PREPARED FOR THE U.S. DEPARTMENT OF ENERGY,
UNDER CONTRACT DE-AC02-76CH03073

PPPL-3798
UC-70

PPPL-3798

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by

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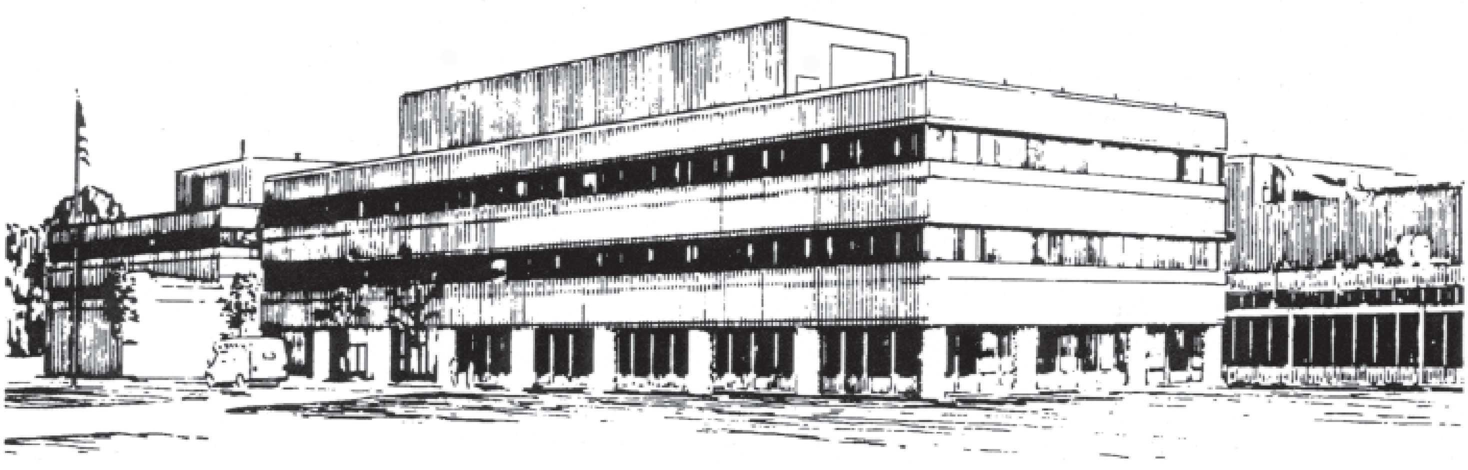
March 2003



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Numerical Loading of a Maxwellian Probability Distribution Function

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Abstract

A renormalization procedure for the numerical loading of a Maxwellian probablity distribution function (PDF) is formulated. The procedure, which involves the solution of three coupled nonlinear equations, yields a numerically-loaded PDF with improved properties for higher velocity moments. This method is particularly useful for low-noise particle-in-cell simulations with electron dynamics.

Pacs: 52.35.Py, 52.30.Jb, 52.55.Fa

1 Introduction

The collective behavior of a hot collisionless plasma is described in kinetic theory by the evolution of the distribution functions of its species $f_e(\mathbf{x}, \mathbf{z}, t)$ and $f_i(\mathbf{x}, \mathbf{z}, t)$ in continuous phase space. In the particle-in-cell (PIC) technique one returns to a discrete representation of the plasma in terms of a small sample of 10^4 to 10^8 'particles' (or markers) [1].

The most common (and natural) initialization of the simulation particles is to load the particle velocities, for example, with random numbers having the desired distribution. This method has obvious advantages; in particular it is in agreement with our physical intuition (that is the numerically-loaded probabliblity distribution function (PDF) for the markers ressembles the random distribution of actual particles). However, one disadvantage of random loading is that higher-order velocity moments are not well represented, and this may impact the long term behavior and the noise level of the simulated plasma.

Recently it has been pointed out by Manuilsky and Lee [2] that the implementation of electron dynamics in existing δf (ion) PIC codes could be best achieved using the so-called split-weight scheme. The basic idea behind the split-weight scheme is that the electron PDF is 'split' into an adiabatic part and a nonadiabatic part; only the phase space evolution associated with the nonadiabatic part of the PDF is dynamically evolved along the marker trajectories. The split-weight scheme, however, requires the evaluation of higher-order velocity moments: the current (first order velocity moment) in the electrostatic version [2]; as well as the pressure and heat flux (second and third order velocity moments, respectively) in the electromagnetic case [3].

In this paper, we present a renormalization procedure which yields Maxwellian probability distribution functions with improved properties for higher-order velocity moments. The paper is organized as follow; in section 2, we discuss the (standard) random loading procedure and its associated weaknesses; in section 3, we describe a renormalization procedure and its numerical implementation; numerical results are presented and discussed in section 4.

2 Random Loading

Let us assume that a Maxwellian PDF, based on a set of N samples (markers), has been (numerically) generated using some arbitrary random technique; the method used can be straightforward methods (for example, Neumann's rejection technique) or more sophisticated methods, such as those based on number theory [4,5]. Some methods based on random number generators tend to introduce a 'background noise' that could be detrimental for the observation of low-amplitude instabilities. Apart from the noise properties associated with the initial PDF, the accuracy of higher-order velocity moments can be also important in some applications. This paper attempt to address some of the issues associated with higher-order velocity moments (irrespective of the loading method of the initial PDF).

The continuous (exact) Maxwellian distribution function $F_M(v)$ satisfies

$$\left\langle v^{2n+1} \right\rangle \equiv \int_{-\infty}^{+\infty} v^{2n+1} F_M(v) dv = 0 \tag{2.1}$$

for $n = 0, 1, 2, ...$ The derivation of the even moments of the Maxwellian PDF are presented in the Appendix. Now consider the moments of the *numerically-loaded* PDF. Since the loading is random, it is sufficient to carry out the velocity space integration using Riemmann sums; the velocity moment of order k, based on a set of N markers, is then defined as

$$M\left(k;N\right) \equiv \frac{1}{N}\sum_{j=1}^{N} {v_j}^k \tag{2.2}$$

where k is a nonnegative integer and j labels the marker. For $N \mapsto \infty$, we expect $M(1,N) \mapsto 0$, $M(2,N) \mapsto 1$ and $M(3,N) \mapsto 0$ and so on (see the Appendix for higher-order moments). The set $\{v_j; j = 1,..,N\}$ will not, in general, satisfy the relations of $\langle v\rangle = \langle v^3\rangle = 0$ and $\langle v^2\rangle = 1$. To remedy to this situation, a simple renormalization through the first-order is often used; upon evaluating

$$\xi = \frac{1}{N}\sum_{j=1}^{N} v_j \tag{2.3}$$

a new set $\{V_j; j = 1,..,N\}$ is generated according to

$$V_j = v_j - \xi \tag{2.4}$$

for $j = 1,...,N$. By construction, the new set of markers satisfies $\langle V\rangle \equiv 0$; however, the accuracy of higher-order velocity moments is not guaranteed with this method.

3 Renormalization Procedure

In this paper, we propose a renormalization procedure of the PDF based on the polynomial given by

$$V_j = v_j - \alpha - \beta v_j - \gamma {v_j}^2 \tag{3.5}$$

where α, β and γ are unknown parameters. Note that for $\beta = \gamma = 0$, we have $\alpha = \xi$, where ξ is given by Eq.(2.3). We demand that the parameters α, β and γ are chosen such that the relations

$$\begin{aligned} \langle V\rangle &= \frac{1}{N}\sum_{j=1}^{N} V_j = 0 \\ \left\langle V^2\right\rangle &= \frac{1}{N}\sum_{j=1}^{N} V_j^2 = 1 \\ \left\langle V^3\right\rangle &= \frac{1}{N}\sum_{j=1}^{N} V_j^3 = 0 \end{aligned} \tag{3.6}$$

are satisfied (see Appendix). Substituting Eq.(3.5) in Eq.(3.6) one gets after some algebra a set of 3 coupled, nonlinear equations for the parameters α, β and γ

$$\begin{aligned} F\left(\alpha,\beta,\gamma\right) &= 0 \\ G\left(\alpha,\beta,\gamma\right) &= 0 \\ H\left(\alpha,\beta,\gamma\right) &= 0 \end{aligned} \tag{3.7}$$

where

$$F(\alpha,\beta,\gamma) \equiv (1-\beta)\langle v\rangle - \alpha - \gamma\left\langle v^2\right\rangle \tag{3.8}$$

$$G(\alpha,\beta,\gamma) \equiv \alpha^2 - \eta\langle v\rangle + \mu\left\langle v^2\right\rangle - \theta\left\langle v^3\right\rangle + \gamma^2\left\langle v^4\right\rangle - 1 \tag{3.9}$$

and

$$H(\alpha,\beta,\gamma) \equiv -\alpha^3 + \lambda\langle v\rangle - \varphi\left\langle v^2\right\rangle + \xi\left\langle v^3\right\rangle - \omega\left\langle v^4\right\rangle + \kappa\left\langle v^5\right\rangle - \gamma^3\left\langle v^6\right\rangle \tag{3.10}$$

In Eqs.(3.8-3.10) we have the following definitions

$$\begin{aligned}
\eta &= 2\alpha(1-\beta)\\
\mu &= 1+\beta^2-2\beta+2\alpha\gamma\\
\theta &= 2\gamma(1-\beta)\\
\lambda &= \alpha\eta+\alpha^2(1-\beta)\\
\varphi &= \alpha^2\gamma+\eta(1-\beta)+\alpha\mu\\
\xi &= \eta\gamma+\mu(1-\beta)+\theta\alpha\\
\omega &= \alpha\gamma^2+\mu\gamma+\theta(1-\beta)\\
\kappa &= \theta\gamma+\gamma^2(1-\beta)
\end{aligned}$$

The renormalization procedure is implemented as follows; for a given set of N markers, one computes the moments $\langle v^p\rangle$ for $p = 1,\cdots,6$ that enter the definitions of the functions F, G and H. Then, starting from an initial guess $\{\alpha_0,\beta_0,\gamma_0\}$, a new set of coefficients is generated through a set of random increments $\Delta\alpha, \Delta\beta$ and $\Delta\gamma$; the sequence takes the general form

$$\begin{aligned}
\alpha_{k+1} &= \alpha_k+\Delta\alpha\\
\beta_{k+1} &= \beta_k+\Delta\beta\\
\gamma_{k+1} &= \gamma_k+\Delta\gamma
\end{aligned}$$

for $k = 0,1,2,...$ (We denote the asymptotic solution as $\{\alpha_\infty,\beta_\infty,\gamma_\infty\}$ although in practise the sequence has a finite number of terms). The new set of coefficients is tested against the constraint $\chi(\alpha,\beta,\gamma) \equiv |FGH| < \epsilon$ (where ϵ is a small tolerance parameter). This algorithm yields a trajectory in 'phase space', as shown in Figure 1. Although there exists more powerful root finding techniques, the computing time required to determine an appropriate set $\{\alpha,\beta,\gamma\}$ represents, in practise, a small fraction of the total computing time of a global PIC simulation. We have compared various other constraints such as

$$|F| < \epsilon_1\ ;\ |G| < \epsilon_2\ ;\ |H| < \epsilon_3\ ,$$

where ϵ_1,ϵ_2 and ϵ_3 are (in general, independent) smallness parameters. As it turns out, the same fixed point in Figure 1 has been found (indicating that the root solution is a strong attractor).

4 Numerical Results

The algorithm described in the previous section has been parallelized using the Message Passing Interface (MPI) for maximum efficiency. In a typical PIC simulations, the computation of the set of coefficients $\{\alpha_\infty, \beta_\infty, \gamma_\infty\}$ is carried out once. Most PIC codes are based on parallel algorithms, and it is therefore meaningful to exploit this parallelism when determining the coefficients necessary for the renormalization of the probability distribution function. The markers are distributed across all processors (PEs), with an equal (or almost equal) number of particles per PE; in the same spirit, one can distribute M different values of $\alpha_J^{(p)}, \beta_J^{(p)}$ and $\gamma_J^{(p)}$, for $p = 1, \cdots, M$ in the phase space volume element

$$\begin{aligned} \alpha &: \ \alpha_J^{(p)} \in [\alpha_k - \Delta\alpha/2, \alpha_k + \Delta\alpha/2] \\ \beta &: \ \beta_J^{(p)} \in \ [\beta_k - \Delta\beta/2, \beta_k + \Delta\beta/2] \\ \gamma &: \ \gamma_J^{(p)} \in [\gamma_k - \Delta\gamma/2, \gamma_k + \Delta\gamma/2] \end{aligned}$$

Here $J = 0, \cdots, N_{PE} - 1$ labels the processor, and N_{PE} is the total number of processors. Therefore the quantity $\chi(\alpha, \beta, \gamma)$ can be evaluated independently on N_{PE} processors; communication between processors is only required in the last step of the computation

$$\chi_{\min} = \mathrm{MIN}\,\{\chi_J\ ;\ J = 0, \cdots, N_{PE}\}$$

In Figures 2-4, the dotted (plain) line show the value of the velocity moments before (after) the renormalization procedure. In order to illustrate the features of the renormalization procedure, we have varied the number of markers N. As expected the properties of the random initialization improve (on average) as the number of markers is increased; although this is true for the first-order moment (Figure 2), the third-order moment (Figure 4) does show strong departure from the exact value. The velocity moments for the remormalized PDF, however, gives a much better agreement with the exact values for all 3 moments.

Figure 5 shows the exact (plain) and the approximate (dotted) Maxwellian PDFs for a set of $N = 2^{16} = 65536$ markers. The differences between the exact and approximate PDFs occur mostly for a group of low-velocity markers ($|V| \leq 0.5$) and a small group of suprathermal ($|V| > 2$) markers.

The renormalization procedure can be generalized so that higher order velocity moments are accurately represented. Furthermore, although the case of a Maxwellian PDF has been considered here, other probability distribution functions can also be renormalized using similar ideas; of course, one must have a knowledge of the analytical expressions of the velocity moments of the continuous (exact) PDF (for a Maxwellian PDF, these moments are given in the Appendix). As discussed above, the root finding procedure can be easily implemented into existing parallel PIC algorithms; furthermore, it is easy to code and and, at the same time, has a good computation/communication performance ratio.

5 Concluding Remarks

We have a presented a simple renormalization procedure for a numerically loaded Maxwellian probabiblity distribution function. The method amounts to a root searching procedure for a set of three coupled nonlinear equations. In the spirit of modern global PIC simulations, the method can be easily implemented as a parallel algorithm; numerical simulations do confirm that higher-order velocity moments are accurately reproduced even for small numbers of markers.

Acknowledgments The author is grateful to Dr W.W. Lee for interesting discussions. This research was supported by Contract No. DE-AC02-CH0-3073 and the Scientific Discovery through Advanced Computing (SciDAC) initiative (U.S. Department of Energy).

Appendix: Velocity Moments of a Maxwellian Probability Distribution Function

In this Appendix, we present a method to calculte the velocity moments of a one-dimensional Maxwellian PDF. The one-dimensional Maxwellian distribution function (for particle species j) is

$$F_{Mj}\left(v_{||}\right)=\frac{n_0}{\sqrt{2\pi}V_{thj}}\ \exp\left(-\frac{v_{||}^2}{2V_{thj}^2}\right) \tag{A.1}$$

where $V_{thj}=\sqrt{T_j/m_j}$ is the thermal velocity. Letting $x\equiv v_{||}/\left(\sqrt{2}V_{thj}\right)$ one has

$$F_{Mj}dv_{||}=\frac{n_0}{\sqrt{\pi}}\ \exp\left(-x^2\right)dx\ . \tag{A.2}$$

Define

$$J\left(\alpha\right)\equiv\int_{-\infty}^{+\infty}\exp\left(-\alpha x^2\right)dx \tag{A.3}$$

for positive α. Using the change of variable $y=\sqrt{\alpha}x$ one obtains

$$J\left(\alpha\right)=\frac{1}{\sqrt{\alpha}}\ \int_{-\infty}^{+\infty}\exp\left(-y^2\right)dy=\sqrt{\pi}\alpha^{-1/2} \tag{A.4}$$

Differentiating Eq.(A.3) with respect to α, we note that

$$\frac{dJ}{d\alpha}\ =-\int_{-\infty}^{+\infty}x^2\exp\left(-\alpha x^2\right)dx$$

and

$$\frac{d^2J}{d\alpha^2}\ =\int_{-\infty}^{+\infty}x^4\exp\left(-\alpha x^2\right)dx$$

from which one can deduce the relation of recurrence given by

$$\int_{-\infty}^{+\infty}x^{2p}\exp\left(-\alpha x^2\right)dx=\left(-1\right)^p\frac{d^pJ}{d\alpha^p} \tag{A.5}$$

for $p=1,2,...$. From Eq.(A.4) we note that $dJ/d\alpha=-1/2\sqrt{\pi}\alpha^{-3/2}$, $d^2J/d\alpha^2=3/4\sqrt{\pi}\alpha^{-5/2}$, or

$$\frac{d^pJ}{d\alpha^p}\ =\sqrt{\pi}\left(-1\right)^p\frac{\left(2p-1\right)\left(2p-3\right)...(5)(3)(1)}{2^p}\ \alpha^{-(2p+1)/2} \tag{A.6}$$

for $p=1,2,...$. Substituting Eq.(A.6) in the right-hand side of Eq.(A.5) we obtain

$$\int_{-\infty}^{+\infty}x^{2p}\exp\left(-\alpha x^2\right)dx=\sqrt{\pi}\frac{\left(2p-1\right)\left(2p-3\right)...(5)(3)(1)}{2^p}\ \alpha^{-(2p+1)/2} \tag{A.7}$$

With these preliminary calculations, we are ready to calculate the velocity moment of order k, defined as

$$M_j\left(k\right)\equiv\int_{-\infty}^{+\infty}F_{Mj}\left(v_{||}\right)v_{||}^kdv_{||} \tag{A.8}$$

The change of variable $x \equiv v_{||}/\left(\sqrt{2}V_{thj}\right)$ and the relation $F_{Mj}dv_{||} = n_0\pi^{-1/2}\exp\left(-x^2\right)dx$ show that the velocity moment (A.8) can be written as

$$M_j(k) = \frac{n_0}{\sqrt{\pi}} \int_{-\infty}^{+\infty} \left(\sqrt{2}V_{thj}\right)^k x^k \exp\left(-x^2\right) dx = n_0 \left(\sqrt{2}V_{thj}\right)^k I\left(k\right) \tag{A.9}$$

where

$$I\left(k\right) \equiv \frac{1}{\sqrt{\pi}} \int_{-\infty}^{+\infty} x^k \exp\left(-x^2\right) dx \tag{A.10}$$

Clearly $I\left(2k-1\right) = 0$ for $k = 1, 2, 3, \ldots$. We use Eq.(A.7) to show that

$$\begin{aligned}
I(2) &= \frac{1}{2} \\
I(4) &= \frac{3}{4} \\
I(6) &= \frac{15}{8} \\
I(8) &= \frac{105}{16} \\
I(10) &= \frac{945}{32} \\
I(12) &= \frac{10395}{64} \\
I(14) &= \frac{135135}{128}
\end{aligned}$$

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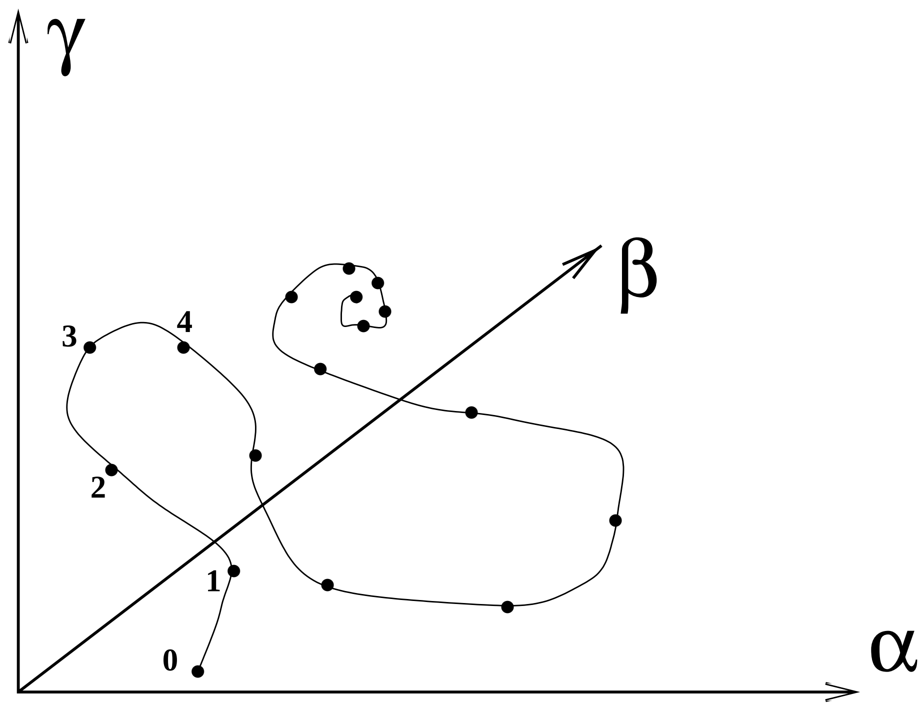

Figure 1: The renormalization procedure requires the computation of an optimal set $\{\alpha, \beta, \gamma\}$. A typical trajectory in parameter space is shown.

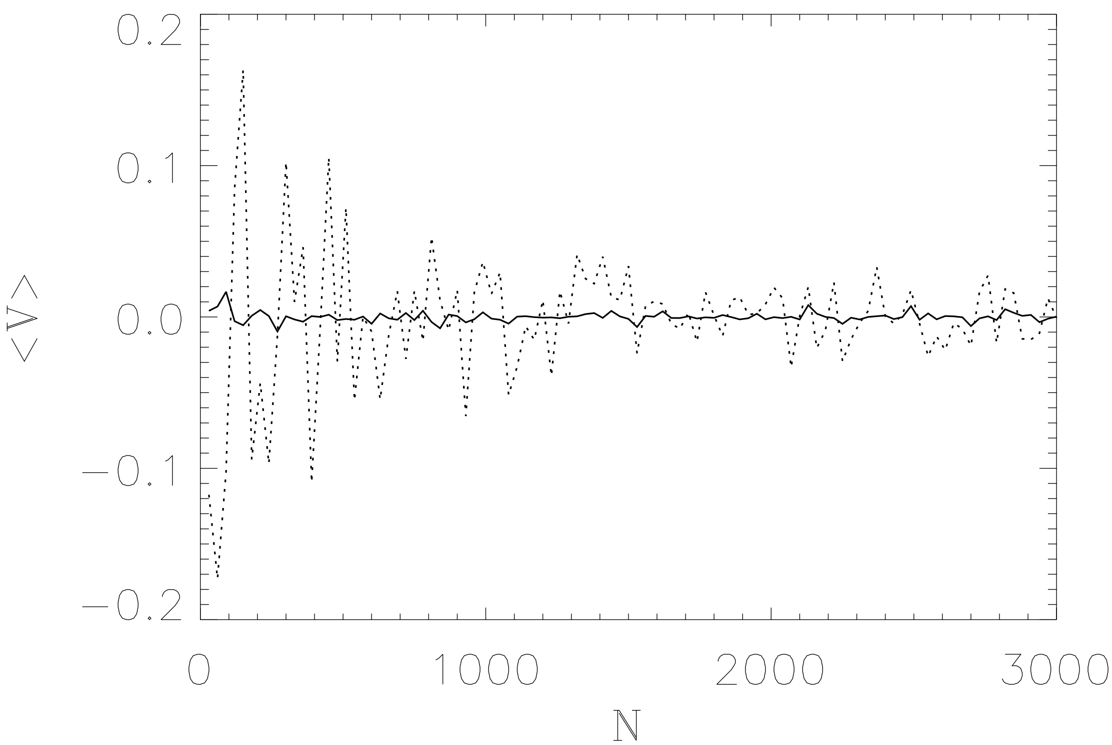

Figure 2: First-order velocity moment $\langle V \rangle$ as a function of number of markers N before (dotted line) and after (plain line) the renormalization procedure. The exact answer corresponds to the $\langle V \rangle = 0$ line.

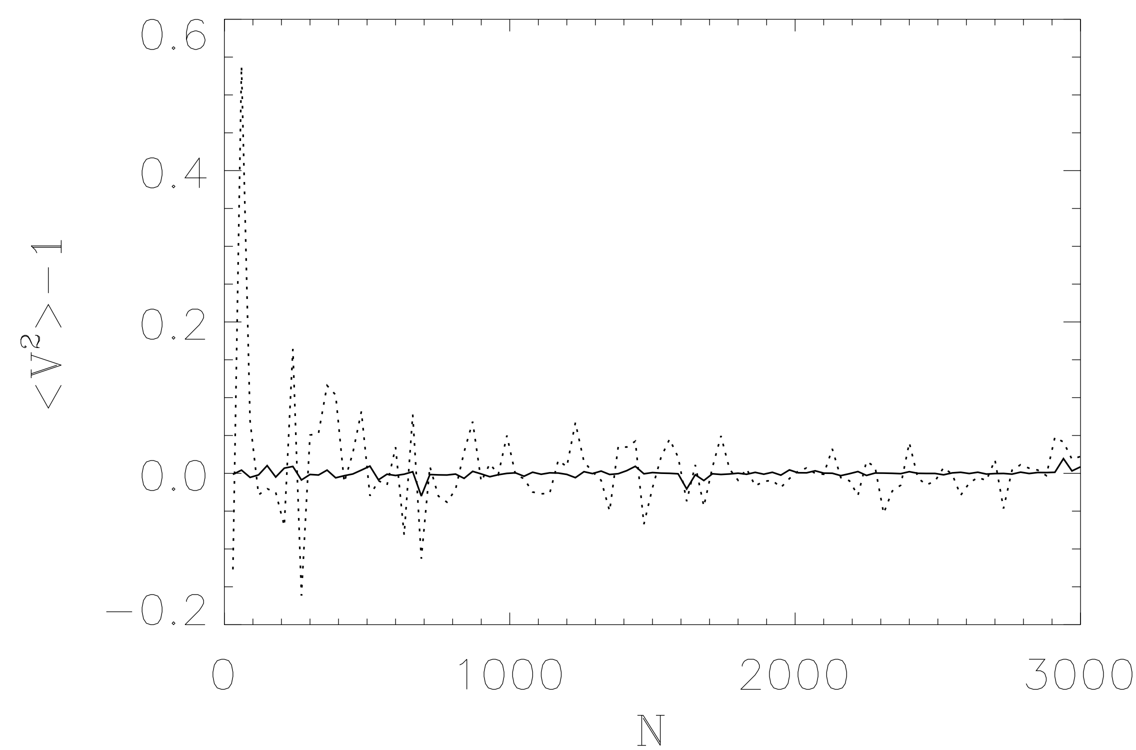

Figure 3: Second-order velocity moment $\langle V^2 \rangle$ as a function of number of markers N before (dotted line) and after (plain line) the renormalization procedure. The exact answer corrresponds to the $\langle V^2 \rangle - 1 = 0$ line.

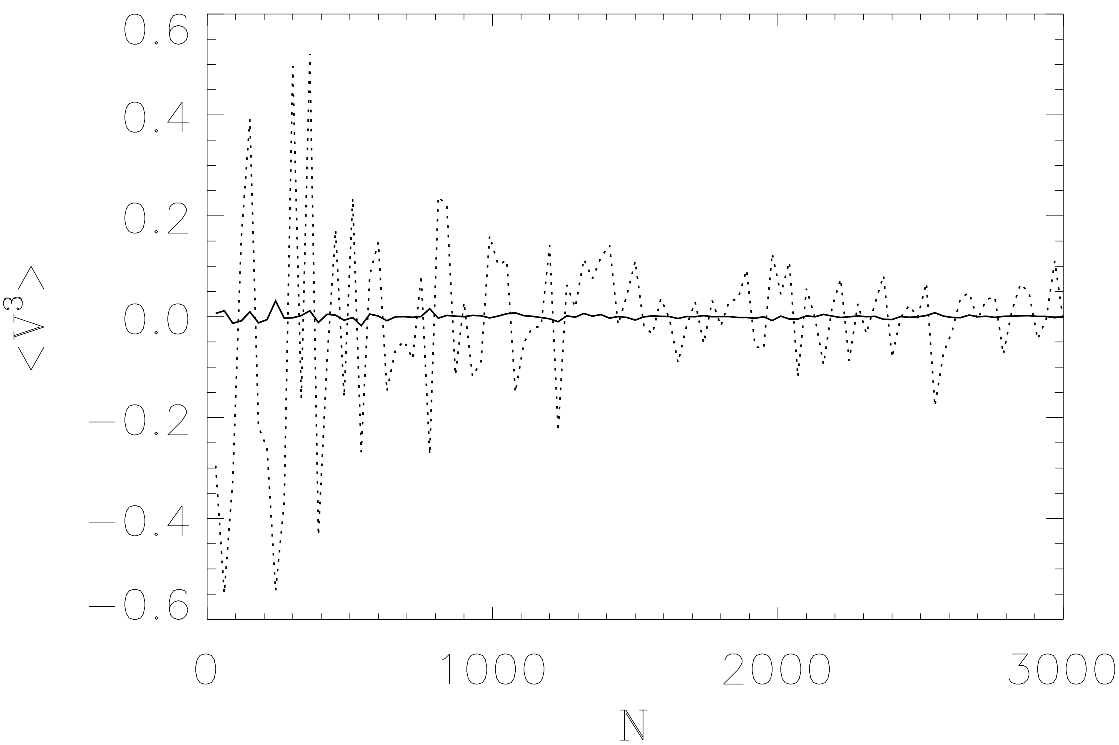

Figure 4: Second-order velocity moment $\langle V^3 \rangle$ as a function of number of markers N before (dotted line) and after (plain line) the renormalization procedure. The exact answer corrresponds to the $\langle V^3 \rangle = 0$ line.

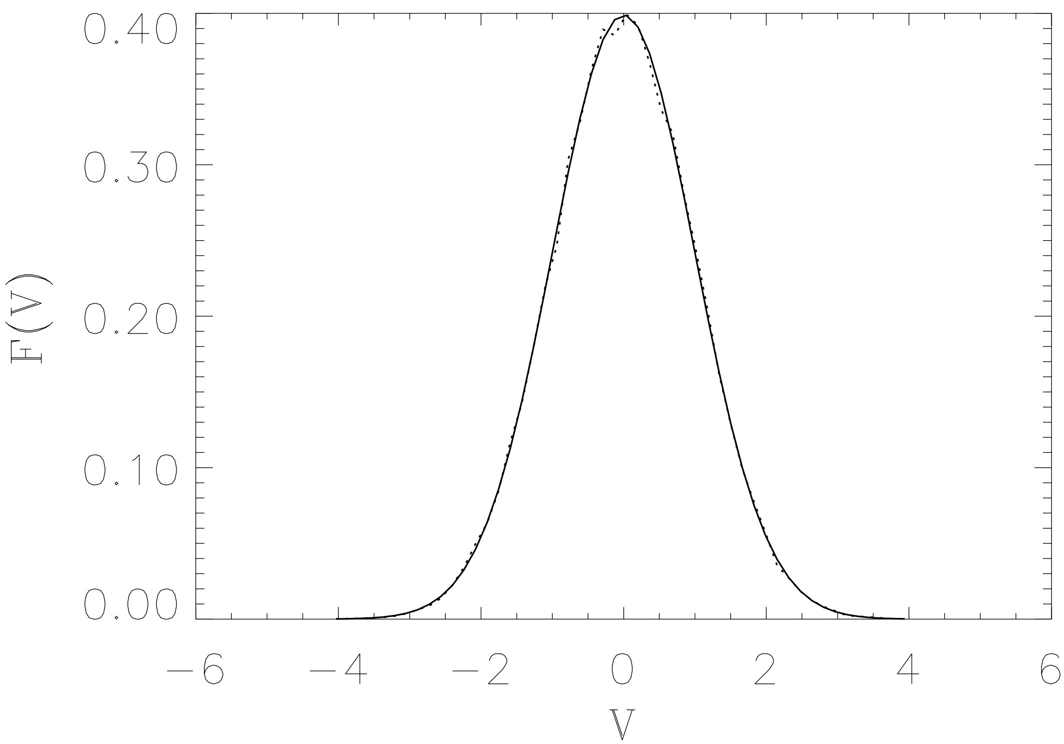

Figure 5: Exact (plain line) and renormalized (dotted) Maxwellian probability function for a set of $N = 2^{16} = 65536$ markers.

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