21st International Symposium on
Mathematical Theory of Networks and Systems
July 7-11, 2014. Groningen, The Netherlands

Structure-preserving discretization for continuum models*

Marc Gerritsma[1]

Abstract— **This paper describes the mathematical setting of continuum models such as elasticity and fluid flow. From this continuous description we derive a discrete formulation which satisfies the conservation laws from the outset. The only approximation required is for the material-dependent constitutive equations.**

Keywords: Structure-preserving, continuum mechanics, elasticity, fluid mechanics

I. INTRODUCTION

Mimetic methods or structure-preserving methods constitute an emerging field of scientific computing. Where in the past a differential equation was solved by approximating all derivatives individually using nodal approximations, the new paradigm considers the governing equations in a more global form. Enzo Tonti, [1], [2], explicitly made a distinction between topological and metric-dependent relations in physical models. The topological relations consist of conservation laws, equilibrium and compatibility conditions, while the metric-dependent part consists – according to Tonti – of phenomenological equations provided by constitutive laws, also referred to as material equations or equations of state. The class of topological equations is further divided into inner-oriented relation and outer-oriented relations. In terms of differential forms this distinction amounts to topological relations between true forms and pseudo-forms, respectively. Tonti classifies nearly all physical theories in terms of their topological and constitutive relations in so-called Tonti-diagrams.

Bossavit, [3], writes the Maxwell equations in terms of differential forms and demonstrates that the Maxwell equations are purely topological. The discrete laws can be fully represented by k-cochains, where the coboundary operator represents the discrete analogue of the exterior derivative in differential geometry. Ampère's law, for instance, $-\partial_t \tilde{d} + \mathrm{d}\tilde{h} = \tilde{j}$, where, $\tilde{d}$, is the electric field intensity represented by a pseudo 2-form, $\tilde{h}$ is the magnetic field represented as an outer-oriented 1-form and $\tilde{j}$ is the current density represented by an outer-oriented 2-form. The twiddles, $\tilde{\cdot}$ indicate that all forms in this equation are pseudo-forms. Faraday's law, on the other hand, takes the form $\partial_t b + \mathrm{d}e = 0$, where b is the 2-form, magnetic induction associated with inner-oriented objects and e denotes the electric induction represented as an inner-oriented 1-form. Using the generalized Stokes Theorem one can represent these equations exactly on two dual grids; on one grid the the discrete pseudo-forms are represented as cochains while on the other grid the true forms are encoded.

[1]Marc Gerritsma is with Faculty of Aerospace Engineering, TU Delft, 2629 HS Delft, The Netherlands `M.I.Gerritsma@tudelft.nl`

In the end we have more (discrete) unknowns than equations and therefore closure relations – constitutive relations – are required. In the example of electromagnetism these closure relations are given by $b = \star_\mu \tilde{h}$, $\tilde{d} = \star_\varepsilon e$ and $\tilde{j} = \star_\sigma e$. These constitutive laws provide the link between the two dual grids. Where the Maxwell equations are *global*, i.e. associated to lines, surfaces and volume, the constitutive relations are *local* and need to be satisfied in each point. In structure-preserving methods, the global, discrete unknowns are interpolated by a suitably chosen set of basis functions and one imposes that the interpolated global unknowns approximate the constitutive relations. The accuracy of the this interpolation determines the overall accuracy of the physical field problem, see [5].

Bossavit, [3], [6] introduced the Whitney forms, [7], as conforming reconstructions. Bochev and Hyman, [8], describe the general requirements for a structure-preserving reconstruction. Whitney forms satisfy these requirements. A very geometric approach towards structure-preserving discretizations is given by discrete exterior calculus (DEC), [9], [10]. Extension to higher order reconstructions can be found in [11], [12], [15].

II. COVECTOR-VALUED DIFFERENTIAL FORMS

The reconstructions mentioned above work well for the approximation of differential forms, but continuum models require higher order tensors for a proper description. While conservation of mass may still be expressed in terms of differential forms, conservation of momentum should be expressed in terms of covector-valued pseudo volume forms. This description of momentum can be found in [16], [17], [18], [19] and [20, Appendix A], although Frankel treats momentum as a *vector*-valued form. The reason for the use of more extended tensors is because in continuum mechanics physics 'is smeared out' over volumes, surfaces and lines. In classical mechanics we have momentum which can be described by a 1-form, but in continuum mechanics we use momentum *per unit volume* which only yields momentum 'after integration over a volume'.

Traditionally, continuum mechanics is described in Euclidean space which allows integration of momentum and forces over volumes, because we can transport vectors from one place to another. This is no longer the case for general manifolds since there is no way to compare vectors assigned to different points in the manifold. So 'integration over a volume' of vector-valued quantities requires a different approach as outlined in [19] and [4] based on virtual power.

A. Displacement, flow and momentum

Displacements in elasticity and velocity in flow problems are described by vector fields, $v = v^i\partial_{x^i}$, i.e. section, $\mathfrak{X}(\mathscr{M})$, of the tangent bundle of a manifold $\mathscr{M}$[1]. Let dim($\mathscr{M}$)= n, then the dual space of vector fields consists of covector-valued pseudo volume forms, $m = m^{(1)} \otimes \widetilde{\mathrm{vol}}^{(n)}$, where $m^{(1)}$ is a true 1-form and $\widetilde{\mathrm{vol}}^{(n)}$ is the standard volume form, under the duality pairing

$$\langle m, v\rangle := \int_{\mathscr{M}} \left\langle m^{(1)}, v\right\rangle_p \widetilde{\mathrm{vol}}^{(n)} \,, \qquad (1)$$

where $\left\langle m^{(1)}, v\right\rangle_p$ denotes duality pairing in the fibers over $p \in \mathscr{M}$, $T_p^*\mathscr{M} \times T_p\mathscr{M} \to \mathbb{R}$, [21]. For momentum to be independent of the orientation of the volume form, momentum is a covector-valued *pseudo*-volume form as indicated by the $\tilde{}$ over the volume form. This means that covector part needs to be represented on the inner-oriented grid, while the volumetric part needs to be represented on the outer-oriented grid. To be compatible with this description of momentum, the velocity field needs to be represented as *vector-valued true-0-form*, [22], in order to ensure that $\langle m, v\rangle$ is independent of the orientation of ambient space.

The space of vector-valued 0-forms, $\mathfrak{X}(\mathscr{M}) \otimes \Lambda^0(\mathscr{M})$ and covector-valued pseudo volume forms, $\Lambda^1(\mathscr{M}) \otimes \tilde{\Lambda}^n(\mathscr{M})$ are isomorphic, where $\Lambda^k(\mathscr{M})$ is the space of true differential k-forms defined on the manifold $\mathscr{M}$ and $\tilde{\Lambda}^k(\mathscr{M})$ is the space of differential pseudo k-forms defined on $\mathscr{M}$. This isomorphism will be denoted by $\star_\rho^\flat : \mathfrak{X}(\mathscr{M}) \otimes \Lambda^0(\mathscr{M}) \to \Lambda^1(\mathscr{M}) \otimes \tilde{\Lambda}^n(\mathscr{M})$ which consists of the musical operator $\flat$ which converts the vector-valued form to a covector-valued form and the Hodge-$\star$ which converts a k-form to a pseudo $(n-k)$-form. This isomorphism depends explicitly on the metric, see also [17]. The inverse of this operation is $\star_{1/\rho}^\sharp$.

B. Rate of strain and stress

Strain in elasticity and the rate of strain in fluid mechanics are given by the intrinsic or covariant derivative, ∇v, which, if the vector field v in a particular local coordinate system is given by $v = v^i\partial_{x^i}$, yields

$$\nabla v = \frac{\partial}{\partial x^i} \otimes \left(\mathrm{d}v^i + \omega^i_k v^k\right) \,, \qquad (2)$$

where the $\omega^i_k = \omega^i_{kj}\,\mathrm{d}x^j$ are the connection 1-forms. The rate of strain ∇v is vector-valued 1-form. The dual space of vector-valued 1-forms consists of covector-valued pseudo $(n-1)$-forms, $\mathrm{d}x^j \otimes \tilde{\tau}^{(n-1)}$, where $\tilde{\tau}^{(n-1)}$ is an outer-oriented $(n-1)$-form. The duality pairing between vector-valued 1-forms. $L = \partial_{x^i} \otimes l^{i,(1)}$ and covector-valued $(n-1)$-forms, $T = \mathrm{d}x^j \otimes \tilde{\tau}_j^{(n-1)}$, is given by

$$\langle L, T\rangle := \int_{\mathscr{M}} \mathrm{d}x^j \left(\frac{\partial}{\partial x^i}\right) l^{i,(1)} \wedge \tau_j^{(n-1)} \,. \qquad (3)$$

[1]We only consider smooth, differentiable manifolds

If $\mathrm{d}x^i$ is a canonical dual basis which satisfies $\mathrm{d}x^i(\partial_{x^j}) = \delta^i_j$ then this reduces to

$$\langle L, T\rangle := \int_{\mathscr{M}} l^{i,(1)} \wedge \tau_i^{(n-1)} \,. \qquad (4)$$

To be compatible with the description of momentum, stress should be expressed as a covector-valued pseudo-$(n-1)$-form, which reflects the fact that stress is associated to *surface* forces. Again, the covector part corresponds to a true covector, while the $(n-1)$-form is a pseudo-form, because if we reverse the transverse orientation through the surface we expect the force to be the same; physics should not depend on our choice of orientation. Therefore, stress fields form the linear functionals acting on rate of strain fields.

The covariant derivative of covector-valued $(n-1)$-forms, ∇T, yield covector-valued volume forms. If the stress tensor is written as

$$\begin{aligned} T \;=\; & \mathrm{d}x^1 \otimes \left(\tau^1_1\,\mathrm{d}x^2\mathrm{d}x^3 + \tau^1_2\,\mathrm{d}x^3\mathrm{d}x^1 + \tau^1_3\,\mathrm{d}x^1\mathrm{d}x^2\right) + \\ & \mathrm{d}x^2 \otimes \left(\tau^2_1\,\mathrm{d}x^2\mathrm{d}x^3 + \tau^2_2\,\mathrm{d}x^3\mathrm{d}x^1 + \tau^2_3\,\mathrm{d}x^1\mathrm{d}x^2\right) + \\ & \mathrm{d}x^3 \otimes \left(\tau^3_1\,\mathrm{d}x^2\mathrm{d}x^3 + \tau^3_2\,\mathrm{d}x^3\mathrm{d}x^1 + \tau^3_3\,\mathrm{d}x^1\mathrm{d}x^2\right) \,. \end{aligned}$$

Then, in the absence of connection 1-forms, ∇T is given by

$$\begin{aligned} \nabla T \;=\; & \mathrm{d}x^1 \otimes \left(\frac{\partial \tau^1_1}{\partial x^1} + \frac{\partial \tau^1_2}{\partial x^2} + \frac{\partial \tau^1_3}{\partial x^3}\right) \mathrm{d}x^1\mathrm{d}x^2\mathrm{d}x^3 + \\ & \mathrm{d}x^2 \otimes \left(\frac{\partial \tau^2_1}{\partial x^1} + \frac{\partial \tau^2_2}{\partial x^2} + \frac{\partial \tau^2_3}{\partial x^3}\right) \mathrm{d}x^1\mathrm{d}x^2\mathrm{d}x^3 + \\ & \mathrm{d}x^3 \otimes \left(\frac{\partial \tau^3_1}{\partial x^1} + \frac{\partial \tau^3_2}{\partial x^2} + \frac{\partial \tau^3_3}{\partial x^3}\right) \mathrm{d}x^1\mathrm{d}x^2\mathrm{d}x^3 \,, \end{aligned}$$

where we recognize the divergence of the stress tensor as usually employed in vector calculus. The main advantage of writing the stress tensor in terms of differential forms, is that it explicitly shows that stress is associated with (hyper)-surfaces.

C. Acceleration and rate of change of momentum

Let the velocity be given by $v = v^i\partial_{x^i}$ the acceleration is given by $a = a^i\partial_{x^i}$, where a^i is given by [18] $\dot{v} + \nabla_v v$

$$a = \frac{dv}{dt} = \left(\frac{\partial v^i}{\partial t} + dv^i(v) + v^k\omega^i_k(v)\right)\partial_{x^i} \,. \qquad (5)$$

The rate of change of momentum is then given by dm/dt

$$\frac{dm}{dt} = \star_\rho^\flat \frac{dv}{dt} = \star^\flat \frac{d}{dt}\left(\star^\sharp m\right) \,. \qquad (6)$$

The presence of $\star^\flat$ and $\star^\sharp$ shows that the rate of change of momentum is a metric concept.

III. The incompressible Navier-Stokes equations

We see from the expression for the rate of strain, (21), and the time rate of change of momentum, (5), that they both depend on the connection coefficients. For a Riemannian manifold the connection can be expressed in terms of the metric tensor g in which case the connection coefficients equal the Christoffel symbols. If we would apply these metric-dependent realtions in conservation of momentum, as is traditionally done, conservation of momentum would be a metric-dependent relation, [17], [18].

In mimetic/structure-preserving methods it is generally assumed that conservation laws and equilibrium relations purely topological relations which are metric-free and all metric is contained in the constitutive relations. This paradigm has many advantages in numerical methods for continuum models. First, discretization of conservation laws is independent of any mesh-quantities, so the discrete representation of the conservation law is exactly the same for a fine and a coarse grid, for a uniform and a non-uniform grid and for an orthogonal grid and highly deformed mesh. More specifically, the exact solution will satisfy these discrete relation and therefore the discrete topological conservation laws are generally referred to as being *exact*.

The approximation, that inevitably takes place when we discretize the continuous equations, therefore has to reside in the constitutive relations, see [1], [5].

A. Conservation laws

1) Conservation of momentum: Conservation of momentum states that the time rate of change of momentum of a material volume equals the resultant force acting on the volume

$$\frac{dm}{dt} = F \,. \tag{7}$$

So both momentum m and force F are associated with a material volume. In addition, both variables have three components, so we will introduce *momentum density* and *force density* as momentum per unit volume and force per unit volume, respectively. Mathematically these physical variables are represented by *covector-valued volume forms*. The force will be split into a volumetric part, the body forces, and forces connected to the surface of a volume, the surface forces.

The force on any sub-volume $\mathscr{R} \subset \mathscr{M}$ will be given by

$$\mathbf{f}_{\mathscr{R}} := \int_{\mathscr{R}} \mathbf{f} \,,$$

in Euclidean space. In more general domains, this integral is not defined, because there is no natural way to compare tangent vectors and covectors located at different points in the manifold. Covector-valued volume forms can also be written as linear maps from the tangent space at a point $p \in \mathscr{M}$ to a volume form at that particular point, i.e. $f \in L(\mathfrak{X}(\mathscr{M}), \Lambda^n(\mathscr{M}))$, which means that $f(w) \in \Lambda^n(\mathscr{M})$ for $w \in \mathfrak{X}(\mathscr{M})$, which can be integrated over a volume. Note that if the vector denotes a displacement then $f(w)$ physically represents the work done by f in the direction w, whereas, when the vector denotes velocity $f(w)$ represents the power exerted by f in the direction w. Here we take any vector field w and then we call it the virtual work (displacements) in solid mechanics or the virtual power (velocities) in fluid mechanics.

In addition to the force per unit volume we also have surface forces given by covector-valued $(n-1)$-forms, T, which can be considered as linear maps from $\mathfrak{X}(\mathscr{M})$ to $\Lambda^{n-1}(\mathscr{M})$, $T \in L(\mathfrak{X}(\mathscr{M}), \Lambda^{n-1}(\mathscr{M}))$. Therefore $T(w)$ is an $(n-1)$-form which can be naturally integrated over the boundary of the volume $\mathscr{R}$. So the total virtual work/power exerted on the sub-volume $\mathscr{R}$ by the body and surface forces is given by

$$F_{\mathscr{R}}(w) = \int_{\mathscr{R}} f(w) + \int_{\partial\mathscr{R}} T(w) \,.$$

The contribution of the surface forces can further split into the deviatoric surface force, σ, and the mean hydrostatic contribution, $T = \sigma - P$

$$P = \mathrm{d}x^1 \otimes p\mathrm{d}x^2\mathrm{d}x^3 + \mathrm{d}x^2 \otimes p\mathrm{d}x^3\mathrm{d}x^1 + \mathrm{d}x^3 \otimes p\mathrm{d}x^1\mathrm{d}x^2 \,,$$

in which case the forces acting on the volume can be written as

$$F_{\mathscr{R}}(w) = \int_{\mathscr{R}} f(w) + \int_{\partial\mathscr{R}} \sigma(w) - \int_{\partial\mathscr{R}} P(w) \,. \tag{8}$$

Note that all these operation are metric-free, it, in fact, consists of the duality pairing and the integration of volume forms which is a metric-free operation.

Similar consideration also apply to momentum density being a covector-valued volume form and therefore we have

$$\frac{d}{dt}\int_{\mathscr{R}} m(w) = \int_{\mathscr{R}} f(w) + \int_{\partial\mathscr{R}} \sigma(w) - \int_{\partial\mathscr{R}} P(w) \,.$$

The time rate of change of momentum can be decomposed into a local time rate of change and a change in momentum due to convection of momentum through the boundary $\partial\mathscr{R}$

$$\int_{\mathscr{R}} \frac{\partial m(w)}{\partial t} + \int_{\partial\mathscr{R}} \iota_v m(w) \,.$$

Also these operations are metric-free. The complete momentum equation in metric-free form is then given by

$$\begin{aligned}\int_{\mathscr{R}} \frac{\partial m(w)}{\partial t} + \int_{\partial\mathscr{R}} \iota_v m(w) = \\ \int_{\mathscr{R}} f(w) + \int_{\partial\mathscr{R}} \tau(w) - \int_{\partial\mathscr{R}} P(w) \,,\end{aligned} \tag{9}$$

$\forall w \in \mathfrak{X}(\mathscr{M})$.

Using the generalized Stokes Theorem, the integral relations (9) van be written as

$$\begin{aligned}\int_{\mathscr{R}} \frac{\partial m(w)}{\partial t} + \int_{\mathscr{R}} \mathrm{d}\iota_v m(w) = \\ \int_{\mathscr{R}} f(w) + \int_{\mathscr{R}} \mathrm{d}\tau(w) - \int_{\mathscr{R}} \mathrm{d}P(w) \,,\end{aligned} \tag{10}$$

which needs to hold for all sub-volumes $\mathscr{R} \subset \mathscr{M}$ and all smooth vector fields $w \in \mathfrak{X}(\mathscr{M})$. As remarked by Segev, [19], this implies that conservation of momentum in its general form not only depends linearly on the vector values w, but also linearly on its derivatives. The integrand is linear in the jet space $j(w)$ of the velocity field.

In Euclidean space one may take for the velocity fields the uniform velocity fields ∂_i. In this case (9) expresses conservation of linear momentum and the integral relation becomes an equation for the momentum density *coefficients*. So the momentum equation, generally employed in computational physics, is a special case of the metric-free momentum equation given by (9). The derivative of the vector field $w = \partial_i$ are zero.

If for an arbitrary point we can also choose the linear vector field $w = (x_0^j - x^j)\partial_{x^i} - (x_0^i - x^i)\partial_{x^j}$ which vector field corresponds to a solid body rotation around the point x_0^i. The resulting conservation law expresses conservation of angular momentum around the point x_0^i. At the continuous level, conservation of linear momentum implies conservation of angular momentum, provided the stress tensor is symmetric. This is no longer the case for the discretized equations for linear momentum. So explicit imposition of conservation of angular momentum in a discretization based on (9) is required. Conservation of angular momentum is vitally important to represent vorticity and helicity correctly in a discrete setting.

In a 2D simulation, in absence of dissipative terms, $\tau \equiv 0$, vorticity and enstrophy are conserved quantities, while in the 3D case helicity is conserved. These relations are purely topological and follow from the more general conservation of momentum as given by (9). When a small amount of dissipation is present, vorticity and enstrophy in the 2D case and helicity in the 3D case, are almost conserved. This is the regime where one encounters turbulent flow, [14] and a proper preservation is related to to energy scales in turbulent flow, [13].

Another special case is obtained when we take $w = v$, where v is the fluid velocity. In this case, (9) expresses the evolution equation for kinetic energy.

Finally, when high order methods are used not only linear momentum and angular momentum will be conserved, but also higher moments of momentum will be conserved. The more physical constraints one imposes on the discrete equations, the more likely the discrete solution will represent a true flow. For high order methods, one could take vector field w which is small in the L^2-norm, but large in H^1-norm, i.e. a small but spatially highly oscillatory vector field. Since (9) also depends on the derivatives of the vector field w, the volume integrals will be small in comparison to the boundary integrals in (9). So for highly oscillating vector fields there is a direct relation between the convective terms on the left and the surface forces on the right side of (9). In the limit for the oscillations going to infinity, this is an equilibrium relation because unsteady behaviour is associated with the volume integral of momentum (the first term in (9)). For smooth, laminar flow the contribution of highly oscillating vector fields is irrelevant, but near transition, separation and in turbulent flow a proper response to spatially highly oscillatory vector fields is important.

Although (9) resembles a weak formulation for linear momentum as commonly used in finite element methods, this is in fact a strong formulation for higher order moments. In the current formulation the tensor unknowns are paired with vector fields and then the conservation law is set up, whereas in finite element methods first the equation for linear momentum is formulated and then a projection on vector fields is performed.

2) Conservation of mass: For conservation of mass we consider an arbitrary sub-volume $\mathscr{V} \subset \mathscr{M}$. Let $\rho \in \Lambda^n(\mathscr{M})$ be the mass density, then the mass of the volume $\mathscr{V}$ is given by

$$M_{\mathscr{V}} = \int_{\mathscr{V}} \rho \; .$$

Since mass can be locally created nor destroyed, any change of mass in the volume is due to a net influx of mass through the boundary $\partial\mathscr{V}$. This can be expressed as

$$\int_{\mathscr{V}} \frac{\partial \rho}{\partial t} + \int_{\partial\mathscr{V}} \iota_v \rho = 0 \; .$$

For incompressible flow the mass density is constant, in which case conservation of mass reduces to

$$\int_{\partial\mathscr{V}} \iota_v \widetilde{\mathrm{vol}}_\rho^{(n)} = 0 \; , \tag{11}$$

with $\rho = \text{const}$. This is equal to

$$\int_{\partial\mathscr{V}} \mathrm{d}\iota_v \widetilde{\mathrm{vol}}_\rho^{(n)} = \int_{\partial\mathscr{V}} \mathscr{L}_v \widetilde{\mathrm{vol}}_\rho^{(n)} = 0 \; ,$$

where $\mathscr{L}_v$ denotes the Lie derivative applied to the volume form $\widetilde{\mathrm{vol}}_\rho^{(n)}$.

Note that (11) was already used in [23] to satisfy conservation of mass point-wise. However, the formulation employed in [23] does not guarantee conservation of momentum, because in that formulation conservation of momentum is somewhat artificially imposed over surfaces instead in volume as is the case with (9).

B. *Constitutive equations*

Equations (11) and (9) constitute 4 equations for $n = 3$ with for 16 unknowns, 3 momentum densities, $m^{i,(n)}$ 3 velocity components, v^i, 1 pressure, p and 9 surface force components $\tau^{i,j}$. This means that we have to find additional relations to close the system of equations. The first constitutive equation is the one relating momentum to velocity, usually expressed as $m = \rho v$, where ρ, the fluid mass density acts as material parameter. While in vector calculus this may seem a trivial relation between vectors, the more geometric approach shows that we want to equate two dual objects, namely momentum (a covector-valued volume form) to velocity (a vector-valued 0-form). This can be expressed as $m = \star_\rho^\flat v$, where the $\flat$-operator 'lowers the index' to convert the vector to a covector and the $\star$ converts the 0-form to an n-form, see also [17]. Alternatively, we can use the inner-product for vector fields (here the metric enters) and use the Riesz representation theorem that states that for any linear function f acting on a linear vector space V, there exists an element $v_f \in V$ such that for $w \in V$ we have

$$\langle f, w \rangle = (v_f, w) \; , \tag{12}$$

where $\langle \cdot, \cdot \rangle$ denotes duality pairing between dual spaces, while $(\cdot, \cdot)$ represents the inner-product on V. Doing this for momentum and velocity gives

$$\langle m, w \rangle = (v, w)_\rho := \int_{\mathscr{M}} (v, w)_p \mathrm{vol}_\rho^{(n)} \; , \quad \forall w \in \mathfrak{X}(\mathscr{M}) \; , \tag{13}$$

where $(\cdot, \cdot)_p$ denotes the points-wise inner-product of vectors at the point $p \in \mathscr{M}$ and ρ acts as integration measure. The relation between momentum and velocity gives us $n = 3$

additional relations. The remaining 9 closure relations are provided by the Newtonian stress-strain relation, $\tau = \mu \nabla v$, where μ is the viscosity coefficient. This is again a relation between dual objects, so one could use $\tau = \star_\mu^\flat \nabla v$ or

$$\langle \tau, \sigma \rangle = (\nabla v, \sigma)_\mu = \int_{\mathscr{M}} (\nabla v, \sigma)_p \mathrm{vol}_\mu^{(n)} \,, \quad \forall \sigma \in \mathfrak{X}(\mathscr{M}) \otimes \Lambda^1(\mathscr{M}) \,.$$

Following [5] the error in the structure-preserving discretization will be completely determined by the accuracy how well we satisfy the two constitutive relation between momentum and velocity and stress and strain.

IV. Structure-preserving discretization

A discrete representation of the mass flux $\iota_v \mathrm{vol}_\rho^{(n)}$ as an outer-oriented $(n-1)$-form on a unit square for $\rho = 1$ was already considered in [11], [12], [25]. For this particular situation the metric tensor $g_{i,j} = \delta_{i,j}$ and the connection forms all vanish.

$$u^{(n-1)} = \iota_v \mathrm{vol}^{(n)} = \sum_{i=0}^{N} \sum_{j=1}^{N} \bar{u}_{i,j} h_i^{(0)}(x) e_j^{(1)}(y) - \sum_{i=1}^{N} \sum_{j=0}^{N} \bar{v}_{i,j} e_i^{(1)}(x) h_j^{(0)}(y) \,, \tag{14}$$

where N is the number of cells in the x- and y-direction , see Figure 1 and the 0-form $h_i^{(0)}(x)$ is a Lagrange polynomial of degree N which satisfies $h_i^{(0)}(x^p) = \delta_i^p$ and the polynomial 1-form $e_i^{(1)}(x)$ of degree $N+1$ which satisfies

$$\int_{x^{j-1}}^{x^j} e_i^{(1)} = \begin{cases} 1 & \text{if} \quad i = j \\ 0 & \text{if} \quad i \neq j \end{cases} \,, \tag{15}$$

and

$$\star e_i^{(1)}(-1) = \star e_i^{(1)}(1) = 0 \,. \tag{16}$$

The expansion coefficients $\bar{u}_{i,j}$ and $\bar{v}_{i,j}$ represent for $n = 2$

$$\bar{u}_{i,j} = \int_{y^{j-1}}^{y^j} u^{(n-1)} \Big|_{x^i} \,, \tag{17}$$

$$\bar{v}_{i,j} = \int_{x^{i-1}}^{x^i} u^{(n-1)} \Big|_{y^j} \,, \tag{18}$$

the mass fluxes for $\rho = 1$. The advantage of writing the mass flux in the form (14) is that conservation of mass reduces to

$$\bar{u}_{i,j} - \bar{u}_{i-1,j} + \bar{v}_{i,j} - \bar{v}_{i,j-1} = 0 \,. \tag{19}$$

Note that this discrete conservation law is purely topological and independent of the size of the grid. Next we sample the discrete representation (14) in points $(x_i, y_{j+1/2})$, $i = 0, \ldots, N$ and $j = 0, \ldots, N-1$ for the x-component u – indicated by the black bullet, $\bullet$, in Figure 1 – and the point $(x_{i+1/2}, y_j)$, $i = 0, \ldots, N-1$ and $j = 0, \ldots, N$ for the y-component v – indicated by the $\times$ in Figure 1. We sample these velocities on the boundary where the tangential velocity is set to zero

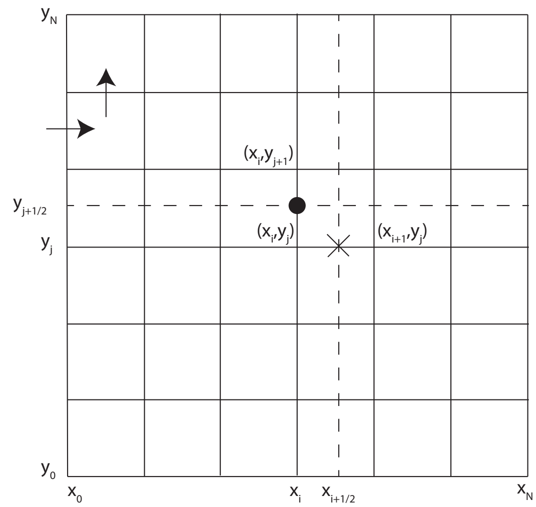

Fig. 1. Layout of the grid. The points (x_i, y_j) form the intersection of the solid lines. The horizontal arrow indicates $\bar{u}_{i,j}$ the velocity flux through the vertical line segments, the vertical arrow indicates the flux $\bar{v}_{i,j}$ through the horizontal line segments. The cross, $\times$ indicates a point where the polynomial expansion (14) for the y-component is sampled, the solid bullet, $\bullet$, indicates a point where the x-component in (14) is sampled.

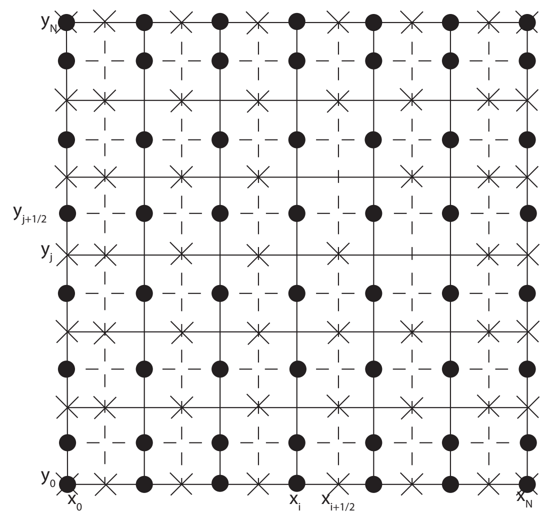

Fig. 2. All points where the x- and y-component of the velocity are sampled.

due to (16). This nodal representation of the velocity is then given by

$$v(x,y) = \sum_{i=0}^{N} \sum_{j=-1}^{N} u_{i,j+1/2} h_i(x) \tilde{h}_{j+1/2}(y) \frac{\partial}{\partial x} + \sum_{i=-1}^{N} \sum_{j=0}^{N} v_{i+1/2,j} \tilde{h}_{i+1/2}(x) h_j(y) \frac{\partial}{\partial y} \,. \tag{20}$$

This is a vector-valued 0-form which assigns to each point (x,y) a vector. Note that $u^\flat = \star u^{(n-1)}$, so going from the flux representation to the vector representation is just an isomorphism (change of basis), $v \to \iota_v \mathrm{vol}^{(n)}$ as required, [24]. We can express this in a matrices which convert $\bar{u}_{i,j} \leftrightarrow u_{i,j+1/2}$ and $\bar{v}_{i,j} \leftrightarrow v_{i+1/2,j}$

With this representation ∇v is given by ($\omega_k^i = 0$)

$$\nabla v = \sum_{i=1}^{N}\sum_{j=-1}^{N}(u_{i,j+1/2} - u_{i-1,j+1/2})\varepsilon_i(x)\tilde{h}_{j+1/2}(y)\frac{\partial}{\partial x}\otimes \mathrm{d}x + \sum_{i=0}^{N}\sum_{j=}^{N}(u_{i,j+1/2} - u_{i,j-1/2})h_i(x)\tilde{\varepsilon}_{j+1/2}(y)\frac{\partial}{\partial x}\otimes \mathrm{d}y + \sum_{i=0}^{N}\sum_{j=0}^{N}(v_{i+1/2,j} - v_{i-1/2,j})\tilde{\varepsilon}_{i+1/2}(x)h_j(y)\frac{\partial}{\partial y}\otimes \mathrm{d}x + \sum_{i=-1}^{N}\sum_{j=1}^{N}(v_{i+1/2,j} - v_{i+1/2,j-1})\tilde{h}_{i+1/2}(x)\varepsilon_j(y)\frac{\partial}{\partial y}\otimes \mathrm{d}y\,. \tag{21}$$

Using (20) and (21) allows us to express $\nabla_v v$. The vector $\nabla_v v$ is again sampled in the bullets and crosses in the grid. This invariably leads to loss of information, but this was to be expected, because conservation of momentum is not a purely topological relation. Therefore some approximation is necessary. We now define momentum as in the volumes surrounding the points where the x-component of the velocity is defined and the points where the y-component of the velocity is defined, see Figure 3 Pressure and stress are discrete represented as in [25]. This gives a one-to-one correspondence between ∇v as represented by (21) and the polynomial stress representation. All these discrete relations can be gathered in one big system of equations which admits a unique solution. The accuracy of the final approximation is determined by the accuracy by which we can satisfy the two constitutive equations $m = \star_\rho^\flat v$ and $\tau = \star_\mu^\flat \nabla v$. This is a common feature of structure-preserving approximations, that is that the discrete error takes place at exactly the same place where the physical model is approximated, namely the constitutive model, [5].

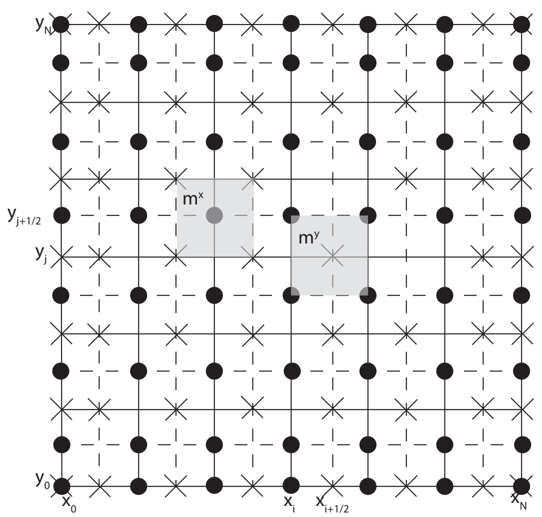

Fig. 3. The volume in which momentum in the x-direction, m^x, is defined around the black bullet where the x-component of the velocity vector is defined and the volume in which y-momentum, m^y, is defined surrounding the crosses where the y-component of the velocity is defined.

V. CONCLUSIONS

In this paper a metric-free formulation for continuum models is described with an emphasis on flow equations. Conservation of momentum is represented as a virtual power formulation, where virtual velocity fields w are introduced to reduce covector-valued differential forms to ordinary differential forms. Once the governing equations are expressed in terms of differential forms mimetic or structure-preserving discretization techniques can be employed, which yield discrete relations which do not involve any mesh-dependent parameters. Special cases of such virtual velocity fields are described: the uniform vector fields which yield conservation of linear momentum, the solid body rotations which result in conservation of angular momentum, the true velocity field which establishes the evolution equation for kinetic energy. The approximation of the exact solution is completely determined by the approximation of the constitutive laws. In case of incompressible flow these constitutive laws are given by the momentum-velocity relation and the rate of strain-stress relation.

REFERENCES

[1] E.Tonti, On the formal structure of physical theories, Prepr. Ital. Natl. Res. Counc.(1975).
[2] E.Tonti, Why starting from differential equations for computational physics?, J. Comp. Physics, 257, pp. 1260–1290, 2014.
[3] A.Bossavit, Whitney forms: A class of finite elements for three-dimensional computations in electromagnetism, IEE Proceedings A: Physical Science. Measurement and Instrumentation. Management and Education. Reviews 135 pt A (8) , pp. 493-500, 1988.
[4] A. Bossavit, Virtual power principle and Maxwell's tensor: Which comes first?, COMPEL - The International Jopurnal for Computation and Mathematics in Electrical and Electronic Engineering, 2011.
[5] P. Bochev and M. Gerritsma, A spectral mimetic least-squares method, submitted to Computers & Mathematics with Applications, 2014.
[6] A. Bossavit, Computational Electromagnetism, Academic Press (Boston), 1998.
[7] H. Whitney, Geometric intergation theory, Princeton Universtity Press, 1957.
[8] P. B. Bochev and J. M. Hyman, Principles of mimetic discretizations of differential equations, Compatible Spatial Discretizations The IMA Volumes in Mathematics and its Applications Volume 142,pp 89-119, 2006.
[9] A.N. Hirani, Discrete exterior calculus, PhD thesis,California Institute of Technology, Pasadena, CA, 2003.
[10] M. Desbrun, A. N. Hirani, M. Leok and J. E. Marsden, Discrete Exterior Calculus, arXiv:math/0508341, 2005.
[11] M. Gerritsma, Edge functions for spectral element methods, in: J. Hesthaven et al. (Eds), Spectral and High Order Methods for Partial Differential Equations, in: Lect. Notes Comput. Sci. Eng., vol. 76, Springer, Berlin, Heidelberg, pp. 199-207, 2011.
[12] J. Kreeft, A. Palha and M. Gerritsma, Mimetic framework on curvilinear quadrilaterals of arbitrary order, arXiv:1111.4304, 2011.
[13] A. Arakawa, Computational Design for Long-Term Numerical Integration of the Equation of Fluid Motion: Two-Dimensional Incompressible Flow. Part I., J. Comput. Phys., 135, pp. 103-114, 1997.
[14] Moffatt, H. K., and A. Tsinober, Helicity in laminar and turbulent flow. Annual review of fluid mechanics 24.1 281-312, 1992.
[15] D. Rufat, G. Mason, P. Mullen and M. Desbrun, The chain collocation method: A spectrally accurate calculus of forms, J. Comput. Physics, 257, pp. 1352-1372, 2014.
[16] E. Kanso, M. Arroyo, Y. Tong, A. Yavari, J.E. Marsdenand M. Desbrun, On the geometric character of stress in continuum mechanics, Zeitschrift fur Angewandte Mathematik und Physik 58 (5) , pp. 843-856, 2007.
[17] A. Yavari, On geometric discretization of elasticity, Journal of Mathematical Physics 49 (2) , art. no. 022901, 2008.

[18] J. E. Marsden and T. J. R. Hughes, Mathematical Foundations of Elasticity, Dover Publications, New York, 1983.
[19] R. Segev, Notes on Metric Independent Analysis of Classical fields, Math. Meth. Appl. Sci., 36, pp. 497 - 566, 2013.
[20] Th. Frankel, The geometry of Physics. An Introduction, 2nd edition, Cambridge University Press, 2004.
[21] D. D. Holm, J. E. Marsden and T. S. Ratiu, The Euler-Poincaré Equations and Semidirect Products with Applications to Continuum Theories, Advances in Mathematics, 137, pp. 1-81, 1998.
[22] A. Bossavit, private communication, 2012 - 2013.
[23] J. Kreeft and M. Gerritsma, Mixed mimetic spectral element method for Stokes flow:A pointwise divergence-free solution, J. Comput. Physics, 240, pp. 284-309, 2013.
[24] B. Khesin, Dynamics of Symplectic Fluids and Point Vortices, Geom. Funct. Anal., Vol. 22, pp. 1444 - 1459, 2012.
[25] D. Toshniwal, R. H. M. Huijsmans and M. I. Gerritsma, A geometric approach towards momentum conservation, Spectral and High Order Methods for Partial Differential Equations - ICOSAHOM 2012, Eds M. Azaiez et al., Lecture Notes in Computational Science and Engineering, Volume 95, pp. 393–402, 2014.