How to train your IMP (Implicit Mid-Point)

Daniel Duque, Javier Calderon-Sanchez
Canal de Ensayos Hidrodinámicos (CEHINAV)
Universidad Politécnica de Madrid (UPM)
Madrid, Spain

Jose Luis Cercos-Pita, Pablo Eleazar-Merino
CoreDigital department
CoreMarine AB
Stavanger, Norway
jlc@core-marine.com

I. Introduction

The implicit mid-point (IMP) Euler scheme has recently been revealed [1] as a privileged time integrator, offering unconditional stability to weakly-compressible SPH (WCSPH) formulations. The IMP is deceptive: it promises stability, but is implicit in nature. In fact, a fixed-point problem must be solved, increasing the computational cost. However, numerical experiments showed that the algorithm converged spectrally to the exact solution, producing residues low enough to keep the simulation stable, with a rather low number of iterations per time step.

It appears that our previous publication [1] was the victim of a mischief: we were lured by the IMP to follow the same strategy with the mid-pint density as with the velocity. Although that did provide unconditional stability to the scheme, it is unfortunately unfeasible to describe the energy due to compressibility as a state variable. It is hereby impossible to take a picture of the IMP, and predict the energy state of the fluid.

It should be highlighted that evaluating the energy due to the compressibility as a state variable is a quite desirable feature, and that several authors have used analytic expressions to achieve this goal. (e.g. [2]). However, it has been impossible until now to check if that state variable accurately predicts the actual energy of the system.

However, the IPM's prank has led to a significant breakthrough: we here introduce a more robust IMP, that utilizes a new expression for the mid-point density — as well as the pressure, which no longer results from a straight evaluation of the equation of state (EOS). The implications on the accuracy within WCSPH are assessed with the normal impact problem.

II. Power, continuum and discrete

Taking into account only pressure forces, it is easy to derive that the specific energy changes according to

$$\frac{\mathrm{d}e}{\mathrm{d}t} = -\frac{1}{\rho}\nabla\cdot(p\boldsymbol{u}). \tag{1}$$

The total energy of the system is $E = \int \rho e \mathrm{d}\boldsymbol{r}$, so that

$$\frac{\mathrm{d}E}{\mathrm{d}t} = \underbrace{-\int \boldsymbol{u}\cdot(\nabla p)\,\mathrm{d}\boldsymbol{r}}_{P_\mathrm{k}} \underbrace{-\int p\,(\nabla\cdot\boldsymbol{u})\,\mathrm{d}\boldsymbol{r}}_{P_\mathrm{c}}, \tag{2}$$

where we have identified the total kinetic power and the total compression power.

In the absence of energy flux across the boundaries or external forces, the total energy does not change. This follows from the integration of (1), using Gauss' theorem. Another way of putting this fact is by asserting that the gradient and divergence operators in (2) are skew-adjoint, as a consequence of integration by parts in several dimensions. We therefore expect $P_\mathrm{k} + P_\mathrm{c} = 0$ in this case.

In a discrete SPH formulation the expressions would be

$$P_\mathrm{k} = -\sum_i \frac{m_i}{\rho_i}\langle\nabla p\rangle_i\cdot\boldsymbol{u}_i \tag{3}$$

$$P_\mathrm{c} = -\sum_i \frac{m_i}{\rho_i} p_i\langle\nabla\cdot\boldsymbol{u}\rangle_i. \tag{4}$$

We use the notation $\langle\cdot\rangle$ for every spatial operator that is approximated by SPH.

A basic requirement for an SPH implementation, in order to ensure the conservation of total energy, is that the discrete gradient and divergence operators are chosen to be skew-adjoint, as their continuum versions are. In a discrete formulation, this means that the powers in (3) and (4) must satisfy $P_\mathrm{k} + P_\mathrm{c} = 0$ for any pressure and velocity values.

III. The IMP in a nutshell

A summary of the mid-point integration in [1] is:

1) Guess a value for the mid-point change of the velocity field, in order to reach the next time step:
$$\boldsymbol{u}_i^m(t_{n+1}) = \boldsymbol{u}_i(t_n) + (\Delta t)\left(\frac{\mathrm{d}\boldsymbol{u}}{\mathrm{d}t}\right)_i^m(t_{n+1/2}), \tag{5}$$
where the guess corresponds to $m = 0$. A similar procedure is carried out for the density field.
2) Use the values of the fields at t_n and t_{n+1} to find mid-point values of the field. This is the main point of this contribution: these are not necessarily arithmetic means!
3) With these mid-point values of the fields, calculate SPH expressions for the changes, and take them into account with a relaxation factor α^m:
$$\left(\frac{\mathrm{d}\boldsymbol{u}}{\mathrm{d}t}\right)_i^{m+1}(t_{n+1/2}) = \alpha^m\left(\frac{\mathrm{d}\boldsymbol{u}}{\mathrm{d}t}\right)_i^m(t_{n+1/2}) + (1-\alpha^m)\left\langle\frac{\mathrm{d}\boldsymbol{u}}{\mathrm{d}t}\right\rangle_i(t_{n+1/2}). \tag{6}$$

Here, the change in velocity is computed from the SPH pressure gradient, through Euler's equation. There is a similar expression for the change in density, which will be related to the SPH velocity divergence, through continuity.

4) Increase m by one and use these updated changes again in step 1, with Eq. (5) now referring to the new iteration. Repeat the procedure, checking for the convergence of the field changes. In particular, the convergence of $(\mathrm{d}\boldsymbol{u}/\mathrm{d}t)_i^{m+1}$ towards $\left\langle \frac{\mathrm{d}\boldsymbol{u}}{\mathrm{d}t} \right\rangle_i$.

IV. IMPish Power

We begin by considering the total kinetic power as we go from time-step t_n to $t_{n+1} = t_n + \Delta t$:

$$\begin{aligned} P_\mathrm{k}(t_{n+1/2}) &= \frac{1}{2\Delta t} \sum_i m_i \left(|\boldsymbol{u}_i(t_{n+1})|^2 - |\boldsymbol{u}_i(t_n)|^2 \right) \\ &= \sum_i m_i \frac{\boldsymbol{u}_i(t_{n+1}) + \boldsymbol{u}_i(t_n)}{2} \cdot \frac{\boldsymbol{u}_i(t_{n+1}) - \boldsymbol{u}_i(t_n)}{\Delta t}. \end{aligned} \tag{7}$$

The expression asks for the following definitions:

$$\boldsymbol{u}_i(t_{n+1/2}) := \frac{\boldsymbol{u}_i(t_{n+1}) + \boldsymbol{u}_i(t_n)}{2} \tag{8}$$

$$\frac{\mathrm{d}\boldsymbol{u}_i}{\mathrm{d}t}(t_{n+1/2}) := \frac{\boldsymbol{u}_i(t_{n+1}) - \boldsymbol{u}_i(t_n)}{\Delta t}. \tag{9}$$

The latter is given by Euler's equation of motion. Inserting it, we find

$$P_\mathrm{k}(t_{n+1/2}) = -\sum_i \frac{m_i}{\rho_i(t_{n+1/2})} \langle \nabla p \rangle_i (t_{n+1/2}) \cdot \boldsymbol{u}_i(t_{n+1/2}), \tag{10}$$

compatible with the general form of (3).

Regarding total compression power, we may write

$$\begin{aligned} P_\mathrm{c}(t_{n+1/2}) &:= -\sum_i p_i(t_{n+1/2}) \frac{V_i(t_{n+1}) - V_i(t_n)}{\Delta t} \\ &= \sum_i \frac{m_i p_i(t_{n+1/2})}{\rho_i(t_{n+1})\rho_i(t_n)} \frac{\rho_i(t_{n+1}) - \rho_i(t_n)}{\Delta t}. \end{aligned} \tag{11}$$

We can also define the density variation rate and associate it with the SPH-computed value, in a similar fashion to the kinetic energy:

$$\frac{\mathrm{d}\rho_i}{\mathrm{d}t}(t_{n+1/2}) = \left\langle \frac{\mathrm{d}\rho}{\mathrm{d}t} \right\rangle_i (t_{n+1/2}) = \frac{\rho_i(t_{n+1}) - \rho_i(t_n)}{\Delta t}. \tag{12}$$

Therefore,

$$P_\mathrm{c}(t_{n+1/2}) = \sum_i \frac{m_i p_i(t_{n+1/2})}{\rho_i(t_{n+1})\rho_i(t_n)} \left\langle \frac{\mathrm{d}\rho}{\mathrm{d}t} \right\rangle_i (t_{n+1/2}). \tag{13}$$

By inserting the continuity equation, this may be written as

$$P_\mathrm{c}(t_{n+1/2}) = -\sum_i \frac{m_i \rho_i(t_{n+1/2})}{\rho_i(t_{n+1})\rho_i(t_n)} p_i(t_{n+1/2}) \langle \nabla \cdot \boldsymbol{u} \rangle_i (t_{n+1/2}), \tag{14}$$

in a form that is compatible with (4) (in the limit of vanishingly small time-steps.)

To ensure energy balance,

$$P_\mathrm{k}(t_{n+1/2}) + P_\mathrm{c}(t_{n+1/2}) = 0. \tag{15}$$

Comparing (10) and (14), and provided that the gradient and divergence operators are skew-adjoint (which, we stress, is needed for energy balance), the mid-point density is:

$$\rho_i(t_{n+1/2}) = \sqrt{\rho_i(t_{n+1})\rho_i(t_n)}. \tag{16}$$

Surprisingly, this is a geometric average, in contrast to the arithmetic average of the mid-point velocity of (8). However, the mid-point pressure still remains undefined.

V. Equation of State

To obtain an expression for the mid-point pressure, we use the equation of state (EOS): a relationship between pressure and density $\mathrm{p} = \mathrm{p}(\rho)$. However, we are interested in deriving a definition that is consistent with the energy evolution, which may not be compatible with a straightforward evaluation of the EOS.

Given a generic EOS,

$$p_i(t) = \mathrm{p}(\rho_i(t)), \tag{17}$$

we can define the compression work done on a particle (per unit mass) at any time as

$$e_\mathrm{c}(\rho) := -\frac{1}{m} \int \mathrm{p}(V)\, \mathrm{d}V = \int \frac{\mathrm{p}(\rho)}{\rho^2}\, \mathrm{d}\rho, \tag{18}$$

Therefore, and for consistency, it should be ensured that

$$P_\mathrm{c}(t_{n+1/2}) = \sum_i m_i \frac{e_\mathrm{c}(t_{n+1}) - e_\mathrm{c}(t_n)}{\Delta t}. \tag{19}$$

Comparing this with the compression power in (11), we can derive an expression for the pressure at the midpoint of the time step:

$$p_i(t_{n+1/2}) = \frac{\rho_i(t_{n+1})\rho_i(t_n)}{m_i} \frac{e_\mathrm{c}(t_{n+1}) - e_\mathrm{c}(t_n)}{\rho_i(t_{n+1}) - \rho_i(t_n)}. \tag{20}$$

For instance, for the usual stiffened EOS,

$$p(\rho) := c_0^2(\rho - \rho_0) \tag{21}$$

the following expression for the pressure at the midpoint results:

$$p_i(t_{n+1/2}) = c_0^2 \left(\frac{\rho_i(t_{n+1})\rho_i(t_n)}{\rho_i(t_{n+1}) - \rho_i(t_n)} \log\left(\frac{\rho_i(t_{n+1})}{\rho_i(t_n)} \right) - \rho_0 \right). \tag{22}$$

The evaluation of the expression above shall be carefully done, as $\rho_i(t_n)$ may be very close to $\rho_i(t_n)$. However, a Taylor series expansion of the log function in terms of $\rho_i(t_{n+1}) - \rho_i(t_n)$ reveals that the expression is not singular. In fact, in this limit, $p_i(t_{n+1/2}) \to c_0^2(\rho_i(t_{n+1}) - \rho_0)$. In practice, it suffices to check that $\rho_i(t_{n+1}) - \rho_i(t_n)$ is larger than the so-called machine epsilon.

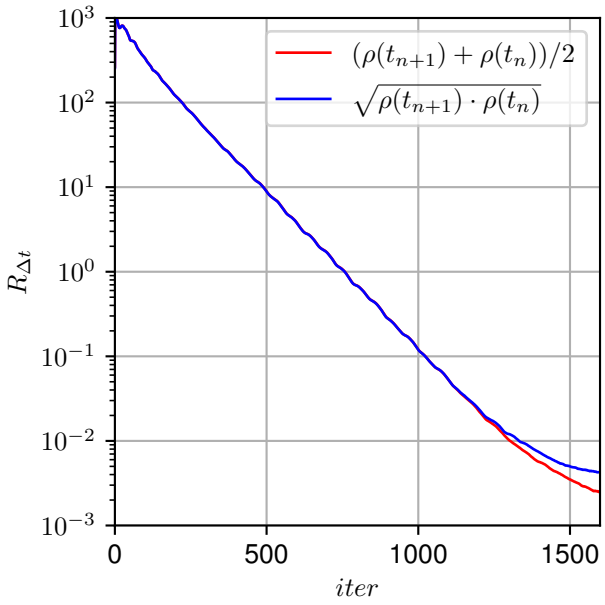

Fig. 1. Residue convergence as a function of iteration number m. Red line: previous IMP, with arithmetic mean for the mid-point density. Blue line: new IMP, with geometric mean.

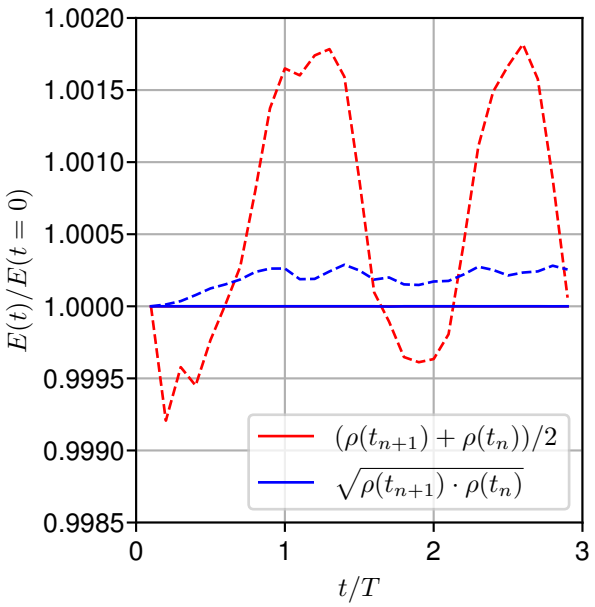

Fig. 2. Total energy profile using both formulations. Solid lines: Total energy integrated from the variation rates. Dashed lines: Total energy evaluated as a state variable. Colors as in 1.

VI. Practical applications

This improved IMP may now be confronted with the old one in a power struggle. To this end, the same normal impact considered in the original manuscript [1] is here considered. Since its introduction [3], such application has revealed itself as a powerful tool to check energy balance (in the absence of boundaries and external forces).

However, in this manuscript, the Courant-Friedich-Lewy (CFL) number has been significantly increased to a value of CFL $= 10$. An IMP with so much power could overreact and become quite unpredictable — thus, the number of inner iterations is increased to 1600, in order to balance the large CFL. The IMP begins heavily relaxed, with a factor $\alpha = 0.99$, which is geometrically increased in order to keep the spectral convergence rate. In Fig. 1 the 95% percentile of the residue is represented at each substep. The convergence rate is seen to be similar on both formulations, although the new IMP lags behind its older adversary at the last iterations of the fixed-problem solution.

However, when the energy integrated from the variation rates is compared against the energy computed as a state variable, the new IMP emerges victorious in the power struggle against its older counterpart, as seen in Fig. 2.

VII. Conclusions

This work is part of an ongoing effort that is aimed at the role of the time integration scheme in SPH (and in WCSPH in particular). It is our opinion that much of the usual doubts about the stability of SPH methods are strongly dependent on this issue, which has received less attention than the spatial operators. The IMP is an attractive method, even if surely not the only option. Nevertheless, we have the feeling that any successful time integrator method must have good energy-conservation features. This is certainly the case in molecular dynamics, where so-called simplectic integrators have reigned for many years.

Bibliography

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