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Particles spatial merging in 2D PIC codes

Particle-In-Cell (PIC) simulations require large machine-time to process particles charge assignment and motion. Moreover coupling such methods with Monte-Carlo-Collisional (MCC) modules causes another expensive computational cost to simulate particle multiple collisions with background gas and domain boundaries. Merging many particles in few particles with increased weights is a widely used accelerating technique. A merging procedure based on charge conservation on a spatial 2D domain is here proposed to avoid an exponentially increasing number of particles per cell during the simulation. Two different strategies are here presented, based on first and second order charge moments conservation. If coupled with a splitting technique, the technique should increase performances of both PIC and MCC module reducing noise in electric field solution and increasing samples representativeness in stochastic calculations.

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Abstract

Particle-In-Cell (PIC) simulations require large machine-time to process particles charge assignment and motion. Moreover coupling such methods with Monte-Carlo-Collisional (MCC) modules causes another expensive computational cost to simulate particle multiple collisions with background gas and domain boundaries. Merging many particles in few particles with increased weights is a widely used accelerating technique. A merging procedure based on charge conservation on a spatial 2D domain is here proposed to avoid an exponentially increasing number of particles per cell during the simulation. Two different strategies are here presented, based on first and second order charge moments conservation. If coupled with a splitting technique, the technique should increase performances of both PIC and MCC module reducing noise in electric field solution and increasing samples representativeness in stochastic calculations.

Contents

1 Introduction

The PIC method is based upon super-particles (or simulation) particles, which represent an ensemble of many real particles. A weight w, equal to the number of real particles represented by the super-particle, can be assigned to each simulation particle in order to account the total charge of the collapsed ensemble and to preserve the charge-mass ratio q/m.

PIC codes require considerably large computation time, since it scales with the number of particles N, which must be kept sufficiently high to reduce the simulation noise (proportional to $1/\sqrt{N}$) [1]. In the case of plasma discharge evolution, the number of charged particles increases exponentially, varying tipically of several orders of magnitude. This consequently leads to an increasing computation time demand. A way to improve considerably the simulation speed is the reduction of the number N of super-particles with a consequent increase of their weight w. Such a procedure has to be performed without the violation of charge and energy conservation laws.

A first rough approach could be based on a typical variance reduction technique of the Monte Carlo methods, called *russian roulette*. When a threshold for N is reached, a survival probability P_s is defined as the ratio between the reduced number N' of super-particle at the next time-step and the actual number N. Cycling on the N simulation particles, a survival probability P_s will be common to each one and a random number R will be extracted from a pseudo-random sequence to check if the particle will die or survive (by comparison with P_s). Moreover, each survived particle ($\sim N'$ in total) will have an increased weigth $w' = wN/N'$. The total charge will be globally conserved if the sample of particles is sufficiently large. Nonetheless, little fluctuations in the mean energy of the charged particles can be observed, since the technique is careless of their energy; locally, any conservation law is not satisfied: lower is the number of particles per cell, greater is the induced error. Finally, the technique isn't optimal from the point of view of the MCC module: if a region of space undergoes a depletion of particles during the simulation, the application of the russian-roulette will further decrease their density and, consequently, the statistics of the events related to those particles will result poorer and poorer.

In the past, particle splitting and shifting methods were developed in one-dimensional systems [2, 3] to overcome the usual problem of particles rise and contemporaneous depletion in the cathode fall region. This method was based on the separation of the particle into two species for the bulk and cathode regions of the system: large-weighted particles are used in the bulk and small-weighted ones in the depleted region. The net effect is a speed-up of the simulation and a reduction of spurious fluctuations.

Shon *et al.* [4] presented an alternative approch aimed to preserve, not only the conservation laws, but also to reduce the time of simulation. If the particle number reaches the limit suggested by a certain criteria, new large-weighted particle species are created by meshing the phase space. The particle number is reduced without discriminating the bulk and cathode fall region. The method was extended to two-dimensional systems: at least two new super-particles are necessary to merge the particles of a cell in order to conserve the

charge densities on the nodes of the grid. Lapenta [5], instead, proposed binary and ternary proceddures for particle rezoning in collisionless PIC with generic spline weighting functions.

In the next section, an analysis of a merging technique for the bidimensional spatial coordinates of the phase space is presented together with an interesting analogy with well-known mechanical properties. Only the PIC bilinear interpolation weighting is studied in this first stage, since it can be successfully applied both in cartesian and cylindrical coordinate systems.

2 Shape factor and grid moments

All the physical quantities related to the particles are weighted on the grid points on through the so called *shape factor* [6, 7]. All the moments of the particle distribution on the grid points are easily defined by [5]

$$M_g = \sum_p q_p S(\vec{x}_g - \vec{x}_p)\vec{f}(\vec{v}_p)\,,$$

where q_p is the particle charge and $\vec{f}(\vec{v}_p)$ is a generic function of the particle velocity. In particular, when $\vec{f}(\vec{v}_p) = 1$, $\vec{v}_p$ and $\vec{v}_p\vec{v}_p$ one obtains the charge density, current density and pressure tensor respectively.

For example, a widely diffuse choice in PIC code is the first order weighting (PIC-CIC); in this case the shape factor assumes the form

$$S(\vec{x}_g - \vec{x}_p) = \begin{cases} \dfrac{\prod_{j=1}^{N_\mathrm{D}} (\Delta x_{g,j} - |x_{p,j} - x_{g,j}|)}{\prod_{j=1}^{N_\mathrm{D}} \Delta x_{g,j}} & \text{if } |x_{p,j} - x_{g,j}| \le \Delta x_{g,j}\ \forall j \\ 0 \quad \text{otherwise} \end{cases} \tag{1}$$

where $\vec{x}_g$ and $\vec{x}_p$ are respectively the grid point and particle positions in N_D dimensions, while $\Delta x_{g,j}$ is the cell width in the j-th direction.

In kinetic PIC codes, the equivalence between two sets of particles is based on two conditions:

- the two ensembles equally contributes to the grid moments appearing indistinguishable;

- the two sets sample the same velocity distribution function.

Only the first criterion will be treated here. Moreover, in electrostatic codes, the only moment involved in electric field calculation is the first order one: in other words, if a set of N particles has to be merged in a set of $N' < N$, the contribution to charge density on grid points must be the same for the two sets. It will be shown that, for linear interpolation weighting in two dimensions, at least two particles are required to merge an ensemble of N particles lying in the same cell.

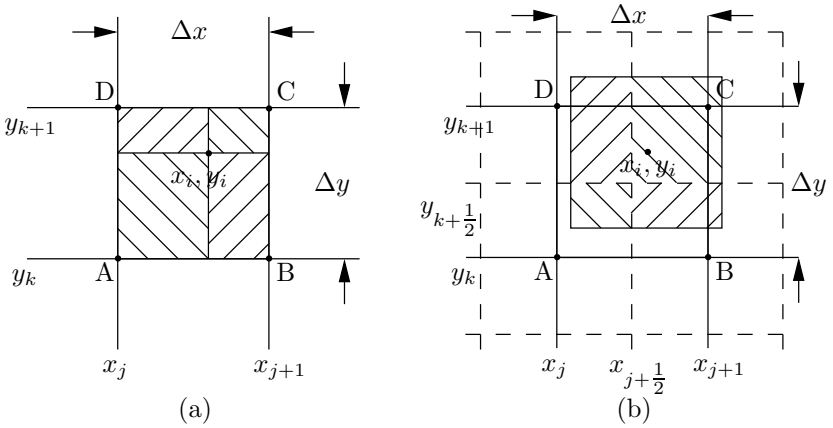

Figure 1: Charge assignment for linear weighting in two dimensions; areas are assigned in the PIC bilinear interpolation interpretation (a) and in the CIC cloud one (b). The two methods lead to the same result in cartesian geometry.

3 Cartesian 2D coordinate systems

It's widely known [1] that linear-weighting (first-order) charge assignment with PIC and CIC logic are equivalent in cartesian coordinates, while they differ in cylindrical and spherical coordinate systems. The shape factor of (1) can be represented in two dimensions (x, y) as shown in figure 1. The two area-weighting methods are completely equivalent, even if based on slightly different interpretations of the particle. The PIC bilinear interpolation is widely used as weighting function both in cartesian and cylindrical coordinate systems.

3.1 Conservation laws

Referring to figure 1-a for variables meaning, the generic i-th particle of local coordinates inside the cell (x_i, y_i), weight w_i and charge q ($q_i = w_i q$ is the effective charge of the simulation particle) contributes to nodes charges on the base of the following fractions:

$$q_{\mathrm{A},i} = w_i q \frac{(\Delta x - x_i)(\Delta y - y_i)}{\Delta x \Delta y} = q w_i \rho_{\mathrm{A},i} \tag{2a}$$

$$q_{\mathrm{B},i} = w_i q \frac{x_i(\Delta y - y_i)}{\Delta x \Delta y} = q w_i \rho_{\mathrm{B},i} \tag{2b}$$

$$q_{\mathrm{C},i} = w_i q \frac{x_i y_i}{\Delta x \Delta y} = q w_i \rho_{\mathrm{C},i} \tag{2c}$$

$$q_{\mathrm{D},i} = w_i q \frac{(\Delta x - x_i) y_i}{\Delta x \Delta y} = q w_i \rho_{\mathrm{D},i}\,. \tag{2d}$$

Assuming a generic subset of N particles in the cell, their total charge contribution to each node P (with P=A,B,C or D) results

$$q_P = q \sum_{i=1}^{N} w_i \rho_{P,i} \,; \tag{3}$$

then, the total charge in the cell is given by

$$\sum_{P=\mathrm{A}}^{\mathrm{D}} q_P = q \sum_{P=\mathrm{A}}^{\mathrm{D}} \sum_{i=1}^{N} w_i \rho_{P,i} = q \sum_{i=1}^{N} w_i \sum_{P=\mathrm{A}}^{\mathrm{D}} \rho_{P,i} = q \sum_{i=1}^{N} w_i \,. \tag{4}$$

The fraction of the total charge to each node can be defined by the ratio between the total charge in P (3) and the total charge in the cell (4):

$$\rho_P = \frac{q_P}{\sum_{P=\mathrm{A}}^{\mathrm{D}} q_P} = \frac{\sum_{i=1}^{N} w_i \rho_{P,i}}{\sum_{i=1}^{N} w_i} \,,$$

which obviously represents a weighted average value.

By definition of $\rho_{P,i}$, it's evident that $\sum_{P=\mathrm{A}}^{\mathrm{D}} \rho_{P,i} = 1$ for each i; then, it follows that

$$\sum_{P=\mathrm{A}}^{\mathrm{D}} \rho_P = \sum_{P=\mathrm{A}}^{\mathrm{D}} \frac{\sum_{i=1}^{N} w_i \rho_{P,i}}{\sum_{i=1}^{N} w_i} = \frac{\sum_{i=1}^{N} w_i \sum_{P=\mathrm{A}}^{\mathrm{D}} \rho_{P,i}}{\sum_{i=1}^{N} w_i} = 1 \,, \tag{5}$$

as foreseeable by reasoning on superposition effects.

Finally, from (2) it arises also the indentity

$$\rho_{\mathrm{A},i} \rho_{\mathrm{C},i} = \rho_{\mathrm{B},i} \rho_{\mathrm{D},i} \,,$$

which cannot be extended by summation to $\rho_{\mathrm{A}} \rho_{\mathrm{C}} = \rho_{\mathrm{B}} \rho_{\mathrm{D}}$, because of crossed products between different particles.

3.2 Non dimensional quantities and change of reference

Generally speaking, in substituting of a set of N particles with a set of N' particles, one should conserve the total charge on each grid node; shifting the problem to the cell and summing the contributions of each cell on the corresponding nodes, the condition can be expressed in terms of conservation of the charge fractions on the cell nodes. For greater convenience, the local coordinates on the cell will be normalized to Δx and Δy as

$$\xi_i = \frac{x_i}{\Delta x}$$
$$\eta_i = \frac{y_i}{\Delta y} \,,$$

with $\xi_i, \eta_i \in [0, 1]$. Moreover, the weigths w_i will be referred to the total weight $\sum_{i=1}^{N} w_i$ introducing

$$\omega_i = \frac{w_i}{\sum_{i=1}^{N} w_i} \,.$$

Making use of the prime to identify the merged particles properties, their coordinates must satisfy the following conditions:

$$\sum_{i=1}^{N} \omega_i(1-\xi_i)(1-\eta_i) = \sum_{i'=1'}^{N'} \omega_{i'}(1-\xi_{i'})(1-\eta_{i'}) = \rho_{\mathrm{A}} \tag{7a}$$

$$\sum_{i=1}^{N} \omega_i\xi_i(1-\eta_i) = \sum_{i'=1'}^{N'} \omega_{i'}\xi_{i'}(1-\eta_{i'}) = \rho_{\mathrm{B}} \tag{7b}$$

$$\sum_{i=1}^{N} \omega_i\xi_i\eta_i = \sum_{i'=1'}^{N'} \omega_{i'}\xi_{i'}\eta_{i'} = \rho_{\mathrm{C}} \tag{7c}$$

$$\sum_{i=1}^{N} \omega_i(1-\xi_i)\eta_i = \sum_{i'=1'}^{N'} \omega_{i'}(1-\xi_{i'})\eta_{i'} = \rho_{\mathrm{D}}\,. \tag{7d}$$

where the leftmost and rightmost sides are known. The normalization condition of (5) makes the four equations linearly dependent. A further condition must be added in order to conserve the total weight of the ensemble:

$$\sum_{i=1}^{N} \omega_i = \sum_{i'=1'}^{N'} \omega_{i'} = 1\,.$$

A total of 4 equations, is obtained for the unknowns $(\omega_{i'}, \xi_{i'}, \eta_{i'})$. One particle is not enough to satisfy all of them: it would indeed introduce a second closure equation given by $\rho'_{\mathrm{A}}\rho'_{\mathrm{D}} = \rho'_{\mathrm{B}}\rho'_{\mathrm{C}}$ which, in general, is not satisfied by an ensemble of more than one particle: $\rho_{\mathrm{A}}\rho_{\mathrm{D}} \neq \rho_{\mathrm{B}}\rho_{\mathrm{C}}$.

Then, at least two particles are necessary to solve the system. Having only 4 equations in 6 unknowns, one can chose arbitrarily 2 of them. While it would be wise to merge N particles into two equally weighted particles, no particular condition can be imposed on the particles coordinates a priori. Only bounding conditions could be used: the two new particles must belong to the same cell of the old set.

Summing (7c) with (7b) and (7d) respectively, the system is simplified in

$$\sum_{i=1}^{N} \omega_i = \sum_{i'=1'}^{N'} \omega_{i'} = 1 \tag{8a}$$

$$\sum_{i=1}^{N} \omega_i\xi_i = \sum_{i'=1'}^{N'} \omega_{i'}\xi_{i'} = \rho_{\mathrm{B}} + \rho_{\mathrm{C}} \tag{8b}$$

$$\sum_{i=1}^{N} \omega_i\eta_i = \sum_{i'=1'}^{N'} \omega_{i'}\eta_{i'} = \rho_{\mathrm{C}} + \rho_{\mathrm{D}} \tag{8c}$$

$$\sum_{i=1}^{N} \omega_i\xi_i\eta_i = \sum_{i'=1'}^{N'} \omega_{i'}\xi_{i'}\eta_{i'} = \rho_{\mathrm{C}}\,. \tag{8d}$$

The first two equations represent the equivalence between the barycenter (or centroid) coordinates of the two sets of particles, since it's easy to show that in the normalized reference they become

$$\xi_{\mathrm{G}} = \frac{1}{\Delta x}\frac{\sum_{i=1}^{N} w_i x_i}{\sum_{i=1}^{N} w_i} = \sum_{i=1}^{N} \omega_i \xi_i$$
$$\eta_{\mathrm{G}} = \frac{1}{\Delta y}\frac{\sum_{i=1}^{N} w_i y_i}{\sum_{i=1}^{N} w_i} = \sum_{i=1}^{N} \omega_i \eta_i \,.$$

This shouldn't astonish the reader since the two terms $\rho_{\mathrm{B}} + \rho_{\mathrm{C}}$ and $\rho_{\mathrm{C}} + \rho_{\mathrm{D}}$ represent respectively the fraction of the total charge in the second horizontal and vertical half of the cell respectively.

Since $\sum_{i=1}^{N} \omega_i = 1$, it's usefull to change the reference shifting it to the barycenter of the ensembles:

$$\sum_{i'=1'}^{N'} \omega_{i'}(\xi'_i - \xi_{\mathrm{G}}) = \sum_{i'=1'}^{N'} \omega_{i'}\zeta_{i'} = 0 \tag{10a}$$
$$\sum_{i'=1'}^{N'} \omega_{i'}(\eta'_i - \eta_{\mathrm{G}}) = \sum_{i'=1'}^{N'} \omega_{i'}\gamma_{i'} = 0\,, \tag{10b}$$

with $\zeta_{i'} \in [-\xi_{\mathrm{G}}, 1-\xi_{\mathrm{G}}]$ and $\gamma_{i'} \in [-\eta_{\mathrm{G}}, 1-\eta_{\mathrm{G}}]$. Working on (8d) in order to obtain ζ_i and γ_i, it follows that

$$\begin{aligned}\rho_{\mathrm{C}} = \sum_{i=1}^{N} \omega_i \xi_i \eta_i &= \sum_{i=1}^{N} \omega_i(\zeta_i\gamma_i + \gamma_i\xi_{\mathrm{G}} + \eta_{\mathrm{G}}\zeta_i + \xi_{\mathrm{G}}\eta_{\mathrm{G}}) = \\ &= \sum_{i=1}^{N} \omega_i\zeta_i\gamma_i + \xi_{\mathrm{G}}\sum_{i=1}^{N}\omega_i\gamma_i + \eta_{\mathrm{G}}\sum_{i=1}^{N}\omega_i\zeta_i - \xi_{\mathrm{G}}\eta_{\mathrm{G}} = \\ &= \sum_{i=1}^{N} \omega_i\zeta_i\gamma_i + \xi_{\mathrm{G}}\eta_{\mathrm{G}}\,,\end{aligned} \tag{11}$$

where (10) have been used. Equation (8d) can then be substitued by

$$\sum_{i=1}^{N} \omega_i\zeta_i\gamma_i = \sum_{i'=1'}^{N'} \omega_{i'}\zeta_{i'}\gamma_{i'} = \rho_{\mathrm{C}} - (\rho_{\mathrm{B}} + \rho_{\mathrm{C}})(\rho_{\mathrm{C}} + \rho_{\mathrm{D}})\,.$$

3.3 The inertia tensor analogy

The total system of equations in the new normalized reference centered in the centroid of charge of the cell is

$$\sum_{i'=1'}^{N'} \omega_{i'} = 1 \tag{12a}$$

$$\sum_{i'=1'}^{N'} \omega_{i'}\zeta_{i'} = 0 \tag{12b}$$

$$\sum_{i'=1'}^{N'} \omega_{i'}\gamma_{i'} = 0 \tag{12c}$$

$$\sum_{i'=1'}^{N'} \omega_{i'}\zeta_{i'}\gamma_{i'} = \rho_{\mathrm{C}} - (\rho_{\mathrm{B}} + \rho_{\mathrm{C}})(\rho_{\mathrm{C}} + \rho_{\mathrm{D}})\,. \tag{12d}$$

The first equation is the condition of conservation of the total charge in the cell. The second and third ones define the coincidence of the barycenter of the two sets of particles. The fourth one is a sort of non-diagonal component of a pseudo-inertia tensor: in classical mechanics, the inertia tensor is defined as a symmetric matrix in the form of

$$\vec{\vec{I}} = \begin{pmatrix} I_{xx} & I_{xy} & I_{xz} \\ I_{yx} & I_{yy} & I_{yz} \\ I_{zx} & I_{zy} & I_{zz} \end{pmatrix},$$

with components I_{jk} given by

$$I_{jk} = \delta_{jk} \sum_{i=1}^{N} w_i (x_{l,i}^2 + x_{m,i}^2) + (\delta_{jk} - 1) \sum_{i=1}^{N} w_i x_{j,i} x_{k,i}\,,$$

where $x_{j,i}$ is the coordinate along the j-th direction (x, y or z) of the generic i-th particle with weight w_i in the system (k, l, m having the same meaning of j); δ_{lm} is the Kroneker delta function. If the moment of inertia tensor has been calculated for rotations about the centroid of the system, it is relatively easy to compute the tensor for rotations offset from the centroid, by the shifting formula (known as *Huygens law*)

$$I_{jk}^{\mathrm{displaced}} = I_{jk}^{\mathrm{centroid}} + w(r^2\delta_{jk} - r_j r_k)\,, \tag{13}$$

$\vec{r} = (r_x, r_y, r_z)$ being the 3D vector by which the rotation axis is displaced from the centroid. Equation (13) explains the meaning of (11) which modifies the $\xi\eta$ component of the inertia tensor changing reference to the barycenter G centered (ζ, γ) one. The mechanical analogy suggests to consider (12d) as describing the particles distribution disuniformity in the cell: its sign depends on the particles distribution in the four quarters defined by the (ζ, γ) axis.

The conservation of the charge fractions on the nodes doesn't require any other condition if a first order interpolation is used. Anyway, inertia moments conservation conditions will be examined in section 5.

4 A first solution: equally weighted particles

The system obtained by imposition of charge conservation on the nodes has multiple acceptable solutions. However, it is wise to chose the lower number of equally weighted merging particles in order to optimize the particles number reduction and to homogenize weights distribution. The choice $N' = 2$ and $\omega_{1'} = \omega_{2'} = 1/2$ allows to reduce the number of unknowns to the 4 particles coordinates.

4.1 The merged particles coordinates

The system of (12) can be easily rewritten for $N' = 2$ equally weighted particles, leading to

$$\begin{aligned} &\zeta_{1'} = -\zeta_{2'} \\ &\gamma_{1'} = -\gamma_{2'} \\ &\frac{1}{2}\zeta_{1'}\gamma_{1'} + \frac{1}{2}\zeta_{2'}\gamma_{2'} = I_{\zeta\gamma}\,. \end{aligned}$$

Having three equations in four unknowns, the system is not closed. One of the particles coordinates can be arbitrarily chosen as a parameter; then the other three will be expressed as functions of it. Moreover, it can be noticed by the first two equations (conservation of the system barycenter) that the particles must lie on a line containing the charge centroid, on opposite sides of it, at the same distance from it. The symmetry of the system allows to reduce the field of variability for the chosen parameter to positive or negative values only. Once fixed $\zeta_{1'} > 0$, the other three coordinates are

$$\zeta_{2'} = -\zeta_{1'} \tag{15a}$$

$$\gamma_{1'} = \frac{I_{\zeta\gamma}}{\zeta_{1'}} \tag{15b}$$

$$\gamma_{2'} = -\frac{I_{\zeta\gamma}}{\zeta_{1'}}\,. \tag{15c}$$

A bounded interval of variability must be defined for $\zeta_{1'}$.

4.2 Cell coordinates limits

The new particles coordinates are not free in the whole 2D space, but must be bounded by the cell limits. For the coordinate systems considered up to now, one has

$$\begin{aligned} &x \in [0, \Delta x]\,, && \xi \in [0, 1]\,, && \zeta \in [-\xi_{\mathrm{G}}, 1 - \xi_{\mathrm{G}}]\,, \\ &y \in [0, \Delta y]\,, && \eta \in [0, 1]\,, && \gamma \in [-\eta_{\mathrm{G}}, 1 - \eta_{\mathrm{G}}]\,. \end{aligned}$$

Working in the (ζ, γ) reference for conveninence, the coordinates limits on $\zeta_{1'}$, $\zeta_{2'}$, $\gamma_{1'}$ and

$\gamma_{2'}$ and the assumptions on $\zeta_{1'}$ affect the restriction limits over $\zeta_{1'}$ as follows

$$\begin{aligned}
&\zeta_{1'} \in [-\xi_G, 1-\xi_G] \quad \Rightarrow \quad \zeta_{1'} \in]0, 1-\xi_G] \\
&\zeta_{2'} \in [-\xi_G, 1-\xi_G] \quad \Rightarrow \quad \zeta_{1'} \in]0, \xi_G] \\
&\gamma_{1'} \in [-\eta_G, 1-\eta_G] \quad \Rightarrow \quad \begin{cases} \zeta_{1'} \in]-\frac{I_{\zeta\gamma}}{\eta_G}, \infty[& \text{if } I_{\zeta\gamma} < 0 \\ \zeta_{1'} \in]\frac{I_{\zeta\gamma}}{(1-\eta_G)}, \infty[& \text{if } I_{\zeta\gamma} \geq 0 \end{cases} \\
&\gamma_{2'} \in [-\eta_G, 1-\eta_G] \quad \Rightarrow \quad \begin{cases} \zeta_{1'} \in]-\frac{I_{\zeta\gamma}}{\eta_G}, \infty[& \text{if } I_{\zeta\gamma} < 0 \\ \zeta_{1'} \in]\frac{I_{\zeta\gamma}}{(1-\eta_G)}, \infty[& \text{if } I_{\zeta\gamma} \geq 0\,. \end{cases}
\end{aligned}$$

The multiple conditions obtained for $\zeta_{1'}$ can be gathered in

$$\zeta_{1'}^{\min} = \max\left\{\frac{|I_{\zeta\gamma}|}{2\eta_G}, \frac{|I_{\zeta\gamma}|}{2(1-\eta_G)}\right\} < \zeta_{1'} < \min\{\xi_G, (1-\xi_G)\} = \zeta_{1'}^{\max}\,,$$

where the module has been used to contract the limits for $I_{\zeta\gamma} \lessgtr 0$, while the min and max functions allow to obtain the smallest variability interval. Since $\xi_G, \eta_G \in [0,1]$, four cases can be distinguished

$$\begin{aligned}
\zeta_{1'}^{\min} &= \begin{cases} \frac{|I_{\zeta\gamma}|}{2(1-\eta_G)} & \text{if } \eta_G \geq \frac{1}{2} \\ \frac{|I_{\zeta\gamma}|}{2\eta_G} & \text{if } \eta_G < \frac{1}{2} \end{cases} \\
\zeta_{1'}^{\max} &= \begin{cases} \xi_G & \text{if } \xi_G < \frac{1}{2} \\ 1-\xi_G & \text{if } \xi_G \geq \frac{1}{2}\,. \end{cases}
\end{aligned}$$

Since the centrigual inertia moment is conserved for both the sets of N and N' particles, it's easy to show (even graphically) that the condition can be reduced to the following four conditions

$[\zeta_{1'}^{\min}, \zeta_{1'}^{\max}] \neq \emptyset$	$\xi_G < \frac{1}{2}$	$\xi_G \geq \frac{1}{2}$
$\eta_G \geq \frac{1}{2}$	$\lvert I_{\zeta\gamma}\rvert < \xi_G(1-\eta_G)$	$\lvert I_{\zeta\gamma}\rvert < (1-\xi_G)(1-\eta_G)$
$\eta_G < \frac{1}{2}$	$\lvert I_{\zeta\gamma}\rvert < \xi_G\eta_G$	$\lvert I_{\zeta\gamma}\rvert < (1-\xi_G)\eta_G$

Once chosen $\zeta_{1'}$ in the allowed interval, all the other coordinates are known from (15). The case of null centrifugal inertia moment leads immediately to $\gamma_{1'} = \gamma_{2'} = 0$ with no lack of generality.

The arbitrarity $\zeta_{1'}$ prevent from obtaining the starting particles when $N = 2$ is considered: even in the case $\omega_1 = \omega_2 = 1/2$ the $N' = 2$ new particles would be placed in different positions inside the cell.

5 An alternative solution

The solution presented in section 4 is self-consistent but allows a degree of freedom in the choice of a particle coordinate. Exploiting the inertia tensor analogy, one could expect that

the conservation of higher order moments allow to determine exactly the position of the two particles in the cell without any arbitratily chosen parameter. Unfortunately, it will be shown that this is not possible and, moreover, particles loose the equal weight property.

5.1 Second order moments for two particles

In section3.3, it was shown that the system (12) is equivalent to total charge, charge centroid and centrifugal pseudo-inertia moment conservation.

The analogy with the inertia tensor and the not closed form of the system suggest to add more inertia moments conservation laws in order to determine univocally all the 6 unknowns. Therefore, three further conditions can be written:

$$\sum_{i=1}^{N} \omega_i \zeta_i^2 = \sum_{i'=1'}^{N'} \omega_{i'} \zeta_{i'}^2 = I_{\gamma\gamma} \tag{16a}$$

$$\sum_{i=1}^{N} \omega_i \gamma_i^2 = \sum_{i'=1'}^{N'} \omega_{i'} \gamma_{i'}^2 = I_{\zeta\zeta} \tag{16b}$$

$$\sum_{i=1}^{N} \omega_i (\zeta_i^2 + \gamma_i^2) = \sum_{i'=1'}^{N'} \omega_{i'} (\zeta_{i'}^2 + \gamma_{i'}^2) = I_{\varsigma\varsigma}\,, \tag{16c}$$

where ς betoken the third direction, perpendicular to the plane (ζ, γ); the other components are all zero since $\varsigma_i = 0\ \forall i$. It's clear that (16) are linearly dependet: for a system of particles lying on a plane, $I_{\varsigma\varsigma}$ is known as polar moment and it represents the invariant of the reduced 2×2 tensor for the ζ and γ components. Then, for $N' = 2$ particles, a system of 6 equations in 6 unknowns is obtained. It can be shown that it is not closed. Indeed, for a system of 2 particles, (12b) and (12c) give immediately

$$\frac{\zeta_{1'}}{\zeta_{2'}} = \frac{\gamma_{1'}}{\gamma_{2'}} = -\frac{\omega_{2'}}{\omega_{1'}}\,,$$

that means the two particles lie on a line passing through the centroid of the system and have distances inversely proportional to their weights, as a gneralization of (15a) and (15b). This condition implies

$$I_{\gamma\gamma} I_{\zeta\zeta} = I_{\zeta\gamma}^2\,, \tag{17}$$

not valid, in general, for a system of $N' > 2$ particles. Then, one must conclude that a system of $N > 2$ particles cannot be replaced by only two particles on the base of total weight, centroid position and inertia moments conservation.

5.2 Polar inertia moment conservation

Since the axial inertia moments cannot be both conserved, one could ask for the conservation of the polar one, at least.

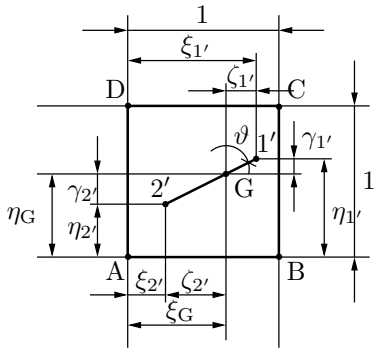

Figure 2: Position of the two merged particles in the normalized reference $(\xi, \eta) - (\zeta, \gamma)$.

If one considers $N' = 2$ and works with $\omega_{1'}$ and $\omega_{1'}$ as parameters, the two particles coordinates would then be given by

$$\zeta_{1'} = -\frac{\omega_{2'}}{\omega_{1'}}\zeta_{2'} \tag{18a}$$

$$\gamma_{1'} = -\frac{\omega_{2'}}{\omega_{1'}}\gamma_{2'} \tag{18b}$$

$$\frac{\omega_{1'}}{\omega_{2'}}\zeta_{1'}\gamma_{1'} = I_{\zeta\gamma} = \rho_C - (\rho_B + \rho_C)(\rho_C + \rho_D) \tag{18c}$$

$$\frac{\omega_{1'}}{\omega_{2'}}(\zeta_{1'}^2 + \gamma_{1'}^2) = I_{\varsigma\varsigma} \tag{18d}$$

where the first two equations define the positions of the two particles as aligned with the centroid on opposite sides of it; the third equation gives the direction in the plane (ζ, γ) of the line connecting the two particles and containing the centroid, while the last equation represents a weighted distance of the particles with respect to their barycenter. Introducing $\varrho_{1'} = \sqrt{\zeta_{1'}^2 + \gamma_{1'}^2} = \sqrt{\frac{\omega_{2'}}{\omega_{1'}} I_{\varsigma\varsigma}}$ and the angle ϑ between the line containing the two particles and the direction of ζ, as represented in figure 2, by trigonometric well-known formulae, (18a) and (18b) are rewritten in the form

$$\zeta_{1'} = -\frac{\omega_{2'}}{\omega_{1'}}\zeta_{2'} = \varrho_{1'}\cos\vartheta \tag{19a}$$

$$\gamma_{1'} = -\frac{\omega_{2'}}{\omega_{1'}}\gamma_{2'} = \varrho_{1'}\sin\vartheta \tag{19b}$$

and, then, (18c) gives

$$I_{\zeta\gamma} = \frac{\omega_{1'}}{\omega_{2'}}\zeta_{1'}\gamma_{1'} = \frac{\omega_{1'}}{\omega_{2'}}\varrho_{1'}^2\cos\vartheta\sin\vartheta = \frac{1}{2}I_{\varsigma\varsigma}\sin(2\vartheta)\,, \tag{20}$$

with $\vartheta \in [-\pi/2, \pi/2[$, due to symmetry reasons. The last equation can be inverted in order to obtain the angle ϑ defined as

$$\vartheta = \frac{1}{2}\arcsin\left(\frac{2I_{\zeta\gamma}}{I_{\varsigma\varsigma}}\right)\,; \tag{21}$$

the sine inverse function is defined only for arguments in the interval $[-1, 1]$, but it is easy to show that

$$\left|\frac{2I_{\zeta\gamma}}{I_{\varsigma\varsigma}}\right| \leq 1 \Leftrightarrow I_{\varsigma\varsigma} \geq \pm 2I_{\zeta\gamma} \Leftrightarrow \sum_{i=1}^{N} \omega_i(\zeta_i^2 + \gamma_i^2) \pm 2\sum_{i=1}^{N} \omega_i \zeta_i \gamma_i \geq 0 \Leftrightarrow$$
$$\Leftrightarrow \sum_{i=1}^{N} \omega_i(\zeta_i \pm \gamma_i)^2 \geq 0$$

is always true for each (ζ_i, γ_i) being a summation of squared terms. Moreover, the angle given by the sine inverse function is inside the interval $[-\pi/2, \pi/2]$ that implies $\vartheta \in [-\pi/4, \pi/4]$.

5.3 The inertia main reference analogy

For a system of two particles, the obtained value of ϑ corresponds to the reference rotation angle which gives the main inertia axis. In general, this doesn't coincide with the reference rotation angle of the initial system containing N particles. The main reference is, indeed, defined as that reference in which the centrifugal inertia moment $I_{\zeta\gamma} = I_{\gamma\zeta}$ is zero; in the rotated reference, the new coordinates are given by

$$\begin{pmatrix} \zeta^* \\ \gamma^* \end{pmatrix} = \begin{pmatrix} \cos\vartheta & \sin\vartheta \\ -\sin\vartheta & \cos\vartheta \end{pmatrix} \begin{pmatrix} \zeta \\ \gamma \end{pmatrix} \qquad \text{with} \qquad \vec{\vec{N}} = \begin{pmatrix} \cos\vartheta & \sin\vartheta \\ -\sin\vartheta & \cos\vartheta \end{pmatrix},$$

and, consequently, the characteristic tensor transformation is

$$\vec{\vec{I^*}} = \vec{\vec{N}}\vec{\vec{I}}\vec{\vec{N}}^T,$$

which leads to

$$I_{\zeta^*\zeta^*} = \frac{I_{\zeta\zeta} + I_{\gamma\gamma}}{2} + \frac{I_{\zeta\zeta} - I_{\gamma\gamma}}{2} - I_{\zeta\gamma}\sin(2\vartheta)$$
$$I_{\gamma^*\gamma^*} = \frac{I_{\zeta\zeta} + I_{\gamma\gamma}}{2} - \frac{I_{\zeta\zeta} - I_{\gamma\gamma}}{2} + I_{\zeta\gamma}\sin(2\vartheta)$$
$$I_{\zeta^*\gamma^*} = \frac{I_{\zeta\zeta} - I_{\gamma\gamma}}{2}\sin(2\vartheta) + I_{\zeta\gamma}\cos(2\vartheta).$$

Note that again $I_{\gamma^*\gamma^*} + I_{\zeta^*\zeta^*} = I_{\gamma\gamma} + I_{\zeta\zeta} = I_{\varsigma\varsigma}$, the polar moment being an invariant of the system. The main reference is obtained by imposing $I_{\zeta^*\gamma^*} = 0$; the conditon gives

$$\tan(2\vartheta) = -\frac{2I_{\zeta\gamma}}{I_{\zeta\zeta} - I_{\gamma\gamma}}, \tag{23}$$

which defines the rotation angle ϑ that nullify the centrifugal moment $I_{\zeta^*\gamma^*}$ and maximize the axial ones $I_{\zeta^*\zeta^*}$ and $I_{\gamma^*\gamma^*}$. It was shown that (17) is always true for a system of 2 particles; then, from (20), applying $\cos(2\vartheta) = \sqrt{1 - \sin^2(2\vartheta)}$, it follows that

$$\tan(2\vartheta) = \frac{\sin(2\vartheta)}{\cos(2\vartheta)} = \frac{2I_{\zeta\gamma}}{\sqrt{I_{\varsigma\varsigma}^2 - 4I_{\zeta\gamma}}},$$

which results equal to (23) if and only if

$$I_{\gamma\gamma} - I_{\zeta\zeta} = \sqrt{I_{\varsigma\varsigma}^2 - 4I_{\zeta\gamma}^2} = \sqrt{I_{\gamma\gamma}^2 + 2I_{\gamma\gamma}I_{\zeta\zeta} + I_{\zeta\zeta}^2 - 4I_{\zeta\gamma}^2} \;\Leftrightarrow\; I_{\gamma\gamma}I_{\zeta\zeta} = I_{\zeta\gamma}^2\,,$$

as previously stated. The conclusion must not surprise, since the main reference for a system of two particles is identified by axis coincident with the line connecting the particles: in this case, it results $I_{\gamma^*\gamma^*} = I_{\zeta^*\gamma^*} = 0$ and only $I_{\zeta^*\zeta^*} \neq 0$ (maximized), while for a system of more than 2 particles the inertia ellipses has two main axes with both $I_{\gamma^*\gamma^*} \neq 0$ and $I_{\zeta^*\zeta^*} \neq 0$. Moreover, it can be noted from (23) that, since the tangent function has a periodicity of π, both ϑ and $\vartheta + \pi/2$ would lead to the same main reference with an inversion of ζ^* and γ^*. In the particular case of two particles, a rotation of $\pi/2$ would nullify the main inertia moment $I_{\zeta^*\zeta^*}$ and maximize $I_{\gamma^*\gamma^*}$.

5.4 The merged particles coordinates

The distances $\varrho_{1'}$ and $\varrho_{2'}$ of the two particles along the main axis are still unknown and strictly dependent on their weights $\omega_{1'}$ and $\omega_{2'}$. Due to the arbitrariness of particles labeling, one can ask the first particle to fall in positive ζ half plane. Paying much attention to the signs, one obtains

$$\begin{aligned}\zeta_{1'} &= \varrho_{1'}\cos\vartheta = \varrho_{1'}\sqrt{1-\sin^2\vartheta}\\ \gamma_{1'} &= \varrho_{1'}\sin\vartheta = \pm\varrho_{1'}\sqrt{1-\cos^2\vartheta}\,,\end{aligned}$$

$\cos\vartheta$ being always positive for each $\vartheta \in [-\pi/2, \pi/2]$ and $\sin\vartheta \geq 0$ only for $\vartheta \in [0, \pi/2]$. Then, working on the squares of sine and cosine, it follows

$$\begin{aligned}\sin^2\vartheta = \frac{1-\cos(2\vartheta)}{2} &\;\Rightarrow\; \cos\vartheta = \sqrt{\frac{1}{2}(1+\cos(2\vartheta))}\\ \cos^2\vartheta = \frac{1+\cos(2\vartheta)}{2} &\;\Rightarrow\; \sin\vartheta = \sqrt{\frac{1}{2}(1-\cos(2\vartheta))}\,.\end{aligned}$$

In order to use (20), the $\cos(2\vartheta)$ has to be converted in $\pm\sqrt{1-\sin^2(2\vartheta)}$ where the positive sign is obtained for $\vartheta \in [-\pi/4, \pi/4]$ and the negative one outside. By substitution, the two coordinates of the first merging particle are

$$\zeta_{1'} = \varrho_{1'}\sqrt{\frac{1}{2}\left(1 \pm \sqrt{1-\sin^2(2\vartheta)}\right)} = \sqrt{\frac{\omega_{2'}}{\omega_{1'}}\frac{I_{\varsigma\varsigma} + \chi\sqrt{I_{\varsigma\varsigma}^2 - 4I_{\zeta\gamma}^2}}{2}} \tag{24a}$$

$$\gamma_{1'} = \pm\varrho_{1'}\sqrt{\frac{1}{2}\left(1 \mp \sqrt{1-\sin^2(2\vartheta)}\right)} = \kappa\sqrt{\frac{\omega_{2'}}{\omega_{1'}}\frac{I_{\varsigma\varsigma} - \chi\sqrt{I_{\varsigma\varsigma}^2 - 4I_{\zeta\gamma}^2}}{2}}\,, \tag{24b}$$

where χ and κ depends on ϑ and modifies only the signs in the expressions as given in the following scheme

$\vartheta \in$	$[-\pi/2, -\pi/4]$	$[-\pi/4, 0]$	$[0, \pi/4]$	$[\pi/4, \pi/2]$
χ	$-$	$+$	$+$	$-$
κ	$-$	$-$	$+$	$+$

The position of the second particle is immediately obtained as

$$\zeta_{2'} = -\frac{\omega_{1'}}{\omega_{2'}}\zeta_{1'} = -\sqrt{\frac{\omega_{1'}}{\omega_{2'}}\frac{I_{\varsigma\varsigma} + \chi\sqrt{I_{\varsigma\varsigma}^2 - 4I_{\zeta\gamma}^2}}{2}} \tag{25a}$$

$$\gamma_{2'} = -\frac{\omega_{1'}}{\omega_{2'}}\gamma_{1'} = -\kappa\sqrt{\frac{\omega_{1'}}{\omega_{2'}}\frac{I_{\varsigma\varsigma} - \chi\sqrt{I_{\varsigma\varsigma}^2 - 4I_{\zeta\gamma}^2}}{2}}\,. \tag{25b}$$

It arises evident that the coordinates expressions are in the form of solutions of an equation of the fourth order directly obtainable from the system of (18).

Looking at the table summarizing the signs of χ and κ, one could complain that the interval for ϑ as obtained from (21) must be $[-\pi/4, \pi/4]$ due to the invertibility of sine function. The ϑ interval of variability can, indeed, be limited to $[-\pi/4, \pi/4]$ without lack of generality: the complementary interval over $[-\pi/2, \pi/2]$ is completely equivalent. Starting from the solution $\{(\zeta_{1'}, \gamma_{1'})_{1'}, (-\omega_{1'}/\omega_{2'}\zeta_{1'}, -\omega_{1'}/\omega_{2'}\gamma_{1'})_{2'}\}$ obtained for $\chi = +1$, the solution for $\pi/2 - \vartheta \in [\pi/4, \pi/2]]$ would lead to $\{(\gamma_{1'}, \zeta_{1'})_{1'}, (-\omega_{1'}/\omega_{2'}\gamma_{1'}, -\omega_{1'}/\omega_{2'}\zeta_{1'})_{2'}\}$, as immediately given by (19); then, one of the two particles falls in the interval $[-\pi/2, -\pi/4] \cup [\pi/4, \pi/2]$ with an authomatic inversion of sign for χ but not for κ. The same equivalence can be pointed out for $\vartheta \in [-\pi/4, 0]$ and $-(\pi/2 - \vartheta) \in [-\pi/2, -\pi/4] \cup [\pi/4, \pi/2]$. In both cases, $|I_{\zeta\gamma}|$ and $I_{\varsigma\varsigma}$ are still conserved. Obviously, inverting the ζ and γ coordinates produces an inversion of $I_{\zeta\zeta}$ and $I_{\gamma\gamma}$, which are not conserved by the system of (18).

Even in this case, then, a set of $N = 2$ particles couldn't be replaced by the same particles univocally: to obtain the same direction one should impose the conservation of one of the two axial moments (automatically both in the two particles case) which would solve the uncertainty on the choice of $\pm\vartheta$ or $\pm(\pi/2 - \vartheta)$. As it will be shown in the next section, the distance from the centroid is still a bounded degree of freedom.

5.5 Unique choice of the rotation angle

The $I_{\gamma\gamma}$ axial moment can be used to determine univocally the rotation angle in $[-\pi/2, \pi/2]$ rather than in $[-\pi/4, \pi/4]$. From (16a) it follows that

$$\omega_{1'}\zeta_{1'} + \omega_{2'}\zeta_{2'} = I_{\gamma\gamma} \qquad \Rightarrow \qquad \zeta_{1'} = \varrho_{1'}^2 \cos^2\vartheta = \frac{\omega_{2'}}{\omega_{1'}} I_{\gamma\gamma}\,;$$

an expression for $\cos\vartheta$ can be immediately derived:

$$\cos\vartheta = \sqrt{\frac{I_{\gamma\gamma}}{I_{\varsigma\varsigma}}}\,. \tag{26}$$

The assumption $\zeta_{1'} > 0$ implies $\cos\vartheta > 0$, which means $\vartheta \in [-\pi/2, \pi/2]$. Therefore, it's enough to evaluate if

$$\cos\vartheta \gtrless \frac{\sqrt{2}}{2}$$

to know if $\vartheta \in [-\pi/4, \pi/4]$ or $\vartheta \in [-\pi/2, -\pi/4[\cup]\pi/4, \pi/2]$ respectively; the sign of $\sin(2\vartheta)$ will then allow to discriminate $\vartheta \gtrless 0$.

Practically speaking, if $\cos\vartheta < \sqrt{2}/2$, then $\sin\vartheta$ and $\cos\vartheta$ has o be exchanges. If $\sin(2\vartheta) < 0$ the new angle is given by $\vartheta' = -\pi/2 + \vartheta < 0$ and, then, also the signs must be inverted; in the opposite case, the new angle is $\vartheta' = \pi/2 - \vartheta > 0$ and no sign exchange is needed. Remembering that $\text{sign}(\sin(2\vartheta)) = \text{sign}(I_{\zeta\gamma})$, it can be sinthetically written

$$\sin\vartheta' = \frac{I_{\zeta\gamma}}{|I_{\zeta\gamma}|}\cos\vartheta \qquad \text{and} \qquad \cos\vartheta' = \frac{I_{\zeta\gamma}}{|I_{\zeta\gamma}|}\sin\vartheta\,.$$

The reader should observe that the exact conservation of $I_{\gamma\gamma}$ (or $I_{\zeta\zeta}$) wouldn't supply any additional information on the particles weights or on their distances from the charge centroid. Moreover, the two angle obtained by conservation of axial moments or centrifugal and polar moments are generally different for a system of more than two particles. Assuming the value of $\cos\vartheta$ from (26), if follows that

$$\sin\vartheta\cos\vartheta = \sqrt{1-\cos^2\vartheta}\cos\vartheta = \sqrt{1-\frac{I_{\gamma\gamma}}{I_{\varsigma\varsigma}}}\sqrt{\frac{I_{\gamma\gamma}}{I_{\varsigma\varsigma}}} = \frac{\sqrt{I_{\zeta\zeta}I_{\gamma\gamma}}}{I_{\varsigma\varsigma}}\,,$$

in general not equal to

$$\frac{1}{2}\sin(2\vartheta) = \frac{I_{\zeta\gamma}}{I_{\varsigma\varsigma}}\,,$$

as obtained in (20) by polar moment conservation. Standing the relation of (17) for systems of two particles, it arises evident that, only in these particular cases the two angles equal. One can conclude, that the rule defined to chose ϑ interval is not equivalent to an axial moment conservation law.

Anyway, the condition on $I_{\gamma\gamma}$ allows to fix univocally th rotation angle ϑ, that, in the case of two starting particles, means to indentify exactly their orientation in the cell. The arbitrariness on weights still remains.

5.6 Cell coordinates limits

Working in the local reference centered in G, each particle position strictly depends on the direction on which it lies, as defined by ϑ. The bounds for $(\zeta_{1'}, \gamma_{1'})$ and $(\zeta_{2'}, \gamma_{2'})$ are summarized in the following table:

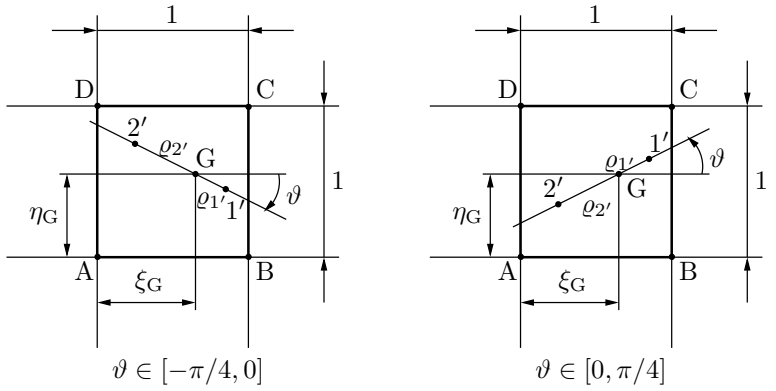

Figure 3: Coordinates limits depending on ϑ and centroid position.

	$\vartheta \in [-\pi/2, 0]$ $(I_{\zeta\gamma} < 0)$	$\vartheta \in [0, \pi/2]$ $(I_{\zeta\gamma} > 0)$
$\zeta_{1'}^{\lim}$	$\min\{1-\xi_G, \eta_G \cot\vartheta\}$	$\min\{1-\xi_G, (1-\eta_G)\cot\vartheta\}$
$\gamma_{1'}^{\lim}$	$\max\{-\eta_G, (1-\xi_G)\tan\vartheta\}$	$\min\{1-\eta_G, (1-\xi_G)\tan\vartheta\}$
$\zeta_{2'}^{\lim}$	$\max\{-\xi_G, -(1-\eta_G)\tan\vartheta\}$	$\max\{-\xi_G, -\eta_G\cot\vartheta\}$
$\gamma_{2'}^{\lim}$	$\min\{1-\eta_G, \xi_G\cot\vartheta\}$	$\max\{-\eta_G, -\xi_G\tan\vartheta\}$

(refer to figure 3 and remember the assumption $\zeta_{1'} > 0$).

Moving from the cartesian (ζ, γ) reference system to the polar (ϱ, ϑ) one with origin in G, the mentioned bounds reflects on $\varrho_{1'}$ and $\varrho_{2'}$, being ϑ fixed by the conservation of centrifugal and polar inertia moments (refer to (20)). The previous summarizing table can, then, be compressed in the following one:

	$\vartheta \in [-\pi/2, 0]$ $(I_{\zeta\gamma} < 0)$	$\vartheta \in [0, \pi/2]$ $(I_{\zeta\gamma} > 0)$
$\varrho_{1'}^{\lim}$	$\min\left\{\dfrac{1-\xi_G}{\cos\vartheta}, -\dfrac{\eta_G}{\sin\vartheta}\right\}$	$\min\left\{\dfrac{1-\xi_G}{\cos\vartheta}, \dfrac{1-\eta_G}{\sin\vartheta}\right\}$
$\varrho_{2'}^{\lim}$	$\min\left\{\dfrac{\xi_G}{\cos\vartheta}, -\dfrac{1-\eta_G}{\sin\vartheta}\right\}$	$\min\left\{\dfrac{\xi_G}{\cos\vartheta}, \dfrac{\eta_G}{\sin\vartheta}\right\}$

(the minus signs is due to $\sin\vartheta < 0$ for $\vartheta < 0$).

In section 5.4 the coordinates of the system of new particles $\{1', 2'\}$ were derived by conservation of centrifugal and polar inertia moments, for weights $\omega_{1'}$ and $\omega_{2'}$ treated as parameters.

It was stated in section 4 thath the assumption of equal weighted merging particles appears a wise decision: unfortunately, this condition is not sufficient to assure both particles fall inside the cell of interest. The conservation laws for $I_{\zeta\gamma}$ and $I_{\varsigma\varsigma}$ fix the rotation angle ϑ; then, the just derived bounding limits on $\varrho_{1'}$ and $\varrho_{2'}$ define a limited interval for the weigths

of the two particles. These conditions must be observed in order to place both of them inside the cell.

Neglecting the (18c) (which is needed only to find ϑ) and adding the total weight conservation, the system of (18) can be rewritten in terms of distances from the barycenter

$$\omega_{1'} + \omega_{2'} = 1 \tag{27a}$$

$$\varrho_{2'} = \frac{\omega_{1'}}{\omega_{2'}} \varrho_{1'} \tag{27b}$$

$$\varrho_{1'}^2 = \frac{\omega_{2'}}{\omega_{1'}} I_{\varsigma\varsigma} \,. \tag{27c}$$

The two distances are easily derivable from the polar inertia moment and particles weights as

$$\varrho_{1'} = \sqrt{\frac{\omega_{2'}}{\omega_{1'}} I_{\varsigma\varsigma}} \qquad \text{and} \qquad \varrho_{2'} = \sqrt{\frac{\omega_{1'}}{\omega_{2'}} I_{\varsigma\varsigma}} \,.$$

Since

$$0 < \varrho_{1'} < \varrho_{1'}^{\lim} \qquad \text{and} \qquad 0 < \varrho_{2'} < \varrho_{2'}^{\lim} \,,$$

(27c) allows to write two conditions for the weights ratio which can be merged in the following one:

$$\frac{I_{\varsigma\varsigma}}{(\varrho_{1'}^{\lim})^2} < \frac{\omega_{1'}}{\omega_{2'}} < \frac{(\varrho_{2'}^{\lim})^2}{I_{\varsigma\varsigma}} \,,$$

and, by subtituting $1 - \omega_{1'}$ to $\omega_{2'}$, it follows that

$$\omega_{1'}^{\min} = \frac{I_{\varsigma\varsigma}}{(\varrho_{1'}^{\lim})^2 + I_{\varsigma\varsigma}} < \omega_{1'} < \frac{(\varrho_{2'}^{\lim})^2}{(\varrho_{2'}^{\lim})^2 + I_{\varsigma\varsigma}} = \omega_{1'}^{\max} \,,$$

where the rightmost-hand of the disequation is greater than the leftomost one, being $\varrho_{1'}^{\lim} \varrho_{2'}^{\lim} > \varrho_{1'} \varrho_{2'}$. Any weight $\omega_{1'} \in [\omega_{1'}^{\min}, \omega_{1'}^{\max}]$ allows to obtain both the new particles inside the cell of interest. Once $\omega_{1'}$ is known, $\omega_{2'}$ comes immediately and (24) – (25) can be used to evaluate the particles coordinates.

6 Concluding remarks

In the present work a particle merging technique to speedup PIC-MCC code has been presented for the PIC bilinear weighting method in cartesian and cylindrical coordinates. It has been shown that an ensemble of N charged particles belonging to the same cell can be merged into two new superparticles. The particles positioning is not univocally defined by conservation of charge densities in the nodes, even if second order moments for the system are considered.

Unfortunately it's not possible to obtain the same set of two particles as blank test. Charge fractions conservation on the cell nodes has the advantage to allow equally weighted merging particles, while pseudo-inertia moments conservation cannot assure this, even allowing to mantain the orientation of the particles in the two particles case.

Two merging algorithm will be soon presented with first spatial merging results in order to decide for the best technique.

The merging procedure will be then extended to the phase space by the application of energy and momentum conservation laws for the merged subset particles. Moreover, a splitting technique will be coupled to the merging one in order to increase the system statistical representativeness, when portion of the space will undergo a particle depletion.

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