Optimal transportation meshfree approximation schemes for fluid and plastic flows

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SUMMARY

We develop an optimal transportation meshfree (OTM) method for simulating general solid and fluid flows, including fluid–structure interaction. The method combines concepts from optimal transportation theory with material-point sampling and max-ent meshfree interpolation. The proposed OTM method generalizes the Benamou–Brenier differential formulation of optimal mass transportation problems to problems including arbitrary geometries and constitutive behavior. The OTM method enforces mass transport and essential boundary conditions exactly and is free from tension instabilities. The OTM method exactly conserves linear and angular momentum and its convergence characteristics are verified in standard benchmark problems. We illustrate the range and scope of the method by means of two examples of application: the bouncing of a gas-filled balloon off a rigid wall; and the classical Taylor-anvil benchmark test extended to the hypervelocity range. Copyright © 2010 John Wiley & Sons, Ltd.

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1. INTRODUCTION

The traditional Eulerian framework for the description of fluid flows becomes awkward when the flow involves variable domains, free-surface boundary conditions, and contact and interactions with highly deformable structures. Furthermore, solid flows require the tracking of the local state of material particles, especially when the response of the solid is history dependent. In a Eulerian setting this tracking necessitates the solution of transport equations, which poses non-trivial numerical challenges. The satisfaction of the divergence-free constraint for incompressible flows poses similar challenges. Moreover, solids can interact by contact and undergo fracture,
fragmentation and other topological transitions, which are exceedingly difficult to capture by means of Eulerian approaches. A number of strategies have been devised with a view to overcoming these difficulties, including: Particle methods such as smooth particle hydrodynamics [1–3]; ghost fluid and immersed boundary methods [4–8]; the material-point method [9–13]; Lagrangian formulations with continuous adaptive remeshing [14, 15] and others. Many appealing features notwithstanding, some of these methods still suffer from a variety of shortcomings, including: the introduction of large numerical diffusion errors; large discretization errors at fluid–solid interfaces; the need for background meshes; difficulties in maintaining monotonicity, positivity and in tracking state variables; lack of strict conservation properties; spurious modes and tensile instabilities; difficulties with separated flows and contact; unknown convergence and stability properties and others. Strictly Lagrangian approaches based on a fix mesh also experience difficulty in dealing with unconstrained flows due to mesh entanglement. A number of strategies have been devised with a view to overcoming this difficulty, including: methods based on continuous remeshing [16–19]; arbitrary-Lagrangian–Eulerian and related formulations [20–24]; the diffuse element method [25]; meshfree methods (see, e. g., [26] for a review); max-ent interpolation schemes [27, 28] and others. Again, some of these methods may still experience a variety of difficulties, including: the need to remesh or rezone arbitrary three-dimensional domains; variable mass matrices; the remapping of state variables; ad hoc transition or blending regions; difficulties in defining numerical integration rules and satisfying essential boundary conditions; spurious modes and tensile instabilities; unknown convergence and stability properties and others.

The objective of this work is the formulation of a meshfree updated-Lagrangian methodology for fluid and solid dynamic flows, possibly involving multiple phases, viscosity and general equations of state, general inelastic and history-dependent constitutive relations, arbitrary variable domains and boundary conditions and the interaction between fluid flows and highly deformable structures. The scheme, which we refer to as the optimal transportation meshfree (OTM) method, is constructed through an integration of optimal transportation theory (cf., [29] for a review) with max-ent meshfree interpolation [27] and material-point sampling. The rationale behind the approach is as follows. We resort to the Benamou–Brenier [30, 31] differential formulation of optimal mass transportation problems and its connection to the Wasserstein distance [32–34] to discretize the inertial action in space and time within a strictly variational framework. The resulting discretization may be regarded as the result of restricting the inertial action to mass measures concentrated on material points undergoing piecewise rectilinear motions. The density of such mass measures and the constrained minimization structure of the problem may be expected to confer the discretization robust convergence properties, e.g. in the sense of Γ-convergence (see [35] for an application of Γ-convergence concepts to finite element approximations). The optimal transportation variational framework also results in: proper mass matrices and inertia forces in the presence of continuously varying spatial interpolation; geometrically exact mass transport and satisfaction of the continuity equation; and exact linear and angular momentum conservation. The introduction of material points serves the additional purposes of: supplying an effective numerical integration rule for the remaining terms of the action, including material terms; and providing sampling points for the local state of the material, which may include internal state variables when the material is inelastic and history dependent. Finally, fields requiring differentiation, such as deformation and velocity fields, are interpolated from nodal values using max-ent shape functions [27]. These shape functions are reconstructed continuously from the nodal set and have the key property of possessing a Kronecker-delta property at the boundary, which enables the direct imposition of displacement boundary conditions. In addition, the max-ent shape functions are affine on the boundary, which
renders them exactly compatible with simplicial finite element interpolation. This property in turn renders the coupling of fluid flows to highly deformable structures straightforward.

The combination of these desirable attributes effectively overcomes many of the difficulties alluded to earlier, thereby supplying a methodology that is well-suited to the simulation of general, possibly coupled, fluid/solid/structural problems. The intended areas of application where the OTM methodology is thought to be potentially advantageous include fluid flows involving free surfaces, fluid flows coupled to very flexible solids and structures, processes involving unconstrained plastic flows and others. Following the description of the approach for the increasingly general cases of mass, fluid and solid flows in Sections 2–5, respectively, the conservation and convergence properties of the OTM method are analyzed in Section 6. Finally, selected numerical examples of application are presented in Section 7 that demonstrate the scope and versatility of the method.

2. THE MASS TRANSPORT PROBLEM

We begin by considering the case of the motion of a fluid of non-interacting particles, which provides the simplest framework for discussing the connection between optimal transportation and the Lagrangian dynamics of a continuous distribution of mass. In particular, we draw on the theory of optimal transportation, specific aspects of which are summarized in Section 2.1, to formulate the kinetic energy of the system and, by extension, its action directly in terms of its mass density. This defines a minimum principle whose minimizers are the time histories of the mass density. In Sections 2.2 and 2.3, we also address matters of temporal and spatial discretization for the simple case of flows of non-interacting particles. These discretization schemes are extended to general fluid and solid flows in subsequent sections.

2.1. Optimal transportation

In this section we summarize the relevant aspects of the theory of optimal transportation that are required for subsequent developments. Optimal transportation theory derives its importance from the fact that it supplies a powerful and useful mathematical foundation for a number of areas in mechanics and physics. A thorough and rigorous account of the theory may be found, e.g. in the monographs of Evans [36] and Villani [29]. For simplicity, here and subsequently we formally use mass densities in lieu of more rigorous measure-theoretical notation, which is nevertheless evident from the expressions and can be found in the above-referenced monographs.

We begin by considering the flow of an inviscid fluid of non-interacting particles in $\mathbb{R}^n$ at zero temperature. The motion of the fluid over a time interval $(a, b)$ is governed by the coupled equations

\begin{align}
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho v) &= 0, \quad (1a) \\
\frac{\partial (\rho v)}{\partial t} + \nabla \cdot (\rho v \otimes v) &= 0, \quad (1b)
\end{align}

where $\rho$ is the mass density of the fluid and $v$ is the velocity field. Equation (1a) is the equation of conservation of mass and Equation (1b) is the equation of conservation of linear momentum.
We assume that the fluid has finite total mass
\[ M = \int \rho \, dx \]
and that mass does not ‘leak to infinity’, i.e.
\[ \lim_{R \to \infty} \int_{B_R} \rho \, v \cdot n \, dx = 0 \]
where \( B_R \) is the ball of radius \( R \). It then follows that the total mass \( M \) of the fluid remains unchanged throughout the flow. Indeed,
\[ \dot{M} = \lim_{R \to \infty} \int_{B_R} \frac{\partial \rho}{\partial t} \, dx = - \lim_{R \to \infty} \int_{B_R} \nabla \cdot (\rho v) \, dx = - \lim_{R \to \infty} \int_{\partial B_R} \rho v \cdot n \, dx = 0 \]

Suppose that, in addition, we specify the initial and final mass densities, namely,
\[ \rho(x, a) = \rho_a(x), \]
\[ \rho(x, b) = \rho_b(x). \]

The problem thus becomes a transportation problem of finding the flow that transports the initial mass density \( \rho_a \) to the final one \( \rho_b \).

The problem just enunciated can be recast as an optimal transportation problem. Thus, Benamou and Brenier [30, 31] noted that Problem (1, 5) admits the variational characterization:
\[ \inf_{(\rho, v) \in X} A(\rho, v) \]
subject to:
\[ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho v) = 0, \]
where
\[ A(\rho, v) = \int_a^b K(\rho, v) \, dt \]
is the action over the time interval \((a, b)\),
\[ K(\rho, v) = \int \frac{\rho}{2} |v|^2 \, dx \]
is the kinetic energy and the natural space of solutions is \( X = \{(\rho, v) \in C((a, b); L^1(\mathbb{R}^n; [0, \infty))) \times C((a, b); L^2(\mathbb{R}^n; \mathbb{R}^n))\} \) (see [29] Section 8.1.1 for a more precise account). We recall that \( L^1(\mathbb{R}^n) \) Lebesgue space of integrable functions over \( \mathbb{R}^n \). Thus \( \{d \mu = \rho \, dx, \rho \in L^1(\mathbb{R}^n; [0, \infty))\} \) is the set of measures that are absolutely continuous with respect to the Lebesgue measure. Physically, the restriction of \( \rho \) to \( L^1(\mathbb{R}^n; [0, \infty)) \) ensures that every subset of \( \mathbb{R}^n \) with a well-defined volume can be assigned a well-defined non-negative mass. In addition, \( L^2(\mathbb{R}^n; \mathbb{R}^n) \) is the Lebesgue space of square-integrable vector-valued functions over \( \mathbb{R}^n \). Physically, restriction of \( v \) to \( L^2(\mathbb{R}^n; \mathbb{R}^n) \), in conjunction with the restriction of \( \rho \) to \( L^1(\mathbb{R}^n; [0, \infty)) \), ensures that the velocity fields have finite kinetic energy. Finally, \( C((a, b); L^1(\mathbb{R}^n; [0, \infty))) \) and \( C((a, b); L^2(\mathbb{R}^n; \mathbb{R}^n)) \) are the space of time-continuous functions taking values in \( L^1(\mathbb{R}^n; [0, \infty)) \) and \( L^2(\mathbb{R}^n; \mathbb{R}^n) \), respectively.
We may formally verify that the minimization (6) is indeed equivalent to (1, 5) by enforcing Hamilton’s principle of stationary action and computing the corresponding Euler–Lagrange equations. However, in taking variations of the action \( A(\rho, v) \) care must be exercised to properly account for the fact that the time-dependent fields \( \rho \) and \( v \) are not independent but are constrained by the continuity Equation (5b). Alternatively, the flow can be described by means of a deformation mapping \( \varphi: \mathbb{R}^n \times (a, b) \to \mathbb{R}^n \). The velocity and mass fields then follow as:

\[
\begin{align*}
v(x, t) &= \frac{\partial \varphi}{\partial t} (\varphi^{-1}(x, t), t), \\
\rho(x, t) &= \rho_a(\varphi^{-1}(x, t))/\det(\nabla \varphi(\varphi^{-1}(x, t), t)),
\end{align*}
\]

which shows that, indeed, \( \rho \) and \( v \) are not independent. Thus, we may regard the deformation mapping as the independent fundamental description of the flow and the velocity and mass fields as derived fields, or we may alternatively treat the velocity and mass fields as fundamental fields constrained by the continuity Equation (6b). Taking variations of (7) taking (9) into account gives

\[
\delta A(\rho, v) = \int_a^b \int \rho v \cdot \frac{D\xi}{Dt} \, dx \, dt
\]

where \( \xi \circ \varphi \) is an admissible variation of \( \varphi \). Integrating by parts and requiring stationarity for all admissible variations we obtain (1b), as required.

The Benamou and Brenier [30] variational characterization (6) of the transport (1,5) admits a compelling reformulation within the context of the Monge–Kantorovich optimal transportation framework. Specifically Benamou and Brenier [29, 30] showed that the minimizers of the action (7) are given in terms of McCann’s displacement interpolation [37]

\[
\varphi(x, t) = \frac{b-t}{b-a} x + \frac{t-a}{b-a} T(x),
\]

through relations (9), where \( T = \varphi(\cdot, b) \) is the optimal transference mass of \( \rho_a \) into \( \rho_b \) in the sense of the cost function

\[
I(T) = \int |T(x) - x|^2 \rho_a(x) \, dx,
\]

i.e.

\[
\mathcal{F}_2(\rho_a, \rho_b) = \inf \{ I(T) : T \text{measurable}, \rho_a(x) = \rho_b(T(x)) \det(\nabla T(x)) \}
\]

\[
= \inf \{ (b-a) A(\rho, v) : (\rho, v) \in V(\rho_a, \rho_b) \},
\]

where \( V(\rho_a, \rho_b) \) is the set of pairs \( (\rho, v) \in X \) such that \( \bigcup_{t \in (a, b)} \text{supp} \rho(\cdot, t) \) is bounded, (1a) is satisfied weakly in a distributional sense, \( \rho(\cdot, a) = \rho_a \) and \( \rho(\cdot, b) = \rho_b \). Here and subsequently, \( \text{supp} f \) denotes the support of a measurable function \( f \). We recall that the minimum cost of transportation (13) can be related to the Wasserstein distance

\[
d_W(\rho_a, \rho_b) = \left\{ \inf_{\sigma \in \Gamma(\rho_a, \rho_b)} \int \int |x-y|^2 \sigma(x, y) \, dx \, dy \right\}^{1/2},
\]
where the infimum is taken over the space of Radon measures of mass $M$ with finite second moments and marginals

$$
\int \sigma(x, y) \, dy = \rho_a(x),
$$

(15a)

$$
\int \sigma(x, y) \, dx = \rho_b(y).
$$

(15b)

Then we have

$$
\mathcal{T}_2(\rho_a, \rho_b) = d_W^2(\rho_a, \rho_b),
$$

(16)

i.e. the cost of transportation is given by the Wasserstein distance between the initial and final mass densities. In applications we shall often need to take variations of the minimum cost of transportation $\mathcal{T}_2(\rho_a, \rho_b)$ with respect to $\rho_b$. Suppose that $\rho_a, \rho_b \in L^1(\mathbb{R}^n; [0, \infty))$ and have finite second moments. Let $\rho(x, t), t \in (b-e, b+e)$ be a path in $L^1(\mathbb{R}^n; [0, \infty))$ of mass densities with finite second moments such that $\rho(\cdot, 0) = \rho_b$ and

$$
\frac{\partial \rho_b}{\partial t} + \mathbf{\nabla} \cdot (\rho \xi) = 0,
$$

(17)

for some $C^1$, globally bounded, velocity field $\xi$. Then, ([29], Theorem 8.13)

$$
\frac{d}{dt} \mathcal{T}_2(\rho_a, \rho)|_{t=0} = 2 \int \langle T(x) - x, \xi(T(x)) \rangle d\rho_a(x),
$$

(18)

where $T$ is the optimal transference mapping from $\rho_a$ to $\rho_b$.

### 2.2. Time discretization

Next, we turn to the question of time discretization of the action (7). To this end, let $t_0 = a < t_1 < \cdots < t_N = b$ be a discretization of the time interval $(a, b)$. Recall that $(\frac{1}{2})d_W^2(\rho_a, \rho_b)/(b-a)$ gives the exact minimum of the action $A(\rho, \nu)$ over the entire time interval $(a, b)$. Building on this identity we can define the semi-discrete action

$$
A_d(\rho_1, \ldots, \rho_N) = \sum_{k=0}^{N-1} \frac{1}{2} \mathcal{T}_2(\rho_k, \rho_{k+1}),
$$

(19)

which is expressed directly in terms of densities. If no further approximation is introduced the infimum of $A_d$ over $\{\rho_1, \ldots, \rho_N\} \in [L^1(\mathbb{R}^n; [0, \infty))]^{N+1}$ to be again $(\frac{1}{2})\mathcal{T}_2(\rho_a, \rho_b)/(b-a)$ and the scheme to be exact. The discrete motion consists of incremental transference maps $\phi_{k \rightarrow k+1}$ transporting $\rho_k$ into $\rho_{k+1}$ over the time interval $[t_k, t_{k+1}]$ optimally with respect to the cost function (12). Time discretizations of functionals of the type (7) based on the Wasserstein distance were introduced by Jordan et al. [32–34] in the context of the Fokker–Planck equation.

The discrete equations of motion now follow by rendering the discrete action stationary. Taking variations of (19) with respect to $\rho_k$ with the aid of (18) gives

$$
\langle \delta A_d, \xi_k \rangle = - \int \left\{ \rho_k \left( \frac{\phi_{k \rightarrow k+1}(x) - x}{t_{k+1} - t_k} + \frac{\phi_{k \rightarrow k-1}(x) - x}{t_k - t_{k-1}} \right) \cdot \xi_k \right\} dx,
$$

(20)
where we write
\[ \varphi_{k \to k-1} = \varphi_{k-1 \to k}^{-1}. \]  
(21)

In (20) \( \varphi_{k \to k+1} \) denotes the optimal transference mapping from \( \rho_k \) to \( \rho_{k+1} \) and, in particular, we have
\[ \rho_{k+1} \circ \varphi_{k \to k+1} = \rho_k / \det(\nabla \varphi_{k \to k+1}). \]  
(22)

We note that these mass density updates differ sharply from those in conventional Eulerian approaches, which rely on some direct time discretization of the continuity equation. In particular, the mass--density update (22) is geometrically exact. Integrating by parts (20) using (3) and enforcing stationarity with respect to all variations \( \xi_k \) we obtain
\[ \rho_k \left( \varphi_{k \to k+1} - \text{id} \overline{t_{k+1} - t_k} + \varphi_{k \to k-1} - \text{id} \overline{t_k - t_{k-1}} \right) = 0, \]  
(23)

where, here and subsequently, \( \text{id} \) denotes the identity mapping. Evidently, these equations are jointly satisfied by setting
\[ \varphi_{k \to k+1}(x) = \varphi(\varphi^{-1}(x, t_k), t_{k+1}), \]  
(24)

where \( \varphi \) is the given McCann’s displacement interpolation (11), which shows that the discretization (20) is indeed exact, as expected.

2.3. Spatial discretization

Finally, we turn to the question of spatial discretization of the semi-discrete action (19). A natural and computationally convenient spatial discretization may be effected by considering mass densities of the type
\[ \rho_{h,k}(x) = \sum_{p=1}^{M} m_{p,k} \delta(x-x_{p,k}), \]  
(25)

where \( x_{p,k} \) represents the position at time \( t_k \) of a material point of mass \( m_p \) and \( \delta(x-x_{p,k}) \) is the Dirac-delta distribution centered at \( x_{p,k} \). A fully discrete action may then be obtained by inserting representation (25) into (19), which defines a discrete transportation problem (cf. e.g. [36]).

We note that, by considering mass distributions of the form (25), we have expanded the original space of solutions \( L^1(\mathbb{R}^n; [0, \infty)) \) to a larger space of \( \mathcal{M}(\mathbb{R}^n) \) of Radon measures. In computing the minimum cost of transportation \( \mathcal{F}_2(\rho_{h,k}, \rho_{h,k+1}) \) between two consecutive discrete mass densities, the incremental optimal transference mappings \( \varphi_{h,k \to k+1} \) transporting \( \rho_{h,k} \) into \( \rho_{h,k+1} \) are simply rearrangements of the point set \( \{x_{1,k}, \ldots, x_{M,k}\} \) into the point set \( \{x_{1,k+1}, \ldots, x_{M,k+1}\} \). In addition, the incremental mass conservation relation (22) must be understood in a weak or distributional sense, i.e. as the requirement that
\[ \int \rho_k(x) \eta(x) \, dx = \int \rho_{k+1}(y) \eta(\varphi^{-1}_{k \to k+1}(y)) \, dy, \]  
(26)
for all continuous test functions $\eta$ with compact support. For discrete mass distributions of the form (25), (26) reduces to
\[
\sum_{p=1}^{M} m_{p,k} \eta(x_{p,k}) = \sum_{p=1}^{M} m_{p,k+1} \eta(x_{p,k}),
\]
(27)
which must be satisfied for all test functions $\eta$ and, hence,
\[
m_{p,k} = m_{p,k+1} = m_p,
\]
(28)
i.e. the material points must have constant mass.

The fully discrete action now takes the form
\[
A_h(\rho_{h,1}, \ldots, \rho_{h,N-1}) = \sum_{k=0}^{N-1} \sum_{p=1}^{M} \frac{m_p}{2} \frac{|x_{p,k+1} - x_{p,k}|^2}{t_{k+1} - t_k},
\]
(29)
which is the semi-discrete action of a system of non-interacting mass particles. The corresponding discrete Euler–Lagrange equations are
\[
\frac{x_{p,k+1} - x_{p,k}}{t_{k+1} - t_k} - \frac{x_{p,k} - x_{p,k-1}}{t_k - t_{k-1}} = 0,
\]
(30)
or, equivalently,
\[
x_{p,k+1} = x_{p,k} + (t_{k+1} - t_k) \frac{x_{p,k} - x_{p,k-1}}{t_k - t_{k-1}},
\]
(31)
which provides an update for the positions of the material points. In this update
\[
v_{p,k} \equiv \frac{x_{p,k} - x_{p,k-1}}{t_k - t_{k-1}}
\]
(32)
may be regarded as the velocity of material point $p$ at time $t_k$, whereupon the update (31) takes the particularly simple form
\[
x_{p,k+1} = x_{p,k} + (t_{k+1} - t_k)v_{p,k}.
\]
(33)
These updates simply define a ballistic motion of the material points from their initial positions $x_{p,0}$ to their final positions $x_{p,N}$.

3. EULER FLUID FLOWS

In this section, we extend the optimal transportation framework developed above to compressible Euler flows. For these systems, inertia competes with free energy in determining the flow of mass. Conveniently, the free energy of a fluid can be expressed directly in terms of its mass density and, as in the case of non-interacting fluids, Equation (19), the resulting semi-discrete action can also be expressed directly in terms of the mass density. Further extensions to solid flows, which require consideration of more general actions, and to viscous and inelastic behavior are pursued in subsequent sections.
3.1. Compressible Euler flows

The motion of a compressible inviscid fluid in a time-dependent domain \( B(t) \subset \mathbb{R}^n \) over a time interval \((a, b)\), part of whose boundary \( \partial_1 B(t) \) is kinematically constrained with the remainder \( \partial_2 B(t) = \partial B(t) \setminus \partial_1 B(t) \) of the boundary either free or acted upon by an applied pressure, is governed by the coupled equations

\[
\begin{align*}
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho v) &= 0 \quad \text{in } \Omega, \\
\frac{\partial (\rho v)}{\partial t} + \nabla \cdot (\rho v \otimes v - pI) &= \rho b \quad \text{in } \Omega, \\
v \cdot n &= w \quad \text{on } \partial_1 \Omega, \\
p &= q \quad \text{on } \partial_2 \Omega,
\end{align*}
\]

where \( \rho \) is the pressure, \( b \) is a body force density per unit mass, \( w \) is the prescribed outward normal velocity of the boundary of the domain, \( n \) is the unit outward normal, \( q \) is the applied pressure, \( \Omega = \bigcup_{t \in (a, b)} B(t) \) is the space time domain swept by the flow, \( \partial_1 \Omega = \bigcup_{t \in (a, b)} \partial_2 B(t) \) is the space time displacement boundary and \( \partial_2 \Omega = \bigcup_{t \in (a, b)} \partial_2 B(t) \) is the space time traction boundary. Here and subsequently we adopt the solid’s sign convention and take a tensile (compressive) pressure to be positive (negative). Equation (34a) enforces conservation of mass and Equation (34b) the conservation of linear momentum.

In order to close the set of governing equations, a material-specific equation of state must be specified. For simplicity, we shall assume that the flow is barotropic. We recall that a flow is said to be barotropic if there is a functional relation between \( p \) and \( \rho \) independent of temperature of the form

\[
p = -\rho^2 \frac{\partial f}{\partial \rho}(\rho),
\]

for some potential function \( f(\rho) \). We shall additionally assume that the body forces derive from a scalar potential \( u \), i.e.

\[
b = \nabla u.
\]

Problem (34) can be given a variational structure—albeit no longer a minimum problem structure—by recourse to Hamilton’s principle of stationary action. The action of the fluid differs from the bare action (7) in that the fluid now has free energy and moves under the action of a body-force potential and either kinematic constraints or an applied pressure at the boundary. Adding the corresponding terms to (7) the action now becomes

\[
A(\rho, v, B) = \int_a^b \left\{ \int_{B(t)} \left[ \frac{\rho}{2} |v|^2 - \rho (f(\rho) - u) + q \right] \, dx \right\} \, dt,
\]

where in this expression \( q \) denotes, at the expense of some abuse of notation, an arbitrary extension of the applied pressure from \( \partial_2 \Omega \) to the entire domain \( \Omega \). We now expect the actual flow to render the action (37) stationary with respect to all admissible variations of the fields. However, as in the case of mass transport in taking variations of the action \( A(\rho, v, B) \) care must be exercised in order...
to account for the fact that $\rho$, $v$ and $B$ are not independent. Again, an irreducible representation of the flow is obtained by introducing a deformation mapping $\varphi(\cdot,t): B_a \to B(t)$, with $\rho$ and $v$ additionally given by (9). Taking variations of (37) taking (9) into account gives

$$
\delta A(\rho, v, B) = \int_B \left\{ \int_{B(t)} \left( \rho v \cdot \frac{D\varphi}{Dt} - \rho \nabla \cdot \xi + \rho b \cdot \xi \right) \, dx + \int_{\partial B(t)} q \xi \cdot n \, d\sigma \right\} \, dt
$$

where we assume that

$$
\varphi(\cdot,a) = \varphi_a(\cdot),
$$

$$
\varphi(\cdot,b) = \varphi_b(\cdot),
$$

are given and $\xi \circ \varphi$ denotes an admissible variation of $\varphi$ such that

$$
\xi(\cdot,a) = 0 \quad \text{in } B_a,
$$

$$
\xi(\cdot,b) = 0 \quad \text{in } B_b,
$$

$$
\xi = 0 \quad \text{on } \partial_1 \Omega.
$$

Evidently, (38) reduces to (10) when $p = 0, u = 0$ and $B(t) = \mathbb{R}^n$. Integrating by parts and requiring stationarity for all admissible variations we obtain (34b) and (34d), as required.

### 3.2. Time discretization

The aim now is to formulate a time-discretized, or semi-discrete, approximate action for compressible Euler flows that extends the semi-discrete action (19) for non-interacting flows. The additional terms to be taken into account in this extension concern the free energy of the fluid and the body forces. Using a trapezoidal rule approximation for the corresponding action terms gives a semi-discrete action of the form

$$
A_d(\rho_1, \ldots, \rho_{N-1}) = \sum_{k=0}^{N-1} \frac{1}{2} \left\{ \int_{B(k)} \frac{1}{2} \left( \frac{\nabla \cdot \varphi_k(x) - x}{t_k + 1 - t_k} + \frac{\nabla \cdot \varphi_{k+1}(x) - x}{t_k + 1 - t_k} \right) \, dx \right\} (t_{k+1} - t_k),
$$

which is expressed directly in terms of densities. In this expression

$$
U(\rho) = \int_{B(t)} [\rho (f(\rho) - u) - q] \, dx,
$$

is the total internal energy of the fluid. The discrete equations of motion now follow by rendering the semi-discrete (41) action stationary. Taking variations of (41) with the aid of (9) and (18) gives

$$
\langle \delta A_d, \xi_k \rangle = - \int_{B_k} \rho_k \left( \frac{\varphi_k \to \varphi_{k+1}(x) - x}{t_{k+1} - t_k} + \frac{\varphi_k \to \varphi_{k-1}(x) - x}{t_k - t_{k-1}} \right) \cdot \xi_k \, dt
$$

$$
+ \frac{t_{k+1} - t_k}{2} \left\{ \int_{B_k} (p_k \nabla \cdot \xi_k + \rho_k b_k \cdot \xi_k) \, dx + \int_{\partial B_k} q_k \xi_k \cdot n \, d\sigma \right\},
$$

where $\varphi_k \to \varphi_{k+1}$ is a transference map transporting $\rho_k$ into $\rho_{k+1}$ optimally over the time interval $[t_k, t_{k+1}]$ and we adopt the notation (21). In particular, identity (22) holds. In addition, in (43)
and in the sequel we write $b_k(\cdot) = b(\cdot, t_k)$, $p_k(\cdot) = p(\cdot, t_k)$ and so on. Integrating by parts (43) we obtain

$$
(\delta A_d, \xi_k) = -\int_{B_k} \rho_k \left( \frac{\varphi_{k \to k+1}(x) - x}{t_{k+1} - t_k} + \frac{\varphi_{k \to k-1}(x) - x}{t_k - t_{k-1}} \right) \cdot \xi_k \\
+ \frac{t_{k+1} - t_{k-1}}{2} \left\{ \int_{B_k} (\nabla p_k + \rho_k b_k) \cdot \xi_k \, dx + \int_{\partial^2 B_k} (q_k - p_k) \xi_k \cdot n_k \, d\sigma \right\} \tag{44}
$$

Enforcing stationarity with respect to all admissible variations $\xi_k$ we obtain

$$
\frac{2\rho_k}{t_{k+1} - t_{k-1}} \left( \frac{\varphi_{k \to k+1} - id}{t_{k+1} - t_k} + \frac{\varphi_{k \to k-1} - id}{t_k - t_{k-1}} \right) = \nabla p_k + \rho_k b_k \quad \text{in} \ B_k, \tag{45a}
$$

$$
p_k = q_k \quad \text{on} \ \partial^2 B_k. \tag{45b}
$$

A comparison of (45), (23) shows that the discrete motion now results from the competition between: inertia, represented by the first term in (45a), which endeavors to transport $\rho_k$ into $\rho_{k+1}$ over the time interval $[t_k, t_{k+1}]$ optimally with respect to the cost function (12); and the internal energy of the fluid, which introduces discrete percussions at the discrete times $t_0 < t_1 < \cdots < t_N$ causing the trajectory to deviate from the optimal transportation path.

3.3. Spatial discretization

In order to obtain a fully discrete action for computations, we proceed to effect a spatial discretization of the semi-discrete action (41). In particular, we wish to carry over to the present setting the material-point formalism introduced in Section 2.3 for non-interacting fluids. Recall that, in that context, material points are introduced by adopting concentrated mass densities of the form (25). The operation of inserting these mass densities into the semi-discrete action (19), or directly into the semi-discrete Euler–Lagrange equation (20), is mathematically well-defined since for a non-interacting fluid the mass density enters the variation of the action linearly, Equation (20). By contrast, for a compressible fluid the mass density enters non-linearly in the variation of the semi-discrete action, Equation (43), and the insertion of representation (25) directly into (43) no longer makes mathematical sense.

In order to overcome this difficulty, we note that representation (25) combines two mathematically distinct operations that become blurred in the context of non-interacting fluids, but which need to be carefully separated for general flows. The first operation is the approximation of the usual Lebesgue measure of volume $\mathcal{L}$ by discrete measures

$$
\mathcal{L}_{h,k} = \sum_{p=1}^{M} v_{p,k} \delta_{x_{p,k}} \tag{46}
$$

concentrated at material points $x_{p,k}$, each of which is assigned a discrete volume $v_{p,k}$. Thus, for any smooth function $f$ we have

$$
\int f \, d\mathcal{L}_{h,k} = \sum_{p=1}^{M} f(x_{p,k}) v_{p,k}. \tag{47}
$$
In addition, the usual push-forward operation for measures,

\[ \int \eta(y) \, dy = \int \eta(\varphi_{k \rightarrow k+1}(x)) \det(\nabla \varphi_{k \rightarrow k+1}(x)) \, dx \]  

now becomes

\[ \sum_{p=1}^{M} \eta(x_{p,k+1}) v_{p,k+1} = \sum_{p=1}^{M} \eta(\varphi_{k \rightarrow k+1}(x_{p,k})) \det(\nabla \varphi_{k \rightarrow k+1}(x_{p,k})) v_{p,k}. \]  

But material points are convected by the flow, i.e.

\[ x_{p,k+1} = \varphi_{k \rightarrow k+1}(x_{p,k}). \]  

Inserting this identity in (49) and noting that \( \eta \) is arbitrary gives

\[ v_{p,k+1} = \det(\nabla \varphi_{k \rightarrow k+1}(x_{p,k})) v_{p,k}, \]  

which defines the material-point volume update.

The second operation subsumed in representation (25) is the identification of discrete mass distributions as measures that are absolutely continuous with respect to the discrete volume measure \( \mathcal{L}_{h,k} \), with Radon–Nykodim density \( \rho_{h,k} \), in the same manner as continuous mass distributions are defined by measures that are absolutely continuous with respect to the usual Lebesgue measure \( \mathcal{L} \) with density \( \rho \). Owing to the discreteness of \( \mathcal{L}_{h,k} \), the corresponding mass densities \( \rho_{h,k} \) are defined simply by assigning mass density values \( \rho_{p,k} \) to every material point, i.e.

\[ \rho_{h,k}(x) = \sum_{p=1}^{M} \rho_{p,k} v_{p,k} \delta(x - x_{p,k}). \]  

Comparing (52) and (25) yields the identity

\[ m_{p} = \rho_{p,k} v_{p,k}, \]  

where have used (28). Equivalently,

\[ \rho_{p,k} = \frac{m_{p}}{v_{p,k}} \]  

relates the mass density at material point \( x_{p,k} \) to its mass and volume.

The identities (50)–(54) provide update formulae for the position, volume and mass density of the material points. However, it should be carefully noted that the gradient of the transference map \( \varphi_{k \rightarrow k+1} \) appears explicitly in (51). Therefore, in contrast to the case of non-interacting fluids, where it suffices to track the motion of the material points, now the transference maps \( \varphi_{h,k \rightarrow k+1} \) must be approximated by conforming interpolations of the form

\[ \varphi_{h,k \rightarrow k+1}(x) = \sum_{a=1}^{N} x_{a,k+1} N_{a,k}(x), \]  

where \( \{x_{a,k+1}, a = 1, \ldots, N\} \) are coordinates of nodes on the configuration at time \( t_{k+1} \) and \( N_{a,k}(x) \) are conforming shape functions defined over the configuration at time \( t_k \). For discrete transference
maps of the form (55), the material-point update (50) becomes

\[ x_{p,k+1} = \sum_{a=1}^{N} x_{a,k+1} N_{a,k}(x_{p,k}). \]  

(56)

We note that we are left with considerable latitude in the choice of shape functions. For instance, in the implementations to date we choose to use meshfree max-ent shape functions [27] computed from the convected nodal coordinates. However, there is no need to convect the nodes by the flow and more general schemes aiming to optimize the nodal positions at the beginning of each time step could in principle be devised, though such extensions of the method will not be pursued here.

By virtue of representations (46)–(55) for the approximate volume measure, mass density and incremental deformation mapping, respectively, it follows that, in the OTM method, all the field information is carried by two sets of points, Figure 1: the nodal points, \( x_{a,k} \), which carry position information, and the material points, which carry volume and material information. We note that the material points are connected to the nodes through the interpolation rule (56). In general, the shape functions \( N_{a,k} \) may be expected to have a finite range, and thus each material point is connected to a finite number of nodes in its environment, Figure 2. The construction of the shape functions \( N_{a,k} \) from the nodal set is a key step in the OTM forward integration procedure and is discussed in detail in [27].

Insertion of the preceding approximations into (41) yields the discrete action

\[ A_k(\rho_{h,1}, \ldots, \rho_{h,N-1}) = \sum_{k=0}^{N-1} \sum_{p=1}^{M} g \left\{ \begin{array}{l} m_p \frac{|x_{p,k+1} - x_{p,k}|^2}{2(t_{k+1} - t_k)^2} \\ - \frac{1}{2} \left[ m_p (f(\rho_{p,k}) - u(x_{p,k})) - q(x_{p,k}) v_{p,k} \\ + m_p (f(\rho_{p,k+1}) - u(x_{p,k+1})) - q(x_{p,k+1}) v_{p,k+1} \right] (t_{k+1} - t_k) \end{array} \right\}. \]  

(57)

Figure 1. Schematic of the OTM approximation scheme, showing two successive configurations \( B_k \) and \( B_{k+1} \) of the body, mapped into each other by the incremental deformation mapping \( \varphi_{k\rightarrow k+1} \) and the corresponding sets of nodal points (white symbols), \( x_{a,k} \) and \( x_{a,k+1} \), and material points (red symbols), \( x_{p,k} \) and \( x_{p,k+1} \), respectively.
Figure 2. Domain of interaction of a material point (red symbol) as determined by the ranges of interaction of the shape functions centered at neighboring nodes (white symbols).

where (54) is tacitly understood to be in force. Taking variations of $A_h$ gives the discrete Euler–Lagrange equations

$$
\langle \delta A_h, \zeta_h \rangle = \sum_{k=0}^{N-1} \sum_{p=1}^M m_p \left( \frac{x_{p,k+1} - x_{p,k}}{t_{k+1} - t_k} + \frac{x_{p,k} - x_{p,k-1}}{t_k - t_{k-1}} \right) \cdot \zeta_{h,k}(x_{p,k})
$$

$$- \frac{t_{k+1} - t_k - 1}{2} \left\{ (p(x_{p,k}) + q(x_{p,k})) \nabla \cdot \zeta_{h,k}(x_{p,k}) + (p(x_{p,k}) + q(x_{p,k})) \cdot \zeta_{h,k}(x_{p,k}) \right\},
$$

where

$$\zeta_{h,k}(x) = \sum_{a=1}^N \zeta_{a,k} N_{a,k}(x)
$$

are discrete admissible virtual displacements. We note that Equation (58) can alternatively be obtained by inserting the spatial discretization into the semi-discrete Euler–Lagrange equations (43) directly. Enforcing stationarity with respect to all admissible variations $\zeta_h$ we obtain

$$
\frac{2}{t_{k+1} - t_k - 1} \left( M_k \frac{x_{k+1} - x_k}{t_{k+1} - t_k} - I_k \right) = f_k,
$$

where $x_k \equiv \{x_{1,k}, \ldots, x_{N,k}\}$ is the nodal coordinate array at time $t_k$,

$$I_{a,k} = \sum_{p=1}^M m_p \frac{x_{p,k} - x_{p,k-1}}{t_k - t_{k-1}} N_{a,k}(x_{p,k})
$$
is the linear momentum of node $a$ at time $t_k$,

$$M_{ab,k} = \sum_{p=1}^{M} m_p N_{a,k}(x_{p,k}) N_{b,k}(x_{p,k}) I$$

(62)

is the consistent mass submatrix for nodes $a$ and $b$ at time $t_k$, and

$$f_{a,k} = \sum_{p=1}^{M} \left[ (p(\rho_{p,k}) + q(x_{p,k}))\nabla N_{a,k}(x_{p,k}) + (\rho_{p,k}b_{k}(x_{p,k}) + \nabla q(x_{p,k}))N_{a,k}(x_{p,k}) \right] v_{p,k}$$

(63)

are the nodal out-of-balance forces. If the shape functions satisfy the consistency conditions

$$\sum_{a=1}^{N} N_{a,k}(x) = 1,$$

(64a)

$$\sum_{a=1}^{N} x_{a,k} N_{a,k}(x) = x,$$

(64b)

and are backward-compatible, i.e. satisfy the identity

$$x_{p,k-1} = \sum_{a=1}^{N} x_{a,k-1} N_{a,k}(x_{p,k}),$$

(65)

then Equation (60) simplifies to

$$\frac{2}{t_{k+1}-t_k} M_k \left( \frac{x_{k+1}-x_k}{t_{k+1}-t_k} - \frac{x_k-x_{k-1}}{t_k-t_{k-1}} \right) = f_k,$$

(66)

which is a central-difference scheme.

The above equations define a finite-dimensional semi-discrete central-difference scheme that can be solved forward explicitly. Algorithm 1 outlines the general structure of the forward solution, which has the usual structure of explicit time-integration schemes, where the updated nodal coordinates are computed directly from the initial conditions at the beginning of the time step. However, as noted earlier, the time-integration algorithm differs sharply from conventional Eulerian algorithms, which rely on some direct time discretization of the continuity equation, where the update of the mass density is geometrically exact. In addition, the discretization of inertia by means of the Wasserstein distance between consecutive mass densities results in the inertia forces appearing in the discrete equation of motion (66), which properly account for the variation of the mass matrix between time steps.

The OTM forward solution scheme also has the usual structure of updated-Lagrangian procedures where the shape functions are continuously updated. This continuous update causes the connectivity between material points and nodes to change dynamically throughout the solution. This dynamic reconnection is akin to that resulting from edge flips in finite element calculations and other similar adaptive strategies for avoiding mesh entanglement (e.g. [38, 39] and references therein). It bears emphasis that in the finite element method the material—or quadrature—points are tied to the triangulation and, consequently, remeshing inevitably necessitates remapping of the information carried by the material points, an operation that is often fraught with difficulty [40]. In contrast, no such remapping operations are required in the OTM method.
Algorithm 1 OTM – COMPRESSIBLE EULER FLOWS

1: Initialization: Set \( k = 0 \), initialize nodal coordinates \( x_{a,-1}, x_{a,0} \), shape functions \( N_{a,0} \), material point coordinates \( x_{p,0} \), volumes \( v_{p,0} \) and densities \( \rho_{p,0} \).
2: Compute mass matrix \( M_k \), linear momenta \( l_k \) and internal forces \( f_k \).
3: Update nodal coordinates:
   \[
   x_{k+1} = x_k + (t_{k+1} - t_k) M_k^{-1} \left( l_k + \frac{t_{k+1} - t_k}{2} f_k \right)
   \]
4: Update material point coordinates:
   \[
   x_{p,k+1} = \varphi_{h,k \rightarrow k+1}(x_{p,k})
   \]
5: Update material point volumes:
   \[
   v_{p,k+1} = \det \nabla \varphi_{h,k \rightarrow k+1}(x_{p,k}) v_{p,k}
   \]
6: Update material point mass densities:
   \[
   \rho_{p,k+1} = \frac{m_p}{v_{p,k+1}}
   \]
7: Recompute shape functions \( N_{a,k+1}(x_{p,k+1}) \) and derivatives \( \nabla N_{a,k+1}(x_{p,k+1}) \) from updated nodal set.
8: Reset \( k \leftarrow k + 1 \). If \( k = N \) exit. Otherwise go to (2).

The OTM approach affords complete flexibility as regards the choice of incremental shape functions, which need not be convected by the flow as in conventional isoparametric interpolation. In particular, the nodal set can be rearranged at the beginning of every time step so as to equilibrate the corresponding configurational forces (e.g. [38, 39] and references therein) and the shape functions can then be reconstructed from the rearranged nodal sets [27]. Evidently, the efficient reconstruction of the shape functions from the nodal set is a key element of the OTM scheme.

An additional advantageous feature of the OTM method as applied to fluids is that it renders trivial the imposition of general boundary conditions, including kinematic boundary conditions as in forced flows, and traction boundary conditions as in free-surface flows. Furthermore, since maxent shape functions are perfectly compatible with finite elements, the treatment of fluid–structure interaction problems involving highly flexible solids and structures is greatly facilitated. These attributes of the OTM method are demonstrated in the examples of application shown in Section 6.

4. ELASTIC SOLIDS

The kinetic energy of a solid is no different from that of a fluid, Equation (8), and can be expressed in terms of the mass density and the velocity field. Therefore, the treatment of the kinetic energy of a solid, including its temporal and spatial discretization, may be effected using the same optimal transportation approach followed for fluids above. Conveniently, the free energy of a compressible barotropic fluid depends solely on its mass density, and the entire action can thus be expressed in terms of the mass density and velocity field. By way of contrast, the free energy density of
a general material-frame indifferent, anisotropic, inelastic solid has a far more complex structure and its evaluation requires additional fields. For simplicity, we start by considering the case of elastic solids. Further extensions to viscous and inelastic behavior are pursued in the next section.

We consider the motion of an elastic solid described by a deformation mapping \( \varphi : B_a \times (a, b) \to B(t) \subset \mathbb{R}^n \). Part of the boundary \( \partial_1 B(t) \) of the solid is kinematically constrained and the remainder \( \partial_2 B(t) = \partial B(t) \setminus \partial_1 B(t) \) of the boundary is either free or acted upon by an applied traction. In an Eulerian framework, the motion of the solid is governed by the coupled equations

\[
\begin{align*}
v \circ \varphi &= \frac{\partial \varphi}{\partial t} \quad \text{in } \Omega, \\
F \circ \varphi &= \nabla \varphi \quad \text{in } \Omega, \\
C &= F^T F \quad \text{in } \Omega, \\
\rho &= \rho_a \circ \varphi^{-1} \quad \text{in } \Omega, \\
\frac{\partial (\rho v)}{\partial t} + \nabla \cdot (\rho v \otimes v - \sigma) &= \rho b \quad \text{in } \Omega, \\
\sigma &= 2 \rho F \frac{\partial f}{\partial C} (C) F^T \quad \text{in } \Omega, \\
v &= w \quad \text{on } \partial_1 \Omega, \\
\sigma n &= q \quad \text{on } \partial_2 \Omega,
\end{align*}
\]

where \( F \) and \( C \) denote the deformation gradient and the right Cauchy–Green deformation tensor expressed as fields over the deformed configuration, respectively, \( f(C) \) is the isothermal free energy density of the solid per unit mass, \( \sigma \) is the Cauchy stress, \( b \) is a body force density per unit mass, \( w \) is the prescribed velocity at the boundary of the domain, \( q \) is the applied traction, \( n \) is the outward unit normal, and, as before, \( \Omega = \bigcup_{t \in (a, b)} B(t) \) is the space time domain swept by the flow, \( \partial_1 \Omega = \bigcup_{t \in (a, b)} \partial_1 B(t) \) is the space time displacement boundary and \( \partial_2 \Omega = \bigcup_{t \in (a, b)} \partial_2 B(t) \) is the space time traction boundary. Equation (67d) enforces conservation of mass, Equation (67c) gives the right Cauchy–Green deformation tensor field in terms of the deformation mapping, Equation (67e) enforces conservation of linear momentum, Equation (67f) gives the Cauchy stress tensor field in terms of the deformation mapping, Equation (67g) enforces kinematic compatibility over the displacement boundary and Equation (67h) the equilibrium of tractions over the traction boundary.

The action of the solid over the time interval \((a, b)\) is now

\[
A(\rho, v, C, B) = \int_a^b \left\{ \int_{B(t)} \left[ \frac{\rho}{2} |v|^2 - \rho (f(C) - u) + \text{tr} \tau \right] \, dx \right\} \, dt,
\]

where \( \tau \) denotes an arbitrary self-equilibrated stress field over \( \Omega \) in equilibrium with the applied tractions over \( \partial_2 \Omega \), i.e.

\[
\begin{align*}
\nabla \cdot \tau &= 0 \quad \text{in } \Omega, \\
\tau n &= q \quad \text{on } \partial_2 \Omega.
\end{align*}
\]
Taking variations of (68) with respect to the deformation mapping taking (67a)–(67d) into account gives
\[ \delta A(\rho, v, C, B) = \int_a^b \left\{ \int_{B(t)} \left( \rho v \cdot \frac{D\xi}{Dt} - \sigma \cdot \nabla \xi + \rho b \cdot \xi \right) \, dx + \int_{\partial B(t)} \sigma \cdot \nabla \xi \, d\sigma \right\} \, dt \]  
(70)

Integrating by parts and requiring stationarity for all admissible variations satisfying (40a)–(40c) we obtain (67e) and (67h), as required.

**Algorithm 2 OTM — Elastic Solid Flows**

1: Initialization: Set \( k = 0 \), initialize nodal coordinates \( x_{a,-1}, x_{a,0} \), shape functions \( N_{a,0} \), material point coordinates \( x_{p,0} \), volumes \( v_{p,0} \), densities \( \rho_{p,0} \) and deformation gradients \( F_{p,0} \).
2: Compute mass matrix \( M_k \), linear momenta \( l_k \) and internal forces \( f_k \).
3: Update nodal coordinates:
\[ x_{k+1} = x_k + (t_{k+1} - t_k) M_k^{-1} \left( l_k + \frac{t_{k+1} - t_{k-1}}{2} f_k \right) \]
4: Update material point coordinates:
\[ x_{p,k+1} = \phi_{h,k \rightarrow k+1}(x_{p,k}) \]
5: Update material point volumes:
\[ v_{p,k+1} = \text{det} \nabla \phi_{h,k \rightarrow k+1}(x_{p,k}) v_{p,k} \]
6: Update material point mass densities:
\[ \rho_{p,k+1} = \frac{m_p}{v_{p,k+1}} \]
7: Update material point deformation gradients and right Cauchy–Green deformation tensors:
\[ F_{p,k+1} = \nabla \phi_{h,k \rightarrow k+1}(x_{p,k}) F_{p,k} \]
\[ C_{p,k+1} = F_{p,k+1}^T F_{p,k+1} \]
8: Recompute shape functions \( N_{a,k+1}(x_{p,k+1}) \) and derivatives \( \nabla N_{a,k+1}(x_{p,k+1}) \) from updated nodal set.
9: Reset \( k \leftarrow k+1 \). If \( k = N \) exit. Otherwise go to (2).

The temporal and spatial discretization of the action (68) can now proceed along the same lines followed for fluid flows. Thus, a temporal discretization of (68) based on an optimal transportation treatment of the kinetic energy is
\[ A_d(C_1, \ldots, C_{N-1}) = \sum_{k=0}^{N-1} \left\{ \frac{1}{2} \mathcal{F}(\rho_k, \rho_{k+1}) - \frac{1}{2} [U(C_k) + U(C_{k+1})] \right\} (t_{k+1} - t_k), \]  
(71)
which is expressed directly in terms of the right Cauchy–Green deformation field. For elastic solids,

\[ U(C) = \int_{B(t)} [\rho(f(C) - u) - \text{tr}\tau] \,dx, \tag{72} \]

Inserting the approximations (46)–(55) into (71) we obtain the fully discrete action

\[ A_h(\varphi_{h,1}, \ldots, \varphi_{h,N-1}) = \sum_{k=0}^{N-1} \sum_{p=1}^{M} g \left\{ \frac{m_p}{2} \frac{|x_{p,k+1} - x_{p,k}|^2}{(t_{k+1} - t_k)^2} - \frac{1}{2} g [m_p (f(C_{p,k}) - u(x_{p,k})) - \text{tr}\tau(x_{p,k})v_{p,k} + m_p (f(C_{p,k+1}) - u(x_{p,k+1})) - \text{tr}\tau(x_{p,k+1})v_{p,k+1}] \right\} (t_{k+1} - t_k), \tag{73} \]

Taking variations of \( A_h \) and enforcing stationarity with respect to all admissible variations of the form (59) gives a discrete equation of motion of the form (66) with

\[ f_{a,k} = \sum_{p=1}^{M} \left[ (\sigma(p_{p,k}) + \tau(x_{p,k}))\nabla N_{a,k}(x_{p,k}) + \rho_{p,k} b_k(x_{p,k}) \right] v_{p,k}, \tag{74} \]

where we assume that (64a), (64b) and (65) are in force.

As in the case of fluid flows, the above equations define a finite-dimensional central-difference scheme that can be solved forward explicitly, cf. Algorithm 2. This forward solution has the usual structure of explicit time-integration and updated-Lagrangian schemes. In particular, all the finite kinematics of the motion, including the mass density and volume updates, are geometrically exact. As in the case of fluid flows, the continuous reconstruction of the shape functions has the effect of automatically reconnecting the material points and the nodal set, with no need of remapping the information carried by the material points. This property of the method is particularly convenient for inelastic materials such as considered in Section 5, whose local material state often includes additional internal variable information.

\section{5. VISCOSITY AND INELASTICITY}

In this section we extend the OTM method developed above to problems involving dissipative and inelastic behavior. Consideration of viscosity and inelasticity enables the application of the OTM method to Navier–Stokes flows, unconstrained plastic flows and other problems of interest. Hamilton’s principle of stationary action can be extended to dissipative systems as the Hamilton–d’Alembert principle (e.g. [41, 42]). We begin by reinterpreting the variational structure of the conservative equations of motion equation (66). To this end, introduce the discrete local action

\[ A_k(x_k) = \frac{(x_{k+1} - x_k)^T M_k (x_{k+1} - x_k)}{2(t_{k+1} - t_k)} + \frac{(x_k - x_{k-1})^T M_k (x_k - x_{k-1})}{2(t_k - t_{k-1})} + \frac{t_{k+1} - t_k - 1}{2} U_k(x_k), \tag{75} \]
where, for simplicity, we work with the fully discretized system, semi-discrete systems being amenable to an entirely similar treatment. In (75), $x_{k-1}$ and $x_{k+1}$ are regarded as fixed and $U_k(x_k)$ denotes the discretized potential energy, with the defining property that

$$f_k = \frac{\partial U_k}{\partial x_k}(x_k),$$

i.e. $U_k(x_k)$ is a potential for the effective forces acting on the nodes. Thus, for inviscid fluids $U_k(x_k)$ follows from the spatial discretization of (42), whereas for elastic solids $U_k(x_k)$ follows from the spatial discretization of (72). In (75), the shape functions $N_k$ at time $t_k$ are regarded as fixed and, hence, so is the corresponding mass matrix $M_k$. A direct calculation then shows that Equation (66) is equivalent to

$$DA_k(x_k) = 0,$$  

provided that $A_k(x_k)$ is differentiable.

Within this discrete Hamilton-d’Alembert framework viscosity can be introduced into the formulation as follows (cf. [14, 15]). Let $\phi(F_{k-1\rightarrow k})$ be any material-frame indifferent function of the incremental deformation gradient $F_{k-1\rightarrow k} = \nabla \varphi_{k-1\rightarrow k}$ such that

$$\langle \mathbf{D}\phi(I) \beta, \beta \rangle = 0$$

and

$$\langle \mathbf{D}^2\phi(I) \beta, \beta \rangle = \frac{\lambda}{2} \text{tr}(\beta)^2 + \mu \|\text{sym}(\beta)\|_2^2,$$

where $\lambda$ and $\mu$ are viscosities. Consider now the discrete local action

$$A_k(x_k) = \frac{(x_{k+1} - x_k)^T M_k (x_{k+1} - x_k)}{2(t_{k+1} - t_k)} + \frac{(x_k - x_{k-1})^T M_k (x_k - x_{k-1})}{2(t_k - t_{k-1})} + \frac{t_{k+1} - t_{k-1}}{2} U_k^{\text{tot}}(x_k),$$

where

$$U_k^{\text{tot}}(x_k) = U_k(x_k) + U_k^{\text{vis}}(x_k)$$

and $U_k^{\text{vis}}(x_k)$ is the spatial discretization of

$$U_k^{\text{vis}}(\varphi_{k-1\rightarrow k}) = \int_{B_k} \frac{\phi(\nabla \varphi_{k-1\rightarrow k})}{t_k - t_{k-1}} \, dx.$$

Then, (77) gives

$$\frac{2}{t_{k+1} - t_{k-1}} M_k \left( \frac{x_{k+1} - x_k}{t_{k+1} - t_k} - \frac{x_k - x_{k-1}}{t_k - t_{k-1}} \right) = f_k^{\text{tot}}(x_k),$$
where

\[ f_k^{\text{tot}}(x_k) = f_k(x_k) + f_k^{\text{vis}}(x_k) \]  \hspace{1cm} (84)

are the viscous forces. A straightforward calculation shows that such viscous forces are indeed consistent with Newton's law of viscosity in the limit of \( \Delta t \to 0 \), provided that condition (79) is satisfied. This leaves considerable latitude in the choice of the increment viscous potential density \( \phi(F_{k-1\to k}) \) since, from a consistency point of view, only the behavior of \( \phi(F_{k-1\to k}) \) about the identity matters. For instance, in the examples presented in this paper \( \phi \) is chosen to be of the Hadamard form, i.e. a neo-Hookean function extended to the compressible range. Conveniently, by the preceding incremental treatment of viscosity the structure of the calculations remains identical to that of an elastic solid, Algorithm 2, the sole effect of viscosity being that of introducing an additional term to the incremental energy functional (75) or, equivalently, and additional set of viscous forces to the force system (76).

Inelastic behavior of the viscoplastic type can also be integrated seamlessly into the discrete Hamilton-d'Alembert framework with the aid of incremental variational updates \[43]. In these updates, all internal processes are optimized incrementally and locally, which results in an effective incremental energy

\[ U_k(C_k) = \int_{B_k} [\rho f_k(C_k) - \mathbf{u_k} - \text{tr}\tau_k] \, dx, \]  \hspace{1cm} (86)

In this energy, the effective incremental energy density \( f_k(C_k) \) is the result of minimizing out the internal variables pointwise from a suitably defined incremental minimum principle. Since this local minimization accounts for kinetic processes, the effective incremental energy density \( f_k(C_k) \) depends parametrically on the initial conditions for the time step at time \( t_{k-1} \). This dependence in turn allows for irreversibility and hysteresis. The corresponding discrete local action then remains of the form (75), with \( U_k(x_k) \) resulting simply from a spatial discretization of (86). Conveniently, the flow of the calculations remains formally identical to the case of elastic solids, Algorithm 2, with the elastic energy density \( f(C_k) \) simply replaced by the effective incremental energy density \( f_k(C_k) \). However, the evaluation of the nodal forces entails an additional local update of the internal variables at all material points. It bears emphasis that, since material points are convected by the flow at all times, no remapping of state variables is required at any time during the calculations.

6. CONSERVATION AND CONVERGENCE PROPERTIES

In this section we assess the convergence properties of the OTM method by means of two standard benchmark tests: the Riemann problem of a long shock tube initially containing a viscous gas in two different states separated by a thin diaphragm; and the shock compression of a viscous gas in a shock tube configuration. Both problems are amenable to exact solutions and therefore provide convenient tests of the accuracy of the OTM method. We also make contact with the theory of variational time integrators (e.g. \[41, 42]\) to establish the conservation properties of the OTM method.
6.1. Conservation properties

The conservation properties of the OTM method follow directly from the standard theory of variational time integrators (e.g. [41, 42]) once it is realized that the OTM method indeed falls within that general framework. To make this connection we rewrite (73) as an action sum

$$A_h(\varphi_{h,1}, \ldots, \varphi_{h,N-1}) = \sum_{k=0}^{N-1} L_d(q_k, q_{k+1})$$

(87)

where the nodal coordinates $q_k = \{x_{a,k}, a = 1, \ldots, N\}$ are now regarded as the generalized coordinates of a Lagrangian system and

$$L_d(q_k, q_{k+1}) = \sum_{p=1}^{M} g \left\{ \frac{m_p}{2} \frac{|x_{p,k+1} - x_{p,k}|^2}{(t_{k+1} - t_k)^2} - \frac{1}{2} g \left[ m_p (f(C_{p,k}) - u(x_{p,k})) - \text{tr} \tau(x_{p,k}) v_{p,k} \right] 
+ m_p (f(C_{p,k+1}) - u(x_{p,k+1})) - \text{tr} \tau(x_{p,k+1}) v_{p,k+1} \right\} (t_{k+1} - t_k),$$

(88)

is a discrete Lagrangian. In (88) we note that the material-point coordinates and the right Cauchy–Green deformation tensor at the material points follow from the nodal coordinates through (56) and step 7 of Algorithm 2, respectively.

As may be recalled, a fundamental property of Lagrangian systems is that symmetries in the system result in the conservation of certain momentum maps along trajectories, a classical result known as Noether’s theorem. The same precise link exists for discrete-time Lagrangian systems governed by the stationarity of action sums of the form (87). Thus, suppose that

$$L_d(q_k, \zeta, q_{k+1}, \zeta) = L_d(q_k, q_{k+1})$$

(89)

for a family of discrete trajectories parameterized by $\zeta \in \mathbb{R}^n$ with $q_{k,0} = q_k$. An invariance of this form is referred to as a symmetry of the discrete Lagrangian. The infinitesimal generator of the symmetry is

$$\eta_k = \frac{\partial q_{k, \epsilon \zeta}}{\partial \epsilon} \bigg|_{\epsilon = 0}.$$  

(90)

Invariance of the discrete Lagrangian implies invariance of the action sum. Thus, if $q_k = q_{k,0}$ is a trajectory of the discrete system we must have

$$0 = \left[ \frac{\partial}{\partial \epsilon} \sum_{k=0}^{N-1} L_d(q_k, \epsilon \zeta, q_{k+1}, \epsilon \zeta) \right]_{\epsilon = 0} = D_1 L_d(q_0, q_1) \cdot \eta_0 + D_2 L_d(q_{N-1}, q_N) \cdot \eta_N,$$

(91)

where we have used the stationarity of the action. Since, in addition,

$$0 = D_1 L_d(q_0, q_1) \cdot \eta_0 + D_2 L_d(q_0, q_1) \cdot \eta_1$$

(92)

by the invariance of $L_d$, we arrive at the identity

$$D_2 L_d(q_{N-1}, q_N) \cdot \eta_N = D_2 L_d(q_0, q_1) \cdot \eta_1,$$

(93)

which may be regarded as a *discrete Noether’s theorem*. Defining the discrete momentum map by the identity

\[ J_d(q_k, q_{k+1}) \cdot \xi = D_2 L_d(q_k, q_{k+1}) \cdot \eta_{k+1} \]  

(94)

and noting that \( \xi \) is arbitrary we can rewrite (93) as

\[ J_d(q_{N-1}, q_N) = J_d(q_0, q_1). \]  

(95)

which shows that the momentum map is conserved along discrete trajectories.

The exact conservation of linear and angular momentum by the OTM method now follow as an application of the discrete Noether’s theorem just outlined. We begin by noting that, for an unforced system, the discrete Lagrangian (88) is invariant under superposed translations, i.e.

\[ L_d(q_k + \xi, q_{k+1} + \xi) = L_d(q_k, q_{k+1}) \]  

(96)

and the preceding machinery applies with \( q_k, \xi = q_k + \xi, \xi \in \mathbb{R}^3 \). The corresponding momentum map is

\[ J_d(q_k, q_{k+1}) = \sum_{a=1}^N \sum_{b=1}^N M_{ab, k+1} \frac{x_{b, k+1} - x_{b, k}}{t_{k+1} - t_k}, \]  

(97)

which gives the total linear momentum of the system. In this expression \( M_{ab, k} \) denotes the consistent mass matrix (62). By material-frame-indifference, for an unforced system we additionally have

\[ L_d(e^{*\xi} q_k, e^{*\xi} q_{k+1}) = L_d(q_k, q_{k+1}) \]  

(98)

where \( *\xi \) is the Hodge dual of \( \xi \in \mathbb{R}^3 \), i.e. the skewsymmetric matrix whose axial vector is \( \xi \). In particular, \( e^{*\xi} \in SO(3) \), i.e. it defines a finite rotation. In this case, the discrete-Noether machinery applies with \( q_k, \xi = e^{*\xi} q_k \). The corresponding momentum map is

\[ J_d(q_k, q_{k+1}) = \sum_{a=1}^N x_{a, k+1} \times \sum_{b=1}^N M_{ab, k+1} \frac{x_{b, k+1} - x_{b, k}}{t_{k+1} - t_k}, \]  

(99)

which gives the total angular momentum of the system. Thus we conclude that the OTM method exactly conserves the total linear and angular momentum of the system as defined by (97) and (99), respectively.

Variational integrators can be made to conserve energy exactly by adapting the time step [44]. In contrast, when a constant time step is used in calculations energy is no longer conserved exactly. This lack of exact conservation notwithstanding, in numerical tests energy is observed to oscillate tightly around a constant value and to exhibit excellent long-term behavior. Exact local conservation of momenta and energy can be achieved by means of *asynchronous* variational integrators [45]. These algorithms derive from a space time form of a discrete version of Hamilton’s principle and permit the local adaption of time steps, which need not bear an integral relation to each other. As a consequence of this variational structure, asynchronous variational integrators conserve local energy and momenta exactly, subject to solvability of the local time steps. Despite their strong appeal, these enhancements are beyond the scope of this paper and will not be pursued here.
6.2. Initialization and set-up

We initialize all subsequent calculations by triangulating the initial domain of analysis in order to set the initial locations of the nodes, which are identified with the nodal set of the triangulation, and of the material points, which are placed at the barycenters of the simplicial cells. However, the initial mesh is subsequently jettisoned and the calculations proceed in a meshfree manner. As already indicated, we choose to convect the nodes by the flow and we interpolate all conforming fields by means of local max-ent interpolation [27]. This choice of shape functions is indeed pivotal to the method, since it furnishes a Kronecker-delta property at the boundary which in turn enables the direct imposition of displacement boundary conditions and furnishes automatic compatibility between fluids and solids or structures. Given the explicit nature of the time-integration scheme, in all calculations we set the time step to a fraction of the stable time step as estimated from a Courant–Friedrichs–Lewy-type (CFL) condition.

6.3. Riemann problem

The classical Riemann problem is widely used as a benchmark test for evaluating the capability and accuracy of gas-dynamics codes or numerical methods (cf., e.g. [46] for an early example in that regard). The Riemann problem tests the accuracy of a method for solving the one-dimensional time-dependent compressible Euler equations with discontinuous initial conditions. The Riemann problem is particularly convenient as a verification test since it has an exact mathematical solution. The Riemann problem concerns a long shock tube initially containing a gas in two different states separated by a thin diaphragm. At the onset of the experiment, the diaphragm is ruptured resulting in three waves: a shock wave, a contact surface, and a fan of expansion wave emanating from the rupture point. Figure 3 depicts the general experimental setup and the resulting wave structure in space time. A complete analysis and presentation of the Riemann problem and traditional numerical analysis are provided elsewhere.

Figure 3. Schematic of the Riemann problem and resulting wave structure.
solvers can be found, e.g., in [47]. We specifically solve the one-dimensional compressible Euler equations formulated in Section 3 for an ideal gas undergoing reversible adiabatic (isentropic) dynamics, which results in the equations of state

\[
\begin{align*}
  f &= \frac{C}{\gamma - 1} \rho^{\gamma - 1}, \\
  p &= -\frac{C}{\gamma - 1} \rho^\gamma,
\end{align*}
\tag{100a, 100b}
\]

where \( C \) and \( \gamma = C_p/C_v \) are constants.

In calculations, we initially partition the domain of analysis \([0, L]\) into \( N \) equal segments separated by nodes and place material points at the center point of each segment. We then use meshfree max-ent shape functions based on the current positions of the nodes for interpolating the nodal fields. As required by the OTM, the material points are advected by the flow. We choose to also advect the nodes with the flow and keep the characteristic max-ent shape-function width constant at a certain multiple of the average mesh size (cf. [27]). Because of the local character of the max-ent shape functions, only the nearest nodes contribute significantly to the value of the shape functions—and, therefore, to the value of the state variables—at a given material point. We note, however, that max-ent shape functions adapt automatically to the local node density and always couple each material point to a minimum of \( d+1 \) nodes, with \( d \) the spatial dimension. When the separation of those \( d+1 \) points is much larger than the characteristic width \( w \) of the max-ent shape functions, the max-ent interpolation ostensibly reduces to simplicial interpolation. This property is in contrast to interpolation schemes based on shape functions of constant width that translate rigidly with the nodes and has the effect of eliminating the well-known tension instabilities of those interpolation schemes.

The time step is set to approximately \( \frac{1}{20} \) of the Courant–Friedrichs–Lewy (CFL) condition. As is standard in shock propagation calculations, we use an artificial viscosity scheme [48] in order to stabilize unresolved shock profiles while keeping the shock propagation speed unchanged. We specifically use the Lagrangian artificial viscosity scheme proposed in [49]. The remaining parameters employed in calculations are summarized in Table I, where \((p_L, \rho_L)\), respectively, \((p_R, \rho_R)\) refer to the initial state of the gas on the left, respectively, right of the diaphragm. This initial state corresponds to a choice of \( C = 1 \) and \( \gamma = 1.661 \) in the equation of state (100).

Figure 4 shows snapshots of the pressure and density profiles at time \( t = 0.25 \) obtained using \( N = 400 \) nodes. The exact solution is also shown in the figure for reference. As is evident from the figure, the OTM profiles are in excellent agreement with the numerical solution.

A more detailed picture of the accuracy and convergence properties of OTM is afforded by the conventional convergence plots, Figure 5. As noted in Section 2, a natural space of solutions for compressible Euler flows is \( C([a, b]; L^1(\mathbb{R}^n; [0, \infty])) \) for the density field. Therefore, we exhibit convergence plots in the norms

\[
\|\rho_h - \rho\| = \max_{t \in [a, b]} \int_0^L |\rho_h(x, t) - \rho(x, t)| \, dx
\tag{101}
\]

| Table I. Parameters used in simulations of Riemann problem. |
|--------------|--------------|--------------|--------------|---|
| \( \rho_L \) | \( \rho_L \) | \( \rho_R \) | \( \rho_R \) | \( L \) |
| -1.0 | 1.0 | -0.1 | 0.25 | 2.0 |

Figure 4. Riemann problem, snapshot of numerical (symbols) and exact (solid curve) solutions at $t = 0.25$:
(a) pressure profile and (b) density profile.

Figure 5. Riemann problem. Convergence plot showing density error vs number of
nodes indicative of linear convergence.

As expected from a low-order method and the presence of strong discontinuities in the solution, the order of convergence of the OTM in the Riemann problem is linear. We note that increased accuracy may be achieved by moving the nodes in a variationally optimal manner, e.g. by recourse to variational $r$-adaption \cite{38, 39, 50} and, additionally, by adapting the width of the shape functions variationally as suggested in \cite{27}. Indeed, the existence of a well-defined incremental minimum
principle conveniently opens the way for variational adaptivity in all its form. However, these enhancements will not be pursued here in the interest of simplicity.

6.4. Shock wave in piston

Planar shock waves in a shock tube configuration, Figure 6, can have sharp profiles and result in large compression ratios, thereby supplying an exacting numerical verification test. The particular case of the isothermal compression of a gas obeying the equation of state

\[ p(J) = \frac{K}{2} (J - J^{-1}) \]  

and exhibiting the Newtonian viscosity (cf. Section 5) can be solved exactly [15] for the steady shock profile. In Equation (102), \( J = \det(\nabla \phi) = \rho_0 / \rho \) and \( K \) is a constant that measures the compressibility of the gas. In Lagrangian coordinates, the steady shock profile is of the form

\[ \varphi(x, t) = x + w f \left( \frac{x - ct}{w} \right), \]  

where \( x \) and \( \varphi \) denote the longitudinal Lagrangian coordinate and deformation mapping in the direction of the shock tube axis,

\[ c = \sqrt{\frac{K}{2 \rho_0} \left( 1 + \frac{1}{J - J^+} \right)}, \]  

is the material propagation speed of the shock, and

\[ w = \frac{8 \eta c}{3 K} \frac{J^+ - J^-}{J^+ - J^-} \]  

measures the width of the shock profile in the Lagrangian configuration. In these expressions, \( \rho_0 \) is a reference gas density, \( \eta \) its Newtonian viscosity and we have appended the boundary conditions

\[ \lim_{x \to \pm \infty} J(x, t) = J^\pm \]  

The exact steady shock profile is

\[ f(\xi) = \left( \frac{J^+ + J^-}{2} - 1 \right) \xi + (J^+ - J^-) \left( \log \cosh \frac{\xi}{2} - \log 2 \right) \]  

The density field follows simply as \( \rho = \rho_0 / J \) and the Lagrangian longitudinal velocity field as

\[ \dot{\varphi}(x, t) = c \left( 2 - (J^+ + J^-) - (J^+ - J^-) \tanh \frac{x - ct}{2w} \right) \]
Table II. Parameters used in simulations of isothermal compression shockwave.

<table>
<thead>
<tr>
<th>( \rho_0 )</th>
<th>( K )</th>
<th>( \eta )</th>
<th>( J^+ )</th>
<th>( J^- )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.0</td>
<td>1.0</td>
<td>0.0025</td>
<td>1.0</td>
<td>0.1</td>
</tr>
</tbody>
</table>

Numerical solutions have been computed using OTM for the parameters listed in Table II using one-, two- and three-dimensional discretizations, Figures 7 and 8. For these parameters, the shock propagation speed is \( C = 2.3452 \) and the shock profile width is \( w = 1.737 \times 10^{-3} \). In calculations we use the time step (e.g. [15])

\[
\Delta t = 0.1 \min \left\{ \frac{h_{\text{min}}}{c}, \frac{\rho_0 h_{\text{min}}^2}{\eta} \right\}
\]

The length of the tube is \( L = 25w \), where \( w \) is the width of the shock. We start the simulation as the center of the shockwave reaches the upstream end of the tube. The initial conditions for the calculation and the subsequent displacement boundary conditions are evaluated from the exact solution. The initial node distribution is taken to be uniform with one material point at the center of each pair of nodes. Figure 9 compares the exact and OTM solutions for a coarse discretization of the domain. The good accuracy of the OTM solution is evident from the figure. A more detail picture of the accuracy and convergence properties of OTM is afforded by conventional convergence plots, Figure 10. As noted in Section 2, a natural space of solutions for compressible Euler flows is \( C([a, b]; L^1(\mathbb{R}^n; [0, \infty])) \) for the density field and \( C([a, b]; L^2(\mathbb{R}^n; \mathbb{R}^n)) \) for the velocity field. Therefore, we exhibit convergence plots in the norms

\[
\| \rho_h - \rho \| = \max_{t \in [a, b]} \int_0^L |\rho_h(x, t) - \rho(x, t)| \, dx
\]

\[
\| \phi_h - \phi \| = \max_{t \in [a, b]} \left( \int_0^L |\phi_h(x, t) - \phi(x, t)|^2 \, dx \right)^{1/2}
\]

The level of accuracy of the OTM revealed by these convergence plots is quite remarkable. Thus, remarkably low errors are obtained even for coarse discretizations. The rate of convergence is quadratic in both density and velocity, although a degradation of convergence is apparent in the former for fine discretizations.

7. EXAMPLES OF APPLICATION

In this section, the range and scope of the OTM method are illustrated by way of selected tests and examples of application. The first example of application concerns the dynamics and fluid–structure interaction of a gas-filled spherical balloon impacting a flat terrain at high speed. This example illustrates the relative ease with which the OTM method can track complex flows in variable domains and couple them to highly flexible structures. The second example of application concerns the classical Taylor-anvil benchmark test, which probes in a simple and effective manner the compressive strength of materials undergoing large plastic deformations at high-strain rates.
Because of its widespread use, the Taylor-anvil test affords comparisons between the OTM and other methods. However, in order to exhibit the full range of the OTM method we extend the Taylor-anvil test to the hypervelocity range, which provides a compelling demonstration of the ability of the method to simulate solid flows under extreme conditions of deformation.
Figure 9. Isothermal compressive shock in shock tube. Comparison of OTM (symbols) and exact velocity, displacement and density fields: (a) velocity field; (b) displacement field; and (c) density field.

Figure 10. Isothermal compressive shock in shock tube: (a) convergence of the velocity field and (b) convergence of the density field. Rates are indicated by the value of $r$.

7.1. Bouncing balloons

Our first example of application concerns the dynamics of a gas-filled spherical balloon impacting a rigid flat terrain at high speed. Examples of engineering applications of such devices include airbag systems for automobile safety, inflatable structures for space applications, hot-air and high-altitude observation balloons and NASA’s recent use of airbag technology to provide the last stage of entry/descent and landing (EDL) in Mars missions. The example demonstrates the ability of the OTM method to couple fluids and highly deformable structures in a particularly seamless and straightforward manner.

The membrane of the balloon is modeled by means of conventional finite-kinematics membrane finite elements. Specifically, we use three-noded simplicial elements and model the material as Neo-Hookean elastic. A plane-stress condition is enforced by minimizing locally the transverse

Table III. Parameters used in simulations of an air-filled Kapton balloon.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reference density</td>
<td>$\rho_{\text{ref}}$ (kg/m$^3$)</td>
</tr>
<tr>
<td>Reference pressure</td>
<td>$p_{\text{ref}}$ (Pa)</td>
</tr>
<tr>
<td>Initial density</td>
<td>$\rho_0$ (kg/m$^3$)</td>
</tr>
<tr>
<td>Initial viscosity</td>
<td>$\mu$ (Pa s)</td>
</tr>
<tr>
<td>Initial radius</td>
<td>$R$ (m)</td>
</tr>
<tr>
<td>Membrane thickness</td>
<td>$t$ (m)</td>
</tr>
<tr>
<td>Membrane density</td>
<td>$\rho_{\text{mem}}$ (kg/m$^3$)</td>
</tr>
<tr>
<td>Membrane stiffness</td>
<td>$E_{\text{mem}}$ (Pa)</td>
</tr>
</tbody>
</table>

Figure 11. Initial configuration of an air-filled Kapton balloon: (a) 4381 nodes, 23,216 material points and 2,016 membrane elements and (b) 42,809 nodes, 246,288 material points and 7,680 membrane elements.

The deformation of the gas is assumed to be isothermal and to obey the ideal-gas law equation of state

$$f(\rho) = \frac{p_{\text{ref}}}{\rho_{\text{ref}}} \log \frac{\rho}{\rho_{\text{ref}}}$$

where $\rho_{\text{ref}}$ is a reference density and $p_{\text{ref}}$ is a reference pressure. The contact with the rigid wall is modeled simply by penalizing the one-sided constraint through a quadratic potential at the largest stiffness that does not reduce the stable time step of the system. The parameters used in simulations are collected in Table III.

Figure 11 depicts two initial configurations of the balloon. As already mentioned, the initial configuration is set up by triangulation of the domain, with the material points placed at the barycenters of the tetrahedral elements. This auxiliary triangulation is employed solely for purposes of initialization and it is jettisoned thereafter. The smallest model used in calculations contains 4381 nodes, 23,216 material points and 2,016 membrane elements, whereas the largest model contains 42,809 nodes, 246,288 material points and 7,680 membrane elements. The time step is set to a fraction of the stable time step.

Figure 12 shows a sequence of snapshots of the collision between the balloon and the terrain for an impact velocity of 10 m/s. The color coding corresponds to the von Mises equivalent stress distribution on the membrane and the pressure distribution in the gas. The von Mises

Figure 12. Sequence of snapshots showing the collision between an air-filled Kapton balloon and a flat rigid terrain at 10 m/s. The color coding corresponds to the von Mises equivalent stress distribution on the membrane and the pressure distribution superposed on the streamlines in the gas: (a) $t = 50$ ms; (b) $t = 99$ ms; (c) $t = 167$ ms; (d) $t = 199$ ms; (e) $t = 236$ ms; and (f) $t = 323$ ms.

equivalent stress field is meant to underscore that the membrane is indeed a true membrane capable of withstanding shear. The large deformations undergone by the balloon are noteworthy. The ability of the OTM method to simulate the flow of the gas bears particular emphasis. It should also be noted that the coupling between the gas and the membrane is completely seamless and straightforward, since the max-ent interpolation employed for the gas reduces naturally to—and is perfectly compatible with—the simplicial interpolation employed for the membrane.
7.2. Taylor anvil test

Our second example of application concerns the standard Taylor-anvil benchmark test \[51\], which consists of a cylindrical copper rod that strikes a rigid wall head-on. The Taylor-anvil test probes in a simple and effective manner the compressive strength of materials undergoing large plastic deformations at high-strain rates. The Taylor-anvil test has been extensively investigated in the past and thus supplies a convenient benchmark test for assessing the performance of the OTM method in problems involving large plastic flows.

Figure 13(a) depicts the initial configuration of the rod. As in all the other examples, the initial configuration is set up by triangulation of the domain, with the material points placed at the barycenters of the tetrahedral elements. This auxiliary triangulation is employed solely for purposes of initialization and it is jettisoned thereafter. The rod has an initial radius of 3.2 mm, a length of 32.4 mm and strikes a rigid frictionless wall head-on at 227 m/s. The model contains 5174 nodes and 26741 material points. The time step is set to a fraction of the stable time step. As discussed in Section 5, the elastic–plastic constitutive relations are integrated in time using variational updates, which confers the OTM method an incremental variational structure. The material constants used in calculations are representative of copper and are tabulated in Table IV. A full three-dimensional simulation is carried out to 80 \(\mu\)s, at which point the rod comes to rest.

Figure 13(b) displays a sequence of snapshots of the nodal distribution at times \(t=20, 40\) and \(80\mu\)s. An incipient rearrangement of the nodes is evident at the late times when the deformations

<table>
<thead>
<tr>
<th>Undeformed mass density (kg/m(^3))</th>
<th>Young’s modulus (GPa)</th>
<th>Poisson ratio</th>
<th>Yield stress (MPa)</th>
<th>Plastic modulus (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>8930</td>
<td>117</td>
<td>0.35</td>
<td>400</td>
<td>100</td>
</tr>
</tbody>
</table>
Figure 14. Taylor-anvil impact test of copper specimen at 227 m/s impact velocity. Distributions of effective plastic strain at 20, 40 and 80 μs.

Table V. Taylor-anvil impact test of copper specimen. Comparison of results.

<table>
<thead>
<tr>
<th></th>
<th>Final length (mm)</th>
<th>Final mushroom radius (mm)</th>
<th>Max. effective plastic strain</th>
<th>Max. von Mises stress (Mpa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>OTM method</td>
<td>21.43</td>
<td>6.8</td>
<td>3.0</td>
<td>474</td>
</tr>
</tbody>
</table>

are high. However, as already noted, in the present implementation of the OTM method no effort is made to optimize the position of the nodes, which are simply convected by the flow. The framework offers ample flexibility to rearrange the nodes at each time step, e.g. variationally or by configurational force equilibrium (cf., e.g. [50]), but these enhancements of the OTM method have not yet been pursued.

Figure 14 depicts snapshots of the distribution of effective plastic strain at times $t = 20$, 40 and 80 μs. The plots serve to illustrate the versatility of the OTM method, which applies equally both to fluid as well as to solid flows, including solid flows involving complex material behavior such as finite-deformation viscoplasticity. As already mentioned, the Taylor-anvil test has been extensively used as a benchmark test and, thus, it provides a basis for comparison to other works. Table V collects the final length of the rod, the final mushroom radius, the maximum effective strain and von Mises stress predicted by the OTM method and by the finite element calculations of Kamoulakis [52], Zhu and Cescotto [53] and Camacho and Ortiz [17]. It should be noted that all the calculations shown for comparison were carried out in the axisymmetric mode. The OTM results are indeed comparable to those from the other works in every measure, which provides a sense of the reliability and robustness of the method.
In order to exhibit the full range of the OTM method, Figure 15 shows a sequence of snapshots at times 7.5, 15 and 28 μs of the deformed shape of a copper rod striking a rigid wall at 750 m/s. The remaining parameters of the simulation are as in the preceding case except for the length of the rod, which in the present case is reduced to 12.8 mm in order to enhance yaw stability throughout the collision. As may be seen from the figure, the projectile completely flattens out by the end of the collision, which demonstrates the ability of the OTM method to deal with extremely large deformation in an effective manner. It also bears emphasis that the flow being simulated is a free-surface flow with traction-free boundary conditions outside the contact region. As is well-known, the simulation of such flows by, e.g., Eulerian methods is exceedingly challenging, whereas the handling of free boundaries and traction boundary conditions comes essentially for free within the OTM framework. Contact conditions likewise challenge Eulerian methods greatly, but are readily enforced within the OTM framework.

8. SUMMARY AND CONCLUSIONS

We have developed an optimal transportation meshfree (OTM) method for simulating general solid and fluid flows, including fluid–structure interaction. The scheme is constructed through an
integration of optimal transportation theory, local max-ent meshfree interpolation and material-point sampling. The tools of optimal transportation theory, in conjunction with material-point sampling, furnish a robust discretization of the action. This discretization may be regarded as an **interior approximation** in which the Benamou–Brenier minimum problem is restricted to mass densities concentrated on piecewise linear trajectories. This strict Rayleigh–Ritz-type approximation, and the minimum-problem structure of the mass transportation problem, bodes well for the application of powerful tools of analysis such as $\Gamma$ convergence. A successful execution of this program has the potential for supplying rigorous convergence proofs in areas of application where such proofs have been generally lacking. The systematic use of local max-ent interpolation renders the OTM scheme meshfree, which entirely sidesteps the need for continuous remeshing. Perhaps more importantly, the boundary Kronecker-delta property of the local max-ent interpolation enables the direct imposition of displacement boundary conditions and furnishes automatic compatibility between fluids and solids or structures. Finally, the use of material-point sampling supplies an effective numerical integration rule as well as the means of tracking the local state of inelastic and history-dependent materials. In addition, since material points are convected by the flow no remapping is required at any time during the calculations despite the continuously shifting local max-ent shape functions. The convergence and conservation properties, scope and versatility that this suite of properties confer the OTM method have been demonstrated by recourse to standard theory of variational time integrators, by means of verification examples and through two examples of application: the bouncing of a gas-filled balloon off a rigid wall; and the classical Taylor-anvil benchmark test extended to the hypervelocity range.

We close by pointing out several possible extensions of the OTM method and directions for further research. As noted in Section 6, we have initialized all the calculations presented in this paper by triangulating the initial domain of analysis in order to set the initial locations of the nodes, which are identified with the nodal set of the triangulation, and of the material points, which are placed at the barycenters of the simplicial cells. An appealing alternative consists of inserting the nodes and material points into the domain without recourse to an auxiliary triangulation of the domain. Schemes such as centroidal Voronoi tessellation [54] immediately suggest themselves as a means of inserting material points in accordance with some suitable optimality criterion. The remaining problem then concerns the optimal insertion of nodes once the distribution of material points is known. Evidently, these operations supply attractive alternatives to conventional triangulation, which is often an onerous task when applied to complex three-dimensional domains.

Efficient implementations of contact, fracture and fragmentation would greatly extend the range of applicability of the OTM method. Some of the automatic contact-detection and enforcement properties of particle-in-cell methods [10] and the material-point method [55] are expected to carry over to the OTM framework, which bodes well for the ability of the OTM method to deal effectively and efficiently with complex contact situations. In addition, fracture and fragmentation schemes such as element erosion [56] and the method of eigenfracture [57] are also expected to carry over to the OTM framework essentially unchanged.

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