Metriplectic Integrators for Dissipative Fluids

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Abstract. Many systems from fluid dynamics and plasma physics possess a so-called metriplectic structure, that is the equations are comprised of a conservative, Hamiltonian part, and a dissipative, metric part. Consequences of this structure are conservation of important quantities, such as mass, momentum and energy, and compatibility with the laws of thermodynamics, e.g., monotonic dissipation of entropy and existence of a unique equilibrium state.
For simulations of such systems to deliver accurate and physically correct results, it is important to preserve these relations and conservation laws in the course of discretisation. This can be achieved most easily not by enforcing these properties directly, but by preserving the underlying abstract mathematical structure of the equations, namely their metriplectic structure. From that, the conservation of the aforementioned desirable properties follows automatically.
This paper describes a general and flexible framework for the construction of such metriplectic structure-preserving integrators, that facilitates the design of novel numerical methods for systems from fluid dynamics and plasma physics.

Keywords: Fluid Dynamics · Geometric Numerical Integration · Metriplectic Dynamics

1 Metriplectic Dynamics

Metriplectic dynamics [12, 11, 14, 15, 16, 6, 7, 8] provides a convenient framework for the description of systems that encompass both Hamiltonian and dissipative parts. The Hamiltonian evolution of such a system is determined by a Poisson bracket $\{\cdot,\cdot\}$ and the Hamiltonian functional $\mathcal{H}$, usually the total energy of the system. The dissipative evolution is determined by a metric bracket $(\cdot,\cdot)$ and some functional $\mathcal{S}$ that evolves monotonically in time, usually some kind of entropy.

Let us denote by $u(t,x) = (u^1, u^2, ..., u^m)^T$ the dynamical variables, defined over the domain $\mathcal{D}$ with coordinates x. The evolution of any functional $\mathcal{F}$ of the dynamical variables u is given by

$$\frac{\mathrm{d}\mathcal{F}}{\mathrm{d}t} = \{\mathcal{F},\mathcal{G}\} + (\mathcal{F},\mathcal{G})\,, \tag{1}$$

with $\mathcal{G} = \mathcal{H} - \mathcal{S}$ a generalised free energy functional, analogous with the Gibb's free energy from thermodynamics, $\{\cdot,\cdot\}$ a Poisson bracket, and $(\cdot,\cdot)$ a metric bracket. The Poisson bracket, describing the ideal, conservative evolution of the system, is a bilinear, anti-symmetric bracket of the form

$$\{\mathcal{A},\mathcal{B}\} = \int_{\mathcal{D}} \frac{\delta\mathcal{A}}{\delta u^i}\,\mathcal{J}^{ij}(u)\,\frac{\delta\mathcal{B}}{\delta u^j}\,\mathrm{d}x, \tag{2}$$

where $\mathcal{A}$ and $\mathcal{B}$ are functionals of u and $\delta\mathcal{A}/\delta u^i$ is the functional derivative, defined by

$$\frac{d}{d\epsilon}\mathcal{A}\big[u^1,\, ...,\, u^i + \epsilon v^i,\, ...,\, u^m\big]\Big|_{\epsilon=0} = \int_{\mathcal{D}} \frac{\delta\mathcal{A}}{\delta u^i}\, v^i \,\mathrm{d}x. \tag{3}$$

The kernel of the bracket, $\mathcal{J}(u)$, is an anti-self-adjoint operator, which has the property that

$$\sum_{l=1}^{m}\left(\frac{\partial\mathcal{J}^{ij}(u)}{\partial u^l}\,\mathcal{J}^{lk}(u) + \frac{\partial\mathcal{J}^{jk}(u)}{\partial u^l}\,\mathcal{J}^{li}(u) + \frac{\partial\mathcal{J}^{ki}(u)}{\partial u^l}\,\mathcal{J}^{lj}(u)\right) = 0 \qquad \text{for} \qquad 1 \leq i,j,k \leq m, \tag{4}$$

ensuring that the bracket $\{\cdot,\cdot\}$ satisfies the Jacobi identity,

$$\{\{\mathcal{A},\mathcal{B}\},\mathcal{C}\} + \{\{\mathcal{B},\mathcal{C}\},\mathcal{A}\} + \{\{\mathcal{C},\mathcal{A}\},\mathcal{B}\} = 0, \tag{5}$$

for arbitrary functionals $\mathcal{A},\mathcal{B},\mathcal{C}$ of u. Apart from that, $\mathcal{J}(u)$ is not required to be of any particular form, and most importantly it is allowed to depend on the fields u. If $\mathcal{J}(u)$ has a non-empty nullspace, there exist so-called Casimir invariants, that is functionals $\mathcal{C}$ for which $\{\mathcal{A},\mathcal{C}\} = 0$ for all functionals $\mathcal{A}$. The monotonic entropy functional $\mathcal{S}$ is usually one of these Casimir invariants.

The metric bracket $(\cdot,\cdot)$, describing non-ideal, dissipative effects, is a symmetric bracket, defined in a similar way as the Poisson bracket by

$$(\mathcal{A},\mathcal{B}) = \int_{\mathcal{D}} \frac{\delta\mathcal{A}}{\delta u^i}\,\mathcal{G}^{ij}(u)\,\frac{\delta\mathcal{B}}{\delta u^j}\,\mathrm{d}x, \tag{6}$$

where $\mathcal{G}(u)$ is now a self-adjoint operator with an appropriate nullspace such that $(\mathcal{H},\mathcal{G}) = 0$. All Casimirs $\mathcal{C}$ of the Poisson bracket should be Casimirs also of the metric bracket, except the entropy functional $\mathcal{S}$ which is explicitly required not to be a Casimir of the metric bracket.

In the following, we choose a convention that dissipates entropy and conserves the Hamiltonian, so that the equilibrium state is reached when entropy is at minimum. For this framework and our conventions to be consistent, it is essential that (i) $\mathcal{H}$ is a Casimir of the metric bracket, (ii) $\mathcal{S}$ is a Casimir of the Poisson bracket, and that (iii) the metric bracket is positive semi-definite. With respect to these choices, we then have

$$\frac{\mathrm{d}\mathcal{H}}{\mathrm{d}t} = \{\mathcal{H},\mathcal{G}\} + (\mathcal{H},\mathcal{G}) = \{\mathcal{H},-\mathcal{S}\} = 0, \qquad \frac{\mathrm{d}\mathcal{S}}{\mathrm{d}t} = \{\mathcal{S},\mathcal{G}\} + (\mathcal{S},\mathcal{G}) = -\,(\mathcal{S},\mathcal{S}) \leq 0, \tag{7}$$

reproducing the First and Second Law of Thermodynamics.

For an equilibrium state u_{eq}, the time evolution of any functional $\mathcal{F}$ stalls and the entropy functional reaches its minimum. If the metriplectic system has no Casimirs, the equilibrium state satisfies an energy principle, according to which the first variation of the free energy vanishes, $\delta\mathcal{G}[u_{eq}] = 0$, and its second variation is strictly positive, $\delta^2\mathcal{G}[u_{eq}] > 0$ (for details see e.g. [10]). If Casimirs $\mathcal{C}_i$ exist, the equilibrium state becomes degenerate, and the energy principle must be modified to account for the existing Casimirs. This leads to the so-called energy--Casimir principle [17]. In this case the the equilibrium state satisfies

$$\delta\mathcal{G}[u_{eq}] + \sum_i \lambda_i \delta\mathcal{C}_i[u_{eq}] = 0, \tag{8}$$

where λ_i act as Lagrange multipliers and are determined uniquely from the values of the Casimirs at the initial conditions for u. Lastly, for each $x \in \mathcal{D}$ the equilibrium state of the free-energy functional

$\mathcal{G}$ is unique. This can be verified by employing a convexity argument, namely if $\mathcal{D}$ is a convex domain and $\mathcal{G}$ is strictly convex, then $\mathcal{G}$ has at most one critical point (see e.g. [5] for details). This is the case if

$$\delta^2(\mathcal{G} + \sum_i \lambda_i \mathcal{C}_i) > 0, \tag{9}$$

for the non-vanishing field u_{eq}.

2 Dissipative Hydrodynamics

Many dissipative systems from fluid dynamics and plasma physics feature a metriplectic structure. Examples include Korteweg-type fluids [9, 20, 19, 21, 22], geophysical fluid flows [3, 4] and extended magnetohydronamics [2]. In the following we consider the example of viscous heat-conductive flows, whose state is described in terms of the variables (ρ, m, σ), where ρ is the mass density, m is the momentum density, and σ is the entropy density. The ideal dynamics of this system are described by the Poisson bracket [18, 1, 9, 17, 19, 21]

$$\begin{aligned}\{\mathcal{A},\mathcal{B}\} = \int_{\mathcal{D}} m(x,t)\cdot\left[\frac{\delta\mathcal{B}}{\delta m}\cdot\nabla\frac{\delta\mathcal{A}}{\delta m} - \frac{\delta\mathcal{A}}{\delta m}\cdot\nabla\frac{\delta\mathcal{B}}{\delta m}\right] + \int_{\mathcal{D}}\rho(x,t)\left[\frac{\delta\mathcal{B}}{\delta m}\cdot\nabla\frac{\delta\mathcal{A}}{\delta\rho} - \frac{\delta\mathcal{A}}{\delta m}\cdot\nabla\frac{\delta\mathcal{B}}{\delta\rho}\right] \\ + \int_{\mathcal{D}}\sigma(x,t)\left[\frac{\delta\mathcal{B}}{\delta m}\cdot\nabla\frac{\delta\mathcal{A}}{\delta\sigma} - \frac{\delta\mathcal{A}}{\delta m}\cdot\nabla\frac{\delta\mathcal{B}}{\delta\sigma}\right],\end{aligned} \tag{10}$$

and the Hamiltonian functional

$$\mathcal{H} = \int_{\mathcal{D}}\left[\frac{1}{\rho}\frac{|m|^2}{2} + \rho\, U(\rho,\sigma/\rho)\right]\mathrm{d}x. \tag{11}$$

Here, U denotes the internal energy, from which the pressure and temperature follow as $p = \rho^2 U_\rho$ and $T = \rho U_\sigma$, respectively. The ideal dynamics preserves the total mass, momentum and entropy,

$$\frac{d\mathcal{M}}{dt} = \{\mathcal{M},\mathcal{H}\} = 0, \qquad \mathcal{M} = \int_{\mathcal{D}}\rho(x,t)\,\mathrm{d}x, \tag{12}$$

$$\frac{d\mathcal{P}}{dt} = \{\mathcal{P},\mathcal{H}\} = 0, \qquad \mathcal{P} = \int_{\mathcal{D}} m(x,t)\,\mathrm{d}x, \tag{13}$$

$$\frac{d\mathcal{S}}{dt} = \{\mathcal{S},\mathcal{H}\} = 0, \qquad \mathcal{S} = \int_{\mathcal{D}}\sigma(x,t)\,\mathrm{d}x, \tag{14}$$

where mass and entropy are Casimir invariants of the Poisson bracket (10), i.e., $\{\mathcal{M},\mathcal{B}\} = 0$ and $\{\mathcal{S},\mathcal{B}\} = 0$ for any $\mathcal{B}$, and conservation of momentum follows from a symmetry of the Hamiltonian (11), i.e., $\{\mathcal{M},\mathcal{H}\} = 0$ only for $\mathcal{H}$ (for details see e.g. Reference [17]). Dissipation due to viscous friction and heat conduction is modelled by the metric bracket [20, 19, 21]

$$\begin{aligned}(\mathcal{A},\mathcal{B}) = \int_{\mathcal{D}} 2\mu\left[T\left\langle\nabla\frac{\delta\mathcal{A}}{\delta m}\right\rangle - \frac{\delta\mathcal{A}}{\delta\sigma}\langle\nabla v\rangle\right] : \left[T\left\langle\nabla\frac{\delta\mathcal{B}}{\delta m}\right\rangle - \frac{\delta\mathcal{B}}{\delta\sigma}\langle\nabla v\rangle\right]\mathrm{d}x \\ + \int_{\mathcal{D}}\lambda\left[T\nabla\cdot\frac{\delta\mathcal{A}}{\delta m} - \frac{\delta\mathcal{A}}{\delta\sigma}\nabla\cdot v\right]\cdot\left[T\nabla\cdot\frac{\delta\mathcal{B}}{\delta m} - \frac{\delta\mathcal{B}}{\delta\sigma}\nabla\cdot v\right]\mathrm{d}x\end{aligned}$$

$$+ \int_{\mathcal{D}} \kappa T^2 \nabla \left[\frac{1}{T}\frac{\delta \mathcal{A}}{\delta \sigma}\right] \cdot \nabla \left[\frac{1}{T}\frac{\delta \mathcal{B}}{\delta \sigma}\right] \mathrm{d}x, \tag{15}$$

and the entropy functional from (14). Here, $v = m/\rho$ denotes the velocity, μ the coefficient of shear viscosity, λ the coefficient of bulk viscosity, κ the thermal conductivity, and $\langle\cdot\rangle$ denotes the projection

$$\langle \nabla v \rangle = \frac{1}{2}(\nabla v + \nabla v^T) - \frac{1}{3}(\operatorname{trace} \nabla v)\mathbb{1}, \tag{16}$$

with $\mathbb{1}$ the 3×3 identity matrix. Note that all of the coefficients μ, λ and κ need to be non-negative for the metric bracket (15) to be positive semi-definite. It is straightforward to verify that the metric bracket (15) preserves mass (12), momentum (13) and energy (11). The equations of motion are computed using (1) for $\mathcal{F} \in \{\rho, m, \sigma\}$ and $\mathcal{G} = \mathcal{H} - \mathcal{S}$ with $\mathcal{H}$ from (11) and $\mathcal{S}$ from (14) as

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot m, \tag{17}$$

$$\frac{\partial m}{\partial t} = -\nabla \cdot (m \otimes v) + \nabla \cdot \left[(\rho \nabla \cdot \xi - p)\mathbb{1} - \nabla\rho \otimes \xi + 2\mu \langle \nabla v \rangle + \lambda(\nabla \cdot v)\mathbb{1}\right], \tag{18}$$

$$\frac{\partial \sigma}{\partial t} = -\nabla \cdot \left[\sigma v - \frac{\kappa \nabla T}{T}\right] + \frac{1}{T}\left[2\mu \langle \nabla v \rangle \cdot \langle \nabla v \rangle + \lambda(\nabla \cdot v)^2 + \frac{\kappa}{T}\left|\nabla T\right|^2\right]. \tag{19}$$

With standard approaches such as finite element or discontinuous Galerkin methods, numerical algorithms are obtained by direct discretisation of these equations. The idea of metriplectic integrators [13] instead is to construct discrete expressions of the brackets (10) and (15) and to obtain semi-discrete equations of motion from the discrete brackets in analogy to (1). The advantage of the latter approach is that important properties like energy conservation and monotonic dissipation of entropy will automatically be preserved.

3 Metriplectic Integrators

In the following, we describe a general framework for the construction of structure-preserving integrators for dissipative fluids and similar systems that have a metriplectic structure. This framework facilitates the construction of novel numerical methods that automatically preserve important physical quantities, such as mass, energy and the laws of thermodynamics, independently of the particular discretisation framework. Due to limited space, we do not go into the details of a specific discretisation technique and we only consider the spatial discretisation and its properties independently of a particular temporal discretisation. The fully discrete setting together with numerical examples will be described elsewhere.

The spatial discretisation consists of the following components: (a) choosing approximations of the function spaces of the dynamical variables, (b) choosing approximations of the inner products on these spaces, (c) choosing an approximation of functionals, (d) choosing a finite-dimensional representation of the functional derivative. The first step implies the choice of an appropriate finite element or similar space. The second as well as the third step tend to boil down to choosing a quadrature formula. And the last step usually amounts to the most simple choice of a plain partial derivative. Apart from these degrees of freedom, the whole construction is systematic and automatic. Everything follows from these choices and the metriplectic structure of the system of equations.

In the following, we explain this methodology using a rather abstract continuous Galerkin approach, where we do not go into the details of an actual discretisation of the domain or a specific choice of basis (that is we do not concretise component (a) from above). This avoids certain technicalities that arise in practical applications and specific frameworks such as discontinuous Galerkin methods, and thus allows us to focus on conveying the general idea of metriplectic integrators. Nonetheless, the following treatment should provide enough insight for applying and adapting the framework to other discretisation techniques. Concrete examples of discretisations using discontinuous Galerkin methods will be discussed in consecutive publications.

Let v and w be elements of $\mathbb{V} = L^2(\mathcal{D})$, that is the space of square integrable functions over $\mathcal{D}$ with scalar product

$$\langle v\,,\, w\rangle_{\mathcal{D}} = \int_{\mathcal{D}} v(x)\, w(x)\,\mathrm{d}x. \tag{20}$$

Let $\mathbb{V}_h \subset \mathbb{V}$ denote some finite dimensional subspace and $\{\varphi_i\}_{i=1}^N$ a basis in $\mathbb{V}_h$. Then $v_h \in \mathbb{V}_h$ can be written as

$$v_h(t,x) = \sum_{i=1}^{N} v_i(t)\,\varphi_i(x). \tag{21}$$

The discretisation of the density ρ, the momentum m and the entropy density σ follow in full analogy with the function spaces $\mathbb{V}$ chosen appropriately. Note that while ρ and σ are scalar quantities, the momentum m is a three-vector.

In simple situations, we can retain the inner product $\langle\cdot\,,\,\cdot\rangle$ on $\mathbb{V}$ and work with the continuous functionals $\mathcal{F}$ evaluated on (ρ_h, m_h, σ_h), however, in many situations the resulting integrals cannot be computed easily. Therefore we introduce an approximate inner product $\langle\cdot\,,\,\cdot\rangle_h$ as well as approximate functionals $\mathcal{F}_h$ by utilising some quadrature rule $\{(b_n, c_n)\}_{n=1}^R$, where c_n denotes the nodes of the quadrature and b_n the weights, such that

$$\langle v_h\,,\, w_h\rangle_h = \sum_{n=1}^{R} b_n v_h(c_n)\, w_h(c_n) = V^T \mathbb{M} W, \tag{22}$$

with $V = (v_1, v_2, ..., v_N)^T$ the coefficient vector of v_h when expressed in the basis $\{\varphi_i\}_{i=1}^N$ according to (21), analogously W for w_h, and $\mathbb{M}$ the mass matrix

$$\mathbb{M}_{ij} = \sum_{n=1}^{R} b_n\, \varphi_i(c_n)\, \varphi_j(c_n). \tag{23}$$

In the same fashion, functionals of (ρ, m, σ) are approximated using the quadrature rule $\{(b_n, c_n)\}_{n=1}^R$, e.g., for the Hamiltonian (11) we obtain

$$\mathcal{H}_h[\rho_h, m_h, \sigma_h] = \sum_{n=1}^{R} b_n \left[\frac{|m_h(c_n)|^2}{2\rho_h(c_n)} + \rho_h(c_n)\, U\big(\rho_h(c_n),\, \sigma_h(c_n)/\rho_h(c_n)\big)\right] \equiv \mathsf{H}(\hat\rho, \hat m, \hat\sigma), \tag{24}$$

for the mass (12), momentum (13), and entropy (14), respectively, we get

$$\mathcal{M}_h[\rho_h] = \sum_{n=1}^{R} b_n\, \rho_h(c_n) = 1_N^T \mathbb{M}^\rho \hat\rho \equiv \mathsf{M}(\hat\rho), \tag{25}$$

$$\mathcal{P}_h[\rho_h] = \sum_{n=1}^{R} b_n \, m_h(c_n) = 1_{3N}^T \mathbb{M}^m \hat{m} \equiv \mathsf{P}(\hat{m}), \tag{26}$$

$$\mathcal{S}_h[\sigma_h] = \sum_{n=1}^{R} b_n \, \sigma_h(c_n) = 1_N^T \mathbb{M}^\sigma \hat{\sigma} \equiv \mathsf{S}(\hat{\sigma}), \tag{27}$$

where $\hat{\rho} = (\rho_1, \rho_2, ..., \rho_N)$ are the coefficients of ρ_h, cf. Equation (21), and analogously $\hat{m} = (m_1, m_2, ..., m_{3N})$ and $\hat{\sigma} = (\sigma_1, \sigma_2, ..., \sigma_N)$ are the coefficients of the discrete momentum m_h and entropy density σ_h. By $1_N \in \mathbb{R}^N$ and $1_{3N} \in \mathbb{R}^{3N}$ we denote the respective vectors with all components being equal to 1, and $\mathbb{M}^a$ denotes the mass matrices for $a \in \{\rho, m, \sigma\}$ corresponding to the respective basis functions φ^a following (23). Finally, we need to construct a discrete equivalent to the functional derivative. To that end, we set $\mathsf{A}(\hat{v}) = \mathcal{A}[v]$ and require that

$$\left\langle \frac{\delta \mathcal{A}}{\delta v}[v_h] \, , \, w_h \right\rangle_h = \left\langle \frac{\partial \mathsf{A}}{\partial \hat{v}} \, , \, \hat{w} \right\rangle_N , \tag{28}$$

where $\langle \cdot \, , \, \cdot \rangle_N$ denotes the inner product in $\mathbb{R}^N$, i.e., the scalar product. The functional derivative $\delta\mathcal{A}/\delta v$ is an element of the dual space $\mathbb{V}^*$ of $\mathbb{V}$. Restricting $\mathcal{A}$ to elements v_h of $\mathbb{V}_h$, we can express $\delta\mathcal{A}/\delta v[v_h]$ in the basis $\{\psi_i\}_{i=1}^N$ of $\mathbb{V}_h^*$ as

$$\frac{\delta \mathcal{A}}{\delta v}[v_h] = \sum_{i=1}^{N} a_i \, \psi_i(x). \tag{29}$$

By the Riesz representation theorem we can express the basis functions ψ_i in terms of the basis $\{\varphi_i\}_{i=1}^N$, and using the duality between the bases, i.e., $\langle \psi_i \, , \, \varphi_j \rangle = \delta_{ij}$, as well as (28), we find that

$$\frac{\delta \mathcal{A}}{\delta v}[v_h] = \sum_{i,j=1}^{N} \frac{\partial \mathsf{A}}{\partial v_i} \, \mathbb{M}_{ij}^{-1} \, \varphi_j(x). \tag{30}$$

In order to obtain a semi-discrete metriplectic system, discretised in space but not yet time, all that needs to be done is replace the functional derivatives in (10) and (15) and replace the integrals with the quadrature rule $\{(b_n, c_n)\}_{n=1}^R$. Setting $\mathsf{A}(\hat{\rho}, \hat{m}, \hat{\sigma}) = \mathcal{A}[\rho_h, m_h, \sigma_h]$ and $\mathsf{B}(\hat{\rho}, \hat{m}, \hat{\sigma}) = \mathcal{B}[\rho_h, m_h, \sigma_h]$, for the Poisson bracket (10) this yields

$$\begin{aligned} \{\mathsf{A}, \mathsf{B}\}_h = \sum_{i,j,k}^{3N} \mathbb{P}_{ijk}^{mm} \, m_k \left[\frac{\partial \mathsf{B}}{\partial m_i} \frac{\partial \mathsf{A}}{\partial m_j} - \frac{\partial \mathsf{A}}{\partial m_i} \frac{\partial \mathsf{B}}{\partial m_j} \right] + \sum_{i}^{3N} \sum_{j,k=1}^{N} \mathbb{P}_{ijk}^{m\rho} \, \rho_k \left[\frac{\partial \mathsf{B}}{\partial m_i} \frac{\partial \mathsf{A}}{\partial \rho_j} - \frac{\partial \mathsf{A}}{\partial m_i} \frac{\partial \mathsf{B}}{\partial \rho_j} \right] \\ + \sum_{i}^{3N} \sum_{j,k=1}^{N} \mathbb{P}_{ijk}^{m\sigma} \, \sigma_k \left[\frac{\partial \mathsf{B}}{\partial m_i} \frac{\partial \mathsf{A}}{\partial \sigma_j} - \frac{\partial \mathsf{A}}{\partial m_i} \frac{\partial \mathsf{B}}{\partial \sigma_j} \right], \end{aligned} \tag{31}$$

with

$$\mathbb{P}_{ijk}^{mm} = \sum_{p,q=1}^{3N} \mathbb{L}_{pqk}^{mm} \, (\mathbb{M}^m)_{ip}^{-1} \, (\mathbb{M}^m)_{qj}^{-1}, \qquad \mathbb{L}_{ijk}^{mm} = \sum_{n=1}^{R} b_n \, \varphi_k^m(c_n) \, \varphi_i^m(c_n) \cdot \nabla \varphi_j^m(c_n), \tag{32}$$

$$\mathbb{P}_{ijk}^{m\rho} = \sum_{p=1}^{3N} \sum_{q=1}^{N} \mathbb{L}_{pqk}^{m\rho} \, (\mathbb{M}^m)_{ip}^{-1} \, (\mathbb{M}^\rho)_{qj}^{-1}, \qquad \mathbb{L}_{ijk}^{m\rho} = \sum_{n=1}^{R} b_n \, \varphi_k^\rho(c_n) \, \varphi_i^m(c_n) \cdot \nabla \varphi_j^\rho(c_n), \tag{33}$$

$$\mathbb{P}^{m\sigma}_{ijk} = \sum_{p=1}^{3N}\sum_{q=1}^{N} \mathbb{L}^{m\sigma}_{pqk} \left(\mathbb{M}^{m}\right)^{-1}_{ip} \left(\mathbb{M}^{\sigma}\right)^{-1}_{qj}, \qquad \mathbb{L}^{m\sigma}_{ijk} = \sum_{n=1}^{R} b_n \, \varphi^{\sigma}_{k}(c_n) \, \varphi^{m}_{i}(c_n) \cdot \nabla \varphi^{\sigma}_{j}(c_n). \tag{34}$$

The discrete bracket (31) is anti-symmetric, but it does not satisfy the Jacobi identity. In the context of metriplectic systems, this is not critical as the full metriplectic bracket does not satisfy the Jacobi identity either. More importantly, the discrete bracket (31) preserves the discrete energy (24) as well as mass (25) and entropy (27), and depending on the actual discretisation possibly also momentum (26). Energy conservation follows immediately from the anti-symmetry of (31), so that $\{\mathsf{H},\mathsf{H}\}_h = 0$. Mass and entropy conservation can be seen by inserting (25) or (27) into (31), e.g.,

$$\{\mathsf{M},\mathsf{B}\}_h = \sum_{i,l}^{3N}\sum_{j,k=1}^{N} \mathbb{L}^{m\rho}_{ijk} \, \rho_k \, \mathsf{1}_j \left(\mathbb{M}^{m}\right)^{-1}_{il} \frac{\partial \mathsf{B}}{\partial m_l} = 0 \qquad \text{as} \qquad \sum_{j=1}^{N} \mathbb{L}^{m\rho}_{ijk} \, \mathsf{1}_j = 0. \tag{35}$$

Note that this holds for any B. Momentum conservation, on the other hand, relies on the specific form of H and is not warranted for any discrete Hamiltonian of the form (24), but only for specific choices of basis functions and quadrature rules.

The discretisation of the metric bracket (15) and the proof of its conservation properties follow exactly along the same lines. The semi-discrete equations of motion are obtained by utilising Equation (1) and thus computing

$$\frac{du}{dt} = \{u,\mathsf{G}\}_h + (u,\mathsf{G})_h \qquad \text{for} \qquad u \in \{\rho_1,...,\rho_N,\, m_1,...,m_{3N},\, \sigma_1,...,\sigma_N\}, \tag{36}$$

where $\mathsf{G} = \mathsf{H} - \mathsf{S}$ approximates the free energy $\mathcal{G}$.

4 Summary

The preceding paper outlines a flexible framework for the construction of structure-preserving algorithms for the numerical integration of dissipative systems from fluid dynamics and plasma physics. This framework is very general with respect to both, the system of equations and the particular numerical method applied. Although here it was applied to the specific example of Korteweg-type fluids, it is equally applicable e.g. to geophysical fluid flows, magnetohydrodynamics or kinetic systems. While in the above construction a continuous Galerkin discretisation was assumed, this approach is equally well applicable to discontinuous Galerkin approximations, isogeometric analysis, spectral methods or even finite differences.

Note that in contrast to typical finite volume or discontinuous Galerkin methods, the metriplectic framework and the conservation properties of the resulting schemes do not depend on the coordinate representation of the system. Although conservative coordinates have been used here, this is not required in order to obtain conservation of the corresponding invariants. The same can have been achieved using, for example, the density ρ, velocity $v = m/\rho$ and entropy $s = \sigma/\rho$ instead.

An important ingredient for a fully discrete algorithm is the temporal discretisation. It has not been discussed here due to the constrained space and will be explained elsewhere, together with a thorough discussion of the discrete conservation laws and the discrete H-theorem.

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