ZAMM · Z. Angew. Math. Mech. **93**, No. 12, 868 – 881 (2013) / **DOI** 10.1002/zamm.201300080

A discrete-mechanical approach for computation of three-dimensional flows

B. Emek Abali[1,*], **Wolfgang H. Müller**[1], **and Dimitri V. Georgievskii**[2]

[1] Technical University of Berlin, Institute of Mechanics, Chair of Continuum Mechanics and Material Theory, Einsteinufer 5, 10587 Berlin, Germany
[2] Moscow State University, Mechanical and Mathematical Department, Moscow, 119899 Russia

Received 2 April 2013, accepted 24 May 2013
Published online 2 July 2013

Communicated by H. Altenbach and C. Wieners

Key words Variational formulation, computational fluid dynamics, balance equations.

Dynamical processes modeled with a suitable set of differential equations can be approximately computed with finite element method. However, especially in fluid dynamics, numerical instabilities may occur. In order to circumvent such problems many techniques have been realized over the last four decades. Often the lack of stability is linked to numerical insufficiency, therefore the solution is sought by tuning functional spaces, cf. [5] or by adding stabilizing terms, cf. [18, 19, 41]. Stabilizing terms are needed and helpful, however, they involve coefficients to be found depending on the underlying problem. The purpose of this work is to propose another approach based on first principles producing similar terms so that the numerical approximation converges without using any other parameter but the material constants, which are measurable. The approach eliminates stability problems, first, by setting the primary variables in a fundamental way and, second, by using the balance equations in their global form in a discrete manner instead of a continuous one. Some applications at the end emphasize the usefulness of the lengthy calculations, which we develop in a straightforward and consistent way.

1 Introduction

We consider a dynamic system to be defined in a finite region in ordinary space. Suppose that the region is a box filled with matter, which we call the "fluid." We shall compute the motion of every fluid particle in that region. Fluid can either enter or leave the region across the boundaries, thus the region is an open system. Each and every particle of the fluid flows with a velocity, however, it is cumbersome to follow each particle simultaneously, which is the case in a LAGRANGEan framework. Hence, we project the equations describing the fluid behavior onto the region. The equation of velocity in that projected region becomes a field function. The concept of such a field in the space employed MAXWELL according to [4] for the first time. We shall call a finite part of the region a domain. It can be thought of as equipped with infinitely many infinitesimally small measurement devices that record the velocity. This is merely a *Gedankenexperiment* and in reality not feasible, however, it is helpful to clarify the meaning of a field function. We can easily extend the experiment by measuring differently many quantities rather than just the velocity. Moreover, we can discretize the (region of) space by using a finite number of measurement devices, which are still infinitesimal. The measurement of a quantity, ϕ, takes place simultaneously on each (finite number of) measurement device, which we call *node*. The values of ϕ in each node can be interpolated and visualized by colors over the (region of) space. This corresponding distribution in space evolves in time: $\phi(\boldsymbol{x}, t)$. There may be many quantities, $\{\phi_1, \phi_2, \dots\}$, which we measure at the same time and may list as an array. We can even take a combination of them, as in the case of motion in three dimensions, and visualize them by an arrow at the nodes.

The interpolation between the nodes can be obtained with a suitable function. For the sake of computational time, we choose linear functions between the nearest neighbor nodes, which is the standard method in finite element analysis. Therefore, in three-dimensional space we define an element of four nodes, which has the shape of a tetrahedron. The field functions are linear within and continuous across each element that is a domain in the (region of) space, Ω. The connection between the nodes builds the configuration of the domain. The union of all domains, $\sum \Omega$, represents the region. Once the nodes and their connections are set, the resulting configuration does not change. Thus, the nodes have the same neighbors

* Corresponding author E-mail: abali@tu-berlin.de

during the simulation time, although the positions of the nodes may change. The collection of nodes, i.e., the mesh, gets its own velocity field $\boldsymbol{w}(\boldsymbol{x}, t)$, independent of the underlying physics. When the mesh velocity vanishes, then the framework is called EULERian. The velocity field may be arbitrary, however, the connectivity of finite elements shall be conserved, i.e., any penetration in the mesh should be omitted. In the next section we will obtain the equations based on first principles, the balances of mass, momenta, energy on the moving mesh.

In continuum mechanics for fluid flows, important assumptions are used to get the well-known differential equations that lead to numerical difficulties. First, the assumption of irrotational motion was proposed by KELVIN. The spin shall vanish in the formulation, which yields to potential flows [42, Sect. 88]. For non-polar media we also suppose that this assumption be true in a continuum consisting of infinitely many nodes. In a discretized space, however, the solution in each node without spin may produce a rotational velocity field inside of the domain. Thus, for the sake of computation, this production should be restricted. We will acquire the latter condition from the balance of angular momentum.

Instead of starting from the conservation laws, conventionally the balance of angular momentum is obtained by starting off a line integral of the tangential component of the velocity vector, as known as the circulation [11, Chap. I, Sect. 1.14.]. Subsequently, by using KELVIN's irrotational motion and HELMHOLTZ's first, second, and third theorems the convection is characterized by means of the CAUCHY's theorem [42, Sect. 134]. In the end, having a symmetric CAUCHY stress tensor implies that the balance of angular momentum is satisfied. This deduction, however, has a built-in condition of circulation preservation. Here, by employing the balance of angular momentum, we describe the rotational motion with respect to the domain–with respect to the midpoint of the finite element. Hence we allow the fluid to perform a circulation by satisfying the balance of angular momentum. Therefore we control the vortex motion regarding to material coefficients (like viscosity). From the extensive work about computational turbulent flow in [17] we learn that numerically induced turbulence starts as a vortex line which grows rapidly. A rapid growing output of a perturbation input might easily lead to (computational) instabilities. Hence it is of importance to include the balance of angular momentum in the calculations.

The flow of a viscous fluid would produce an energy due to internal friction between the particles. A simple application for purely viscous fluids demonstrates this fact in [30]. However, in many processes this production of energy is negligible. When no heat energy fluxes over the boundaries, i.e., adiabatic boundaries, and if the initial temperature distribution is homogeneous, we expect an isothermal flow. We only implement isothermal processes for the sake of comparison to the successful finite element modelings in fluid dynamics as in [8,17,20,37]. Quite often, the presumption of an isothermal state (no temperature gradients) is interpreted such that the energy equation is also numerically fulfilled. On the contrary, the production term in the energy equation may lead to numerical instabilities. Although we will not compute the temperature distribution, the induced production term may be necessary to regulate the flow. The physical example of this was realized by BENARD in 1900, by heating over one boundary and thus creating a temperature gradient in a stable fluid which induces a flow to homogenize the temperature, although the phenomenon was already realized by RUMFORD (1797) and THOMSON (1882) (for a detailed study refer to [6, Chap. II]).

In what follows, we introduce conserved quantities and their balance laws for open systems, which hold universally. It is worthwhile pointing out that we immediately handle the balance equations in a discrete sense rather than within a continuum framework. Thereafter the constitutive relations will be outlined in a mathematically consistent way. Finally, by using variational formulation, the generic form is represented. For the sake of completeness, some flow problems in three-dimensions, which are numerically complicated, are solved and their codes are published in [1] to be used under GNU Public License, cf. [15], for convenience.

2 Formulation

Throughout this work we will use the symbol "$(\cdot)^\bullet$" to denote the material time derivative for a field related to a particle. The configuration, i.e., the connection between the nodes, is a HILBERT configuration as defined in [16] and we use linear interpolation functions between the adjacent nodes, which form the elements, Ω.

As for each point in a continuum mechanics' sense, there are conserved quantities, Ψ_i, in each domain Ω, i.e., in each finite element. We can track their evolution over time, following a path inside the domain or crossing its boundaries. A generic balance equation inside the element Ω over its boundaries $\partial\Omega$ can be written such that the change of each conserved quantities Ψ_α in the interior of the element Ω is due to the appropriate supplies $\mathcal{Z}_\alpha$, convective fluxes $\mathcal{F}_\alpha$, as well as the non-convective fluxes Φ_α across the boundary $\partial\Omega$:

$$\begin{aligned} (\Psi_\alpha)^\bullet &= \mathcal{Z}_\alpha + \mathcal{F}_\alpha + \Phi_\alpha \,, \\ \left(\int_\Omega \mathrm{d}\Psi_\alpha\right)^\bullet &= \int_\Omega z_\alpha \,\mathrm{d}V + \int_{\partial\Omega} (f_\alpha + \phi_\alpha)\,\mathrm{d}A \,. \end{aligned} \tag{1}$$

The index α denotes different conserved quantities. The supply term, z_α, is a volume density and the flux terms, f_α, ϕ_α, are areal densities. The conserved quantities are mass, M, linear momentum, $P_i = (P_1, P_2, P_3)$, angular momentum, $A_i = (A_1, A_2, A_3)$, and total energy, E. The list of $\Psi_\alpha = \{M, P_i, A_i, E\}$ consists of eight field functions in three-dimensional space $x^i \in \mathbb{R}^3$. For all of these the balance equations for open systems will now be introduced. For a more detailed discussion the reader is referred to [31, 32].

2.1 Supply and fluxes

The corresponding supply and fluxes for a fluid without electric charge has been collected in Tab. 1, where, and henceforth, EINSTEIN's summation convention over repeated indices is applied.

Table 1 Supplies and fluxes of conserved quantities.

α	Ψ_α	z_α	f_α	ϕ_α
1	M	$-$	$\rho(w_i - v_i)n^i$	$-$
2	P_i	ρg_i	$p_i(w_j - v_j)n^j$	t_i
3	A_i	$\rho s_i + \rho g_{in}\epsilon^{njk}x_j g_k$	$\rho s_i(w_j - v_j)n^j + g_{in}\epsilon^{njk}x_j p_k(w_l - v_l)n^l$	$-l_i + g_{in}\epsilon^{njk}x_j t_k$
4	E	$\rho r + g_i p^i$	$\rho e(w_j - v_j)n^j$	$-q + t_k v^k$

In the case of the balance of mass, M, and its density, ρ, the flux term is purely convective. The mass flux across the boundary, oriented outwards in its normal, n^i, is caused by particles having a velocity relative to the motion of boundary. The field w_i is the velocity of the boundary and the field v_i is the velocity of the particle.

For the linear momentum, P_i, and its density, p_i, the supply term is of gravitational or electro-magnetic origin. Since the fluid lacks electric charge electro-magnetic forces induce no motion. Thus, only the volumetric (specific, per mass) force of gravitation, g_i, may exist. Here we assume that the traction forces, t_i, caused by the non-convective fluxes are much greater than the forces due to the supplies, thus g_i for linear momentum is neglected. The traction vector, $t_i = n^j\sigma_{ji}$, is given by the CAUCHY stress tensor σ_{ij} according to the CAUCHY's tetrahedron argument [42, Sect. 203].

Angular momentum, written as an axial vector, A_i, is the sum of the spin, S_i, and of the moment of momentum, $\epsilon_i^{\ jk}x_j P_k$, with respect to mid-point of the domain Ω. Same holds for the axial angular momentum density, a_i, spin density, s_i, and moment of momentum density, $\epsilon_i^{\ jk}x_j p_k$ with respect to mid-point of the domain Ω. Hence x_j denotes the position of a particle with respect to the mid-point of the finite element, Ω. In the case of a continuum, Ω collapses into a point and thus the moment of momentum vanishes since $x_j \to 0$. In the discrete case, however, it may produce a vortex motion. In order to see this, first we need to bring the balance of momenta to the local form by using the GAUSS-OSTOGRADSKIY's theorem, which implies the continuity of the stress, σ_{ij}. Second, we multiply the balance of linear momentum with $\epsilon_n^{\ jk}x_j$; third, we subtract the result from the balance of angular momentum. The rest written as a balance equation leads to a balance of spin with a non-convective flux term: l_i, and a production term: $-\epsilon_i^{\ jk}\sigma_{jk}$, cf. [29, p. 31]. We already stated that the fluid in this work is a non-polar medium. Thus, the spin will vanish, $s_i = 0$. By choosing a symmetric stress tensor, $\sigma_{ij} = \sigma_{ji}$, we exclude a production of spin, $\epsilon_i^{\ jk}\sigma_{jk} = 0$. Since no spin exists and is also not produced, the non-convective flux of spin, l_i, disappears, too. The metric of the space, g_{ij}, will be defined by choosing a coordinate system in the next section.

In the case of the total energy, E, we assume an isothermal state. This means that there is no heat conducting in the domain, $q = 0$. We can control the radiation term, thus we choose: $r = 0$. Since g_i is neglected, zero kinetic supply follows for energy. Moreover, the flux term of the angular momentum vanishes on a closed domain integration, as a consequence of ignoring the spin production (symmetric stress tensor).

2.2 Rate of conserved quantities

We have defined the supplies and fluxes for the conserved quantities for a fluid without electric charge, cf. Table 1, and then assumed some simplifications such as: neglecting the gravity, expecting no spin, presuming an isothermal state. Equations (1) are now specified in a domain, Ω:

$$\begin{aligned}
\left(\int_\Omega \mathrm{d}M\right)^\bullet &= \int_{\partial\Omega} \rho(w_i - v_i) n^i \,\mathrm{d}S\,,\\
\left(\int_\Omega \mathrm{d}P_i\right)^\bullet &= \int_{\partial\Omega} n^j \Big(\sigma_{ji} + p_i w_j - p_i v_j\Big)\,\mathrm{d}S\,,\\
\left(\int_\Omega \mathrm{d}A_i\right)^\bullet &= \int_{\partial\Omega} g_{in}\epsilon^{njk} x_j \Big(\sigma_{lk} + p_k w_l - p_k v_l\Big) n^l \,\mathrm{d}S\,,\\
\left(\int_\Omega \mathrm{d}E\right)^\bullet &= \int_{\partial\Omega} \Big(n^l \sigma_{lk} v^k + e(w_i - v_i) n^i\Big)\,\mathrm{d}S\,.
\end{aligned} \tag{2}$$

We define the following quantities:

$$M = \rho V\,,\ P_i = M v_i\,,\ A_i = S_i + g_{ij}\epsilon^{jkl} x_k P_l\,,\ E = U + K\,, \tag{3}$$

where the mass density ρ is a field per volume of the domain, V, and $S_i, \epsilon^{jkl} x_k P_l, U, K$ denote spin, moment of momentum, internal, and kinetic energy, respectively. We already excluded spin by assuming a non-polar media, thus $S_i \equiv 0$. Internal and kinetic energies U, K are usually defined as specific (per unit mass) quantities, i.e., $U = uM, K = kM$. We choose cartesian coordinate system for numerical reasons, cf. Sect. 3. Therefore $g_{ij} \equiv \delta_{ij}$ and the metric is everywhere (in Ω) the same, i.e., $\frac{\partial g_{ij}}{\partial x^k} \equiv \frac{\partial \delta_{ij}}{\partial x^k} = 0 \Rightarrow \mathrm{d}g_{ij} \equiv \mathrm{d}\delta_{ij} = 0$. We refrain from distinguishing between co-and contravariant notation in the following since they are the same in cartesian coordinates. We restrict ourselves to small finite elements, $\Omega \to 0$, so that the approximation $\mathrm{d}x_i = 0$ holds. However, we insist on $\mathrm{d}v_i \neq 0$ because we cannot control the velocities directly. Now, we write the conserved quantities as differentials in space:

$$\begin{aligned}
&\mathrm{d}M = \mathrm{d}\left(\frac{M}{V}V\right) = \mathrm{d}(\rho V) = \rho\,\mathrm{d}V\,,\ \mathrm{d}P_i = \mathrm{d}(M v_i) = \mathrm{d}M\, v_i + M\,\mathrm{d}v_i = \rho\,\mathrm{d}V v_i + M\,\mathrm{d}v_i\,,\\
&\mathrm{d}A_i = \epsilon_{ikl} x_k\,\mathrm{d}P_l\,,\ \mathrm{d}E = \mathrm{d}uM + u\,\mathrm{d}M + \mathrm{d}k\,M + k\,\mathrm{d}M\,.
\end{aligned} \tag{4}$$

The densities are quantities per volume of space and thus they can be treated like constants in the differential element. The specific quantities, $\mathrm{d}u$, $\mathrm{d}k$, are quantities per mass of fluid and their values change regarding the differential element. In the continuum $\mathrm{d}v_i$ also vanishes under the assumption that in an infinitesimal space the velocity is constant. However, in a finite domain Ω this is not the case, unless polynomial elements of order zero, like in finite volume method or discontinuous elements with order zero, are used. This might be a simple explanation of (numerically) more stable results by using one of these methods.

The internal energy may depend on the elastic deformation and on the temperature deviation from the reference temperature. The latter will not exist under the assumption of an isothermal state assumption. The elastic deformation in a viscous fluid is assumed to be caused by the mechanical pressure. The mechanical pressure is equivalent to the thermodynamical pressure under some restrictions [10, Sect. 48], which we will discuss later and fulfill them. This leads to a simple, but nevertheless for many cases of simple fluids well working approximation for the specific internal energy $u = p/(\alpha\rho)$, where p denotes the pressure and α is a matter dependent constant parameter. Because of its constancy, we have $\mathrm{d}\alpha = 0$. Pressure is force per unit area, i.e., it is also a (areal) density. Since p, α, ρ lack differentials, $\mathrm{d}u$ vanishes, too.

The kinetic energy is defined as $K = \frac{1}{2} M v_k v_k$. Thus the specific (per mass) kinetic energy, $k = \frac{1}{2} v_k v_k$, has a differential such that $\mathrm{d}k = v_k\,\mathrm{d}v_k$ holds.

The integration holds on one finite element domain Ω and the sum of all the domains represents the region. The mass $M = m$ and volume V denote the mass and volume of one single element Ω.

2.3 Balance equations

Consequently the balance of mass:

$$\int_\Omega \Big((\rho)^\bullet\ \mathrm{d}V + \rho\,(\,\mathrm{d}V)^\bullet \Big) = \int_{\partial\Omega} \rho(w_i - v_i) n_i\,\mathrm{d}S\,, \tag{5}$$

the balance of linear momentum:

$$\int_\Omega \Big((\rho v_i)^\bullet\ \mathrm{d}V + \rho v_i\,(\,\mathrm{d}V)^\bullet + (m)^\bullet\ \mathrm{d}v_i + m\,(\,\mathrm{d}v_i)^\bullet \Big) = \int_{\partial\Omega} \Big(n_j \sigma_{ji} + n_j w_j \rho v_i - n_j v_j \rho v_i\Big)\,\mathrm{d}S\,, \tag{6}$$

the balance of angular momentum:

$$\int_\Omega \Big(\epsilon_{ikl} w_k(\rho v_l \,\mathrm{d}x + m\,\mathrm{d}v_l) + \epsilon_{ikl} x_k \left(\rho v_l \,\mathrm{d}x + m\,\mathrm{d}v_l\right)^\bullet\Big) = \int_{\partial\Omega} \epsilon_{ijk} x_j \Big(\sigma_{lk} + \rho v_k w_l - \rho v_k v_l\Big) n_l \,\mathrm{d}S\,, \tag{7}$$

the balance of total energy:

$$\begin{aligned}\int_\Omega \Bigg(\left(\frac{p}{\alpha\rho}\rho\,\mathrm{d}V\right)^\bullet + (m v_i\,\mathrm{d}v_i)^\bullet + v_n\,(v_n)^\bullet\,\rho\,\mathrm{d}V + \frac{1}{2} v_n v_n\,(\rho)^\bullet\,\mathrm{d}V + \frac{1}{2} v_n v_n \rho\,(\mathrm{d}V)^\bullet \Bigg) \\ = \int_{\partial\Omega} \Big(n_l \sigma_{lk} v_k + \frac{1}{2}\rho v_k v_k n_i w_i - \frac{1}{2}\rho v_k v_k n_i v_i\Big)\,\mathrm{d}S\,,\end{aligned} \tag{8}$$

need to be satisfied for an isothermal flow of a viscous flow without charge. As already mentioned, the coordinates of the nodes may change in time, thus the moving mesh has a velocity, w_i. In order to evaluate the velocity we need a static observer. We will start from a zero velocity with an initial mesh, which we can choose as the reference frame. By employing a reference frame $\mathrm{d}X_i$ that does not evolve in time, i.e., $\left(\mathrm{d}X_j\right)^\bullet = 0$, the rate of the element frame is derived

$$(\mathrm{d}x_i)^\bullet = \left(\frac{\partial x_i}{\partial X_j}\,\mathrm{d}X_j\right)^\bullet = \frac{\partial w_i}{\partial X_j}\,\mathrm{d}X_j = \mathrm{d}w_i\,, \tag{9}$$

where w_i is the velocity field of the domain Ω with respect to the static reference frame. The underlying physics does not change upon the mesh velocity. By using Eq. (9), the rate of the volume element can be found,

$$\begin{aligned}(\mathrm{d}V)^\bullet &= (\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z)^\bullet = (\mathrm{d}x)^\bullet\,\mathrm{d}y\,\mathrm{d}z + \mathrm{d}x\,(\mathrm{d}y)^\bullet\,\mathrm{d}z + \mathrm{d}x\,\mathrm{d}y\,(\mathrm{d}z)^\bullet \\ &= \left(\frac{(\mathrm{d}x)^\bullet}{\mathrm{d}x} + \frac{(\mathrm{d}y)^\bullet}{\mathrm{d}y} + \frac{(\mathrm{d}z)^\bullet}{\mathrm{d}z}\right)\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z = \frac{(\mathrm{d}x_i)^\bullet}{\mathrm{d}x_i}\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z = \frac{\mathrm{d}w_i}{\mathrm{d}x_i}\,\mathrm{d}V \\ &= \Big(\frac{\partial w_i}{\partial x_i} + \frac{\partial w_i}{\partial t}\frac{\mathrm{d}t}{\mathrm{d}x_i}\Big)\,\mathrm{d}V = \frac{\partial w_i}{\partial x_i}\,\mathrm{d}V\,,\end{aligned} \tag{10}$$

where we utilized that the time, t, is absolute. By applying the GAUSS-OSTROGRADSKIY theorem, by using the material time rate $(\cdot)^\bullet = \frac{\partial}{\partial t} + \frac{\mathrm{d}x_i}{\mathrm{d}t}\frac{\partial}{\partial x_i} = \frac{\partial}{\partial t} + w_i\frac{\partial}{\partial x_i}$ and by recalling that the mass, volume of one element is m, V, respectively, the residuals denoted by "R," which are left-hand sides minus right-hand sides, of the balance Eqs. (5), (6), (7), (8) read

$$\mathrm{Rm} = \int_\Omega \mathrm{d}V\Big(\frac{\partial \rho}{\partial t} + w_i\frac{\partial \rho}{\partial x_i} + \rho\frac{\partial w_i}{\partial x_i} - \frac{\partial}{\partial x_i}(\rho(w_i - v_i))\Big)\,, \tag{11}$$

$$\begin{aligned}\mathrm{Rp}_i = &\int_\Omega \mathrm{d}V\Big(\frac{\partial \rho}{\partial t}v_i + w_j\frac{\partial \rho}{\partial x_j}v_i + \rho\frac{\partial v_i}{\partial t} + \rho w_j\frac{\partial v_i}{\partial x_j} + \rho v_i\frac{\partial w_k}{\partial x_k} - \frac{\partial}{\partial x_j}\Big(\sigma_{ji} + w_j\rho v_i - v_j\rho v_i\Big)\Big) \\ &+ \int_\Omega \mathrm{d}v_i\Big(\frac{\partial \rho}{\partial t}V + w_i\frac{\partial \rho}{\partial x_i}V + \rho\,(V)^\bullet\Big) + \int_\Omega m\,(\mathrm{d}v_i)^\bullet\,,\end{aligned} \tag{12}$$

$$\begin{aligned}\mathrm{Ra}_i = &\int_\Omega \mathrm{d}V\Big(\epsilon_{ikl}w_k\rho v_l + \epsilon_{ikl}x_k v_l\Big(\frac{\partial \rho}{\partial t} + w_i\frac{\partial \rho}{\partial x_i}\Big) + \epsilon_{ikl}x_k\rho\Big(\frac{\partial v_l}{\partial t} + w_i\frac{\partial v_l}{\partial x_i}\Big) + \epsilon_{ikl}x_k\rho v_l\frac{\partial w_i}{\partial x_i} \\ &- \frac{\partial}{\partial x_l}\Big(\epsilon_{ijk}x_j\big(\sigma_{lk} + w_l\rho v_k - v_l\rho v_k\big)\Big)\Big) + \int_\Omega \mathrm{d}v_l\epsilon_{ikl}\Big(w_k\rho V + x_k\frac{\partial \rho}{\partial t}V + x_k w_j\frac{\partial \rho}{\partial x_j}V \\ &+ x_k\rho\,(V)^\bullet\Big) + \int_\Omega \epsilon_{ikl}x_k m\,(\mathrm{d}v_l)^\bullet\,,\end{aligned} \tag{13}$$

$$\begin{aligned}\mathrm{Re} = &\int_\Omega (m)^\bullet\, v_i \,\mathrm{d}v_i + \int_\Omega m\,(v_i)^\bullet \,\mathrm{d}v_i + \int_\Omega m v_i\,(\mathrm{d}v_i)^\bullet + \int_\Omega \mathrm{d}V\Big(\frac{1}{\alpha}\Big(\frac{\partial p}{\partial t} + w_i\frac{\partial p}{\partial x_i}\Big) + \frac{1}{\alpha}p\frac{\partial w_i}{\partial x_i}\\ &+ \rho v_n\Big(\frac{\partial v_n}{\partial t} + w_i\frac{\partial v_n}{\partial x_i}\Big) + \frac{1}{2}v_n v_n\Big(\frac{\partial \rho}{\partial t} + w_i\frac{\partial \rho}{\partial x_i}\Big) + \frac{1}{2}v_n v_n\rho\frac{\partial w_i}{\partial x_i}\\ &- \frac{\partial}{\partial x_l}\Big(\sigma_{lk}v_k + \frac{1}{2}\rho v_k v_k w_l - \frac{1}{2}\rho v_k v_k v_l\Big)\Big)\,. \end{aligned} \tag{14}$$

2.4 Remarks

This lengthy but straightforward discrete derivation shows the clear distinction to the continuous case. If the derivation would have been started from the continuum, i.e., local conservation laws in every point instead of global ones in a finite element, there would be many terms missing in the end. The missing terms may cause numerical instabilities. This can be demonstrated for each balance equation. Assume that the space, or better the mesh has no velocity, $w_i = 0$, then the Eq. (11) takes the form of the usual local balance of mass

$$\int_\Omega \mathrm{d}V\Big(\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x^i}(\rho v_i)\Big) = 0 \Rightarrow \frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x^i}(\rho v_i) = 0\,. \tag{15}$$

Suppose that the element volume is constant in time $(V)^\bullet = 0$. Additionally the volume gets infinitesimal, $V \to 0$, then the corresponding terms from the balance of linear and angular momentum will vanish

$$\begin{aligned}&\int_\Omega \mathrm{d}v_i\Big(\frac{\partial \rho}{\partial t}V + w^i\frac{\partial \rho}{\partial x^i}V + \rho\,(V)^\bullet\Big) = 0\,,\\ &\int_\Omega \mathrm{d}v_l\epsilon_i^{kl}\Big(w_k\rho V + x_k\frac{\partial \rho}{\partial t}V + x_k w^j\frac{\partial \rho}{\partial x^j}V + x_k\rho\,(V)^\bullet\Big) = 0\,.\end{aligned} \tag{16}$$

Moreover, we have acquired many terms with a directed measure, $\mathrm{d}v_i$. The phenomenon of numerical instabilities is known for a long time. A thorough overview of various approaches, i.e., stabilization techniques, can be found in [28]. Roughly speaking, stabilization techniques propose to add terms in direction of the velocity and appeared for the first time in [18,19]. In our formulation, the terms with $\mathrm{d}v_i$ maintain a similar effect since

$$\int_\Omega \mathrm{d}v_i = \int_\Omega \frac{v_i}{\|v_j\|}\,\mathrm{d}V \tag{17}$$

proposes that only the term projected onto the velocity direction shall be integrated. Here we have obtained such terms in Eqs. (12) and (13) by starting from balance equations in a finite element in global forms. Now it is obvious why the balance of angular momentum and balance of energy are included in the formulation. The first one stabilizes the velocity and the second the mass density (or pressure). The advantage of this approach is that we only need to know the material constants–they do not depend on the process.

3 Variational formulation

We are going to discretize in time and space separately. In order to discretize in time, we choose an implicit backwards finite difference scheme

$$\frac{\partial(\cdot)}{\partial t} = \frac{(\cdot) - (\cdot)^0}{\mathrm{d}t}\,,\ \ \mathrm{d}t = t - t^0\,, \tag{18}$$

which is a stable (for real valued problems) method. The upper index "0" denotes to the value from the last time position, i.e., to the solution at the last time step. We use and implement constant time steps, $\mathrm{d}t$, for all applications in Sect. 3.3.

In order to discretize in space, we employ the finite element method. The unknown fields[1] are $u_i = (\rho, v_i)$ and spans a four-dimensional HILBERT space of order one, $\mathcal{H}^1$, in one single node. Formally the space is a SOBOLEV space $\mathcal{H}^1_s$ where the differentiation operation is defined. In the domain Ω with many nodes, the HILBERT space is of higher dimensions. In that space, the approximation with finite element method is based on a weak formulation. In order to obtain a weak formulation we multiply each residual in Eqs. (11)–(14) with an appropriate test function

$$\int_\Omega \mathrm{d}V q\Big(\frac{\rho-\rho^0}{\mathrm{d}t} + w_i\frac{\partial\rho}{\partial x_i} + \rho\frac{\partial w_i}{\partial x^i} - \frac{\partial}{\partial x_i}(\rho(w_i - v_i))\Big) = 0\,, \tag{19}$$

$$\begin{aligned}\int_\Omega \mathrm{d}V \varpi_i\Big(&\frac{\rho-\rho^0}{\mathrm{d}t}v_i + w_j\frac{\partial\rho}{\partial x_j}v_i + \rho\frac{v_i - v_i^0}{\mathrm{d}t} + \rho w^j\frac{\partial v_i}{\partial x_j} + \rho v_i\frac{\partial w_k}{\partial x_k} - \frac{\partial}{\partial x_j}\Big(\sigma_{ji} + w_j\rho v_i - v_j\rho v_i\Big)\\ &+ \frac{v_i}{\|v_k\|}\frac{\rho-\rho^0}{\mathrm{d}t}V + \frac{v_i}{\|v_k\|}w_i\frac{\partial\rho}{\partial x_i}V + \frac{v_i}{\|v_k\|}\rho\frac{1}{\mathrm{d}t}(V-V^0) + \frac{1}{\mathrm{d}t}\Big(\frac{v_i}{\|v_k\|} - \frac{v_i^0}{\|v_k^0\|}\Big)\rho V\Big) = 0\,,\end{aligned} \tag{20}$$

$$\begin{aligned}\int_\Omega \mathrm{d}V \varpi_i\Big(&\epsilon_{ikl}w_k\rho v_l + \epsilon_{ikl}x_k v_l\Big(\frac{\rho-\rho^0}{\mathrm{d}t} + w_i\frac{\partial\rho}{\partial x_i}\Big) + \epsilon_{ikl}x_k\rho\Big(\frac{v_l - v_l^0}{\mathrm{d}t} + w_i\frac{\partial v_l}{\partial x_i}\Big)\\ &+ \epsilon_{ikl}x_k\rho v_l\frac{\partial w_i}{\partial x_i} - \frac{\partial}{\partial x_l}\Big(\epsilon_{ijk}x_j\big(\sigma_{lk} + w_l\rho v_k - v_l\rho v_k\big)\Big) + \frac{v_l}{\|v_p\|}\epsilon_{ikl}\Big(w_k\rho V + x_k\frac{\rho-\rho^0}{\mathrm{d}t}V\\ &+ x_k w_j\frac{\partial\rho}{\partial x_j}V + x_k\rho\frac{1}{\mathrm{d}t}(V-V^0)\Big) + \frac{1}{\mathrm{d}t}\Big(\frac{v_l}{\|v_p\|} - \frac{v_l^0}{\|v_p^0\|}\Big)\epsilon_{ikl}x_k\rho V\Big) = 0\,,\end{aligned} \tag{21}$$

$$\begin{aligned}\int_\Omega \mathrm{d}V q\Big(&\frac{\rho-\rho^0}{\mathrm{d}t}Vv_i\frac{v_i}{\|v_k\|} + \rho V\frac{v_i - v_i^0}{\mathrm{d}t}\frac{v_i}{\|v_k\|} + \rho V v_i\frac{1}{\mathrm{d}t}\Big(\frac{v_i}{\|v_k\|} - \frac{v_i^0}{\|v_k^0\|}\Big) + \rho V v_i\frac{v_i}{\|v_k\|}\frac{\partial w_j}{\partial x_j}\\ &+ \frac{1}{\alpha}\Big(\frac{p-p^0}{\mathrm{d}t} + w_i\frac{\partial p}{\partial x_i}\Big) + \frac{1}{\alpha}p\frac{\partial w^i}{\partial x^i} + \rho v_n\Big(\frac{v_n - v_n^0}{\mathrm{d}t} + w_i\frac{\partial v_n}{\partial x_i}\Big) + \frac{1}{2}v_n v_n\Big(\frac{\rho-\rho^0}{\mathrm{d}t} + w_i\frac{\partial\rho}{\partial x_i}\Big)\\ &+ \frac{1}{2}v_n v_n\rho\frac{\partial w_i}{\partial x_i} - \frac{\partial}{\partial x_l}\Big(\sigma_{lk}v_k + \frac{1}{2}\rho v_k v_k w_l - \frac{1}{2}\rho v_k v_k v_l\Big)\Big) = 0\,.\end{aligned} \tag{22}$$

The test functions $\bar{u}_i = (q, \varpi_j)$ can be chosen from any space, there exists a unique solution according to the RIESZ representation theorem, cf. [38]. We choose them from the same space as the unknowns, which is the GALERKIN method, so that the variational formulation reads

$$\min\Big(q\mathrm{Rm} + \varpi_i\mathrm{Rp}_i + \varpi_i\mathrm{Ra}_i + q\mathrm{Re}\Big)\,,\ \forall u_i, \bar{u}_i \in \mathcal{H}^1_s\,. \tag{23}$$

The residuals are weighted by appropriate functions, i.e., they are contracted into scalar values, which are invariants in the HILBERT space, cf. [33, 34]. The HILBERT space as defined in [16] has the PHYTAGORAS length definition, therefore

$$\|v_i\| = \sqrt{v_j\delta_{ji}v_i} = (v_i v_i)^{1/2}\,. \tag{24}$$

Since the whole region consists of the union of domains, we can sum up the integrals

$$\sum_{\text{Elements}}\int_\Omega \ldots\,\mathrm{d}V\,, \tag{25}$$

where each integral is to be computed with GAUSS quadrature. The GAUSS points and weights are known in orthonormal set of coordinates, this is the reason of having chosen the cartesian coordinates for the space.

[1] We omit to represent the discretized functions differently from the continuous ones in order not to overload the notation.

The mesh velocity is arbitrary and only useful in case of a fluid structure interaction. For our purposes in Sect. 3.3 a static mesh is appropriate, thus $w_i = 0$ that implies $V = V^0$. The final formulation reads

$$\begin{aligned}
&\sum_{\text{Elements}} \int_\Omega \mathrm{d}V \Big(q\frac{\rho-\rho^0}{\mathrm{d}t} + q\frac{\partial \rho}{\partial x_i} + q\rho\frac{\partial v_i}{\partial x_i} + \varpi_i \frac{\rho-\rho^0}{\mathrm{d}t} v_i + \varpi_i \rho \frac{v_i - v_i^0}{\mathrm{d}t} - \varpi_i \frac{\partial}{\partial x_j}\Big(\sigma_{ji} - v_j \rho v_i\Big) \\
&+ \varpi_i \frac{v_i}{\|v_k\|}\frac{\rho-\rho^0}{\mathrm{d}t} V + \varpi_i \frac{1}{\mathrm{d}t}\Big(\frac{v_i}{\|v_k\|} - \frac{v_i^0}{\|v_k^0\|}\Big)\rho V + \varpi_i \epsilon_{ikl} x_k v_l \frac{\rho-\rho^0}{\mathrm{d}t} + \varpi_i \epsilon_{ikl} x_k \rho \frac{v_l - v_l^0}{\mathrm{d}t} \\
&- \varpi_i \frac{\partial}{\partial x_l}\Big(\epsilon_{ijk} x_j \big(\sigma_{lk} - v_l \rho v_k\big)\Big) + \varpi_i \frac{v_l}{\|v_p\|}\epsilon_{ikl} x_k \frac{\rho-\rho^0}{\mathrm{d}t} V + \varpi_i \frac{1}{\mathrm{d}t}\Big(\frac{v_l}{\|v_p\|} - \frac{v_l^0}{\|v_p^0\|}\Big)\epsilon_{ikl} x_k \rho V \\
&+ q\frac{\rho-\rho^0}{\mathrm{d}t} V v_i \frac{v_i}{\|v_k\|} + q\rho V \frac{v_i - v_i^0}{\mathrm{d}t}\frac{v_i}{\|v_k\|} + q\rho V v_i \frac{1}{\mathrm{d}t}\Big(\frac{v_i}{\|v_k\|} - \frac{v_i^0}{\|v_k^0\|}\Big) + q\frac{p-p^0}{\alpha\,\mathrm{d}t} + q\rho v_n \frac{v_n - v_n^0}{\mathrm{d}t} \\
&+ q\frac{1}{2} v_n v_n \frac{\rho-\rho^0}{\mathrm{d}t} - q\frac{\partial}{\partial x_l}\Big(\sigma_{lk} v_k - \frac{1}{2}\rho v_k v_k v_l\Big)\Big) = 0\,. \qquad (26)
\end{aligned}$$

Minimization of this relation will lead to the solution $u_i = (\rho, v_j)$ uniquely. But first we need to define an appropriate material equation, stress σ_{ij}, as well as suitable boundary conditions.

3.1 Constitutive relation

There exists many different approaches to find a constitutive relation. One of them is a polynomial approximation in the arguments as in [10, Chap. 5, Sect. 49], which reads for the case that σ_{ij} depends on $\partial v_{(i}/\partial x_{j)}$

$$\sigma_{ij} = a\delta_{ij} + b\frac{\partial v_{(i}}{\partial x_{j)}} + c\frac{\partial v_{(i}}{\partial x_{k)}}\frac{\partial v_{(k}}{\partial x_{j)}}\,,\ \frac{\partial v_{(i}}{\partial x_{j)}} = \frac{1}{2}\Big(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i}\Big)\,. \qquad (27)$$

This is the most general constitutive equation for a tensor of second rank depending solely on one second rank tensor as an argument, cf. [40]. The symmetric part of the velocity gradients, $\partial v_{(i}/\partial x_{j)}$, ensures that the CAUCHY stress tensor becomes symmetric. The coefficients a, b, c are scalar functions depending on the invariants of the argument; read according to HAMILTON-CAYLEY theorem

$$\begin{aligned}
&a = \hat{a}(I, II, III)\,,\ b = \hat{b}(I, II, III)\,,\ c = \hat{c}(I, II, III)\,, \\
&I = \frac{\partial v_i}{\partial x_i}\,,\ II = \frac{\partial v_i}{\partial x_j}\frac{\partial v_j}{\partial x_i}\,,\ III = \frac{\partial v_i}{\partial x_j}\frac{\partial v_j}{\partial x_k}\frac{\partial v_k}{\partial x_i}\,.
\end{aligned} \qquad (28)$$

The well-known NAVIER-STOKES equation emerges by using a first-order relation, i.e., $c = 0$ and $b = \mu = \text{const}$, and by choosing the first coefficient as $a = -p + \lambda I$. In this thermodynamically admissible case p is the thermodynamic pressure, which is important for the approximation of internal energy by the pressure.

From a physical point of view, the dependence of the stress may be extended so that besides velocity gradients also acceleration gradients take part in it. By using the latter scheme the number of coefficients depends on polynomials of their invariants; and, thus, the total number of material constants will increase potentially to more than a measurable amount. Therefore another approach, starting from retarded motions in [7] for incompressible, isotropic matter has been found useful. This model reads

$$\sigma_{ij} = -p\delta_{ij} + \mu A_{ij}^{(1)} + \gamma A_{ij}^{(2)} + \beta A_{ik}^{(1)} A_{kj}^{(1)}\,, \qquad (29)$$

where μ, γ, β are real scalar values, i.e., material constants and the RIVLIN-ERICKSEN tensors, cf. [39], are defined as

$$A_{ij}^{(1)} = \frac{\partial v_{(i}}{\partial x_{j)}}\,,\ A_{ij}^{(2)} = \frac{\partial A_{ij}^{(1)}}{\partial t} + \frac{\partial A_{ij}^{(1)}}{\partial x_k} v_k + A_{ik}^{(1)}\frac{\partial v_k}{\partial x_j} + \frac{\partial v_k}{\partial x_i} A_{kj}^{(1)}\,. \qquad (30)$$

Especially its ability on the second-order effects with three-parameters makes this model popular in polymer science. However, there are some drawbacks coming with such models. A closed form solution of flows of such non-linear flows is only possible for very special cases, an example can be found in [13]. Moreover, the material parameters cannot be determined easily, for a discussion of it cf. [14]. From a thermodynamic point of view there are some restrictions to the

material parameters, cf. [9], but also [12]. We will choose: $\mu \geq 0, \beta \geq 0, \gamma + \beta = 0$, and implement this model to the variational form. In order to clarify the terms with second-order derivatives in space, we decompose the stress as $\sigma_{ij} = -p\delta_{ij} + \tau_{ij}$. Hence τ_{ij} includes all the terms involving velocity gradients. By recasting the latter into variational form (26), we obtain

$$\begin{aligned}
&\sum_{\text{Elements}} \int_\Omega \mathrm{d}V \Bigg(q\frac{\rho-\rho^0}{\mathrm{d}t} + q\frac{\partial \rho}{\partial x_i}v_i + q\rho\frac{\partial v_i}{\partial x_i} + \varpi_i\frac{\rho-\rho^0}{\mathrm{d}t}v_i + \varpi_i\rho\frac{v_i-v_i^0}{\mathrm{d}t} + \varpi_i\frac{\partial p}{\partial x_j}\delta_{ji} \\
&- \varpi_i\frac{\partial \tau_{ji}}{\partial x_j} + \varpi_i\frac{\partial v_j}{\partial x_j}\rho v_i + \varpi_i v_j\frac{\partial \rho}{\partial x_j}v_i + \varpi_i v_j\rho\frac{\partial v_i}{\partial x_j} + \varpi_i\frac{v_i}{\|v_k\|}\frac{\rho-\rho^0}{\mathrm{d}t}V + \varpi_i\frac{1}{\mathrm{d}t}\Big(\frac{v_i}{\|v_k\|} - \frac{v_i^0}{\|v_k^0\|}\Big)\rho V \\
&+ \varpi_i\epsilon_{ikl}x_k v_l\frac{\rho-\rho^0}{\mathrm{d}t} + \varpi_i\epsilon_{ikl}x_k\rho\frac{v_l-v_l^0}{\mathrm{d}t} + \varpi_i\epsilon_{ijk}\delta_{jl}p\delta_{lk} + \varpi_i\epsilon_{ijk}x_j\frac{\partial p}{\partial x_l}\delta_{lk} \\
&- \varpi_i\epsilon_{ijk}\delta_{jl}\tau_{lk} - \varpi_i\epsilon_{ijk}x_j\frac{\partial \tau_{lk}}{\partial x_l} + \varpi_i\epsilon_{ijk}\delta_{jl}v_l\rho v_k + \varpi_i\epsilon_{ijk}x_j\frac{\partial v_l}{\partial x_l}\rho v_k + \varpi_i\epsilon_{ijk}x_j v_l\frac{\partial \rho}{\partial x_l}v_k \\
&+ \varpi_i\epsilon_{ijk}x_j v_l\rho\frac{\partial v_k}{\partial x_l} + \varpi_i\frac{v_l}{\|v_p\|}\epsilon_{ikl}x_k\frac{\rho-\rho^0}{\mathrm{d}t}V + \varpi_i\frac{1}{\mathrm{d}t}\Big(\frac{v_l}{\|v_p\|} - \frac{v_l^0}{\|v_p^0\|}\Big)\epsilon_{ikl}x_k\rho V \\
&+ q\frac{\rho-\rho^0}{\mathrm{d}t}Vv_i\frac{v_i}{\|v_k\|} + q\rho V\frac{v_i-v_i^0}{\mathrm{d}t}\frac{v_i}{\|v_k\|} + q\rho V v_i\frac{1}{\mathrm{d}t}\Big(\frac{v_i}{\|v_k\|} - \frac{v_i^0}{\|v_k^0\|}\Big) + q\frac{p-p^0}{\alpha\,\mathrm{d}t} + q\rho v_n\frac{v_n-v_n^0}{\mathrm{d}t} \\
&+ q\frac{1}{2}v_n v_n\frac{\rho-\rho^0}{\mathrm{d}t} + q\frac{\partial p}{\partial x_l}\delta_{lk}v_k + qp\delta_{lk}\frac{\partial v_k}{\partial x_l} - q\frac{\partial \tau_{lk}}{\partial x_l}v_k - q\tau_{lk}\frac{\partial v_k}{\partial x_l} + q\frac{1}{2}\frac{\partial \rho}{\partial x_l}v_k v_k v_l \\
&+ q\rho\frac{\partial v_k}{\partial x_l}v_k v_l + q\frac{1}{2}\rho v_k v_k\frac{\partial v_l}{\partial x_l}\Bigg) = 0\,. \qquad (31)
\end{aligned}$$

Although the stress tensor looks complicated, it is still symmetric. Since the first RIVLIN-ERICKSEN tensor, $A_{ij}^{(1)}$, is symmetric, the first and the second terms of the second RIVLIN-ERICKSEN tensor, $A_{ij}^{(2)}$, in Eq. $(30)_2$ are also symmetric. Even though the third term in Eq. $(30)_2$ is not necessarily symmetric the addition of fourth term implies symmetricity in $A_{ij}^{(2)}$. Hence $\epsilon_{ijk}\tau_{jk} = 0$ and related terms vanish. Moreover $v_j v_k = v_k v_j$ which implies: $\epsilon_{ijk}v_j v_k = 0$.

We have chosen $\mathcal{H}_s^1$ and therefore linear shape functions within the elements. Thus any space-derivative higher than order one vanishes identically in the formulation. This includes any derivative of τ_{ij}, since it already consists of velocity gradients (of first-order). The second-order derivatives, which identically vanish due to shape functions of polynomial-degree one, can be weakened by performing integration by parts, This, however, produces some boundary terms that can be related to boundary conditions as follows

$$\int_\Omega \mathrm{d}V\Big(-\varpi_i\epsilon_{ijk}x_j\frac{\partial \tau_{lk}}{\partial x_l}\Big) = \int_\Omega \mathrm{d}V\Big(\frac{\partial(\varpi_i\epsilon_{ijk}x_j)}{\partial x_l}\tau_{lk}\Big) - \oint_{\partial\Omega}\mathrm{d}s\Big(n_l\varpi_i\epsilon_{ijk}x_j\tau_{lk}\Big)\,. \qquad (32)$$

Subsequently the boundary terms can be rewritten, for example

$$-\oint_{\partial\Omega}\mathrm{d}s\Big(n_l\varpi_i\epsilon_{ijk}x_j\tau_{lk}\Big) = -\oint_{\partial\Omega}\mathrm{d}s\Big(n_l\varpi_i\epsilon_{ijk}x_j\big(\sigma_{lk}+p\delta_{lk}\big)\Big)\,. \qquad (33)$$

The boundary conditions can thus be included in the variational formulation in a natural way. We exclude any ROBIN type boundary conditions and implement a NEUMANN type condition on a part of the boundary, $\partial\Omega_N$. Suppose that the remaining part is covered by conditions of the DIRICHLET type that gives the values of the unknowns on the boundaries $\partial\Omega_D$. Since on $\partial\Omega_D$ the values are known, we remove them from the variational formulation and implement directly. Hence we construct a problem where only one type of condition exists, namely NEUMANN condition, i.e., $\partial\Omega = \partial\Omega_N \cup \partial\Omega_D$ and $\partial\Omega_N \cap \partial\Omega_D = \{\}$. Now the boundary part of the variational form is rewritten with the known traction vector $\hat{t}_i = n_j\sigma_{ji}$ in the example as

$$-\int_{\partial\Omega_N}\mathrm{d}s\Big(\varpi_i\epsilon_{ijk}x_j\big(\hat{t}_k + n_k p\big)\Big)\,. \qquad (34)$$

Here the pressure field p is given and the mass density ρ is the unknown variable. Therefore the pressure p is known on the boundary. We can simply change this so that ρ is given and p is sought. Then $p = \hat{p}$ should be defined as a boundary

condition. Moreover by using Eq. (30) in Eq. (29) the viscous part of the stress τ_{ij} in the time-discretized fashion becomes

$$\tau_{ij} = \mu \frac{\partial v_{(i}}{\partial x_{j)}} + \frac{\gamma}{\mathrm{d}t} \frac{\partial (v_{(i} - v^0_{(i)})}{\partial x_{j)}} + \gamma \frac{\partial^2 v_{(i}}{\partial x_k \partial x_{j)}} v_k + \gamma \frac{\partial v_{(i}}{\partial x_{k)}} \frac{\partial v_k}{\partial x_j} + \gamma \frac{\partial v_k}{\partial x_i} \frac{\partial v_{(k}}{\partial x_{j)}} + \beta \frac{\partial v_{(i}}{\partial x_{k)}} \frac{\partial v_{(k}}{\partial x_{j)}} \,. \tag{35}$$

Finally, after couple of integrations by parts and by using $\epsilon_{ikk} = 0$, the form to be computed reads

$$\begin{aligned}
&\sum_{\text{Elements}} \int_\Omega \mathrm{d}V \Big(q \frac{\rho - \rho^0}{\mathrm{d}t} + q \frac{\partial \rho}{\partial x_i} v_i + q \rho \frac{\partial v_i}{\partial x_i} + \varpi_i \frac{\rho - \rho^0}{\mathrm{d}t} v_i + \varpi_i \rho \frac{v_i - v_i^0}{\mathrm{d}t} + \varpi_i \frac{\partial p}{\partial x_i} \\
&+ \frac{\partial \varpi_i}{\partial x_j} \mu \frac{\partial v_{(j}}{\partial x_{i)}} + \frac{\partial \varpi_i}{\partial x_j} \frac{\gamma}{\mathrm{d}t} \frac{\partial (v_{(j} - v^0_{(j)})}{\partial x_{i)}} + \frac{\partial \varpi_i}{\partial x_j} \gamma \frac{\partial^2 v_{(j}}{\partial x_k \partial x_{i)}} v_k + \frac{\partial \varpi_i}{\partial x_j} \gamma \frac{\partial v_{(j}}{\partial x_{k)}} \frac{\partial v_k}{\partial x_i} + \frac{\partial \varpi_i}{\partial x_j} \gamma \frac{\partial v_k}{\partial x_j} \frac{\partial v_{(k}}{\partial x_{i)}} \\
&+ \frac{\partial \varpi_i}{\partial x_j} \beta \frac{\partial v_{(j}}{\partial x_{k)}} \frac{\partial v_{(k}}{\partial x_{i)}} + \varpi_i \frac{\partial v_j}{\partial x_j} \rho v_i + \varpi_i v_j \frac{\partial \rho}{\partial x_j} v_i + \varpi_i v_j \rho \frac{\partial v_i}{\partial x_j} + \varpi_i \frac{v_i}{\|v_k\|} \frac{\rho - \rho^0}{\mathrm{d}t} V \\
&+ \varpi_i \frac{1}{\mathrm{d}t} \Big(\frac{v_i}{\|v_k\|} - \frac{v_i^0}{\|v_k^0\|} \Big) \rho V + \varpi_i \epsilon_{ikl} x_k v_l \frac{\rho - \rho^0}{\mathrm{d}t} + \varpi_i \epsilon_{ikl} x_k \rho \frac{v_l - v_l^0}{\mathrm{d}t} + \varpi_i \epsilon_{ijk} x_j \frac{\partial p}{\partial x_k} \\
&+ \frac{\partial \varpi_i}{\partial x_l} \epsilon_{ijk} x_j \mu \frac{\partial v_{(l}}{\partial x_{k)}} + \frac{\partial \varpi_i}{\partial x_l} \epsilon_{ijk} x_j \frac{\gamma}{\mathrm{d}t} \frac{\partial (v_{(l} - v^0_{(l)})}{\partial x_{k)}} + \frac{\partial \varpi_i}{\partial x_l} \epsilon_{ijk} x_j \gamma \frac{\partial^2 v_{(l}}{\partial x_m \partial x_{k)}} v_m \\
&+ \frac{\partial \varpi_i}{\partial x_l} \epsilon_{ijk} x_j \gamma \frac{\partial v_{(l}}{\partial x_{m)}} \frac{\partial v_m}{\partial x_k} + \frac{\partial \varpi_i}{\partial x_l} \epsilon_{ijk} x_j \gamma \frac{\partial v_m}{\partial x_l} \frac{\partial v_{(m}}{\partial x_{k)}} + \frac{\partial \varpi_i}{\partial x_l} \epsilon_{ijk} x_j \beta \frac{\partial v_{(l}}{\partial x_{m)}} \frac{\partial v_{(m}}{\partial x_{k)}} \\
&+ \varpi_i \epsilon_{ijk} x_j \frac{\partial v_l}{\partial x_l} \rho v_k + \varpi_i \epsilon_{ijk} x_j v_l \frac{\partial \rho}{\partial x_l} v_k + \varpi_i \epsilon_{ijk} x_j v_l \rho \frac{\partial v_k}{\partial x_l} + \varpi_i \frac{v_l}{\|v_p\|} \epsilon_{ikl} x_k \frac{\rho - \rho^0}{\mathrm{d}t} V \\
&+ \varpi_i \frac{1}{\mathrm{d}t} \Big(\frac{v_l}{\|v_p\|} - \frac{v_l^0}{\|v_p^0\|} \Big) \epsilon_{ikl} x_k \rho V + q \frac{\rho - \rho^0}{\mathrm{d}t} V v_i \frac{v_i}{\|v_k\|} + q \rho V \frac{v_i - v_i^0}{\mathrm{d}t} \frac{v_i}{\|v_k\|} \\
&+ q \rho V v_i \frac{1}{\mathrm{d}t} \Big(\frac{v_i}{\|v_k\|} - \frac{v_i^0}{\|v_k^0\|} \Big) + q \frac{p - p^0}{\alpha \, \mathrm{d}t} + q \rho v_n \frac{v_n - v_n^0}{\mathrm{d}t} + q \frac{1}{2} v_n v_n \frac{\rho - \rho^0}{\mathrm{d}t} + q \frac{\partial p}{\partial x_k} v_k + q p \frac{\partial v_k}{\partial x_k} \\
&+ \frac{\partial q}{\partial x_l} v_k \mu \frac{\partial v_{(l}}{\partial x_{k)}} + \frac{\partial q}{\partial x_l} v_k \frac{\gamma}{\mathrm{d}t} \frac{\partial (v_{(l} - v^0_{(l)})}{\partial x_{k)}} + \frac{\partial q}{\partial x_l} v_k \gamma \frac{\partial^2 v_{(l}}{\partial x_m \partial x_{k)}} v_m + \frac{\partial q}{\partial x_l} v_k \gamma \frac{\partial v_{(l}}{\partial x_{m)}} \frac{\partial v_m}{\partial x_k} \\
&+ \frac{\partial q}{\partial x_l} v_k \gamma \frac{\partial v_m}{\partial x_l} \frac{\partial v_{(m}}{\partial x_{k)}} + \frac{\partial q}{\partial x_l} v_k \beta \frac{\partial v_{(l}}{\partial x_{m)}} \frac{\partial v_{(m}}{\partial x_{k)}} + q \frac{1}{2} \frac{\partial \rho}{\partial x_l} v_k v_k v_l + q \rho \frac{\partial v_k}{\partial x_l} v_k v_l + q \frac{1}{2} \rho v_k v_k \frac{\partial v_l}{\partial x_l} \Big) \\
&+ \int_{\partial \Omega_N} \mathrm{d}s \Big(- \varpi_i (\hat{t}_i + n_i p) - \varpi_i \epsilon_{ijk} x_j (\hat{t}_k + n_k p) - q v_k (\hat{t}_k + n_k \hat{p}) \Big) = 0 \,.
\end{aligned} \tag{36}$$

Due to the stress definition, some terms consist of second-order derivatives in space. Formally it is possible to use elements of polynomial-degree two. However, the smoothness between the elements should be confined such that the first-order derivatives match even on the facet between adjacent (neighbor) elements. This is possible but computationally costly and therefore we leave it to further study. The form above is quite general and should represent any process if the material constants $\alpha, \mu, \gamma, \beta$ are known. Unfortunately the problem is highly non-linear with respect to the unknowns. Therefore a linearization procedure at the partial differential equations' level will be given next.

3.2 Linearization

The form (36) is non-linear in its arguments. Conventionally the form is written in the discrete matrix form and a linearization based on NEWTON-RAPHSON scheme is undertaken at the linear algebra level. However, we present a linearization at the partial differential level, which can handle any type and any order of non-linearities with the same ease. Since Eq. (36) is lengthy, we write the form as a functional of (the set of) unknowns u_i and test functions $\bar{u}_i$ such that

$$F(u_i, \bar{u}_j) = 0 \,. \tag{37}$$

Suppose that we have calculated a set of u_i for a time step. For the next time step the u_i will not be correct, therefore a greater value (a positive value other than zero) is going to be evaluated from the same functional F. If the time step is

sufficiently small then the correct values in the next time shall be close to the u_i such that the small update δu_i upon the correct values from the last time step, u_i, leads to the correct values at the next time step, $u_i \leftarrow u_i + \delta u_i$. Of course the update δu_i is not known but we can determine them by trial and error. We search for the trial functions δu_i that minimizes the functional, F, in the next time step. Minimization yields to the functional, $F(u_i + \delta u_i, \bar{u}_j)$, evaluated with $u_i + \delta u_i$ being smaller than the functional, $F(u_i, \bar{u}_j)$ when evaluated with u_i. Hence, by using a directional GATEAUX differentiation formulation

$$\begin{aligned}
&\lim_{\varepsilon\to 0} \frac{F(u_i + \varepsilon\delta u_i, \bar{u}_j) - F(u_i, \bar{u}_j)}{\varepsilon} \leq 0\,,\\
&\lim_{\varepsilon\to 0} \frac{F(u_i + \varepsilon\delta u_i, \bar{u}_j) - F(u_i + \varepsilon\delta u_i - \varepsilon\delta u_i, \bar{u}_j)}{\varepsilon} \leq 0\,,\\
&\lim_{\varepsilon\to 0} \frac{+F(u_i + \varepsilon\delta u_i - \varepsilon\delta u_i, \bar{u}_j) - F(u_i + \varepsilon\delta u_i, \bar{u}_j)}{\varepsilon} \geq 0\,,\\
&-\frac{\partial}{\partial\varepsilon} F(u_i + \varepsilon\delta u_i, \bar{u}_j)\Big|_{\varepsilon=0} = -J_k(u_i, \bar{u}_j)\delta u_k \geq 0\,,
\end{aligned} \tag{38}$$

we get the JACOBI array J_i, which reaches zero from below, and hence, a maximization problem. By employing both

$$F(u_i, \bar{u}_j) \geq 0\,,\ -J_k(u_i, \bar{u}_j)\delta u_k \geq 0\,, \tag{39}$$

and solving them simultaneously

$$F(u_i, \bar{u}_j) - J_k(u_i, \bar{u}_j)\delta u_k \geq 0\,, \tag{40}$$

another minimization problem results, which is linear in δu_i. Solving this in δu_i and subsequently updating the unknowns $u_i + \delta u_i$ incrementally

$$\underset{\text{w.r.t. } \delta u_i}{\arg\min}\Big(F(u_i, \bar{u}_j) - J_k(u_i, \bar{u}_j)\delta u_k\Big)\,,\ u_i \leftarrow u_i + \delta u_i\,, \tag{41}$$

we solve the set of unknowns in each time step. This is a NEWTON-RAPHSON linearization at the level of partial differential equations and the directional derivation is achieved with symbolic novel packages automatically, cf. [3]. We present applications to demonstrate the power and versatility of the proposed formulation and linearization in the next section.

3.3 Computation

All computational work has been realized by employing the FEniCS project, cf. [26], which is a collection of efficient and highly optimized open source codes, cf. [22–25, 35]. The supply codes, using SciPy, cf. [21], with the unified form language, cf. [2], imported via Dolfin, cf. [27], of the examples below can be found in [1] and used under GNU Public License, cf. [15]. All post-processing is handled within Mayavi, cf. [36].

3.3.1 Flow over a rigid obstacle

First, a computationally difficult example is going to be discussed in order to demonstrate the strength of the explained procedure. Water at 20°C is modeled as an incompressible NEWTONian fluid according to the NAVIER-STOKES constitutive equation. This is a simplified version of Eq. (30) by using $\gamma = 0$ and $\beta = 0$. The viscosity $\mu = 1001.6 \cdot 10^{-6}$ kg/(s m) is taken from VDI-Wärmeatlas [43, Dba2] and implemented for $\alpha = 5.1$.

Since the model is incompressible, a volume change is not permitted. Therefore, from a algebraic point of view, the terms multiplied by $\partial v_i/\partial x_i$ may be omitted. However, we have seen that these terms are important for the sake of numerical stability, thus we compute the form with these terms. Another important issue is that the terms with $\partial p/\partial x_i$ are not transformed by integration by parts. Although there is no need to do that, since the first-order derivative of pressure is admissible within the linear elements, many FEM codes for fluid dynamics are implemented that way. This might be the reason of the success by choosing different-order functional spaces for velocity and pressure, known as the LADYZHENSKAYA-BABUSKA-BREZZI condition, for a mathematical view of this condition cf. [5]. We are neither using different weights nor any stabilization techniques and achieve incompressibility by employing simply a constant mass density field, i.e.,

$\rho = 998.21$ kg/m^3. Instead of calculating the mass density, we compute the pressure field p for the flow over a rigid obstacle. A three-dimensional channel of dimensions 1 m $\times$ 0.5 m $\times$ 0.5 m is filled up with water which is at rest and under 1 bar (10^5 Pa) of pressure at the beginning. The DIRICHLET boundaries on left and right

$$p = 250t + 10^5 \text{ Pa on } \partial\Omega_{\text{left}} ,$$
$$p = -250t + 10^5 \text{ Pa on } \partial\Omega_{\text{right}} , \tag{42}$$

which yields 500 Pa pressure difference in a 1 m length within one second by an outer pressure of 1 bar (10^5 Pa). In the channel a rigid obstacle is positioned, on which the fluid particles have zero velocity and thus the solution is numerically challenging. A solution in three-dimensions without stabilization appears to be new and can be seen in Figs. 1, 2 where the velocity and pressure distributions are visualized under a pressure difference of 500 Pa reached after 1 second by the transient solution in constant time steps[2] of 0.001 seconds. The obstacle is 0.1 m $\times$ 0.1 m $\times$ 0.35 m in size so that a $\bar{v} = 0.1$ m/s mean velocity denotes approximately a REYNOLD's number of $\mathrm{Re} = \rho\bar{v}0.1/\mu = 10^4$.

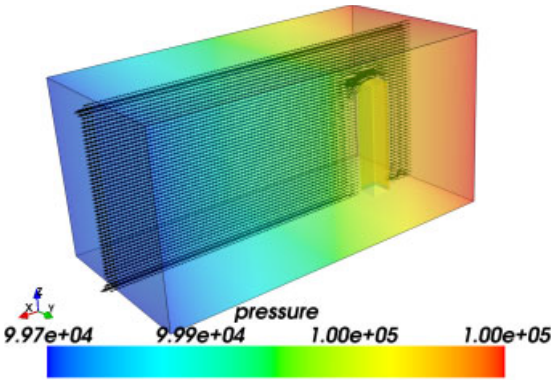

Fig. 1 After 1.0 s pressure field as colors and velocity field represented by arrows on a cut plane.

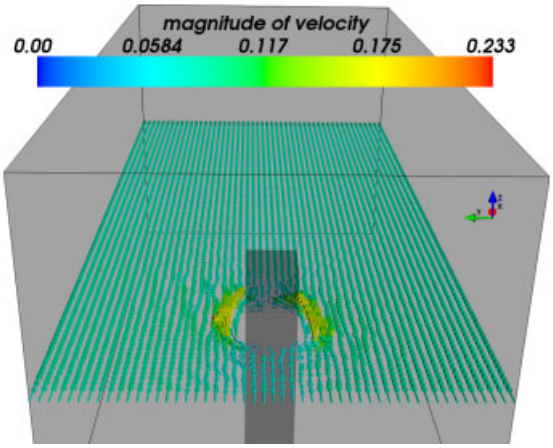

Fig. 2 Velocity field after 1.0 s represented by arrows on a cut plane colored with their magnitude.

3.3.2 Lid driven cavity

A three-dimensional lid driven cavity is used as a standard benchmark test of the numerical procedure. A cubic box of 1 m in each of three directions is filled with a fictitious fluid that has the following material constants and mass density: $\alpha = 1,\ \mu = 100$ kg/(s m), $\beta = \gamma = 0,\ \rho = 1$ kg/m^3. The simulation starts from the rest, i.e., $v_i(x_j, t = 0) = 0$, and from the given pressure $p(x_j, t = 0) = 10^5$ Pa. The fluid accelerates due to the transient velocity at the top. After 1 second the top gains the velocity 0.1 m/s. The computation continues one more second. The result is obtained by solving with constant time step[3] of 0.005 s and the REYNOLD's number reads 10. The pressure and the velocity fields at the $t = 2$ s can be seen in Figs. 3, 4.

3.3.3 Shear flow

We perform a shear flow, in order to visualize one of the effects of the non-linear terms. The box of dimensions 10 mm $\times$ 2 mm $\times$ 10 mm is filled with a fictitious fluid of $\alpha = 1,\ \mu = 1000$ g/(s mm), $\beta = 1$ g/mm, $\gamma = -1$ g/mm, $\rho = 1$ g/mm^3. On top a given velocity is applied and at the bottom the fluid is resting. In case of a NEWTONian fluid, i.e., $\gamma = \beta = 0$, the velocity profile results in a linear function starting from the velocity on top to the velocity at the bottom. In Fig. 5 the velocity profile is curved due to the γ, β terms. Instead of the pressure distribution, the mass density has been calculated, which is initially homogeneous and remains the same, cf. Fig. 6. The process is solved with constant time steps[4] of 0.01 s.

[2] The matrix $137,632 \times 137,632$ solved in approximately 470 s in every time step by using Epetra solver without preconditioning on a single Intel$^{\text{TM}}$ core of 3003.0 MHz processor.

[3] The matrix $530,604 \times 530,604$ solved in approximately 927.3 s in every time step by using uBLAS Krylov solver with ILU preconditioner on a single Intel$^{\text{TM}}$ core of 3003.0 MHz processor.

[4] The matrix $60,516 \times 60,516$ solved in approximately 1200 s in every time step by using uBLAS Krylov solver with ILU preconditioner on a single Intel$^{\text{TM}}$ core of 3003.0 MHz processor.

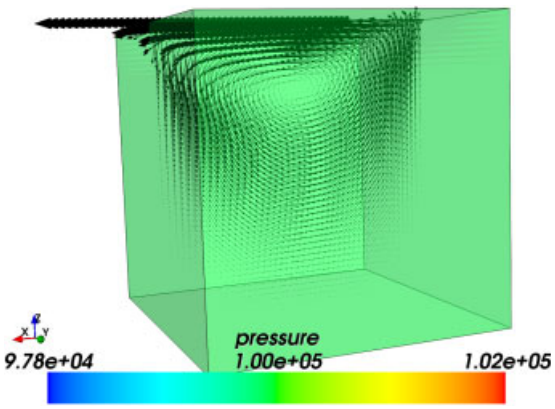

Fig. 3 After 2.0 s pressure field as colors and velocity field represented by arrows on a cut plane.

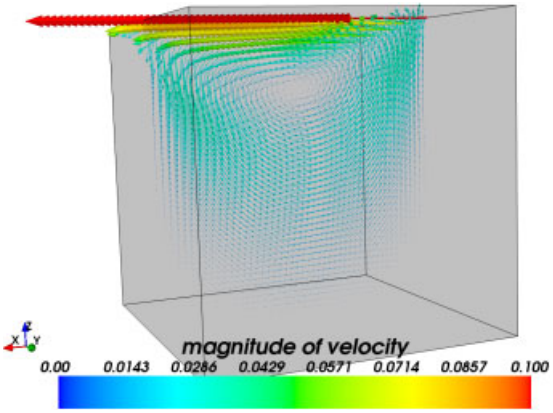

Fig. 4 After 2.0 s velocity field represented by arrows on a cut plane colored with their magnitude.

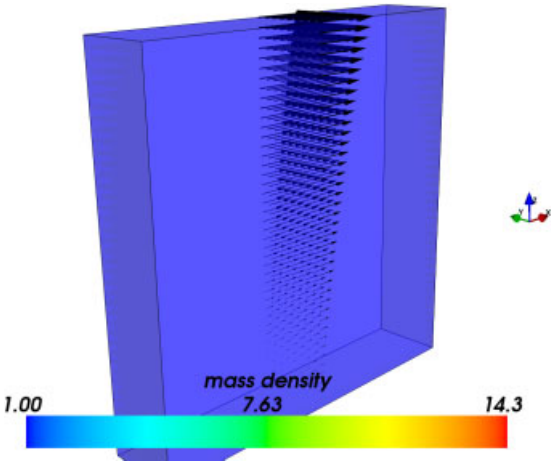

Fig. 5 After 1.0 s mass density as colors and velocity field as arrows on a cut plane.

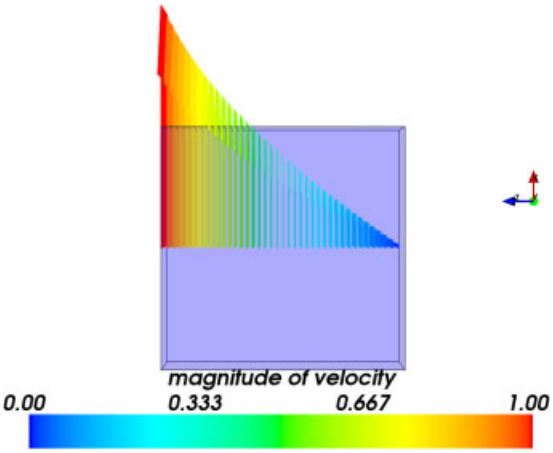

Fig. 6 After 1.0 s velocity field as arrows on a cut plane colored with the magnitude.

4 Conclusion

We have presented a complete variational formulation to compute the flow of non-linear fluids from a discrete point of view. The formulation herein seems promising in the sense that numerical stabilizing parameters are not needed. We have programmed and solved different processes in three dimensions by using open-source codes. The results look qualitatively correct. In order to encourage further studies we publish in [1] the codes of the corresponding applications showed in Sect. 3.3 under GNU Public License, cf. [15]. We have left a quantitative analysis regarding experiments and analytic solutions, as well as a generalization of the formulation to include the non-isothermal case to the future research.

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