On determining the smoothing length in the Smoothed Particle Hydrodynamics (SPH) description of fluids

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The Smoothed Particle Hydrodynamic is a meshless, Lagrangian (particle) method that is useful to simulate fluid flows. It is also a free boundary method although special methods can be used to introduce solid boundaries. The original implementation of the method dates back to 1977 when Bob Gingold and J. J. Monaghan [1] and independently by Leon Lucy [2] performed simulations of astrophysical objects. Three particularly attractive features of the method are to be mentioned: the spatial gradients can be calculated without a grid; it is easy to arrange for the resolution to change automatically; it is also easy to incorporate complex physics [3]. The difficult physical systems, which the SPH analyse well, include the study of fragmented gaseous region producing dense clumps surrounded by less dense material or the volcanic outbursts where the hot gas rises up and expands while the dust it carries eventually sinks to the ground. We present an equilibrium study of the Euler fluid equation to determine an upper bound to the arbitrary smoothing length introduced by the decomposition of the fluid into SPH particles. Thermodynamically, this upper bound corresponds to a transition from the gaseous phase to a liquid phase.

A fluid of constant mass M is decomposed in N mass elements (index a) such that $M = \sum_{a=1}^{N} m_a$ characterized by four parameters, mass, density, position and velocity: $\{m_a, \rho_a, r_a, v_a\}$. These parameters are obtained by a smoothing of the identity $A(r) = \int A(r') \delta(r - r') \, dr'$ with the delta function replaced by a kernel function W(r-r',h) (normalized to one) that depends on a smoothing length h: $A(r) = \int \frac{A(r')}{\rho(r')} W(r - r') \rho(r') \, dr'$. Recognizing that $\rho(r') \, dr' \approx m$ is the mass element, the integral can readily be approximated by a summation $A(r) \propto \sum_{b=1}^{N} m_b \frac{A_b}{\rho_b} W(r - r_b; h)$. Particles are then placed in the fluid volume according to the

expression $A_a(r_a) \propto \sum_{b=1}^{N} m_b \frac{A_b}{\rho_b} W(r_a - r_b; h)$. The SPH describes a fluid by replacing its

continuum properties with locally (smoothed) quantities at discrete Lagrangian locations.

The set of valid kernels include $W(r, h) = \frac{1}{\pi^{n/2} h^n} e^{-q^2}$ for a n-Dimensional systems where

$q = r / h$, and $r = |\mathbf{r}_a - \mathbf{r}_b|$. The behaviour of a system of N-SPH particles is as follows:

particles too far apart (compared to h) do not interact while too many particles in interaction

lead to a freezing of the dynamics. This behaviour suggests a phase transition between a

gaseous and a liquid phase. Since the transition parameter is the smoothing length we find

here a way to derive an upper bound to h guaranteeing the simulation applies to the gaseous

phase.

Equilibrium estimate of the smoothing length h

The Euler fluid is used as a model to derive a physical constraint on the smoothing length h.

The analysis of this parameter relies on the equilibrium properties of the fluid. It is known

that the Euler fluid can be represented by a Lagrangian

$L\left(q, \dot{q}\right) = \sum_{b=1}^{N} m_b \left(\frac{1}{2} \dot{q}_b^2 - u(\rho_b(q)) \right)$ with $u(\rho(q))$ the thermal energy per unit mass. The

canonical variable $p_a = \partial L\left(q, \dot{q}\right) / \partial \dot{q}_a = m_a \dot{q}_a$ together with $q = \{q_1, ..., q_N\}$,

$\dot{q} = \left\{ \dot{q}_1, ..., \dot{q}_N \right\}$, and $p = \{p_1, ..., p_N\}$ permit to define a N–particles Hamiltonian

as $H_N(q, p) = \sum_{b=1}^{N} \left(\frac{1}{2m_b} p_b^2 + m_b \, u(\rho_b(q)) \right)$. Thermodynamics implies a relation between u

and the pressure P: $u(\rho) = u(0) - \frac{P}{\rho}$. It is now easy to define a Liouville equation by

introducing a normalized distribution function F(q,p) such that $\int dq dp \, F(q, p) = N$. The

evolution of the distribution function is given by the classical

expression $\partial_t F(q, p) = [H_N(q, p), F(q, p)]$ where $H_N(q, p) = H^0(p) + V(q)$

with $V(q) = \sum_{b=1}^{N} m_b \, u(\rho_b)$ and $H^0(p) = \sum_{b=1}^{N} \frac{1}{2m_b} p_b^2$. The N-particles equilibrium distribution

function $\rho_N^{eq} = \frac{\exp(-\beta H_N)}{Z'_N}$ depends only on the Hamiltonian and its normalization

introduces the partition function $Z'_N = \int dqdp \exp(-\beta H_N)$. Averages are performed using the expression $<A>^{eq} = \int dqdp \, A \, \rho_N^{eq}$. One quantity of interest is the pressure given by $\beta^{-1} \dfrac{\partial \ln Z'_N}{\partial \Omega} = p$ which will be used below to derive an upper value to the smoothing length h. The partition function can be computed analytically with great accuracy. Considering only the interaction part of the partition function $Q = \int dq \exp(-\beta V) = \int dq \exp\left(-\beta \sum_{b=1}^{N} m_b \, u(\rho_b)\right)$ and assuming $m_i = m$, we get $Q = e^{-N \beta m u_b(0)} \int dq \exp\left\{\beta P \sum_{b=1}^{N} \left(\sum_{a=1}^{N} W_{ab}\right)^{-1}\right\}$. For a one dimensional system (the extension to a n-Dimensional system is trivial), with $u_i(0) = u(0), W_{ab} = W_{ba}$, we get $Q = e^{-2\beta m u(0)} \int dq_1 \, dq_2 \exp\left\{\dfrac{2\beta P}{W_0}\left(1+\dfrac{W_{12}}{W_0}\right)^{-1}\right\}$. With the smoothing kernel introduced previously, the argument of the exponential reduces to $X_2 = \dfrac{2\beta P}{W_0 \left(1+\frac{W_{12}}{W_0}\right)} = \dfrac{2\beta P}{W_0}$ when the two particles are within the interaction range, and to $X_2 \approx \dfrac{2\beta P}{W_0\left(1+1-\left(\frac{r_{12}}{h}\right)^2\right)}$ when the two particles are far apart. The two quantities X_2 are equal at $\frac{L_0}{2} \equiv r_{12} = h$. Using this distance as boundary condition for the integral, we get $Q_L = \left(2\left(L-h\right)\right)^N e^{-N\beta\left(m u(0) - \frac{P}{N W_0}\right)} e^{\frac{(N-1)\beta P}{W_0}}$ at large distances, and $Q_S = e^{-N\beta\left(m u(0) - \frac{P}{N W_0}\right)} \left(\dfrac{N}{\sqrt{\alpha}} e^{\left(\sqrt{\alpha}\frac{L_0}{N}\right)^2} D\left(\sqrt{\alpha} \, \frac{L_0}{N}\right)\right)^N$ at short distances. Here D(x) is Dawson function $D(x) = \exp(-x^2)\int_0^x \exp(t^2) dt$ and $\alpha = \dfrac{\beta P}{2 h^2 W_0}$. The equation of state $\beta^{-1} \dfrac{\partial \ln Z'_N}{\partial \Omega} = P$, which satisfies the pressure equation $u(\rho) = u(0) - \dfrac{P}{\rho}$, is a non-linear equation in X: $X \equiv \dfrac{\beta P L}{N} = \dfrac{1}{(1-\varepsilon)} \dfrac{1}{\left(1+\frac{Q_S}{Q_L}\right)}$ with $\varepsilon = h/L$. When $\frac{Q_S}{Q_L} \ll 1$ we get $X = \dfrac{1}{(1-\varepsilon)}$; whereas when $\frac{Q_S}{Q_L} \gg 1$, we get $X \to 0$. Depending on the value of the smoothing length h, the equation of state gives one or multiple solutions. Since only the

gaseous phase is of interest to us, the smoothing length has to be taken small enough to avoid the transition to the non gaseous phase. For example, defining $Y = \dfrac{2\beta P}{N^2 W_0} = \dfrac{2\sqrt{\pi}}{N} \varepsilon X$,

we get the equation of state in the form $\varepsilon^{-1} \dfrac{N}{2\sqrt{\pi}} Y = X = \dfrac{1}{(1-\varepsilon)} \dfrac{1}{(1+Q(Y;N,\varepsilon))}$. Then the

phase transition for a system of five SPH particles happens at h=0.68 (See Fig.1: the oblique line (curved line) corresponds to the left (right) hand side of the equation of state). This result indicates that the interaction length cannot exceed 68% of the system characteristic length. Obviously, the higher is the number of particles the lower is the critical h.

Fig. 1: Transition point N=5 h=0.68

Conclusions

An estimate of the smoothing length has been obtained from equilibrium arguments. The understanding of this limit permits to avoid unphysical local condensate of SPH particles where only gaseous solutions are expected. Also, the theory can be used to analyse the thermodynamics of SPH systems of particles such as the stability $\left(\dfrac{\partial p}{\partial V}\right)_{T,N} < 0$. Applications to MHD instabilities, in particular to the

classical tearing instability, can now be studied using SPH for a range of more physically relevant smoothing lengths. It will be shown elsewhere that SPH simulations of MHD systems compare well with analytical and other simulation results (e.g. from the spectral TURBO code).

[1] Gingold, R. A., & Monaghan, J. J. 1977, Mon. Not. R. Astron. Soc., 181, 375

[2] Lucy, L. B. 1977, Astron. J., 82, 1013

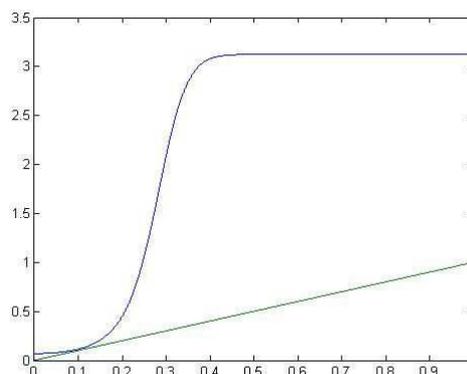[3] Monaghan J., 1992, Ann. Rev. Astron. Astrophys. 30, 543