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Noise minimization by bias-variance optimization in particle-based plasma simulation methods

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Variational Lagrangian Particle Methods

The 1D Vlasov-Poisson system is formulated with Low's Lagrangian:

$$L = L_p + L_{int} + L_f$$

with

$$L_p = \frac{1}{2}\int dx_0\, dv_0 f_0(x_0, v_0)\left(\frac{\partial x(x_0, v_0, t)}{\partial t}\right)^2$$

$$L_f = \frac{1}{2}\int dx|\nabla\phi|^2$$

$$L_{int} = -\int dx_0\, dv_0 f_0(x_0, v_0)\phi(x, t)$$

$$f(x, y, t) = f_0(x_0(x, v, t), v_0(x, v, t), 0)$$

Variation with respect to x and ϕ gives (for electron species, assuming immobile ions)

$$\ddot{x} = \nabla\phi = -E(x), \quad \frac{\partial^2\phi}{\partial x^2} = \varrho - \varrho^{\text{ion}},$$

where $\varrho(x) = \int dv f(x, y, t)$ and $\int_0^1 dx\,\varrho(x) = \int_0^1 dx\,\varrho^{\text{ion}}(x)$.

Density Estimation

Assume N_p (macro) particles in the system and uniform grid on $0 \le x \le 1$. Write a charge deposition function in terms of a fundamental "kernel" as

$$\rho(x) = \frac{1}{h} K\left(\frac{x}{h}\right).$$

where h is the particle width, not necessarily related to the grid spacing. Some commonly used kernels are:

$$K_0(x) = U\left(x - \frac{1}{2}\right) U\left(\frac{1}{2} - x\right) \quad \text{(fundamental kernel)}$$

with U the step function; then derived kernels as

$$K_1 = K_0 * K_0,$$
$$K_2 = K_1 * K_0 = K_0 * K_0 * K_0, \text{ etc.} \quad \text{(derived kernels)}$$

where $K * \tilde{K}(x) = \int K(y)\tilde{K}(x-y)dy$.
The estimated electron density is obtained as (using ξ_α for particle positions)

$$\varrho_{est}(x) = \sum_{\alpha=1}^{N_p} q_\alpha \rho(x - \xi_\alpha).$$

(Note: $\rho(x)$ is denoted as $S(x)$ in traditional texts such as the book by Birdsall & Langdon.)

Statistical Analysis

Restricting x to grid values, x_i, we can estimate the density on the grid:

$$\varrho_{est}(x_i) = \sum_{\alpha=1}^{N_p} q_\alpha \rho(x_i - \xi_\alpha) \equiv \sum_{\alpha=1}^{N_p} q_\alpha \rho_i(\xi_\alpha)$$

For a periodic and charge neutral system, we also assume $\int \varrho(x)dx = 1$. Suppose the particles are distributed with a position distribution $f(\xi)$; then

$$\langle \varrho(x_i) \rangle = \sum_{\alpha=1}^{N_p} q_\alpha \langle \rho(x_i - \xi_\alpha) \rangle = \int d\xi \, \rho(x_i - \xi) f(\xi).$$

Assuming $\varrho(x) = \bar{\varrho}(x) + \tilde{\varrho}(x)$, where $\bar{\varrho}_i = \langle \varrho_i \rangle$ is average over the distribution of particles and $\tilde{\varrho}_i$ the fluctuating part due to the particle noise, we have

$$\varrho_i = \bar{\varrho}_i + \tilde{\varrho}_i \, .$$

Next, we write

$$\langle \varrho(x_i)\varrho(x_j) \rangle = \langle \bar{\varrho}(x_i) \rangle \langle \bar{\varrho}(x_j) \rangle + \langle \tilde{\varrho}(x_i)\tilde{\varrho}(x_j) \rangle$$

If we define the covariance matrix as $C_{ij} = \langle \tilde{\varrho}(x_i)\tilde{\varrho}(x_j) \rangle$, we see that

$$C_{ij} = \sum_{\alpha,\beta}^{N_p} q_\alpha q_\beta \langle \rho(x_i - \xi_\alpha)\rho(x_j - \xi_\beta) \rangle - \langle \bar{\varrho}(x_i) \rangle \langle \bar{\varrho}(x_j) \rangle \, .$$

Correlations in a Uniform Density Distribution

For uniform density we set $f(\xi) = 1$. First consider the kernel $K^{(0)}$ corresponding to *nearest grid point* (NGP) charge deposition, $\rho = \rho^{(0)}$. The particle width equals the grid spacing $h = \Delta = 1/N_g$. For $i = j$ we have

$$\begin{aligned}
\langle \varrho(x_i)\varrho(x_i)\rangle &= \sum_{\alpha=\beta} \left\langle \rho^{(0)}(x_i - \xi_\alpha)\right\rangle \left\langle \rho^{(0)}(x_i - \xi_\beta)\right\rangle q_\alpha q_\beta \\
&+ \sum_{\alpha\neq\beta} \left\langle \rho^{(0)}(x_i - \xi_\alpha)\right\rangle \left\langle \rho^{(0)}(x_i - \xi_\beta)\right\rangle q_\alpha q_\beta \\
&= \frac{1}{N_p} \int \left[\rho^{(0)}(x_i - \xi)\right]^2 d\xi \\
&+ \frac{N_p^2 - N_p}{N_p^2} \int \rho^{(0)}(x_i - \xi)\rho^{(0)}(x_i - \xi')\, d\xi\, d\xi'.
\end{aligned}$$

Using $\int \left[\rho^{(0)}(\xi)\right]^2 d\xi = (1/\Delta) \int K_0(\eta)^2\, d\eta = (1/\Delta)$ and $\int \rho^{(0)}(x_i - \xi)\rho^{(0)}(x_i - \xi')\, d\xi\, d\xi' = \int \rho^{(0)}(x_i - \xi)\, d\xi \int \rho^{(0)}(x_i - \xi')\, d\xi' = 1$,

$$\langle \varrho(x_i)\varrho(x_i)\rangle = \frac{1}{N_{ppc}} + 1 - \frac{1}{N_p},$$

where $N_{ppc} = \Delta\, N_p = N_p/N_g$, $\eta = (\xi - x)/h$, and

Correlations in a Uniform Density Distribution (cont'd)

We find for $i = j$

$$C_{ij} = \frac{1-\Delta}{N_{ppc}}.$$

For $j \neq j$ we have

$$\langle \varrho(x_i)\varrho(x_i)\rangle = \sum_{\alpha} \left\langle \rho^{(0)}(x_i - \xi_\alpha)\right\rangle \left\langle \rho^{(0)}(x_j - \xi_\beta)\right\rangle q_\alpha^2$$

$$+ \sum_{\alpha\neq\beta} \left\langle \rho^{(0)}(x_i - \xi_\alpha)\right\rangle \left\langle \rho^{(0)}(x_j - \xi_\beta)\right\rangle q_\alpha q_\beta .$$

The kernels $\rho^{(0)}(x_i - \xi_\alpha)$ and $\rho^{(0)}(x_j - \xi_\beta)$ do not overlap for $i \neq j$, so the first term is zero. The second term is

$$\frac{N_p^2 - N_p}{N_p^2} \int \rho^{(0)}(x_i - \xi)\, d\xi \int \rho^{(0)}(x_j - \xi')\, d\xi' = 1 - \frac{1}{N_p}$$

leading to

$$C_{ij} = -\frac{\Delta}{N_{ppc}}.$$

Combining we find

$$C_{ij} = \frac{1}{N_{ppc}}\delta_{ij} - \frac{\Delta}{N_{ppc}}$$

Note: the factor $-\Delta/N_{ppc}$ is small but should not be neglected because it is present in *all* terms of C_{ij} (see page 8 below).

Correlations with Higher Order Particle Shapes (Uniform Density)

Similar calculations give the following correlations (again, *uniform density* is assumed):

$$C_{ij}^{(0)} = \begin{cases} \frac{2}{3N_{ppc}} - \frac{\Delta}{N_{ppc}} & \text{for} \quad i = j \\ \frac{1}{6N_{ppc}} - \frac{\Delta}{N_{ppc}} & \text{for} \quad i = j \pm 1 \end{cases} \quad \text{(linear charge deposition)}$$

and

$$C_{ij}^{(0)} = \begin{cases} \frac{11}{20N_{ppc}} - \frac{\Delta}{N_{ppc}} & \text{for} \quad j = i \\ \frac{13}{60N_{ppc}} - \frac{\Delta}{N_{ppc}} & \text{for} \quad j = i \pm 1 \\ \frac{1}{120N_{ppc}} - \frac{\Delta}{N_{ppc}} & \text{for} \quad j = i \pm 2 \end{cases} \quad \text{(quadratic charge deposition)}$$

Negative Correlations

We notice that, in addition to the diagonal part of C_{ij} equal to $1/N_{ppc}$, there is a part of C_{ij} equal to $-\Delta/N_{ppc}$ for all i, j. This overall negative correlation is due to the fact that the total number of particles N_p is fixed. Specifically, for $\rho^{(0)}$ (NGP) we see that

$$\sum_i \varrho_{est}(x_i)\Delta = \frac{1}{N_p}\sum_{\alpha=1}^{N_p}\left(\sum_{i=1}^{N_g}\rho^{(0)}(x_i-\xi_\alpha)\Delta\right) = 1$$

because for fixed α the quantity $\rho^{(0)}(x_i - \xi_\alpha) = 1$ for the nearest x_i and 0 elsewhere. This means that

$$\sum_i \tilde{\varrho}(x_i) = 0$$

Therefore we conclude that $\left\langle \tilde{\varrho}(x_i)^2 \right\rangle + \sum_{i\neq j} \langle \tilde{\varrho}(x_i)\tilde{\varrho}(x_j)\rangle = 0$ for each i or

$$\sum_j C_{ij} = 0;$$

We can also directly verify that $\sum_j C_{ij} = 0$ for all particle shapes.

Numerical Monte Carlo Simulations of Correlations in Uniform Density Distribution

We use the normalized quantities for *linear charge deposition*:

$$\widetilde{C}_{ii} \equiv C_{ii} \times N_{ppc} = \frac{2}{3} - h = 0.666\ldots - h$$

$$\widetilde{C}_{i,i\pm1} \equiv C_{i,i\pm1} \times N_{ppc} = \frac{1}{6} - h = 0.166\ldots - h$$

N_p	M	$\widetilde{C}_{ii}$		$\widetilde{C}_{i,i\pm1}$	
		theoretical	numerical	theoretical	numerical
250	100,000	0.6266...	0.6269	0.1266...	0.1267
2500	10,000		0.6256		0.1251
25,000	1000		0.6208		0.1252
250,000	100		0.6673		0.1827

Table: Monte Carlo simulation results; M is the number of samples in the averages.

Numerical simulations have also confirmed the theoretical results for quadratic charge deposition (not shown).

Nonuniform Density Estimate: Bias

Consider now the more general case of $\varrho(x) \neq \text{const}$. For a particle shape given by a symmetric kernel $K(x)$ we find:

$$\langle \varrho_{est}(x) \rangle = \sum_{\alpha} q_\alpha \langle \rho(x - \xi_\alpha) \rangle$$

$$= \left(\sum_{\alpha} q_\alpha \right) \int d\xi \rho(x - \xi) \varrho(\xi) = \int d\xi \frac{1}{h} K\left(\frac{x - \xi}{h} \right) \varrho(\xi).$$

Since we assume $\sum q_\alpha = 1$, we ca rewrite

$$\langle \varrho_{est}(x) \rangle = \int d\eta K(\eta) \varrho(x + h\eta) \approx \varrho(x) + \frac{\varrho''(x) h^2}{2} \int d\eta K(\eta) \eta^2$$

by assuming the density varies over a length long compared to h and expanding in series. The term with $\varrho'(x)$ equals zero because $K(x)$ is assumed symmetric. The second term represents the bias:

$$\langle \varrho_{est}(x) \rangle = \varrho(x) + B$$

or

$$B = \frac{\varrho''(x) h^2}{2} \int d\eta K(\eta) \eta^2.$$

Non-uniform Density Estimate: Variance

Consider now the variance of the density estimate. We have

$$\left\langle \varrho_{est}(x)^2 \right\rangle = \sum_{\alpha=\beta} q_\alpha^2 \left\langle \rho(x-\xi_\alpha) \right\rangle + \sum_{\alpha\neq\beta} q_\alpha q_\beta \left\langle \rho_\alpha(x-\xi_\alpha)\rho(x-\xi_\beta) \right\rangle .$$

Again, assuming slow density variation and expanding, we find:

$$\left\langle \varrho_{est}(x)^2 \right\rangle \approx \frac{\varrho(x)}{N_p h} \int d\eta K(\eta)^2 + \left(1 - \frac{1}{N_p}\right) \left\langle \varrho_{est}(x) \right\rangle^2$$

The variance of the density estimate is $V = \left\langle \varrho_{est}(x)^2 \right\rangle - \left\langle \varrho_{est}(x) \right\rangle^2$, or

$$V \approx \frac{\varrho(x)}{N_p h} \int d\eta K(\eta)^2 - \frac{1}{N_p} \varrho(x)^2.$$

Finally, neglecting the second term (N_p is usually very large) we have for the variance:

$$V \approx \frac{\varrho(x)}{N_p h} \int d\eta K(\eta)^2.$$

Bias vs. Variance Optimization: Optimal Particle Width

The variance relative to the ***actual*** density is

$$Q = \left\langle \left(\varrho_{est}(x) - \varrho(x)\right)^2 \right\rangle = \left\langle \varrho_{est}(x)^2 \right\rangle - 2\varrho(x) \left\langle \varrho_{est}(x) \right\rangle + \varrho(x)^2 .$$

Using $\left\langle \varrho_{est}(x)^2 \right\rangle = V + \left\langle \varrho_{est}(x) \right\rangle^2$ and $\left\langle \varrho_{est}(x) \right\rangle = \varrho(x) + B$ we obtain

$$Q = V + B^2.$$

An approximate theoretical calculation of the optimal particle width can be done by averaging over the domain and defining $C_1 = \left(\int dx\, \varrho''(x)^2\right) \left[\int d\zeta\, K(\zeta)\zeta^2\right]^2 /4$ and $C_2 = \left(\int dx\, \varrho(x)\right) \int d\zeta\, K(\zeta)^2$; then

$$Q(h) \approx C_1 h^4 + \frac{C_2}{N_p h}.$$

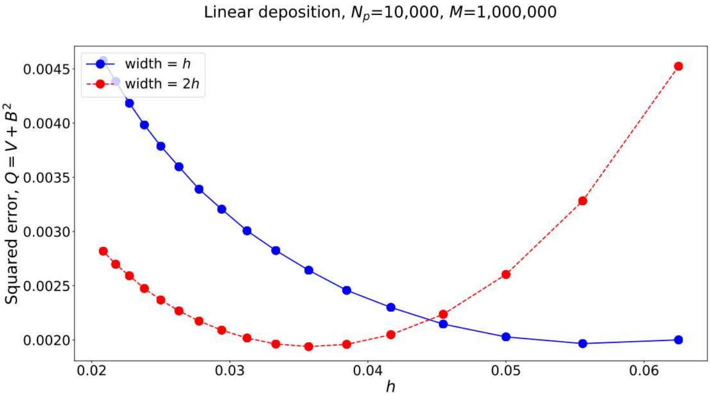
Optimizing with respect to h yields:

$$h_{\rm opt} = \left(\frac{C_2}{4 C_1 N_p}\right)^{1/5} \quad \text{and} \quad Q_{\rm min} = \frac{5 C_1^{1/5} C_2^{4/5}}{4^{4/5} N_p^{4/5}} \sim \frac{1}{N_p^{4/5}}.$$

Bias vs. Variance Optimization: Numerical Results

Theory predicts that optimal particle width results from a balance between two trends:

- *Wider* particle shape would *increase the bias* while *decreasing the variance.*
- *Narrower* particle shape would *increase the variance* while *decreasing the bias.*



Characterization of Noise in the Electric Field (Uniform Density)

The noise in the density is of importance because it affects the electric field, which in turn affects the particle orbits. For a periodic charge-neutral system we can calculate the electric field form the density as

$$\frac{dE(x)}{dx} = -\varrho(x) \quad \text{or} \quad E(x) = E(0) - \int_0^x dx' \, \varrho(x').$$

Using the *charge neutrality condition* $\int dx' \varrho(x') = 0$ and *zero applied potential*, $\int_0^1 dx \, E(x) = 0$, we obtain

$$E(0) = -\int_0^1 dx' \, x' \varrho(x')$$

and therefore

$$E(x) = -\int_0^1 dx' \, x' \varrho(x') - \int_0^x dx' \, \varrho(x') \, .$$

Characterization of Noise in the Electric Field (cont'd) (Uniform Density)

For the discrete form of the electric field we have (and staggered E_i and ϱ_i.)

$$E_i = E_0 - \Delta \sum_{j=0}^{i-1} \varrho_{j+1/2},$$

Using the discrete form of the charge neutrality $\Delta \sum_{i=0}^{N_g} E_i = 0$ we obtain

$$E_i = \Delta^2 \sum_{j=0}^{N_g-2} \varrho_{j+1/2}(N_g - 1 - j) - \Delta \sum_{j=0}^{i-1} \varrho_{j+1/2}.$$

The noise in $\varrho_{j_1/2}$ leads to noise in the electric field:

$$\widetilde{E}_i = \Delta^2 \sum_{j=0}^{N_g-2} \tilde{\varrho}_{j+1/2}(N_g - 1 - j) - \Delta \sum_{j=0}^{i-1} \tilde{\varrho}_{j+1/2} = \tilde{E}_i^{(1)} + \tilde{E}_i^{(2)}$$

and the charge neutrality condition gives

$$\sum_{j=0}^{N_g-1} \tilde{\varrho}_{j+1/2} = 0.$$

Correlations for the Electric Field (Uniform Density)

The simplest treatment is that for a the particle shape $\rho^{(0)}$ (NGP). We calculate

$$D_{ij}^{(1,1)} \equiv \left\langle \tilde{E}_i^{(1)} \tilde{E}_j^{(1)} \right\rangle = \Delta^4 \sum_{k=0}^{N_g-2} \sum_{l=0}^{N_g-2} (N_g - 1 - k)(N_g - 1 - l) \left\langle \tilde{\varrho}_{k+1/2} \tilde{\varrho}_{l+1/2} \right\rangle ,$$

$$\begin{aligned} D_{ij}^{(1,2)} &= \left\langle \tilde{E}_i^{(1)} \tilde{E}_j^{(2)} \right\rangle + \left\langle \tilde{E}_i^{(2)} \tilde{E}_j^{(1)} \right\rangle \\ &= -\Delta^3 \sum_{k=0}^{N_g-1} (N_g - 1 - k) \sum_{l=0}^{i-1} \left\langle \tilde{\varrho}_{k+1/2} \tilde{\varrho}_{l+1/2} \right\rangle \\ &\quad -\Delta^3 \sum_{l=0}^{N_g-1} (N_g - 1 - l) \sum_{l=0}^{j-1} \left\langle \tilde{\varrho}_{l+1/2} \tilde{\varrho}_{k+1/2} \right\rangle , \end{aligned}$$

$$D_{ij}^{(2,2)} = \left\langle \tilde{E}_i^{(2)} \tilde{E}_j^{(2)} \right\rangle = \Delta^2 \sum_{k=0}^{i-1} \sum_{l=0}^{i-1} \left\langle \tilde{\varrho}_{k+1/2} \tilde{\varrho}_{l+1/2} \right\rangle .$$

Random Walk vs. Brownian Bridge (Uniform Density)

A uniform random distribution is given is given by a Poisson density distribution with a parameter $\lambda = 1/N_{ppc}$. The correlation matrix in this case is $C_{ij} = \sigma^2 \delta_{ij}$ with $\sigma^2 = q/N_{ppc}$. Such distribution leads to correlations

$$\left\langle \tilde{E}_i^{(2)} \tilde{E}_j^{(2)} \right\rangle = \Delta^2 \sum_{k=0}^{i} \sum_{l=0}^{j} \left\langle \tilde{\varrho}_{k+1/2}^{P} \tilde{\varrho}_{l+1/2}^{P} \right\rangle = \Delta^2 \sigma^2 \sum_{k=0}^{i} \sum_{l=0}^{j} \delta_{kl} = \Delta^2 \sigma_2 \mathrm{Min}(i,j)$$

or

$$D_{ij} = D_{ij}^{(2,2)} = \Delta \sigma^2 \mathrm{Min}(x_i, x_j), \qquad \text{(random walk)}$$

Which is the covariance matrix for a random walk. Now we use the *modified Poisson density*, for which we have derived $C_{ij} = \sigma^2(\delta_{ij} - \Delta)$. We find

$$D_{ij} = D_{ij}^{(2,2)} = \Delta^2 \sigma^2 \mathrm{Min}(i,j) - \Delta^3 \sigma^2 ij$$

or

$$D_{ij} = D_{ij}^{(2,2)} = \Delta \sigma^2 \mathrm{Min}(x_i, x_j)\,(1 - \mathrm{Max}(x_i, x_j)) \quad \text{(Brownian Bridge).}$$

This modification to the random walk is called Brownian Bridge and results because N_p=const (so is N_{ppc}=const) is a fixed rather than expected number (as is for Poisson distribution).

Random Walk vs. Brownian Bridge (Uniform Density)

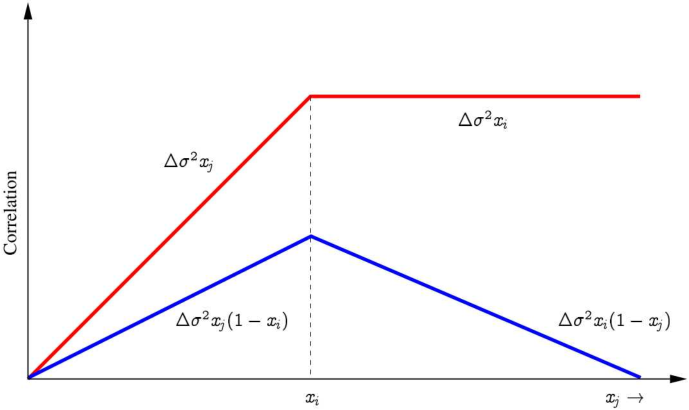


Figure: Illustration of random walk (red) vs. Brownian Bridge (blue).

Conclusions

- With a fixed number of particles, a non-Poisson distribution is appropriate in describing the noise (error) in particle simulations.
- Fixed number of particles leads to negative correlations in the covariance matrix.
- Optimization of bias-variance leads to minimizing noise in density estimations via an optimal particle width.
- Particle width — but not smoothness — important for density estimations.
- A non-Poisson distribution leads to a modification — Brownian bridge for the electric field versus random walk for the Poisson distribution — because the total number of particles is fixed.