Investigation of a novel numerical scheme for high-pressure supercritical fluids turbulence

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High-pressure supercritical turbulence simulations are strongly susceptible to numerical instabilities. The multi-scale nature of the flow, in conjunction with the nonlinear thermodynamics and the strong density gradients across the pseudo-boiling line can trigger spurious pressure oscillations and unbounded amplification of aliasing errors. A wide variety of regularization approaches have been traditionally utilized by the community, including upwind-biased schemes, artificial dissipation, and/or high-order filtering, where stability is achieved at the expense of suppressing part of the turbulent energy spectrum. In this work, a novel numerical scheme based on the paradigm of physics-compatible discretizations is investigated. In particular, the proposed method discretely enforces kinetic-energy conservation (by convection) as well as preservation of pressure equilibrium; the former is achieved using proper splitting of the convective terms, whereas the latter is obtained by directly evolving an equation for pressure. The simultaneous enforcement of these two properties can lead to stable and physically consistent scale-resolving simulations of supercritical turbulence without the need for any form of artificial stabilization. The novel method is preliminarly assessed on two benchmark cases, with numerical results supporting the theoretical findings.

1. Introduction

Supercritical fluids are substances operating at temperatures and pressures above their critical values (T_c, P_c), where no clear phase separation is present. However, within this region, they can be distinguished between (i) supercritical fluids with gas-like density and transport coefficients and (ii) liquid-like fluids with a large density and transport coefficients similar to those of a liquid (Jofre & Urzay 2020). These peculiar thermophysical characteristics present very interesting properties that can be fine-tuned for several purposes. For instance, they can be leveraged to achieve turbulent regimes in microfluidic devices (Bernades & Jofre 2022), which is of remarkable interest for energy applications given the enhanced mixing and transfer rates of turbulent flows.

Although numerical simulations can be an invaluable tool to elucidate the underlying physics of high-pressure supercritical turbulence, they also come with remarkable challenges. At supercritical conditions, the thermodynamic relations can become strongly nonlinear. In particular, the rapid variations of density, viscosity, and thermal conductivity across the pseudo-boiling region can result in spurious pressure oscillations that can contaminate the numerical solution and even lead to solution divergence (Ma *et al.* 2017). Additionally, the multi-scale nature of the flow necessitates methods that are simultaneously able to capture the vast range of flow scales and to avoid unbounded amplification of aliasing errors. Therefore, the numerical solution of supercritical fluids turbulence ultimately requires methods that are (i) able to represent the wide range of turbulent scales

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(non-dissipative), (ii) nonlinearly stable, (iii) free of artificial pressure oscillations, and (iv) computationally fast (efficient), as introduced by Bernades *et al.* (2022).

Several numerical strategies have been developed to deal with turbulent flows at supercritical conditions. Abgrall & Karni (2000) proposed the concept of double-flux modeling, where internal energy is frozen within the time-integration step to artificially enforce pressure equilibrium at a material interface. This method has been recently employed for transcritical flows by Ma *et al.* (2017). In the same context, Terashima & Koshi (2012) and Kawai *et al.* (2015), among others, proposed to evolve an equation for pressure, rather than for, e.g., total energy, to prevent pressure oscillations, at the expense of total energy conservation. Lacaze *et al.* (2019) compared pressure-, enthalpy- and total-energy-based formulations in terms of stability and pressure behavior. In the above-mentioned works, the conservative formulation of the Navier-Stokes equations is discretized, and nonlinear stability is achieved by either filtering (Visbal & Gaitonde 2002) or upwind-biased methods, such as HLLC (Toro 2009) or WENO (Shu 1999) schemes.

In this work, a novel approach inspired by the paradigm of physics-compatible discretizations is proposed and preliminarily assessed. The scheme is based on discretely mimicking two properties: (i) kinetic-energy preservation (KEP) by convection, via splitting of the convective terms (Coppola *et al.* 2019*a*,*b*), and (ii) pressure-equilibrium preservation (PEP), i.e., the property of maintaining constant pressure when both pressure and velocity are initially uniform. The latter was recently achieved for ideal- and stiffened-gas thermodynamics using a careful splitting for internal energy fluxes (Shima *et al.* 2021; Jain & Moin 2022); here, PEP is enforced by evolving an equation for pressure. The simultaneous enforcement of KEP and PEP can lead to stable and reliable simulations of supercritical turbulence without the need for any form of artificial stabilization.

The objectives of this work are twofold: (i) introduce the novel KEP and PEP scheme, and (ii) assess its properties and overall behavior with respect to several state-of-the-art methods. Hence, the paper is organized as follows. First, in Section 2, the flow physics modeling of supercritical fluids is presented. Next, the discretization frameworks considered in this work are described and numerically analyzed in Section 3. Then, the numerical results are presented in Section 4. Finally, in Section 5, the work is concluded, and future directions are proposed.

2. Flow physics modeling

The framework utilized for studying supercritical fluids turbulence in terms of (i) equations of fluid motion and (ii) real-gas thermodynamics is described below.

2.1. *Equations of fluid motion*

The turbulent flow motion of supercritical fluids is generally described by the following set of conservation equations of mass, momentum, and total energy

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0, \tag{2.1}$$

$$\frac{\partial (\rho \mathbf{v})}{\partial t} + \nabla \cdot (\rho \mathbf{v}\mathbf{v}) = -\nabla P + \nabla \cdot \boldsymbol{\tau}, \tag{2.2}$$

$$\frac{\partial (\rho E)}{\partial t} + \nabla \cdot (\rho \mathbf{v} E) = -\nabla \cdot \boldsymbol{q} - \nabla \cdot (P\mathbf{v}) + \nabla \cdot (\boldsymbol{\tau} \cdot \mathbf{v}), \tag{2.3}$$

where ρ is the density, $\mathbf{v}$ is the velocity vector, P is the pressure, $\boldsymbol{\tau}$ is the viscous stress tensor for Newtonian fluids, E is the total energy, and $\boldsymbol{q}$ is the Fourier heat conduction.

2.2. *Real-gas thermodynamics*

The thermodynamic space of solutions for the state variables pressure P, temperature T, and density ρ of a single substance is described by an equation of state. One popular choice for systems at high pressures, which is used in this study, is the Peng-Robinson equation of state (Peng & Robinson 1976) written as

$$P = \frac{R_u T}{\bar{v} - b} - \frac{a}{\bar{v}^2 + 2b\bar{v} - b^2}, \tag{2.4}$$

with R_u the universal gas constant, $\bar{v} = W/\rho$ the molar volume, and W the molecular weight. The coefficients a and b take into account real-gas effects related to attractive forces and finite packing volume, respectively, and depend on the critical temperatures T_c, critical pressures P_c, and acentric factors ω. They are defined as

$$a = 0.457\frac{(\mathrm{R_u}T_c)^2}{P_c}\left[1 + c\left(1 - \sqrt{T/T_c}\right)\right]^2 \quad \text{and} \quad b = 0.078\frac{\mathrm{R_u}T_c}{P_c}, \tag{2.5}$$

where coefficient c is provided by

$$c = \begin{cases} 0.380 + 1.485\omega - 0.164\omega^2 + 0.017\omega^3 & \text{if } \omega > 0.49, \\ 0.375 + 1.542\omega - 0.270\omega^2 & \text{otherwise.} \end{cases} \tag{2.6}$$

The Peng-Robinson real-gas equation of state needs to be supplemented with the corresponding high-pressure thermodynamic variables based on departure functions calculated as a difference between two states. In particular, their usefulness is to transform thermodynamic variables from ideal-gas conditions (low pressure—only temperature dependent) to supercritical conditions (high pressure). The ideal-gas parts are calculated with the NASA 7-coefficient polynomial (Burcat & Ruscic 2005), while the analytical departure expressions to high pressures are derived from the Peng-Robinson equation of state, as detailed in Jofre & Urzay (2021).

2.3. *Pressure-based formulation*

Eq. (2.3) for total energy can be equivalently substituted by the evolution equation of another thermodynamic variable using the equation of state and basic rules of calculus. Here, the focus is placed on the pressure equation, which can be derived by properly expanding the material derivative, as in, e.g.,

$$\frac{DP}{Dt} = \left(\frac{\partial P}{\partial \rho}\right)_e \frac{D\rho}{Dt} + \left(\frac{\partial P}{\partial e}\right)_\rho \frac{De}{Dt}, \tag{2.7}$$

where e is the internal energy. Upon properly deriving the material derivative of density, momentum and internal energy from Eqs. (2.1)–(2.3), the pressure evolution equation can be finally written as

$$\frac{\partial P}{\partial t} + \mathbf{v}\cdot\nabla P + \rho c^2 \nabla\cdot\mathbf{v} = \frac{1}{\rho}\frac{\beta_v}{c_v\beta_T}(\boldsymbol{\tau} : \nabla\otimes\mathbf{v} - \nabla\cdot\boldsymbol{q}), \tag{2.8}$$

where $c = 1/\sqrt{\rho\beta_s}$ is the speed of sound, with $\beta_s = -(1/v)\left(\partial v/\partial P\right)_s$ the isentropic compressibility and $v = 1/\rho$ the specific volume; $\beta_v = (1/v)\left(\partial v/\partial T\right)_P$ is the volume expansivity; c_v is the isochoric specific heat capacity; and $\beta_T = -(1/v)\left(\partial v/\partial P\right)_T$ is the isothermal compressibility. The system constituted by Eqs. (2.1)–(2.2) and Eq. (2.8) is formally equivalent to the one presented in Section 2.1 but has different discrete properties, as outlined in the subsequent sections.

3. Discretization frameworks

This section describes the discretization method of (i) the proposed KEP and PEP scheme introduced in Section 1 and of (ii) several existing methods utilized for trans- and supercritical fluids turbulence.

3.1. *Novel kinetic-energy- and pressure-equilibrium-preserving scheme*

The equations of fluid motion introduced in Section 2.1 are numerically tackled by adopting a standard semi-discretization procedure, i.e., they are first discretized in space and then integrated in time. Spatial differential operators are treated using centered finite-differencing formulas; a second-order centered scheme is used in this paper, although the results can be easily generalized to formulas of any order that satisfy a discrete summation-by-parts rule. The temporal errors that arise due to the time-integration scheme (in this case a Runge-Kutta method) are assumed to be kept under control by using sufficiently small time steps (Capuano *et al.* 2017*a*).

As reported in Section 1, the novel scheme is based on two main properties: KEP and PEP. With regards to KEP, the convective terms of Eqs. (2.1)–(2.3) can be rewritten with a common divergence (conservative) structure as

$$C^D = \frac{\partial \rho u_j \phi}{\partial x_j}, \tag{3.1}$$

where ϕ is the transported scalar. The derivation of a family of KEP methods relies on the preliminary observation that the general convective term in Eq. (3.1) can be equivalently expressed as follows, using the product rule (Coppola *et al.* 2019*b*)

$$C^\phi = \phi \frac{\partial \rho u_j}{\partial x_j} + \rho u_j \frac{\partial \phi}{\partial x_j}, \tag{3.2}$$

$$C^u = u_j \frac{\partial \rho \phi}{\partial x_j} + \rho \phi \frac{\partial u_j}{\partial x_j}, \tag{3.3}$$

$$C^\rho = \rho \frac{\partial u_j \phi}{\partial x_j} + \phi u_j \frac{\partial \rho}{\partial x_j}, \tag{3.4}$$

$$C^L = \rho \phi \frac{\partial u_j}{\partial x_j} + \rho u_j \frac{\partial \phi}{\partial x_j} + \phi u_j \frac{\partial \rho}{\partial x_j}. \tag{3.5}$$

Any linear combination of Eqs. (3.1)–(3.5) is a consistent formulation; for instance, the convective terms for mass ($\phi = 1$) and momentum ($\phi = u_i$) can be expressed as

$$\mathcal{M} = \xi \mathcal{M}^D + (1 - \xi)\mathcal{M}^A, \tag{3.6}$$

$$C = \alpha C^D + \beta C^\phi + \gamma C^u + \delta C^\rho + \epsilon C^L, \tag{3.7}$$

where ξ is an arbitrary coefficient and $\alpha + \beta + \gamma + \delta + \epsilon = 1$, and $\mathcal{M}^D$ and $\mathcal{M}^A$ are the divergence and advective forms for the continuity equation, respectively. It can be shown that, upon enforcing discrete conservation of global kinetic energy by convection, a two-parameter family of energy-preserving formulations is found (Coppola *et al.* 2019*b*). Here the attention will be focused on the so-called KGP (proposed by Kennedy & Gruber (2008) and later shown to be energy-preserving by Pirozzoli (2010)) split form, which is obtained by setting $\epsilon = 0$ (sufficient condition for local conservation) and $\alpha = \beta = \gamma = \delta = 1/4$. When applied to the continuity and momentum equations, the KGP scheme preserves kinetic energy by convection and has proved to be particularly robust in previous works, compared to other kinetic-energy-preserving splittings (Coppola *et al.*

2019*b*). Hereinafter, the scheme obtained by evolving Eqs. (2.1)–(2.3), with the KGP split applied to all the convective terms, will be referred to as KGP-Et.

The second component of the novel scheme is the enforcement of the PEP property. PEP refers to a property of the Euler equations, according to which, if pressure and velocity are initially constant in space, then pressure (and velocity) remains uniform and constant in time (Abgrall 1996). The property is easily shown by considering a one-dimensional inviscid version of the general pressure evolution equation, Eq. (2.8),

$$\frac{\partial P}{\partial t} = -\frac{\partial Pu}{\partial x} - (\rho c^2 - P)\frac{\partial u}{\partial x}, \tag{3.8}$$

as well as the one-dimensional velocity-evolution equation that can be derived by subtracting the mass equation multiplied by velocity from the momentum equation, yielding

$$\frac{\partial u}{\partial t} = -\frac{1}{\rho}\left(\frac{\partial \rho uu}{\partial x} + \frac{\partial P}{\partial x} - u\frac{\partial \rho u}{\partial x}\right). \tag{3.9}$$

Based on Eqs. (3.8)–(3.9), it can be immediately deduced that when the initial pressure and velocity are spatially constant (with density varying in space), then neither pressure nor velocity change in time; it is therefore highly desirable that this equilibrium is also discretely preserved in numerical simulations, leading to the concept of PEP schemes. Nonetheless, numerical methods generally fail to reproduce this property discretely, even in the context of ideal-gas thermodynamics.

Recently, Shima *et al.* (2021) and Jain & Moin (2022) proposed a flux formulation for internal energy (while keeping, e.g., KGP splitting for momentum) able to ensure PEP for compressible flows with ideal-gas equations of state. This method will be hereinafter referred to as PEP-IG. The extension of this approach to real-gas thermodynamics involves nonlinear departure functions and the real-gas equation of state, which makes the analytical derivation of a PEP splitting particularly involved. In this work, the PEP property is instead enforced by directly transporting an evolution equation for pressure, i.e., Eq. (2.8) instead of total energy, Eq. (2.3). It is easily shown that when pressure and velocity are initially uniform (with density varying in space), the discretization of Eq. (2.8) inherently satisfies $\partial P/\partial t = 0$.

The novel approach, labeled as KGP-Pt, is therefore based on the combinations of (i) KGP convective scheme applied to mass and momentum, Eqs. (2.1)–(2.2) and (ii) the solution of the pressure equation, Eq. (2.8).

3.2. *Alternative methods for high-pressure turbulent flows*

This section covers other standard numerical state-of-the-art approaches employed for solving the equations of fluid motion for compressible flow considered and tested in this study for comparison with the novel scheme.

– Divergence (D): Discretization of the conservative formulation of convection, as defined in Eq. (3.7). The divergence form usually suffers from nonlinear instability and leads to simulation blow-up, hence it is usually coupled with a stabilization scheme.

– Filtering (D + F4): This work focuses on the implicit filter F4 with $\alpha_f = 0.495$, as proposed by Visbal & Gaitonde (2002), which filters the conservative variables of the solution provided by the method D. These filters introduce numerical dissipation but are generally successful in stabilizing the solution (when a nonlinearly unstable scheme

is used). However, as reported by Lacaze *et al.* (2019), filtering can amplify pressure oscillations due to the interaction with thermodynamic nonlinearities, particularly across the pseudo-boiling line. The filter is defined as

$$\alpha_f \bar{\varphi}_{i-1} + \bar{\varphi} + \alpha_f \bar{\varphi}_{i+1} = \sum_{n=0}^{N} \frac{a_n}{n} (\varphi_{i+n} + \varphi_{i-n}), \tag{3.10}$$

where $\bar{\varphi}$ is the filtered variable and a_n the filter coefficient parameters. Even though increasing the order of the filter obviously leads to a less dissipative simulation, here the stencil is limited to a four-point function for efficiency purposes; indeed, increasing the stencil width is known to significantly deteriorate the parallel performances, especially when dealing with implicit spatial schemes (Capuano *et al.* 2017*b*).

– Upwind-biased scheme (UB, H): These methods have been often used to capture shocks and stabilize compressible simulations, either alone or in the context of hybrid methods [i.e., in conjunction with non-dissipative schemes (H), with sensor-based switching as proposed by Ducros *et al.* (1999)]. Nevertheless, they are supposed to be unsuitable for turbulence due to the high levels of artificial dissipation introduced. To this end, Section 4 will use for comparison both UB (HLLC) and H (KGP + HLLC).

– Double-flux (Df): The double-flux approach (Abgrall & Karni 2000) was recently extended by Ma *et al.* (2017) to transcritical fluids. In this method, the internal energy is fixed within the time-integration step to artificially enforce pressure equilibrium, at the expense of modifying the thermodynamics. Assuming a generalized relationship of type $e = (P\,v)/(\gamma^* - 1) + e_0^*$, where e_0^* and γ^* are nonlinear functions of the thermodynamic states, in this approach γ^* and e_0^* are forced to be frozen both in space and time during each time step. By doing so, the solution is exempt from spurious pressure oscillations. This method is usually coupled with the HLLC scheme (Ma *et al.* 2017), labeled hereinafter as UB-Df. However, for the purpose of comparison, the Df will also be assessed with the KGP scheme, here denoted as KGP-Df.

4. Numerical results

In this section, the numerical methods presented in Section 3 are comparatively assessed and the results are presented for a one-dimensional inviscid advective test both for (i) an ideal-gas and (ii) a real-gas framework.

4.1. *One-dimensional advection test (ideal-gas thermodynamics)*

As proposed by Shima *et al.* (2021), nonlinear one-dimensional advection is a useful test to numerically assess pressure equilibrium and the generation of spurious pressure-velocity oscillations. The sinusoidal density profile $\rho = (\rho_{min} + \rho_{max})/2 + (\rho_{max} - \rho_{min})/2 \cdot \sin(2\pi\, x)$ is advected at constant velocity $v_0 = 1\,\mathrm{m/s}$ and pressure $P_0 = 1\,\mathrm{Pa}$, where $\rho_{min} = 1\,\mathrm{kg/m^3}$ and $\rho_{max} = 3\,\mathrm{kg/m^3}$, with reference $\rho_0 = 2\,\mathrm{kg/m^3}$, on a domain of length $L = 1\,\mathrm{m}$ discretized with 41 grid points and $CFL = 0.3$. The flow is advanced up to $11 \cdot t/t_c$ ($t_c = 1s$) with a standard fourth-order Runge-Kutta time integrator. Two main conclusions can be extracted from the results shown in Figure 1. First, only three schemes are free from pressure oscillations: D (which however is not KEP and unstable for multi-dimensional flows), PEP-IG and the novel KGP-Pt. The KGP-Et suffers from spurious oscillations, which in fact affect the thermophysical quantities. However, dissipative methods minimize these oscillations, although not completely, as

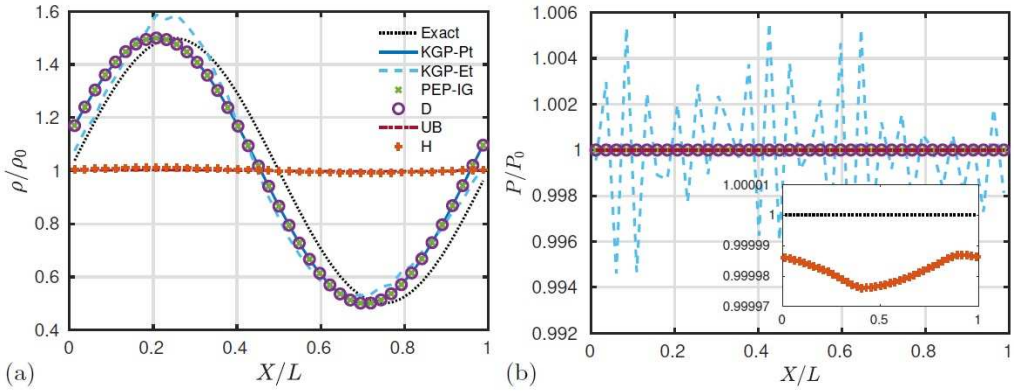

FIGURE 1. One-dimensional advection test under ideal-gas conditions ($\gamma = 1.4$), at $t/t_c = 11$ for KGP-Pt (solid blue line), KGP-Et (dashed cyan line), PEP-IG (green cross), D (purple circle), UB (red dashed-dotted line), and H (orange plus sign) with the black dotted line being the exact solution. Shown are normalized (a) density and (b) pressure.

seen for H in the inset to Figure 1(b). Second, the UB scheme leads to dissipation of the density wave, while the H scheme is dissipating at a slightly lower rate, although the sensor is generally switched on due to these oscillations, and the upwind-biased scheme is governing the convective term. In any case, it is unable to prevent pressure wiggles. All schemes suffer from density lag due to dispersion errors.

4.2. *One-dimensional advection test (real-gas thermodynamics)*

Similar to the ideal-gas advection test, a transcritical one-dimensional advection test is performed for the real-gas framework as proposed by Ma *et al.* (2017). The test is performed with the same domain length, mesh size, and time integrator as in the ideal-gas case. In this case, N_2 is the supercritical fluid operating at a bulk (constant) pressure of $P_0 = 5\,\mathrm{MPa}$ and advected at an initial constant velocity of $\mathbf{v}_0 = 1\,\mathrm{m/s}$. The smooth density profile is given by the harmonic wave $\rho = (\rho_{min} + \rho_{max})/2 + (\rho_{max} - \rho_{min})/2 \cdot \sin(2\pi x)$, with $\rho_{min}/\rho_c = 0.182$ ($T = 300\,\mathrm{K}$) and $\rho_{max}/\rho_c = 2.531$ ($T = 100\,\mathrm{K}$) with reference density $\rho_0/\rho_c = 0.305$ ($T = 200\,\mathrm{K}$).

Numerical results are depicted in Figure 2. Note that the schemes that did not attain PEP under ideal-gas conditions have not been assessed for this case, as this property will not be satisfied under transcritical conditions either. To this extent, the proposed method KGP-Pt is compared against D+F4 (the divergence form coupled with implicit filter), PEP-IG and the double-flux-based schemes. Four main conclusions can be extracted from the results: (i) the PEP-IG, scheme is no longer PEP under transcritical conditions, as demonstrated in the inset to Figure 2(b); (ii) the Df formulation is able to prevent the spurious oscillations only if it is coupled with UB method, whereas when used with KGP, the PEP property is not accomplished; (iii) filtering is unable to suppress pressure oscillations, and oscillations are particularly severe when crossing the pseudo-boiling line at $X/L \approx 0.65-0.85$, in accordance with previous results showing that filters may amplify pressure oscillations due to the interaction with nonlinear thermodynamics (Lacaze *et al.* 2019); and (iv) dissipative methods are clearly altering the thermodynamic properties [i.e., density in Figure 2(a)], especially UB-Df. A small amount of dissipation is present even when utilizing a low-dissipative filter, D+F4.

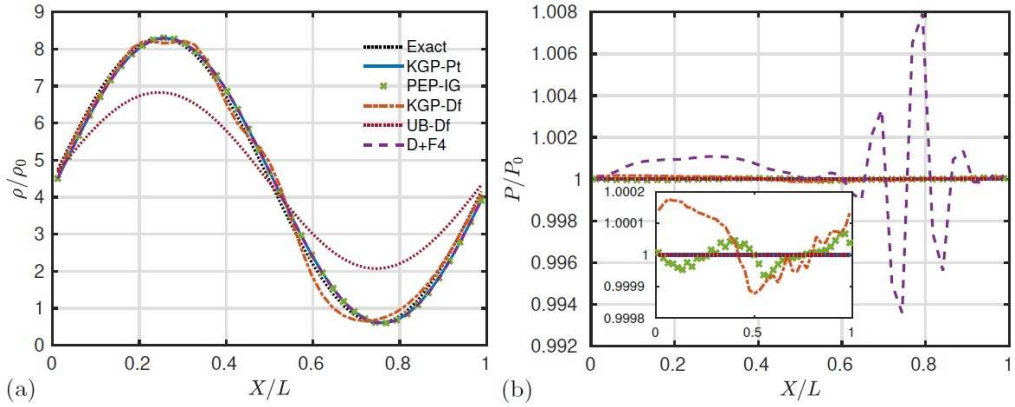

FIGURE 2. One-dimensional advection test under transcritical thermodynamic conditions, at $t/t_c = 10^{-2}$ for KGP-Pt (solid blue line), PEP-IG (green cross), KGP-Df (orange dashed-dotted line), UB-Df (red dotted line) and D+F4 (purple dashed line) with black-dotted line being the exact solution. Shown are normalized (a) density and (b) pressure.

	D	D+F4	KGP-Et	PEP-IG	UB	H	KGP-Pt	KGP-Df	UB-Df
KEP	×	×	⊙	⊙	×	×	⊙	⊙	×
PEP	○	○	×	○	○	○	⊙	×	⊙

TABLE 1. Summary of numerical schemes assessment; ○ property applies only to ideal gas, ⊙ property applies also to real gas, × property is not satisfied in any framework.

4.3. *Assessment summary*

Table 1 summarizes the KEP and PEP properties satisfied in ideal- and real-gas frameworks for the schemes assessed within this work. It can be observed that the attainment of both KEP and PEP properties under transcritical conditions is only accomplished by KGP-Pt scheme. Other state-of-the-art schemes cannot guarantee these requirements, as they are either contaminated by pressure oscillations, numerically dissipative, or globally unstable.

5. Conclusions

This work has focused on proposing a novel scheme for supercritical fluids turbulence and to comparatively assessing its performances with respect to several numerical schemes commonly used in the literature. The novel scheme is based on the enforcement of two main properties: (i) pressure equilibrium preservation, for stability against spurious pressure oscillations resulting from the inherent nonlinearities of real-gas thermodynamics, and (ii) kinetic-energy preservation by convection, to allow for low-dissipative simulations and to prevent unbounded amplification of aliasing errors. The KEP and PEP novel numerical method is proposed to be able to obtain stable and accurate transcritical turbulent simulations without the need for any form of artificial stabilization.

The proposed scheme has been assessed with respect to several state-of-the-art numerical schemes in a one-dimensional inviscid advection test. This test has been previously proved to be particularly challenging in terms of both (i) preservation of pressure equilib-

rium and (ii) nondissipative behavior. The results showed that the strategies specifically developed for this class of problems, like the double-flux scheme, are able to mitigate pressure oscillations but at the expense of requiring artificial dissipation based on upwind-biased schemes and/or additional terms in the equations of mass and momentum. However, KEP methods generally preserve kinetic energy for ideal- and real-gas conditions, although they are not able to avoid spurious pressure oscillations in either framework (ideal- or real-gas conditions), eventually yielding instability and even blow-up of the computations. In this regard, the novel scheme attains pressure equilibrium preservation while simultaneously conserving kinetic energy and, as a result, it is an ideal candidate for scale-resolving supercritical turbulence simulations.

These preliminary results motivate the authors to continue a careful assessment of this method, particularly to (i) evaluate its global and local conservation properties and (ii) comparatively test its behavior in a complex three-dimensional turbulent case.

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REFERENCES

Abgrall, R. 1996 How to prevent pressure oscillations in multicomponent flow calculations: A quasi conservative approach. *J. Comput. Phys.* **125**, 150–160.

Abgrall, R. & Karni, S. 2000 Computations of compressible multifluids. *J. Comput. Phys.* **169**, 594–623.

Bernades, M., Capuano, F., Trias, F. X. & Jofre, L. 2022 Energy-preserving stable computations of high-pressure supercritical fluids turbulence. In *9th European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS)*, pp. 1–12.

Bernades, M. & Jofre, L. 2022 Thermophysical analysis of microconfined turbulent flow regimes at supercritical fluid conditions in heat transfer applications. *J. Heat Transf.* **144**, 082501.

Burcat, A. & Ruscic, B. 2005 Third millennium ideal gas and condensed phase thermochemical database for combustion with updates from active thermochemical tables. *Tech. Rep.*, Argonne National Laboratory.

Capuano, F., Coppola, G., Rández, L. & de Luca, L. 2017*a* Explicit RungeKutta schemes for incompressible flow with improved energy-conservation properties. *J. Comput. Phys.* **328**, 86–94.

Capuano, F., Mastellone, A. & Angelis, E. D. 2017*b* A conservative overlap method for multi-block parallelization of compact finite-volume schemes. *Computers & Fluids* **159**, 327–337.

Coppola, G., Capuano, F. & de Luca, L. 2019*a* Discrete energy-conservation properties in the numerical simulation of the Navier-Stokes equations. *Appl. Mech. Rev.* **71**, 010803.

Coppola, G., Capuano, F., Pirozzoli, S. & de Luca, L. 2019*b* Numerically stable formulations of convective terms for turbulent compressible flows. *J. Comput. Phys.* **382**, 86–104.

Ducros, F., Ferrand, V., Nicoud, F., Weber, C., Darracq, D., Gacherieu, C.

& Poinsot, T. 1999 Large-eddy simulation of the shock/turbulence interaction. *J. Comput. Phys.* **1252**, 517–549.

Jain, S. S. & Moin, P. 2022 A kinetic energy–and entropy-preserving scheme for compressible two-phase flows. *J. Comput. Phys.* **464**, 111307.

Jofre, L. & Urzay, J. 2020 A characteristic length scale for density gradients in supercritical monocomponent flows near pseudoboiling. *Annual Research Briefs*, Center for Turbulence Research, Stanford University, pp. 277–282.

Jofre, L. & Urzay, J. 2021 Transcritical diffuse-interface hydrodynamics of propellants in high-pressure combustors of chemical propulsion systems. *Prog. Energy Combust. Sci.* **82**, 100877.

Kawai, S., Terashima, H. & Negishi, H. 2015 A robust and accurate numerical method for transcritical turbulent flows at supercritical pressure with an arbitrary equation of state. *J. Comput. Phys.* **300**, 116–135.

Kennedy, C. A. & Gruber, A. 2008 Reduced aliasing formulations of the convective terms within the NavierStokes equations for a compressible fluid. *J. Comput. Phys.* **227**, 1676–1700.

Lacaze, G., Schmitt, T., Ruiz, A. & Oefelein, J. 2019 Comparison of energy-, pressure- and enthalpy-based approaches for modeling supercritical flows. *Comput. Fluids* **181**, 35–56.

Ma, P. C., Lv, Y. & Ihme, M. 2017 An entropy-stable hybrid scheme for simulations of transcritical real-fluid flows. *J. Comput. Phys.* **340**, 330–357.

Peng, D. Y. & Robinson, D. B. 1976 A new two-constant equation of state. *Ind. Eng. Chem. Fundam.* **15**, 59–64.

Pirozzoli, S. 2010 Generalized conservative approximations of split convective derivative operators. *J. Comput. Phys.* **229**, 7180–7190.

Shima, N., Kuya, Y., Tamaki, Y. & Kawai, S. 2021 Preventing spurious pressure oscillations in split convective form discretization for compressible flows. *J. Comput. Phys.* **427**, 110060.

Shu, C. 1999 High order ENO and WENO schemes for computational fluid dynamics. *Lect. Notes Comput. Sci. Eng.* **9**, 439–582.

Terashima, H. & Koshi, M. 2012 Approach for simulating gas-liquid-like flows under supercritical pressures using a high-order central differencing scheme. *J. Comput. Phys.* **231**, 6907–6923.

Toro, F. 2009 *Riemann Solvers and Numerical Methods for Fluid Dynamics*, 3rd ed. Springer-Verlag, Berlin.

Visbal, M. R. & Gaitonde, D. V. 2002 On the use of higher-order finite-difference schemes on curvilinear and deforming meshes. *J. Comput. Phys.* **181**, 155–185.