TITLE: A WEIGHT (CHARGE) CONSERVING IMPORTANCE-WEIGHTED COMB FOR MONTE CARLO

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NOTICE

A WEIGHT (CHARGE) CONSERVING IMPORTANCE-WEIGHTED COMB
FOR MONTE CARLO

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ABSTRACT

Importance-weighted combing techniques can be used to control particle populations throughout a problem with widely varying importances. However, a naive importance-weighted comb does not preserve the total particle weight. This is generally unimportant for neutron and photon transport. However, this can be very important in simulations of charged particles where the particles are generating the electric field that they are being transported through. From a Monte Carlo standpoint, preserving the expected weight by a combing technique produces an unbiased result. However, there may be a serious degradation to the physics of the problem if total charge is not exactly conserved. This paper describes a combing method that preserves the total weight and hence the total charge.

I. INTRODUCTION

Combing techniques for particle population control are well-known in the particle transport field, although the author has been unable to find a suitable publication to reference for the combing technique. Combing techniques have been employed for particle population control for over 30 years at the Lawrence Livermore National Laboratory, and probably elsewhere under different names.

A simple comb replaces $K$ particles of varying weights that sum to $W$ with $M$ particles, each of weight $W/M$. (This process will be explained below.) An importance-weighted comb of $K$ particles produces $M$ particles with weights inversely proportional to a user-specified importance function. However, an importance-weighted comb ordinarily does not preserve the precomb total weight. That is, the expected postcomb total weight is equal to the precomb total weight, but there is a fluctuation in the postcomb total weight introduced by the importance-weighted comb.

For those instances when it is important to exactly preserve the total weight, a small modification to an importance-weighted comb is necessary. For instance total charge conservation is important in the transport of charged particles in semiconductor modeling. This paper describes
a modification to the importance-weighted comb that will exactly preserve total weight, and hence the total charge.

II. A SIMPLE COMB

Suppose that one has $K$ particles and one decides that one would rather follow $M$ particles. The $K$ particles are “combed” into $M$ particles using an $M$-toothed comb. Figure 1 shows a comb with $K = 6$ and $M = 4$. The length of the comb is the sum of the particle weights

$$W = \sum_{i=1}^{K} w_i$$

The comb teeth are equally spaced with the position of the teeth randomly ($\xi$ is a uniform random number on $(0,1)$) selected as

$$t_m = \xi \frac{W}{M} + (m - 1) \frac{W}{M} \quad m = 1, \ldots, M$$

Each time a tooth hits interval $i$, the $i^{th}$ particle is duplicated and assigned a weight

$$w'_i = \frac{W}{M} = \text{postcombed weight}$$

Defining the integer $j$ by

$$j < \frac{w_i}{W/M} \leq j + 1$$

one sees that either $j$ or $j + 1$ teeth of a comb with a pitch of $W/M$ will hit an interval of length $w_i$. In particular,

$$p_{i,j} = j + 1 - \frac{w_i}{W/M} \quad \text{is the probability of } j \text{ teeth in interval } i$$

$$p_{i,j+1} = \frac{w_i}{W/M} - j \quad \text{is the probability of } j + 1 \text{ teeth in interval } i$$

Let $C_i$ be the total weight from the $i^{th}$ particle after combing. Then the expected weight after combing is using Eqs. 3 and 5

$$E[C_i] = p_{i,j} j \frac{W}{M} + p_{i,j+1} (j + 1) \frac{W}{M} = \frac{w_i}{W/M} \frac{W}{M} = w_i$$
Note that this combing exactly preserves the total weight because the output of the combing is always $M$ particles of weight $W/M$.

III. AN IMPORTANCE-WEIGHTED COMB

An importance-weighted comb is just like the simple comb described above with importance times weight taking the place of weight in the simple comb. This is shown in Fig 2. In particular, combing $K$ particles into $M$ and defining

$$I_i = \text{user selected importance of } i^{th} \text{ particle} \tag{7}$$

$$u_i = I_i w_i \tag{8}$$

$$U = \sum_{i=1}^{K} u_i \tag{9}$$

Define the importance weighted $M$-toothed comb by

$$t_m = \xi \frac{U}{M} + (m - 1) \frac{U}{M} \quad m = 1, \ldots, M \tag{10}$$

Defining $j$ by

$$j < \frac{u_i}{U/M} \leq j + 1 \tag{11}$$

one sees that either $j$ or $j + 1$ teeth of a comb with a pitch of $U/M$ will hit an interval of length $u_i$. In particular,

$$p_{i,j} = j + 1 - \frac{u_i}{U/M} \quad \text{is the probability of } j \text{ teeth in interval } i \tag{12}$$

$$p_{i,j+1} = \frac{u_i}{U/M} - j \quad \text{is the probability of } j + 1 \text{ teeth in interval } i \tag{13}$$

Note that the the weights are obtained by noting that the average number of particles of type $i$ selected by the comb is $M(u_i/U)$. Thus to conserve the expected weight before and after combing requires that for all particles selected

$$\text{precomb weight} = w_i = w_i m_i M(u_i/U) = \text{expected postcomb weight} \tag{13}$$
where $m_i$ is the weight multiplication for combed particles derived from particle $i$. Solving Eq. 13 for $m_i$, one finds

$$m_i = U/(Mu_i)$$

(14)

is the weight multiplication for each combed particle derived from the $i^{th}$ precombed particle. Thus the postcombed weight of all particles derived from the $i^{th}$ precombed particle is using Eqs. 14 and 8

$$w_i' = m_i w_i = w_i U/(Mu_i) = U/(MI_i)$$

(15)

The expected total weight is conserved because each of the individual expected weights are conserved by construction. More formally, let

$$n_i = \text{the number of hits of the } i^{th} \text{ interval}$$

(16)

then using Eq. 15

$$W' = \sum_{i=1}^{K} n_i \frac{U}{MI_i}$$

(17)

Taking the expectation of Eq. 17 and using Eq. 12 yields

$$E[W'] = E[\sum_{i=1}^{K} n_i \frac{U}{MI_i}] = \sum_{i=1}^{K} \frac{U}{MI_i} (j_{pi,j} + (j + 1)_{pi,j+1})$$

$$= \sum_{i=1}^{K} \frac{U}{MI_i} (j(j + 1) - \frac{u_i}{U/M})$$

(18)

$$+ (j + 1)(\frac{u_i}{U/M} - j) = \sum_{i=1}^{K} \frac{U}{MI_i} \frac{u_i}{U/M} = \sum_{i=1}^{K} w_i = W$$

Unfortunately, unlike the simple comb, the total weight is not conserved. The next section addresses a possible solution to this problem when it is required to exactly preserve the weight and an importance-weighted comb is desired.
IV. A COMBING PROCEDURE THAT EXACTLY PRESERVES PARTICLE WEIGHT

Rather than applying a comb to the entire set of particles, this method combs a fraction of the particles and adjusts the weight of the uncombed fraction so that the total weight is exactly conserved on each combing.

First, consider the combed particles.

1. Let $w_i$ be the precomb weight of the $i^{th}$ combed particle.
2. Let $K$ be the total number of particles before comb
3. Let $M$ be the desired number of particles after combing
4. Let $I_i$ be the importance of the $i^{th}$ particle
5. Let

$$W = \sum_{i=1}^{K} w_i \quad (19)$$

6. Let

$$U = \sum_{i=1}^{K} w_i I_i \quad (20)$$

Now consider the uncombed particles.

7. Let $v_j$ be the weight of the $j^{th}$ uncombed particle.
8. Let $L$ be the total number of uncombed particles.
9. Let

$$V = \sum_{j=1}^{L} v_j \quad (21)$$

From Eq. 18, the combing technique preserves the expected weight of the first $K$ particles as these $K$ particles are combed into $M$ particles. Readjust the weights of the $L$ uncombed particles to

$$v'_j = v_j \frac{V - (W' - W)}{V} \quad (22)$$
Letting $V'$ be the adjusted weight of the uncombed particles then

$$V' = \sum_{j=1}^{L} v'_j = \sum_{j=1}^{L} v_j \frac{V - (W' - W)}{V} = \frac{V - (W' - W)}{V} \sum_{j=1}^{L} v_j = V - (W' - W)$$  \hspace{1cm} (23)

where the last equality follows by Eq. 21. (It is shown later how to ensure $V' > 0$.) The combined total weight of the combed and uncombed particles using Eq. 23 is thus

$$W' + V' = W' + V - (W' - W) = W + V$$  \hspace{1cm} (24)

That is, the total weight is exactly conserved.

The expected adjusted weight of the uncombed particles from Eq. 22 is

$$E[v'_j] = E[v_j \frac{V - (W' - W)}{V}] = v_j \frac{V + W}{V} - \frac{v_j}{V} E[W'] = v_j$$  \hspace{1cm} (25)

where the last equality follows from Eq. 18.

In deriving Eq. 23, discussion was deferred about how to ensure that

$$V' = V - (W' - W) > 0$$  \hspace{1cm} (26)

To do this, one can find an upper bound for $W'$. Suppose that one orders the particles by importance with the high importance particles to the left. Note from Fig. 3 and Eq. 15 that the upper combing represents the maximum possible $W'$ and that the lower combing represents the minimum possible $W'$. (This is because of the ordering by importance.) Note that the difference between the maximum and minimum possible $W'$ is easy to compute because with the exception of the first and last teeth, all other teeth are common between the two cases. That is, defining

$$W'_{high} = \text{maximum possible } W'$$  \hspace{1cm} (27)

$$W'_{low} = \text{minimum possible } W'$$  \hspace{1cm} (28)

Then from Fig. 3 and Eq. 15 we see that

$$W'_{high} - W'_{low} = \frac{U}{MI_M} - \frac{U}{MI_1}$$  \hspace{1cm} (29)
From Eq. 18 $E[W'] = W$, and noting that the maximum that $W'$ can deviate its mean is bounded by $W_{\text{high}}' - W_{\text{low}}'$, one gets

$$W' < W + W_{\text{high}}' - W_{\text{low}}'$$  \hspace{1cm} (30)

Thus using Eqs. 30 and 29

$$W' - W < W_{\text{high}}' - W_{\text{low}}' = \frac{U}{MI_M} - \frac{U}{MI_1}$$  \hspace{1cm} (31)

Thus as long as the total weight of the uncombed particles is

$$V > \frac{U}{MI_M} - \frac{U}{MI_1}$$  \hspace{1cm} (32)

then by Eq. 3 $V' > 0$ and the method will not result in any negative weights. Note that Eq. 32 can usually be satisfied with a single uncombed particle ($L = 1$) of large weight in an unimportant region.

Suppose that one does not wish to order the particles by importance? Can one still ensure that $V' > 0$? Let

$$j = \text{integer}(u_iM/U)$$  \hspace{1cm} (33)

On average

$$j - 1 < u_iM/U \leq j$$  \hspace{1cm} (34)

copies of the $i^{th}$ particle are taken each with weight

$$\frac{u_iU}{Mu_i}$$  \hspace{1cm} (35)

The total weight after combing must satisfy
Thus Eq. 26 will be true if

\[ W' \leq \sum_{i=1}^{K} \text{integer}(u_i M/U + 1) \frac{w_i U}{M u_i} \leq \sum_{i=1}^{K} (u_i M/U + 1) \frac{w_i U}{M u_i} \]

\[ = \sum_{i=1}^{K} w_i + \frac{U}{M} \sum_{i=1}^{K} \frac{1}{I_i} = W + \frac{U}{M} \sum_{i=1}^{K} \frac{1}{I_i} \]

Thus Eq. 26 will be true if

\[ V \geq \frac{U}{M} \sum_{i=1}^{K} \frac{1}{I_i} \]  

(37)

Note that Eq. 37 will be easily satisfied if one starts combing the higher importance particles first. One could roughly divide the particles in half and comb the first half and adjust the weight of the second half via Eq. 22. Then one could divide this adjusted part by two and comb the top part and adjust the weights of the bottom part. This process repeats until all the particles that can be combed have been combed.

V. SUMMARY

This paper has generalized the combing technique to allow an importance-weighted comb that precisely preserves the total weight and therefore the total charge. Thus, for those charged particle transport applications where a simple comb is useful for particle population control, the generalized combing technique not only provides population control but also provides an importance-weighted population.

REFERENCE

make 1 copy of particle 1 with weight \( W/M \)
make 0 copies of particle 2
make 2 copies of particle 3 with weight \( W/M \)
make 0 copies of particle 4
make 1 copy of particle 5 with weight \( W/M \)
make 0 copies of particle 6

Fig. 1. Simple Comb.

\[
\begin{align*}
\text{make 1 copy of particle 1 with weight } & \frac{w_1}{Mu_1} \\
\text{make 0 copies of particle 2} & \\
\text{make 2 copies of particle 3 with weight } & \frac{w_3}{Mu_3} \\
\text{make 0 copies of particle 4} & \\
\text{make 1 copy of particle 5 with weight } & \frac{w_5}{Mu_5} \\
\text{make 0 copies of particle 6} & \\
\end{align*}
\]

Fig. 2. Importance-Weighted Comb.
decreasing importance, increasing combed weight

maximum total combed weight configuration

minimum total combed weight configuration

\[
U = u_1 + u_2 + u_3 + u_4 + u_5 + u_6
\]

Fig. 3. Ordered. Importance-Weighted Comb.