An algorithm for reducing PIC ensembles with exact conservation of
distribution functions and conservation laws

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We propose an algorithm for reducing the number of macro-particles in PIC simulations
in such a way that an arbitrary number of conservation laws can be preserved exactly and all
the distribution functions are not modified in any other way than due to the statistical noise.

Accounting for processes like ionization$^1$ and electron-positron pair production$^{2-7}$ in Particle-In-Cell (PIC) codes requires adding macro-particles, possible causing a drastic increase of their
number. This can lead not only to a largely inefficient use of computational resources but also to
a strong restriction due to reaching an allocation limit for the computer memory. Dynamically in-
creasing the statistical weights of the macro-particles (i.e. the number of real particles associated
with the macro-particle) can provide a way to reduce their number while keeping a sufficiently
detailed representation of real particles. There are two well-known approaches for this proce-
dure also referred as resampling: thinning$^{2,8,9}$ and merging$^{6,10}$. The approach of thinning implies
removing a random particle and redistributing evenly its statistical weight among the remaining
ones of the same type. (Hereafter for the sake of shortness, we write particles instead of macro-
particles.) In such a way, the thinning procedure does not change the total number of real particles
for any specific type. However, generally the procedure obviously does not preserve other conser-
vation laws such as total energy or total momentum. Even though the deviation should be inversely
proportional to the number of particles, which is typically very large, the conservation laws might
be significantly affected in the vicinity of the removed particle. This kind of inaccuracies might
lead to various numerical artefacts such as numerical heating or the destruction of some features
of the distribution functions originating from particular conservation laws. Another problem is
that removing particles in a region where they are abundantly produced affects all particles in the
whole region of simulation. One can avoid this by using the procedure of merging. This procedure
implies that if in the coordinate-momentum space a set of particles densely populates a region of
the size below some certain threshold, then the set of particles is replaced with a single particle. As was pointed out in the recent paper of Vranic et al.\(^5\), this procedure cannot provide preserving the conservation laws. As was also proposed in this paper, this issue can be perfectly resolved in case of replacing the set of particles with two particles instead of one. However, for all kinds of merging algorithms the procedure inevitable causes at least tiny modification of distribution functions. For example, the merging procedure would lead to merging of two physically different particle beams if they are closer in the coordinate-momentum space than the merging threshold. The merging procedure can also lead to an artificial reduction of the particles spread for a single beam. Certainly, one can always choose a sufficiently small threshold to avoid these negative effects, but this requires some knowledge about the typical scales. Thus, in some cases, it might be valuable to use a procedure that does not affect the distribution functions in any other way than due to the statistical noise. For example, as one can show, the thinning procedure can have this feature, but, as mentioned above, it does not preserves the conservation laws. Here we present a new simple algorithm simultaneously solving both issues.

We formulate the problem for a set of \(n\) particles of the same type. Because of the outlined properties the algorithm can be applied either to the whole ensemble of particles or to any subset of particles, such as all particles in a certain region or a cell of the grid. Suppose before applying the method the \(i\)-th particle has the statistical weight \(w_i\). The related description of the ensemble can be associated with an \(n\)-dimensional vector \(w_{\text{before}} = (w_1, w_2, \ldots, w_n)\). We also define a set of unit vectors \(w_i\), pointing in \(i\)-direction. Applying the method implies determining the vector \(w_{\text{after}}\), which has at least one component equal to zero. The particle, which corresponds to this component, is then removed from the ensemble while others are assigned with new weights that are equal to the corresponding components of the vector \(w_{\text{after}}\).

In this notation, the scalar product of the vector \(w\) and a vector \(1 = (1, \ldots, 1)\) is equal to the total statistical weight of all the particles:

\[
W = (w, 1) = \sum_{i=1}^{i=n} w_i.
\] (1)

The requirement that the method conserves the total number of real particles is equivalent to the requirement, that this scalar product remains the same before and after applying the method. Preserving an arbitrary conservation law in the particle ensemble is equivalent to the conservation
of the scalar product:

\[(\mathbf{w}, \mathbf{e}) = \sum_{i=1}^{i=n} e_i w_i = E, \]

where each component of the vector \( \mathbf{e} = (e_1, e_2, \ldots, e_n) \) is defined as the corresponding characteristic of the related particle (for example, energy). We can also define the value of center mass \( e_C \) for any vector \( \mathbf{w} \) in terms of every particular characteristic (or conservation law) as the ratio of the scalar product (2) to the total statistical weight (1):

\[ e_C = \frac{(\mathbf{w}, \mathbf{e})}{(\mathbf{w}, \mathbf{1})} = \frac{E}{W}. \]

For the method to not affect any distribution function, the choice of the vector \( \mathbf{w}_{after} \) has to be probabilistic. Developing the novel algorithm then requires defining a set of possible vectors and finding the respective probabilities of choosing one of them. Preserving all distribution functions is then equivalent to the average final weight of each particle being equal to its initial weight. For shortness, we refer to this property of an algorithm as ”statistics preserving”. In this notation, the problem statement for the paper is to find an algorithm that preserves statistics and a number of conservation laws.

For sake of simplicity, we first consider the case of \( n = 3 \) and just two conservation laws: for the total number of real particles (1) and for one additional characteristic (2). The description of the algorithm for the general case is similar and is discussed in the end of the paper.

We assume that all the particles have different values \( e_1 \neq e_2 \neq e_3 \). This is easy to achieve by choosing a set of particles for the reduction. If all the particles have one of two values, the problem becomes trivial.

At least one of the values has to be from each side of the center mass related to the characteristic (2). Without restriction generality we may assume \( e_1 < e_2 < e_C < e_3 \). (The case of the center mass to be equal to one of the values \( e_i \) is also considered below.) We define two vectors

\[ \mathbf{v}_1 = (e_3 - e_C) \mathbf{w}_1 + (e_C - e_1) \mathbf{w}_3, \]
\[ \mathbf{v}_2 = (e_3 - e_C) \mathbf{w}_2 + (e_C - e_2) \mathbf{w}_3. \]

As one can see both vectors have the same center mass \( e_C \), i.e. \((\mathbf{v}_k, \mathbf{e}) / (\mathbf{v}_k, \mathbf{1}) = e_C \) for \( k = 1, 2 \). This feature pertains even when multiplying the vectors by an arbitrary non-zero scalar number.
Apart from this, all non-zero components of both vectors are positive. In case $e_2 = e_C$ we define the vector $v_2 = w_2$, which provides the same features.

One can see that the vector

$$v = (e_3 - e_2) v_1 - (e_3 - e_1) v_2$$

has the same center mass $e_C$ and also has the total weight equal to zero. Again, both features pertain when multiplying it by an arbitrary non-zero scalar number. Note that the first component of this vector is always positive, the second one is always negative and the third one can be positive, negative or equal to zero depending on the values of $e_i$. To fix the problem let us assume that the third component is positive, which implies

$$(e_3 - e_2)(e_C - e_1) > (e_3 - e_1)(e_C - e_2).$$

The consideration of other cases is similar.

Next, we define the vector

$$p(\alpha) = w_{before} + \alpha v. \tag{7}$$

This vector, being used as $w_{after}$, provides exact conservation of both conservation laws for all values of scalar factor $\alpha$. As it is easy to understand, when increasing the value of $\alpha$ from zero, all components increase except the second one which decreases. The second component becomes zero for

$$\alpha_1 = \frac{w_2}{(e_3 - e_C)(e_3 - e_1)}. \tag{8}$$

When decreasing the value of $\alpha$ from zero, the second component increases, while the first and the third one decrease. We define $\alpha_2$ as the value that provides one of those components to reach zero while keeping the second one still positive:

$$\alpha_2 = \max (\alpha_2^1, \alpha_2^3), \tag{9}$$

where

$$\alpha_2^1 = -\frac{w_1}{(e_3 - e_2)(e_3 - e_C)}, \quad \alpha_2^3 = -\frac{w_3}{(e_3 - e_2)(e_C - e_1)(e_3 - e_1)}, \tag{10}$$

Now we can define our algorithm in the following way. With the probability $\alpha_2 / (\alpha_2 - \alpha_1)$ we apply $w_{after} = p(\alpha_1)$ and with the probability $\alpha_1 / (\alpha_1 - \alpha_2)$ we apply $w_{after} = p(\alpha_2)$. As it is easy to calculate, the average expected value for each component coincides exactly with the component
before applying the procedure. The proposed algorithm thus provides an exact solution of the stated problem.

Now it is obvious how to construct the solution for the case of arbitrary number of particles and an arbitrary number of conservation laws. We start from skipping the conservation law for the number of real particles. First, we consider all the pairs of particles, in which one particle is smaller and one particle is greater than the center mass in terms of the second conservation law (i.e. lying on different sides of the center mass). For each pair we construct the vector that has the same center mass as all the particles have in terms of this conservation law. Particles lying on different sides of the center mass ensures all vectors to have only positive components. However, the algorithm only requires a set of linearly independent vectors. We can gradually add these vectors to a set excluding the ones that can be expressed as a linear combination of the previously added vectors. Next, we consider all the pairs of vectors in the obtained set that have their center masses lying on different sides of the center mass of all initial particles in terms of the third conservation law. We construct vectors that have the same center mass as all initial particles have in terms of the third conservation law. These vectors will also have only positive components. We do so for all the conservation laws except the first one, which is for the total number of real particles. In the end we need at least two vectors to construct the vector $\mathbf{v}$ that has zero value of the total weight. Next we find the smallest positive $\alpha_1$ and the largest negative $\alpha_2$ that provide at least one component of the $\mathbf{p}(\alpha)$ to be equal to zero. The remaining description of the algorithm remains the same. Certainly, the more conservation law we want to preserve the larger number of particles we need. However, this number is obviously reasonable in terms of typical needs. In particular, as it is shown above, for two conservation laws we need only 3 particles.

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