Arbitrary-Lagrangian-Eulerian Finite-Element Hydrodynamics

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Contents

Chapter 1

The Lagrangian Step

1.1 Lagrangian governing equations

We consider Lagrangian fluid particles, for which we define their position $\mathbf{x}^+ = \mathbf{x}^+(t, \mathbf{y})$, density $\rho^+ = \rho^+(t, \mathbf{y})$, velocity $\mathbf{u}^+ = \mathbf{u}^+(t, \mathbf{y})$, and internal energy $e^+ = e^+(t, \mathbf{y})$. The vector $\mathbf{y}$ is the location of each fluid particle at time zero and thus serves to differentiate between the different particles. The Eulerian counterparts for the density, velocity, and internal energy are, respectively, $\rho = \rho(t, \mathbf{x})$, $\mathbf{u} = \mathbf{u}(t, \mathbf{x})$, and $e = e(t, \mathbf{x})$. The vector $\mathbf{x}$ is a location in Eulerian space. Also consider the volume Ω_0 as the set of all $\mathbf{y}$ vectors that make up the initial domain. The control volume $\Omega^+ = \Omega^+(t, \Omega_0)$ is then defined by

$$\Omega^+ = \{\mathbf{x}^+ : \mathbf{y} \in \Omega_0\}. \tag{1.1}$$

Note that $\Omega^+(0, \Omega_0) = \Omega_0$.

The governing equations for the Lagrangian fluid particles are derived in my flow-physics notes. These are shown below

$$\frac{\partial \mathbf{x}^+}{\partial t} = \mathbf{u}^+, \tag{1.2}$$

$$\frac{\partial \eta_\alpha^+}{\partial t} = \alpha^+, \tag{1.3}$$

$$\frac{\partial \eta_\alpha^+ \rho_\alpha^+}{\partial t} = -\eta_\alpha^+ \rho_\alpha^+ \left(\nabla \cdot \mathbf{u}\right)_{\mathbf{x}=\mathbf{x}^+}, \tag{1.4}$$

$$\rho^+ \frac{\partial \mathbf{u}^+}{\partial t} = \left(\nabla \cdot \sum_\alpha \eta_\alpha \boldsymbol{\sigma}_\alpha\right)_{\mathbf{x}=\mathbf{x}^+}, \tag{1.5}$$

$$\eta_\alpha^+ \rho_\alpha^+ \frac{\partial e_\alpha^+}{\partial t} = \left(\eta_\alpha \boldsymbol{\sigma}_\alpha : \nabla \mathbf{u}\right)_{\mathbf{x}=\mathbf{x}^+} - \left(\bar{p}\alpha_\alpha\right)_{\mathbf{x}=\mathbf{x}^+}. \tag{1.6}$$

In the above, η_α, α_α, and $\boldsymbol{\sigma}_\alpha = \boldsymbol{\sigma}(t, \mathbf{x})_\alpha$ are the volume fraction, closure model, and the stress tensor of material α. The term $\bar{p}$ is the common pressure across all materials.

A note on notation. The products that involve a tensor $\boldsymbol{\tau}$ can be expressed in Einstein notation as

$$\nabla \cdot \boldsymbol{\tau} = \frac{\partial \tau_{ij}}{\partial x_j},$$

$$\boldsymbol{\tau} \cdot \nabla f = \tau_{ij} \frac{\partial f}{\partial x_j},$$

$$\mathbf{g} \cdot \boldsymbol{\tau} \cdot \nabla f = g_i \tau_{ij} \frac{\partial f}{\partial x_j},$$

$$\boldsymbol{\tau} : \nabla \mathbf{g} = \tau_{ij} \frac{\partial g_i}{\partial x_j}.$$

where f is a scalar and $\mathbf{g}$ a vector. In these notes we'll mostly be using indices i and j for FE expansions, rather than for Einstein notation.

1.2 Lagrangian finite elements

We introduce a Lagrangian basis function $\Phi_i^+ = \Phi_i^+(t, \mathbf{y})$ and an Eulerian basis function $\Phi_i = \Phi_i(t, \mathbf{x})$. These are related to each other as any other Lagrangian-Eulerian pair, namely

$$\Phi_i^+(t, \mathbf{y}) = \Phi_i(t, \mathbf{x}^+(t, \mathbf{y})). \tag{1.7}$$

We now introduce the Lagrangian variable $f^+ = f^+(t, \mathbf{y})$ and the Eulerian counterpart $f = f(t, \mathbf{x})$, and they also satisfy

$$f^+(t, \mathbf{y}) = f(t, \mathbf{x}^+(t, \mathbf{y})). \tag{1.8}$$

The expansion of an Eulerian variable in terms of basis functions is as follows

$$f = \sum_i^n F_i \Phi_i, \tag{1.9}$$

where $F_i = F_i(t)$. Plugging in $\mathbf{x}^+$ for $\mathbf{x}$ in the above, and using eqs. (1.7) and (1.8) gives

$$f^+ = \sum_i^n F_i \Phi_i^+. \tag{1.10}$$

Thus, both the Lagrangian and Eulerian variables share the same finite-element coefficients F_i.

As shown in my fluid mechanics notes, we also have

$$\frac{\partial \Phi_i^+}{\partial t} = \left(\frac{\partial \Phi_i}{\partial t} + \mathbf{u} \cdot \nabla \Phi_i \right)_{\mathbf{x}=\mathbf{x}^+}, \tag{1.11}$$

where $\mathbf{u} = \mathbf{u}(t, \mathbf{x})$ is the Eulerian counterpart to $\mathbf{u}^+$. We'll introduce the restriction that Φ_i^+ is constant in time, that is $\partial \Phi_i^+ / \partial t = 0$, which gives

$$\frac{\partial \Phi_i}{\partial t} + \mathbf{u} \cdot \nabla \Phi_i = 0. \tag{1.12}$$

Thus, F_i in eq. (1.10) accounts for the time dependence of F^+, whereas Φ_i^+ accounts for the dependence on $\mathbf{y}$.

1.3 Finite element expansion

We introduce the coefficients $\hat{\mathbf{x}}_i = \hat{\mathbf{x}}_i(t)$, $\hat{\mathbf{u}}_i = \hat{\mathbf{u}}_i(t)$ and $\hat{e}_i = \hat{e}_i(t)$, as well as the Lagrangian basis functions $\phi_i^+ = \phi_i^+(\mathbf{y}) \in L^2$, and $w_i^+ = w_i^+(\mathbf{y}) \in H^1$. We note that $\hat{\mathbf{x}}_i$ and $\hat{\mathbf{u}}_i$ are each vectors, e.g., the components of $\hat{\mathbf{u}}_i$ are $\hat{u}_{i,\alpha} = \hat{u}_{i,\alpha}(t)$ for $\alpha = x, y, z$. We also note that ϕ_i^+ and w_i^+ have Eulerian counterparts $\phi_i = \phi_i(t, \mathbf{x})$ and $w_i = w_i(t, \mathbf{x})$, respectively. The coefficients are used in the following expansions

$$\mathbf{x}^+ = \sum_j^{N_w} \hat{\mathbf{x}}_j w_j^+, \tag{1.13}$$

$$\mathbf{u}^+ = \sum_j^{N_w} \hat{\mathbf{u}}_j w_j^+, \tag{1.14}$$

$$e_\alpha^+ = \sum_j^{N_\phi} \hat{e}_{\alpha,j} \phi_j^+. \tag{1.15}$$

We note that the expansion coefficients are the same for the Lagrangian and Eulerian variables, as shown in section 1.2. For example, for the Eulerian velocity, we have

$$\mathbf{u} = \sum_j^{N_w} \hat{\mathbf{u}}_j w_j. \tag{1.16}$$

1.4 Semi-discrete Lagrangian governing equations

1.4.1 Position and Jacobian

Plugging in eqs. (1.13) and (1.14) in eq. (1.2) gives

$$\sum_j^{N_w} \frac{d\hat{\mathbf{x}}_j}{dt} w_j^+ = \sum_j^{N_w} \hat{\mathbf{u}}_j w_j^+.$$

To satisfy the equation above, we'll require

$$\frac{d\hat{\mathbf{x}}_j^+}{dt} = \hat{\mathbf{u}}_j.$$

We now introduce the vectors $\mathbf{X}$ and $\mathbf{U}$, whose components are $\hat{\mathbf{x}}_i$ and $\hat{\mathbf{u}}_i$, respectively. Thus, the above is written as

$$\frac{d\mathbf{X}}{dt} = \mathbf{U}. \tag{1.17}$$

1.4.2 Density

We introduce the Jacobian matrix $\mathbf{J}^+ = \mathbf{J}^+(t, \mathbf{y})$, which is defined as

$$\mathbf{J}^+ = \frac{\partial \mathbf{x}^+}{\partial \mathbf{y}}. \tag{1.18}$$

It's determinant is denoted by $J^+ = J^+(t, \mathbf{y})$, and it satisfies the following equation

$$\frac{\partial J^+}{\partial t} = J^+ \left(\nabla \cdot \mathbf{u}\right)_{\mathbf{x}=\mathbf{x}^+}. \tag{1.19}$$

Thus, Equation (1.4) can be re-written as

$$\frac{1}{\eta_\alpha^+ \rho_\alpha^+} \frac{\partial \eta_\alpha^+ \rho_\alpha^+}{\partial t} = -\frac{1}{J^+} \frac{\partial J^+}{\partial t},$$

or

$$\frac{\partial \eta_\alpha^+ \rho_\alpha^+ J_\alpha^+}{\partial t} = 0. \tag{1.20}$$

Since $J^+ = 1$ at the initial time, we obtain the density according to

$$\eta_\alpha^+ \rho_\alpha^+ = \frac{\eta_{\alpha,0}^+ \rho_{\alpha,0}^+}{J^+}, \tag{1.21}$$

where $\rho_0^+ = \rho^+(0, \mathbf{y})$. Note that summing over all α gives

$$\rho^+ = \frac{\rho_0^+}{J^+}. \tag{1.22}$$

To compute J^+, we first plug in eq. (1.13) in the definition of the Jacobian matrix, which gives

$$\mathbf{J}^+ = \frac{\partial}{\partial \mathbf{y}} \sum_j^{N_w} \hat{\mathbf{x}}_j w_j^+ = \sum_j^{N_w} \hat{\mathbf{x}}_j \nabla_{\mathbf{y}} w_j^+.$$

We then simply compute the determinant of the above to obtain J^+. Note that for any function $\mathbf{x}^+$ and its corresponding $\mathbf{u}^+$, whether it be an exact analytical expression or a finite-element expansion as given by eq. (1.13), one obtains eq. (1.19). Thus, the derivation of eq. (1.20) from eq. (1.4) still holds whether one plans to represent J^+ using an analytical expression or a finite-element expansion.

1.4.3 Velocity

Plugging in eq. (1.22) in eq. (1.5) we get

$$\rho_0^+ \frac{\partial \mathbf{u}^+}{\partial t} = \left(\nabla \cdot \sum_\alpha \eta_\alpha \boldsymbol{\sigma}_\alpha\right)_{\mathbf{x}=\mathbf{x}^+} J^+.$$

We then multiply both sides of the above by the basis functions for velocity and integrate over all space to obtain

$$\int_{\Omega_0} \rho_0^+ \frac{\partial \mathbf{u}^+}{\partial t} w_i^+ \, dV_y = \int_{\Omega_0} \left(\nabla \cdot \sum_\alpha \eta_\alpha \boldsymbol{\sigma}_\alpha\right)_{\mathbf{x}=\mathbf{x}^+} w_i^+ J^+ \, dV_y.$$

For the left-hand side we have

$$\begin{aligned}\int_{\Omega_0} \rho_0^+ \frac{\partial \mathbf{u}^+}{\partial t} w_i^+ \, dV_y &= \int_{\Omega_0} \rho_0^+ \sum_j^{N_w} \frac{d\hat{\mathbf{u}}_j}{dt} w_j^+ w_i^+ \, dV_y, \\ &= \sum_j^{N_w} \frac{d\hat{\mathbf{u}}_j}{dt} \int_{\Omega_0} \rho_0^+ w_i^+ w_j^+ \, dV_y, \\ &= \sum_j^{N_w} \frac{d\hat{\mathbf{u}}_j}{dt} m_{\mathcal{V},ij},\end{aligned}$$

where

$$m_{\mathcal{V},ij} = \int_{\Omega_0} \rho_0^+ w_i^+ w_j^+ \, dV_y \tag{1.23}$$

is a mass bilinear form (which is independent of time). For the right-hand side we have

$$\begin{aligned}\int_{\Omega_0} \left(\nabla \cdot \sum_\alpha \eta_\alpha \boldsymbol{\sigma}_\alpha \right)_{\mathbf{x}=\mathbf{x}^+} w_i^+ J^+ \, dV_y &= \int_{\Omega_0} \left[\nabla \cdot \left(\sum_\alpha \eta_\alpha \boldsymbol{\sigma}_\alpha \right) w_i \right]_{\mathbf{x}=\mathbf{x}^+} J^+ \, dV_y \\ &= \int_{\Omega^+} \nabla \cdot \left(\sum_\alpha \eta_\alpha \boldsymbol{\sigma}_\alpha \right) w_i \, dV_x \\ &= - \int_{\Omega^+} \sum_\alpha \eta_\alpha \boldsymbol{\sigma}_\alpha \cdot \nabla w_i \, dV_x.\end{aligned}$$

The second equality above follows from integration by substitution. Combining results we have

$$\sum_j^{N_w} \frac{d\hat{\mathbf{u}}_j}{dt} m_{\mathcal{V},ij} = - \int_{\Omega^+} \sum_\alpha \eta_\alpha \boldsymbol{\sigma}_\alpha \cdot \nabla w_i \, dV_x. \tag{1.24}$$

We introduce the matrix $\mathbf{M}_\mathcal{V}$, whose components are $m_{\mathcal{V},ij}$. Thus, the left-hand side of eq. (1.24) can be written as $\mathbf{M}_\mathcal{V} \, d\mathbf{U}/dt$. We also introduce the vector bilinear form

$$\mathbf{f}_{ij,\alpha} = \int_{\Omega^+} \eta_\alpha \boldsymbol{\sigma}_\alpha \cdot \nabla w_i \phi_j \, dV_x. \tag{1.25}$$

This is a *vector* bilinear form since $\mathbf{f}_{ij,\alpha}$ has components $f_{ij,\alpha,a} = f_{ij,\alpha,a}(t)$, for $a = x, y, z$, where a denotes the first index of $\boldsymbol{\sigma}_\alpha$. We introduce the force matrix $\mathbf{F}_\alpha$, whose components are $\mathbf{f}_{ij,\alpha}$. We also expand the field with constant value of one as follows

$$1 = \sum_i^{N_\phi} \hat{1}_i \phi_i.$$

If we define the vector $\hat{\mathbf{1}}$ as that with components $\hat{1}_i$, we can show that

$$\begin{aligned}
\mathbf{F}_\alpha \hat{\mathbf{1}} &= \sum_j^{N_\phi} \mathbf{f}_{ij,\alpha} \hat{1}_j \\
&= \sum_j^{N_\phi} \int_{\Omega^+} \eta_\alpha \boldsymbol{\sigma}_\alpha \cdot \nabla w_i \phi_j \, dV_x \hat{1}_j \\
&= \int_{\Omega^+} \eta_\alpha \boldsymbol{\sigma}_\alpha \cdot \nabla w_i \left(\sum_j^{N_\phi} \hat{1}_j \phi_j \right) dV_x \\
&= \int_{\Omega^+} \eta_\alpha \boldsymbol{\sigma}_\alpha \cdot \nabla w_i \, dV_x.
\end{aligned}$$

Thus, eq. (1.24) can now be written as

$$\mathbf{M}_\mathcal{V} \frac{d\mathbf{U}}{dt} = -\sum_\alpha \mathbf{F}_\alpha \hat{\mathbf{1}}. \tag{1.26}$$

We note that since both the Lagrangian and Eulerian velocities share the same coefficients $\mathbf{U}$, we now have a solution for both.

1.4.4 Energy

Plugging in eq. (1.21) in eq. (1.6) we get

$$\eta^+_{\alpha,0} \rho^+_{\alpha,0} \frac{\partial e^+_\alpha}{\partial t} = (\eta_\alpha \boldsymbol{\sigma}_\alpha : \nabla \mathbf{u})_{\mathbf{x}=\mathbf{x}^+} J^+ - (\bar{p}\alpha_\alpha)_{\mathbf{x}=\mathbf{x}^+} J^+.$$

We then multiply both sides of the above by the basis functions for energy and integrate over all space to obtain

$$\int_{\Omega_0} \eta^+_{\alpha,0} \rho^+_{\alpha,0} \frac{\partial e^+_\alpha}{\partial t} \phi^+_i \, dV_y = \int_{\Omega_0} (\eta_\alpha \boldsymbol{\sigma}_\alpha : \nabla \mathbf{u})_{\mathbf{x}=\mathbf{x}^+} \phi^+_i J^+ \, dV_y - \int_{\Omega_0} (\bar{p}\alpha_\alpha)_{\mathbf{x}=\mathbf{x}^+} \phi^+_i J^+ \, dV_y.$$

For the left-hand side we have

$$\begin{aligned}
\int_{\Omega_0} \eta^+_{\alpha,0} \rho^+_{\alpha,0} \frac{\partial e^+_\alpha}{\partial t} \phi^+_i \, dV_y &= \int_{\Omega_0} \eta^+_{\alpha,0} \rho^+_{\alpha,0} \sum_j^{N_\phi} \frac{d\hat{e}_{\alpha,j}}{dt} \phi^+_j \phi^+_i \, dV_y, \\
&= \sum_j^{N_\phi} \frac{d\hat{e}_{\alpha,j}}{dt} \int_{\Omega_0} \eta^+_{\alpha,0} \rho^+_{\alpha,0} \phi^+_j \phi^+_i \, dV_y, \\
&= \sum_j^{N_\phi} \frac{d\hat{e}_{\alpha,j}}{dt} m_{\mathcal{E},ij,\alpha}
\end{aligned}$$

where

$$m_{\mathcal{E},ij,\alpha} = \int_{\Omega_0} \eta^+_{\alpha,0} \rho^+_{\alpha,0} \phi^+_j \phi^+_i \, dV_y \tag{1.27}$$

is a mass bilinear form (which is independent of time). For the first term on right-hand side we have

$$\int_{\Omega_0} (\eta_\alpha \boldsymbol{\sigma}_\alpha : \nabla \mathbf{u})_{\mathbf{x}=\mathbf{x}^+} \phi_i^+ J^+ \, dV_y = \int_{\Omega_0} (\eta_\alpha \boldsymbol{\sigma}_\alpha : \nabla \mathbf{u} \phi_i)_{\mathbf{x}=\mathbf{x}^+} J^+ \, dV_y$$
$$= \int_{\Omega^+} \eta_\alpha \boldsymbol{\sigma}_\alpha : \nabla \mathbf{u} \phi_i \, dV_x.$$

For the second term on the right hand side we have

$$\int_{\Omega_0} (\bar{p}\alpha_\alpha)_{\mathbf{x}=\mathbf{x}^+} \phi_i^+ J^+ \, dV_y = \int_{\Omega_0} (\bar{p}\alpha_\alpha \phi_i)_{\mathbf{x}=\mathbf{x}^+} J^+ \, dV_y$$
$$= \int_{\Omega^+} \bar{p}\alpha_\alpha \phi_i \, dV_x.$$

Combining results we have

$$\sum_j^{N_\phi} \frac{d\hat{e}_{\alpha,j}}{dt} m_{\mathcal{E},ij} = \int_{\Omega^+} \eta_\alpha \boldsymbol{\sigma}_\alpha : \nabla \mathbf{u} \phi_i \, dV_x - \int_{\Omega^+} \bar{p}\alpha_\alpha \phi_i \, dV_x.$$

We no show that

$$\eta_\alpha \boldsymbol{\sigma}_\alpha : \nabla \mathbf{u} = \eta_\alpha \boldsymbol{\sigma}_\alpha : \nabla \left(\sum_k^{N_w} \hat{\mathbf{u}}_k w_k \right) = \sum_k^{N_w} \hat{\mathbf{u}}_k \cdot \eta_\alpha \boldsymbol{\sigma}_\alpha \cdot \nabla w_k,$$

and hence the previous result is written as

$$\sum_j^{N_\phi} \frac{d\hat{e}_{\alpha,j}}{dt} m_{\mathcal{E},ij} = \sum_k^{N_w} \hat{\mathbf{u}}_k \cdot \int_{\Omega^+} \eta_\alpha \boldsymbol{\sigma}_\alpha \cdot \nabla w_k \phi_i \, dV_x - \int_{\Omega^+} \bar{p}\alpha_\alpha \phi_i \, dV_x.$$

The above is finally re-written as

$$\sum_j^{N_\phi} \frac{d\hat{e}_{\alpha,j}}{dt} m_{\mathcal{E},ij} = \sum_k^{N_w} \hat{\mathbf{u}}_k \cdot \mathbf{f}_{ki,\alpha} - c_{\alpha,i}, \tag{1.28}$$

where

$$c_{\alpha,i} = \int_{\Omega^+} \bar{p}\alpha_\alpha \phi_i \, dV_x \tag{1.29}$$

Note that in eq. (1.28) there is a dot product in first term of the right-hand side. To see this, we expand this term as follows

$$\sum_k^{N_w} \hat{\mathbf{u}}_k \cdot \mathbf{f}_{ki,\alpha} = \sum_k^{N_w} \sum_{a=x,y,z} \hat{u}_{k,a} f_{ki,\alpha,a}.$$

We now introduce the vector $\mathbf{E}_\alpha$ whose components are $\hat{e}_{\alpha,i}$, the matrix $\mathbf{M}_{\mathcal{E},\alpha}$ whose components are $m_{\mathcal{E},ij,\alpha}$, and the vector $\mathbf{C}_\alpha$ whose components are $c_{\alpha,i}$. Thus, eq. (1.28) can be succinctly written as

$$\mathbf{M}_{\mathcal{E},\alpha} \frac{d\mathbf{E}_\alpha}{dt} = \mathbf{F}_\alpha^T \cdot \mathbf{U} - \mathbf{C}_\alpha. \tag{1.30}$$

Note again that the first term on the right-hand side above has a matrix-vector product *and* a dot product. We also note that since both the Lagrangian and Eulerian internal energies share the same coefficients $\mathbf{E}_\alpha$, we now have a solution for both.

1.5 Momentum and energy conservation

We'll now define the internal energy $IE = IE(t)$, the kinetic energy $KE = KE(t)$, and the momentum $P_{\mathbf{n}} = P_{\mathbf{n}}(t)$ along a constant $\mathbf{n}$ direction.

$$\begin{aligned}
IE &= \int_{\Omega^+} \rho e \, dV_x \\
&= \int_{\Omega_0} \rho^+ e^+ J^+ \, dV_y \\
&= \int_{\Omega_0} \rho_0^+ e^+ \, dV_y \\
&= \int_{\Omega_0} \rho_0^+ \sum_j^{N_\phi} \hat{e}_j \phi_j^+ \, dV_y \\
&= \int_{\Omega_0} \rho_0^+ \sum_j^{N_\phi} \hat{e}_j \phi_j^+ \left(\sum_i^{N_\phi} \hat{1}_i \phi_i^+ \right) dV_y \\
&= \sum_i^{N_\phi} \sum_j^{N_\phi} \hat{1}_i \int_{\Omega_0} \rho_0^+ \phi_i^+ \phi_j^+ \, dV_y \hat{e}_j \\
&= \sum_i^{N_\phi} \sum_j^{N_\phi} \hat{1}_i m_{\mathcal{E},ij} \hat{e}_j \\
&= \hat{\mathbf{1}}^T \mathbf{M}_{\mathcal{E}} \mathbf{E}
\end{aligned} \tag{1.31}$$

$$\begin{aligned}
KE &= \int_{\Omega^+} \frac{1}{2} \rho \mathbf{u} \cdot \mathbf{u} \, dV_x \\
&= \int_{\Omega_0} \frac{1}{2} \rho^+ \mathbf{u}^+ \cdot \mathbf{u}^+ J^+ \, dV_y \\
&= \int_{\Omega_0} \frac{1}{2} \rho_0^+ \mathbf{u}^+ \cdot \mathbf{u}^+ \, dV_y \\
&= \int_{\Omega_0} \frac{1}{2} \rho_0^+ \left(\sum_i^{N_w} \hat{\mathbf{u}}_i w_i^+ \right) \cdot \left(\sum_j^{N_w} \hat{\mathbf{u}}_j w_j^+ \right) dV_y \\
&= \sum_i^{N_w} \sum_j^{N_w} \frac{1}{2} \hat{\mathbf{u}}_i \cdot \int_{\Omega_0} \rho_0^+ w_i^+ w_j^+ \, dV_y \hat{\mathbf{u}}_j \\
&= \sum_i^{N_w} \sum_j^{N_w} \frac{1}{2} \hat{\mathbf{u}}_i \cdot m_{\mathcal{V},ij} \hat{\mathbf{u}}_j \\
&= \frac{1}{2} \mathbf{U}^T \cdot \mathbf{M}_{\mathcal{V}} \mathbf{U}.
\end{aligned} \tag{1.32}$$

$$
\begin{aligned}
P_{\mathbf{n}} &= \int_{\Omega^+} \rho \mathbf{u} \cdot \mathbf{n} \, dV_x \\
&= \int_{\Omega_0} \rho^+ \mathbf{u}^+ \cdot \mathbf{n} J^+ \, dV_y \\
&= \int_{\Omega_0} \rho_0^+ \mathbf{u}^+ \cdot \mathbf{n} \, dV_y \\
&= \int_{\Omega_0} \rho_0^+ \left(\sum_j^{N_w} \hat{\mathbf{u}}_j w_j^+ \right) \cdot \left(\sum_i^{N_w} \hat{\mathbf{n}}_i w_i^+ \right) \, dV_y \\
&= \sum_i^{N_w} \sum_j^{N_w} \hat{\mathbf{n}}_i \cdot \int_{\Omega_0} \rho_0^+ w_i^+ w_j^+ \, dV_y \hat{\mathbf{u}}_j \\
&= \sum_i^{N_w} \sum_j^{N_w} \hat{\mathbf{n}}_i \cdot m_{\mathcal{V},ij} \hat{\mathbf{u}}_j \\
&= \mathbf{N}^T \cdot \mathbf{M}_{\mathcal{V}} \mathbf{U}.
\end{aligned} \tag{1.33}
$$

The total energy is conserved, as shown below

$$
\begin{aligned}
\frac{d}{dt}(IE + KE) &= \hat{\mathbf{1}}^T \mathbf{M}_{\mathcal{E}} \frac{d\mathbf{E}}{dt} + \mathbf{U}^T \cdot \mathbf{M}_{\mathcal{V}} \frac{d\mathbf{U}}{dt} \\
&= \hat{\mathbf{1}}^T \mathbf{F}^T \cdot \mathbf{U} - \mathbf{U}^T \cdot \mathbf{F} \hat{\mathbf{1}} \\
&= 0.
\end{aligned} \tag{1.34}
$$

The momentum along a constant direction is conserved, as shown below

$$
\begin{aligned}
\frac{dP_{\mathbf{n}}}{dt} &= \mathbf{N}^T \cdot \mathbf{M}_{\mathcal{V}} \frac{d\mathbf{U}}{dt} \\
&= -\mathbf{N}^T \cdot \mathbf{F} \hat{\mathbf{1}} \\
&= -\sum_i^{N_w} \sum_j^{N_\phi} \hat{\mathbf{n}}_i \cdot \mathbf{f}_{ij} \hat{1}_j \\
&= -\sum_i^{N_w} \sum_j^{N_\phi} \hat{\mathbf{n}}_i \cdot \int_{\Omega^+} \boldsymbol{\sigma} \cdot \nabla w_i \phi_j \, dV_x \hat{1}_j \\
&= -\int_{\Omega^+} \boldsymbol{\sigma} : \nabla \mathbf{n} \, dV_x \\
&= 0.
\end{aligned} \tag{1.35}
$$

1.6 The reference element

We introduce the reference element as the unit square in 2D or the unit cube in 3D. The domain of this reference element is labelled as Ω_r and it doesn't change with time. We introduce the function

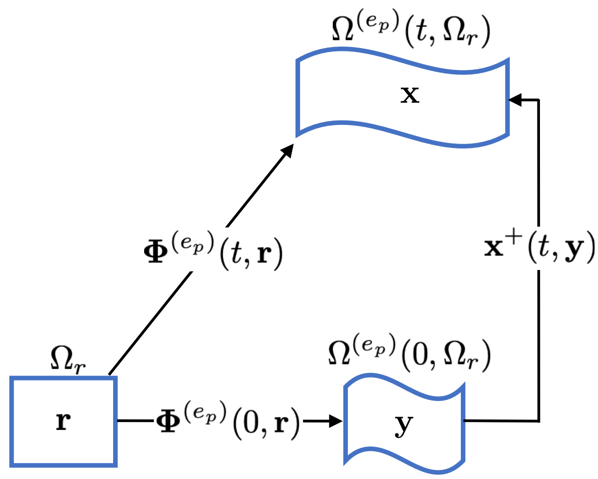

Figure 1.1: Schematic of the three domains Ω_r, $\Omega^{(e_p)}(t,\Omega_r)$, $\Omega^{(e_p)}(0,\Omega_r)$.

$\boldsymbol{\Phi}^{(e_p)} = \boldsymbol{\Phi}^{(e_p)}(t,\mathbf{r})$, which maps from points $\mathbf{r}$ in Ω_r to points in the finite element e_p of the physical space. The evolving domain of the finite element e_p is giving by the function $\Omega^{(e_p)} = \Omega^{(e_p)}(t,\Omega_r)$. A depiction of these domains and their mappings is shown in fig. 1.1. Whereas for Ω^{+} we had $\Omega^{+}(0,\Omega_0) = \Omega_0$, for $\Omega^{(e_p)}$ the analogue does not hold, that is, $\Omega^{(e_p)}(0,\Omega_r) \neq \Omega_r$.

The mapping functions $\boldsymbol{\Phi}^{(e_p)}$ and $\mathbf{x}^{+}$ are related to each other as follows

$$\boldsymbol{\Phi}^{(e_p)}(t,\mathbf{r}) = \mathbf{x}^{+}(t,\boldsymbol{\Phi}^{(e_p)}(0,\mathbf{r})). \tag{1.36}$$

The Jacobian $\mathbf{J}^{(e_p)} = \mathbf{J}^{(e_p)}(t,\mathbf{r})$ is defined as

$$\mathbf{J}^{(e_p)} = \frac{\partial \boldsymbol{\Phi}^{(e_p)}}{\partial \mathbf{r}}, \tag{1.37}$$

with its determinant labeled as $J^{(e_p)} = J^{(e_p)}(t,\mathbf{r})$. Using eq. (1.36) in the definition of $\mathbf{J}^{(e_p)}$ we get

$$\begin{aligned}\mathbf{J}^{(e_p)} &= \left(\frac{\partial \mathbf{x}^{+}}{\partial \mathbf{y}}\right)_{\mathbf{y}=\boldsymbol{\Phi}^{(e_p)}(0,\mathbf{r})} \frac{\partial \boldsymbol{\Phi}^{(e_p)}(0,\mathbf{r})}{\partial \mathbf{r}} \\ &= \left(\mathbf{J}^{+}\right)_{\mathbf{y}=\boldsymbol{\Phi}^{(e_p)}(0,\mathbf{r})} \mathbf{J}_0^{(e_p)},\end{aligned}$$

where $\mathbf{J}_0^{(e_p)} = \mathbf{J}^{(e_p)}(0,\mathbf{r})$. Taking the determinant of the above gives

$$J^{(e_p)} = \left(J^{+}\right)_{\mathbf{y}=\boldsymbol{\Phi}^{(e_p)}(0,\mathbf{r})} J_0^{(e_p)}, \tag{1.38}$$

where $J_0^{(e_p)} = J^{(e_p)}(0,\mathbf{r})$.

As a reminder, a Lagrangian variable $f^{+} = f^{+}(t,\mathbf{y})$ is related to $f = f(t,\mathbf{x})$ according to

$$f^{+}(t,\mathbf{y}) = f(t,\mathbf{x}^{+}(t,\mathbf{y})).$$

In an analogous manner, $f^{(e_p)} = f^{(e_p)}(t,\mathbf{r})$ is related to $f = f(t,\mathbf{x})$ according to

$$f^{(e_p)}(t,\mathbf{r}) = f(t,\boldsymbol{\Phi}^{(e_p)}(t,\mathbf{r})). \tag{1.39}$$

Examples of these reference-element functions include those for density $\rho^{(e_p)} = \rho^{(e_p)}(t, \mathbf{r})$, velocity $\mathbf{u}^{(e_p)} = \mathbf{u}^{(e_p)}(t, \mathbf{r})$, and internal energy $e^{(e_p)} = e^{(e_p)}(t, \mathbf{r})$. Using integration by substitution and then eq. (1.39) we show

$$\begin{aligned}\int_{\Omega^{(e_p)}} f dV_x &= \int_{\Omega_r} f(t, \mathbf{\Phi}^{(e_p)}(t, \mathbf{r}))J^{(e_p)}\, dV_r \\ &= \int_{\Omega_r} f^{(e_p)} J^{(e_p)}\, dV_r.\end{aligned}$$

In other words, integrals over elements at any time can be computed as integrals over the reference space.

If the integrand contains a derivative, a bit of extra care is required. To show this, we'll use index notation for the sake of clarity. Consider as an example a term of the form

$$(\boldsymbol{\sigma} \cdot \nabla f)_{\mathbf{x}=\mathbf{\Phi}^{(e_p)}} = \left(\sigma_{ij} \frac{\partial f}{\partial x_j}\right)_{\mathbf{x}=\mathbf{\Phi}^{(e_p)}} = \sigma_{ij}^{(e_p)} \left(\frac{\partial f}{\partial x_j}\right)_{\mathbf{x}=\mathbf{\Phi}^{(e_p)}}.$$

We first note that

$$\frac{\partial f^{(e_p)}}{\partial r_k} = \left(\frac{\partial f}{\partial x_i}\right)_{\mathbf{x}=\mathbf{\Phi}^{(e_p)}} \frac{\partial x_i^{(e_p)}}{\partial r_k} = \left(\frac{\partial f}{\partial x_i}\right)_{\mathbf{x}=\mathbf{\Phi}^{(e_p)}} J_{ik}^{(e_p)}.$$

Upon multiplying both sides by the inverse of $\mathbf{J}^{(e_p)}$, we get

$$\left(\frac{\partial f}{\partial x_j}\right)_{\mathbf{x}=\mathbf{\Phi}^{(e_p)}} = \frac{\partial f^{(e_p)}}{\partial r_k} \left(J^{(e_p)}\right)_{kj}^{-1}.$$

Thus, we now have

$$(\boldsymbol{\sigma} \cdot \nabla f)_{\mathbf{x}=\mathbf{\Phi}^{(e_p)}} = \sigma_{ij}^{(e_p)} \frac{\partial f^{(e_p)}}{\partial r_k} \left(J^{(e_p)}\right)_{kj}^{-1} = \sigma_{ij}^{(e_p)} \left[\left(J^{(e_p)}\right)^{-1}\right]_{jk}^{T} \frac{\partial f^{(e_p)}}{\partial r_k}.$$

In vector/tensor notation, the above is written as

$$(\boldsymbol{\sigma} \cdot \nabla f)_{\mathbf{x}=\mathbf{\Phi}^{(e_p)}} = \boldsymbol{\sigma}^{(e_p)} \cdot \left[\left(\mathbf{J}^{(e_p)}\right)^{-1}\right]^{T} \cdot \nabla_{\mathbf{r}} f^{(e_p)}.$$

Thus, for the force matrix $\mathbf{f}_{ij}$ we can now write

$$\begin{aligned}\int_{\Omega^{(e_p)}} \boldsymbol{\sigma} \cdot \nabla w_i \phi_j \, dV_x &= \int_{\Omega_{\mathbf{r}}} (\boldsymbol{\sigma} \cdot \nabla w_i \phi_j)_{\mathbf{x}=\mathbf{\Phi}^{(e_p)}} J^{(e_p)}\, dV_r \\ &= \int_{\Omega_{\mathbf{r}}} \boldsymbol{\sigma}^{(e_p)} \cdot \left[\left(\mathbf{J}^{(e_p)}\right)^{-1}\right]^{T} \cdot \nabla_{\mathbf{r}} w_i^{(e_p)} \phi_j^{(e_p)} J^{(e_p)}\, dV_r.\end{aligned}$$

We also note that we can evaluate eq. (1.21) at $\mathbf{y} = \mathbf{\Phi}^{(e_p)}(0, \mathbf{r})$ to obtain

$$\rho^{(e_p)} = \frac{\rho_0^{(e_p)} J_0^{(e_p)}}{J^{(e_p)}}. \tag{1.40}$$

As with the other variables, we can define a reference basis function $w^{(e_p)}$ so that it satisfies

$$w_j^{(e_p)}(t,\mathbf{r}) = w_j^{+}(t,\mathbf{\Phi}^{(e_p)}(0,\mathbf{r})). \tag{1.41}$$

Now, as mentioned earlier, the Lagrangian basis functions are independent of time, and as a result the reference basis functions are so as well. That is, $w^{(e_p)} = w^{(e_p)}(\mathbf{r})$. Consider the expansion in eq. (1.13). Plugging in $\mathbf{\Phi}^{(e_p)}(0,\mathbf{r})$ for $\mathbf{y}$ gives

$$\mathbf{\Phi}^{(e_p)} = \sum_j^{N_w} \hat{\mathbf{x}}_j w_j^{(e_p)}. \tag{1.42}$$

Thus, both the Lagrangian and reference variables share the same finite-element coefficients.

1.7 Temporal integration

We now integrate forward in time the semi-discrete eqs. (1.17), (1.26) and (1.30), which we repeat below for convenience

$$\mathbf{M}_{\mathcal{V}}\frac{d\mathbf{U}}{dt} = -\mathbf{F}\hat{\mathbf{1}}. \tag{1.26}$$

$$\mathbf{M}_{\mathcal{E}}\frac{d\mathbf{E}}{dt} = \mathbf{F}^T\cdot\mathbf{U}. \tag{1.30}$$

$$\frac{d\mathbf{X}}{dt} = \mathbf{U}. \tag{1.17}$$

The equations are integrated using the RK2-average scheme of Dobrev et al. [2012], which consists of the following for the first stage

$$\begin{aligned}
\mathbf{U}^{n+1/2} &= \mathbf{U}^n - \frac{\Delta t}{2}\left(\mathbf{M}_{\mathcal{V}}\right)^{-1}\mathbf{F}^n\hat{\mathbf{1}},\\
\mathbf{E}^{n+1/2} &= \mathbf{E}^n + \frac{\Delta t}{2}\left(\mathbf{M}_{\mathcal{E}}\right)^{-1}\left(\mathbf{F}^n\right)^T\cdot\mathbf{U}^{n+1/2},\\
\mathbf{X}^{n+1/2} &= \mathbf{X}^n + \frac{\Delta t}{2}\mathbf{U}^{n+1/2},
\end{aligned} \tag{1.43}$$

and the following for the second stage

$$\begin{aligned}
\mathbf{U}^{n+1} &= \mathbf{U}^n - \Delta t\left(\mathbf{M}_{\mathcal{V}}\right)^{-1}\mathbf{F}^{n+1/2}\hat{\mathbf{1}},\\
\mathbf{E}^{n+1} &= \mathbf{E}^n + \Delta t\left(\mathbf{M}_{\mathcal{E}}\right)^{-1}\left(\mathbf{F}^{n+1/2}\right)^T\cdot\bar{\mathbf{U}}^{n+1/2},\\
\mathbf{X}^{n+1} &= \mathbf{X}^n + \Delta t\bar{\mathbf{U}}^{n+1/2}.
\end{aligned} \tag{1.44}$$

In the above, $\bar{\mathbf{U}}^{n+1/2} = \left(\mathbf{U}^n + \mathbf{U}^{n+1}\right)/2$. In particular, this scheme is used since it conserves total energy, that is, $(IE+KE)^{n+1} - (IE+KE)^n = 0$. To prove this we first show that for the internal energy we have

$$\begin{aligned}
IE^{n+1} - IE^n &= \hat{\mathbf{1}}^T\mathbf{M}_{\mathcal{E}}\left(\mathbf{E}^{n+1} - \mathbf{E}^n\right)\\
&= \Delta t\hat{\mathbf{1}}^T\left(\mathbf{F}^{n+1/2}\right)^T\cdot\bar{\mathbf{U}}^{n+1/2}
\end{aligned} \tag{1.45}$$

For the kinetic energy we have

$$
\begin{aligned}
KE^{n+1} - KE^{n} &= \frac{1}{2}\left[\left(\mathbf{U}^{n+1}\right)^{T}\cdot\mathbf{M}_{\mathcal{V}}\mathbf{U}^{n+1} - \left(\mathbf{U}^{n}\right)^{T}\cdot\mathbf{M}_{\mathcal{V}}\mathbf{U}^{n}\right]\\
&= \frac{1}{2}\left[\left(\mathbf{U}^{n+1}\right)^{T}\mathbf{M}_{\mathcal{V}}\cdot\mathbf{U}^{n+1} - \left(\mathbf{U}^{n}\right)^{T}\mathbf{M}_{\mathcal{V}}\cdot\mathbf{U}^{n}\right]\\
&= \frac{1}{2}\left(\mathbf{U}^{n+1} - \mathbf{U}^{n}\right)^{T}\mathbf{M}_{\mathcal{V}}\cdot\left(\mathbf{U}^{n+1} + \mathbf{U}^{n}\right)\\
&= \left(\mathbf{U}^{n+1} - \mathbf{U}^{n}\right)^{T}\mathbf{M}_{\mathcal{V}}\cdot\bar{\mathbf{U}}^{n+1/2}\\
&= \left[-\Delta t\left(\mathbf{M}_{\mathcal{V}}\right)^{-1}\mathbf{F}^{n+1/2}\hat{\mathbf{1}}\right]^{T}\mathbf{M}_{\mathcal{V}}\cdot\bar{\mathbf{U}}^{n+1/2}\\
&= -\Delta t\hat{\mathbf{1}}^{T}\left(\mathbf{F}^{n+1/2}\right)^{T}\left[\left(\mathbf{M}_{\mathcal{V}}\right)^{-1}\right]^{T}\mathbf{M}_{\mathcal{V}}\cdot\bar{\mathbf{U}}^{n+1/2}\\
&= -\Delta t\hat{\mathbf{1}}^{T}\left(\mathbf{F}^{n+1/2}\right)^{T}\left[\left(\mathbf{M}_{\mathcal{V}}\right)^{T}\right]^{-1}\mathbf{M}_{\mathcal{V}}\cdot\bar{\mathbf{U}}^{n+1/2}\\
&= -\Delta t\hat{\mathbf{1}}^{T}\left(\mathbf{F}^{n+1/2}\right)^{T}\left(\mathbf{M}_{\mathcal{V}}\right)^{-1}\mathbf{M}_{\mathcal{V}}\cdot\bar{\mathbf{U}}^{n+1/2}\\
&= -\Delta t\hat{\mathbf{1}}^{T}\left(\mathbf{F}^{n+1/2}\right)^{T}\cdot\bar{\mathbf{U}}^{n+1/2}. \qquad (1.46)
\end{aligned}
$$

Thus, adding eq. (1.45) and eq. (1.46) leads to total energy conservation.

Chapter 2

The Re-mesh Step

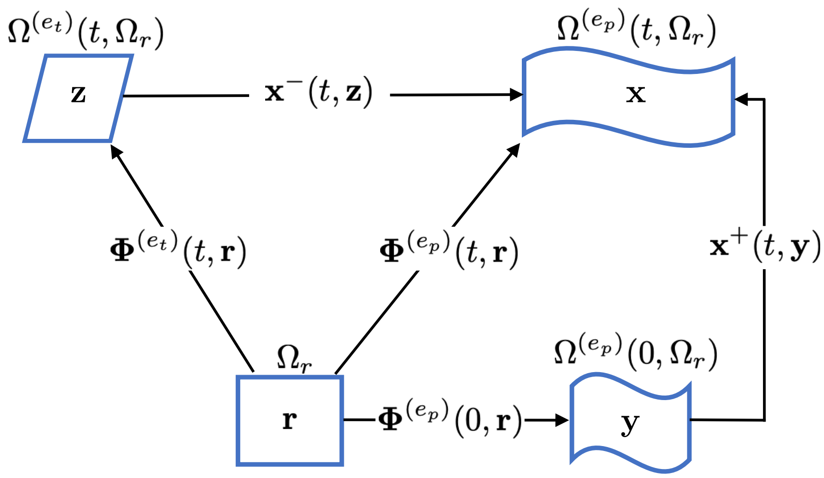

Figure 2.1: Schematic of the four domains Ω_r, $\Omega^{(e_p)}(t, \Omega_r)$, $\Omega^{(e_p)}(0, \Omega_r)$, $\Omega^{(e_t)}(t, \Omega_r)$.

We introduce a new space, the target space, which is divided into target elements, where each corresponds to a physical element e_p. Consider a mapping $\mathbf{\Phi}^{(e_t)} = \mathbf{\Phi}^{(e_t)}(t, \mathbf{r})$ from a point $\mathbf{r}$ in the reference element to a point in the target element. Also consider the mapping $\mathbf{x}^- = \mathbf{x}^-(t, \mathbf{z})$ from a point $\mathbf{z}$ in the target space to a point in the physical space. Note that $\mathbf{\Phi}^{(e_p)}$, $\mathbf{\Phi}^{(e_t)}$, and $\mathbf{x}^-$ are related to each other according to

$$\mathbf{\Phi}^{(e_p)}(t, \mathbf{r}) = \mathbf{x}^-(t, \mathbf{\Phi}^{(e_t)}(t, \mathbf{r})). \tag{2.1}$$

We define the Jacobeans as follows

$$\mathbf{J}^{(e_t)} = \frac{\partial \mathbf{\Phi}^{(e_t)}}{\partial \mathbf{r}}, \tag{2.2}$$

$$\mathbf{J}^- = \frac{\partial \mathbf{x}^-}{\partial \mathbf{z}}. \tag{2.3}$$

where $\mathbf{J}^{(e_t)} = \mathbf{J}^{(e_t)}(t, \mathbf{r})$ and $\mathbf{J}^- = \mathbf{J}^-(t, \mathbf{z})$. Taking the derivative of eq. (2.1) we get

$$\frac{\partial \mathbf{\Phi}^{(e_p)}}{\partial \mathbf{r}} = \left(\frac{\partial \mathbf{x}^-}{\partial \mathbf{z}}\right)_{\mathbf{z}=\mathbf{\Phi}^{(e_t)}} \frac{\partial \mathbf{\Phi}^{(e_t)}}{\partial \mathbf{r}},$$

which we write as

$$\mathbf{J}^{(e_p)} = \left(\mathbf{J}^{-}\right)_{\mathbf{z}=\mathbf{\Phi}^{(e_t)}} \mathbf{J}^{(e_t)}.$$

Multiplying both sides by the inverse of $\mathbf{J}^{(e_t)}$ we finally get

$$\left(\mathbf{J}^{-}\right)_{\mathbf{z}=\mathbf{\Phi}^{(e_t)}} = \mathbf{J}^{(e_p)} \left(\mathbf{J}^{(e_t)}\right)^{-1}. \tag{2.4}$$

Combining eq. (1.36) and eq. (2.1) we get

$$\mathbf{x}^{-}(t, \mathbf{\Phi}^{(e_t)}(t, \mathbf{r})) = \mathbf{x}^{+}(t, \mathbf{\Phi}^{(e_p)}(0, \mathbf{r})). \tag{2.5}$$

We also define a target basis function $w^{(e_t)} = w^{(e_t)}(t, \mathbf{z})$ so that it satisfies

$$w^{-}(t, \mathbf{\Phi}^{(e_t)}(t, \mathbf{r})) = w^{+}(t, \mathbf{\Phi}^{(e_p)}(0, \mathbf{r})). \tag{2.6}$$

Consider the expansion in eq. (1.13). Plugging in $\mathbf{\Phi}^{(e_p)}(0, \mathbf{r})$ for $\mathbf{y}$ gives

$$\mathbf{x}^{-}(t, \mathbf{\Phi}^{(e_t)}(t, \mathbf{r})) = \sum_{j}^{N_w} \hat{\mathbf{x}} w^{-}(t, \mathbf{\Phi}^{(e_t)}(t, \mathbf{r})).$$

Assuming this holds for any $\mathbf{\Phi}^{(e_t)}$ we get

$$\mathbf{x}^{-} = \sum_{j}^{N_w} \hat{\mathbf{x}} w^{-}. \tag{2.7}$$

Thus, both the Lagrangian and the target variables share the same finite-element coefficients.

To obtain the relaxed mesh, one minimizes the following function

$$F(\mathbf{X}) = \sum_{e_t \in \mathcal{M}_t} \int_{\Omega^{(e_t)}} \mu(\mathbf{J}^{-})\, dV_z \tag{2.8}$$

Chapter 3

The Re-map Step

Bibliography

V. A. Dobrev, T. V. Kolev, and R. N. Rieben. High-order curvilinear finite element methods for Lagrangian hydrodynamics. *SIAM Journal on Scientific Computing*, 34(5), 2012. doi: https://doi.org/10.1137/120864672.