Fire and Explosions in Avatar: The Way of Water Supplemental Technical Document

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1 GOVERNING EQUATIONS

Let us recall the main continuum mechanics equations for compressible fluids. For more in-depth exposition we refer the reader to [Gonzalez and Stuart 2008].

Conservation of momentum. Or effectively the second Newton's law stating that the rate of change in momentum is equal to the sum of all forces

$$\rho \frac{D\boldsymbol{u}}{Dt} = -\nabla p + \rho \boldsymbol{g}, \tag{1}$$

for a fluid with density ρ, velocity $\boldsymbol{u}$, and pressure p in the presence of gravity $\boldsymbol{g}$. Here $\frac{D}{Dt} \equiv \frac{\partial}{\partial t} + \boldsymbol{u} \cdot \nabla$ is the *material derivative* operator. We ignore viscosity effects for simplicity.

Conservation of mass. Also known as the continuity equation describing the evolution of density ρ in velocity field $\boldsymbol{u}$

$$\frac{D\rho}{Dt} = -\rho \nabla \cdot \boldsymbol{u}. \tag{2}$$

Note that for incompressible fluids this simplifies to zero-divergence condition $\nabla \cdot \boldsymbol{u} = 0$, which together with equation (1) forms the system of Navier-Stokes equations.

Equation of state. For compressible fluids we need to establish a dependency between density and other state variables. We use the *ideal gas law* to relate density ρ to pressure p, molar mass M, and temperature T

$$\rho = \frac{pM}{RT}, \tag{3}$$

where R is the thermodynamic constant.

Temperature evolution. There is another advection-diffusion equation describing the evolution of temperature

$$\rho C \frac{DT}{Dt} = \kappa \nabla^2 T + W, \tag{4}$$

which together with equations (1), (2) and (3) forms a closed system in variables $\boldsymbol{u}$, p, ρ, and T. W represents additional energy sources that in our case are the result of chemical reactions, κ is thermal conductivity of the fluid, and C is its specific heat capacity. The heat capacity value depends on the fluid evolution regime. For instance, one may distinguish between isobaric, adiabatic, or other thermodynamic variations.

1.1 Assumptions and simplifications

The system of equations (1), (2), (3), and (4) has severe stability limitations associated with compressibility, and is non-trivial to integrate numerically. Similar to [Nielsen et al. 2022] we replace

Figure 1: An explosion simulated with our solver. ©Wētā FX.

variable p with fixed atmospheric pressure $p_{\text{atm}} = 101.3\text{KPa}$ in equation (3) and also consider temperature evolution in equation (4) to be isobaric (happening at constant atmospheric pressure). This simplification is based on the assumption that local variations in pressure ∇p driving mechanical evolution of the fluid are small enough not to introduce a considerable disturbance to the large absolute pressure of the atmospheric layer. It eliminates the possibility of shock waves and constrains simulatable scenarios to relatively slow contractions and expansions, but also makes the problem much easier to deal with numerically. Thus, the system of continuous equations to be solved becomes

$$\begin{cases} \rho \dfrac{D\boldsymbol{u}}{Dt} &=& -\nabla p + \rho \boldsymbol{g}, \\[2mm] \nabla \cdot \boldsymbol{u} &=& -\dfrac{1}{\rho} \dfrac{D\rho}{Dt}, \\[2mm] \rho &=& \dfrac{p_{\text{atm}} M}{RT}, \\[2mm] \rho C_p \dfrac{DT}{Dt} &=& \kappa \nabla^2 T + W. \end{cases} \tag{5}$$

Note the use of specific heat capacity at constant pressure C_p.

1.2 Operator splitting

A common approach to solve (5) is to use operator splitting. It allows separating advection/convection into its own step of temporal integration. With that, the temperature evolution equation (4) becomes a parabolic heat diffusion and can also be solved on its own, assuming fixed density. So in what follows, we will consider it solved for, and the temperature field to be predefined. Molar mass

evolution can be considered predefined as well, as a result of the combustion/chemistry step. Consequently, we are left with solving

$$
\begin{cases}
\rho \dfrac{D\boldsymbol{u}}{Dt} &= -\nabla p + \rho \boldsymbol{g}, \\[2mm]
\nabla \cdot \boldsymbol{u} &= -\dfrac{1}{\rho}\dfrac{D\rho}{Dt}, \\[2mm]
\rho &= \dfrac{p_{\text{atm}} M}{RT}.
\end{cases}
\tag{6}
$$

2 DIFFERENTIAL EXPANSION

Following [Nielsen et al. 2022] we compute the time derivative of the last equation in system (6)

$$
\frac{D\rho}{Dt} = \frac{p_{\text{atm}}}{RT}\left(\frac{DM}{Dt} - \frac{M}{T}\frac{DT}{Dt}\right),
\tag{7}
$$

and substitute it into the second equation of system (6) to get

$$
\begin{cases}
\rho \dfrac{D\boldsymbol{u}}{Dt} &= -\nabla p + \rho \boldsymbol{g}, \\[2mm]
\nabla \cdot \boldsymbol{u} &= -\dfrac{p_{\text{atm}}}{\rho RT}\left(\dfrac{DM}{Dt} - \dfrac{M}{T}\dfrac{DT}{Dt}\right).
\end{cases}
\tag{8}
$$

The latter can be solved as a regular pressure projection with pre-determined velocity divergence, representing expansion. Note that M generally depends on time as it represents the molar mass of a mixture of gases and may change due to a chemical reaction.

Limitations. The problem with the approach outlined above is in the differential nature of equation (7). It assumes the ideal gas equation in system (6) is satisfied at the beginning of each integration step, and attempts to have it satisfied at the end of the step as well via incremental updates to density given M and T changes. While being precise in the continuous setting, it is prone to error accumulation and drift when integrated numerically. Moreover, the assumption that the ideal gas law is satisfied at the beginning of the simulation may not be valid, as there is typically limited control over the input data provided by an artist. Finally, there could be additional phenomena contributing to density evolution, such as density diffusion, each of which would need to be manually added to equation (7) to be properly accounted for. In the next section we propose our new integral approach to handling expansion, which resolves the aforementioned issues.

3 INTEGRAL EXPANSION

Rather than considering density evolution in differential form (7) we enforce ideal gas law as a constraint directly. Let ρ_{prev}, M, and T be density, molar mass, and temperature of the simulated fluid. Note that the combination may not necessarily satisfy the ideal gas law with pressure p_{atm}, indicating a potential for expansion or contraction. We can however determine the density that would satisfy it as

$$
\rho_{\star} = \frac{p_{\text{atm}} M}{RT}.
\tag{9}
$$

The change in density from ρ_{prev} to the desired $\rho_{\star}$ over the duration of a timestep δt determines the expansion

$$
-\frac{1}{\rho}\frac{D\rho}{Dt} = -\frac{D\ln\rho}{Dt} \simeq -\frac{1}{\delta t}(\ln\rho_{\star} - \ln\rho_{\text{prev}}) = -\frac{1}{\delta t}\ln s,
\tag{10}
$$

where we have introduced density scaling

$$
s = \frac{\rho_{\star}}{\rho_{\text{prev}}}.
\tag{11}
$$

With that system (6) becomes

$$
\begin{cases}
\rho \dfrac{D\boldsymbol{u}}{Dt} &= -\nabla p + \rho \boldsymbol{g}, \\[2mm]
\nabla \cdot \boldsymbol{u} &= -\dfrac{1}{\delta t}\ln s,
\end{cases}
\tag{12}
$$

and can be solved using a standard pressure projection.

3.1 Measure of concentration

While being reasonable from a physics/chemistry standpoint, density [kg/m^3] or even moles per unit volume [1/m^3] are not the most convenient quantities for artists to deal with when it comes to specifying the amount of a chemical contained in a region of space. We introduce a new dimensionless relative measure

$$
c = \frac{\rho}{\rho_{\text{atm}}},
\tag{13}
$$

which we call *concentration*. Here ρ is the current density of a chemical with molar mass M, and ρ_{atm} is the density of that same chemical at the thermodynamic equilibrium

$$
\rho_{\text{atm}} = \frac{p_{\text{atm}} M}{RT_{\text{atm}}},
\tag{14}
$$

with pressure p_{atm} and room temperature $T_{\text{atm}} = 288.15$K. Substituting (14) into (13) gives

$$
c = \frac{\rho RT_{\text{atm}}}{p_{\text{atm}} M}.
\tag{15}
$$

Concentration is intuitive for artists to use as $c = 1$ means a chemical is exactly at the thermodynamic equilibruim with $p = p_{\text{atm}}$ and $T = T_{\text{atm}}$, and values greater and less than 1 indicate expansion and contraction respectively.

Chemical mixtures. Given chemicals with concentrations c^i and equilibrium densities ρ^i_{atm}, the density of the mixture is then

$$
\rho = \sum_i c^i \rho^i_{\text{atm}}.
\tag{16}
$$

With this, concentrations are similar to chemical fractions in [Nielsen et al. 2022], but they do not necessarily add up to 1, with the sum $c = \sum_i c^i$ serving as an indicator of a potential expansion or contraction. If molar masses of the chemicals are M^i, the molar mass of the mixture can be computed as

$$
M = \frac{1}{c}\sum_i c^i M^i_{\text{atm}}.
\tag{17}
$$

It is then easy to check that equation (15) holds for mixtures of chemicals as well.

3.2 Concentration change with expansion

Previously we have connected expansion to density change via equations (10) and (11). We can now rewrite it in terms of concentration and temperature. Assuming $c_{\star}$ and c_{prev} correspond to $\rho_{\star}$ and ρ_{prev} as per equation (15), respectively

$$
s = \frac{\rho_{\star}}{\rho_{\text{prev}}} = \frac{c_{\star}}{c_{\text{prev}}} = \frac{1}{c_{\text{prev}}}\frac{\rho_{\star}RT_{\text{atm}}}{p_{\text{atm}} M} = \frac{1}{c_{\text{prev}}}\frac{T_{\text{atm}}}{T}.
\tag{18}
$$

The computation within the solver timestep enforcing expansion and mass/concentration conservation then proceeds as follows:

(1) Perform combustion reaction and diffusion to update temperature and concentrations of all chemicals.
(2) Compute the sum c_{prev} of all concentrations.
(3) Scale c_{prev} by $\frac{T}{T_{\text{atm}}}$ and invert to obtain s.
(4) Perform pressure projection with divergence $-\frac{1}{\delta t} \ln s$.
(5) Multiply all concentrations by s to account for expansion.
(6) Advect concentrations of all chemicals.

4 ARTISTIC CONTROLS

We have introduced a set of artistic controls that were particularly useful when tuning the size and timing of explosions, such as the one shown in Figure 1.

Expansion scaling. Similar to [Nielsen et al. 2022] we allow our users to scale the expansion term $-\frac{1}{\delta t} \ln s$ arbitrarily to achieve more or less expansion. We note however that this operation in general breaks conservation of mass, since such correction to expansion is effectively achieved through creating or destroying fluid.

Relaxation time. Instead of performing immediate expansion to achieve the equilibruim concentration $c_\star$, one may wish to spread the effect over a period of time. We introduce a new parameter τ called *relaxation time*, and rather than aiming for $c_\star$ by the end of a timestep we choose to target

$$\tilde{c} = c_\star + \left(c_{\text{prev}} - c_\star \right) \exp\left(-\frac{\delta t}{\tau} \right). \tag{19}$$

This makes fluid concentration approach $c_\star$ exponentially, reducing the discrepancy by a factor of e over time τ. The corresponding update to the algorithm in Section 3.2 is to replace scaling s in steps 4 and 5 with

$$\tilde{s} = \frac{\tilde{c}}{c_{\text{prev}}} = \frac{1 + \left(\frac{c_{\text{prev}} T}{T_{\text{atm}}} - 1 \right) \exp\left(-\frac{\delta t}{\tau} \right)}{\frac{c_{\text{prev}} T}{T_{\text{atm}}}}. \tag{20}$$

REFERENCES

Oscar Gonzalez and Andrew M. Stuart. 2008. *A First Course in Continuum Mechanics.* Cambridge University Press. https://doi.org/10.1017/CBO9780511619571

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