ORTHOGONAL BASIS FUNCTION APPROXIMATION OF PARTICLE DISTRIBUTION IN NUMERICAL SIMULATIONS OF BEAMS *

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Abstract

Numerical simulations of charged particle beams require an approximation to the particle distribution being simulated. We present a mathematical formalism for approximating two-dimensional (2D) particle distribution using a basis composed of scaled and translated Gauss-Hermite (STGH) functions. It is computationally efficient, because it only requires the values of the particle distribution at $(N+1)\times(M+1)$ nodes, where N and M are the highest basis function retained in the expansion in each coordinate. After outlining the mathematical formalism for the expansion, we compare it to the cosine expansion which is currently used in a code simulating coherent synchrotron radiation. The advantages of the STGH approximation over the cosine expansion are demonstrated by comparing the computational costs and execution times, as well as manifesting that unphysical fluctuations in the tail of the approximation which plague cosine expansion are not a factor in the new method. All these features make the STGH approximation valuable for N-body codes simulating the dynamics of multiparticle systems.

INTRODUCTION

The normalized Gauss-Hermite functions are given by

$$\psi_n(v) = \frac{1}{\sqrt{2^n n!\sqrt{\pi}}} H_n(v) e^{-v^2}, \qquad (1)$$

where the $H_n(v)$ are the Hermite polynomials. They are orthonormal on $(-\infty,\infty)$ with the weight $w(v)=e^{v^2}$:

$$\int_{-\infty}^{\infty} \psi_n(v)\psi_m(v)e^{v^2}dv = \delta_{nm}, \qquad (2)$$

where δ_{nm} is a Kronecker delta. The basis composed of Gauss-Hermite functions $\{\psi_n\}_{n=0}^N$ are often used in various areas of physics, because of their relationship to normal distribution. The Gauss-Hermite spectral methods, while possessing some useful properties, only yield good approximation when scaled. Scaled Gauss-Hermite functions have been used earlier in the context of beam simulations [1, 2, 3]. While most of our motivation and justification for using scaled Gauss-Hermite function coincides with theirs, the mathematical formalism and computational implementation we present here are different. In the new method: (i) no underlying ellipsoidal distributions are assumed; (ii) the computation of the scaled Gauss-Hermite expansion here is done in a more direct and efficient way; (iii) the Poisson equation and the self-fields are directly obtained, without an expensive multidimensional integration. The results reported in the earlier work – most notably appreciable increase in accuracy and computational efficiency over the existing particle-in-cell (PIC) codes – gives us a reasonable expectation that the approach we present here is indeed superior to the existing gridless approaches. The efforts to integrate this 2D formalism into an existing 2D beam simulation code, as well as extending it to 3D and implementing a full 3D gridless N-body code as an alternative to PIC codes, are currently underway [4].

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SCALED AND TRANSLATED GAUSS-HERMITE BASIS

The 2D gaussian-type functions (i.e., functions which decay at infinity at least like $\exp\left(-px^2-qy^2\right)$, with p,q some positive constants) can be well-approximated by a finite Gauss-Hermite expansion

$$f(x,y) = \sum_{n=0}^{N}\sum_{m=0}^{M} a_{nm}\psi_n(\alpha_1(x-\bar{x}))\psi_m(\alpha_2(y-\bar{y})), \qquad (3)$$

where $\alpha_1,\alpha_2>0$ and $\bar{x}$, $\bar{y}$ are constants. In solving differential equations, it is important to be able to express derivatives of the function in the same basis. This is achieved via recurrence relations of Gauss-Hermite polynomials [6]:

$$\begin{aligned} H_{k+1}(z) &= 2zH_k(z) - 2kH_{k-1}(z), \qquad (4)\\ H_k'(z) &= 2zH_{k-1}(z). \end{aligned}$$

This ability to express coefficients of the derivatives of the function in terms of coefficients of the function itself renders solving the Poisson equation in this basis trivial.

In pseudo-spectral methods, such as the collocation method used in [5], the optimal pseudo-spectral points are the roots of the $H_{N+1}(x)$ and $H_{M+1}(y)$, denoted by $\{\gamma_j\}_{j=0}^N$ and $\{\beta_k\}_{k=0}^M$, respectively. The collocation points are arranged in descending order, i.e., $\gamma_0>\gamma_1>...>\gamma_N$ and $\beta_0>\beta_1>...>\beta_M$. If the eq. (3) is satisfied at the collocation points, then it can be written as

$$f(\tilde{\gamma}_j,\tilde{\beta}_k) = \sum_{n=0}^{N}\sum_{m=0}^{M} a_{nm}\psi_n(\gamma_j)\psi_m(\beta_k), \qquad (5)$$

where $0\le j\le N$, $0\le j\le M$, and

$$\tilde{\gamma}_j = \frac{\gamma_j}{\alpha_1}+\bar{x}, \qquad \tilde{\beta}_k = \frac{\beta_k}{\alpha_2}+\bar{y}. \qquad (6)$$

It is now convenient to take advantage of the following relation for Hermite polynomials [6]:

$$\sum_{k=0}^{n} \frac{H_k(x)H_k(y)}{2^k k!} = \frac{H_{n+1}(x)H_n(y) - H_n(x)H_{n+1}(y)}{2^{n+1} n!(x-y)}, \tag{7}$$

which, for $0 \le i, j \le N$ and $0 \le k, l \le M$, leads to

$$\sum_{n=0}^{N} \psi_n(\gamma_i)\psi_n(\gamma_j) \sum_{m=0}^{M} \psi_m(\beta_k)\psi_m(\beta_l) = C_{ik}\delta_{ij}\delta_{kl}. \tag{8}$$

From eq. (8) it follows for $0 \le i \le N$ and $0 \le k \le M$:

$$C_{ik} = \sum_{n=0}^{N} \left[\psi_n(\gamma_i)\right]^2 \sum_{m=0}^{M} \left[\psi_m(\beta_k)\right]^2 \tag{9}$$

after which we finally we obtain the expression for coefficients a_{nm}, with $0 \le n \le N$ and $0 \le m \le M$:

$$a_{nm} = \sum_{j=0}^{N}\sum_{k=0}^{M} \frac{1}{C_{jk}} f(\tilde{\gamma}_j, \tilde{\beta}_k)\psi_n(\gamma_j)\psi_m(\beta_k). \tag{10}$$

By utilizing the property in eq. (7), evaluation of the expansion coefficients a_{nm} no longer requires integration over the entire distribution function, but only its value at the nodes. Combining eqs. (5) and (10) yields a STGH approximation to function f.

The scaling factors α_1 and α_2 for the normalized distribution function f are computed from the standard deviation in x- and y-coordinates:

$$\alpha_1 = \frac{1}{\sqrt{2}\sigma_x}, \qquad \alpha_2 = \frac{1}{\sqrt{2}\sigma_y}, \tag{11}$$

while $\bar{x}$ and $\bar{y}$ are simply first moments of the DF in x- and y-coordinates, respectively.

APPLICATION TO SIMULATIONS OF MULTIPARTICLE SYSTEMS

The STGH expansion is well-suited in the context where one needs an analytical approximation to the microscopic Klimontovich density distribution:

$$f(x,y) = \frac{1}{N_{\text{part}}} \sum_{i=1}^{N_{\text{part}}} \delta(x - x_i)\delta(y - y_i), \tag{12}$$

where N_{part} is the number of macroparticles. The STGH expansion can be tailored to the 2D gridless N-body simulation of charged-particle beams [7, 8] in which:

1. discretely-sampled macroparticle distribution is analytically approximated by a cosine expansion;
2. the Poisson equation is solved to obtain corresponding potential and forces acting on each macroparticle;
3. each macroparticle is advanced a small time-step Δt.

The STGH seeks to improve on computationally expensive cosine expansion in Step 1, while providing an efficient way to compute the potential and forces.

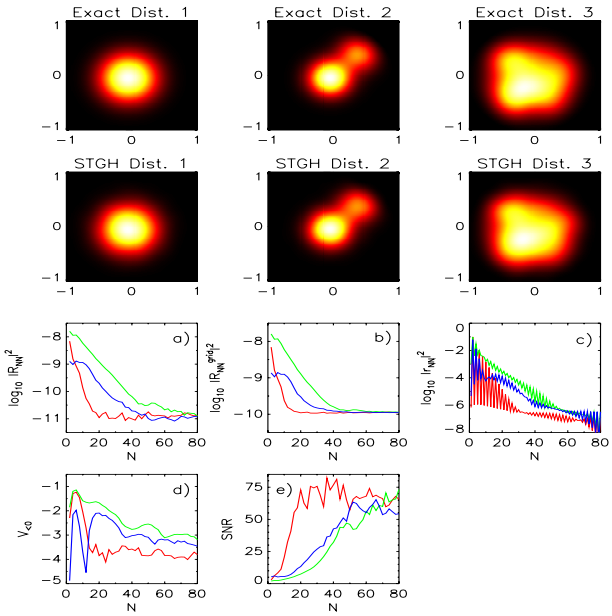

Figure 1: Three "toy" analytical distributions (superpositions of 1, 2 and 50 gaussians): exact (top row); approximated by STGH with $N = M = 80$ (second row); convergence estimators $|R_{NM}|^2$, $\left|R^{\text{grid}}_{NM}\right|^2$, $|r_{NM}|^2$ versus the number of expansion coefficients $N = M$; fraction of negative volume (panel d) and signal-to-noise ratio (panel e).

STGH Algorithm Outline

The STGH algorithm for computing coefficients a_{nm} can be outlined as follows:

1. tabulate unchanging quantities $\frac{\psi_n(\gamma_j)\psi_m(\beta_k)}{C_{ik}}$;
2. compute scaling and translation factors $\bar{x}$, $\bar{x}$, α_1, α_2;
3. evaluate $f\left(\tilde{\gamma}_j, \tilde{\beta}_k\right)$;
4. compute coefficients a_{lm} [eq. (10)].

Steps 2-4 are repeated at each time-step of the simulation. Evaluation of $f\left(\tilde{\gamma}_j, \tilde{\beta}_k\right)$ in Step 3 is the key to the STGH approximation. It can be done by counting the number of particles in some small neighborhood of the node (*shifted histogram estimator*), and normalizing it. We also tested alternative adaptive estimators, but the difference was not appreciable enough to warrant substantial increase in computational effort.

Convergence and Accuracy of the STGH

Convergence and accuracy of the STGH can be quantified using several quantities.

When the exact distribution is known:

(i) L_2-norm of the difference between the exact and approximated distributions:
$R_{NM}(x,y) = f^{\text{apx}}_{NM}(x,y) - f^{\text{ex}}(x,y)$;
(ii) signal-to-noise ratio (SNR):

$$SNR \equiv \left[\sum_{i=1}^{K_x}\sum_{j=1}^{K_y}\left(f_{ij}^{\mathrm{apx}}\right)^2\right]^{\frac{1}{2}}\left[\sum_{i=1}^{K_x}\sum_{j=1}^{K_y}\left(f_{ij}^{\mathrm{ex}}-f_{ij}^{\mathrm{apx}}\right)^2\right]^{-\frac{1}{2}}.$$

(Figure 1 shows these for three analytical "toy" distributions.)

When the exact distribution is not *known:*

(i) L_2-norm of the difference between the approximated and gridded distributions:
$R_{NM}^{\mathrm{grid}}(x,y) = f_{NM}^{\mathrm{apx}}(x,y) - f^{\mathrm{g}}(x,y)$;
(ii) correction to the expansion from one step to another: $r_{NM}(x,y) = f_{N-1M-1}^{\mathrm{apx}}(x,y) - f_{NM}^{\mathrm{apx}}$.

STGH VS. COSINE EXPANSION: ACCURACY AND EFFICIENCY

We compare the cosine and STGH expansion on a set of particle distributions containing 10^6 macroparticles, generated from realistic simulation [9].

Accuracy: As quantified by $|R_{NM}^{g}|^2$, $|r_{NM}|^2$, the STGH is at least as accurate as the cosine expansion (Fig. 2, second and third row).

Efficiency: STGH expansion is considerably faster than cosine expansion – by about 5-25 times – because it does not require expensive trigonometric function evaluations, and each coefficient does not require integration (summation) over all particles in the distribution (Fig. 2, fourth row).

Unphysical "wiggles" in the particle distribution: Fraction of negative particle distribution for STGH expansion is considerably lower – by at least an order of of magnitude (Fig. 2, fifth row; Fig. 3). This is because the cosine basis functions are non-decaying, while the STGH basis functions decay exponentially.

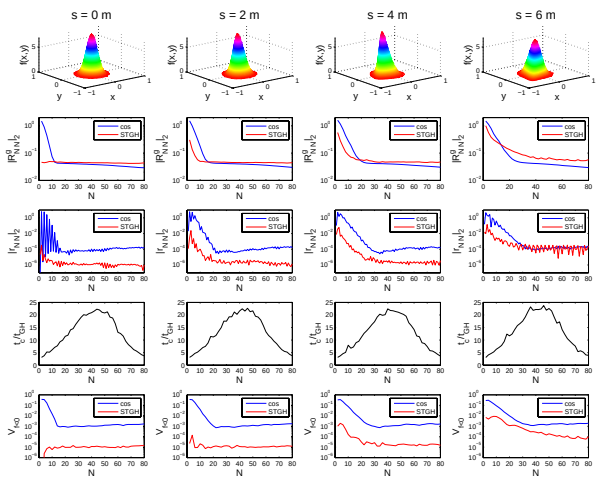

Figure 2: Particle distribution from a beam simulation with $N_{\mathrm{part}} = 10^6$ macroparticles at $s = 0, 2, 4, 6$m, gridded on a 128×128 grid. For the cosine (blue lines) and the STGH (red) expansion: second and third rows show convergence estimators $\left|R_{NM}^{\mathrm{grid}}\right|^2$, $|r_{NM}|^2$; fourth ratio of execution speeds; and fifth fraction of negative volume.

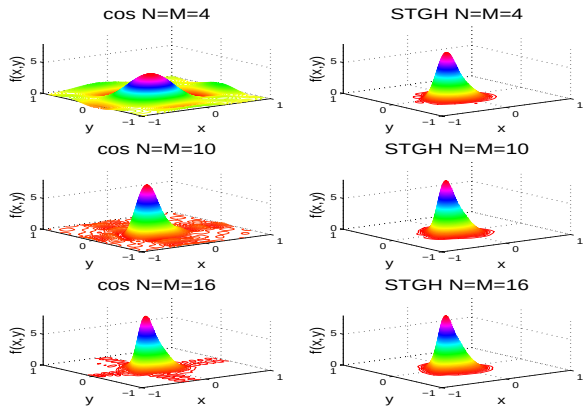

Figure 3: Approximations to the particle distribution from a beam simulation with $N_{\mathrm{part}} = 10^6$ macroparticles at $s = 4$m with the cosine expansion (left column) and the STGH (right column), with $N = M = 4$ (first row), $N = M = 10$ (second row), $N = M = 16$ (second row).

CONCLUSION

We presented the STGH expansion which is well-suited when an analytical approximation of the distribution sampled by N_{part} macroparticles is needed. We have shown that in the context of simulations of charged particle beams, the STGH approximation is more accurate and about an order of magnitude faster than the cosine approximation. It is also immune to a problem of unphysical wiggles in the tails of the distribution, which is intrinsic to cosine expansion. Therefore, the STGH provides a more accurate approximation in the tails of the distribution, which is of pivotal importance to beam halo simulations. Overall, the STGH represents a significant improvement over the existing analytic approximations used in beam simulation codes.

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