Equation of State Solver for Smoothed Particle Hydrodynamics

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$$\frac{D\vec{\boldsymbol{v}}}{Dt} = -\frac{1}{\rho}\nabla p + \nu\,\nabla^2\vec{\boldsymbol{v}} + \vec{\boldsymbol{b}}^{ext}$$

The Navier-Stokes momentum equation for incompressible flow. This tile page itself is used as a simulation domain in which this equation is solved, highlighting the solver's ability to handle complex boundary conditions and resolve details while maintaining low levels of compression (here: $\rho_{err}^{max} < 0.1\%$ for $N > 250k$ particles).

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Governing Equations of Fluid Flow

In an attempt to create a numerical solver for fluid dynamics problems, the governing equations of the underlying physical process must first be understood and formulated. Only then can an appropriate discretization be applied to numerically solve for desired properties of a system. In this chapter, the abstractions of continuum mechanics are used as a framework to describe incompressible flow. Physical principles such as conservation of mass and momentum are used to derive the continuity and momentum equations which encode them, then augmented by constitutive relations which describe properties of Newtonian fluids to finally yield the Navier-Stokes equations as governing equations.[1][2]

The particular form of these equations will favour a Lagrangian view of the system, in which the frame of reference in which quantities are described is advected along with the flow of the fluid itself, which will seamlessly integrate with the discretization scheme later used to derive workable numerical algorithms.

2.1 Lagrangian and Eulerian Continuum Mechanics

The purpose of our mathematical modelling of fluids is to simulate fluid dynamics at macroscopic scales with numerical methods. We know that fluids consist of innumerable molecules, and smaller yet quarks, interacting in complex ways, which give rise to emergent properties that we observe on a macroscopic scale. Instead of resolving all scales and simulating from quantum mechanical principles up, we content with modelling the emergent properties themselves, focusing on the question of how fluids behave instead of asking why. Our macroscopic scale is so many orders of magnitude larger than the discrete, physical reality, that we can reasonably assume quantities describing the fluid to be continuous and tackle them with the tools of calculus. This gives rise to the field of **Continuum Mechanics**.
In the following derivations, two major points of view can be taken, which produce different but equivalent forms of equations: the Eulerian or conservation forms, and the Lagrangian or nonconservation forms of the equations[1].

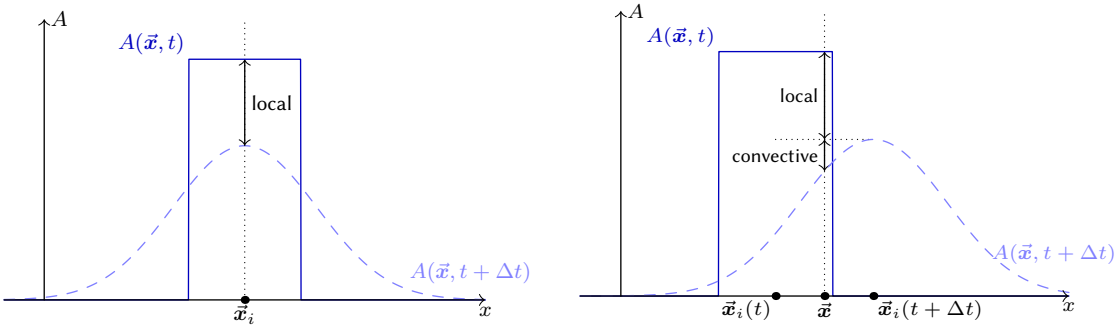
Using the assumption from continuum mechanics that quantities of our fluid are continuously distributed in space and asserting that they be differentiable, we can define derivatives on them. The two major forms of equations arise from a different interpretation of the so-called substantial derivative[1] or material derivative[2] $\frac{D}{Dt}$. This operator describes the instantaneous time rate of change of a quantity of a continuum element as it moves through space[1]. This movement through space however can be observed from different frames of reference:

- a frame that is advected along with the flow of the fluid, in which the continuum element observed is constant
- a frame that is constant in space at a fixed point, observing the flow of the fluid as continuum elements move through it

For both frames of reference, it can be derived that the material derivative in vector notation is[1]:

$$\frac{D}{Dt} = \underbrace{\frac{\partial}{\partial t}}_{\text{local derivative}} + \underbrace{(\vec{\boldsymbol{v}} \cdot \nabla)}_{\text{convective derivative}} \tag{2.1}$$

where $\vec{\boldsymbol{v}}$ is the velocity of the element and ∇ denotes the differential operator $\left(\frac{\partial}{\partial x_0}, \frac{\partial}{\partial x_1}, \ldots, \frac{\partial}{\partial x_n}\right)^T$ in n dimensions[1]. If an Eulerian view is chosen, there is an additional term for the convective derivate, which describes a rate of change of a quantity at a fixed point due to movement of the fluid. If a Lagrangian view is taken, the reference frame is advected with the velocity $\vec{\boldsymbol{v}}$, precisely such that the convective derivative



(a) Lagrangian view (b) Eulerian view

Figure 2.1: A field quantity A in one dimension is shown at some time t and a later time $t + \Delta t$ where the distribution of A has changed due to some diffusive process and the quantity was advected in positive x-direction. In the Lagrangian view, changes in a quantity A are evaluated at the advected position $\vec{x}_i$ at any point in time and only the local derivative is needed to describe the change in A. In the Eulerian view there are two reasons for A at a point $\vec{x}$ fixed in space to change: the local derivative due to the diffusive process and the convective derivative due to the advection of the quantity with the velocity field.

is zero and the material derivative simply becomes the total time derivative of a quantity. The difference between the two views is illustrated in Figure 2.1. In a way, the Lagrangian frame of reference is chosen precisely such that only local derivatives suffice to describe material derivatives by using a coordinate transformation defined by the velocity field.

How this simpler, Lagrangian form can be used largely depends on the later choice of discretization: discretizing space and tracking the fluid that moves through it favours an Eulerian framework, while discretizing the continuum into particles and sampling quantities only at advected particle positions makes the Lagrangian view applicable.

As is common for SPH discretizations, we will elect the Lagrangian view since it holds additional desirable properties such as making conservation of mass trivial to implement and enables solving the Navier-Stokes equations for primitive quantities instead of flux quantities that may cause drift instead of oscillations due to numerical inaccuracy. We state all following equations in the Lagrangian, nonconservation form.

2.2 The Continuity Equation

Using the Lagrangian view of continuum mechanics, we can apply laws of conservation to derive equations that express invariants of each fluid element with respect to time, which is an important step towards describing the dynamics of the system as time evolves. One such equation is the **CONTINUITY EQUATION**, which expresses conservation of mass:

Consider an infinitesimally small volume element $\delta\mathcal{V}$ with density ρ. The mass of the volume δm is simply[1]:

$$\delta m = \rho \delta \mathcal{V} \tag{2.2}$$

and is invariant under the material derivative in the Lagrangian reference frame[1]:

$$\frac{D\delta m}{Dt} = 0 \qquad \textit{conservation of mass} \tag{2.3}$$

$$= \frac{D\rho\delta\mathcal{V}}{Dt} \qquad \textit{identity 2.2} \tag{2.4}$$

$$= \delta\mathcal{V}\frac{D\rho}{Dt} + \rho\frac{D\delta\mathcal{V}}{Dt} \qquad \textit{product rule of calculus} \tag{2.5}$$

$$= \frac{D\rho}{Dt} + \rho\left(\frac{1}{\delta\mathcal{V}}\frac{D\delta\mathcal{V}}{Dt}\right) \qquad \textit{divide by } \delta\mathcal{V} \tag{2.6}$$

We can now apply the **DIVERGENCE THEOREM** to relate $\frac{D\mathcal{V}}{Dt}$ to the divergence of the velocity across the volume of the element, where $\partial\mathcal{V}$ is its surface and $\vec{n}$ the corresponding unit normal vector[1]:

$$\frac{D\mathcal{V}}{Dt} = \oint_{\partial\mathcal{V}} \vec{v}\cdot\vec{n}\, dS = \int_{\mathcal{V}} (\nabla\cdot\vec{v})\, d\mathcal{V} \tag{2.7}$$

As the volume $\mathcal{V}$ approaches the infinitesimal volume element $\delta\mathcal{V}$ of interest, the velocity in the volume becomes constant, the integral vanishes, and it holds that[1]:

$$\frac{D(\delta\mathcal{V})}{Dt} = (\nabla \cdot \vec{v})\,\delta\mathcal{V} \tag{2.8}$$

Substituting Equation 2.8 into Equation 2.6 we finally obtain the continuity equation:

$$\boxed{\frac{D\rho}{Dt} + \rho\,(\nabla \cdot \vec{\boldsymbol{v}}) = 0} \tag{2.9}$$

This is one of the Navier-Stokes equations in its derivative form, as opposed to the more general integral form[1]. When we additionally assume that the fluid is incompressible across a wide range of pressures, as is often done when simulating hydrodynamics, we can assert that the density of the fluid element in a Lagrangian reference frame is constant, meaning $\frac{D\rho}{Dt} = 0$ and therefore the velocity field of the flow for constant density is divergence-free[3]:

$$\nabla \cdot \vec{\boldsymbol{v}} = 0 \tag{2.10}$$

In the following sections, the fluid will generally be assumed to be incompressible.

An alternative derivation of the continuity equation uses the **Reynolds Transport Theorem**, which describes the material derivative of a scalar or tensor quantity $q(\vec{\boldsymbol{x}}, t)$ integrated over a volume as the sum of its time rate of change within the volume and the flux of the quantity through the volume's surface[3]:

$$\frac{D}{Dt}\int_{\mathcal{V}} q(\vec{\boldsymbol{x}}, t)\,dV = \int_{\mathcal{V}} \frac{\partial q(\vec{\boldsymbol{x}}, t)}{\partial t}\,dV + \oint_{\partial\mathcal{V}} q(\vec{\boldsymbol{x}}, t)(\vec{\boldsymbol{v}} \cdot \vec{\boldsymbol{n}})\,dS \tag{2.11}$$

This derivation goes as follows[3]:

$$0 = \frac{D}{Dt}\int_{\mathcal{V}} \rho\,dV \qquad \textit{conservation of mass} \tag{2.12}$$

$$= \int_{\mathcal{V}} \frac{\partial\rho}{\partial t}\,dV + \oint_{\partial\mathcal{V}} \rho(\vec{\boldsymbol{v}} \cdot \vec{\boldsymbol{n}})\,dS \qquad \textit{Reynolds Transport Theorem} \tag{2.13}$$

$$= \int_{\mathcal{V}} \frac{\partial\rho}{\partial t}\,dV + \int_{\mathcal{V}} \nabla \cdot (\rho\vec{\boldsymbol{v}})\,dV \qquad \textit{Divergence Theorem} \tag{2.14}$$

$$= \int_{\mathcal{V}} \left(\frac{\partial\rho}{\partial t} + \nabla \cdot (\rho\vec{\boldsymbol{v}})\right) dV \qquad \textit{combine integrals} \tag{2.15}$$

$$= \int_{\mathcal{V}} \left(\frac{D\rho}{Dt} + \rho\nabla \cdot \vec{\boldsymbol{v}}\right) dV \qquad \textit{constant density, Lagrangian framework} \tag{2.16}$$

$$\overset{\forall\mathcal{V}}{\Longrightarrow} \frac{D\rho}{Dt} + \rho\,(\nabla \cdot \vec{\boldsymbol{v}}) = 0 \qquad \textit{integral holds for all } \mathcal{V} \tag{2.17}$$

This use of the Reynolds Transport Theorem is very similar to the derivation that follows in section 2.3, which is why this alternative formulation was stated.

2.3 The Cauchy Momentum Equation

Mass is not the only conserved quantity that can be formulated in terms of a volume integral which can be transformed into a more convenient form using Reynolds Transport Theorem: a vital step in the derivation of the Navier-Stokes equations comes from applying the same concept to the conservation of momentum. In fact, the **Cauchy momentum equation**, which is the general case of the more specific momentum equation used in the Navier-Stokes equations, can be derived similarly to section 2.2, additionally using the continuity equation itself and Newton's second law.

We begin by observing that the change of momentum of a fluid volume $\mathcal{V}$ can be defined as the material derivative of the momentum $\int_{\mathcal{V}}(\rho\vec{\boldsymbol{v}})\,dV$ and simplify the resultant expression[3]:

$$\frac{D}{Dt}\int_{\mathcal{V}}(\rho\vec{\boldsymbol{v}})\,dV \qquad \textit{define change in momentum} \tag{2.18}$$

$$=\int_{\mathcal{V}}\frac{\partial(\rho\vec{\boldsymbol{v}})}{\partial t}\,dV+\oint_{\partial\mathcal{V}}\rho\vec{\boldsymbol{v}}(\vec{\boldsymbol{v}}\cdot\vec{\boldsymbol{n}})\,dS \qquad \textit{Reynolds Transport Theorem 2.11} \tag{2.19}$$

$$=\int_{\mathcal{V}}\frac{D}{Dt}(\rho\vec{\boldsymbol{v}})\,dV+\int_{\mathcal{V}}(\rho\vec{\boldsymbol{v}})\nabla\cdot\vec{\boldsymbol{v}}\,dV \qquad \textit{Divergence Theorem} \tag{2.20}$$

$$=\int_{\mathcal{V}}\rho\frac{D\vec{\boldsymbol{v}}}{Dt}+\vec{\boldsymbol{v}}\frac{D\rho}{Dt}+(\rho\vec{\boldsymbol{v}})\nabla\cdot\vec{\boldsymbol{v}}\,dV \qquad \textit{product rule on first integral} \tag{2.21}$$

$$=\int_{\mathcal{V}}\rho\frac{D\vec{\boldsymbol{v}}}{Dt}+\vec{\boldsymbol{v}}\underbrace{\left(\frac{D\rho}{Dt}+\rho\nabla\cdot\vec{\boldsymbol{v}}\right)}_{\text{continuity equation}=0}dV \qquad \textit{factor out } \vec{\boldsymbol{v}} \tag{2.22}$$

$$=\int_{\mathcal{V}}\rho\frac{D\vec{\boldsymbol{v}}}{Dt}\,dV \tag{2.23}$$

Then, we use Newton's second law, best known in its form $F=m\vec{\boldsymbol{a}}$, to assert that this change in momentum $m\vec{\boldsymbol{a}}$ is equal to the sum of forces exerted on the fluid volume, which can be decomposed into body forces $\vec{\boldsymbol{b}}^{ext}$ per unit mass[3] that act on the entire fluid mass homogeneously 'at a distance'[1], like gravity for example, and into surface forces described by stress vectors $\vec{\boldsymbol{t}}$ integrated over the fluid element's surface[3]:

$$\int_{\mathcal{V}}\rho\frac{D\vec{\boldsymbol{v}}}{Dt}\,dV=\oint_{\partial\mathcal{V}}\vec{\boldsymbol{t}}\,dS+\rho\vec{\boldsymbol{b}}^{ext} \tag{2.24}$$

One can define the **Cauchy stress tensor** $\mathbb{T}$ (sometimes referred to as σ) for the material such that it satisfies $\mathbb{T}\vec{\boldsymbol{n}}=\vec{\boldsymbol{t}}$[3]. Then, the divergence theorem may be applied again and the total forces acting on the fluid element written as:

$$\int_{\mathcal{V}}\nabla\cdot\mathbb{T}\,dV+\rho\vec{\boldsymbol{b}}^{ext} \tag{2.25}$$

Setting the expressions for total force in Equation 2.25 and total change of momentum in Equation 2.23 equal according to Newton's Law, we obtain:

$$\int_{\mathcal{V}}\rho\frac{D\vec{\boldsymbol{v}}}{Dt}-\nabla\cdot\mathbb{T}-\rho\vec{\boldsymbol{b}}^{ext}\,dV=0 \tag{2.26}$$

From this, we have obtained the **Cauchy Momentum Equation** as our equation of motion[2]:

$$\boxed{\rho\frac{D\vec{\boldsymbol{v}}}{Dt}=\nabla\cdot\mathbb{T}+\rho\vec{\boldsymbol{b}}^{ext}} \tag{2.27}$$

2.4 The Lagrangian Navier-Stokes Equations

With the Cauchy momentum equation we have reached the end of what can be modelled using general physical principles and continuum mechanics and is valid for a range of materials. To close the system of equations for fluid flow, generality must be given up and specific assumptions about the behaviour of fluids must be used to model the specific stress tensor $\mathbb{T}$ representing incompressible, linearly viscous or Newtonian fluids. In order to derive the form of the tensor, we make the further assumptions about the fluid that will later be clarified:

1. Fluids cannot sustain shear stresses when in rigid body motion.
2. Viscosity depends on the symmetric component of the gradient of velocity, it is linearly proportional to the rate of deformation tensor.

All remaining terms of the Cauchy momentum equation are clear, only the stress tensor $\mathbb{T}$ needs to be elaborated upon. First, it can be noted that $\mathbb{T}$ is a linear transformation[3] and that the tensor is symmetric[3], as in equal to its transpose $\mathbb{T}^T=\mathbb{T}$ or $\mathbb{T}_{ij}=\mathbb{T}_{ji}$. This means that in three dimensions for example, only six degrees of freedom actually exist in this tensor[4].

The element $\mathbb{T}_{ij}$ expresses a stress along some axis $\vec{e_i}$ acting on a plane perpendicular to $\vec{e_j}$, which means that the diagonal elements $\mathbb{T}_{ii}$ are normal stresses called *tensile stresses* for negative values and *compressive stresses* for positive values of $\mathbb{T}_{ii}$[3], while $\forall i \neq j : \mathbb{T}_{ij}$ refer to *shear stresses*[1].

To make this tensor more tractable, it can be assumed that a fluid is a material which cannot sustain shear stresses when in rigid body motion, including rest[3] (assumption 1) - this means that when in rigid body motion, the stress vector on any plane is normal to that plane[3], the stress is therefore isotropic and $\mathbb{T}$ must be represented by the only isotropic second order tensor $\lambda\mathbb{1}$ or $\lambda\delta_{ij}$ for some $\lambda \in \mathbb{R}$ where δ_{ij} is the Kronecker delta[5]. This motivates a decomposition of $\mathbb{T}$ for any general motion into a sum of an isotropic tensor describing *volumetric stress* caused by pressure forces and the *deviatoric stress* $\mathbb{V}$ which simply describes deviation of the total stress $\mathbb{T}$ from the volumetric stress[6]:

$$\mathbb{T} = \mathbb{V} - p\mathbb{1} \tag{2.28}$$

Conventionally, the pressure p is defined such that a positive pressure causes a negative stress, meaning the pressure acts normal to the surface and is directed into the fluid volume $\mathcal{V}$[4]. For a fluid at rest $\mathbb{V}_{ij} = 0$ holds and the normal stress is isotropically $-p$ according to *Pascal's law*[5]. Equation 2.28 decomposes stresses into a part caused by pressure and one caused by viscosity, which is why $\mathbb{V}$ is sometimes referred to as the *viscous stress tensor*[4]. Viscosity can be thought of as internal friction in a fluid or its resistance to deformation.

The remaining term $\mathbb{V}$ is caused by viscosity and modelled according to assumption 2 in terms of the gradient of the velocity. This makes intuitive sense: where the velocity is homogeneous, and the gradient is zero, there is no friction between fluid elements - where the velocity differs greatly, there is more friction. Since velocity is a vector quantity, the gradient $\nabla\vec{v}$ is a tensor[4]:

$$(\nabla\vec{v})_{ij} = \partial_j v_i = \frac{\partial v_i}{\partial x_j} \tag{2.29}$$

As always, we can decompose this tensor $\mathbb{L} := \nabla\vec{v}$ into a sum of a symmetric and an antisymmetric part[3]:

$$\mathbb{L} = \mathbb{D} + \mathbb{W} \tag{2.30}$$

$$\mathbb{D} = \frac{1}{2}\left(\mathbb{L} + \mathbb{L}^T\right) \tag{2.31}$$

$$\mathbb{W} = \frac{1}{2}\left(\mathbb{L} - \mathbb{L}^T\right) \tag{2.32}$$

$$\tag{2.33}$$

$\mathbb{D}$ is referred to as the **RATE OF DEFORMATION TENSOR** and $\mathbb{W}$ is called the **SPIN TENSOR**.

This decomposition is convenient since the spin tensor does not contribute to viscosity and only the rate of deformation tensor may be focused on. Note that since the deviatoric stress $\mathbb{V}$ we are trying to approximate is symmetric, and it only makes sense to use the symmetric component of the velocity gradient to model it.

Intuitively, the spin tensor encodes the rotational component of the velocity gradient, and a steadily rotating fluid (where $\mathbb{D} =$) is like a rigid body rotation: the relative positions of the fluid elements do not change, only their orientation with respect to a fixed reference frame, and therefore there is no friction. There is a vector $\vec{\omega}$ such that for any $\vec{v}$ it holds that $\mathbb{W}\vec{v} = \vec{\omega} \times \vec{v}$, where $\vec{\omega}$ points in the axis of rotation with a length of the angular velocity[3]. This is why the spin tensor is closely related to the vorticity tensor $2\mathbb{W}$[3]. In fact, enforcing that viscosity shall not affect the rotational component of velocity gradients and preserving accurate vorticity is key to accurately simulating turbulences in incompressible flows and conserving angular momentum[7].

Focusing further on the rate of deformation tensor, assumption 2 can now fully be appreciated. One defining characteristic of Newtonian fluids is the assumption dating back to Isaac Newton that viscosity depends *linearly* on the rate of deformation tensor[1]. This means that terms of an order higher than linear may be neglected for small velocity gradients[4] and constant terms cannot occur since shear stress is only proportional to the rate of deformation, not the state thereof[3]: if a shear stress is applied to a fluid it will eventually continuously deform at some non-zero rate but will remain in that deformed state if the

stress is removed, unlike purely elastic materials[3]. In other words $\mathbb{V}$ must vanish when the velocity is homogeneous since there is no friction in that case[4].

We now know that for incompressible fluids $\mathbb{V}$ is of the form[4]:

$$\mathbb{V} = 2\mu\mathbb{D} + \lambda(\nabla\cdot\vec{\boldsymbol{v}})\mathbb{1} \tag{2.34}$$

$$= \frac{2\mu}{2}\left((\nabla\vec{\boldsymbol{v}}) + (\nabla\vec{\boldsymbol{v}})^T\right) + \underbrace{\lambda(\nabla\cdot\vec{\boldsymbol{v}})\mathbb{1}}_{\text{incompressibility} = 0} \tag{2.35}$$

$$= \mu\left((\nabla\vec{\boldsymbol{v}}) + (\nabla\vec{\boldsymbol{v}})^T\right) \tag{2.36}$$

where μ is the dynamic viscosity[1] or first-order viscosity[4]. A second-order viscosity λ exists for compressible flows[1], but can be neglected here.

Combining the deviatoric stress with the volumetric stress, the **CONSTITUTIVE RELATION** for the stress tensor $\mathbb{T}$ of an incompressible, Newtonian fluid is finally obtained[2]:

$$\boxed{\mathbb{T} = -p\mathbb{1} + \mu\left((\nabla\vec{\boldsymbol{v}}) + (\nabla\vec{\boldsymbol{v}})^T\right)} \tag{2.37}$$

With the constitutive relation in hand, the Cauchy momentum equation can be revisited, and Equation 2.37 can be inserted into Equation 2.27:

$$\rho\frac{D\vec{\boldsymbol{v}}}{Dt} = \nabla\cdot\left(-p\mathbb{1} + \mu\left((\nabla\vec{\boldsymbol{v}}) + (\nabla\vec{\boldsymbol{v}})^T\right)\right) + \rho\vec{\boldsymbol{b}}^{ext} \qquad \textit{insert Eq. 2.37 into Eq. 2.27} \tag{2.38}$$

$$\rho\frac{D\vec{\boldsymbol{v}}}{Dt} = \nabla\cdot(-p\mathbb{1}) + \mu\nabla\cdot\left((\nabla\vec{\boldsymbol{v}}) + (\nabla\vec{\boldsymbol{v}})^T\right) + \rho\vec{\boldsymbol{b}}^{ext} \qquad \nabla\cdot \textit{ is linear} \tag{2.39}$$

$$\frac{D\vec{\boldsymbol{v}}}{Dt} = -\frac{1}{\rho}\nabla p + \nu\nabla\cdot\left((\nabla\vec{\boldsymbol{v}}) + (\nabla\vec{\boldsymbol{v}})^T\right) + \vec{\boldsymbol{b}}^{ext} \qquad \nabla\cdot(-p\mathbb{1}) = -\nabla p\textit{, divide by } \rho \tag{2.40}$$

$$\frac{D\vec{\boldsymbol{v}}}{Dt} = -\frac{1}{\rho}\nabla p + \nu\left(\underbrace{\nabla\cdot(\nabla\vec{\boldsymbol{v}})}_{=\nabla^2\vec{\boldsymbol{v}}} + \underbrace{\nabla\cdot(\nabla\vec{\boldsymbol{v}})^T}_{=0}\right) + \vec{\boldsymbol{b}}^{ext} \qquad \nabla\cdot \textit{ is linear} \tag{2.41}$$

$$\frac{D\vec{\boldsymbol{v}}}{Dt} = -\frac{1}{\rho}\nabla p + \nu\,\nabla^2\vec{\boldsymbol{v}} + \vec{\boldsymbol{b}}^{ext} \qquad \square \tag{2.42}$$

A few things of note happen in this derivation:

- The kinematic viscosity ν is defined as $\frac{\mu}{\rho}$ and inserted in Equation 2.40
- The identity $\nabla\cdot(-p\mathbb{1}) = -\nabla\cdot\begin{bmatrix}p & 0 & 0\\ 0 & p & 0\\ 0 & 0 & p\end{bmatrix} = -\begin{bmatrix}\partial p/\partial x\\ \partial p/\partial y\\ \partial p/\partial y\end{bmatrix} = -\nabla p$ is used in Equation 2.40.
- For sufficiently smooth $\vec{\boldsymbol{v}}$ and $\nabla\cdot\vec{\boldsymbol{v}} = 0$ one can show using the Theorem of Schwarz that $\nabla\cdot(\nabla\vec{\boldsymbol{v}}) = \nabla^2\vec{\boldsymbol{v}}$ as annotated in Equation 2.41[4].
- Similarly, in Equation 2.41 $\nabla\cdot(\nabla\vec{\boldsymbol{v}}^T) = \nabla(\nabla\cdot\vec{\boldsymbol{v}}) = 0$ is used[4], since the continuity equation for fluids of homogeneous density implies $\nabla\cdot\vec{\boldsymbol{v}} = 0$.

With all this, the final Navier-Stokes momentum equation for incompressible Newtonian fluids in Lagrangian form is obtained in step 2.42:

$$\boxed{\frac{D\vec{\boldsymbol{v}}}{Dt} = -\frac{1}{\rho}\nabla p + \nu\,\nabla^2\vec{\boldsymbol{v}} + \vec{\boldsymbol{b}}^{ext}} \tag{2.43}$$

2.5 Equations of State

Although the momentum equation typically takes centre stage when discussing the Navier-Stokes equations, it is important to realize that the complete Navier-Stokes equations actually refer to a set of equations and the momentum equation cannot function on its own. At the very least, the continuity equation should be included, sometimes accompanied by an energy balance equation which is crucial to heat transport problems and formulates conservation of energy in viscous flows[1]. For the dynamics of the systems

considered here, the continuity and momentum equations appear to be sufficient, but one field quantity remains elusive until now: We have yet to discuss how to compute pressure.

When incompressibility is strongly enforced, the continuity equation is a constraint on the momentum equation that p can be chosen to fulfil, making it a Lagrange multiplier to the equation[2]. Since strongly enforced incompressibility generally requires solving a system to solve the Poisson equation for pressure and can be more involved, a more straightforward first approach is to employ an **Equation of State** to couple pressure to known quantities. Such an equation of state can be thought of intuitively as relating strain and stress, or a deformation of a material and the potential caused by this deformation, the negative gradient of which is a force. In this case a deviation of the fluid from its rest density ρ_0 or volume V_0 causes a pressure potential, the negative gradient of which is a pressure force that counteracts the deformation, in this case compression, as demonstrated in the hydrostatic case.

There are many such equations of state to choose from. While this choice indeed encodes different physical assumption about the fluid, choice at times appears to be rather motivated by discretization and implementation details for practical reasons than general physical principles. The equation of state should be chosen with the goal of weak compressibility and well-behavedness of the system in mind and options include:

1. $p = k\rho$ or $p = k(\rho - \rho_0)$ from the ideal gas equation[8]
2. $p = k(\frac{\rho}{\rho_0} - 1)^\gamma$ from Tait's equation[8][9]
3. $p = \max(0, k(\rho - \rho_0))$ or $p = \max\left(0, k\left(\frac{\rho}{\rho_0} - 1\right)^\gamma\right)$ to prevent negative pressure values[2]

Option 3 in particular is used to penalize relative deviations from rest density while preventing negative pressure values that may cause undesired clumping artefacts when using SPH discretizations. In the implementation used for this report, $p = \max\left(0, k\left(\frac{\rho}{\rho_0} - 1\right)\right)$ was chosen by inserting $\gamma = 1$ into Tait's equation.

While the equation of state does allow the computation of the unknown pressure, it does not appear to help close the Navier-Stokes equations, since the problem was only pushed back to the seemingly arbitrary choice or some parameter k representing stiffness. It is important to note that this parameter does not however govern the magnitude of pressure per se, but only the compressibility of the fluid[2], where larger values of k yield higher incompressibility but also higher pressure accelerations and therefore demand a higher resolution of time discretization to remain numerically stable[2] and satisfy the Courant-Friedrichs-Lewy condition[10], decreasing computational efficiency. In order to ensure that the assumption of incompressibility made in the derivation of the Navier-Stokes momentum equations hold, a sufficiently large stiffness k should be chosen for a given setting, such that compressibility becomes negligible.

Approximations for the choice of k in Tait's equation such as $k \approx \frac{\rho_0 c_s}{\gamma}$ exist, where c_s is the speed of sound and relates to the speed of flow $\vec{v}_f$[8]. Other methods such as Predictive-Corrective Incompressible SPH (PCISPH for short) approximate a globally constant k specifically for SPH discretizations such that a more optimal trade-off of incompressibility and time step size might be realized. Generally, k might need to be tuned depending on the simulated scenario in a fluid solver employing an equation of state.

Chapter 3

Smoothed Particle Hydrodynamics

In chapter 2, the governing equations of fluid flow were derived in their Lagrangian differential form for continuous field quantities. To make the simulation of fluids tractable, these equations must now be discretized in space and time so that the evolution of the system can be numerically calculated.

The temporal domain is commonly discretized into global time steps Δt that propagate the solution of the system into the future. Numerically integrating the acceleration $\vec{\boldsymbol{a}}_i(t) = \frac{D\vec{\boldsymbol{v}}_i(t)}{Dt}$ from the left-hand side of the momentum equation (Equation 2.43) twice with respect to time yields a change in position $\Delta\vec{\boldsymbol{x}}$ that can be used to advect quantities. Symplectic Euler time integration (also referred to as semi-implicit Euler or Euler-Cromer) is very commonly used to achieve this[2]:

$$\vec{\boldsymbol{v}}_i(t + \Delta t) = \vec{\boldsymbol{v}}_i(t) + \Delta t\vec{\boldsymbol{a}}_i(t) \tag{3.1}$$

$$\vec{\boldsymbol{x}}_i(t + \Delta t) = \vec{\boldsymbol{x}}_i(t) + \Delta t\vec{\boldsymbol{v}}_i(t + \Delta t) \tag{3.2}$$

The subscript i in these equations indicates that quantities are evaluated at respective particle positions $\vec{\boldsymbol{x}}_i$, which are advected with the velocity field. This is why the Lagrangian form is applicable, and the material derivative can be implemented as a total derivative with respect to time.

The spatial discretization of the problem is less straightforward and yields different methods depending on the scheme chosen.

3.1 Spatial Discretization of the Continuum

The discretization chosen here makes use of **Smoothed Particle Hydrodynamics** or **SPH** for short, which was devised independently by Lucy[11] as well as Gingold and Monaghan[12] in 1977. Despite its name, this scheme has little to do with Hydrodynamics per se and does not even strictly require a particle representation of quantities to work, but rather is a general framework for the interpolation of field quantities stored at discrete locations to obtain a smooth function that can be evaluated at any location.

Since the Lagrangian framework tends to favour discretizing the continuum itself over the space it exists within, regions of the continuum are here represented by so-called particles with a singular position that represent some volume or, equivalently in the incompressible case with homogeneous density, mass. It is important to keep in mind that the word *particle* in this context refers not to a physical, elementary particle or a spherical object, but rather an abstract representation of a discrete, shapeless parcel of the continuum.

SPH can be derived by considering that these particles represent a sampling of the continuous fluid domain at singular points and can be expressed as Dirac-δ functions weighted by some quantity. The δ-function can be defined as a normalized function:

$$\int \delta(\vec{\boldsymbol{x}})\, dV = 1 \tag{3.3}$$

which obeys $\vec{\boldsymbol{x}} \neq \vec{\mathbf{0}} \implies \delta(\vec{\boldsymbol{x}}) = 0$. This results in a function that is zero everywhere but at a singularity at the origin, where a spike of undefined height shoots up and only the integral of the function across that spike is well-defined. The Dirac-δ can be thought of as the limit of a Gaussian distribution as the variance approaches zero and the distribution becomes ever higher and narrower[2], or as the limit of a box of fixed unit area as the width of the box approaches zero.
For this function representing the particles, the identity holds that for any continuous, compactly supported function $A(\vec{\boldsymbol{x}})$[2]:

$$A(\vec{\boldsymbol{x}}) = (A * \delta)(\vec{\boldsymbol{x}}) = \int A(\vec{\boldsymbol{x}}')\delta(\vec{\boldsymbol{x}} - \vec{\boldsymbol{x}}')dV' \tag{3.4}$$

or the convolution of A with δ is A itself. This can be explained by the product in the integral being zero everywhere but at the origin, where the value of A can be taken as constant since it is a singular point, pulled out of the integral and multiplied by one, which the integral of the δ is defined to be.

The same identity can be explained from the perspective of signal theory and Fourier analysis, where the δ can be defined as the constant unit function in Fourier space and therefore $\delta = \mathcal{F}^{-1}(1)$. Since the convolution theorem applies, it then holds that a convolution in the spatial domain is equivalent to a multiplication in the frequency domain and vice-versa, resulting in a multiplication by one in the case of the convolution with a δ-distribution real space, and therefore an identity.

The key insight to SPH is that the δ-function can be approximated by more well-behaved function with desirable properties such as smoothness, while approximately retaining the above identity. Such a function is referred to in SPH as a **Kernel function** W, *smoothing kernel*[2] or *broadening function*[11], since it broadens and smooths out the Dirac-δ distribution. With this, one can then derive[2]:

$$
\begin{aligned}
A(\vec{\boldsymbol{x}}) &= (A * \delta)(\vec{\boldsymbol{x}}) && \text{Equation 3.4} && (3.5)\\
&\approx (A * W)(\vec{\boldsymbol{x}}) && \text{approximate } \delta \text{ with } W && (3.6)\\
&= \int A(\vec{\boldsymbol{x}}')W(\vec{\boldsymbol{x}} - \vec{\boldsymbol{x}}')dV' && \text{Definition of a convolution} && (3.7)\\
&= \int \frac{A(\vec{\boldsymbol{x}}')}{\rho(\vec{\boldsymbol{x}}')}W(\vec{\boldsymbol{x}} - \vec{\boldsymbol{x}}')\underbrace{\rho(\vec{\boldsymbol{x}}')dV'}_{=dm'} && \text{multiply by } \frac{\rho(\vec{\boldsymbol{x}}')}{\rho(\vec{\boldsymbol{x}}')} = 1 && (3.8)\\
&\approx \sum_{\vec{\boldsymbol{x}}_j \in \mathcal{S}} A_j \frac{m_j}{\rho_j} W(\vec{\boldsymbol{x}} - \vec{\boldsymbol{x}}_j) && \text{approximate Integral with discrete samples} && (3.9)
\end{aligned}
$$

where subscripts denote the position where a quantity is evaluated as in $A_j := A(\vec{\boldsymbol{x}}_j)$ and $\mathcal{S}$ is a set of fluid samples. This leads to the general SPH approximation for any field quantity A[2]:

$$A_i = \sum_j A_j \frac{m_j}{\rho_j} W_{ij} \tag{3.10}$$

where the sample set $\mathcal{S}$ is implicit in the notation and $W_{ij} := W(\vec{\boldsymbol{x}}_i - \vec{\boldsymbol{x}}_j)$.

Note in particular that the mass density $\rho_i = \sum_j m_j W_{ij}$ is simply a sum over kernel functions weighted by the respective mass of samples[2]. Since mass can be perfectly conserved in a Lagrangian framework, this lends itself to fluid solvers that enforce density invariance as opposed to minimizing velocity divergence and the errors of which therefore result in volume oscillations rather than loss of volume and drift - this trade-off might be desirable but is not required by the SPH scheme in general.

As briefly mentioned before, SPH simply employs the kernel function W to perform a smoothing, thereby interpolating discrete samples, and does not necessarily have to be applied only to locations that coincide with particle positions, although finding the value of field quantities at a particle position is certainly desirable in a Lagrangian fluid simulation.

Further, note that since the gradient is a linear operator it can be pulled into the sum in Equation 3.10, resulting in[2]:

$$\nabla A_i = \sum_j A_j \frac{m_j}{\rho_j} \nabla W_{ij} \tag{3.11}$$

such that the gradient of a field can conveniently be computed simply by evaluating the function ∇W instead of W.

3.2 Kernel Functions and Properties

So far it has been left unspecified what form exactly the kernel function W takes, although some of its required properties were alluded to. Furthermore, W is often parameterized in its support radius $\hbar$ and smoothing length h, which we will assume to be equal in the following, yielding $W(\vec{\boldsymbol{x}}_{ij}, h)$, where $\vec{\boldsymbol{x}}_{ij} = \vec{\boldsymbol{x}}_i - \vec{\boldsymbol{x}}_j$. Properties of this function shall be enumerated in the following[2]:

1. **Normalization** $\int_{\mathcal{V}} W(\vec{\boldsymbol{x}}_{ij}, h) d\vec{\boldsymbol{x}}_j = 1$
   is required for the approximation to be consistent.

2. **Dirac-δ Condition** $\lim_{h\to 0} W(\vec{\boldsymbol{x}}_{ij}, h) = \delta(h)$
   is the motivation for the scheme in the first place and required for $A = (A * \delta) = (A * W)$ to hold in the limit.

3. **Compact Support** $\forall\, ||\vec{\boldsymbol{x}}_{ij}|| > \hbar : W(\vec{\boldsymbol{x}}_{ij}, h) = 0$
   reduces the SPH sum from $\mathcal{O}(n^2)$-complexity in n particles to potentially $\mathcal{O}(n)$

4. **Sufficient Smoothness** $W \in C^n, n \geq 2$
   it is desirable for the first few derivatives of W to be continuous for discretizations such as in Equation 3.11 to be viable and for second order partial differential equations to be handled with ease[2]

5. **Positivity** $\forall \vec{\boldsymbol{x}}_{ij} : W(\vec{\boldsymbol{x}}_{ij}, h) \geq 0$
   while negative values of the kernel are permitted[11] and even desired in rare cases such as when modelling surface tension[13], they are typically avoided since they might yield unphysical results at suboptimal sampling

6. **Symmetry** $W(\vec{\boldsymbol{x}}_{ij}, h) = W(\vec{\boldsymbol{x}}_{ji}, h)$
   is typically desired, even if just for lack of better assumptions about the structure of the interpolated field - indeed most kernels are spherically symmetric and only depend on the distance $||\vec{\boldsymbol{x}}_{ij}||$ between two points

A very typical choice for such a function is one that is similar to a Gaussian distribution in shape but has compact support, as demanded above. There are a few intuitions as to why a Gaussian-like kernel is a very natural choice for this problem: in terms of signal theory, where SPH can be derived from the convolution theorem applied to discrete samples - it is natural to apply a Gaussian filter to a signal in order to smoothen it and reduce high-frequency noise, allowing for better interpolation. In fact, a Gaussian filter can be thought of as the optimal way to filter a signal: it does not overshoot when approximating step functions and minimizes spatial spread while maximizing the damping of high frequencies. The Gaussian is special in the sense that its Fourier transformation is again a Gaussian, and it is the only function to attain minimum uncertainty in the uncertainty principle, minimizing dispersion about zero in both the real and frequency domains. Seen from this perspective, SPH is literally nothing more than a filtering operation.

Another perspective on the usefulness of the Gaussian and SPH in general is given by a probabilistic perspective on the problem. Interestingly, the original authors of SPH independently derive it from a stochastic point of view, both groups even referencing the same book on Monte Carlo techniques[14].

Chapter 4

Solving for Incompressibility

4.1 Weakly Compressible SPH

4.2 Operator Splitting and Iterative Solver

Chapter 5

Boundary and Initial Conditions

5.1 Non-Uniform Single Layer Boundaries

5.2 Jittered Initialization and Lattices

5.3 Solving for Equilibrated Density

Chapter 6

Analysis

6.1 Oscillation Frequency and Error as a Function of Speed of Sound

6.2 Stability as a Function of Viscosity, Stiffness and Timestep

6.3 Stability over Viscosity and Stiffness

Chapter 7

Conclusion

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