OLD - A Riemann solver application to inviscid SPH method to improve shock structure resolution / NEW - A Riemann solver application to inviscid SPH method: consequences on the state equation G. Lanzafame INAF-OAC (Ct)

- SPH is a Lagrangian numerical scheme;
- SPH origin to be found in Lucy (1977) + Monaghan (from 1977 up to today - in particular 1992);
- PM methods vs. SPH: in SPH, spatial interpolations are performed on particles themselves; SPH is a Mesh-Free method;
- SPH is widely adopted also in laboratory flow simulations or in solidbody collision simulations (Astrophysical and Engineering);
- SPH provides very good results in simulations of flow discontinuities and/or convective fows;

• In SPH, $A_i = \int A_j W_{ij} d^3 r_{ij}$ (interpolation or convolution integral)

• where
$$\underline{r}_{ij} = \underline{r}_i - \underline{r}_j$$

• Kernel $W_{ij} = W(r_i, r_j, h) = W(\underline{r_{ij}}, h) - \text{smooth function: cubic spline or Gaussian function;}$

• Normalization:
$$\int W_{ij} d^3 r = 1$$

$$1 = \sum_{j} W_{ij} / n_{j} = \sum_{j} m_{j} W_{ij} / \rho_{j}$$

- In computational discretization, $A_i = \sum_j A_j W_{ij} / n_j = \sum_j m_j A_j W_{ij} / \rho_j$
- $m_j = SPH$ particle mass.



ideal gas state equation (1)

- continuity equation (2)
- momentum equation (3)

energy equation (4)

- kinematic equation (5)
- In SPH framework, all spatial derivatives of physical quantities transform in Kernel spatial derivatives. SPH particle mass is known. Therefore SPH particle density can be computed by definition as:
- $\rho_i = \sum_j m_j W_{ij}$ (SPH equiv. of the time integral of continuity eq. 2)
- Or via temporal integration of direct SPH conversion of eq. (2):

•
$$\frac{d\rho_i}{dt} = -\sum_j m_j \underline{v}_{ij} \cdot \nabla_i W_{ij}$$

continuity equation (6)

• The SPH conversion of momentum equation and energy equation in non-viscous modelling is:

•
$$\frac{d\underline{v}_i}{dt} = -\sum_j m_j \left(\frac{p_i}{\rho_i^2} + \frac{p_j}{\rho_j^2}\right) \nabla_i W_{ij} - \nabla \Phi_i$$
 momentum equation (7)

•
$$\frac{d\varepsilon_i}{dt} = \sum_j m_j \frac{p_j}{\rho_j^2} \underline{v}_{ij} \cdot \nabla_i W_{ij}$$

• $\frac{d\varepsilon_i}{dt} = \frac{1}{2} \sum_i m_j \left(\frac{p_i}{\rho_i^2} + \frac{p_j}{\rho_i^2} \right) \underline{v}_{ij} \cdot \nabla_i W_{ij}$

energy equation (8a)

energy equation (8b)

$$\underline{v}_{ij} = \underline{v}_i - \underline{v}_j$$

• As a "shock capturing method", in SPH an artificial viscosity term: η_{ij} is introduced to handle shock and flow discontinuities. It is effective only when particles approach with each other. Otherwise it is zero.

(9)

•
$$\frac{p_i}{\rho_i^2} = \frac{p_i}{\rho_i^2} \bigg|_{gas} \left(1 + \eta_{ij}\right) \qquad \eta_{ij} = \alpha \mu_{ij} + \beta \mu_{ij}^2$$

- $\mu_{ij} = \frac{2\pi v_{ij} \cdot r_{ij}}{(c_{si} + c_{sj})(r_{ij}^2 + \zeta^2)}$ c_{si}, c_{sj} , sound velocities
- $\underline{r}_{ij} = \underline{r}_i \underline{r}_j$; $\zeta^2 \ll h^2$ to prevent a singularity when particles collide.
- $\hat{\beta}$ is a Von Néumann-Richtmyer-like viscosity contribution;
- Despite the role of artificial viscosity pressure terms are marginal, compared to physical pressure terms, artificial viscosity looks like not suitable to reveal weak shocks, especially if rotational flows are involved. For strong shocks, typically $\alpha \approx 1$ and $\beta \approx 1-2$.
- Papers of Molteni et al. (1991), Lanzafame et al. (1992), Meglicki et al. (1993), Yukawa et al. (1997), as to accretion discs in close binaries, both in high compressibility ($\gamma = 1.01$) and in low compressibility ($\gamma = 5/3$) conditions, outline such SPH difficulties.
- In particular, Meglicki et al. (1993) adopted $\alpha = 0.04$ and $\beta = 0$, obtaining a very turbulent disc without any spiral shock.

• Viscous pressure terms can also be written as:

$$\frac{p_i}{\rho_i^2}\Big|_{gas}\eta_{ij} = -\frac{\alpha h \underline{v}_{ij} \cdot \underline{r}_{ij}}{\overline{\rho_{ij}} |\underline{r}_{ij}|^2} \left(\overline{c_{sij}} - 2\frac{h \underline{v}_{ij} \cdot \underline{r}_{ij}}{|\underline{r}_{ij}|^2}\right)$$

- Where $\overline{c_{sij}} = 0.5(c_{si} + c_{sj})$ and $\overline{\rho_{ij}} = 0.5(\rho_i + \rho_j)$
- The term involving the speed of sound is based on the viscosity of a gas. The term involving $(v_{ij} \cdot r_{ij})^2$ is introduced to prevent particle penetration of high Mach number collisions by producing an artificial pressure term proportional to ρv^2 . In the continuum limit, this artificial viscosity gives both bulk and shear viscosity components. Strong shocks require $\alpha \approx 1$. However, for weak shocks and for small Mach number flows, the fluid becomes "too viscous" and angular momentum and vorticity are transferred unphysically.
- Several solutions are proposed to solve such a problem:

 1) Balsara (1995) - formulation of a "limiter", multiplying only the artificial pressure terms:

$$\overline{f_{ij}} = 0.5(f_i + f_j) \qquad \qquad f_i = \frac{|\nabla \cdot \underline{v}_i|}{|\nabla \cdot \underline{v}_i| + |\nabla \times \underline{v}_i| + \sigma c_{si}/h}$$

$$\nabla \cdot \underline{v}_{i} = \sum_{j} \frac{m_{j}}{\rho_{j}} \underline{v}_{ji} \cdot \nabla_{i} W_{ij} \qquad \nabla \times \underline{v}_{i} = \sum_{j} \frac{m_{j}}{\rho_{j}} \underline{v}_{ji} \times \nabla_{i} W_{ij} \qquad \sigma \approx 0.1 - 0.2$$

- It reduces the unphysical spread of angular momentum in discs up to 20 times. It is nearly equal to one for planar shocks. It decreases whenever and wherever the tangential shear kinematics is relevant.
- 2) Morris & Monaghan (1997) a switch to reduce artificial viscosity:
- In this hypothesis, the α parameter evolves according to a decay equation, including also a source term: $\alpha^* = 0.1$

$$\frac{d\alpha_i}{dt} = -\frac{\alpha_i - \alpha^*}{\tau} + S_i \qquad S_i = f_i \max(-\nabla \cdot \underline{v}_i, 0)$$
$$\tau_i = \frac{h}{\zeta c_{si}} \qquad \varsigma \approx 0.1 - 0.2$$

 3) Monaghan (1997) – reformulation of artificial viscosity according to the Riemann Problem as a numerical approximation of the Riemann solution, to be used in the momentum equation:

•
$$\left(\frac{p_i}{\rho_i^2}\Big|_{gas} + \frac{p_j}{\rho_j^2}\Big|_{gas}\right)\eta_{ij} = -\frac{Kv_{sig,ij}\underline{v}_{ij} \cdot \underline{j}}{\overline{\rho_{ij}}}$$
 better if $\eta_{ij} \to \eta_{ij} h/|\underline{r}_{ij}|$
• Where, $\underline{j} = \frac{\underline{r}_{ij}}{|\underline{r}_{ij}|}$ $K \approx 1$ $v_{sig,ij} = c_{si} + c_{sj} - \underline{v}_{ij} \cdot \underline{j}$

• Instead, as far as the energy equation is concerned,

• being
$$e_i = \frac{1}{2} \left(\underline{v}_i \cdot \underline{j} \right)^2 + \varepsilon_i$$

$$\frac{de_i}{dt} = \frac{1}{2} \sum_j m_j \left(\frac{p_i \underline{v}_j}{\rho_i^2} + \frac{p_j \underline{v}_i}{\rho_j^2} - \frac{K v_{sig,ij}}{\rho_{ij}} \left(e_i - e_j \right) \underline{j} \right) \cdot \nabla_i W_{ij}$$

• $V_{sig,ij}$ must also be considered in the CFL condition.

- 4) Parshikov & Medin (2002) the key concept in SPH approximation is to substitute the velocity and stresses determined at a contact point by 1D Riemann solution, instead of SPH values between velocities and stresses of basic and companion particles. So doing, there is no need to use any artificial viscosity. The scheme sets a contact point between the basic particle and each companion along the line joining them.
- The main SPH equations of the Euler equations modify as follow:

$$\frac{d\rho_{i}}{dt} = -\sum_{j} m_{j} \underline{v}_{ij} \cdot \nabla_{i} W_{ij} \rightarrow \frac{d\rho_{i}}{dt} = \sum_{j} \frac{m_{j}}{h} (v_{i}^{R} - v_{j}^{R}) W_{ij}$$

$$\frac{d\underline{v}_{i}}{dt} = -\sum_{j} m_{j} \left(\frac{p_{i}}{\rho_{i}^{2}} + \frac{p_{j}}{\rho_{j}^{2}} \right) \nabla_{i} W_{ij} \rightarrow \frac{d\underline{v}_{i}}{dt} = \sum_{j} \frac{m_{j}}{h} \left(\frac{p_{i}}{\rho_{i}^{2}} + \frac{p_{j}}{\rho_{j}^{2}} \right) \frac{\underline{r}_{ji}}{|\underline{r}_{ji}|} W_{ij}$$

$$\frac{d\varepsilon_{i}}{dt} = \frac{1}{2} \sum_{j} m_{j} \left(\frac{p_{i}}{\rho_{i}^{2}} + \frac{p_{j}}{\rho_{j}^{2}} \right) \underline{v}_{ij} \cdot \nabla_{i} W_{ij} \rightarrow \frac{d\varepsilon_{i}}{dt} = -\frac{1}{2} \sum_{j} \frac{m_{j}}{h} \left(\frac{p_{i}}{\rho_{i}^{2}} + \frac{p_{j}}{\rho_{j}^{2}} \right) (v_{i}^{R} - v_{j}^{R}) W_{ij}$$
• This reformulation is done when $\nabla_{i} W_{ij} \left(\frac{|\underline{r}_{ij}|}{h} \right) = W_{ij} \frac{\underline{r}_{ij}}{h|\underline{r}_{ij}|}$

• In these expressions
$$v_i^R = \underline{v}_i \cdot \frac{\underline{r}_{ji}}{h|\underline{r}_{ij}|}$$

• In the acoustic approximation,

$$v_{ij}^{*R} = \frac{v_{j}^{R} \rho_{j} c_{sj} + v_{i}^{R} \rho_{i} c_{si} - p_{j} + p_{i}}{\rho_{j} c_{sj} + \rho_{i} c_{si}}$$
$$p_{ij}^{*R} = \frac{p_{j} \rho_{i} c_{si} + p_{i} \rho_{j} c_{sj} - \rho_{j} c_{sj} \rho_{i} c_{si} \left(v_{j}^{R} - v_{i}^{R} - v_{j}^{R} -$$

• Substituting in the previous equations

$$\frac{1}{2} \left(v_i^R + v_j^R \right) \rightarrow v_{ij}^{*R} \quad \frac{1}{2} \left(p_i + p_j \right) \rightarrow p_{ij}^{*R}$$

• We get:
$$\frac{d\rho_i}{dt} = -2\sum_j \frac{m_j}{h} \left(v_i^R - v_{ij}^{*R} \right) W_{ij}$$

•
$$\frac{d\underline{v}_i}{dt} = \sum_j \frac{m_j}{h} \left(\frac{p_{ij}^{*R}}{\rho_i^2} + \frac{p_{ij}^{*R}}{\rho_j^2} \right) W_{ij} \frac{\underline{r}_{ji}}{|\underline{r}_{ji}|}$$

•
$$\frac{d\varepsilon_i}{dt} = -\sum_j \frac{m_j}{h} \left(\frac{p_{ij}^{*R}}{\rho_i^2} + \frac{p_{ij}^{*R}}{\rho_j^2} \right) \left(v_i^R - v_{ij}^{*R} \right) W_{ij}$$

continuity equation

momentum equation

energy equation

5) Inutsuka (2002) – SPH is reformulated according to the original convolution, determining the force acting on each particle by solving the 1D Riemann problem according to the 2° (MUSCL) and 3° (PPM) Godunov method. In such reformulation, the general SPH interpolation:

•
$$A_i = \sum_j \frac{m_j}{\rho_j} A_j W_{ij}$$
 modifies in: $A_i = \sum_j \int \frac{m_j}{\rho_k} A_k W_{ik} W_{jk} d\underline{r}_k$
• Ensuring that $\sum_j \frac{m_j}{\rho_j} W_{ij} = 1$ and $\sum_j m_j \nabla_i \left(\frac{W_{ij}}{\rho_i}\right) = 0$

 According to these concepts, the SPH momentum and the energy equations become:

$$\frac{d\underline{v}_i}{dt} = -\sum_j m_j \int \frac{p_k}{\rho_k^2} \left(\nabla_i - \nabla_j \right) W_{ik} W_{jk} d\underline{r}_k$$

$$\frac{d\varepsilon_i}{dt} = \sum_j m_j \int \frac{p_k}{\rho_k^2} \underline{v}_{ki} \cdot \left(W_{jk} \nabla_i W_{ik} - W_{ik} \nabla_j W_{jk} \right) d\underline{r}_k$$

- Spatial integrals are computer knowing the spatial distribution of the density along the 1D direction (s) joining particles i (basic) and j (companion). To do this, either linear or cubic spline interpolation techniques are involved.
- Numerical solutions through a Godunov scheme: S^{*} are introduced in the momentum and in the energy equations, taking into account of the midpoint between the ith and the jth particles. Such numerical solutions are used at each cell interface in the calculation of the numerical flux. Therefore, momentum and energy equations are:

$$\frac{d\underline{v}_{i}}{dt} = -\sum_{j} m_{j} p_{ij}^{*R} \int \frac{1}{\rho_{k}^{2}} \left(\frac{\partial}{\partial s_{i}} - \frac{\partial}{\partial s_{j}} \right) W_{ik} W_{jk} ds_{k} = -2\sum_{j} m_{j} p_{ij}^{*R} V_{ij}^{2} \frac{\partial}{\partial s_{i}} W_{ij}^{*}$$
$$\frac{d\varepsilon_{i}}{dt} = -\sum_{j} m_{j} p_{ij}^{*R} \left(\underline{v}_{ij}^{*R} - \underline{v}_{i} \right) \int \frac{1}{\rho_{k}^{2}} \left(\frac{\partial}{\partial s_{i}} - \frac{\partial}{\partial s_{j}} \right) W_{ik} W_{jk} ds_{k} = 2\sum_{j} m_{j} p_{ij}^{*R} \left(\underline{v}^{*R} - \underline{v}_{i} \right) V_{ij}^{2} \frac{\partial}{\partial s_{i}} W_{ij}^{*}$$
$$\bullet \quad \text{Where} \quad W_{ij}^{*} = W \left(r_{ij}, \sqrt{2}h \right) \quad \text{and} \quad V_{ij} = V(s) = 1/\rho(s)$$

 6) Molteni & Bilello (2003) – the Lagrangian Van Leer Godunov technique is adopted to solve the 1D Riemann problem along the line joining particles i and j. Pressure and velocity of the Riemann problem are computed at the two "equivalent interface distances" both "ahead" and "behind" the basic particle i. Such values are the used to calculate spatial derivatives relative to particle i:

•
$$\frac{\underline{r}_{ij}}{|\underline{r}_{ij}|} = \underline{j}$$
 $V_{ij} = \underline{V}_i \cdot \underline{j}$ $\begin{cases} W_{ij}^{ah} = W_{ij} \cos \theta_{ij} & \text{if } \cos \theta_{ij} > 0 \\ W_{ij}^{ah} = 0 & \text{otherwise} \end{cases}$

- \mathcal{G}_{ij} is the angle between \underline{r}_{ij} and \underline{x}_q , q = 1, 2, 3
- Solution of the Riemann problem are: p_{ii}^{*R} and v_{ij}^{*R}

$$\begin{cases} W_{ij}^{be} = W_{ij} \cos \vartheta_{ij} & \text{if } \cos \vartheta_{ij} < 0 \\ W_{ij}^{be} = 0 & \text{otherwise} \end{cases}$$

The "equivalent interface distance"

•
$$s_{i,q}^{ah} = \frac{\sum_{j} \frac{m_j}{\rho_j} \left| \underline{r}_{ji} \cdot \underline{x}_q \right| W_{ij}^{ah}}{M_{0i}^{ah}}$$
 where $M_{0i}^{ah} = \sum_{j} \frac{m_j}{\rho_j} W_{ij}^{ah}$

$$p_{iq}^{ah} = \frac{\sum_{j} \frac{m_{j}}{\rho_{j}} p_{ij}^{*R} W_{ij}^{ah}}{M_{0i}^{ah}} \qquad v_{iq}^{ah} = \frac{\sum_{j} \frac{m_{j}}{\rho_{j}} v_{ij}^{*R} (\underline{r}_{ij} \cdot \underline{x}_{q}) W_{ij}^{ah}}{M_{0i}^{ah}}$$

• Spatial derivatives found are:

$$\nabla \cdot \underline{v}_{i} = 2 \sum_{q=1}^{3} \frac{v_{iq}^{ah} - v_{iq}^{be}}{s_{i,q}}$$

$$\nabla p_{iq} = 2 \frac{p_{iq}^{ah} - p_{iq}^{be}}{s_{i,q}}$$

$$\nabla \cdot \left(p\underline{v}\right)_{i} = 2 \sum_{q=1}^{3} \frac{p_{iq}^{ah} v_{iq}^{ah}}{s_{i,q}} - \frac{p_{iq}^{be} v_{iq}^{be}}{s_{i,q}} \quad \text{where} \quad s_{i,q} = s_{i,q}^{ah} + s_{i,q}^{be}$$

• To be used in the integration of the Euler equations:

$$\rho_i^{n+1} = \rho_i^n - \rho_i^n (\nabla \cdot \underline{v})_i \Delta t$$

$$\underline{v}_i^{n+1} = \underline{v}_i^n - \frac{\nabla p_i}{\rho_i^n} \Delta t \qquad e_i^{n+1} = e_i^n - \frac{\nabla \cdot (p \underline{v})_i}{\rho_i^n} \Delta t$$

 7) Lanzafame (200?) – The treatment of the Riemann problem in the Euler equations involves a dissipation either via an explicit artificial viscosity contribution or via a native dissipation in the Godunov solver themselves (Park & Kwon 2003). The key concept is that the physical interpretation of the application of such a dissipation in the pressure terms corresponds to a reformulation of the equation of state (EOS) for inviscid ideal flows, whose equation:

$$p^{(G)} = (\gamma - 1)\rho\varepsilon$$

• Is strictly applied in fluid dynamics only to describe either equilibrium conditions or "quasi-static" trasformations. In the case of gas collisions, it modifies as:

$$p^* = (\gamma - 1)\rho\varepsilon + other$$

• The further term, within the pressure expression, takes into account the velocity of perturbation propagation (Monaghan 1997). This velocity equals the ideal gas sound velocity c_s whenever we treat static or rarefying gases. Instead, it includes the "compression velocity" term: $\underline{v}_{ij} \cdot \underline{r}_{ij} / |\underline{r}_{ij}|$ in the case of shocks. In the first case, we write the EOS for inviscid gases as:

$$p^{(G)} = \frac{\rho}{v} c_s^2$$

• Where $c_s^{\gamma} = (\gamma p / \rho)^{1/2} = (\gamma (\gamma - 1)\varepsilon)^{1/2}$ Instead, in the second case, the

• New formulation for the EOS is:

•
$$p^* = \begin{cases} \frac{\rho}{\gamma} c_s^2 \left(1 - \frac{v_{shock}}{c_s}\right)^2 & \text{if } v_{shock} < 0 \\ \frac{\rho}{\gamma} c_s^2 & \text{if } v_{shock} \ge 0 \end{cases}$$

• In the SPH, being:
$$p_i^* = \frac{\rho_i}{\gamma} c_{si}^2 \left(1 - \frac{v_{shock}}{c_{si}}\right)^2$$

•
$$v_{shock} = \begin{cases} \frac{\underline{v}_{ij} \cdot \underline{r}_{ij}}{|\underline{r}_{ij}|} & \text{if } \underline{v}_{ij} \cdot \underline{r}_{ij} < 0\\ 0 & \text{otherwise} \end{cases}$$

- This formulation introduces the "shock pressure term": $\rho \left(v_{shock}^2 2v_{shock}c_s \right) / \gamma$ whose dependence on linear and quadratic power on $v_{ij} \cdot \underline{r}_{ij} / |\underline{r}_{ij}|$ is analogue to both the linear and quadratic components of the artificial viscosity • term (9). These contributions involve a dissipation, whose effect correspond to an increase of the gas pressure. Adopting the reformulated pressure p_i^* within the SPH formulation of the momentum and energy equations, we get:



- A dissipation is always necessary to solve the hyperbolic Euler equation • system either through an explicit artificial viscosity, or through an always dissipative Godunov solver (Park & Kwon 2003).
- Therefore, it could be time to consider a reformulation of the perfect flow EOS • including a physical dissipation due to the presence of discontinuities in the flow producing non-reversible compressions.

• To give an empirical more general EOS,

$$p^* = \frac{\rho}{\gamma} c_s^2 \left(1 - C \frac{v_R}{c_s} \right)^2$$

• where $C \to 1$ for $v_R = \underline{v}_{ij} \cdot \underline{r}_{ij} / |\underline{r}_{ij}| < 0$, while $C \to 0$ otherwise.

• As for C we propose:

$$C = \frac{1}{\pi} \cot^{-1} \left(R \frac{v_R}{c_s} \right)$$

- Where R >> 1. $R \approx \lambda/d$ where λ is the mean free path and d is the mean linear dimension of molecules.
- Tests as far as the1D shock tube are concerned are accomplished for $\gamma = 5/3$ and $\underline{v} = 0$ at time T=0. Results are compared with "analytical" ones.
- Very impressive results on both 1D and 2D simulations:



Applications: Accretion Discs in Close Binaries

 $M_1 = 1M; M_2 = 0.25, 0.5, 1, 2, 2.5M_{\odot}$

- $r_{12} \approx 10^6$ Km in our models
- Non-dimensional equations Normalization factors:

$$M = M_1 + M_2 = 1$$
$$r = r_{12} = 1$$
$$\omega_{orbit} = 1$$

Free boundary conditions at disc inner and outer edges

• Disc inner edge:

Particle free fall onto the primary star. Particle are simply eliminated when their radial distance from the primary star $r_1 \le r_{in} \ge 2h$

• Disc outer edge:

Particle are lost in the outer space. Particle are eliminated when their radial distance from the primary star $r_1 > r_{out} \cong r_{L1}$, where r_{L1} is the radial distance of the inner Lagrangian point L1.

Stationary state disc models

• Stationary state disc configuration is fulfilled when the total number of disc particles is statistically constant (balance among particles injected, accreted and ejected).









- Balsara, D.S., 1995, JCoPh 121, 357.
- Inutsuka, S., 2002, JCoPh 179, 238.
- Lucy, A., 1977, AJ 82, 1013.
- Meglicki, Z., Wickramasinghe, D. & Bicknell, G.V., 1993, MNRAS 264, 691
- Molteni, D. & Bilello, C., MSAIS 2003, 1, 36.
- Monaghan, J.J., 1997, JCoPh 136, 298.
- Monaghan, J.J., 1992, ARAA 30, 543.
- Morris, J.P. & Monaghan, J.J., 1997, JCoPh 136, 41.
- Parshikov, A.N. & Medin, S.A., 2002, JCoPh 180, 358.
- Park, S.H. & Kwon, J.H., 2003, JCoPh 188, 524.