Particle Control in Phase Space by Global K-Means Clustering

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We devise and explore an iterative optimization procedure for controlling particle populations in particle-in-cell (PIC) codes via merging and splitting of computational macro-particles. Our approach, is to compute an optimal representation of the global particle phase space structure while decreasing or increasing the entire particle population, based on k-means clustering of the data. In essence the procedure amounts to merging or splitting particles by statistical means, throughout the entire simulation volume in question, while minimizing a 6-dimensional total distance measure to preserve the physics. Particle merging is by far the most demanding procedure when considering conservation laws of physics; it amounts to lossy compression of particle phase space data. We demonstrate that our k-means approach conserves energy and momentum to high accuracy, even for high compression ratios, \( R \approx 4 \) — i.e., \( N_f \lesssim 0.25 N_i \). Interestingly, we find that the most intuitive naïve approach to particle splitting does not yield accurate results over hundreds of simulation time steps. Rather, a more complex particle splitting procedure is superior. Implementation and testing is done using an electromagnetic PIC code, the Photon-Plasma code. Nonetheless, the k-means framework is general; it is not limited to Vlasov-Maxwell type PIC codes. We discuss advantages and drawbacks of this optimal phase space reconstruction.

Keywords: particle-in-cell codes, particle merging, plasmas, magnetic fields, k-means, vector compression

I. INTRODUCTION

Control of computational macro-particle (CMP) populations in Particle-In-Cell (PIC) codes is particularly desirable in at least two situations:

Population Runaway: Monte Carlo realizations of collisional processes in PIC codes, for example, often involve fractionation of CMPs into "parents" and "children" for enhanced statistical resolution of the collision processes. This results in explosion of CMP populations, and a memory bounded simulation longevity.

Load balancing: in PIC codes relies on the ability to redistribute CMPs among computational processes (e.g. in MPI domain decomposed models) at runtime to maintain similar execution times of the computational processes, and preserve statistical resolution of continuous phase space.

CMP de-population (re-population) of domains that are progressively filled (depleted) can be achieved through deletion (addition) of CMPs – for those domains which are oversampled (undersampled), while attempting to maintain physical quantities locally conserved. Single particle deletion (addition) CMPs is detrimental with respect to the conservation of the physical properties of the system being modeled. It is necessary to merge (split) several CMPs to conserve both momentum and energy from the phase space information available.

An algorithm that can achieve this goal in a robust and efficient manner will benefit a wide range of problems in laboratory and astrophysical settings. Many physical processes naturally lead to runaway CMP populations (time domain), and extreme CMP concentrations (spatial domain), e.g.

Load: High-intensity laser-plasma wakefield acceleration of electrons, Beck (also Figure 1).

Runaway: Gamma-Ray Burst wakefield plasma acceleration, under the influence of detailed Compton scattering, Frederiksen.

Load: Streaming instabilities and agglomeration of planetesimals leading to planet formation, Johansen and Youdin.

Runaway & load: High-energy radiative processes and pair cascades in pulsar magnetospheres, Timokhin and Arons.

Load: Streams and caustics in the evolution of dark matter structures in cosmological simulations, Vogelsberger and White.

All these cases (and many others) demand an efficient CMP population control and/or redistribution in large-scale numerical simulations.

Several strategies for CMP merging have been visited in the literature over the last few decades, changing in order of complexity, cost and accuracy. Lapenta and...
Brackbill[10], also later Lapenta[11], considered the problem of merging/splitting on a single particle basis, e.g., 2 ↔ 1, 3 ↔ 2, and cell-based N_{cell} ↔ M_{cell} approaches, (Lapenta and Brackbill[11]), with N and M small. More recently, more complex algorithms have emerged such as agglomerate clustering[13] and resampling, and also oct-tree reconstruction[12] in momentum space.

Commonly, those previous strategies used means of algebraic reconstruction to ensure that physical field quantities, represented on the PIC discrete mesh (in r-space) would be conserved exactly. Some were investigated in reduced-dimensional systems, e.g. 1D3V (Martin and Cambier[12]), although their method was not strictly constrained to 1D. Others further applied a reconstruction procedure which decomposed 6D phase space, \( f(\mathbf{r}, \mathbf{p}, t) \), in to 3D subspaces, \( f_x(\mathbf{r}, t) \) and \( f_y(\mathbf{p}, t) \), employing strict algebraic reconstruction on r-space, while retaining the solution found by agglomerate clustering in p-space (Grasso et al.[8]). Any decomposition of phase space, \( \mathbb{R}^D \), into phase subspaces \( \mathbb{R}^B \) and \( \mathbb{R}^C \), with \( B+C=D \) (for our case \( D=6 \)), removes information contained in possible cross-correlation between the subspaces. It is conceivable that such correlations should be preserved.

In a view alternative to previous strategies, we consider the problem of reducing (increasing) particle phase space resolution by merging (splitting) CMPs, as an optimization problem in 6 dimensions. Our approach randomly selects existing particles as a global best guess at a solution for the clustering, with the objective to either merge or split them into a new imitative set of particles. Subsequently, a K-means iterative minimization of a global intra-cluster distance measure successively drives the merged (split) solution towards a reduced (increased) CMP population, with the same physical properties.

In Section II we describe the natural relationship between k-means clustering and the PIC code phase space representation. We then describe the details of our global k-means procedure; initialization, distance measure, particle merging and splitting, as well as an important edge-preserving measure to circumvent k-means artifacts on bounded domain decompositions. Section III outlines our test simulation setup and presents a few crucial tests of our k-means clustering procedure. Discussion and conclusions are given in Section IV.

II. K-MEANS CLUSTERING IN THE PIC CODES

Generally, in electromagnetic PIC codes, the source terms in Maxwell’s equations, \( \rho_e(\mathbf{r}, t) \) and \( \mathbf{J}(\mathbf{r}, \mathbf{p}, t) \), are constructed from interpolated accumulation of a large number of computational macro-particles (CMPs) onto a computational mesh. These CMPs are distributed in continuous real space and momentum space, and given a continuous weight to signify the particle statistical influence. For very large numbers of CMPs, we can approximately describe the computational plasma everywhere by a distribution function, \( f(\mathbf{r}, \mathbf{p}, t) \equiv \sum_i f_i(\mathbf{r}, \mathbf{p}, t) \), hereafter phase space density, where the subscript ‘s’ denotes particle species.

In the Photon-Plasma code[6], for the most complete case of 3D3V simulations, the CMP is represented by a six-tuplet of real numbers, \( \bar{\mathbf{r}} \equiv \{ r_x, r_y, r_z, p_x, p_y, p_z \} \), which positions the particle in 6-dimensional phase space (the tilde signifies a 6D vector). Further each CMP \( \bar{\mathbf{r}} \) is given a statistical weight, \( w_i \), which dictates a relative strength of the particle with respect to either the number of physical particles, or a scaled amount of physical particles. Relativistic momentum is \( \mathbf{p} \equiv m_0 \gamma(v) \mathbf{v} \), with \( \gamma \equiv \sqrt{1 - \beta^2} \), \( \beta \equiv v/c \), and in the Photon-Plasma code we most naturally keep the CMPs’ relativistic 3-velocity, \( \mathbf{p}/m_0 \). For example \( p_z = v_z(1 - \beta_z^2)^{-1/2} \) with \( \beta_z \equiv v_z/c^2 \). This renders direct addition and subtraction of particle momenta, vectorially, physically meaningful. Consequently, we may view the particle ensemble phase space as a collection of points in 6-dimensional Euclidian affine space, with a well defined algebra consisting of addition (e.g. \( p_{z,i} + p_{z,j} = p_{z,k} \)) and a distance measure, \( d^2(\bar{\mathbf{r}}_i, \bar{\mathbf{r}}_j) = (x_i - x_j)^2 + \ldots + (p_{z,i} - p_{z,j})^2 \).

Particles can then be vectorially added or subtracted, and we can find a distance between them in this affine space. We can also construct an arithmetic mean, or for weighted particles, a weighted arithmetic mean of any ensemble, or cluster center point, of particles

\[
\bar{\mathbf{r}} = \frac{\sum_i w_i \bar{\mathbf{r}}_i}{\sum_i w_i} \quad \Leftrightarrow \quad \bar{\mathbf{r}}_{\text{cl}} = \frac{\sum_i w_i \bar{\mathbf{r}}_i}{\sum_i w_i}, \quad w_{\text{cl}} \equiv \sum_i w_i, \quad (1)
\]

where now barred vectors, i.e. \( \bar{\mathbf{r}} \), denotes cluster points.

FIG. 1. Early stage in ultra-high intensity laser pulse interacting with a quiescent homogenous plasma plume, showing electron CMP number density (colors not to scale). A bubble (dark central region), evacuated of electrons, is created by the highly non-linear disturbance from the laser field pulse (green, right), which is propagating to right. A hot-spot (yellow, left) in the wake of the laser pulls electrons along, at close to the speed of light. The highly inhomogeneous density, ranging from \( N_{e,\text{min}} \approx 1 \) to \( N_{e,\text{max}} \approx 300 \) severely affects load balancing. Our method can alleviate this problem to speed up the simulation by a significant factor.
These simple facts form the basis of this paper and the justification of global k-means clustering as a way of optimal phase space reconstruction in, for example, PIC codes.

A. Weighted k-means clustering

Multivariate, multidimensional, data can be analyzed and manipulated using vector compression. K-Means[13] belongs to this general class of vector compression algorithms, and can be used to either refine or coarsen multivariate data manifolds. The k-means objective is simple: from a set of M data points, \{\vec{r}_1, ..., \vec{r}_M\}, with weights \{w_1, ..., w_M\}, in D-dimensional space, \mathbb{R}^D, find K cluster centers, \{\vec{r}_1, ..., \vec{r}_K\}, with weights \{w_1, ..., w_K\}, also in \mathbb{R}^D, which partition the original data in the optimal way. This is defined as that partitioning which minimizes the total global intra-cluster distance,

$$
\min(\tilde{D}_{tot}) \equiv \min \left( \sum_{j=1}^{K} \sum_{\vec{r}_i \in \vec{r}_j} ||w_i \vec{r}_i - w_{cl,j} \tilde{\vec{r}}_j||^2 \right), \quad (2)
$$

with \vec{r}_j and \tilde{w}_{cl,j} defined as the j'th cluster center and j'th cluster weight by equation 1 (left), respectively (right).

We choose to work in this paper in normalized data space, such that \{r_x, ..., p_z\} \rightarrow \{r_x/L_x, ..., p_z/L_{p_z}\}, where \{L_x, ..., L_{p_z}\} \equiv \{\max(r_x) - \min(r_x), ..., \max(p_z) - \min(p_z)\}; this choice is specific to our problem, since we cannot a priori assume that certain directions in phase space are more important than others with respect to the physics, if we want the procedure to be generally applicable and fast.

In signal compression theory, the original data set to be compressed or inflated in k-means is often denoted ‘training vectors’ while the solution (the clustered data set) is called the ‘codebook vectors’. We adopt this terminology henceforth.

1. Computational Effort of K-means

Finding the global minimum for any data set in higher dimensions in k-means is an NP-hard task. For given values of M, K and D, the computational effort is approximately \(O(M^{K+1} \log M)\) which is intractable for almost any PIC code problem we want to consider. If we — on the other hand — accept the solution to be only approximate we can find acceptable alternatives in finite time, and even quite fast. Equivalently, an approximate solution amounts to a local minimum rather than the global minimum described by Equation 2.

2. K-Means Clustering, Lloyd-Forgy algorithm

A variety of heuristic algorithms exist; commonly they use iterative processes to find a local minimum solution to Equation 2. The simplest brute force heuristic algorithm, which is also the most expensive, is Lloyd’s algorithm[12] with Forgys initial conditions[13]. We will use "Lloyd’s” algorithm and "k-means” interchangeably, even though the "k-means” term and a more general treatment of vector quantization originates from MacQueen[13]. Lloyd-Forgy, or k-means clustering optimization goes through three basic steps:

1. Initial condition: a first guess as to a solution is made by placing the initial codebook vector set. Forgys method at random selects K training vectors as the initial codebook. This often (but not always) is better than for example choosing random points within the data space.

2. Cluster assignment: training vectors are assigned each to their nearest codebook vector (cluster center). This is effectively a Voronoi tessellation step.

3. codebook replacement: by calculating the weighted arithmetic mean (Equation 1), based on within-cluster associated training vectors, new codebook centers are found to replace those codebook vectors found in 2) during the previous iteration.

Steps 2 and 3 are repeated until some defined convergence threshold is met; for example, as in this paper, when the ratio in total error (eqn. 2) between successive iterations changes by less than 1% is a common criterion[12]. Figure 1 illustrates the algorithm for a two-dimensional case.

The effect of successively tessellating and cluster re-centering, respectively, reduces the computational effort
to $\mathcal{O}(M \times K \times D \times i)$, with $i$ the number of iterations to convergence. Nonetheless, even when employing Lloyd-Forgy, the computational expense becomes increasingly prohibitive for large values of $M$, $K$ and $D$. Hence, we might expect to discard k-means as feasible for CMP code applications undesirable property of k-means — in Figure 3 for $D=2$.

For PIC codes which are parallelized over computational processes via domain decomposition in real space ($r = \{r_x, r_y, r_z\}$) this is problematic because a given volume will experience edge artifacts in charge density, $\rho_c(r)$, and current density, $J(r)$, namely a reduction of particles’ contribution to those physical quantities. Domain decomposition is often employed in PIC codes, making such an edge-preserving step indispensable.

To alleviate this problem we devise a simple "quick-and-dirty" edge-preserving correction scheme, which is illustrated in Figure 5. The idea is simply to let the clustered codebook solution approach the original training vector set on the domain boundaries. The boundary thickness is presently defined as equal to two cells of width. Is this way we ensure that edges are left untouched. In terms of computation, this leads to an extra iteration which we estimate at effort $O(M \times K)$, thus not severe (yet not ignorable) in the total budget. Furthermore, the final number of codebook vectors will be slightly larger than the target value for large volumes and approach the original number of training vectors when the volume in question approaches PIC code cell size.

This mock edge-preserving procedure is simple; after having found a codebook solution on the entire domain (including the boundary region), the codebook vectors in the domain boundary are deleted, and the training vectors kept here instead. On the interior of the domain (excluding boundaries), the codebook is reduced if the cluster falls inside but has training vector members in the domain boundary. If a codebook vector resides on the interior and has all training vector members on the interior as well, the codebook is kept as-is and the training vector members are deleted.

In Section 3 we demonstrate that, despite its simplicity this edge-preserving scheme manages to suppress significantly and adequately the edge-effects introduced by the contractive artifacts of k-means clustering, as should be appreciated from Figure 4.
4. Particle Merging — Employing K-Means

From the previous section, merging particles many-to-many, globally (or semi-globally) in the volume now becomes obvious; after the k-means operation, the codebook will contain all the necessary phase space information needed to preserve the physics in the continued simulation.

We need only delete the original particle data (the training vectors) and replace them with the new reduced particle data set (the codebook)

\[
\{\tilde{r}_1, ..., \tilde{r}_M\}_{\{s, tr\}} \rightarrow \{\tilde{r}_1, ..., \tilde{r}_K\}_{\{s, cb\}},
\]

while conserving total charge, globally, by preserving the total weight of the CMPs, pre- and post-compression:

\[
\sum_j \sum_{i=1}^K w_{cb,j} = \sum_{i=1}^M w_{tr,i},
\]  

(3)

One further constraint is

\[
w_{cb} = \sum_{i=1}^N w_{tr,i},
\]

(4)

for all \(N\) intra-cluster particles. Here 'cb' ('tr') denoting codebook (training) vectors, respectively, and 's' denoting species.

Several schemes exploit the additive properties of phase space, and they can be classified according to the approaches mentioned in the Introduction. The advantage of a many-to-many \((M \rightarrow K, M,K \gg 1)\) iterative optimizing approach, like ours, is that we do not have to consider specifically, nor analytically, conservation of physical properties, e.g. energy, momentum, space charge density, current density or any higher order moments of the distribution.

The many degrees of freedom ensures total conservation of the physics to any desired precision\cite{5}. The quality of the iterative solution will however be practically constrained by computational expense, and by demands on the number of particles (needed to resolve the physics) in the simulation.

5. Particle splitting, a symmetry argument

An accurate method for splitting particles is also needed; when the particle number in a cell falls below some given threshold, an increase in phase space resolution becomes imperative — even for physical reasons. Simply on-top splitting into many new particles\cite{5,51} is fast, and seemingly precise at the time of splitting. However, it turns out that the simple on-top split may not necessarily be the best choice. We will demonstrate this in a stress test of particle splitting procedures (Section III).

Counter-intuitively, we choose to exploit a symmetry of the k-means procedure. Increasing statistical resolution by adding particles can be achieved as accurately as merging by keeping all training vectors, and adding the codebook vectors

\[
\{\tilde{r}_1, ..., \tilde{r}_M\}_{\{s, tr\}} \rightarrow \{\tilde{r}_1, ..., \tilde{r}_M\}_{\{s, tr\}} + \{\tilde{r}_1, ..., \tilde{r}_K\}_{\{s, cb\}}.
\]

Effectively, all new particles (codebook vectors), are placed precisely on the 6D phase space manifold, but at positions different from those of the original particles (training vectors), in 6D phase space. This amounts to a k-means phase space inflation of type \(M \rightarrow K \Rightarrow M+K\), in terms of number of CMPs. A split which could have been simply \(O(K)\), now becomes a rather expensive — as expensive as k-means for merging — \(O(M \times K \times D \times i)\) once again. Why do this?

The only difference from merging is that we need to redistribute the total weight of the original particle data,
on both training vectors and codebook vectors

\[ \sum_{j}^{K} w_{cb} + \sum_{i}^{M} w_{tr} = \sum_{i}^{M} w_{tr}, \]

where now the \( \prime \) (prime) denotes values before performing k-means. Practically, the re-distribution of weights in our k-means based splitting scheme is done by sharing the weights between training vectors and their associated codebook vector in proportion to the training vectors’ weights. The total amount of weight, \( w_{cb} \), given to a codebook (cluster center), is the average value of those intra-cluster training vectors,

\[ w_{cb} \equiv \langle w_{cl} \rangle \frac{w_{l}}{w_{cb}}, \quad \langle w_{cl} \rangle \equiv \frac{w_{cl} N_{cl}}{N_{cl}} \]

is the mean weight in that cluster, and

\[ w_{cl} \equiv \sum_{i}^{N_{cl}} w_{i}, \]

and \( w_{l} \) are the individual weights of the \( N_{cl} \) training vectors in that cluster. This is done under constraints of the edge-preserving scheme described above (Section IIA3).

When taking into account an accelerated k-means algorithm (Malý et al.), the computational cost issue is relaxed, and we can afford the extra care taken in oversampling phase space for increased statistical resolution.

III. PROOF OF CONCEPT: ‘barbara’ TESTS

We proceed to demonstrate k-means based merging/splitting feasibility in terms of preservation of physics with heavily varying particle numbers.

All tests in the remainder of this article have been performed using a slightly modified setup of a simple 2D3V relativistic two-stream simulation, used for tests of the Photon-Plasma code. A relativistic neutral electron-ion beam is streaming through a neutral electron-ion background at \( \Gamma_{\text{beam}} = 3 \), with density ratio \( n_{e}/n_{bg} = 1/3 \). The dynamics are thought to be of relevance in cases such as Gamma-Ray-Burst afterglow shocks in a circumburst medium.

Our reference ‘barbara’ case in the present paper has grid size \( N_{x,z} = 128, N_{y} = 1 \), physical size \( L_{x,z} = 12\Delta_{x} = 3\Delta_{y}, L_{y} = 1.2\Delta_{x} = 0.3\Delta_{y} \), \( m_{i}/m_{e} = 16 \), beam Lorentz factor \( \Gamma_{b} = 3 \), beam-to-background density \( n_{b}/n_{bg} = 1/3 \), \( \omega_{pe} \approx 0.0856 \), so \( \delta_{x}/\Delta_{x} \approx 8.6 \). Time step \( \Delta t = 0.00391, \tau_{\text{end}} = 10.0 \approx 120\omega_{pe}^{-1} \approx 30\omega_{pe}^{-1}, N_{p} = 30 \) in the background and \( N_{b} = 10 \) in the beam plasma per cell/species; a total of 80 particles/cell.

The detailed reference simulation setup is not important for our tests; the only objective is to see how well we preserve the physics w.r.t. a reference case. Throughout this Section, the ‘reference run’ denotes the instance of ‘barbara’ which is devoid of performing merging and splitting.

Although our simulations are setup in a quasi-2D3V reduced dimensionality, but this does not influence our k-means tests, since particles still have a single cell’s degree of freedom, even in the \( Y \)-coordinate. When we take into account the normalization of data space (see Section IIA), we will have a truly 3D3V phase space manifold to work with.

The simulations were all done on a 4x4 MPI domain decomposed geometry, using simply the MPI processes as our k-means domains. Still, domain sizes are not limited in any way, except for a lower bound on volume of a few cells in each spatial dimension. This is because the edge-preserving scheme will make the solution approach the original phase space density for very small volumes of order a few cells, \( V_{\text{kmeans}} \equiv k\Delta_{x}\Delta_{y}\Delta_{z} \), where \( \{k, l, m\} \to \{1, 1, 1\} \).

We have verified the binary authenticity of successive reference runs, and that runs of ‘barbara’, using actual merging/splitting, were also binarily identical to the reference run – up to the point of first k-means, of course.

A. Pure particle merging & splitting stress test

A severe stress test was performed to ascertain the quality and longevity of clustered solutions under what we defined as ‘extreme’ conditions.

Multiple merges (or splits), only, were performed successively until the solution were no longer meaningful when comparing with the (constant particle number) reference run. After running the simulation for about 400 iterations \((33\omega_{pe}^{-1})\), we either merged or only split the total particle number four times over the course of an additional 260 iterations \((22\omega_{pe}^{-1})\).

The merging stress test successively removed 2/3 of the former number of particles, for all species, on all MPI processes. Thus, from the first merge to the last merge, the number of particles would be \( N_{f}/N_{i} = (1/3)^{4} \approx 0.01 \), had the fraction been exactly \( 1/3 \). However, since we employed the mock edge-preserving scheme (see Section IIA3) included which limits the boundaries to the true solution CMP number density, the remaining particle number fraction in each merging step was somewhat higher than 1/3. In fact the final-to-initial CMP total particle number was rather \( N_{f}/N_{i} \approx 0.1 \).

In a similar fashion, we conducted a splitting test, which of course is less severe, which successively added 1/3 of the former number of particles, for all species, on all MPI processes, to the new solution. We emphasize our use of the expensive on-manifold k-means based splitting (see Section IIA3), the cheap on-top split yielded meaningless results — see also Section IIA1.

Now, instead, the number of particles would have increased to \( N_{f}/N_{i} = (4/3)^{4} \approx 3.2 \), had the added fraction been exactly \( 1/3 \). Again, the mock edge-preserving scheme limited the true solution total number of CMPs to \( N_{f}/N_{i} \approx 2.8 \).

The resulting evolution of the merged and split cases
are worth comparing for a quantity which is solved for by integration, rather than comparing Maxwell’s source terms, $J$ and $\rho_c$, formed by the particle data, directly. In Figure 7 and Figure 8 we compare $B_y(x, z)$ for splitting (left panel), reference (middle panel) and merging (right panel) cases, for two splits (or merges) over 65 iterations, and four splits (or merges) over 260 iterations, respectively. In the latter case, the last merge was done 100 iterations prior to the snapshot shown in the figure. All three panels are contoured on the same color scale, in each of the figures separately; they are directly comparable.

Not surprisingly, the splitting produces a perfect match with respect to the reference case, for all cases. Everything is preserved at close to machine precision. Also as expected, the merged simulation shows increased levels of Poisson noise in the field as the number of CMPs is reduced. Still, after having removed more than 75% of the original data set, and after several tens of iterations, the solution is still very good. Even after having removed more than 90% of the particles over an additional 200 iterations, although the noise levels have risen considerably the overall. The global evolution is well preserved. Although high-$k$ noise has been introduced, the total energy and momentum are conserved to better than $\sim 0.1\%$ and the global field structure is intact. We have checked the Fourier spectra which show this behavior as well; high-$k$ modes are rising during a merge stage, but the spectrum remains largely unaltered for low- and intermediate-$k$ wavenumbers.

This stress test sets limits on the severity of compression parameters and resilience of compressed solutions. Much like image compression, we see that a reduction works well even for very high compression ratios, like 100%, although the compression algorithms for images are likely more sophisticated in the latter case.

A first, back-of-the-envelope quantification of validity of compression solutions hints that we should not compare the solutions by $\|\text{output} - \text{reference}\|$ (A). Naïve versus $k$-means splitting test

More surprisingly, however, comparing the expensive $k$-means splitting procedure with naïve on-top splitting (copy particles, $\tilde{r}_i' \equiv \tilde{r}_i$ and sharing weights, $w_i' + w_i \equiv w_i$), we find that the solutions are nowhere near to being similar. A fraction of the particles for all three cases are plotted in real subspace, $\tilde{r}_{2D} = \{x, z\}$ for on-top split (left panel), reference (middle panel) and $k$-means on-manifold splitting (right panel), in Figure 9. The $k$-means on-manifold split solution traces the reference solution extremely well, while the on-top split does not even begin to compare with reference, the solution is gone.

A plot of differences in position on the phase position subspace manifold, $\tilde{r}_{1DV} = \{z, p_z\}$, for three different times, $\Delta t \approx 0.17\omega_{pe}^{-1}$, $\Delta t \approx 1.0\omega_{pe}^{-1}$, $\Delta t \approx 1.83\omega_{pe}^{-1}$ – proceeding a single split (no other influence) – reveals a strong growth in dissimilarity for the on-top naïve split. This behavior we did not observe for the on-manifold (expensive) $k$-means split described in section IIA5. On a note: the discrepancy seems to be bigger, perhaps even to emanate from, the forefront of the phase space waves (middle panel) of the streaming instability. Thus we could speculate as to a physical artifact of a PIC code formulation origin of this in the on-top splitting method.

To test this in the extreme limit of many iterations post-split, we ran the single split test for a total of 200 iterations in both the on-top and on-manifold splitting cases, and then looked at the difference with respect to

![FIG. 7. Comparison of $B_y(x, z)$ for a hard stress test of merge (right panel) and split (left panel) with the reference case (middle panel), at time $t \sim 23\omega_{pe}^{-1}$. The number of particles has been merged (split) twice, into $N_f/N_i \approx 4/17$ ($N_f/N_i \approx 32/19$). The simulation subsequently ran for 65 iterations. Total energy and momentum conservation is better than $\sim 0.01\%$.](image1)

![FIG. 8. Same as Figure 7, but now, at time $t \sim 32\omega_{pe}^{-1}$. The total number of particles has been merged (split) into $31/8$ ($51/11$) in four steps over the course of 260 iterations. The stress test has severely increased noise. Global field structure and power is unaffected. Energy and momentum is still conserved to about $\sim 0.1\%$, despite the noise introduced by reduced statistics.](image2)
FIG. 9. 4% of the beam electrons (barbara species 3) plotted immediately following the last of eight splits – $t=3.910$, $N_f/N_i = 7.82$ – as function of position in $\{x, z\}$ phase subspace. The complex split procedure makes the phase space inflation follow the reference phase space manifold almost exactly. The simple split solution is meaningless at this stage.

FIG. 10. Deterioration of simple split solution w.r.t. time. After +20 iterations from split, the solution is significantly altered. The difference between all particles in the reference run and the simple one-split only run has been taken in $\{z, p_z\}$ phase subspace the reference case. The result is given in Figure 10, where it is clearly seen that the on-top split produces a solution which deviates not only significantly, but even so detrimentally, from the reference — the on-manifold split exhibits no appreciable dissimilarities, yielding an almost flat field.

B. Edge-preserving mock scheme tests

As previously explained, the k-means procedure possesses an intrinsic and undesired property when it comes to preserving the physics in PIC simulations. Since any calculation exploiting arithmetic means will produce volumes smaller than the original one, a domain decomposed PIC simulation will suffer boundary effects in the domain decomposition dimensions. For our case of the Photon-Plasma code, this is in phase subspace $\tilde{r}_3D = \{x, y, z\}$ (see also Section II.A3). In fact, it will even suffer this constraint in the domain non-decomposed dimensions (here momentum phase subspace, $\tilde{r}_{3V} = \{p_x, p_y, p_z\}$).

The 3D boundaries completely predictable, and it makes sense to counter-balance convexity issues of the k-means based procedure based on a spatial filtering of the real space coordinate boundaries. We regard $\tilde{r}_{3D} = \{x, y, z\}$ as correctable. Momentum subspace boundaries, $\tilde{r}_{3V} = \{p_x, p_y, p_z\}$, are regarded as non-correctable since in any trivial – they will generally not be regular. This is clearly depicted in Figure 10, where the boundaries in the $z$-direction are very regular. In the $p_z$-direction, however, things are not so predictable. We stress that we have not decoupled 6D phase space reconstruction by this procedure, only, we have ensured the convergence of the compressed (or inflated) k-means solution in a subset of dimensions. We have introduced no decoherence between position and momentum at all by this edge-preserving correction.

Two tests were performed to check the mock edge-preserving scheme performance

**Thermal cases:** with little or no bulk flow which leads to little or no replenishment of domain boundaries, keeping the domain boundaries quasi-static in terms of phase space evolution.

**Streaming cases:** the well evolved two-stream simulations would produce extreme replenishment of domain boundaries which will test the scheme’s ability to render advection across boundaries transparent.

These two extreme dynamics are often realized in PIC codes, even simultaneously.

The test results from the thermal case are shown in Figure 12. We performed a single merge (split) — and
nothing else — using the ‘raw’ non-corrected k-means algorithm, and a single merge (split) with our mock edge-preserving correction added to the k-means solver. The MPI domain boundaries are clearly visible. As expected the effect is more severe in the merging case since a split retains clusters with in-boundary particles whereas merging removes them. Still, even for merging, our edge-preserving correction yields significantly improved conservation properties. In both cases, not surprisingly, splitting was almost perfect. Particle merging naturally showed a minor decay in the solution across the merge step since it is a case of lossy compression. Still, the solution following several integrations would not decay rapidly. This result was reinforced by the streaming test case showing no appreciable discontinuities and ability to smooth away the boundary ‘shadows’ introduced by the contractive aspect of k-means arithmetic averaging.

C. Full scale automated merge/split test

We conducted two tests with the full scale automated MPI-domain based merging-splitting activated: a “wide” and “narrow” tolerance range test would decide how well, and how often splitting and merging should be employed.

”Wide”: tolerance yielded splitting when, for any MPI domain, \( N_p < N_{low} \equiv 0.667N_{opt} \) and merging when \( N_p > N_{high} \equiv 1.333N_{opt} \).

”Narrow”: tolerance yielded splitting when, for any MPI domain, \( N_p < N_{low} \equiv 0.9N_{opt} \) and merging when \( N_p > N_{high} \equiv 1.1N_{opt} \).

Due to the more restricted tolerance, the “narrow” test case yielded about twice as many splits and merges during the entire simulation, therefore also twice as many passes through the domain boundary edge-filtering. We have plotted the differences w.r.t. reference when running raw, respectively edge-preserving, k-means in Figure 14 for the “narrow” (panels ‘A’=raw and ‘B’=edge-preserving) respectively ”wide” (panels ‘C’=raw and ‘D’=edge-preserving) tests. The effect of the more frequent splits/merges for the ”narrow” case shows that traces of the MPI boundaries are visible in both the raw and edge-preserving cases, albeit the quality of the edge-preserving scheme still is superior by about a factor of \( \sim 5-10 \).

For the ”wide” tolerance case, the infrequent need for splits/merges both show improvement in handling the domain boundaries, again the edge-preserving scheme is justified by a factor 5-10 improvement. For the remainder we will concentrate on the ”wide” tolerance case. More than 900 iterations, 100 merges, and 100 splits, were performed (6 splits and 6 merges for each MPI domain). The splitting/merging kicks in at approximately the end of the integration cycle completely omitted; the pure effect of the algorithm, and a single merge (split) with our mock edge-preserving correction yields significantly improved conservation properties — both spectral and spatial. In Figure 14 is plotted the difference, \( \Delta E(\text{ref,edge}) \equiv E_{\text{ref}}(t) - E_{\text{edge}}(t) \), \( \Delta E(\text{ref,raw}) \), in total electromagnetic field energy, and the negative difference, \( \Delta E(\text{edge,ref}) \), in total particle energy, between the reference and ”wide” test cases. Although the drift in EM energy is relatively large over time (about \( 1 \cdot 10^{-4}/2 \cdot 10^{-4} \sim 0.05 = 5.0\% \)), this energy drift is compensated by an anti-correlated drift in the total particle energy (see Figure 14). This particle energy drift is partially due to the convex artifacts of k-means, operating in momentum space — which leads to a small artificial cooling. For a single split or merge, energy and momentum is conserved almost to machine precision. The total energy deviates less than 0.5\% from reference in the case of wide tolerance range at the end of the simulation, after more than 200 merges and splits over more than 2000 iterations.
Momentum conservation

Likewise, we can study the total momentum evolution, but it would yield little new information since the total momentum is still conserved to about machine precision (or at least k-means tolerance levels). Rather, it would make sense to look at a "critical" component of the momentum; the ion beam momentum in the streaming direction. We have plotted the time evolution for this quantity in Figure 15. It is unnecessary to plot any other histograms in phase subspace since all directions are equally valuable in the k-means optimization procedure; they will show comparative accuracy. There is a slight shift of the k-means treated runs (red curve) in the histograms as time progresses. We interpret this in connection with the conclusions concerning energy as a loss of energy transfer between particles and fields, which leads to a slower slow-down of the ion beam.

Particle weight distribution evolution

Figure 16 plots the evolution of particle weights (all particles) as the simulation progresses. From an initial constant weight, $w_{\text{init}} = 0.3$, weights become distributed in a uniform manner over a wide range of values, as new generations of particles appear due to merging and splitting. This is desirable in terms of statistical evolution; phase space information is now spread over a wide range in weights, and not only in phase space position. We can more safely destroy particles at random without risking serious biasing effects on the physics in the process.

Figure 18 compares the beam ion density at the very last time step, after 2553 iterations and more than 100 splits and 100 merges. The result demonstrates that the solution stays stable for rather long times. There is a tendency for the particles to clump due to the frequent merges; the edge-preserving performs slightly better in avoiding clumps, and better preserves large scale structure and flow — by a marginal measure.
FIG. 17. Phase subspace \( \{ x, z, \log_{10}(w) \} \), for illustrative purposes. Yellow dots are late generation particles, size shows weight, while blue particles show concurrent reference run. Minor discrepancies in the local number density is due to a 1/100 stridden sampling — and, to some degree, the collapse of phase space from 6D to 2D. This plot can be compared directly with Figures 18 and 16.

IV. DISCUSSION & CONCLUDING REMARKS

It is important to realize that our k-means compression and inflation of CMP data in PIC codes is a global method, which ‘feels’ all modes present in the volume at hand. Thus, the method will preserve all modes increasingly well for decreasing wavenumbers considered. This contrasts the local methods, mentioned during the Introduction, which effort the conservation of the physics locally, rather. We briefly discuss here some obvious limitations of the k-means scheme. We then discuss how these limitations may not be too severe, considering a range of applications for which a global domain method can be utilized.

Applicability limitations on domain sizes

There is a trade-off between the size of domains on which the method is deployed (here sizable MPI domains) and the speed at which the procedure can be executed.

\( V_{\text{kmeans}} \rightarrow V_{\text{cell}} \): In this case, our model approaches the full solution pre-merge/-split. We cannot go to cell sized domains due to the convexity issue, which then becomes either detrimental to conservation of the physics, or becomes nullified due to retention of the full training vector set in question.

\( V_{\text{kmeans}} \rightarrow V_{\text{total}} \): In this case, the edge effects approaches a negligible contribution. We can encompass the entire domain; even though super-linear scaling becomes prohibitive for performance this is only a practical limitation, not a physical one. Also, the compression ratio parameter is relieved of any restrictions imposed by convexity in this limit.

While the latter limit can be remedied by accelerated algorithms or hardware acceleration (see below), the former cannot. We are bound by a lower limit on domain volumes to obtain a reasonable compression factor. The domain volume boundary thickness, \( W_{\text{bound}} \) must be small compared with the domain interior, along all dimensions. \( W_{\text{bound}} \equiv 1\Delta x \ll L_x = 32\Delta x \) (per MPI domain) in our study above. Still, a domain volume granularity leading to \( W_{\text{bound}} = 1\Delta x \lesssim L_x \equiv [ \text{a few} ] \cdot \Delta x \) should be possible.

Demands for memory

The biggest drawback of the current implementation is memory overhead; worst case, we need simultaneous storage for the codebook, as well as training-to-codebook vector mapping of particle IDs, and count of training vectors-per-codebook vector. The total overhead then becomes \((7[\text{real}] + 7/3[\text{integer}])N_{\text{opt}}\) which should be compared with the normal need for a PIC representation (when not employing merging/splitting) of simply \(7[\text{real}]N_{\text{opt}}\) particles: an overhead which doubles the memory need.

Careful implementation and re-use of allocated space can reduce the need for memory, but at present we see no way to remove the need for storage of the full codebook vector data set for the ‘k-means’ scheme. This could improve in the future.

One quite obvious way to remove the problem of overhead in connection with the codebook, as well as training-to-codebook vector mapping of particle IDs, and count of training vectors-per-codebook vector. The total overhead then becomes \((7[\text{real}] + 7/3[\text{integer}])N_{\text{opt}}\) which should be compared with the normal need for a PIC representation (when not employing merging/splitting) of simply \(7[\text{real}]N_{\text{opt}}\) particles: an overhead which doubles the memory need.

Careful implementation and re-use of allocated space can reduce the need for memory, but at present we see no way to remove the need for storage of the full codebook vector data set for the ‘k-means’ scheme. This could improve in the future.

Acceleration of K-Means clustering

The standard Lloyd’s k-means is too slow, even prohibitively so. We cannot obtain a process which is faster than about \(O(M \times K \times D \times i)\), with \(D\) the dimensionality (which is 6 for 3D3V) and \(i\) is the number of iterations to convergence. For our test case, the time spent in k-means calculations exceeded the entire simulation time by several factors. An accelerated method is clearly needed. To gain sufficient speed in the computation, we need an approximate factor of 40 in speed-up. This
FIG. 18. Comparison between three runs of “Barbara” in the "wide" test case. Contour plots show beam ion density, during automatic merging and splitting on the wide tolerance interval. Approximately 100 merging and 100 splitting events occurred in total on the 16 MPI domains, for an average of about 12 splitting and merging events per domain. We have outlined the lowest level contour (thin white lines) to augment the finest level differences clearly. Number of contour levels is 256, \( \max(\rho_{b,i}) \approx 21.0, \min(\rho_{b,i}) \approx 0.0 \). Left panel: raw k-means, no edge filtering. Middle panel: reference simulation (no k-means), Right panel: edge filtered k-means. The edge-preserving method does perform slightly better, but the differences are very small.

is only possible using more efficient algorithms or more efficient hardware, for the same problem size.

In a separate project, we have investigated acceleration by introducing a KD-Tree method, which seems promising when keeping calculations on CPU. Hardware acceleration is also an option; a GPGPU kernel (in OpenCL) was implemented, with considerable speed-up, on-core. However, the copying of data to-and-fro the GPGPU is costly, and only for large data sets does the hardware accelerated method become feasible. The question of algorithmically accelerated versus hardware accelerated k-means will be treated in a subsequent publication (in preparation).

For our “BARBARA” test, a typical accelerated k-means step executed about as fast as a typical simulation timestep, making the procedure competitive for several important applications (see Introduction).

With this article we have given an account for a global k-means based phase space compression method, for PIC codes we have assessed the physical conservation properties without at glance to computational effort. In a forthcoming article (Malý et al. \[\text{in preparation}\]) the question of computational cost is addressed in two different ways; by algorithmic acceleration (KD-Tree algorithm optimization with MPI+OpenMP support), and by hardware acceleration (Lloyd’s brute force on GPGPU). Both methods are affirmative towards using our procedure for realistic problems.

**Generality of K-Means Merging & Splitting**

Particle phase space compression and inflation is not limited to electromagnetic PIC codes. Any system which can be modeled by a discretized particle distribution function, \( f(\tilde{r}(t), t) \), in a D-dimensional space \( (\tilde{r}(t) \in \mathbb{R}^D) \) can be manipulated by the k-means optimization scheme described in this article. This means that

1. the number of particles must be high enough to consider the particle population(s) as approximating a continuous distribution within a given volume selected for merging, and

2. that the intrinsic noise in the non-reduced solution must outweigh the noise introduced by the reduction of the particle data set.

The specific values for these constraints are of course problem dependent, the determination of which are beyond the scope of this paper. This question is deferred to future work.

Nonetheless, to give an example here, we have verified the method in one other case of a particle-in-cell based code, by Johansen et al. \[\text{in preparation}\], which has shown promising results as well. At a well evolved point in time, in a simulation of the formation of streaming instabilities in a proto-planetary disk, a total of 2.4 million particles were merged into 1.2 million, and the simulation was restarted with the reduced codebook solution. Figure 19 shows a comparison between a reference simulation (black) and the compressed phase space simulation (yellow). The quantity plotted is the (global) maximum CMP number
density, $\max[N_{\text{cell}}(t)]$, which is a very sensitive measure. Coherence is almost perfect after 25 iterations and still reasonable after almost 100, even for a reduction by half the particle ensemble. The instance of our k-means algorithm used in this stand-alone test was an early stage implementation, originally employing the Linde-Buzo-Gray algorithm\cite{12}, rather than Lloyd-Forgy’s. Also, we did not employ our edge-preserving procedure. The agreement plotted here is likely to improve in the future.

Concluding Remark

Without the ability to make a direct comparison by benchmark, it is difficult to assess the range of validity, conservation abilities, computational cost, and possible domain boundary constraints, of the methods mentioned in the Introduction. When we consider the problem from a global PIC domain perspective, the issue of memory overhead associated with performing an analytical match of charge and current densities (without the tensor conservation) could possibly approach that associated with our k-means procedure when $M \lesssim K$. We therefore encourage a comparison of merging methods, in particular between more recent methods\cite{5,10}, and the statistical k-means based optimization scheme introduced in the present article.

The clustering merge/split code used for this publication may be requested by emailing the author\cite{20}.

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Note 1. Formally, the original formulation considered only evenly spaced points in one dimension, but the algorithm is not limited to specific point data densities nor one dimension.

Note 2. Note that this does not imply that the solution physics is only good to 1%, it is much better as can be seen from section on tests.

Note 3. We do not need an exact solution, only one good enough to subside the Poisson noise in the original CMP ensemble.

Note 4. Proper citation of this article (or co-authorship) should follow application, transcript or re-engineering of the acquired code.

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