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STRUCTURE-PRESERVING MULTIPHYSICS SIMULATIONS USING PORTABLE ALGEBRAIC KERNELS

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Abstract. Modern HPC systems are enabling scale-resolving multiphysics CFD at increasingly realistic levels of complexity. Exploiting this capability requires discretizations that remain physically consistent while yielding portable and efficient implementations on heterogeneous architectures. In multiphysics problems, kinetic energy continuously exchanges with other energy forms; hence, these transfers must be represented consistently. We revisit structure-preserving discretizations from this energy-exchange viewpoint and show how compatible transport operators determine the corresponding forces in the momentum equation. Since the resulting formulation is algebraic by construction, it can be assembled from a reduced set of portable kernels, providing a natural route towards maintainable high-performance multiphysics solvers on modern HPC systems.

1 INTRODUCTION

Modern HPC systems are making scale-resolving CFD feasible for increasingly complex multiphysics configurations. Exploiting this capability requires more than just larger and larger computations: discretizations must represent the coupled physics consistently, while implementations must remain portable, efficient and maintainable on heterogeneous architectures. This is especially relevant for DNS and LES, where the computational cost is high and small numerical inconsistencies may accumulate over long-time integrations.

In multiphysics flows, kinetic energy exchanges with potential, internal, surface, elastic or magnetic energy. Structure-preserving discretizations have traditionally focused on the conservation of kinetic energy and other quadratic invariants [1, 2]. Nevertheless, these conservation properties are not enough to ensure correct multiphysics couplings since spurious transfers between individual reservoirs may still occur.

Here, we use the consistency of these exchanges as a guiding principle. Given a transported field and its associated energy, the corresponding force in the momentum equation is obtained by requiring exact exchange with kinetic energy. Imposing the same idea at the discrete level leads to compatible transport and coupling operators. Since the formulation is algebraic by construction, it naturally connects with portable kernel-based implementations [3].

2 STRUCTURE-PRESERVING DISCRETIZATION OF MULTIPHYSICS

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

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

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

coupled with the following generic transport equation

$$\frac{\partial \phi}{\partial t} + \mathcal{L}_{\boldsymbol{u}}\phi = 0 \quad \text{where} \quad \left\{ \begin{array}{ll} \mathcal{L}_{\boldsymbol{u}}\phi = (\boldsymbol{u}\cdot\nabla)\phi & \text{if } \phi \text{ is a scalar (0-form)} \\ \mathcal{L}_{\boldsymbol{u}}\phi = \nabla\cdot(\boldsymbol{u}\phi) & \text{if } \phi \text{ is a density-like (3-form)} \end{array} \right. \tag{3}$$

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

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

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

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

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

$$\frac{d}{dt}(E_k + E^{\phi}) = 0 \overset{(4)(5)}{\longrightarrow} (\boldsymbol{u}, \boldsymbol{f}^{\phi}) = (\mu^{\phi}, \mathcal{L}_{\boldsymbol{u}}\phi) \overset{(3)}{\longrightarrow} \boldsymbol{f}^{\phi} = \left\{ \begin{array}{ll} \mu^{\phi}\nabla\phi & \text{if } \phi \text{ is a scalar} \\ -\phi\nabla\mu^{\phi} & \text{if } \phi \text{ is a density} \end{array} \right. \tag{6}$$

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

$$\boxed{\{E^{\phi}, \mathcal{L}_{\boldsymbol{u}}\} \quad \longrightarrow \quad \boldsymbol{f}^{\phi}} \tag{7}$$

The same principle emerges at discrete level. Namely, given a definition of the discrete associated energy, E_h^{ϕ}, and the discrete transport term of $\boldsymbol{\phi}_c$, it yields the discretization of the force $\boldsymbol{f}_h^{\phi}$. A clear example thereof is the potential energy (with gravity $\boldsymbol{g} = -g\boldsymbol{e}_z$)

$$E^{\rho} \equiv \int_\Omega \rho g z \quad \overset{(5)}{\longrightarrow} \quad \mu^{\rho} = gz \quad \overset{(6)}{\longrightarrow} \quad \boldsymbol{f}^{\rho} = -\rho\nabla\mu^{\rho} = -\rho g \boldsymbol{e}_z, \tag{8}$$

whereas at discrete level, and following the same notation used in [4], the discrete transport equation for the cell-centered density field, $\boldsymbol{\rho}_c$, reads

$$\Omega_c \frac{d\boldsymbol{\rho}_c}{dt} + \mathsf{C}(\boldsymbol{u}_s)\,\boldsymbol{\rho}_c = \boldsymbol{0}_c, \tag{9}$$

where Ω_c is a diagonal matrix containing the cell volumes and $\mathsf{C}(\boldsymbol{u}_s)$ is the convective operator discretized in divergence form as follows

$$\mathsf{C}(\boldsymbol{u}_s) = \mathsf{M}\mathsf{U}_s\Pi^{\rho}_{c\to s}, \tag{10}$$

where M is the face-to-cell divergence operator in integral form, $\mathsf{U}_s \equiv \mathrm{diag}(\boldsymbol{u}_s)$ is a diagonal matrix containing the face velocities, $\boldsymbol{u}_s$, and $\Pi^{\rho}_{c\to s}$ is the cell-to-face interpolation. Then, we define the discrete potential energy and its corresponding discrete conjugate variable

$$E^{\rho}_h \equiv g\boldsymbol{\rho}_c \cdot \Omega_c \boldsymbol{z}_c \quad \longrightarrow \quad \mu^{\rho}_c = g\boldsymbol{z}_c, \tag{11}$$

where $\boldsymbol{z}_c$ is a cell-centered column vector containing the z-coordinate of the cells. Then, assuming that the momentum equation is solved using a staggered arrangement, which is the standard approach for canonical buoyancy-driven configurations [5], the time evolution of the total discrete kinetic energy, $E_{k,s} = \frac{1}{2}\boldsymbol{u}_s \cdot \Omega_s(\boldsymbol{\rho}_s \odot \boldsymbol{u}_s)$ reads

$$\frac{dE_{k,s}}{dt} = \boldsymbol{u}_s \cdot \Omega_s \boldsymbol{f}^{\rho}_s, \tag{12}$$

which is the discrete counterpart of Eq.(4) and Ω_s is a diagonal matrix containing the staggered volumes associated with $\boldsymbol{u}_s$. Here, we also assume an inviscid flow with vanishing contributions from the domain boundary. Likewise the continuous case (see Eq. 6), the discretization of the force $\boldsymbol{f}^{\rho}_s$ arises from the total energy conservation at discrete level

$$\begin{aligned}
\frac{d}{dt}(E_{k,s} + E^{\rho}_h) = 0 \overset{(10)(12)}{\longrightarrow}\ \boldsymbol{u}_s \cdot \Omega_s \boldsymbol{f}^{\rho}_s &= \mu^{\rho}_c \mathsf{M}\mathsf{U}_s \Pi^{\rho}_{c\to s}\boldsymbol{\rho}_c = -\mu^{\rho}_c \mathsf{G}^T \Omega_s((\Pi^{\rho}_{c\to s}\boldsymbol{\rho}_c) \odot \boldsymbol{u}_s) \\
&= -((\mathsf{G}\mu^{\rho}_c) \odot (\Pi^{\rho}_{c\to s}\boldsymbol{\rho}_c))\Omega_s \boldsymbol{u}_s \\
&\overset{(11)}{=} -g(\mathsf{N}_{s,z}\Pi^{\rho}_{c\to s}\boldsymbol{\rho}_c)\cdot \Omega_s \boldsymbol{u}_s \rightarrow \boxed{\boldsymbol{f}^{\rho}_s = -g\mathsf{N}_{s,z}\Pi^{\rho}_{c\to s}\boldsymbol{\rho}_c}
\end{aligned} \tag{13}$$

where $\mathsf{G} = -\Omega_s^{-1}\mathsf{M}^T$ is the discrete gradient operator and $\mathsf{N}_{s,z}$ is a diagonal matrix containing the z-components of the face normal vector.

Remark 1 *The key consequence of Eq. (13) is that the cell-to-face interpolation of the density, $\boldsymbol{\rho}_c$, is not arbitrary: it must be the same operator $\Pi^{\rho}_{c\to s}$ used in the density transport equation (see Eqs. 9 and 10).*

3 PORTABLE ALGEBRAIC KERNELS

All the discrete operations described above can be expressed as algebraic operations on sparse matrices and vectors. This leads to a separation between numerical formulation and hardware-dependent implementation: the structure-preserving properties are encoded in the sparse matrix coefficients, while portability and optimization are handled at the kernel level. This algebraic point-of-view is consistent with the minimal-kernel strategy previously proposed for DNS and LES [3]: CFD algorithms must then be reformulated in terms of a few portable operations, mainly SpMV, dot products and vector updates. Such

a restriction improves maintainability across heterogeneous platforms, but also exposes challenges: the low arithmetic intensity of SpMV must be addressed, and flux limiters, boundary conditions and eigenvalue bounds for time-step control [4] must be recast within the same algebraic framework. When the same sparse operator is applied to several variables, components, time slices, multiple SpMV operations can be grouped into a sparse matrix-matrix product (SpMM), increasing data reuse and arithmetic intensity without changing the underlying discrete formulation [6].

4 CONCLUSIONS

We have outlined a structure-preserving approach for multiphysics CFD in which the force coupled to the momentum equation is derived from the transported field and its associated energy. At the discrete level, this requirement determines compatible transport and coupling operators, preventing spurious transfers between energy reservoirs. Since the formulation is algebraic by construction, it can be implemented through a reduced set of portable kernels, linking physical consistency with high-performance multiphysics solvers on modern HPC systems. Results for several multiphysics problems, together with performance analyses on different HPC systems, will be presented at the conference.

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