g_1 + g_2)$ on $e = K_1 \cap K_2$, and n_i is the outward unit normal to K_i .

Thanks to the following proposition, it follows that to each vector field $u \in H_0(\text{div}, \Omega)$ we can associate an element in the Lie algebra \mathfrak{g}_h^r of the discrete diffeomorphism group.

Proposition 3.2. For all $u \in H_0(\text{div}, \Omega) \cap L^p(\Omega)$, $p > 2$, we have

$$A_u \mathbf{1} = 0 \text{ and } \langle A_u f, g \rangle + \langle f, A_u g \rangle + \langle f, (\text{div} u) g \rangle = 0 \quad (14)$$

for all $f, g \in V_h^r$.

From the previous result, we get a well-defined linear map

$$\begin{aligned} \mathbf{A} : H_0(\operatorname{div}, \Omega) \cap L^p(\Omega)^n &\rightarrow \mathfrak{g}_h^r \subset L(V_h^r, V_h^r), \\ u &\mapsto \mathbf{A}(u) = A_u, \quad p > 2, \end{aligned} \quad (15)$$

with values in the Lie algebra $\mathfrak{g}_h^r = \{A \in L(V_h^r, V_h^r) \mid \mathbf{A}1 = 0\}$ of $G_h^r = \{q \in GL(V_h^r) \mid q1 = 1\}$.

3.3 Relation with Raviart-Thomas finite element spaces

We define below the subspace S_h^r of \mathfrak{g}_h^r consisting of all Lie algebra elements that represent a vector field $u \in H_0(\operatorname{div}, \Omega)$.

Definition 3.2. For $r \geq 0$ an integer, we define the subspace $S_h^r \subset \mathfrak{g}_h^r \subset L(V_h^r, V_h^r)$ as

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

The next result identifies a subspace of $H_0(\operatorname{div}, \Omega)$ isomorphic to S_h^r . This result is a key step in the development of our variational finite element approach.

Proposition 3.3. Let $r \geq 0$ be an integer. The space $S_h^r \subset \mathfrak{g}_h^r$ is isomorphic to the Raviart-Thomas space of order $2r$

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

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

Note that only the Lie algebra elements in the subspace $S_h^r \subset \mathfrak{g}_h^r$ correspond to discrete vector fields, and note also that S_h^r is not a Lie subalgebra of \mathfrak{g}_h^r . As we will see below, S_h^r is treated as a nonholonomic constraint in the semidiscrete variational principle.

3.4 The Lie algebra-to-vector fields map

We define a Lie algebra-to-vector fields map that associates to a matrix $A \in L(V_h^r, V_h^r)$ a vector field on Ω . Such a map is needed to define in a general way the semidiscrete Lagrangian associated to a given continuous Lagrangian.

Since any $A \in S_h^r$ is associated to a unique vector field $u \in RT_{2r}(\mathcal{T}_h)$, one could think that the correspondence $A_u \in S_h^r \rightarrow u \in RT_{2r}(\mathcal{T}_h)$ can be used as a Lie algebra-to-vector fields map. However, to apply the variational principle with a nonholonomic constraint the Lagrangian must be defined on a larger space than the constraint space S_h^r , namely, at least on $S_h^r + [S_h^r, S_h^r]$. This is why such a Lie algebra-to-vector fields map is needed.

Definition 3.3. For $r \geq 0$ an integer, we consider the **Lie algebra-to-vector field map** $\widehat{\cdot} : L(V_h^r, V_h^r) \rightarrow [V_h^r]^n$ defined by

$$\widehat{A} := \sum_{k=1}^n A(I_h^r(x^k))e_k, \quad (16)$$

where $I_h^r : L^2(\Omega) \rightarrow V_h^r$ is the L^2 -orthogonal projector onto V_h^r , $x^k : \Omega \rightarrow \mathbb{R}$ are the coordinate maps, and e_k the canonical basis for \mathbb{R}^n .

The idea leading to the definition (16) is the following. On one hand the component u^k of a general vector field $u = \sum_k u^k e_k$, can be understood as the derivative of the coordinate function x^k in the direction u , i.e. $u^k = \nabla_u x^k$. On the other hand, from the definition of the

discrete diffeomorphism group, the linear map $f \mapsto Af$ for $f \in V_h^r$ is understood as a derivation, hence (16) is a natural candidate for a Lie algebra-to-vector field map. The following result is needed to describe the finite element scheme, as it describes explicitly the Lie bracket of two elements in S_h^r , in terms of vector fields in $H_0(\operatorname{div}, \Omega)$.

Proposition 3.4. For all $u, v \in H_0(\operatorname{div}, \Omega) \cap L^p(\Omega)$, $p > 2$, and $r \geq 1$, we have

$$\begin{aligned} \langle \widehat{[A_u, A_v]}^k, g \rangle &= \sum_K \int_K (\nabla \bar{v}^k \cdot u - \nabla \bar{u}^k \cdot v) g dx \\ &\quad - \sum_{e \in \mathcal{E}_h^n} \int_e (u \cdot n[\bar{v}^k] - v \cdot n[\bar{u}^k]) \{g\} ds, \end{aligned}$$

for $k = 1, \dots, n$, for all $g \in V_h^r$, where $\bar{u}^k = I_h^r(u^k) \in V_h^r$ and $\bar{v}^k = I_h^r(v^k) \in V_h^r$. The convention is such that if n is pointing from K_- to K_+ , then $[\bar{v}^k] = \bar{v}_-^k - \bar{v}_+^k$.

4. FINITE ELEMENT VARIATIONAL INTEGRATOR

4.1 Semidiscrete Euler-Poincaré equations

Given a continuous Lagrangian $\ell(u, \rho)$, the associated discrete Lagrangian $\ell_d : \mathfrak{g}_h^r \times V_h^r \rightarrow \mathbb{R}$ is defined with the help of the Lie algebra-to-vector fields map as

$$\ell_d(A, \rho_h) := \ell(\widehat{A}, \rho_h), \quad (17)$$

where $\rho_h \in V_h^r$ is the discrete density. Exactly as in the continuous case, the right action of G_h^r on discrete densities is defined by duality as

$$\langle \rho_h \cdot q, \sigma_h \rangle = \langle \rho_h, q\sigma_h \rangle, \quad \forall \sigma_h \in V_h^r. \quad (18)$$

The corresponding action of \mathfrak{g}_h^r on ρ_h is given by

$$\langle \rho_h \cdot B, \sigma_h \rangle = \langle \rho_h, B\sigma_h \rangle, \quad \forall \sigma_h \in V_h^r. \quad (19)$$

The semidiscrete equations are derived by mimicking the variational formulation of the continuous equations in §2, namely, by using the Euler-Poincaré principle applied to ℓ_d . As we have explained earlier, only the Lie algebra elements in $\operatorname{Im} \mathbf{A} = S_h^r$ actually represent a discretization of continuous vector fields. This condition is included in the Euler-Poincaré principle by imposing S_h^r as a nonholonomic constraint, and hence applying the Euler-Poincaré-d'Alembert principle. As we will see later, one needs to further restrict the constraint S_h^r to a subspace $\Delta_h^R \subset S_h^r$.

For a given constraint $\Delta_h^R \subset \mathfrak{g}_h^r$, a given Lagrangian ℓ_d , and a given duality pairing $\langle \cdot, \cdot \rangle$ between elements $K \in (\mathfrak{g}_h^r)^*$ and $A \in \mathfrak{g}_h^r$, the Euler-Poincaré-d'Alembert principle seeks $A(t) \in \Delta_h^R$ and $\rho_h(t) \in V_h^r$ such that

$$\delta \int_0^T \ell_d(A, \rho_h) dt = 0,$$

for

$$\delta A = \partial_t B + [B, A] \quad \text{and} \quad \delta \rho_h = -\rho_h \cdot B,$$

for all $B(t) \in \Delta_h^R$ with $B(0) = B(T) = 0$. The expressions for δA and $\delta \rho_h$ are deduced from the relations $A(t) = \dot{q}(t)q(t)^{-1}$ and $\rho_h(t) = \varrho_{h0} \cdot q(t)^{-1}$, with ϱ_{h0} the initial value of the density, as in the continuous case in (4)–(5).

The critical condition associated to this principle is

$$\left\langle \left\langle \frac{\delta \ell_d}{\delta A}, B \right\rangle \right\rangle + \left\langle \left\langle \frac{\delta \ell_d}{\delta A}, [A, B] \right\rangle \right\rangle + \left\langle \frac{\delta \ell_d}{\delta \rho_h}, \rho_h \cdot B \right\rangle = 0, \quad (20)$$

for all $t \in (0, T)$, for all $B \in \Delta_h^R$. The differential equation for ρ_h follows from differentiating $\rho_h(t) = \varrho_{h0} \cdot q(t)^{-1}$ to obtain $\partial_t \rho_h = -\rho_h \cdot A$, or, equivalently,

$$\langle \partial_t \rho_h, \sigma_h \rangle + \langle \rho_h, A \sigma_h \rangle = 0, \quad \forall t \in (0, T), \quad \forall \sigma_h \in V_h^r. \quad (21)$$

A sufficient condition for (20) to be a solvable system for T small enough is that the map

$$\Delta_h^R \ni A \mapsto \frac{\delta \ell_d}{\delta A}(A, \rho_h) \in (\mathfrak{g}_h^r)^* / (\Delta_h^R)^\circ \quad (22)$$

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

4.2 The compressible fluid

From (17), the discrete Lagrangian associated to (3) is

$$\ell_d(A, \rho_h) := \ell(\widehat{A}, \rho_h) = \int_{\Omega} \left[\frac{1}{2} \rho_h |\widehat{A}|^2 - \rho_h e(\rho_h) \right] dx. \quad (23)$$

We have

$$\frac{\delta \ell_d}{\delta A} = I_h^r(\rho_h \widehat{A})^\flat, \quad (24)$$

where the linear map $\flat : ([V_h^r]^n)^* = [V_h^r]^n \rightarrow (\mathfrak{g}_h^r)^*$ is defined as the dual map to $\widehat{\cdot} : \mathfrak{g}_h^r \rightarrow [V_h^r]^n$. Denote by R_h the subspace of $RT_{2r}(\mathcal{T}_h)$ corresponding to Δ_h^R via the isomorphism $RT_{2r}(\mathcal{T}_h) \ni u \mapsto A_u \in S_h^r$ shown in Proposition 3.3. We have the following result.

Proposition 4.1. *The kernel of (22) is zero if and only if R_h is a subspace of $[V_h^r]^n \cap H_0(\text{div}, \Omega) = BDM_r(\mathcal{T}_h)$, the Brezzi-Douglas-Marini finite element space of order r .*

The diagram below illustrates the situation that we consider.

$$\begin{array}{ccccc} H_0(\text{div}, \Omega) & \xrightarrow{A} & S_h^r & \hookrightarrow & \mathfrak{g}_h^r \xrightarrow{\widehat{\cdot}} [V_h^r]^n \\ \uparrow & \swarrow & \uparrow & & \\ RT_{2r}(\mathcal{T}_h) & & \Delta_h^R & & \\ \uparrow & \swarrow & \uparrow & & \\ R_h & & & & \end{array}$$

Using the expressions of the functional derivatives of (23), the Euler-Poincaré equations (20) are equivalent to

$$\begin{aligned} & \langle \partial_t(\rho_h \widehat{A}), \widehat{B} \rangle + \langle \rho_h \widehat{A}, \widehat{[A, B]} \rangle \\ & + \left\langle I_h^r \left(\frac{1}{2} |\widehat{A}|^2 - e(\rho_h) - \rho_h \frac{\partial e}{\partial \rho_h} \right), \rho_h \cdot B \right\rangle = 0, \end{aligned} \quad (25)$$

for all $t \in (0, T)$, for all $B \in \Delta_h^R$.

To relate (25) and (21) to more traditional finite element notation, let us denote $u_h = -\widehat{A}$ and $v_h = -\widehat{B}$. Then, using Proposition 3.4, the identities $\widehat{A_{u_h}} = -\widehat{A}$ and $\widehat{A_{v_h}} = -\widehat{B}$, and the definition (13) of A_u , we see that (25) and (21) are equivalent to seeking $u_h \in R_h$ and $\rho_h \in V_h^r$ such that

$$\begin{cases} \langle \partial_t(\rho_h u_h), v_h \rangle + a_h(w_h, u_h, v_h) - b_h(v_h, f_h, \rho_h) = 0 \\ \langle \partial_t \rho_h, \sigma_h \rangle - b_h(u_h, \sigma_h, \rho_h) = 0, \end{cases}$$

for all $v_h \in R_h$ and for all $\sigma_h \in V_h^r$, where

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

$$\begin{aligned} a_h(w, u, v) &= \sum_{K \in \mathcal{T}_h} \int_K w \cdot (v \cdot \nabla u - u \cdot \nabla v) dx \\ &+ \sum_{e \in \mathcal{E}_h^0} \int_e (v \cdot n[u] - u \cdot n[v]) \cdot \{w\} ds, \\ b_h(w, f, g) &= \sum_{K \in \mathcal{T}_h} \int_K (w \cdot \nabla f) g dx - \sum_{e \in \mathcal{E}_h^0} w \cdot \llbracket f \rrbracket \{g\} ds. \end{aligned}$$

4.3 The incompressible fluid with variable density

In the incompressible case, the same developments as before can be carried out with the finite dimensional Lie group approximation of $\text{Diff}_{\text{vol}}(\Omega)$ given by

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

with Lie algebra

$$\begin{aligned} \mathfrak{g}_h &= \{A \in L(V_h, V_h) \mid A\mathbf{1} = 0, \\ &\langle Af, g \rangle + \langle f, Ag \rangle = 0, \forall f, g \in V_h\}. \end{aligned}$$

The variational setting yields, with R_h chosen as $BDM_r(\mathcal{T}_h)$, the following scheme: seek $u_h \in BDM_r(\mathcal{T}_h)$, $\rho_h \in V_h^r$, $p_h \in V_h^{r-1} \cap L_{f=0}^2(\Omega)$, such that

$$\begin{cases} \langle \partial_t(\rho_h u_h), v_h \rangle + a_h(w_h, u_h, v_h) \\ \quad - b_h(v_h, f_h, \rho_h) = \langle p_h, \text{div } v_h \rangle \\ \langle \partial_t \rho_h, \sigma_h \rangle - b_h(u_h, \sigma_h, \rho_h) = 0 \\ \langle \text{div } u_h, q_h \rangle = 0, \end{cases} \quad (26)$$

for all $v_h \in BDM_r(\mathcal{T}_h)$, $\sigma_h \in V_h^r$, and $q_h \in V_h^{r-1} \cap L_{f=0}^2(\Omega)$, where $L_{f=0}^2(\Omega) = \{p \in L^2(\Omega) \mid \int_{\Omega} p dx = 0\}$,

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

The geometric finite element scheme has the following conservative properties.

Proposition 4.2. *For every t , the solution of the scheme satisfies $\text{div } u_h = 0$ and*

$$\frac{d}{dt} \int_{\Omega} \rho_h dx = 0, \quad \frac{d}{dt} \int_{\Omega} \rho_h^2 dx = 0, \quad \frac{d}{dt} \int_{\Omega} \frac{1}{2} \rho_h |u_h|^2 dx = 0.$$

4.4 Temporal discretization

The variational character of compressible fluid equations can be exploited also at the temporal level, by deriving the temporal scheme via a discretization in time of the Euler-Poincaré variational principle. Alternatively, it also admits a time discretization that exactly preserves the total energy. Both approaches are described in details in Gawlik and Gay-Balmaz (2020b). Regarding the incompressible fluid with variable density, a time discretization can be developed that allows to preserve all the quantities in Proposition 4.2.

Proposition 4.3. *Consider the following temporal discretization of (26): seek $u_k \in BDM_r(\mathcal{T}_h)$, $\rho_k \in V_h^r$, $p_k \in V_h^{r-1} \cap L_{f=0}^2(\Omega)$ such that*

$$\left\{ \begin{array}{l} \langle \frac{\rho_{k+1}u_{k+1} - \rho_k u_k}{\Delta t}, v \rangle + a_h((\rho u)_{k+1/2}, u_{k+1/2}, v) \\ \quad - b_h(v, I_h^r(\frac{1}{2}u_k \cdot u_{k+1}), \rho_{k+1/2}) = \langle p_{k+1}, \operatorname{div} v \rangle \\ \langle \frac{\rho_{k+1} - \rho_k}{\Delta t}, \sigma \rangle - b_h(u_{k+1/2}, \sigma, \rho_{k+1/2}) = 0 \\ \langle \operatorname{div} u_{k+1}, q \rangle = 0, \end{array} \right.$$

for all $v \in \text{BDM}_r(\mathcal{T}_h)$, $\sigma \in V_h^r$, and $q \in V_h^{r-1} \cap L_{f=0}^2(\Omega)$, with

$$u_{k+1/2} = \frac{u_k + u_{k+1}}{2}, \quad \rho_{k+1/2} = \frac{\rho_k + \rho_{k+1}}{2}$$

$$(\rho u)_{k+1/2} = \frac{\rho_k u_k + \rho_{k+1} u_{k+1}}{2}.$$

Then, the solution satisfies, for all k , the conservative properties

$$\int_{\Omega} \rho_{k+1} dx = \int_{\Omega} \rho_k dx, \quad \int_{\Omega} \rho_{k+1}^2 dx = \int_{\Omega} \rho_k^2 dx,$$

$$\int_{\Omega} \frac{1}{2} \rho_{k+1} |u_{k+1}|^2 dx = \int_{\Omega} \frac{1}{2} \rho_k |u_k|^2 dx, \quad \operatorname{div} u_k = 0.$$

5. RAYLEIGH-TAYLOR INSTABILITY

For this test, we consider a fully (or baroclinic) compressible fluid, whose energy depends on both the mass density ρ and the entropy density s . The Lagrangian is

$$\ell(u, \rho, s) = \int_{\Omega} \left[\frac{1}{2} \rho |u|^2 - \rho e(\rho, \eta) - \rho \phi \right] dx, \quad (27)$$

where $\eta = \frac{s}{\rho}$ is the specific entropy. We take e equal to the internal energy for a perfect gas $e(\rho, \eta) = K e^{\eta/C_v} \rho^{\gamma-1}$, where $\gamma = 5/3$ and $K = C_v = 1$, and we use a gravitational potential $\phi = -y$, which corresponds to an upward gravitational force. The developments recalled in §4 can be adapted to this case by including the entropy density as an additional advected quantity. We initialize

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

$$u(x, y, 0) = \left(0, -\frac{1}{40} \sqrt{\frac{\gamma p(x, y)}{\rho(x, y, 0)}} \cos(8\pi x) e^{-\frac{(y-0.5)^2}{0.09}}\right),$$

$$s(x, y, 0) = C_v \rho(x, y, 0) \log\left(\frac{p(x, y)}{(\gamma - 1)K \rho(x, y, 0)^\gamma}\right),$$

where

$$p(x, y) = 1.5y + 1.25 + (0.25 - 0.5y) \tanh\left(\frac{y - 0.5}{0.02}\right).$$

We implemented our variational finite element scheme with $\Delta t = 0.01$ and with the finite element spaces $R_h = \text{RT}_0(\mathcal{T}_h)$ and V_h^1 on a uniform triangulation \mathcal{T}_h of $\Omega = (0, 1/4) \times (0, 1)$ with maximum element diameter $h = 2^{-8}$. We incorporated upwinding by using the strategy detailed in Gawlik and Gay-Balmaz (2020b), which retains the scheme's energy-preserving property. We programmed the scheme using the finite element software package FEniCS, Alnaes et al. (2015). Plots of the computed mass density at various times t are shown in Fig. 1, which shows that all the typical characteristics of the Rayleigh-Taylor instability are faithfully represented. Total energy was checked to be preserved exactly up to roundoff errors during the whole instability test.

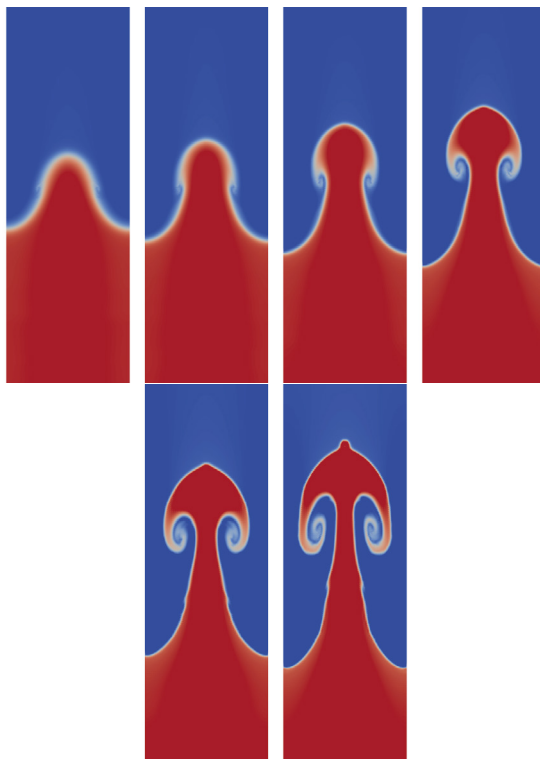


Fig. 1. Contours of the mass density at $t = 1.0, 1.2, 1.4, 1.6, 1.8, 2.0$ in the Rayleigh-Taylor instability simulation.

REFERENCES

- M. S. Alnaes, J. Blechta, J. Hake, A. Johansson, B. Kehlet, A. Logg, C. Richardson, J. Ring, M. E. Rognes, and G. N. Wells. The FEniCS Project Version 1.5. *Archive of Numerical Software*, 3, 2015.
- W. Bauer and F. Gay-Balmaz. Towards a geometric variational discretization of compressible fluids: the rotating shallow water equations. *J. Comp. Dyn.*, 16(1), 1–37, 2019.
- E. S. Gawlik and F. Gay-Balmaz. A conservative finite element method for the incompressible Euler equations with variable density. *J. Comp. Phys.* 412, 109439, 2020.
- E. S. Gawlik and F. Gay-Balmaz. A variational finite element discretization of compressible flow. *Found. Comput. Math.*, 2020.
- J. Guzman, C. W. Shu, and A. Sequeira. H(div) conforming and DG methods for incompressible Euler's equations. *IMA J. Num. Anal.*, 37(4), 1733–71, 2016.
- E. Hairer, C. Lubich, and G. Wanner. *Geometric Numerical Integration: Structure-Preserving Algorithms for Ordinary Differential Equations*. Springer Series in Computational Mathematics, 31, Springer-Verlag, 2006.
- B. Liu, G. Mason, J. Hodgson, Y. Tong and M. Desbrun. Model-reduced variational fluid simulation. *ACM Trans. Graph. (SIG Asia)*, 34, Art. 244, 2015.
- J. E. Marsden and M. West. Discrete mechanics and variational integrators. *Acta Numer.*, 10, 357–514, 2001.
- A. Natale and C. Cotter. A variational H(div) finite-element discretization approach for perfect incompressible fluids. *IMA J. Num. Anal.*, 38(2), 1084, 2018.
- D. Pavlov, P. Mullen, Y. Tong, E. Kanso, J. E. Marsden and M. Desbrun. Structure-preserving discretization of incompressible fluids. *Physica D*, 240, 443–458, 2010.