Low-dissipation finite element strategy for low Mach number reacting flows

A. Both^{a,*}, O. Lehmkuhl^a, D. Mira^a, M. Ortega^b

^a*Barcelona Supercomputing Center (BSC), Barcelona, Spain*

^b*Universitat Politècnica de Catalunya (UPC), ESEIAAT, Terrassa, Barcelona, Spain*

Abstract

The present paper extends the conservative finite element convective scheme proposed by Charnyi et al. (Journal of Computational Physics 337, 2017, 289 - 308) originally formulated for incompressible flows to the low Mach regime. Similar to Lehmkuhl et al. (Journal of Computational Physics 390, 2019, 51 - 65) stabilisation is only introduced for the continuity equation by means of a non-incremental fractional-step method, modified in order to account for variable density flows. The final scheme preserves momentum and angular momentum for variable density flows. The error of kinetic energy conservation is of order $\mathcal{O}(\delta t h^{k+1})$, thus dissipation is limited. Standard stabilised finite elements are used for the scalars. Time integration is carried out by means of an explicit third order Runge-Kutta scheme for all equations. The proposed strategy is tested on a set of relevant cases with available reference data using large-eddy simulations. First, an anisothermal turbulent channel flow is assessed. Later, a technically premixed turbulent flame in a swirl-stabilized configuration is considered. And finally, a turbulent jet

*Corresponding author

Email address: `ambrus.both@bsc.es` (A. Both)

diffusion flame in a low-velocity co-flow has been studied. In all cases the performance of the presented low Mach formulation is fairly good, showing better accuracy than skew-symmetric like strategies.

Keywords: Low Mach, Finite element, Large-eddy simulation, Combustion, Low dissipation schemes

1. Introduction

Modelling of combustion problems of practical interest is a complex task as it involves the solution of chemically reactive flows interacting with turbulence. The multicomponent flow is characterised by high density ratios as a consequence of heat release and the kinetic energy has to be correctly dissipated by viscous forces [1]. This aspect motivates the seek for low-dissipation strategies that can be used to solve turbulent reactive flow calculations with high accuracy.

In practice, flame propagation is typically a slow process, thus the flow velocities are kept moderate to ensure flame stability, and to provide sufficient residence time for the reactions to complete. These processes are characterised by moderate to high Reynolds numbers, but usually take place at low Mach numbers, for instance stationary gas turbines or aero-engines operate at these conditions [2, 3]. Thus, it is known, that turbulence has a strong effect on the flow, but compressibility can be negligible when the burners operate at these conditions. Therefore, low Mach number approximations of the Navier-Stokes equations are commonly used to model the flow on these applications, since they can be solved more efficiently from the numerical point of view.

20 It has been demonstrated that large-eddy simulation (LES) is a powerful
21 tool for solving problems of industrial interest, and it has been extensively
22 applied in the numerical analysis of turbulent reacting flows at the low Mach
23 number limit. LES addresses highly unsteady phenomena that characterises
24 these turbulent problems. It has been successfully applied using different
25 combustion models on various reactive cases [1, 2, 4]. A collective require-
26 ment for the numerical methods irrespective of the choice of combustion
27 model, is the accurate prediction of the velocity field, since advection plays
28 a major role in the transport of the reacting components.

29 One of the key aspects in achieving high-fidelity predictions of the veloc-
30 ity field, is the formulation of the discrete operator applied for the convective
31 transport of momentum. This topic has been extensively studied in incom-
32 pressible [5, 6, 7] and compressible [8, 9, 10, 11, 12] flows likewise. The
33 different operators are characterised by whether they inherently adhere to
34 the conservation of physical quantities like kinetic energy, or momentum.
35 More specifically, in the case of finite elements, it is well established, that
36 kinetic energy conservation can be ensured by devising the convective term
37 of the momentum equation such, that it preserves skew-symmetry at the dis-
38 crete level [13]. Charnyi et al. [5] introduced a discretization strategy for
39 this term, that ensures the conservation of linear and angular momentum
40 besides kinetic energy. Their method is developed for incompressible flows
41 using mixed finite elements to stabilise pressure. Recently, this method has
42 been extended to equal order finite elements by Lehmkuhl et al. [14] and
43 it has been tested in fully turbulent incompressible flows with success. Re-
44 cently Coppola et al. [12] classified a family of commonly used discretization

45 strategies that stem from the splitting of the convective term. The present
 46 paper uses a different splitting method detailed below.

47 This study further extends the energy, momentum, and angular momen-
 48 tum conserving (EMAC) scheme to the low Mach regime. The underlying
 49 idea is to use a change of variables to preserve the fundamental properties
 50 of the incompressible implementation. In this case $\mathbb{A} \equiv \sqrt{\rho}\mathbf{u}$ is used in or-
 51 der to express the momentum flux as a vector product of two equal terms:
 52 $\rho\mathbf{u} \otimes \mathbf{u} = \mathbb{A} \otimes \mathbb{A}$. Such $\sqrt{\rho}$ formalism, appears in many studies related to
 53 variable density flows. Van Driest [15] introduced a scaling law for turbulent
 54 thermal boundary layers applying this transformation. Various studies used
 55 the formalism to study the effects of compressibility on forced and decaying
 56 turbulence in ideal gas [16, 17, 18]. More recently Rozema et al. [11] devel-
 57 oped a conservative discretization scheme for compressible flows using finite
 58 volume method by using a $\sqrt{\rho}$ formalism in the state vector. In the present
 59 study we introduce a scheme, where the transport of $\mathbb{A}$ is not required.

60 Similar to Lehmkuhl et al. [14] the pressure stabilization is done with
 61 a non-incremental fractional-step method, however here, the approach of
 62 Nicoud [8] is used to incorporate variable density effects. Scalar equations
 63 are solved by means of stabilised finite elements to describe the thermo-
 64 chemical state of the fluid. The final set of equations is time integrated using
 65 an explicit third order Runge-Kutta method.

66 The next section introduces the low Mach equations in the weak form, fol-
 67 lowed by the derivation of the EMAC formulation for variable density flows.
 68 Then, we present a comprehensive analysis of the conservation properties of
 69 the EMAC operator in thermally coupled flows. In the results section, we test

70 the developed scheme in representative cases of thermal flows with increased
71 complexity: a fully developed channel flow with different temperature walls,
72 a turbulent premixed swirling flame, and a non-premixed jet flame. Finally,
73 conclusions are drawn.

74 2. Low Mach number approximation

75 In the low Mach number limit, the fully compressible Navier-Stokes equa-
76 tions can be simplified to decouple the thermochemical state of the flow
77 from the momentum equation [19]. This splitting technique removes the
78 acoustic modes forcing the flow to behave as incompressible, where the den-
79 sity can change due to temperature and composition variations. This can
80 be achieved by a decomposition of the pressure into a spatially homoge-
81 neous thermodynamic pressure, and a hydrodynamic pressure: $P(x, y, z, t) =$
82 $P_0(t) + p(x, y, z, t)$.

The thermodynamic pressure $P_0(t)$ is used in the equation of state, such
as the ideal gas law:

$$\rho = P_0 \frac{W}{R_u T}, \quad (1)$$

where W , R_u and T represent the molecular weight, specific gas constant and
temperature respectively. The hydrodynamic pressure $p(x, y, z, t)$ is used in
the momentum equation and is determined by mass conservation. In closed
domains, the thermodynamic pressure is time dependent such, that global
mass conservation is ensured. In the case of the ideal gas law, the temporal
evolution of thermodynamic pressure is calculated as:

$$P_0(t) = \frac{M_{t_0} R_u}{\int_{\Omega} \frac{W}{T} dV}, \quad (2)$$

83 where $M_{t_0} = \int_{\Omega} \rho dV$ is the initial mass in the domain. In open domains, the
 84 thermodynamic pressure is a known constant.

Considering a fluid flow in the low Mach number regime with variable composition, the problem consists of finding a velocity $\mathbf{u}$, a hydrodynamic pressure p , and scalars ξ_k in domain Ω with boundary Γ for the time interval (t_0, t_f) . In conservative form:

$$\partial_t \rho + \nabla \cdot (\rho \mathbf{u}) = 0 \quad \text{on } \Omega \times (t_0, t_f), \quad (3)$$

$$\partial_t (\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) + \nabla p - \nabla \cdot \boldsymbol{\tau}(\mathbf{u}) = \mathbf{f} \quad \text{on } \Omega \times (t_0, t_f), \quad (4)$$

$$\partial_t (\rho \xi_k) + \nabla \cdot (\rho \xi_k \mathbf{u}) + \nabla \cdot \boldsymbol{\Phi}_k = S_k \quad \text{on } \Omega \times (t_0, t_f), \quad (5)$$

85 where $\boldsymbol{\tau}(\mathbf{u}) = 2\mu \mathbf{S}^D(\mathbf{u})$ is the viscous stress tensor with the deviatoric part
 86 of the strain rate: $\mathbf{S}^D(\mathbf{u}) = \frac{1}{2}(\nabla \mathbf{u} + \nabla^T \mathbf{u}) - \frac{1}{3}(\nabla \cdot \mathbf{u})\mathbf{I}$, $\mathbf{f}$ is the body force,
 87 and $\boldsymbol{\Phi}_k = -\rho D_k \nabla \xi_k$ and S_k are the molecular flux and volumetric source
 88 term of scalar k respectively. The system is closed using the equation of
 89 state (1). The temperature T , the molecular weight W , the dynamic viscos-
 90 ity μ , and the diffusivity D_k are known functions of the solved scalars ξ_k .
 91 The selection of transported scalars depends on the physics of the problem
 92 and will be introduced in the application cases. Note, that for the ideal
 93 gas law considered here, the density only depends on these scalars and the
 94 thermodynamic pressure.

The problem has to be appended with appropriate initial and boundary conditions. The initial conditions are:

$$\mathbf{u} = \mathbf{u}_0, \quad \xi_k = \xi_{k,0} \quad \text{on } \Omega \times \{t_0\} \quad (6)$$

and

$$P_0 = P_0^0 \quad (\text{for closed systems}). \quad (7)$$

Dirichlet and Neumann boundary conditions are defined for the velocity $\mathbf{u}$ on $\Gamma_{\mathbf{u},D}$ and $\Gamma_{\mathbf{u},N}$, and for the k^{th} scalar ξ_k on $\Gamma_{\xi_k,D}$ and $\Gamma_{\xi_k,N}$ respectively such, that $\Gamma_{\mathbf{u},D} \cup \Gamma_{\mathbf{u},N} = \Gamma$ and $\Gamma_{\xi_k,D} \cup \Gamma_{\xi_k,N} = \Gamma$,

$$\mathbf{u} = \mathbf{u}_D \quad \text{on } \Gamma_{\mathbf{u},D} \times (t_0, t_f), \quad (8)$$

$$(-p\mathbf{I} + \boldsymbol{\tau}(\mathbf{u})) \cdot \mathbf{n} = 0 \quad \text{on } \Gamma_{\mathbf{u},N} \times (t_0, t_f), \quad (9)$$

$$\xi_k = \xi_{k,D} \quad \text{on } \Gamma_{\xi_k,D} \times (t_0, t_f), \quad (10)$$

$$\nabla \xi_k \cdot \mathbf{n} = 0 \quad \text{on } \Gamma_{\xi_k,N} \times (t_0, t_f). \quad (11)$$

95 The following definitions are needed to obtain the weak form of the gov-
 96 erning equations. $\mathbf{V}_D = \mathbf{H}_D^1(\Omega)$, $\mathbf{V}_0 = \mathbf{H}_0^1(\Omega)$, $Q = L^2(\Omega)/\mathfrak{R}$, $E_{D,k} =$
 97 $H_D^1(\Omega)$, and $E_{0,k} = H_0^1(\Omega)$ are introduced, where $L^2(\Omega)$ is the square inte-
 98 grable function space. $H^1(\Omega)$ is a subspace of $L^2(\Omega)$, such that the deriva-
 99 tives of functions in $H^1(\Omega)$ are elements of $L^2(\Omega)$. Finally the 0 and D
 100 subscripts mark the subspace of $H^1(\Omega)$ that is constant 0 on the boundary
 101 Γ , or satisfy the Dirichlet conditions on boundary Γ respectively. $\mathbf{H}_0^1(\Omega)$ and
 102 $\mathbf{H}_D^1(\Omega)$ are their 2 or 3 dimensional vector counterparts. $(\cdot, \cdot)$ is the L^2 inner
 103 product.

For temporally evolving problems, the above mentioned function spaces are extended with a temporal component: $\mathbf{V}_t \equiv L^2(t_0, t_f; \mathbf{V}_D)$, $Q_t \equiv \mathcal{D}'(t_0, t_f; Q)$, and $E_{t,k} \equiv L^2(t_0, t_f; E_{D,k})$, where $L^p(t_0, t_f; X)$ is the space of time dependent functions in a normed space X such that $\int_{t_0}^{t_f} \|f\|_X^p dt < \infty$, $1 \leq p \leq \infty$, and Q_t consists of mappings whose Q -norm is a distribution in time. The weak form of equations (3), (4), and (5) is defined as: find $\mathbf{u} \in \mathbf{V}_t$, $p \in Q_t$,

and $\xi_k \in E_{t,k}$ such that:

$$(\partial_t \rho, q) + (\nabla \cdot (\rho \mathbf{u}), q) = 0, \quad (12)$$

$$(\partial_t (\rho \mathbf{u}), \mathbf{v}) + (C(\rho, \mathbf{u}), \mathbf{v}) - (p, \nabla \cdot \mathbf{v}) + (\boldsymbol{\tau}(\mathbf{u}), \nabla \mathbf{v}) = (\mathbf{f}, \mathbf{v}), \quad (13)$$

$$(\partial_t (\rho \xi_k), \eta_k) + (\nabla \cdot (\rho \xi_k \mathbf{u}), \eta_k) + (\rho D_k \nabla \xi_k, \nabla \eta_k) = (S_k, \eta_k), \quad (14)$$

for all $(q, \mathbf{v}, \eta_k) \in Q_0 \times \mathbf{V}_0 \times E_{0,k}$, where $C(\rho, \mathbf{u})$ is the convective term of the momentum equation.

3. Convection of momentum in variable density flows

The discretization strategy of $C(\rho, \mathbf{u})$ is a critical feature of flow simulation algorithms, since the convection term should not introduce numerical dissipation [14]. A widely used discretized form for this term is the skew-symmetric formulation, which is preferred for its kinetic energy conserving nature,

$$C_{skew}(\rho, \mathbf{u}) = (\rho \mathbf{u} \cdot \nabla) \mathbf{u} + \frac{1}{2} (\nabla \cdot (\rho \mathbf{u})) \mathbf{u}. \quad (15)$$

Below we extend the Energy, Momentum, and Angular momentum Conserving (EMAC) formulation of Charnyi et al. [5] to variable density flows. The following definitions are used: For $\mathbf{u}, \mathbf{v}, \mathbf{w} \in \mathbf{H}^1(\Omega)$ we define the trilinear form $b : \mathbf{H}^1(\Omega) \times \mathbf{H}^1(\Omega) \times \mathbf{H}^1(\Omega) \rightarrow \mathbb{R}$ as:

$$b(\mathbf{u}, \mathbf{v}, \mathbf{w}) = (\mathbf{u} \cdot \nabla \mathbf{v}, \mathbf{w}). \quad (16)$$

The following identities hold assuming $\mathbf{u} \in \mathbf{H}_0^1(\Omega)$. They follow directly from integration by parts,

$$b(\mathbf{u}, \mathbf{v}, \mathbf{w}) = -b(\mathbf{u}, \mathbf{w}, \mathbf{v}) - ((\nabla \cdot \mathbf{u}) \mathbf{v}, \mathbf{w}), \quad (17)$$

$$b(\mathbf{u}, \mathbf{w}, \mathbf{w}) = -\frac{1}{2} ((\nabla \cdot \mathbf{u}) \mathbf{w}, \mathbf{w}). \quad (18)$$

Furthermore, by definition, the trilinear form can be also written as:

$$b(\mathbf{u}, \mathbf{v}, \mathbf{w}) = ((\nabla \mathbf{v}) \mathbf{u}, \mathbf{w}) = \left((\nabla \mathbf{v})^T \mathbf{w}, \mathbf{u} \right). \quad (19)$$

Additionally the symmetric part of the gradient is denoted as $\nabla_s \mathbf{u} \equiv \mathbf{D}(\mathbf{u}) = \frac{\nabla \mathbf{u} + (\nabla \mathbf{u})^T}{2}$, while the skew-symmetric part is: $\nabla_n \mathbf{u} \equiv \frac{\nabla \mathbf{u} - (\nabla \mathbf{u})^T}{2}$. For $\mathbf{u}, \mathbf{v} \in \mathbf{H}^1(\Omega)$ the following holds,

$$(\nabla_n \mathbf{u}) \mathbf{v} = \frac{1}{2} (\nabla \times \mathbf{u}) \times \mathbf{v}, \quad (20)$$

$$(\mathbf{u} \cdot \nabla) \mathbf{u} = (\nabla \times \mathbf{u}) \times \mathbf{u} + \frac{1}{2} \nabla |\mathbf{u}|^2, \quad (21)$$

$$(\nabla \mathbf{u}) \mathbf{u} = (\nabla_s \mathbf{u}) \mathbf{u} + (\nabla_n \mathbf{u}) \mathbf{u} = \mathbf{D}(\mathbf{u}) \mathbf{u} + \frac{1}{2} (\nabla \times \mathbf{u}) \times \mathbf{u}. \quad (22)$$

Furthermore (22) implies that,

$$(\mathbf{D}(\mathbf{u}) \mathbf{u}, \mathbf{u}) = ((\nabla \mathbf{u}) \mathbf{u}, \mathbf{u}) = b(\mathbf{u}, \mathbf{u}, \mathbf{u}). \quad (23)$$

Using (20), (21), and (22) we get,

$$(\mathbf{u} \cdot \nabla) \mathbf{u} = 2\mathbf{D}(\mathbf{u}) \mathbf{u} - \frac{1}{2} \nabla |\mathbf{u}|^2. \quad (24)$$

Next we introduce the notation $\mathbb{A} \equiv \sqrt{\rho} \mathbf{u}$. This change of variables allows us to preserve the symmetric properties used in the incompressible formulation of Charnyi et al. [5]. The nonlinear term can be written as:

$$C = \nabla \cdot (\mathbb{A} \otimes \mathbb{A}) = (\nabla \cdot \mathbb{A}) \mathbb{A} + (\mathbb{A} \cdot \nabla) \mathbb{A}. \quad (25)$$

Using (24) yields the proposed EMAC formulation for variable density flows,

$$C_{emac}(\rho, \mathbf{u}) \equiv 2\mathbf{D}(\mathbb{A}) \mathbb{A} + (\nabla \cdot \mathbb{A}) \mathbb{A} - \frac{1}{2} \nabla |\mathbb{A}|^2. \quad (26)$$

107 These two discretizations of the convective term will be considered for
 108 analysis in turbulent conditions for flows with variable density and composi-
 109 tion.

110 4. Conservation properties

111 This section presents an analysis of the conservation properties of the
 112 convective operators described above also referred as skew-symmetric and
 113 EMAC respectively.

114 4.1. Kinetic energy

The kinetic energy is defined as: $E = \frac{1}{2}(\rho \mathbf{u}, \mathbf{u}) = \frac{1}{2} \int_{\Omega} \rho |\mathbf{u}|^2 d\Omega$. We formulate the equation of kinetic energy conservation using the weak form of the momentum equation. Testing (13) with $\mathbf{v} = \mathbf{u}$ yields:

$$(\partial_t(\rho \mathbf{u}), \mathbf{u}) + (C(\rho, \mathbf{u}), \mathbf{u}) - (p, \nabla \cdot \mathbf{u}) + (\boldsymbol{\tau}(\mathbf{u}), \nabla \mathbf{u}) = (\mathbf{f}, \mathbf{u}). \quad (27)$$

The pressure term of (27) expresses the volumetric work of the hydrodynamic pressure, which vanishes in the incompressible limit and corresponds to the work of dilatation otherwise. (E.g.: the flow accelerating due to heat release.) This can be shown by reformulating the continuity equation (3) as:

$$\left(\frac{1}{\rho} (\partial_t \rho + \mathbf{u} \cdot \nabla \rho), q \right) = - (q, \nabla \cdot \mathbf{u}). \quad (28)$$

Testing (28) with $q = p$ and introducing the notation of material derivative $\frac{D\rho}{Dt} = \partial_t \rho + \mathbf{u} \cdot \nabla \rho$ gives the term:

$$- (p, \nabla \cdot \mathbf{u}) = \left(\frac{1}{\rho} \frac{D\rho}{Dt}, p \right). \quad (29)$$

Using the common interpretation of the material derivative, this expression indicates, that if the density of fluid particles change, the hydrodynamic pressure is doing work on the fluid. From (27) the temporal evolution of the

total kinetic energy in the domain Ω is:

$$\frac{1}{2} \frac{d}{dt} \|\rho \mathbf{u}^2\| = - (C(\rho, \mathbf{u}), \mathbf{u}) - \left(\frac{1}{\rho} \frac{D\rho}{Dt}, p \right) - (2\mu \mathbf{S}^D(\mathbf{u}), \nabla \mathbf{u}) + (\mathbf{f}, \mathbf{u}). \quad (30)$$

115 To study the effect of the discretization strategy on the kinetic energy trans-
 116 port we consider a non-reacting ($\frac{D\rho}{Dt} = 0$), inviscid ($\mu = 0$) flow without body
 117 force ($\mathbf{f} = \mathbf{0}$) on a periodic domain. Thus the kinetic energy over the whole
 118 periodic domain is preserved by the convective operator if: $(C(\rho, \mathbf{u}), \mathbf{u}) = 0$.

We can prove that the skew-symmetric formulation of the convective term is kinetic energy preserving, by using (18) to get,

$$\begin{aligned} (C_{skew}(\rho, \mathbf{u}), \mathbf{u}) &= ((\rho \mathbf{u} \cdot \nabla) \mathbf{u}, \mathbf{u}) + \left(\frac{1}{2} (\nabla \cdot (\rho \mathbf{u})) \mathbf{u}, \mathbf{u} \right) \\ &= b(\rho \mathbf{u}, \mathbf{u}, \mathbf{u}) - b(\rho \mathbf{u}, \mathbf{u}, \mathbf{u}) = 0. \end{aligned} \quad (31)$$

For the EMAC formulation the proof is the following:

$$(C_{emac}(\rho, \mathbf{u}), \mathbf{u}) = 2 \left(\mathbf{D}(\mathbb{A}) \mathbb{A}, \frac{\mathbb{A}}{\sqrt{\rho}} \right) + \left((\nabla \cdot \mathbb{A}) \mathbb{A}, \frac{\mathbb{A}}{\sqrt{\rho}} \right) - \left(\frac{1}{2} \nabla |\mathbb{A}|^2, \frac{\mathbb{A}}{\sqrt{\rho}} \right). \quad (32)$$

The first term of (32) is transformed using (19) and the definition of the trilinear form,

$$\begin{aligned} 2 \left(\mathbf{D}(\mathbb{A}) \mathbb{A}, \frac{\mathbb{A}}{\sqrt{\rho}} \right) &= \left((\nabla \mathbb{A}) \mathbb{A}, \frac{\mathbb{A}}{\sqrt{\rho}} \right) + \left((\nabla \mathbb{A})^T \frac{\mathbb{A}}{\sqrt{\rho}}, \mathbb{A} \right) \\ &= 2b \left(\mathbb{A}, \mathbb{A}, \frac{\mathbb{A}}{\sqrt{\rho}} \right) = 2 \left((\mathbb{A} \cdot \nabla) \mathbb{A}, \frac{\mathbb{A}}{\sqrt{\rho}} \right) \\ &= 2 \left((\mathbb{A} \cdot \nabla) \frac{\mathbb{A}}{\sqrt[4]{\rho}} \frac{\mathbb{A}}{\sqrt[4]{\rho}} \right) = 2b \left(\mathbb{A}, \frac{\mathbb{A}}{\sqrt[4]{\rho}}, \frac{\mathbb{A}}{\sqrt[4]{\rho}} \right). \end{aligned} \quad (33)$$

Using (18) the second term of (32) is:

$$\left((\nabla \cdot \mathbb{A}) \mathbb{A}, \frac{\mathbb{A}}{\sqrt{\rho}} \right) = \left((\nabla \cdot \mathbb{A}) \frac{\mathbb{A}}{\sqrt[4]{\rho}}, \frac{\mathbb{A}}{\sqrt[4]{\rho}} \right) = -2b \left(\mathbb{A}, \frac{\mathbb{A}}{\sqrt[4]{\rho}}, \frac{\mathbb{A}}{\sqrt[4]{\rho}} \right). \quad (34)$$

119 Finally the last term of (32) is zero on the periodic domain, as it is the
 120 volume integral of the gradient of a scalar. Thus the EMAC formulation is
 121 kinetic energy conserving: $(C_{emac}(\rho, \mathbf{u}), \mathbf{u}) = 0$.

122 4.2. Momentum

The linear momentum is defined as: $\mathbf{M} = \int_{\Omega} \rho \mathbf{u} d\Omega$. To prove its conservation, we are testing (12) and (13) with $\mathbf{v} = \chi(\mathbf{e}_i)$ and $q = 0$, where $\chi(\mathbf{e}_i)$ is a function such that:

$$\chi(\mathbf{e}_i) = \begin{cases} \mathbf{e}_i & \text{on } \hat{\Omega}, \\ \mathbf{g} \in \mathbf{H}_0^1(\Omega) & \text{on } S = \Omega \setminus \hat{\Omega}, \end{cases} \quad (35)$$

where $\mathbf{g}$ is an arbitrary function satisfying zero boundary conditions, and $\hat{\Omega}$ is a strictly interior subdomain. Testing with this function yields,

$$(\partial_t(\rho \mathbf{u}), \mathbf{e}_i) + (C(\rho, \mathbf{u}), \mathbf{e}_i) - (p, \nabla \cdot \mathbf{e}_i) + (\boldsymbol{\tau}(\mathbf{u}), \nabla \mathbf{e}_i) = (\mathbf{f}, \mathbf{e}_i). \quad (36)$$

The terms $(p, \nabla \cdot \mathbf{e}_i)$ and $(\boldsymbol{\tau}(\mathbf{u}), \nabla \cdot \mathbf{e}_i)$ vanish, as $\mathbf{e}_i$ is constant. Thus (36) simplifies to:

$$\frac{d}{dt}(\rho \mathbf{u}, \mathbf{e}_i) + (C(\rho, \mathbf{u}), \mathbf{e}_i) = (\mathbf{f}, \mathbf{e}_i), \quad (37)$$

and linear momentum is conserved if $(\mathbf{f}, \mathbf{e}_i) = 0$ and $(C(\rho, \mathbf{u}), \mathbf{e}_i) = 0$. Latter term in the skew-symmetric formulation is non-zero. Using (17), the definition of the trilinear form, and the fact that the derivatives of $\mathbf{e}_i$ are

zero, we get:

$$\begin{aligned}
(C_{skew}(\rho, \mathbf{u}), \mathbf{e}_i) &= ((\rho \mathbf{u} \cdot \nabla) \mathbf{u}, \mathbf{e}_i) + \left(\frac{1}{2} (\nabla \cdot (\rho \mathbf{u})) \mathbf{u}, \mathbf{e}_i\right) \\
&= b(\rho \mathbf{u}, \mathbf{u}, \mathbf{e}_i) + \frac{1}{2} ((\nabla \cdot (\rho \mathbf{u})) \mathbf{u}, \mathbf{e}_i) \\
&= -b(\rho \mathbf{u}, \mathbf{e}_i, \mathbf{u}) - \frac{1}{2} ((\nabla \cdot (\rho \mathbf{u})) \mathbf{u}, \mathbf{e}_i) \\
&= -\frac{1}{2} ((\nabla \cdot (\rho \mathbf{u})) \mathbf{u}, \mathbf{e}_i) \neq 0,
\end{aligned} \tag{38}$$

hence the skew-symmetric formulation does not conserve linear momentum. For the EMAC formulation the momentum conservation is proven as follows,

$$(C_{emac}(\rho, \mathbf{u}), \mathbf{e}_i) = 2(\mathbf{D}(\mathbb{A}) \mathbb{A}, \mathbf{e}_i) + ((\nabla \cdot \mathbb{A}) \mathbb{A}, \mathbf{e}_i) - \left(\frac{1}{2} \nabla |\mathbb{A}|^2, \mathbf{e}_i\right). \tag{39}$$

The first term of (39) is rearranged using (17) and (19),

$$\begin{aligned}
2(\mathbf{D}(\mathbb{A}) \mathbb{A}, \mathbf{e}_i) &= ((\nabla \mathbb{A}) \mathbb{A}, \mathbf{e}_i) + \left((\nabla \mathbb{A})^T \mathbb{A}, \mathbf{e}_i\right) \\
&= b(\mathbb{A}, \mathbb{A}, \mathbf{e}_i) + b(\mathbf{e}_i, \mathbb{A}, \mathbb{A}) \\
&= -b(\mathbb{A}, \mathbf{e}_i, \mathbb{A}) - ((\nabla \cdot \mathbb{A}) \mathbb{A}, \mathbf{e}_i) - \frac{1}{2} ((\nabla \cdot \mathbf{e}_i) \mathbb{A}, \mathbb{A}) \\
&= -((\nabla \cdot \mathbb{A}) \mathbb{A}, \mathbf{e}_i),
\end{aligned} \tag{40}$$

123 which cancels the second term. While the third term of (39) is constant 0 on
124 a periodic domain using integration by parts. Thus, it is proved the EMAC
125 formulation conserves linear momentum: $(C_{emac}(\rho, \mathbf{u}), \mathbf{e}_i) = 0$.

126 4.3. Angular momentum

The angular momentum is defined as: $\mathbf{M}_{\mathbf{x}} = \int_{\Omega} \rho \mathbf{u} \times \mathbf{x} d\Omega$, where $\mathbf{x}$ is the position vector. We are testing (12) and (13) with $\mathbf{v} = \chi(\phi_i)$ and $q = 0$, where $\phi_i \equiv \mathbf{x} \times \mathbf{e}_i$,

$$(\partial_t(\rho \mathbf{u}), \phi_i) + (C(\rho, \mathbf{u}), \phi_i) - (p, \nabla \cdot \phi_i) + (\boldsymbol{\tau}(\mathbf{u}), \nabla \phi_i) = (\mathbf{f}, \phi_i). \tag{41}$$

The pressure term vanishes since $\nabla \cdot \phi_i = 0$, and in inviscid cases without source terms the requirement for angular momentum conservation is $(C(\rho, \mathbf{u}), \phi_i) = 0$, similarly to above. For the skew-symmetric formulation, using the same arguments as for (40) yields:

$$(C_{skew}(\rho, \mathbf{u}), \phi_i) = -\frac{1}{2}((\nabla \cdot (\rho \mathbf{u})) \mathbf{u}, \phi_i) \neq 0, \quad (42)$$

thus the skew-symmetric formulation does not conserve angular momentum. For the EMAC formulation,

$$(C_{emac}(\rho, \mathbf{u}), \phi_i) = 2(\mathbf{D}(\mathbb{A})\mathbb{A}, \phi_i) + ((\nabla \cdot \mathbb{A})\mathbb{A}, \phi_i) - \left(\frac{1}{2}\nabla |\mathbb{A}|^2, \phi_i\right), \quad (43)$$

the last term is 0 by the same argument as for Linear momentum. The remaining terms can be transformed using (19), and (17),

$$\begin{aligned} (C_{emac}(\rho, \mathbf{u}), \phi_i) &= 2(\mathbf{D}(\mathbb{A})\mathbb{A}, \phi_i) + ((\nabla \cdot \mathbb{A})\mathbb{A}, \phi_i) \\ &= b(\mathbb{A}, \mathbb{A}, \phi_i) + b(\phi_i, \mathbb{A}, \mathbb{A}) + ((\nabla \cdot \mathbb{A})\mathbb{A}, \phi_i) \\ &= b(\mathbb{A}, \mathbb{A}, \phi_i) + ((\nabla \cdot \mathbb{A})\mathbb{A}, \phi_i) \\ &= -b(\mathbb{A}, \phi_i, \mathbb{A}) = 0, \end{aligned} \quad (44)$$

127 since $\nabla \cdot \phi_i = 0$. Thus, it is shown, that the EMAC operator conserves also
128 angular momentum.

129 5. Numerical methods

130 This section introduces a low-dissipation discretization strategy for vari-
131 able density flows in the low Mach number limit within the finite element con-
132 text. It includes the spatial discretization of the governing equations, where
133 the stabilization of the pressure in the momentum equation comes from the

134 numerical dissipation of the fractional step scheme [14], while stabilized-finite
 135 elements are used for scalar transport. An explicit third-order Runge-Kutta
 136 temporal scheme is used for the momentum and scalar transport.

137 5.1. Spacial discretization

Finite elements are used to construct the spacial discretization. The following piecewise linear subspaces are approximating the continuous subspaces: $\mathbf{V}_{D,h} \subset \mathbf{V}_D$, $\mathbf{V}_{0,h} \subset \mathbf{V}_0$, $Q_h \subset Q$, $E_{D,k,h} \subset E_{D,k}$, and $E_{0,k,h} \subset E_{0,k}$. The discretized problem is: find $\mathbf{u}_h^{n+1} \in \mathbf{V}_{D,h}$, $p_h^{n+1} \in Q_h$, and $\xi_{k,h}^{n+1} \in E_{D,k,h}$ such that:

$$(\partial_t \rho_h, q_h) + (\nabla \cdot (\rho_h \mathbf{u}_h), q_h) = 0, \quad (45)$$

$$\begin{aligned} (\partial_t (\rho_h \mathbf{u}_h), \mathbf{v}_h) + (C(\rho_h, \mathbf{u}_h), \mathbf{v}_h) - (p_h, \nabla \cdot \mathbf{v}_h) \\ + (\boldsymbol{\tau}(\mathbf{u}_h), \nabla \mathbf{v}_h) = (\mathbf{f}, \mathbf{v}_h), \end{aligned} \quad (46)$$

$$\begin{aligned} (\rho_h \partial_t \xi_{k,h}, \eta_{k,h}) + (\rho_h \mathbf{u}_h \cdot \nabla \xi_{k,h}, \eta_{k,h}) + (\rho D_k \nabla \xi_{k,h}, \nabla \eta_{k,h}) \\ + \sum_{e=1}^{n_{el}} \tau_e (\rho_h \mathbf{u}_h \cdot \nabla \xi_{k,h} + \nabla \cdot (\rho D_k \nabla \xi_{k,h}) - S_k, \mathbf{u}_h \cdot \nabla \eta_{k,h}) = (S_k, \eta_{k,h}), \end{aligned} \quad (47)$$

for all $(q_h, \mathbf{v}_h, \eta_{k,h}) \in Q_h \times \mathbf{V}_{0,h} \times E_{0,k,h}$. Note, that the scalars are transported using the advective form, and stabilization is introduced where n_{el} is the number of elements, and τ_e is a local timescale for the stabilization in accordance with Codina et al.[13]. The discretized equations are used in matrix form, hereafter,

$$\mathbf{M} \partial_t \mathcal{D} + \mathbf{D} [\mathcal{D} \mathbf{U}] = \mathbf{R}_c, \quad (48)$$

$$\mathbf{M} \mathbf{I} \partial_t [\mathcal{D} \mathbf{U}] + \mathbf{K}_m \mathbf{U} + \mathbf{G} \mathbf{P} = \mathbf{R}_m, \quad (49)$$

$$\mathbf{M} \mathcal{D} \partial_t \Xi_k + \mathbf{K}_k \Xi_k = \mathbf{R}_k. \quad (50)$$

138 We use a, b for the node indices, and i, j for the space indices. The shape
 139 function of node a is N^a . The following notation is adapted in matrix form:
 140 $\mathbf{M}^{ab} = (N^b, N^a)$ is the mass matrix of the elements, $\mathbf{D}_j^{ab} = (\partial_j N^b, N^a)$ is
 141 the discrete divergence operator, $\mathbf{G}_i^{ab} = -(N^b, \partial_i N^a)$ is the discrete gradient
 142 operator, and $\mathbf{I}_{ij} = \delta_{ij}$ is the identity tensor, with δ_{ij} being the Dirac-delta.
 143 $\mathcal{D}$, $\mathbf{U}$, $\mathbf{P}$, and Ξ_k stand for the matrices of density, velocity, pressure, and k^{th}
 144 scalar respectively.

$\mathbf{K}_m = \mathbf{K}_m^{\text{CONV}} + \mathbf{K}_m^{\text{VISC}}$ is the matrix of convective and viscous terms in the
 momentum equation. The viscous term is discretized as,

$$\mathbf{K}_m^{\text{VISC}ab} = (\boldsymbol{\tau}(N^b), \nabla N^a) \delta_{ij}, \quad (51)$$

while the convective term with the skew-symmetric and EMAC operators are
 respectively,

$$\mathbf{K}_{m,\text{skew}}^{\text{CONV}ab} = (\mathcal{D}\mathbf{U} \cdot \nabla N^b, N^a) \delta_{ij} + \frac{1}{2} ((\nabla \cdot (\mathcal{D}\mathbf{U})) N^b, N^a) \delta_{ij}, \quad (52)$$

$$\begin{aligned} \mathbf{K}_{m,\text{emac}}^{\text{CONV}ab} = & \sqrt{\mathcal{D}} [(\mathbb{A}_h \cdot \nabla N^b, N^a) \delta_{ij} + (\partial_i N^b \mathbb{A}_h^j, N^a) \\ & + ((\nabla \cdot \mathbb{A}_h) N^b, N^a) \delta_{ij} - \frac{1}{2} (\partial_i \mathbb{A}_h^j N^b, N^a)] . \end{aligned} \quad (53)$$

For the scalar transport, the convective and diffusive terms are repre-
 sented by $\mathbf{K}_k = \mathbf{K}_k^{\text{CONV}} + \mathbf{K}_k^{\text{DIFF}}$ matrix similarly. The two terms are discretized
 as,

$$\begin{aligned} \mathbf{K}_k^{\text{DIFF}ab} = & \mathcal{D} \mathcal{D}_k (\nabla N^b, \nabla N^a) \\ & - (\nabla (\mathcal{D} \mathcal{D}_k) \cdot \nabla N^b + \mathcal{D} \mathcal{D}_k \Delta N^b, \tau_e \mathbf{U} \cdot \nabla N^a), \end{aligned} \quad (54)$$

$$\mathbf{K}_k^{\text{CONV}ab} = \mathcal{D} (\mathbf{U} \cdot \nabla N^b, N^a) + \mathcal{D} (\mathbf{U} \cdot \nabla N^b, \tau_e \mathbf{U} \cdot \nabla N^a). \quad (55)$$

Note the stabilization terms are included in the matrix forms. The residuals of the equations are treated as,

$$\mathbf{R}_c^a = 0, \quad (56)$$

$$\mathbf{R}_{m_i}^a = \mathbf{f}_i N^a, \quad (57)$$

$$\mathbf{R}_k^a = S_k (N^a + \tau_e \mathbf{U} \cdot \nabla N^a). \quad (58)$$

145 5.2. Temporal discretization

The time integration of the discretised governing equations is done using the standard 3rd order Runge-Kutta scheme. For scalars, the ℓ^{th} Runge-Kutta substep ($\ell = 2..3$) is accomplished as:

$$\Xi_k^\ell = \Xi_k^n + \delta t (\mathbf{M}\mathcal{D}^n)^{-1} \sum_{m=1}^{\ell} a_{\ell m} (-\mathbf{K}_k^n \Xi_k^m + \mathbf{R}_k^n), \quad (59)$$

where δt is the time step. The complete time step uses the linear combination of the right-hand-sides of the substeps,

$$\Xi_k^{n+1} = \Xi_k^n + \delta t (\mathbf{M}\mathcal{D}^n)^{-1} \sum_{\ell=1}^s b_\ell (-\mathbf{K}_k^n \Xi_k^\ell + \mathbf{R}_k^n). \quad (60)$$

For the time marching of the velocity field, the fractional step method is incorporated in the Runge-Kutta steps. First the convective, viscous, and force terms are considered to calculate $\mathbf{U}^{\ell,*}$,

$$\mathbf{U}^{\ell,*} = \mathbf{U}^n + \delta t (\mathbf{M}\mathcal{I}\mathcal{D}^n)^{-1} \sum_{m=1}^{\ell} a_{\ell m} (-\mathbf{K}_m(\mathbf{U}^m, \mathcal{D}^n) \mathbf{U}^m + \mathbf{R}_m^n). \quad (61)$$

Then, the pressure equation is solved utilizing the discrete continuity equation (48) thus ensuring mass conservation,

$$\mathbf{D} [(\mathbf{M}\mathbf{I})^{-1} \mathbf{G}\Phi^\ell] = \frac{1}{c_\ell \delta t} (\mathbf{D} [\mathcal{D}^n \mathbf{U}^{\ell,*}] + \mathbf{M} \partial_t \mathcal{D}^\ell - \mathbf{R}_c^\ell), \quad (62)$$

where $\Phi = P + \mathcal{O}(\delta t)$ is the pseudo-pressure: a first order approximation of the pressure. Optionally the pseudo-pressure in the substep can be approximated using the method of Capuano et al.[20]. By omitting the solution of the Poisson equation (Eq.(62)) in the substeps, the computational time is reduced significantly. Finally the velocity field of the next substep is calculated as:

$$\mathbf{U}^\ell = \mathbf{U}^{\ell,*} - c_\ell \delta t (\text{MID}^n)^{-1} \mathbf{G}\Phi^\ell. \quad (63)$$

The complete Navier-Stokes time step is calculated similarly using the linear combination of the right-hand-sides to obtain $\mathbf{U}^{n+1,*}$. Note that the computed pseudo-pressure for the time-step ensures mass conservation.

$$\mathbf{U}^{n+1,*} = \mathbf{U}^n + \delta t (\text{MID}^n)^{-1} \sum_{\ell=1}^s b_\ell (-\mathbf{K}_m(\mathbf{U}^\ell, \mathcal{D}^n) \mathbf{U}^\ell + \mathbf{R}_m^n), \quad (64)$$

$$\text{D}[(\text{MI})^{-1} \mathbf{G}\Phi^{n+1}] = \frac{1}{\delta t} (\text{D}[\mathcal{D}^n \mathbf{U}^{n+1,*}] + \text{MI} \partial_t \mathcal{D}^{n+1} - \mathbf{R}_c^{n+1}), \quad (65)$$

$$\mathbf{U}^{n+1} = \mathbf{U}^{n+1,*} - \delta t (\text{MID}^n)^{-1} \mathbf{G}\Phi^{n+1}, \quad (66)$$

where $a_{\ell m}$, b_ℓ , and $c_\ell = \sum_m a_{\ell m}$ are the Runge-Kutta coefficients. The time derivative of the density is approximated based on the known values,

$$\partial_t \mathcal{D}^{n+1} = \frac{\mathcal{D}^n - \mathcal{D}^{n-1}}{\delta t}. \quad (67)$$

146 5.3. Approximation of the discrete Laplacian

As the use of the discrete Laplacian $(\text{D}(\text{MI})^{-1} \mathbf{G})$ is a rather expensive operation, the use of an approximated Laplacian can reduce substantially the computational cost of the algorithm. Hence, the Laplacian is approximated as:

$$\text{D}(\text{MI})^{-1} \mathbf{G} = \mathbf{L}, \quad \text{with} \quad \mathbf{L}^{ab} = -(\nabla N^b, \nabla N^a). \quad (68)$$

A stabilizing effect is introduced to the pressure equation by this approximation. Denoting the difference between the discrete and continuous operators with $\mathbf{B} = \mathbf{D} (\mathbf{M}\mathbf{I})^{-1} \mathbf{G} - \mathbf{L}$, and using the approximation in equations (62) and (65) for the pseudo-pressure,

$$\mathbf{L}\Phi^\ell = \frac{1}{c_\ell \delta t} (\mathbf{D} [\mathcal{D}^n \mathbf{U}^{\ell,*}] + \mathbf{M} \partial_t \mathcal{D}^\ell - \mathbf{R}_c^\ell), \quad (69)$$

$$\mathbf{L}\Phi^{n+1} = \frac{1}{\delta t} (\mathbf{D} [\mathcal{D}^n \mathbf{U}^{n+1,*}] + \mathbf{M}\mathbf{I} \partial_t \mathcal{D}^{n+1} - \mathbf{R}_c^{n+1}). \quad (70)$$

Furthermore re-arranging (63) into:

$$\mathcal{D}^n \mathbf{U}^{\ell,*} = \mathcal{D}^n \mathbf{U}^\ell + c_\ell \delta t (\mathbf{M}\mathbf{I})^{-1} \mathbf{G}\Phi^\ell, \quad (71)$$

re-introduced to (69) we obtain,

$$c_\ell \delta t \mathbf{L}\Phi^\ell = \mathbf{D} [\mathcal{D}^n \mathbf{U}^\ell + c_\ell \delta t (\mathbf{M}\mathbf{I})^{-1} \mathbf{G}\Phi^\ell] - \mathbf{R}_c^\ell, \quad (72)$$

$$\mathbf{M} \partial_t \mathcal{D}^\ell + \mathbf{D} [\mathcal{D}^n \mathbf{U}^\ell] + c_\ell \delta t \mathbf{B}\Phi^\ell = \mathbf{R}_c^\ell. \quad (73)$$

Similarly for the time step,

$$\mathbf{M} \partial_t \mathcal{D}^{n+1} + \mathbf{D} [\mathcal{D}^n \mathbf{U}^{n+1}] + \delta t \mathbf{B}\Phi^{n+1} = \mathbf{R}_c^{n+1}. \quad (74)$$

147 Codina & Blasco [21] showed that error introduced by $\mathbf{B}\Phi^{n+1}$ is the same
 148 order as the pressure interpolation error: $\mathcal{O}(h^{k+1})$, where k is the order of
 149 the elements. Using the stabilization term in (28), yields a kinetic energy
 150 dissipation term of $(\delta t \mathbf{B}\Phi, \Phi)$. Thus the stabilization term introduces an
 151 error of $\mathcal{O}(\delta t h^{k+1})$ in the kinetic energy conservation.

152 5.4. Overview of the algorithm

153 The complete approach is summarised in Algorithm 1. The time step is
 154 calculated as the minimum of the time step of the scalar and the momentum

155 equations. For the scalar equations, the standard CFL condition is applied,
 156 while the self-adaptive strategy of Trias & Lehmkuhl [22] is used for the
 157 momentum equations. Then the scalars are transported using stabilized
 158 finite elements, and the new velocity field is calculated with the fractional step
 159 method. For the momentum transport the convective operator is assembled
 160 according to (52) or (53) for the skew-symmetric and EMAC discretizations
 161 respectively using the density ($\mathcal{D}^n$) of the previous time step, and velocity
 162 ($\mathbf{U}^n$) of the substeps. There is no need to solve a transport equation for $\mathbb{A}$.

$t = t_0;$
while $t \leq t_f$ **do**
 Evaluate $\delta t;$
 $t = t + \delta t;$
 $\ell = 2;$
 $\Xi_k^1 = \Xi_k^n;$
 while $\ell \leq s$ **do**
 Evaluate Ξ_k^ℓ using (59) ;
 $\ell = \ell + 1 ;$
 end
 Evaluate Ξ_k^{n+1} using (60);
 $\ell = 2;$
 $\mathbf{U}^1 = \mathbf{U}^n;$
 while $\ell \leq s$ **do**
 Evaluate $\mathbf{U}^{\ell,*}$ using (61) ;
 Evaluate Φ^ℓ solving (69) or approximate Φ^ℓ [20];
 Evaluate $\mathbf{U}^\ell$ using (63) ;
 end
 Evaluate $\mathbf{U}^{n+1,*}$ using (64);
 Evaluate Φ^{n+1} solving (70) ;
 Evaluate $\mathbf{U}^{n+1}$ using (66) ;
 Evaluate $\mathcal{D}^{n+1}$ using (1) and evaluate other material properties;
end

163

Algorithm 1: Overview of the algorithm

164 6. Numerical tests

165 The developed algorithm has been extensively tested in incompressible
166 conditions. A set of dedicated test cases has been published in the recent
167 work of Lehmkuhl et al. [14]. The included tests are: the inviscid and vis-
168 cous Taylor-Green vortex, a turbulent channel flow, flow past a sphere, and
169 flow around an Ahmed body. Using the inviscid Taylor-Green vortex, it has
170 been shown, that the kinetic energy dissipation introduced by the numer-
171 ical scheme is indeed scaling as $\mathcal{O}(\delta t h^{k+1})$. It is important to note, that
172 the same code is used in the present study by adding the scalar transport
173 equations, and the state dependent material properties, and by including
174 the $\partial_t \mathcal{D}$ term in (69) and (70). Thus the results of Lehmkuhl et al. [14] are
175 retained in the incompressible limit with the present formulation. This sec-
176 tion presents three application cases with increasing complexity to evaluate
177 the proposed low Mach number discretization strategy for thermally coupled
178 flows subjected to chemical reactions. The first test case corresponds to an
179 anisothermal turbulent channel flow at constant composition with a rela-
180 tively low density ratio. The second case is a turbulent premixed flame, that
181 is represented by the transport of a reactive scalar also referred as progress
182 variable that describes the thermochemical state of the flame. Finally, the
183 third case corresponds to a turbulent diffusion flame, where a passive scalar
184 also referred as mixture fraction is added as an additional variable to the
185 progress variable to account for the effects of fuel/air mixing. Further details
186 of these modelling approaches and description of the subgrid terms required
187 for LES are given in the corresponding subsections.

188 6.1. Anisothermal channel flow

189 The effect of density gradients is tested in an isolated manner with the
 190 anisothermal channel flow case of Toutant and Bataille [23] using LES with
 191 Favre-averaged quantities [1]. Fig.1 illustrates the domain, which has the
 192 dimensions $L_x = 2\pi h$, $L_y = 2h$, and $L_z = \pi h$ in the streamwise, wall-
 193 normal, and spanwise directions respectively, where $h = 1$ m was chosen
 194 as the channel half-height. Toutant and Bataille [23] showed, that the two
 195 point correlations diminish over these distances, and these dimensions can be
 196 considered adequate for the problem. The domain is periodic in the spanwise
 197 and streamwise directions.

Figure 1: Channel geometry

In this case, the only transported scalar is the temperature. The governing equation substituting (5) using Favre-averaged quantities is:

$$c_p \bar{\rho} \partial_t \tilde{T} + c_p \bar{\rho} \tilde{\mathbf{u}} \cdot \nabla \tilde{T} + \nabla \cdot \left(- \left(\lambda + \frac{c_p \mu^{SGS}}{Pr_t} \right) \nabla \tilde{T} \right) = \frac{dP_0}{dt}, \quad (75)$$

198 where λ is the thermal conductivity, and $c_p = 1005 \frac{\text{J}}{\text{kgK}}$ is the specific heat.
 199 The material properties are representing realistic gas-like behaviour. The
 200 filtering of the continuity and momentum equations (3) and (4) is taken
 201 using a standard LES closure based on Boussinesq [1] with the subgrid scale
 202 turbulent viscosity given by Vreman [24]. Here, the model constant is set to

203 $C = 0.1$, as it is the value recommended by the author for complex cases. The
 204 equation of state (1) is used with a specific gas constant of $R = \frac{R_u}{W} = 287 \frac{\text{J}}{\text{kgK}}$,
 205 the dynamic viscosity is set by Sutherland's law: $\mu = \frac{T^{3/2}}{T+111 \text{ K}} 1.461 \cdot 10^{-6} \frac{\text{Pas}}{\sqrt{\text{K}}}$,
 206 the thermal conductivity is calculated using a constant molecular Prandtl
 207 number: $\lambda = \frac{\mu c_p}{Pr}$ with $Pr = 0.71$, and a turbulent Prandtl number of $Pr_t =$
 208 0.9 is set as proposed by Toutant and Bataille [23].

The mean flow is induced by applying a constant artificial pressure gradient ($\mathbf{f}_x$) in the x direction. Following the convention of incompressible channel simulations the flow is characterised by the wall Reynolds number, however the material properties are evaluated at the corresponding wall temperature,

$$Re_\tau = \frac{\rho_w u_\tau h}{\mu_w}, \quad (76)$$

where "w" indicates the wall state ($\rho_w = \rho(P_0, T_w)$, $\mu_w = \mu(T_w)$), and u_τ is the friction velocity: $u_\tau = \sqrt{\frac{\langle \tau_w \rangle}{\rho_w}}$ with $\langle \tau_w \rangle$ being the mean wall shear stress calculated as:

$$\langle \tau_w \rangle = \frac{1}{\Delta t} \sum_{t_0}^{t_0 + \Delta t} \frac{|\mathbf{F}_{w,x}^n|}{A_w} \delta t^n, \quad (77)$$

209 where $\mathbf{F}_{w,x}^n$ is the friction force exerted on the wall in the streamwise direction
 210 at time step n , A_w is the wall surface, Δt is length of the averaging interval,
 211 and δt^n is the time step size.

The two walls have different wall Reynolds numbers for non-unity temperature ratios (Tr). The usual approach to reach different temperature ratios is keeping the cold wall at room temperature while increasing the temperature of the hot wall. If Sutherland's law is applied, the viscosity at the hot wall increases, and the wall Reynolds number decreases. However, the cases can

be characterised by the average wall Reynolds number,

$$Re_\tau = \frac{Re_{\tau,c} + Re_{\tau,h}}{2}, \quad (78)$$

" c " and " h " indicating the cold and hot walls respectively. There are numerous approaches in the literature for comparing different temperature ratios. The DNS database considered in this work imposes a volumetric force term such that the average wall Reynolds number is defined ($Re_\tau = 395$) [23]. The force term is expressed as:

$$\mathbf{f}_x = \frac{\tau_c + \tau_h}{2h} = \frac{\frac{Re_{\tau,c}^2 \mu_c^2}{\rho_c} + \frac{Re_{\tau,h}^2 \mu_h^2}{\rho_h}}{2h^3}. \quad (79)$$

To calculate the force term in the $Tr = 2$ case, the two wall Reynolds numbers are taken *a priori* from the DNS [23] as: $Re_{\tau,c} = Re_{\tau,c}^{DNS} = 235$ and $Re_{\tau,h} = Re_{\tau,h}^{DNS} = 565$. A structured hexahedral mesh is applied with homogeneous size in x and z . The mesh is refined in the wall-normal direction according to:

$$y_i = h \left\{ 1 + \frac{1}{\alpha} \tanh \left[\text{atanh}(\alpha) \left(\frac{2i}{N_{ey}} - 1 \right) \right] \right\}, \quad i = 0..N_{ey}, \quad (80)$$

212 where N_{ey} is the number of elements in y , and α is a parameter expressing
 213 the level of refinement. A coarse and a fine mesh are considered to evaluate
 214 the effects of resolution on the discretization strategy and the parameters of
 215 relevance for each mesh are listed in Tab.1.

Finally, the temperature scaling is based on the wall heat flux ($\dot{q}_w$) and the friction temperature can be defined as:

$$T_\tau = \frac{\dot{q}_w}{\rho_w c_p u_\tau}. \quad (81)$$

Figure 2: Comparison of mean and RMS properties of the case: $Re_\tau = 395, Tr = 2$ on the cold side, a: mean stream-wise velocity, b: stream-wise velocity RMS, c: wall-normal velocity RMS, d: span-wise velocity RMS, e: mean temperature $\left(T^+ = \frac{T_w - \langle T \rangle}{T_\tau}\right)$, f: temperature RMS; squares: DNS of Toutant and Bataille [23] (truncated at $y^+ = 200$), dashed blue line: EMAC on coarse mesh, dotted orange line: skew-symmetric on coarse mesh, dash-dotted blue line: EMAC on fine mesh, solid red line: skew-symmetric on fine mesh

Figure 3: Comparison of mean and RMS properties of the case: $Re_\tau = 395, Tr = 2$ on the hot side, a: mean stream-wise velocity, b: stream-wise velocity RMS, c: wall-normal velocity RMS, d: span-wise velocity RMS, e: mean temperature $\left(T^+ = \frac{T_w - \langle T \rangle}{T_\tau}\right)$, f: temperature RMS; squares: DNS of Toutant and Bataille [23] (truncated at $y^+ = 200$), dashed blue line: EMAC on coarse mesh, dotted orange line: skew-symmetric on coarse mesh, dash-dotted blue line: EMAC on fine mesh, solid red line: skew-symmetric on fine mesh

	N_{ex}	N_{ey}	N_{ez}	α	Δ_x^+	$\Delta_{y,min}^+$	$\Delta_{y,max}^+$	Δ_z^+	DoF
Coarse	70	66	39	0.9933	35.5	0.50	34.2	31.8	180k
Fine	165	123	82	0.9830	15.0	0.54	15.5	15.1	1.66M

Table 1: Channel flow mesh size based on $Re_\tau = 395$

216 Results for the mean and RMS profiles of the present LES simulations
 217 with the DNS of Toutant and Bataille [23] are shown in Figs. 2 and 3 for
 218 comparison. The plots indicate a good level of correlation overall with the
 219 reference data for the cold and hot sides of the channel. In particular, the
 220 results in the cold side are in good agreement for the first-order statistics
 221 (normalized streamwise velocity and temperature), while the second-order
 222 statistics show a higher dependency with the mesh resolution. On the hot
 223 side, the correlation with the reference data is substantially improved when
 224 compared to the cold side, and show less dependency on the resolution. The
 225 reason behind this different behaviour can be explained by the flow Reynolds
 226 number. The flow in the cold side is characterised by higher density than the
 227 hot side, and hence, it features a higher Reynolds number. As the mesh was
 228 constructed with the same refinement law along the wall-normal direction,
 229 the momentum and thermal boundary layer thicknesses are not as well re-
 230 solved on the cold side as on the hot one. The results also indicate, that there
 231 are no significant differences between the skew-symmetric and the EMAC dis-
 232 cretizations under these conditions. The wall Reynolds numbers predicted
 233 by the present work are listed in Tab.2, and they agree well with the DNS
 234 values in all cases.

	EMAC, coarse	Skew, coarse	EMAC, fine	Skew, fine	DNS[23]
Cold	553 (−2.1%)	560 (−0.9%)	571 (+1.1%)	580 (+2.7%)	565
Hot	239 (+1.7%)	236 (+0.4%)	238 (+1.3%)	235 (0%)	235

Table 2: Wall Reynolds numbers on the hot and cold sides at different cases, and the relative error compared to DNS[23]

235 6.2. Turbulent premixed swirling flame

236 The second test case corresponds to a technically premixed turbulent
237 flame in a swirl-stabilized bluff-body configuration also known as PREC-
238 CINSTA burner. The operating point to be investigated corresponds to an
239 equivalence ratio of $\phi = 0.75$ that burns in stable operation at Reynolds
240 number $Re = 35000$ (based on the swirler outer diameter). Experimental
241 measurements of this burner [25] and previous LES results [26] suggest the
242 perfectly premixed assumption holds for this operating point and the burn-
243 ing of a homogeneous methane/air mixture can be considered to describe
244 the reacting process. The flame exhibits a constant temperature ratio of
245 $Tr \approx 6$ with fluctuations around the adiabatic unstretched value caused
246 by turbulence/chemistry interactions. This test poses an additional degree
247 of complexity as the density ratio is substantially increased respect to the
248 previous case, and small fluctuations of density will appear influencing the
249 turbulent burning velocity, which is the key element to be predicted here.
250 Furthermore the heat release in the reacting layer causes thermal dilatation,
251 that effectively acts as a volumetric momentum source through the $\partial_t \mathcal{D}$ term.
252 The results available for this operating point correspond to mean and fluctu-
253 ations of velocity, and those will be used for comparison with the proposed

254 discretization strategies.

The turbulent combustion model used for this problem is based on flamelet modelling. The governing equations of the problem in the context of LES using Favre-average filtering include the scalar equations for enthalpy ($\tilde{h}$), scaled progress variable ($\tilde{C}$), and its subscale variance (C_v), where the notation ($\tilde{}$) is used for density-weighted variables. The resulting system of equations for scalar transport reads:

$$\partial_t (\bar{\rho} \tilde{h}) + \nabla \cdot (\bar{\rho} \tilde{h} \tilde{\mathbf{u}}) + \nabla \cdot \mathbf{q} = \frac{dP_0}{dt}, \quad (82)$$

$$\partial_t (\bar{\rho} \tilde{C}) + \nabla \cdot (\bar{\rho} \tilde{C} \tilde{\mathbf{u}}) + \nabla \cdot \mathbf{\Phi}_C = \overline{\dot{\omega}_C}, \quad (83)$$

$$\partial_t (\bar{\rho} C_v) + \nabla \cdot (\bar{\rho} C_v \tilde{\mathbf{u}}) + \nabla \cdot \mathbf{\Phi}_{C_v} = -\bar{\rho} \chi_{C_v}^{SGS} - 2\mathbf{\Phi}_C^{SGS} \cdot \nabla \tilde{C} + \overline{\dot{\omega}_{C_v}}, \quad (84)$$

255 where the filtered continuity and momentum equations, as well as the subgrid
 256 scale turbulent viscosity corresponds to the ones of the previous case. Here,
 257 the constant of the Vreman model is also set to $C = 0.1$, as before. The
 258 diffusive fluxes are: $\mathbf{q} = -\bar{\rho} (D + D^{SGS}) \nabla \tilde{h}$, $\mathbf{\Phi}_C = -\bar{\rho} (D + D^{SGS}) \nabla \tilde{C}$,
 259 $\mathbf{\Phi}_{C_v} = -\bar{\rho} (D + D^{SGS}) \nabla C_v$. The subscale Schmidt number is: $Sc^{SGS} = 0.7$.

260 The flamelet database was generated with the GRI3.0 mechanism [27]
 261 using a single unstretched adiabatic premixed flamelet at the global equiva-
 262 lence ratio of $\phi = 0.75$. In this case the β -FPDF was applied on the scaled
 263 progress variable to account for turbulence-chemistry interaction [28].

264 The computation domain and measurement locations are presented in
 265 Fig.4. The domain includes the plenum, swirler and combustion chamber.
 266 A hybrid mesh of 4M DoF is applied with boundary layer refinement on the
 267 walls and tetrahedral mesh in the bulk flow. The base mesh size is 1.5 mm
 268 with 1 mm refinement in the combustion chamber up to 55 mm from the

Figure 4: Sketch of domain configuration with measurement locations on top flame visualization with temperature iso-lines: $T \in \{800, 1000, 1200, 1600, 1800, 2000\}$ K using EMAC discretization

269 swirler outlet. Another refinement region with mean mesh size of 0.5 mm
 270 is enclosing the reacting layers. For this problem a single and optimised
 271 mesh is used to evaluate the low Mach discretization strategy and the two
 272 discretization strategies for the convective term.

273 The numerical results are compared to the measurements of Meier et al.[25]
 274 and are shown in Fig.5 and Fig.6 for analysis. The results indicate the pro-
 275 posed discretization strategy with the two convective term operators provide
 276 reasonably good correlation with the experimental data. At upstream loca-
 277 tions, the mean values of the three components of the velocity match fairly
 278 well the measurements, see first column of Fig.5. The flow in this location, is
 279 highly influenced by the anchoring of the flame between the central and cor-
 280 ner recirculation zones. The flame is located within the refinement region,
 281 and the prediction of velocity is in good agreement. As the flow develops
 282 downstream and the mesh is coarsened, the differences between the results

283 with the two operators increase. The case with EMAC discretization predicts
 284 better the magnitude of the reverse flow of the central recirculation zone, and
 285 also the peak values of the axial velocity at the two downstream locations,
 286 see Fig.5 a,b. However, the trends are well predicted by the two operators
 287 and show the validity of the proposed low dissipation strategy to solve com-
 288 plex reacting flows. The fluctuating components show the impact of the
 289 discretization of the convective term more clearly. While the predicted RMS
 290 values at the upstream location are rather similar, the impact of the EMAC
 291 discretization at downstream locations is evident, see Fig.6. The EMAC
 292 approximation, with enhanced conservative properties with respect to the
 293 skew-symmetric operator, show better prediction of the Reynolds stresses in
 294 regions with lower resolution.

295 The relation between the presence of heat release and the worse perfor-
 296 mance of the skew-symmetric operator can be better understood considering
 297 (38). The error in momentum conservation is proportional to $-\nabla \cdot (\rho \mathbf{u})$,
 298 which is equal to $\partial_t \rho$ in accordance with mass conservation. Thus in the
 299 presence of unsteady reacting layers ($|\partial_t \rho| \gg 0$), the error introduced by the
 300 skew-symmetric discretization is magnified. The EMAC discretization does
 301 not have this error. This difference between the two operators is apparent in
 302 the downstream measurement locations.

303 *6.3. DLR-A non-premixed jet flame*

304 The final case for validation corresponds to a turbulent jet diffusion flame
 305 in a low-velocity coflow. This case incorporates certain aspects of the pre-
 306 vious case, as it requires solving a reacting flow field subjected to density
 307 variations caused by heat release. However in this case, these variations

Figure 5: Comparison of mean velocity profiles in the PRECCINSTA burner at three axial locations: $x \in \{2.5, 15, 35\}$ mm; a: mean axial velocity, b: mean radial velocity, c: mean tangential velocity; squares: measurement of Meier et al. [25], dash-dotted blue line: EMAC, solid red line: skew-symmetric

Figure 6: Comparison of RMS velocity profiles in the PRECCINSTA burner at three axial locations: $x \in \{2.5, 15, 35\}$ mm; a: axial velocity RMS, b: radial velocity RMS, c: tangential velocity RMS; squares: measurement of Meier et al. [25], dash-dotted blue line: EMAC, solid red line: skew-symmetric

308 are caused by differences in fuel/air concentration and mixing, so different
 309 burning and combustion characteristics are expected in this problem. While
 310 in the previous case, the density variation is function of the progress vari-
 311 able ranging from unreacted to fully reacted mixture, the density is direct
 312 function of the fuel/air ratio and the progress variable in this problem. In
 313 diffusion-dominated conditions, composition variations can be described by
 314 the use of an additional transport equation, that is the mixture fraction.
 315 Note that fluctuations of mixture fraction are expected to play an impor-
 316 tant role here as the thermochemical state of the flow is characterised by
 317 two controlling variables. This test represents the second fundamental type
 318 of regime found in combustion applications, and it has great relevance in
 319 practical applications.

320 The test case considered here is the well-established DLR-A jet flame
 321 for which reliable experimental data was generated by DLR and Sandia
 322 Labs. [29]. This is a turbulent round jet of a fuel mixture of $\text{CH}_4/\text{H}_2/\text{N}_2$
 323 burning in a low-velocity air coflow. The fuel nozzle has a diameter of 8 mm,
 324 the jet is composed of 22.1% CH_4 , 33.2% H_2 , and 44.7% N_2 by volume, and
 325 is supplied at a Reynolds number of 15200. The temperature ratio at stoi-
 326 chiometric conditions is $Tr_{st} = 7$, which is quite similar to the previous case,
 327 though this temperature changes also with the mixture fraction to account
 328 for fuel/air mixing. The results available for this operating point correspond
 329 to mean and fluctuations of velocity, mixture fraction and temperature, and
 330 those will be used for comparison with the proposed discretization strategies.

A flamelet model based on diffusion flamelets is used to describe the
 combustion process in this case, and the filtered scalar transport equations

to be solved along with Eqs. (3) and (4) reads:

$$\partial_t (\bar{\rho} \tilde{h}) + \nabla \cdot (\bar{\rho} \tilde{h} \tilde{\mathbf{u}}) + \nabla \cdot \mathbf{q} = \frac{dP_0}{dt}, \quad (85)$$

$$\partial_t (\bar{\rho} \tilde{Z}) + \nabla \cdot (\bar{\rho} \tilde{Z} \tilde{\mathbf{u}}) + \nabla \cdot \Phi_Z = 0, \quad (86)$$

$$\partial_t (\bar{\rho} Z_v) + \nabla \cdot (\bar{\rho} Z_v \tilde{\mathbf{u}}) + \nabla \cdot \Phi_{Z_v} = -\bar{\rho} \chi_{Z_v}^{SGS} - 2\Phi_Z^{SGS} \cdot \nabla \tilde{Z}, \quad (87)$$

$$\partial_t (\bar{\rho} \tilde{Y}_c) + \nabla \cdot (\bar{\rho} \tilde{Y}_c \tilde{\mathbf{u}}) + \nabla \cdot \Phi_{Y_c} = \overline{\dot{\omega}_{Y_c}}, \quad (88)$$

where h , Z , Z_v , and Y_c are the enthalpy, filtered mixture fraction, subscale mixture fraction variance, and filtered progress variable respectively, with diffusive fluxes: $\mathbf{q} = -\bar{\rho} (D + D^{SGS}) \nabla \tilde{h}$, $\Phi_Z = -\bar{\rho} (D + D^{SGS}) \nabla \tilde{Z}$, $\Phi_{Z_v} = -\bar{\rho} (D + D^{SGS}) \nabla Z_v$, $\Phi_{Y_c} = -\bar{\rho} (D + D^{SGS}) \nabla \tilde{Y}_c$. The molecular diffusivity is $\bar{\rho} D = \frac{\lambda}{c_p}$ assuming unity Lewis number, and $\bar{\rho} D^{SGS} = \frac{\mu^{SGS}}{Sc_t}$ is the subscale diffusivity, where the subscale Schmidt number is constant: $Sc^{SGS} = 0.7$. The subscale mixture fraction variance has a dissipation term: $\chi_{Z_v}^{SGS} = 2 \frac{Z_v}{\tau_t}$ associated with the time scale of the subgrid turbulence: $\tau_t = \left(C_\epsilon^2 \nu_t \frac{|\mathbf{S}|^2}{\Delta^2} \right)^{-1/3}$ where $C_\epsilon = 3.24$ is a modelling constant of the subgrid model, ν_t is the subgrid viscosity, S is the strain rate tensor, and Δ is the element size.

Opposing diffusion flamelets are computed using the GRI3.0 mechanism [27] for generating the flamelet tables. The turbulence-chemistry interaction is considered with β -function as the Filtered Probability Density Function (FPDF) of the mixture fraction. The necessary material properties, and the source term of the progress variable are integrated with the FPDF a-priori and tabulated as function of $\tilde{Z}$, Z_v , and $\tilde{C} = \frac{\tilde{Y}_c - \tilde{Y}_c^0(\tilde{Z}, Z_v)}{\tilde{Y}_c^{eq}(\tilde{Z}, Z_v) - \tilde{Y}_c^0(\tilde{Z}, Z_v)}$, where $\tilde{C}$ is the scaled progress variable, $\tilde{Y}_c^0$ and $\tilde{Y}_c^{eq}$ are the minimum and maximum of progress variable at given $\tilde{Z}$ and Z_v .

Two unstructured meshes are used to simulate this case, named coarse

Figure 7: DLR-A jet flame measurement locations, the jet is visualized with temperature iso-lines: $T \in \{800, 1000, 1200, 1600, 1800, 2000\}$ K on the fine mesh using EMAC discretization

and fine. The jet axis is in the x direction. A zoomed section of the computational domain with iso-contours of temperature are shown in Fig.7 along with the studied measurement locations. This section of interest corresponds to the refinement region in the two meshes. The main properties of the two meshes are listed in Tab.3. The coarse one is a rectangular domain, with a width of 1.4 m and a length of 2 m. A fully tetrahedral unstructured mesh is applied in this case, an element size of 60 mm is set in the far field, the mesh around the jet is refined in 3 steps, with a mesh size of 4 mm up to $x/D = 125$, 2 mm up to $x/D = 45$, and 1 mm up to $x/D = 22.5$. The refinement regions are following the expected jet spreading angle.

The fine mesh has a reduced domain size with a width of 0.24 m and a length of 0.48 m. Up to $x/D = 30$ the mesh is extruded from the plane of the inlet with a size of 0.5 mm in the axial direction. The remaining part ($x/D > 30$) is a buffer region with unstructured mesh. The inlet plane is meshed with a base size of 5 mm, it has a refinement region with a 0.06 m

radius with a size of 1 mm, that decreases to 0.25 mm in the vicinity of the nozzle.

	Δ_{axial}	Δ_{radial}	DoF
Coarse	1.0 mm	1.0 mm	970k
Fine	0.5 mm	0.2 .. 1.0 mm	6.9M

Table 3: DLR-A jet mesh size

In order to ensure the correct boundary conditions using the two meshes, the same surface mesh is applied for the fuel inlet in the two cases, so that the same turbulent boundary condition is imposed. The center of the inlet is meshed with a size of 0.2 mm and is refined near the edge of the inlet. The synthetic turbulent inlet strategy of [30] is adapted. In an *a priori* sensitivity study, we found the adequate turbulent length scale to be 3.5% of the diameter. A fully developed turbulent pipe flow profile is imposed for the mean and RMS values. The mean profile is reconstructed from the log-law using second order continuous polynomial interpolation in the core and buffer regions, while the RMS profiles are taken from the DNS data of [31].

The results of the present LES calculation with comparison of the measurement data of Meier et al. [29] are shown in Fig.8 and Fig.9 for analysis. The results show similar trends as those observed in the previous cases, but with more clear evidence of the influence of the discretization of the convective term. The results using the EMAC operator have shown improved predictions for fluctuating quantities, but also for mean values in this case. At upstream locations ($x/D = 5$) the axial velocity and mixture fraction are

Figure 8: Comparison of mean profiles in the DLR A jet flame at three axial locations: $x \in \{5D, 10D, 20D\}$; a: mean axial velocity, b: mean mixture fraction, c: mean temperature; suquares: measurement of Meier et al.[29], dashed blue line: EMAC on coarse mesh, dotted orange line: skew-symmetric on coarse mesh, dash-dotted blue line: EMAC on fine mesh, solid red line: skew-symmetric on fine mesh

Figure 9: Comparison of RMS profiles in the DLR A jet flame at three axial locations: $x \in \{5D, 10D, 20D\}$; a: axial velocity RMS, b: mixture fraction RMS, c: temperature RMS; squares: measurement of Meier et al.[29], dashed blue line: EMAC on coarse mesh, dotted orange line: skew-symmetric on coarse mesh, dash-dotted blue line: EMAC on fine mesh, solid red line: skew-symmetric on fine mesh

385 in good agreement with experimental data. Jet penetration and spreading
 386 are well captured at this distance, which results in an accurate prediction of
 387 the temperature. The impact of the mesh resolution for EMAC at this axial
 388 location is quite low, though it becomes more relevant at downstream loca-
 389 tions. In this test case, the EMAC discretization is clearly superior on both
 390 meshes. The mean profiles are predicted considerably well even on the coarse
 391 mesh except the edge of the jet at the $x/D = 10$ axial location (Fig.8). The
 392 refinement corrects this discrepancy, and improves the RMS values (Fig.9).
 393 The skew-symmetric operator is found to be quite sensitive to the mesh res-
 394 olution, but the results even with the fine mesh are still poor compared to
 395 those with EMAC, see Fig.8 a,b. At more downstream locations, see Fig. 8 at
 396 $x/D = 10$ and $x/D = 20$, the same trend is maintained and the penetration
 397 of the jet is better predicted by EMAC. As the axial velocity exhibits a fast
 398 decay when using the skew-symmetric approximation, the mixture fraction
 399 deviates substantially from the reference values with flattened profiles. This
 400 results in large over-predictions of the flame temperature and jet spreading.
 401 The results using EMAC show an excellent correlation of velocity and mix-
 402 ture faction at all locations for mean and fluctuating quantities, and therefore
 403 predicts all flow parameters better.

404 Analysing the momentum conservation of the skew-symmetric operator
 405 in this case gives further insight on this issue. The jet shows self similar
 406 properties in the measurement for axial velocity and mixture fraction. These
 407 two properties are also similar to each other in the studied locations for the
 408 measurement and the EMAC operator (Fig.8 a,b). However the fluctuating
 409 heat release in the reacting layer surrounding the jet induces the momentum

410 loss in the skew-symmetric case. The discrepancies in the mixture fraction
 411 profile are a consequence of the error in velocity, thus the similarity between
 412 the two quantities is broken.

413 7. Conclusions

414 In this study, we present a low-dissipation finite element scheme for low
 415 Mach number flows in the context of large-eddy simulation using an explicit
 416 third order Runge-Kutta method in conjunction with appropriate subgrid
 417 models.

418 The low Mach number approximation of the Navier-Stokes equations have
 419 been introduced in the weak form. We derived the energy, momentum, and
 420 angular momentum conserving formulation of the non-linear term of the mo-
 421 mentum equation for variable density flows. The symmetry properties of
 422 the original incompressible implementation are preserved by introducing a
 423 change of variables: $\mathbb{A} \equiv \sqrt{\rho} \mathbf{u}$. The conservation properties of the EMAC
 424 and the well-known skew-symmetric operator are derived for specific test
 425 conditions, where mass conservation is not strictly imposed. As postulated,
 426 by writing in terms of $\mathbb{A}$, the EMAC formulation preserves its conservative
 427 properties for variable density flows.

428 The complete spatio-temporal discretization scheme using finite elements
 429 and explicit time integration is presented. We exploit the stabilizing effect
 430 introduced by using an approximate Laplacian to stabilize the pressure equa-
 431 tion. Otherwise no additional stabilization is introduced for the mass and
 432 momentum conservation. The error of kinetic energy conservation is of order
 433 $\mathcal{O}(\delta t h^{k+1})$, thus dissipation is limited.

434 The strategy has been tested on three physical problems: a fully de-
 435 veloped anisothermal channel flow, a premixed swirling flame, and a non-
 436 premixed jet flame. Both the skew-symmetric and the EMAC operators
 437 perform well in the anisothermal channel flow. The difference between the
 438 two strategies is minor. In general we observe higher discrepancies on the
 439 cold side, where the Reynolds number is higher, since a symmetric mesh is
 440 applied. Mesh refinement is shown to improve the results with both opera-
 441 tors.

442 In the reacting cases, the EMAC discretization clearly performs better. It
 443 captures well both the velocity peaks and the central recirculation zone of the
 444 swirling flame. The skew-symmetric strategy produces high discrepancies in
 445 these locations, and it consistently underpredicts the fluctuations. In general
 446 it appears to give a more diffusive solution. In the DLR-A jet flame the
 447 level of complexity of the problem is increased. The results with the EMAC
 448 operator agree very well with the measurements, and mesh refinement leads
 449 to a clear improvement. On the other hand the error introduced by the
 450 skew-symmetric formulation breaks the relationship between the scalar and
 451 velocity fields of the jet, thus the error in the fluctuating properties is less
 452 deterministic.

453 Overall the proposed low-dissipation scheme with the EMAC discretiza-
 454 tion shows good agreement with the reference data in all test cases. The
 455 benefit of using the EMAC discretization with respect the classical skew-
 456 symmetric is more relevant in the reacting cases. We postulate this is caused
 457 by the lack of volumetric source term in anisothermal channel flow case.
 458 Specifically the heat release from combustion causes high density variations

459 in a Lagrangian frame of reference, this effect is lacking in the channel case,
460 where the density of a fluid particle is primarily modified by molecular and
461 subgrid thermal diffusion. To conclude, in all three cases the performance
462 of the proposed strategy is rather good and it has been capable of repro-
463 ducing the results with excellent accuracy outperforming the classical skew-
464 symmetric approach.

465 **Acknowledgements**

466 This project has received funding from the Spanish Ministry of Economy
467 and Competitiveness in the frame of the CHEST project (TRA2017-89139-
468 C2-2-R) and from the European Union’s Horizon 2020 research and inno-
469 vation programme under the Marie Skłodowska-Curie grant agreement No.
470 713673. Ambrus Both has received financial support from ”la Caixa” Funda-
471 tion (ID 100010434). The fellowship grant code is LCF/BQ/IN17/11620032.
472 Conflict of Interest: Daniel Mira acknowledges the Juan de la Cierva personal
473 grant IJCI-2015-26686.

474 **References**

475 **References**

- 476 [1] T. Poinso, D. Veynante, Theoretical and numerical combustion, RT
477 Edwards, Inc., 2005.
- 478 [2] P. Moin, S. V. Apte, Large-eddy simulation of realistic gas turbine
479 combustors, AIAA journal 44 (2006) 698–708.

- 480 [3] D. Mira, M. Vázquez, G. Houzeaux, S. Gövert, J. W. Kok, E. Mahiques,
481 L. Panek, Study of the wall thermal condition effect in a lean-
482 premixed downscaled can combustor using large-eddy simulation, in:
483 ASME. Turbo Expo: Power for Land, Sea, and Air, Volume 5B: Heat
484 Transfer, GT2016-58016, American Society of Mechanical Engineers, p.
485 V05BT17A018.
- 486 [4] H. Pitsch, Large-eddy simulation of turbulent combustion, *Annu. Rev.*
487 *Fluid Mech.* 38 (2006) 453–482.
- 488 [5] S. Charnyi, T. Heister, M. A. Olshanskii, L. G. Rebholz, On conservation
489 laws of navier–stokes galerkin discretizations, *Journal of Computational*
490 *Physics* 337 (2017) 289–308.
- 491 [6] R. Verstappen, A. Veldman, Symmetry-preserving discretization of tur-
492 bulent flow, *Journal of Computational Physics* 187 (2003) 343–368.
- 493 [7] J. Reiss, A family of energy stable, skew-symmetric finite difference
494 schemes on collocated grids, *Journal of Scientific Computing* 65 (2015)
495 821–838.
- 496 [8] F. Nicoud, Conservative high-order finite-difference schemes for low-
497 mach number flows, *Journal of Computational Physics* 158 (2000) 71–
498 97.
- 499 [9] Y. Morinishi, Skew-symmetric form of convective terms and fully con-
500 servative finite difference schemes for variable density low-mach number
501 flows, *Journal of Computational Physics* 229 (2010) 276–300.

- 502 [10] J. Brouwer, J. Reiss, J. Sesterhenn, Conservative time integrators of
503 arbitrary order for finite-difference discretization of compressible flow,
504 Computers & Fluids 100 (2014) 1–12.
- 505 [11] W. Rozema, R. W. Verstappen, A. E. Veldman, J. C. Kok, Low-
506 dissipation simulation methods and models for turbulent subsonic flow,
507 Archives of Computational Methods in Engineering (2018) 1–32.
- 508 [12] G. Coppola, F. Capuano, S. Pirozzoli, L. de Luca, Numerically sta-
509 ble formulations of convective terms for turbulent compressible flows,
510 Journal of Computational Physics 382 (2019) 86–104.
- 511 [13] R. Codina, J. Principe, M. Ávila, Finite element approximation of tur-
512 bulent thermally coupled incompressible flows with numerical sub-grid
513 scale modelling, International Journal of Numerical Methods for Heat
514 & Fluid Flow 20 (2010) 492–516.
- 515 [14] O. Lehmkuhl, G. Houzeaux, H. Owen, G. Chrysokentis, I. Rodriguez, A
516 low-dissipation finite element scheme for scale resolving simulations of
517 turbulent flows, Journal of Computational Physics 390 (2019) 51–65.
- 518 [15] E. R. Van Driest, Turbulent boundary layer in compressible fluids,
519 Journal of Aeronautical Sciences 18 (1951) 145–160.
- 520 [16] C.-S. Yih, A transformation for non-homentropic flows, with an appli-
521 cation to large-amplitude motion in the atmosphere, Journal of Fluid
522 Mechanics 9 (1960) 68–80.
- 523 [17] S. Kida, S. A. Orszag, Energy and spectral dynamics in decaying com-
524 pressible turbulence, Journal of Scientific Computing 7 (1992) 1–34.

- 525 [18] A. W. Cook, Y. Zhou, Energy transfer in rayleigh-taylor instability,
526 Physical Review E 66 (2002) 026312.
- 527 [19] Y. V. Peet, S. K. Lele, Computational framework for coupling compress-
528 ible and low mach number codes, AIAA journal 46 (2008) 1990–2001.
- 529 [20] F. Capuano, G. Coppola, M. Chiatto, L. de Luca, Approximate pro-
530 jection method for the incompressible navier–stokes equations, AIAA
531 Journal 54 (2016) 2179–2182.
- 532 [21] R. Codina, J. Blasco, A finite element formulation for the stokes problem
533 allowing equal velocity-pressure interpolation, Computer Methods in
534 Applied Mechanics and Engineering 143 (1997) 373–391.
- 535 [22] F. Trias, O. Lehmkuhl, A self-adaptive strategy for the time integration
536 of navier-stokes equations, Numerical Heat Transfer, Part B: Funda-
537 mentals 60 (2011) 116–134.
- 538 [23] A. Toutant, F. Bataille, Turbulence statistics in a fully developed chan-
539 nel flow submitted to a high temperature gradient, International Journal
540 of Thermal Sciences 74 (2013) 104–118.
- 541 [24] A. Vreman, An eddy-viscosity subgrid-scale model for turbulent shear
542 flow: Algebraic theory and applications, Physics of fluids 16 (2004)
543 3670–3681.
- 544 [25] W. Meier, P. Weigand, X. Duan, R. Giezendanner-Thoben, Detailed
545 characterization of the dynamics of thermoacoustic pulsations in a lean
546 premixed swirl flame, Combustion and Flame 150 (2007) 2–26.

- 547 [26] S. Gövert, D. Mira, J. B. Kok, M. Vázquez, G. Houzeaux, The effect of
548 partial premixing and heat loss on the reacting flow field prediction of
549 a swirl stabilized gas turbine model combustor, *Flow, turbulence and*
550 *combustion* 100 (2018) 503–534.
- 551 [27] G. P. Smith, D. M. Golden, M. Frenklach, N. W. Moriarty, B. Eiteneer,
552 M. Goldenberg, C. T. Bowman, R. K. Hanson, S. Song, W. Gardiner Jr,
553 et al., *Gri-mech 3.0*, 1999, URL http://www.me.berkeley.edu/gri_mech
554 (2011).
- 555 [28] S. Gövert, D. Mira, J. B. Kok, M. Vázquez, G. Houzeaux, Turbulent
556 combustion modelling of a confined premixed jet flame including heat
557 loss effects using tabulated chemistry, *Applied energy* 156 (2015) 804–
558 815.
- 559 [29] W. Meier, R. Barlow, Y.-L. Chen, J.-Y. Chen, *Raman/rayleigh/lif*
560 *measurements in a turbulent ch₄/h₂/n₂ jet diffusion flame: experimen-*
561 *tal techniques and turbulence–chemistry interaction*, *Combustion and*
562 *Flame* 123 (2000) 326–343.
- 563 [30] A. Kempf, M. Klein, J. Janicka, Efficient generation of initial-and inflow-
564 conditions for transient turbulent flows in arbitrary geometries, *Flow,*
565 *Turbulence and combustion* 74 (2005) 67–84.
- 566 [31] G. K. El Khoury, P. Schlatter, A. Noorani, P. F. Fischer, G. Brethouwer,
567 A. V. Johansson, Direct numerical simulation of turbulent pipe flow at
568 moderately high reynolds numbers, *Flow, turbulence and combustion*
569 91 (2013) 475–495.