Notes on energy conservation in hydro simulations

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1 Aims

- Conserve energy (bulk kinetic+thermal+gravitational potential) to machine precision.
- This was done without particles so that gravitational PE is only due to self-gravity by Jiang et al. (2013); see also Pen (1998).
- Now we want to do this with point particles included.
- Below we follow the procedure of Jiang et al. (2013) but generalize it to include the particle-gas potential energy terms.

2 Equations

Eq. (5) of Jiang et al. (2013) is generalized as

$$E_{\rm tot} = E + \tfrac{1}{2}\rho\phi_{\rm self} + \rho\phi_{\rm part} \tag{1}$$

The energy equation (3) of Jiang et al. (2013) becomes

$$\frac{\partial E}{\partial t} + \boldsymbol{\nabla}\cdot[(E+P)\boldsymbol{v}] = -\rho\boldsymbol{v}\cdot\boldsymbol{\nabla}(\phi_{\rm self}+\phi_{\rm part}). \tag{2}$$

This can be rewritten as (c.f. Eq. (9) of Jiang et al. 2013)

$$\frac{\partial}{\partial t}\left(E + \tfrac{1}{2}\rho\phi_{\rm self} + \rho\phi_{\rm part}\right) + \boldsymbol{\nabla}\cdot[(E+P)\boldsymbol{v} + \boldsymbol{F}_{\rm g}] = 0. \tag{3}$$

We want to derive an expression for $\boldsymbol{F}_{\rm g}$, which was already done in Jiang et al. (2013) for the case $\phi_{\rm part} = 0$.

3 Calculation

Using Eq. (2), Eq. (3) can be written as

$$\frac{\partial}{\partial t}\left(\tfrac{1}{2}\rho\phi_{\rm self} + \rho\phi_{\rm part}\right) + \boldsymbol{\nabla}\cdot\boldsymbol{F}_{\rm g} = \rho\boldsymbol{v}\cdot(\boldsymbol{\nabla}\phi_{\rm self} + \boldsymbol{\nabla}\phi_{\rm part}). \tag{4}$$

The continuity equation is

$$\dot{\rho} = -\boldsymbol{\nabla}\cdot(\rho\boldsymbol{v}). \tag{5}$$

Solving for $\boldsymbol{F}_{\rm g}$ in Eq. (4) and using Eq. (5), we obtain (c.f. Eq. (11) of Jiang et al. 2013)

$$\boldsymbol{\nabla}\cdot\boldsymbol{F}_{\rm g} = \boldsymbol{\nabla}\cdot(\rho\boldsymbol{v})\left(\tfrac{1}{2}\phi_{\rm self} + \phi_{\rm part}\right) + \rho\boldsymbol{v}\cdot\boldsymbol{\nabla}(\phi_{\rm self}+\phi_{\rm part}) - \rho\left(\tfrac{1}{2}\dot{\phi}_{\rm self} + \dot{\phi}_{\rm part}\right). \tag{6}$$

Poisson's equation is

$$\nabla^2\phi_{\rm self} = 4\pi G\rho, \tag{7}$$

and differentiating this equation with respect to time we obtain (c.f. Eq. (12) of Jiang et al. 2013)

$$\nabla^2\dot{\phi}_{\rm self} = 4\pi G\dot{\rho}. \tag{8}$$

First, let's break up the first term in Eq. (6) to write

$$\nabla \cdot \boldsymbol{F}_{\rm g} = \nabla \cdot (\rho \boldsymbol{v})\phi_{\rm self} - \tfrac{1}{2}\nabla \cdot (\rho \boldsymbol{v})\phi_{\rm self} + \nabla \cdot (\rho \boldsymbol{v})\phi_{\rm part} + \rho \boldsymbol{v} \cdot \nabla(\phi_{\rm self} + \phi_{\rm part}) - \rho \left(\tfrac{1}{2}\dot{\phi}_{\rm self} + \dot{\phi}_{\rm part}\right). \quad (9)$$

Now, using Eqs. 7 and (8), Eq. (9) can be written as

$$\nabla \cdot \boldsymbol{F}_{\rm g} = \nabla \cdot (\rho \boldsymbol{v})\phi_{\rm self} + \rho(\boldsymbol{v} \cdot \nabla)\phi_{\rm self} + \frac{1}{8\pi G}(\phi_{\rm self}\nabla^2\dot{\phi}_{\rm self} - \dot{\phi}_{\rm self}\nabla^2\phi_{\rm self}) + \nabla \cdot (\rho \boldsymbol{v})\phi_{\rm part} + \rho \boldsymbol{v} \cdot \nabla \phi_{\rm part} - \rho\dot{\phi}_{\rm part}. \quad (10)$$

Now

$$\nabla \cdot (\phi_{\rm self}\nabla\dot{\phi}_{\rm self} - \dot{\phi}_{\rm self}\nabla\phi_{\rm self}) = \nabla\phi_{\rm self} \cdot \nabla\dot{\phi}_{\rm self} + \phi_{\rm self}\nabla^2\dot{\phi}_{\rm self} - \nabla\dot{\phi}_{\rm self} \cdot \nabla\phi_{\rm self} - \dot{\phi}_{\rm self}\nabla^2\phi_{\rm self} = \phi_{\rm self}\nabla^2\dot{\phi}_{\rm self} - \dot{\phi}_{\rm self}\nabla^2\phi_{\rm self}$$

and

$$\nabla \cdot (\rho \boldsymbol{v}\phi_{\rm self}) = \nabla \cdot (\rho \boldsymbol{v})\phi_{\rm self} + \rho \boldsymbol{v} \cdot \nabla\phi_{\rm self},$$

and similarly for $\phi_{\rm part}$. Using these relations in Eq. (10) we obtain

$$\begin{aligned}\nabla \cdot \boldsymbol{F}_{\rm g} &= \nabla \cdot \left[\rho \boldsymbol{v}\phi_{\rm self} + \frac{1}{8\pi G}(\phi_{\rm self}\nabla\dot{\phi}_{\rm self} - \dot{\phi}_{\rm self}\nabla\phi_{\rm self})\right] + \nabla \cdot (\rho \boldsymbol{v})\phi_{\rm part} + \rho \boldsymbol{v} \cdot \nabla\phi_{\rm part} - \rho\dot{\phi}_{\rm part} \\ &= \nabla \cdot \left[\rho \boldsymbol{v}(\phi_{\rm self} + \phi_{\rm part}) + \frac{1}{8\pi G}(\phi_{\rm self}\nabla\dot{\phi}_{\rm self} - \dot{\phi}_{\rm self}\nabla\phi_{\rm self})\right] - \rho\dot{\phi}_{\rm part}.\end{aligned} \quad (11)$$

This is in the form of a divergence of a flux density *except* for the last term. So we now focus on that term. Using the Poisson equation (7) we can write

$$\begin{aligned}-\rho\dot{\phi}_{\rm part} &= -\frac{1}{4\pi G}\dot{\phi}_{\rm part}\nabla^2\phi_{\rm self} = -\frac{1}{4\pi G}\left[\nabla \cdot (\dot{\phi}_{\rm part}\nabla\phi_{\rm self}) - \nabla\dot{\phi}_{\rm part} \cdot \nabla\phi_{\rm self}\right] \\ &= \frac{1}{4\pi G}\left[\nabla \cdot (\phi_{\rm self}\nabla\dot{\phi}_{\rm part} - \dot{\phi}_{\rm part}\nabla\phi_{\rm self}) - \phi_{\rm self}\nabla^2\dot{\phi}_{\rm part}\right].\end{aligned} \quad (12)$$

This leaves us with

$$\begin{aligned}\nabla \cdot \boldsymbol{F}_{\rm g} =& \nabla \cdot \left[\rho \boldsymbol{v}(\phi_{\rm self} + \phi_{\rm part}) + \frac{1}{8\pi G}(\phi_{\rm self}\nabla\dot{\phi}_{\rm self} - \dot{\phi}_{\rm self}\nabla\phi_{\rm self}) + \frac{1}{4\pi G}(\phi_{\rm self}\nabla\dot{\phi}_{\rm part} - \dot{\phi}_{\rm part}\nabla\phi_{\rm self})\right] \\ &- \frac{1}{4\pi G}\phi_{\rm self}\nabla^2\dot{\phi}_{\rm part}\end{aligned} \quad (13)$$

Now, this last term is equal to zero for true point particles since

$$\nabla^2\dot{\phi}_{\rm part} = \frac{\partial}{\partial t}\nabla^2\phi_{\rm part} = \frac{\partial}{\partial t}\nabla^2\left(\sum_i^N \frac{GM_i}{|\boldsymbol{r} - \boldsymbol{r}_i|}\right) = -4\pi G\sum_i^N \frac{\partial}{\partial t}\left[M_i\delta^3(\boldsymbol{r} - \boldsymbol{r}_i)\right] = 0 \quad (14)$$

where the last equality follows from the fact that $\boldsymbol{r}$ is never precisely equal to $\boldsymbol{r}_i$, i.e. there is no gas at the exact location of the particle. Therefore, for true point particles we would finally have

$$\nabla \cdot \boldsymbol{F}_{\rm g} = \nabla \cdot \left[\rho \boldsymbol{v}(\phi_{\rm self} + \phi_{\rm part}) + \frac{1}{4\pi G}\left(\phi_{\rm self}\nabla(\dot{\phi}_{\rm part} + \tfrac{1}{2}\dot{\phi}_{\rm self}) - (\dot{\phi}_{\rm part} + \tfrac{1}{2}\dot{\phi}_{\rm self})\nabla\phi_{\rm self}\right)\right], \quad (15)$$

and $\boldsymbol{F}_{\rm g}$ can be chosen to equal the quantity in the square brackets. This expression reduces to Eq. (13) of Jiang et al. (2013) for $\phi_{\rm part} = \dot{\phi}_{\rm part} = \nabla\phi_{\rm part} = 0$, as required.

However, the particles in the simulation are *not* true point particles because they have spline potentials. Let $u = |\boldsymbol{r} - \boldsymbol{r}_i|/h$, with h the softening radius. Then the spline potential is given by

$$\phi_{\rm part} = -\frac{GM_i}{h}\begin{cases} -\frac{16}{3}u^2 + \frac{48}{5}u^4 - \frac{32}{5}u^5 + \frac{14}{5}, & \text{if } 0 \le u < 0.5; \\ -\frac{1}{15u} - \frac{32}{3}u^2 + 16u^3 - \frac{48}{5}u^4 + \frac{32}{15}u^5 + \frac{48}{15}, & \text{if } 0.5 \le u < 1; \\ \frac{1}{u}, & \text{if } u \ge 1. \end{cases} \quad (16)$$

Now

$$\nabla^2\dot{\phi}_{\rm part} = \frac{\partial}{\partial t}\nabla^2\phi_{\rm part} = \frac{\partial}{\partial t}\nabla \cdot \nabla\phi_{\rm part} = -\frac{\partial}{\partial t}\nabla \cdot \boldsymbol{g},$$

For $\boldsymbol{g} = -\boldsymbol{\nabla}\phi_{\rm part} = -(\partial\phi_{\rm part}/\partial u)(\partial u/\partial r)\boldsymbol{\nabla} r = -(1/h)(\partial\phi_{\rm part}/\partial u)\hat{\boldsymbol{r}}$ one obtains

$$\boldsymbol{g} = -\frac{GM_i}{h^2}\hat{\boldsymbol{r}} \begin{cases} \frac{32}{3}u - \frac{192}{5}u^3 + 32u^4, & \text{if } 0 \le u < 0.5; \\ -\frac{1}{15u^2} + \frac{64}{3}u - 48u^2 + \frac{192}{5}u^3 - \frac{32}{3}u^4, & \text{if } 0.5 \le u < 1; \\ \frac{1}{u^2}, & \text{if } u \ge 1. \end{cases} \tag{17}$$

Using the divergence formula in spherical coordinates $\boldsymbol{\nabla}\cdot\boldsymbol{g} = (1/r^2)[\partial(r^2 g_r)/\partial r]$, I compute

$$\nabla^2\phi_{\rm part} = -\frac{GM_i}{h^3} \begin{cases} 32 - 192u^2 + 192u^3, & \text{if } 0 \le u < 0.5; \\ 64 - 192u + 192u^2 - 64u^3, & \text{if } 0.5 \le u < 1; \\ 0, & \text{if } u \ge 1. \end{cases} \tag{18}$$

We see then that for $r \ge h$, the extra term $-\frac{1}{4\pi G}\phi_{\rm self}\nabla^2\dot{\phi}_{\rm part}$ vanishes, but otherwise it does not. This implies that for gas *inside* the softening radius, one cannot use this conservative approach. For gas outside the softening spheres of the particles, the conservative approach summarized by Eq. (15) is applicable.

References

Jiang, Y.-F., Belyaev, M., Goodman, J., & Stone, J. M. 2013, New Astron., 19, 48

Pen, U.-L. 1998, ApJS, 115, 19