

CONSISTENT ENERGY-EXCHANGE DISCRETIZATIONS FOR MULTIPHYSICS FLOWS

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Summary. *Structure-preserving discretizations for CFD have traditionally focused on the conservation of kinetic energy and other quadratic invariants. In multiphysics flows, however, kinetic energy is continuously exchanged with other energy reservoirs, such as potential, surface, elastic or magnetic energy. In this work, we formulate an operator-based principle for constructing compatible coupling forces. Given a transported field ϕ , an associated energy $E^\phi[\phi]$, and a transport operator $\mathcal{L}_u\phi$, the force coupled to the momentum equation is obtained by requiring exact energy exchange between kinetic energy and $E^\phi[\phi]$. The same principle is imposed at the discrete level. Once the discrete energy, transport operator and variable arrangement are fixed, the compatible discrete force follows from the corresponding discrete work identity. This links transport and coupling operators through discrete adjoint relations. The framework is developed for both staggered and collocated formulations and illustrated with buoyancy-driven flows and multiphase flows with surface tension.*

1 INTRODUCTION

Large-scale DNS and LES are increasingly applied to multiphysics flows in which kinetic energy continuously exchanges with other energy forms, such as potential, internal, surface, or electromagnetic energy. Classical energy-preserving and symmetry-preserving discretizations have primarily focused on the conservation of quadratic invariants [1, 2], most notably kinetic energy, in order to control numerical dissipation and improve robustness [3, 4]. While this property is essential, it is not sufficient for multiphysics simulations, where the correct representation of energy exchanges between different physical fields is often more relevant than the preservation of a single invariant.

In this work, we revisit symmetry-preserving discretizations of the incompressible Navier–Stokes equations from the perspective of discrete energy exchanges. We show that preserving fundamental operator symmetries at the discrete level not only guarantees the conservation of quadratic invariants, but also provides a consistent and physically meaningful framework for

coupling kinetic energy with other energy reservoirs. Importantly, a numerical method may conserve total energy while still producing spurious inter-energy transfers, leading to qualitatively incorrect multiphysics dynamics.

This viewpoint is particularly relevant for buoyancy-driven flows [5–8], multiphase systems with surface tension [9–12], and magnetohydrodynamic problems [13], where artificial energy exchanges can severely contaminate the solution. Emphasis is placed on formulations suitable for complex physics and complex geometries, requiring unstructured collocated meshes and robust pressure–velocity coupling strategies.

The proposed approach highlights consistent energy-exchange preservation as a guiding principle for the design of artificial-dissipation-free, stable, and physically consistent discretizations for multiphysics flows on unstructured grids.

2 CONTINUOUS FORMULATION

2.1 Continuous energy exchange principle

Let us consider the Navier–Stokes equations for a Newtonian fluid

$$\frac{\partial(\rho\mathbf{u})}{\partial t} + \nabla \cdot (\rho\mathbf{u} \otimes \mathbf{u}) = \nabla \cdot (2\mu\mathbf{S}) - \nabla p + \mathbf{f}^\phi, \quad (1)$$

$$\frac{\partial\rho}{\partial t} + \nabla \cdot (\rho\mathbf{u}) = 0, \quad (2)$$

coupled with the following generic transport equation

$$\frac{\partial\phi}{\partial t} + \mathcal{L}_\mathbf{u}\phi = 0 \quad \text{with} \quad \begin{cases} \mathcal{L}_\mathbf{u}\phi = (\mathbf{u} \cdot \nabla)\phi & \text{if } \phi \text{ is a scalar (0-form)} \\ \mathcal{L}_\mathbf{u}\phi = \nabla \cdot (\mathbf{u}\phi) & \text{if } \phi \text{ is a density-like (3-form)} \end{cases} \quad (3)$$

where $\mathcal{L}_\mathbf{u}$ is the Lie derivative. Assuming an inviscid flow with no contributions from the domain boundaries, $\partial\Omega$, the evolution of the total kinetic energy, $E_k \equiv \frac{1}{2}(\mathbf{u}, \rho\mathbf{u})$, reads

$$\frac{dE_k}{dt} = (\mathbf{u}, \mathbf{f}^\phi), \quad (4)$$

where $(a, b) = \int_\Omega abd\Omega$ is the usual innerproduct of functions. Then, the force $\mathbf{f}^\phi(\mathbf{x}, t)$ in Eq.(1) follows from the transport equation of the scalar field $\phi(\mathbf{x}, t)$ and the definition of the associated energy $E^\phi[\phi]$. To do so, we first need to define the conjugate variable μ^ϕ

$$\mu^\phi \equiv \frac{\delta E^\phi[\phi]}{\delta\phi} \longrightarrow \frac{dE^\phi}{dt} = (\mu^\phi, \partial_t\phi) \stackrel{(3)}{=} -(\mu^\phi, \mathcal{L}_\mathbf{u}\phi), \quad (5)$$

which is the variational derivative of $E^\phi[\phi]$ with respect to ϕ . Therefore, the force $\mathbf{f}^\phi$ follows from the conservation of (total) energy, *i.e.*

$$\frac{d}{dt}(E_k + E^\phi) = 0 \stackrel{(4)(5)}{\longrightarrow} (\mathbf{u}, \mathbf{f}^\phi) = (\mu^\phi, \mathcal{L}_\mathbf{u}\phi) \stackrel{(3)}{\longrightarrow} \mathbf{f}^\phi = \begin{cases} \mu^\phi \nabla \phi & \text{if } \phi \text{ is a scalar} \\ -\phi \nabla \mu^\phi & \text{if } \phi \text{ is a density} \end{cases} \quad (6)$$

Hence, the main message is that the force $\mathbf{f}^\phi$ follows from the definition of the associated energy, $E^\phi[\phi]$, and the Lie derivative, $\mathcal{L}_u$, in the transport equation of the scalar field ϕ

$$\boxed{\{E^\phi, \mathcal{L}_u\} \longrightarrow \mathbf{f}^\phi} \quad (7)$$

At this point, it is relevant to emphasize the difference between the transport of scalars versus densities (or 0-forms versus 3-forms using the terminology of differential forms). In the first case, where $\mathcal{L}_u\phi = (\mathbf{u} \cdot \nabla)\phi$, the definition of the force $\mathbf{f}^\phi$ follows straightforwardly

$$(\mu^\phi, \mathcal{L}_u\phi) = \int_\Omega \mu^\phi (\mathbf{u} \cdot \nabla)\phi d\Omega = \int_\Omega \mathbf{u} \cdot (\mu^\phi \nabla\phi) d\Omega = (\mathbf{u}, \mu^\phi \nabla\phi) \longrightarrow \boxed{\mathbf{f}^{\phi,[0]} = \mu^\phi \nabla\phi} \quad (8)$$

where the superscript in brackets indicates the form degree used in the transport equation. Thus, $\mathbf{f}^{\phi,[k]}$ denotes the force associated with the transport of ϕ as a k -form. For density-like quantities, or 3-forms, integration by parts gives

$$\begin{aligned} (\mu^\phi, \mathcal{L}_u\phi) &= \int_\Omega \mu^\phi \nabla \cdot (\mathbf{u}\phi) d\Omega = (\mu^\phi, \nabla \cdot (\mathbf{u}\phi)) = -(\nabla\mu^\phi, \mathbf{u}\phi) \\ &= - \int_\Omega \mathbf{u} \cdot \phi \nabla\mu^\phi d\Omega = -(\mathbf{u}, \phi \nabla\mu^\phi) \longrightarrow \boxed{\mathbf{f}^{\phi,[3]} = -\phi \nabla\mu^\phi} \end{aligned} \quad (9)$$

where boundary contributions have been omitted. Notice that the two force expressions differ by a gradient term,

$$\mathbf{f}^{\phi,[0]} = \mathbf{f}^{\phi,[3]} + \nabla(\phi\mu^\phi). \quad (10)$$

Hence, for incompressible flows they are dynamically equivalent up to pressure redefinition.

2.2 Practical examples

A key quantity in the previous analysis is the conjugate variable, μ^ϕ , defined in Eq.(5) as the variational derivative of the associated energy, $E^\phi[\phi]$, with respect to ϕ , *i.e.*

$$\left. \frac{d}{d\varepsilon} E^\phi[\phi + \varepsilon\eta] \right|_{\varepsilon=0} = (\mu^\phi, \eta), \quad (11)$$

for all admissible perturbations η . Let us first compute two generic examples

Energy form 1 (Local energy). Let us consider that the total associated energy is given by

$$E^\phi[\phi] \equiv \int_\Omega F(\phi) d\Omega, \quad (12)$$

where $F(\phi)$ is a well-posed function of $\phi(\mathbf{x}, t)$. Then, using Eq.(11) and recalling Leibniz's integral rule leads to

$$\begin{aligned} \left. \frac{d}{d\varepsilon} E^\phi[\phi + \varepsilon\eta] \right|_{\varepsilon=0} &= \frac{d}{d\varepsilon} \int_\Omega F(\phi + \varepsilon\eta) d\Omega \Big|_{\varepsilon=0} = \int_\Omega F'(\phi) \eta d\Omega \\ &= (F'(\phi), \eta) \longrightarrow \boxed{\mu^\phi = F'(\phi)} \quad \text{where } F'(\phi) = \partial F / \partial \phi. \end{aligned} \quad (13)$$

Energy form 2 (Total-variation energy). Let us consider that the total associated energy is

$$E^\phi[\phi] \equiv \int_{\Omega} |\nabla \phi| d\Omega. \quad (14)$$

In this case, Eq.(11) yields

$$\begin{aligned} \left. \frac{d}{d\varepsilon} E^\phi[\phi + \varepsilon \eta] \right|_{\varepsilon=0} &= \left. \frac{d}{d\varepsilon} \int_{\Omega} |\nabla(\phi + \varepsilon \eta)| d\Omega \right|_{\varepsilon=0} = \left. \frac{d}{d\varepsilon} \int_{\Omega} \sqrt{(\nabla \phi + \varepsilon \nabla \eta)^2} d\Omega \right|_{\varepsilon=0} \\ &= \left. \int_{\Omega} \frac{(\nabla \phi + \varepsilon \nabla \eta) \cdot \nabla \eta}{\sqrt{(\nabla \phi + \varepsilon \nabla \eta)^2}} d\Omega \right|_{\varepsilon=0} = \left(\frac{\nabla \phi}{|\nabla \phi|}, \nabla \eta \right) \end{aligned} \quad (15)$$

$$= -(\nabla \cdot \left(\frac{\nabla \phi}{|\nabla \phi|} \right), \eta) \longrightarrow \boxed{\mu^\phi = -\nabla \cdot \left(\frac{\nabla \phi}{|\nabla \phi|} \right)} \quad (16)$$

These two energy forms can now be connected with two common applications in CFD: buoyancy-driven flows (examples thereof can be found in Refs. [5–7]) and multiphase flows with surface tension (examples thereof can be found in Refs. [9–12]).

Physical case 1 (Buoyancy-driven flows). Based on Energy form 1.

In this case, the (mass) density field, $\rho(x, t)$, is associated with the *potential energy* given by

$$E^\rho[\rho] \equiv \int_{\Omega} \rho g z d\Omega. \quad (17)$$

Here, the gravitational field is assumed to point downward in the z -direction. This case corresponds to the Energy form 1 (see Eq. 13) with $F(\rho) = \rho g z$ and $F'(\rho) = g z$, leading to

$$\boxed{\mu^\rho = g z} \quad (18)$$

Similarly, for Boussinesq buoyancy, the *potential energy* is then defined as

$$E^T = - \int_{\Omega} T \mathbf{e}_z \cdot \mathbf{x} d\Omega = - \int_{\Omega} T z d\Omega, \quad (19)$$

leading to

$$\boxed{\mu^T = -z} \quad (20)$$

In this case, the associated scalar is the (mass) density, which is a 3-form. Therefore, the induced force reads

$$\boxed{\mathbf{f}^\rho \stackrel{(9)}{=} -\rho \nabla \mu^\rho \stackrel{(18)}{=} -\rho \nabla (g z) \stackrel{g=cte}{=} -\rho g \mathbf{e}_z} \quad (21)$$

which is the standard gravitational force. On the other hand, the Boussinesq buoyancy leads to

$$\boxed{\mathbf{f}^T \stackrel{(9)}{=} -T \nabla \mu^T \stackrel{(20)}{=} T \nabla z = T \mathbf{e}_z} \quad (22)$$

Physical case 2 (Surface tension). *Based on Energy form 2.* In multiphase flows, the energy associated with the interface area is given by the Helmholtz-free-energy

$$dF = \gamma dA, \quad (23)$$

where γ is the surface tension, *i.e.*, the reversible cost of creating one unit of interfacial area, A . Assuming constant temperature, volume and surface tension, the associated energy reads

$$E^\theta[\theta] \equiv \int_{\Omega} \gamma |\nabla \theta| d\Omega \stackrel{\gamma=cte}{=} \gamma \int_{\Omega} |\nabla \theta| d\Omega, \quad (24)$$

where $0 \leq \theta(x, t) \leq 1$ is the interface marker function. Notice that this corresponds to the Energy form 2 (see Eq. 16). Therefore, the corresponding conjugate variable reads

$$\mu^\theta = \gamma \kappa \quad \text{where} \quad \kappa = -\nabla \cdot \mathbf{n} \quad \text{and} \quad \mathbf{n} = \frac{\nabla \theta}{|\nabla \theta|}, \quad (25)$$

where κ and $\mathbf{n}$ are the surface curvature and the interface normal, respectively. In this case, the associated scalar is the interface marker, which is a 0-form. Therefore, the induced force reads

$$\boxed{\mathbf{f}^\theta \stackrel{(8)}{=} \mu^\theta \nabla \theta \stackrel{(25)}{=} \gamma \kappa \nabla \theta} \quad (26)$$

3 STRUCTURE-PRESERVING DISCRETIZATION OF MULTIPHYSICS FLOWS

3.1 Introduction

The same principles discussed above apply at discrete level. Namely, given a definition of the discrete associated energy $E_h^\phi[\phi_c]$ and a discrete transport operator for ϕ_c , the compatible discretization of the force $\mathbf{f}_h^\phi$ is obtained by enforcing the corresponding discrete energy exchange. In what follows, discrete quantities are denoted using the subscripts c and s , which refer respectively to cell-centered quantities and quantities staggered at the cell faces. Unless otherwise stated, we follow the notation used in Refs. [3, 14].

Therefore, in the next subsections, we replicate the analysis at discrete level. First, we define the discrete counterparts of the associated energies and their conjugate variables. Then, we combine these definitions with the discrete transport operator used for the advection of the associated scalar field in order to derive the corresponding discrete force. In this second part of the analysis, we need to consider two different scenarios, depending on whether the momentum equation is solved using a collocated arrangement [3] or a face-staggered one [15].

3.2 Discrete conjugate variables

Discrete form of Physical case 1 (Buoyancy-driven flows). The discrete counterpart of the *potential energy* defined in Eq.(17) reads

$$E_h^\rho[\rho_c] \equiv \rho_c \cdot \Omega_c (g_c \circ z_c), \quad (27)$$

where Ω_c is a diagonal matrix containing the cell volumes, $\circ$ denotes the Hadamard product, and ρ_c , g_c and z_c are column vectors containing the cell-centered density, gravitational acceleration and z -coordinate, respectively. As before, the gravitational field is assumed to point downward in the z -direction. Then, likewise the continuous case, the discrete conjugate variable is the variational derivative of $E_h^\rho[\rho_c]$ with respect to ρ_c ,

$$\left. \frac{d}{d\varepsilon} E_h^\rho[\rho_c + \varepsilon \eta_c] \right|_{\varepsilon=0} = \eta_c \cdot \Omega_c (g_c \circ z_c) \longrightarrow \boxed{\mu_c^\rho = g_c \circ z_c} \quad (28)$$

which is the discrete counterpart of Eq.(18).

Similarly, for the Boussinesq buoyancy, the *potential energy* is defined as follows

$$E_h^T \equiv -T_c \cdot \Omega_c z_c, \quad (29)$$

where T_c is a cell-centered temperature field. Then, the discrete conjugate variable yields

$$\left. \frac{d}{d\varepsilon} E_h^T[T_c + \varepsilon \eta_c] \right|_{\varepsilon=0} = -\eta_c \cdot \Omega_c z_c \longrightarrow \boxed{\mu_c^T = -z_c} \quad (30)$$

which is the discrete counterpart of Eq.(20).

Discrete form of Physical case 2 (Surface tension). In this case, the discrete Helmholtz-free-energy associated with the cell-centered interface marker, θ_c , is given by

$$E_h^\theta[\theta_c] \equiv \gamma \mathbf{1}_c \cdot \Omega \sqrt{g_x^\theta \circ g_x^\theta + g_y^\theta \circ g_y^\theta} = \gamma \mathbf{1}_c \cdot \Omega |G_c \theta_c|, \quad (31)$$

which is the discrete counterpart of Eq. (24). Here, $\Omega \equiv \mathbf{l}_d \otimes \Omega_c$, where $\mathbf{l}_d$ is the identity matrix of order d and d is the number of spatial dimensions. Functions of vectors are understood component-wise; in particular, $\sqrt{a}$ denotes the vector with entries $\sqrt{(a)_i}$, while $|\cdot|$ denotes the local magnitude of a discrete vector field. In the present two-dimensional setting, $d = 2$, and g_x^θ and g_y^θ are the cell-centered gradients of the interface marker in the x - and y -directions, respectively. The extension to three dimensions is straightforward. In this case,

$$\begin{pmatrix} g_x^\theta \\ g_y^\theta \end{pmatrix} = G_c \theta_c = \Gamma_{s \rightarrow c} G \theta_c \quad \text{where} \quad g_x^\theta = G_x \theta_c \quad \text{and} \quad g_y^\theta = G_y \theta_c, \quad (32)$$

where G is the standard cell-to-face gradient and $\Gamma_{s \rightarrow c}$ is the face-to-cell vector interpolation. For details, the reader is referred to Refs. [3, 14]. Then, the discrete conjugate variable follows

$$\left. \frac{d}{d\varepsilon} E_h^\theta[\theta_c + \varepsilon \eta_c] \right|_{\varepsilon=0} = \gamma \mathbf{1}_c \cdot \Omega_c \frac{(G_x \eta_c) \circ (G_x \theta_c) + (G_y \eta_c) \circ (G_y \theta_c)}{\sqrt{g_x^\theta \circ g_x^\theta + g_y^\theta \circ g_y^\theta}} = \gamma \frac{G_c \theta_c}{|G_c \theta_c|} \Omega G_c \eta_c. \quad (33)$$

Then, recalling the definition of the cell-to-cell discrete gradient, G_c , given in Eq.(32), and the fundamental relation between face-to-cell, $\Gamma_{s \rightarrow c}$, and cell-to-face, $\Gamma_{c \rightarrow s}$, momentum interpolations (see previous works [3, 4, 14], for details)

$$\Gamma_{s \rightarrow c} = \Omega^{-1} \Gamma_{c \rightarrow s}^T \Omega_s, \quad (34)$$

we obtain

$$\left. \frac{d}{d\varepsilon} E_h^\theta[\boldsymbol{\theta}_c + \varepsilon \boldsymbol{\eta}_c] \right|_{\varepsilon=0} = \gamma \frac{\mathbf{G}_c \boldsymbol{\theta}_c}{|\mathbf{G}_c \boldsymbol{\theta}_c|} \Gamma_{c \rightarrow s}^T \Omega_s \mathbf{G} \boldsymbol{\eta}_c = \gamma \left(\Gamma_{c \rightarrow s} \frac{\mathbf{G}_c \boldsymbol{\theta}_c}{|\mathbf{G}_c \boldsymbol{\theta}_c|} \right) \Omega_s \mathbf{G} \boldsymbol{\eta}_c \quad (35)$$

$$\stackrel{(37)}{=} -\gamma \left(\Gamma_{c \rightarrow s} \frac{\mathbf{G}_c \boldsymbol{\theta}_c}{|\mathbf{G}_c \boldsymbol{\theta}_c|} \right) \mathbf{M}^T \boldsymbol{\eta}_c = -\gamma \Omega_c^{-1} \mathbf{M} \left(\Gamma_{c \rightarrow s} \frac{\mathbf{G}_c \boldsymbol{\theta}_c}{|\mathbf{G}_c \boldsymbol{\theta}_c|} \right) \cdot \Omega_c \boldsymbol{\eta}_c, \quad (36)$$

where $\mathbf{M}$ is the integrated discrete divergence operator, which is related to the discrete gradient through the standard duality pairing,

$$\mathbf{M}^T = -\Omega_s \mathbf{G}. \quad (37)$$

Therefore, the discrete conjugate variable reads

$$\boxed{\boldsymbol{\mu}_c^\theta = -\gamma \Omega_c^{-1} \mathbf{M} \left(\Gamma_{c \rightarrow s} \frac{\mathbf{G}_c \boldsymbol{\theta}_c}{|\mathbf{G}_c \boldsymbol{\theta}_c|} \right)} \quad (38)$$

which is the discrete counterpart of Eq.(25).

3.3 Discrete Lie derivative

Once the discrete associated energy $E_h^\phi[\phi_c]$ has been defined for a cell-centered scalar field ϕ_c , its corresponding conjugate variable $\boldsymbol{\mu}_c^\phi$ follows from the discrete variational derivative. The second key ingredient is the discrete Lie derivative, namely the transport operator used to advect ϕ_c . Let us consider the following discrete transport equation

$$\Omega_c \frac{d\phi_c}{dt} + \mathbf{C}_c(\mathbf{u}_s) \phi_c = \mathbf{0}_c, \quad (39)$$

where $\mathbf{C}_c(\mathbf{u}_s)$ is the convective operator discretized in divergence form

$$\mathbf{C}_c(\mathbf{u}_s) = \mathbf{M} \mathbf{U}_s \Pi_{c \rightarrow s}^\phi, \quad (40)$$

where $\mathbf{U}_s \equiv \text{diag}(\mathbf{u}_s)$ and $\Pi_{c \rightarrow s}^\phi$ is the cell-to-face interpolation, which can be split as follows

$$\Pi_{c \rightarrow s}^\phi = \Pi_{c \rightarrow s}^{\text{SP}} + \frac{1}{2} \text{sign}(\mathbf{U}_s) (\mathbf{I}_s - \boldsymbol{\Psi}_s) \mathbf{T}_{cs}, \quad (41)$$

where $\mathbf{T}_{cs}$ is the cell-to-face incidence matrix. Furthermore, $\boldsymbol{\Psi}_s$ is a diagonal matrix that is used to define the level of local *upwinding* for a given face f , e.g. $[\boldsymbol{\Psi}_s]_f = 1$ (symmetry-preserving, SP) and $[\boldsymbol{\Psi}_s]_f = 0$ (upwind). Finally, $\Pi_{c \rightarrow s}^{\text{SP}} = \frac{1}{2} |\mathbf{T}_{cs}|$ is the standard unweighted interpolation, i.e. $[\phi_s]_f = \frac{1}{2} ([\phi]_{c1} + [\phi]_{c2})$ where $c1$ and $c2$ are the two cells adjacent to the face f . For further details, the reader is referred to Refs. [3, 14]. For the sake of simplicity, hereafter, we use the following notation

$$\Pi_{c \rightarrow s}^\phi = \Pi_{c \rightarrow s}^{\text{SP}} + \Upsilon_{c \rightarrow s}^\phi \quad \text{where} \quad \Upsilon_{c \rightarrow s}^\phi = \frac{1}{2} \text{sign}(\mathbf{U}_s) (\mathbf{I}_s - \boldsymbol{\Psi}_s) \mathbf{T}_{cs}. \quad (42)$$

In this way, any possible scheme (upwind, hybrid, flux limiter,..) can be easily represented in this framework, except those schemes that may involve cell values different than those adjacent to the face. At this point, it is relevant to remark that

$$\mathbf{C}_c^{\text{SP}}(\mathbf{u}_s) \equiv \mathbf{M}\mathbf{U}_s\Pi_{c\rightarrow s}^{\text{SP}}, \quad (43)$$

is skew-symmetric *iff* the incompressibility constraint $\mathbf{M}\mathbf{u}_s = \mathbf{0}_c$ is exactly satisfied, *i.e.*

$$\mathbf{C}_c^{\text{SP}}(\mathbf{u}_s) + (\mathbf{C}_c^{\text{SP}}(\mathbf{u}_s))^T = \text{diag}(\mathbf{M}\mathbf{u}_s). \quad (44)$$

Therefore, a strictly skew-symmetric convective matrix can be constructed if we remove its diagonal entries as follows

$$\mathbf{C}_c^{\text{SSP}}(\mathbf{u}_s) = \mathbf{C}_c^{\text{SP}}(\mathbf{u}_s) - \frac{1}{2}\text{diag}(\mathbf{M}\mathbf{u}_s). \quad (45)$$

Then, the convective operator defined in Eq.(40) can be split into a strictly symmetry-preserving (SSP) part, a dilatational part, and a symmetric (diffusive-like) operator. Namely,

$$\begin{aligned} \mathbf{C}_c(\mathbf{u}_s) &= \mathbf{M}\mathbf{U}_s\Pi_{c\rightarrow s}^\phi \stackrel{(42)}{=} \mathbf{M}\mathbf{U}_s\Pi_{c\rightarrow s}^{\text{SP}} + \mathbf{M}\mathbf{U}_s\Upsilon_{c\rightarrow s}^\phi \stackrel{(43)}{=} \mathbf{C}_c^{\text{SP}}(\mathbf{u}_s) + \mathbf{M}\tilde{\Lambda}_s\mathbf{G} \\ &\stackrel{(45)}{=} \mathbf{C}_c^{\text{SSP}}(\mathbf{u}_s) + \frac{1}{2}\text{diag}(\mathbf{M}\mathbf{u}_s) + \mathbf{M}\tilde{\Lambda}_s\mathbf{G}, \end{aligned} \quad (46)$$

where $\tilde{\Lambda}_s \equiv \frac{1}{2}\text{sign}(\mathbf{U}_s)(\mathbf{I}_s - \Psi_s)\Delta_s$ and Δ_s is a diagonal matrix containing the distances between cells adjacent to a face. For the sake of clarity, we can rewrite previous equation as follows

$$\boxed{\mathbf{C}_c(\mathbf{u}_s) = \mathbf{C}_c^{\text{SSP}}(\mathbf{u}_s) + \Sigma_c^C(\mathbf{u}_s) + \mathbf{D}_c^C(\mathbf{u}_s)} \quad (47)$$

where

$$\mathbf{C}_c^{\text{SSP}}(\mathbf{u}_s) = \mathbf{C}_c^{\text{SP}}(\mathbf{u}_s) - \Sigma_c^C(\mathbf{u}_s), \quad (48)$$

$$\Sigma_c^C(\mathbf{u}_s) = \frac{1}{2}\text{diag}(\mathbf{M}\mathbf{u}_s), \quad (49)$$

$$\mathbf{D}_c^C(\mathbf{u}_s) = \mathbf{M}\tilde{\Lambda}_s\mathbf{G} \stackrel{(46)}{=} \mathbf{M}\mathbf{U}_s\Upsilon_{c\rightarrow s}^\phi. \quad (50)$$

3.4 Discrete adjoint formulation of the force

Finally, for the discrete formulation of the coupling force, we need to distinguish two scenarios: a face-staggered formulation of the momentum equation and a collocated one.

3.4.1 Staggered formulation

Let us begin with the scenario where the momentum equation is solved at the cell faces. Hence, we need to compute the staggered force $\mathbf{f}_s^\phi$. We will need to consider two situations:

namely, when the transported quantity is a (i) scalar (0-form) field (see Eq. 8) and a (ii) density-like (3-form) field. In this second case, the force $\mathbf{f}_s^\phi$ must have the form given in Eq.(9).

First of all, the evolution of the total energy at discrete level reads

$$\frac{d}{dt}(E_{k,s} + E_h^\phi) = \mathbf{u}_s \cdot \Omega_s \mathbf{f}_s^\phi + \left(\frac{\delta E_h^\phi}{\delta \phi_c} \right)^T \cdot \Omega_c \frac{d\phi_c}{dt} \stackrel{(5)(39)}{=} \mathbf{u}_s \cdot \Omega_s \mathbf{f}_s^\phi - \boldsymbol{\mu}_c^\phi \cdot \mathbb{C}_c(\mathbf{u}_s) \phi_c. \quad (51)$$

where $E_{k,s} \equiv \frac{1}{2} \rho \mathbf{u}_s \cdot \Omega_s \mathbf{u}_s$. Hence, energy conservation yields the following relation

$$\boxed{\mathbf{u}_s \cdot \Omega_s \mathbf{f}_s^\phi = \boldsymbol{\mu}_c^\phi \cdot \mathbb{C}_c(\mathbf{u}_s) \phi_c} \quad (52)$$

which is the discrete counterpart of Eq.(6). Let us now rewrite the r.h.s. in such a way that resembles the form of the l.h.s.,

$$\boldsymbol{\mu}_c^\phi \cdot \mathbb{C}_c(\mathbf{u}_s) \phi_c \stackrel{(40)(37)}{=} -\boldsymbol{\mu}_c^\phi G^T \Omega_s \mathbb{U}_s \Pi_{c \rightarrow s}^\phi \phi_c = -((G\boldsymbol{\mu}_c^\phi) \circ (\Pi_{c \rightarrow s}^\phi \phi_c)) \cdot \Omega_s \mathbf{u}_s. \quad (53)$$

Hence, the staggered force reads

$$\boxed{\mathbf{f}_s^{\phi,[3]} \equiv -((G\boldsymbol{\mu}_c^\phi) \circ (\Pi_{c \rightarrow s}^\phi \phi_c))} \quad (54)$$

Thus, in this case, the cell-centered scalar field, ϕ_c , must be interpolated to the faces using the same interpolation used for its advection (see Eqs. 39 and 40).

Let us now consider the first case (i), where the force must take the form given in Eq.(8). Recalling the splitting of the convective term given in Eq.(47) and taking its transpose,

$$\mathbb{C}_c^T(\mathbf{u}_s) \stackrel{(40)}{=} (\Pi_{c \rightarrow s}^\phi)^T \mathbb{U}_s \mathbb{M}^T \stackrel{(47)}{=} -\mathbb{C}_c^{\text{SSP}}(\mathbf{u}_s) + \Sigma_c^C(\mathbf{u}_s) + \mathbb{D}_c^C(\mathbf{u}_s). \quad (55)$$

Then, plugging this result and Eq.(48) into the r.h.s. of Eq.(52) leads to

$$\begin{aligned} \boldsymbol{\mu}_c^\phi \cdot \mathbb{C}_c(\mathbf{u}_s) \phi_c &= \phi_c \cdot \mathbb{C}_c^T(\mathbf{u}_s) \boldsymbol{\mu}_c^\phi \stackrel{(55)}{=} \phi_c \cdot (-\mathbb{C}_c^{\text{SSP}}(\mathbf{u}_s) + \Sigma_c^C(\mathbf{u}_s) + \mathbb{D}_c^C(\mathbf{u}_s)) \boldsymbol{\mu}_c^\phi \\ &\stackrel{(48)}{=} \phi_c \cdot (-\mathbb{C}_c^{\text{SP}}(\mathbf{u}_s) + 2\Sigma_c^C(\mathbf{u}_s) + \mathbb{D}_c^C(\mathbf{u}_s)) \boldsymbol{\mu}_c^\phi. \end{aligned} \quad (56)$$

Then, recalling the definitions given in Eq.(43) and Eqs.(48)-(50), and the duality pairing between the gradient and the divergence operator given in Eq.(37), we can rearrange the three terms in the r.h.s. of previous expression as follows

$$-\phi_c \cdot \mathbb{C}_c^{\text{SP}}(\mathbf{u}_s) \boldsymbol{\mu}_c^\phi \stackrel{(43)(37)}{=} \phi_c \cdot G^T \Omega_s \mathbb{U}_s \Pi_{c \rightarrow s}^{\text{SP}} \boldsymbol{\mu}_c^\phi = ((G\phi_c) \circ (\Pi_{c \rightarrow s}^{\text{SP}} \boldsymbol{\mu}_c^\phi)) \cdot \Omega_s \mathbf{u}_s, \quad (57)$$

$$2\phi_c \cdot \Sigma_c^C(\mathbf{u}_s) \boldsymbol{\mu}_c^\phi \stackrel{(49)}{=} (\phi_c \circ \boldsymbol{\mu}_c^\phi) \cdot \mathbb{M} \mathbf{u}_s \stackrel{(37)}{=} - (G(\phi_c \circ \boldsymbol{\mu}_c^\phi)) \cdot \Omega_s \mathbf{u}_s, \quad (58)$$

$$\phi_c \cdot \mathbb{D}_c^C(\mathbf{u}_s) \boldsymbol{\mu}_c^\phi \stackrel{(50)(37)}{=} -\phi_c \cdot G^T \Omega_s \mathbb{U}_s \Upsilon_{c \rightarrow s}^\phi \boldsymbol{\mu}_c^\phi = -((G\phi_c) \circ (\Upsilon_{c \rightarrow s}^\phi \boldsymbol{\mu}_c^\phi)) \cdot \Omega_s \mathbf{u}_s, \quad (59)$$

finally, leading to

$$\boldsymbol{\mu}_c^\phi \cdot \mathbf{C}_c(\mathbf{u}_s) \boldsymbol{\phi}_c = ((\mathbf{G}\boldsymbol{\phi}_c) \circ ((\Pi_{c \rightarrow s}^{\text{SP}} - \Upsilon_{c \rightarrow s}^\phi) \boldsymbol{\mu}_c^\phi)) \cdot \Omega_s \mathbf{u}_s - (\mathbf{G}(\boldsymbol{\phi}_c \circ \boldsymbol{\mu}_c^\phi)) \cdot \Omega_s \mathbf{u}_s. \quad (60)$$

Hence, in this case, the conjugate variable, $\boldsymbol{\mu}_c^\phi$, must be interpolated with $\Pi_{c \rightarrow s}^{\text{SP}} - \Upsilon_{c \rightarrow s}^\phi$; that is, reversing the sign of the *upwinding part* of the cell-to-face interpolation used in the transport of the scalar field (see Eqs. 39 to 42). The same result was obtained in Ref. [10] in the context of multiphase simulations using a conservative level-set method [16]. Hence, in this case, the staggered force reads

$$\boxed{\mathbf{f}_s^{\phi, [0]} \equiv (\mathbf{G}\boldsymbol{\phi}_c) \circ ((\Pi_{c \rightarrow s}^{\text{SP}} - \Upsilon_{c \rightarrow s}^\phi) \boldsymbol{\mu}_c^\phi) - \mathbf{G}(\boldsymbol{\phi}_c \circ \boldsymbol{\mu}_c^\phi)} \quad (61)$$

Notice that this extra gradient term is the discrete counterpart of the rightmost term in Eq.(10). The reason behind this extra force is that we are using the divergence-form for the advection even though it is a 0-form. Nevertheless, for incompressible flows this extra term has no effect on the flow dynamics.

3.4.2 Collocated formulation

Let us finally consider the collocated formulation. It is essentially the same as the staggered one studied above but with the momentum equation solved at the cells. Therefore, at the end, we should reach the following equality

$$\boxed{\mathbf{u}_c \cdot \Omega \mathbf{f}_c^\phi = \boldsymbol{\mu}_c^\phi \cdot \mathbf{C}_c(\mathbf{u}_s) \boldsymbol{\phi}_c} \quad (62)$$

where $\Omega \equiv \mathbf{I}_d \otimes \Omega_c$ is the diagonal matrix containing the cell volumes associated with the cell-centered velocity components, $\mathbf{u}_c = (\mathbf{u}_1^T, \mathbf{u}_2^T, \mathbf{u}_3^T)^T$. Let us consider that both velocities are related via the standard cell-to-face momentum interpolation, $\Gamma_{c \rightarrow s}$, plus a projection, $\mathbf{F}_s$, to make the staggered velocity field incompressible,

$$\mathbf{u}_s = \mathbf{F}_s \Gamma_{c \rightarrow s} \mathbf{u}_c = (\mathbf{I} - \mathbf{G}\mathbf{L}^{-1}\mathbf{M}) \Gamma_{c \rightarrow s} \mathbf{u}_c \quad \longrightarrow \quad \mathbf{M}\mathbf{u}_s = \mathbf{0}_c. \quad (63)$$

where $\mathbf{L} \equiv \mathbf{M}\mathbf{G}$ is the discrete Laplacian. Then, plugging this into Eq.(52) leads to

$$\begin{aligned} \boldsymbol{\mu}_c^\phi \cdot \mathbf{C}_c(\mathbf{u}_s) \boldsymbol{\phi}_c &= \mathbf{f}_s^\phi \cdot \Omega_s (\mathbf{I} - \mathbf{G}\mathbf{L}^{-1}\mathbf{M}) \Gamma_{c \rightarrow s} \mathbf{u}_c \stackrel{(34)}{=} \mathbf{f}_s^\phi \cdot \Gamma_{s \rightarrow c}^T \Omega \mathbf{u}_c - \mathbf{f}_s^\phi \cdot \Omega_s \mathbf{G}\mathbf{L}^{-1}\mathbf{M} \Gamma_{c \rightarrow s} \mathbf{u}_c \\ &\stackrel{(37)}{=} \mathbf{f}_s^\phi \cdot (\Gamma_{s \rightarrow c}^T \Omega - \mathbf{M}^T \mathbf{L}^{-1} \mathbf{G}^T \Omega_s \Gamma_{c \rightarrow s}) \mathbf{u}_c \stackrel{(34)}{=} (\Gamma_{s \rightarrow c} (\mathbf{I} - \mathbf{G}\mathbf{L}^{-1}\mathbf{M}) \mathbf{f}_s^\phi) \cdot \Omega \mathbf{u}_c \end{aligned} \quad (64)$$

Therefore, in this case, if we assume that $\mathbf{u}_s$ is a projection of $\Gamma_{c \rightarrow s} \mathbf{u}_c$, then the collocated force is the projected staggered force interpolated to the cells,

$$\boxed{\mathbf{f}_c^\phi = \Gamma_{s \rightarrow c} \mathbf{F}_s \mathbf{f}_s^\phi} \quad (65)$$

where $\mathbf{F}_s \equiv \mathbf{I} - \mathbf{G}\mathbf{L}^{-1}\mathbf{M}$ is the projection operator onto a divergence-free space.

Field type	$\mathcal{L}_u \phi$	f^ϕ Eqs. (8)-(9)	f_s^ϕ Eqs. (61)-(54)	f_c^ϕ Eq. (65)
Scalar (0-form)	$(\mathbf{u} \cdot \nabla) \phi$	$\mu^\phi \nabla \phi$	$(\mathbf{G} \phi_c) \circ ((\Pi_{c \rightarrow s}^{\text{SP}} - \Upsilon_{c \rightarrow s}^\phi) \mu_c^\phi) - \mathbf{G}(\phi_c \circ \mu_c^\phi)$	$f_c^\phi = \Gamma_{s \rightarrow c} \mathbf{F}_s f_s^\phi,$
Density-like (3-form)	$\nabla \cdot (\mathbf{u} \phi)$	$-\phi \nabla \mu^\phi$	$-\left((\mathbf{G} \mu_c^\phi) \circ (\Pi_{c \rightarrow s}^\phi \phi_c)\right)$	if $\mathbf{u}_s = \mathbf{F}_s \Gamma_{c \rightarrow s} \mathbf{u}_c$

Table 1: Continuous and discrete coupling forces obtained from the energy-exchange principle.

Physical case	Field	Form	$E^\phi[\phi]$	$E_h^\phi[\phi_c]$	μ^ϕ	μ_c^ϕ
Buoyancy	ρ	3-form	$\int_{\Omega} \rho g z \, d\Omega$	$\rho_c \cdot \Omega_c (g_c \circ z_c)$	$g z$	$g_c \circ z_c$
Boussinesq buoyancy	T	3-form	$-\int_{\Omega} T z \, d\Omega$	$-\mathbf{T}_c \cdot \Omega_c z_c$	$-z$	$-z_c$
Surface tension	θ	0-form	$\gamma \int_{\Omega} \nabla \theta \, d\Omega$	$\gamma \mathbf{1}_c \cdot \Omega \mathbf{G}_c \theta_c $	$\gamma \kappa = -\gamma \nabla \cdot \left(\frac{\nabla \theta}{ \nabla \theta } \right)$	$-\gamma \Omega_c^{-1} \mathbf{M} \left(\Gamma_{c \rightarrow s} \frac{\mathbf{G}_c \theta_c}{ \mathbf{G}_c \theta_c } \right)$

Table 2: Associated energies and conjugate variables for the physical examples considered in this work.

4 SUMMARY AND APPLICATIONS

The paper can be summarized by the central message given in Eq. (7):

$$\boxed{\{E^\phi, \mathcal{L}_u\} \longrightarrow f^\phi}$$

Once the associated energy, E^ϕ , and transport operator, $\mathcal{L}_u$, of a field, ϕ , are fixed, the compatible coupling force, f^ϕ , follows from exact exchange with kinetic energy. At the continuous level, this yields the force expressions associated with scalar (0-form) and density-like (3-form) transport. At the discrete level, the same idea becomes a work identity linking the discrete energy, transport operator and variable arrangement through adjoint relations. Tables 1 and 2 summarize the resulting forces, associated energies and conjugate variables for the examples considered in this work. Thus, buoyancy, Boussinesq buoyancy and surface-tension forces are obtained from the same energy-exchange principle, providing a common framework for multiphysics flows involving potential, interfacial, elastic or electromagnetic energy reservoirs. Detailed numerical tests will be addressed in forthcoming studies.

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