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Meshfree particle model for kinetic plasma simulations

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Abstract

We revisit a meshfree particle model for kinetics of a 1D electrostatic plasma, using kernel density estimation and a similar method for the electric field E. The translationally invariant kernel $K(x-y)$ represents the macroparticle charge distribution. Two length scales enter, the width w of K and the interparticle spacing l. This model conserves momentum and energy. Similarly, continuity is satisfied exactly, and the Gauss's law and Ampere's law formulations are exactly equivalent. A unified analysis is used for numerical stability and noise properties. The force can be computed directly using the convolution $K_2 = K * K$, and K_2 is positive definite. We discuss the analogy in the presence of a grid. We can specify a single kernel K_2 , related to the 'kernel trick' of machine learning. Numerical instability can occur unless K_2 is positive definite, related to a breakdown in energy conservation. For the noise analysis, the covariance matrix for the electric field shows a plasma dispersion function modified by w and l. The number of particles per cell does not enter, and the noise is characterized by the number of particles per kernel width, i.e. w/l. We present the bias-variance optimization (BVO) for the electric field, and compare it to the density BVO.

Outline

– Meshfree Vlasov-Gauss and Vlasov-Ampère formulations

– Moment equations; conservation properties

– 'Kernel trick' – preventing instabilities and ensuring energy conservation

– Linearized equations for numerical stability and noise response for a cold plasma

– Linearized equations for numerical stability and noise response for a warm plasma

– Bias-variance optimization for the electric field

The model

One-dimensional electrostatic particle method, immobile ions.
Periodic boundary conditions $0 \leq x \leq 1$
Kernel density estimation to obtain the electron density
The kernel (particle shape) $K(x-y)$ is the local charge density within the macroparticle

As in E. G. Evstatiev, J. M. Finn, B. A. Shadwick, N. Hengartner, "Noise and error analysis and optimization in particle-based kinetic plasma simulations", JCP 440, 110394 (2021).

Related kernel-like method to obtain the estimated electric field $E(x)$ and the electrostatic potential $\phi(x)$
The force on a macroparticle: integrate $F(x) = \int E(y)K(y-x)dy$
Same kernel for particle positions $\rightarrow E(x)$ and for $E(x) \rightarrow F(x)$.
Source and target – charge distribution same. Leads to $K * K$ and a positive definite kernel

The model

$$f(x, v, t) = \sum_{\alpha=1}^{N} q_\alpha K(x - \xi_\alpha(t))\delta(v - v_\alpha(t))$$

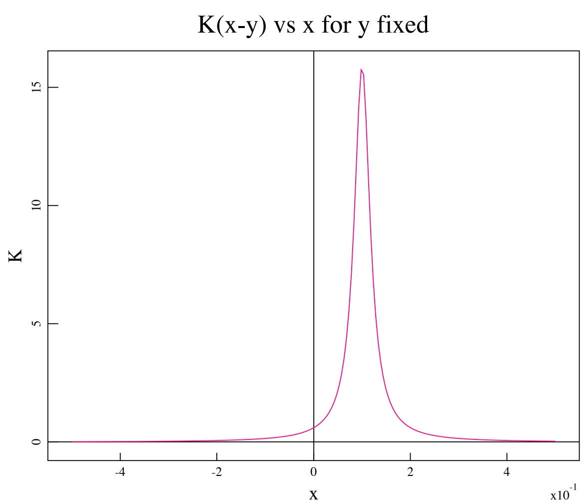
$$K(x) = \frac{1}{w} K_f\left(\frac{x}{w}\right) \qquad K_{per}(x) = \sum_{n=-\infty}^{\infty} K(x - n)$$

$$\rho(x, t) = \sum_\alpha q_\alpha K(x - \xi_\alpha(t))$$

$$E(x, t) = \sum_\alpha q_\alpha G(x - \xi_\alpha(t)); \;\; G'(x) = 1 - K(x)$$

$$\phi(x, t) = \sum_\alpha q_\alpha \Phi(x - \xi_\alpha(t)); \;\; \Phi'(x) = -G(x)$$

The kernel $K(x-y)$ and $G(x-y)$



The model

$G'(x) = 1 - K(x)$ (Gauss); $\int_0^1 G(x)dx = 0$. (zero potential difference.)
$q_\alpha G(x - \xi_\alpha)$...electric field due to single (macro)particle at ξ_α.
Length scales: w, $\lambda = 1/N$. Ratio $w/\lambda = Nw$ – particles per kernel width.

$$\frac{d\xi_\alpha}{dt} = v_\alpha$$

$$\frac{dv_\alpha}{dt} = -F(\xi_\alpha, t), \quad F(x,t) = \int E(y)K(y-x)dy$$

Same kernel K.

Note

It is possible to calculate the force directly by

$$F(x,t) = E(x,t) = \sum_{\alpha} q_\alpha G_2(x - \xi_\alpha(t))$$

$G_2' = 1 - K_2'$ and $K_2(x) = \int K(y)K(x-y)dy$.

This is a *positive definite kernel*! More later.

***The kernel trick*: just choose a positive definite kernel for K_2**
(Then $K = \sqrt{K_2}$, but you do not need K.)

Meshfree Vlasov-Gauss/Vlasov-Poisson and Vlasov-Ampere

$$\rho(x,t)u(x,t) = \sum_\alpha q_\alpha K(x-\xi_\alpha(t))v_\alpha(t) \quad f(v|x,t) = f(x,v,t)/\rho(x,t)$$

and (conditional expectation) $u(x,t) = \int f(v|x,t)vdv$.
$\partial_t \rho(x,t) + \partial_x(\rho(x,t)u)$

$$= -\sum_\alpha q_\alpha K'(x-\xi_\alpha(t))\dot{\xi}_\alpha(t) + \sum_\alpha q_\alpha K'(x-\xi_\alpha(t))v_\alpha(t) = 0$$

The continuity equation is satisfied exactly

$$u(x,t) = \frac{1}{\rho}\sum_\alpha q_\alpha K(x-\xi_\alpha(t))v_\alpha(t) = \sum_\alpha q_\alpha W(x,t)v_\alpha(t)$$

Nadayara-Watson non-parametric regression

$$W(x,\xi_\alpha(t),t) = \frac{K(x-\xi_\alpha(t))}{\rho(x,t)} = \frac{K(x-\xi_\alpha(t))}{\sum_\beta q_\beta K(x-\xi_\beta(t))}$$ Partition of unity

Conservation properties

- Momentum is conserved exactly because, with no mesh, translational invariance is exact
- Energy is conserved exactly – related to the $K_2 = K * K$ issue above. (Time step $h \to 0$)
- Vlasov-Ampère $\partial_t E = -j = \rho u$. V-A and V-G (V-P) are equivalent because the continuity equation holds exactly
- The model consists of N macroparticles with charge distributed according to K, with the force computed from K_2

Linearized equations, cold plasma – numerical stability

Introduce a lattice *just for the linearized calculations*
$x_\alpha = (\alpha - 1)\Delta$, $\xi_\alpha = x_\alpha + \delta\xi_\alpha$

$$\tilde{E}(x,t) = -\Delta \sum_\alpha G'(x - x_\alpha)\delta\xi_\alpha(t) = \Delta \sum_\beta \left(K(x - x_\beta) - 1\right)\delta\xi_\beta(t)$$

$$\delta\ddot{\xi}_\alpha = -\omega^2\delta\xi_\alpha = \tilde{F}(\xi_\alpha(t), t) = -\Delta \sum_\beta \left(K_2(x_\alpha - x_\beta)\cancel{-1}\right)\delta\xi_\beta(t)$$

$$\omega_k^2 = \hat{K}_f(kw), \quad \omega_k^2 \rightarrow_{w \rightarrow 0} \hat{K}_f(0) = 1\,(= \omega_{pe}^2)$$

$\omega_k^2 > 0$ if $K(x - y)$ is positive definite. If using the kernel trick (choosing K_2), **be sure that K_2 is positive definite.**

Positive definite kernels

Energy conservation also requires K_2 to be positive definite.

If $B(x)$ is the boxcar kernel, $B * B$=tent or linear is pos def. $B * B * B$= quadratic spline is *not*.

This numerical instability seems to be the first connection between kernels for density estimation and positive definite (reproducing) kernels.

Linearized equations, cold plasma – noise

$$\langle \hat{E}(k_1,\omega_1)^* \hat{E}(k_2,\omega_2)\rangle =$$

$$\frac{\sigma^2 l_c}{2\pi} \frac{\hat{K}(k_1)}{\hat{K}_2(k_1)-\omega_1^2} \frac{\hat{K}(k_1)}{\hat{K}_2(k_1)-\omega_2^2} (1+\omega_1\omega_2)\,\delta(k_1-k_2)$$

$1/\left(\hat{K}_2(k_1)-\omega_1^2\right)$ propagator for plasma oscillation

- Includes decay of initial conditions (ballistic term) – terms off $D(k,\omega)=0$
- Shows that a plasma oscillation ($D(k,\omega)\approx 0$) persists after the ballistic term decays

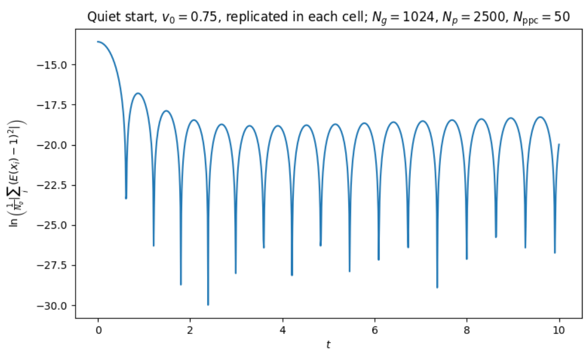
Warm plasma

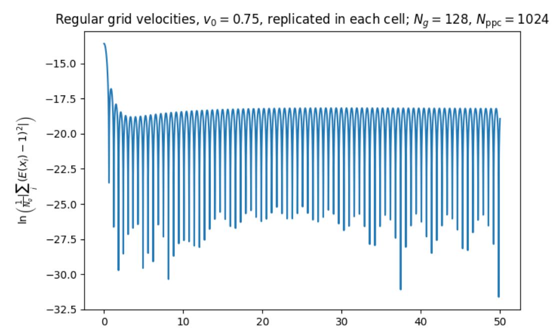
Linear stability for $f_0(v) = \Theta(v_0^2 - v^2)/2v_0$: Langmuir wave (without Landau damping) has

$$\omega^2 = \hat{K}_2(k) + k^2 v_0^2$$

Thermal term ameliorates the instability if the kernel trick is used and K_2 is not positive definite

In $\langle \hat{E}(k_1, \omega_1)^* \hat{E}(k_2, \omega_2) \rangle$: propagator for the Langmuir wave $1/\left(\hat{K}_2(k_1) - \omega_1^2 - k^2 v_0^2\right)$ w/o Landau damping. Ballistic term damps, leaving (non-Landau damped) Langmuir waves.





Bias-variance optimization for $E(x,t)$ and $F(x,t)$

$\partial_x E = 1 - \rho$, so $E(x)$ is smoother – variance should be lower.

BVO for the density was computed in E. G. Evstatiev, J. M. Finn, B. A. Shadwick, N. Hengartner, "Noise and error analysis and optimization in particle-based kinetic plasma simulations", JCP 440, 110394 (2021). Density: diagnostic. $F_e(x) = \sum_\alpha q_\alpha G_2(x - \xi_\alpha)$ enters

$$\text{Bias: } \langle F_e(x) \rangle = F(x) + B(x) + O(w^4),$$

$$B(x) = \frac{C_2 w^2}{2} F''(x), \;\; C_2 = \int \zeta^2 K_f(\zeta) d\zeta$$

Error is $Q = B^2 + V$

$$Q(w) \approx \frac{\rho(x)}{12 N_p} - \frac{2w\rho(x)C_3}{N_p} + \frac{C_2^2 w^4}{4} E''(x)^2$$

Bias-variance optimization

(MISE)

$$Q_2(w) = \frac{1}{12N_p} - \frac{2wC_3}{N_p} + \frac{C_2^2 w^4}{4} R$$

Minimize:

$$w = \left(\frac{2C_3}{C_2^2 R N_p} \right)^{1/3}, \quad Q_{2,min} = \frac{1}{12N_p} - \frac{3}{4(C_2^2 R)^{1/3}} \left(\frac{2C_3}{N_p} \right)^{4/3}.$$

$$w_{min} \sim N_p^{-1/5}(\text{density}); \quad w_{min} \sim N_p^{-1/3}(\text{force})$$

For non-compact support kernels (e.g. Gaussian), computation time scales as N^2. With compact support, like $N(Nw_{min}) \sim N^{5/3}$ (density: $\sim N^{9/5}$ – worse)

Conclusions

- Particles per cell does not enter (meshfree.) *Particles per kernel width* replaces it. Comparison with a PIC code with $\Delta \to 0$ gives agreement.
- Exact energy conservation occurs for $h \to 0$: for finite h, use a symplectic integrator like leapfrog (symplectic Euler) – good energy conservation properties.
- With K in source of $E(x)$ and in integrating $E(x)$ over target particle, the same K should be used and $K_2 = K * K$ can be used to compute $F(x, t)$ directly, without computing $E(x)$. The *kernel trick* means that a positive definite kernel can be used in place of K_2.
- If a non-positive definite kernel is used in the kernel trick, it can give numerical stability as well as lack of energy conservation.
- BVO: If the optimal w_{min} is chosen, the computation time scales as $N^{5/3}$ – better than N^2 but not $N \log N$.