On a Closure for Hamiltonian Particle Mesh Methods —Vlasov-Poisson Dynamics

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1. Introduction

1D Vlasov-Poisson equations:

- *Time evolution of PDF* under electric/gravitational field in space-velocity phase space
- *Collisionless Boltzmann-Poisson*: self-gravitating stellar system; evolution pdf of star density in phase space
- *Kinetic plasmas*: numerical solution plays role in nonlinear behavior of plasmas; control of fusion dynamics

Numerical methods:

- *Grid based*: problematic extension to 3D yielding 6D case
- *Particle based*: problem is **numerical noise**
- *Particle-mesh*: particle in cell, density on grid
- *Hamiltonian particle mesh method*: current topic

Why Hamiltonian?

Hamiltonian particle mesh method (HMM):

- *Compatible scheme*: adhering to Hamiltonian structure of Vlasov-Poisson equations
- *E.g. in fluids*: compressible Euler, incompressible 2D streamfunction-vorticity, shallow water equations, hydrostatic equations (e.g. Frank et al. 2002, . . .)
- *Consistent long-time statistics of HMM*: due to preservation (integral) conservation laws (Dubinkina and Frank 2010)
- *Goal*: design and test a closure for Hamiltonian finite element method for Vlasov-Poisson (& fluid) systems to overcome numerical noise.

2. Hamiltonian Parcel Vlasov-Poisson Dynamics

Equations of motion, dimensionless:

$$\partial_t \mathcal{D} + \zeta \partial_x \mathcal{D} - (\partial_x \phi)\partial_\zeta \mathcal{D} = 0 \qquad (1)$$

$$\partial_{xx}\phi = 1 - \int_{-\infty}^{\infty} \mathcal{D}(x,\zeta,t)\mathrm{d}\zeta \equiv 1 - \rho \qquad (2)$$

- PDF $\mathcal{D}(x,\zeta,t)$, potential $\phi(x,t)$ & density $\rho(x,t)$
- space-velocity dimensions (x,ζ) and time t
- partial derivatives $\partial_x = \partial/\partial x$ and $\partial_\zeta = \partial/\partial\zeta$
- second order derivative $\partial^2\phi/\partial x^2 = \partial_{xx}\phi = \phi_{xx}$
- Characteristics: on

$$\mathrm{d}x/\mathrm{d}t = \zeta, \quad \mathrm{d}\zeta/\mathrm{d}t = -\partial_x\phi \quad \text{we find} \quad \mathrm{d}\mathcal{D}/\mathrm{d}t = 0$$

Coupled Hyperbolic-Elliptic System

- The hyperbolic part can be solved on the characteristics

$$\mathrm{d}x/\mathrm{d}t = \zeta, \quad \mathrm{d}\zeta/\mathrm{d}t = -\partial_x \phi \tag{3}$$

- such that the PDF satisfies:

$$\begin{aligned} \mathrm{d}\mathcal{D}/\mathrm{d}t =& \partial_t \mathcal{D} + \frac{\mathrm{d}x}{\mathrm{d}t}\partial_x \mathcal{D} + \frac{\mathrm{d}\zeta}{\mathrm{d}t}\partial_\zeta \mathcal{D} \\ =& \partial_t \mathcal{D} + \zeta \partial_x \mathcal{D} - \partial_x \phi \partial_\zeta \mathcal{D} = 0 \end{aligned} \tag{4}$$

- Hence, it is frozen along characteristics:

$$\mathcal{D}(x, \zeta, 0) = \mathcal{D}_0(x_0, \zeta_0) \tag{5}$$

- The potential ϕ follows from the elliptic equation:

$$\begin{aligned} \partial_{xx}\phi =& 1 - \int_{-\infty}^{\infty} \mathcal{D}(x, \zeta, t)\mathrm{d}\zeta \\ =& 1 - \int_{-\infty}^{\infty}\int_0^L \mathcal{D}_0(x_0, \zeta_0)\, \delta\big(x - X(x_0, \zeta_0, t)\big)\, \mathrm{d}x_0 \mathrm{d}\zeta_0. \end{aligned} \tag{6}$$

Hamiltonian Formulation

Hamiltonian parcel formulation

$$\frac{\mathrm{d}X}{\mathrm{d}t} = \frac{\partial H}{\partial V} = V \quad \& \quad \frac{\mathrm{d}V}{\mathrm{d}t} = -\frac{\partial H}{\partial X} = -(\partial_x \phi)_{x=X} \tag{7a}$$

$$\partial_{xx}\phi = 1 - \rho \tag{7b}$$

$$\rho(x,t) = \int_{-\infty}^{\infty} \mathcal{D}(x,\zeta,t)\mathrm{d}\zeta = \int_{-\infty}^{\infty}\int_0^L \mathcal{D}_0(x_0,\zeta_0)\,\delta\big(x - X(x_0,\zeta_0,t)\big)\,\mathrm{d}x_0\mathrm{d}\zeta_0 \tag{7c}$$

- initial conditions $X(x_0,\zeta_0,0) = x$ & $V(x_0,\zeta_0,0) = \zeta$
- parcel PDF $\mathcal{D}(x,\zeta,0) = \mathcal{D}_0(x_0,\zeta_0)$ on labels (x_0,ζ_0)
- non-autonomous 1-parcel system (7) with Hamiltonian

$$H = H(X,V,t) = \frac{1}{2}V^2 + \phi(X,t) \tag{8}$$

Constrained Variational Principle

Variational principle (VP):

$$
\begin{aligned}
0 =& \int_0^T \mathcal{L}[X, V, \phi]\mathrm{d}t \\
=& \delta \int_0^T \int_{-\infty}^{\infty} \int_0^L \mathcal{D}_0 V \frac{\mathrm{d}X}{\mathrm{d}t} - \frac{1}{2}\mathcal{D}_0 V^2 \mathrm{d}x_0 \mathrm{d}\zeta_0 + \int_0^L \frac{1}{2}(\partial_x \phi)^2 \mathrm{d}x + \\
& \int_0^L \phi \left(1 - \int_0^L \int_{-\infty}^{\infty} \mathcal{D}_0 \delta(x - X(x_0, \zeta_0, t)) \mathrm{d}x_0 \mathrm{d}\zeta_0 \right) \mathrm{d}x \mathrm{d}t
\end{aligned}
$$

- Thanks to Mark Peletier who removed the Lagrange multiplier in an earlier approach.
- *Discretize VP* consistently, to obtain compatible scheme.

3. Hamiltonian Particle FEM

Discrete approximations ϕ_h, ρ_h and test function φ_h:

$$\frac{\mathrm{d}X_k}{\mathrm{d}t} = \frac{\partial H_k}{\partial V_k} = V_k \tag{9a}$$

$$\frac{\mathrm{d}V_k}{\mathrm{d}t} = -\frac{\partial H_k}{\partial X_k} = -\partial_x \phi_h(x,t)\big|_{x=X_k}$$

$$X_k(0) = x_k \quad \text{and} \quad V_k(0) = \zeta_k \tag{9b}$$

$$-\int \partial_x \varphi_h(x) \partial_x \phi_h(x,t)\mathrm{d}x = \int \varphi_h(x)\mathrm{d}x - \int \varphi_h(x)\rho_h(x,t)\mathrm{d}x$$

$$\int \varphi_h(x)\rho_h(x,t)\mathrm{d}x = \sum_k \varphi_h(X_k)\mathcal{D}_{0k} w_{0k} \Delta_k \tag{9c}$$

- for $k = 1, \dots, N_k$; x_k, ζ_k quadrature points with
- weights w_{0k} and 2D finite element area Δ_k

...FEM

Global energy H is conserved.

- Multiplication, differentiation & substitution of basis functions $\phi_h = \phi_j \varphi_j$ and test function $\varphi_h = \phi_h$ ...yields:

$$
\begin{aligned}
0 =& \frac{\mathrm{d}}{\mathrm{d}t} \sum_k \frac{1}{2} \mathcal{D}_{0k} w_{0k} \Delta_k V^2 + \sum_k \mathcal{D}_{0k} w_{0k} \Delta_k (\partial_x \phi_h)_{x=X_k} \frac{\mathrm{d}X_k}{\mathrm{d}t} \\
=& \frac{\mathrm{d}}{\mathrm{d}t} \left\{ \sum_k \frac{1}{2} \mathcal{D}_{0k} w_{0k} \Delta_k V^2 + \int_0^L \frac{1}{2} (\partial_x \phi_h)^2 \mathrm{d}x \right\} \\
=& \frac{\mathrm{d}H}{\mathrm{d}t}
\end{aligned}
$$

...FEM

Take $\varphi_h(x,t) = \varphi_i(x)$ and $\phi_h(x,t) = \phi_j(t)\varphi_j(x)$, and obtain differential-algebraic system:

$$\frac{\mathrm{d}X_k}{\mathrm{d}t} = V_k \quad \& \quad \frac{\mathrm{d}V_k}{\mathrm{d}t} = -\,\phi_j(\partial_x\varphi_j)|_{x=X_k} \tag{10a}$$

$$-S_{ij}\phi_j = R_i - M_{ij}\rho_j \tag{10b}$$

$$M_{ij}\rho_j = \sum_k \varphi_i(X_k)\mathcal{D}_{0k}w_{0k}\Delta_k \tag{10c}$$

- vector $R_i = \int \varphi_i \mathrm{d}x$
- mass matrix $M_{ij} = \int \varphi_i\varphi_j \mathrm{d}x$
- "Laplace" matrix $S_{ij} = \int \partial_x\varphi_i\partial_x\varphi_j \mathrm{d}x$ ...also for splines!

Eulerian FEM & Lagrangian Particles

- HPM consists of a Lagrangian part:

$$\frac{\mathrm{d}X_k}{\mathrm{d}t} = V_k \quad \& \quad \frac{\mathrm{d}V_k}{\mathrm{d}t} = -\,\phi_j(\partial_x\varphi_j)|_{x=X_k} \tag{11a}$$

- and Eulerian part:

$$-S_{ij}\phi_j = R_i - M_{ij}\rho_j, \tag{11b}$$

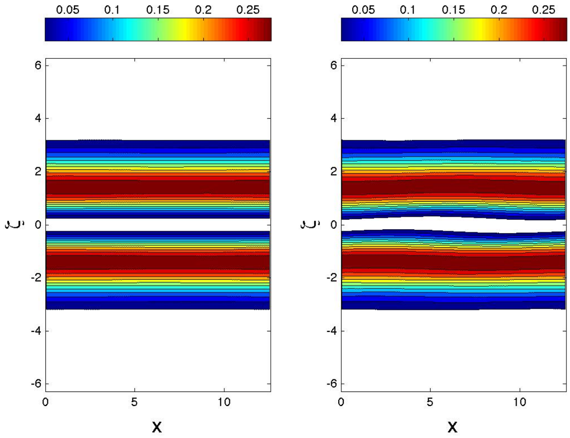
- joined together with a hybrid part:

$$M_{ij}\rho_j = \sum_k \varphi_i(X_k)\mathcal{D}_{0k}w_{0k}\Delta_k \tag{11c}$$

- with Eulerian vector R_i, mass M_{ij} & "Laplace" S_{ij} matrices.

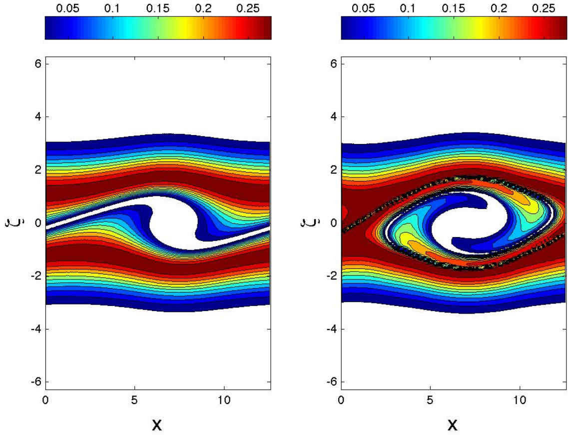
4. Numerical Results

Test $\mathcal{D} = \zeta^2 e^{-\zeta^2/(2\pi)}(1 + \alpha\cos(kx))/(2\pi)$; unstable for $k < 1$:



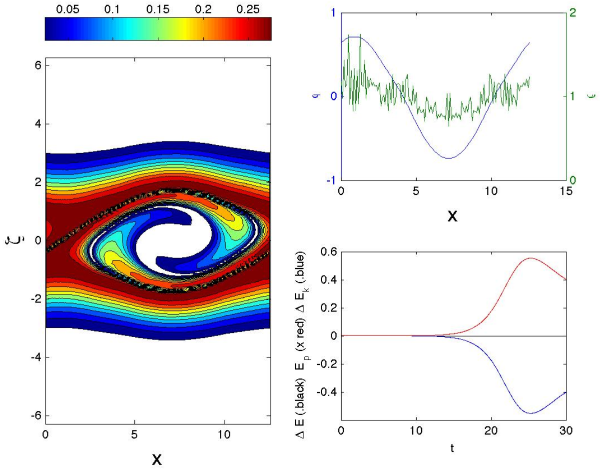
. . . Results

$t = 0, 10 \ldots t = 20, 30 \ldots$ in agreement . . . :



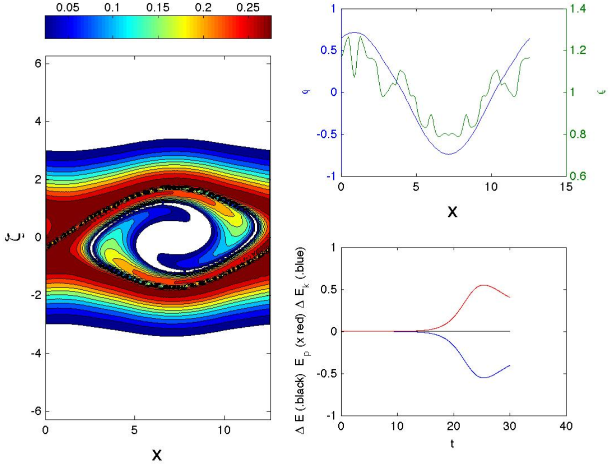
Numerical Results

$t = 30$:



Numerical Results

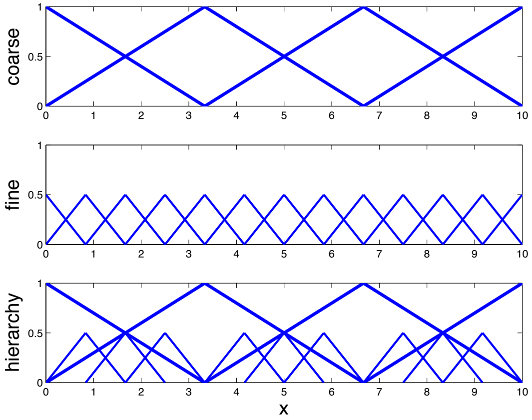
Hamiltonian smoothing, cf. "remeshing" $t = 30$:



5. Eulerian Closure: Hierarchical Basis Functions

Divide fine expansion $\phi_h = \phi_{j'}\varphi_{j'}$ into coarse- and fine-scale basis functions $\phi_h = \phi_I\varphi_I + \phi_\alpha\tilde{\varphi}_\alpha$:

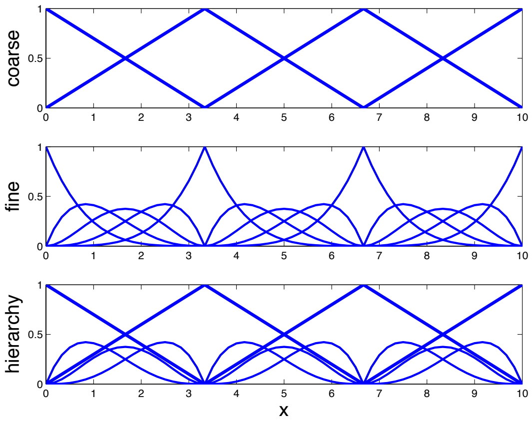
- e.g., top-hat spline/FE basis function:



Hierarchical Basis Functions

Divide fine expansion $\phi_h = \phi_{j'}\varphi_{j'}$ into coarse- and fine-scale basis functions $\phi_h = \phi_l\varphi_l + \phi_\alpha\tilde{\varphi}_\alpha$:

- e.g., Bernstein polynomials:



Hierarchical Orthonormal Basis Functions

Cubic spline fine & coarse expansion
$\phi_h = \phi_{j'}\varphi_{j'} = \phi_I\varphi_I + \phi_\alpha\tilde{\varphi}_\alpha$:

- Refine by steps of two, with projection matrices Q $(N_s \times N_f)$ and W $((N_f - N_s) \times N_f)$, such that:

$$\varphi_I = Q_{Ij'}\varphi_{j'} \quad \text{and} \quad \tilde{\varphi}_\alpha = W_{\alpha j'}\varphi_{j'} \qquad (12)$$

- Define the fine spline projection matrix A on the grid: $A = diag(1/6, 2/3, 1/6)$ (a $N_f \times N_f$ matrix).
- Using A, find complementary matrix WA as follows:

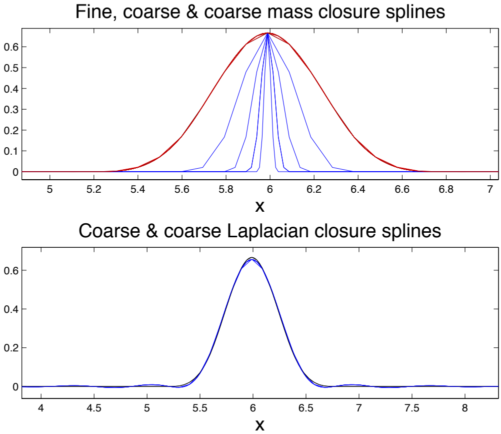
$$P(QA)^T = (QA)^T \quad \Longrightarrow P = (QA)^T(QA(QA)^T)^{-1}(QA)$$
$$P = Id + \tilde{P} \quad \text{with} \quad \tilde{P}(QA)^T = 0 \qquad (13)$$

- Then

$$WA = null(P) = null(\tilde{P}) \quad \text{and} \quad W = (WA)A^{-1}. \qquad (14)$$

Hierarchical Orthonormal Basis Functions

- Refined $(2\times, 4\times, 8\times, 16\times)$, fixed coarse, and closed mass $\tilde{\rho}_l$ and Laplace spline Φ_l basis functions:



Reformulation: Recall

Take $\varphi_h(x,t)=\varphi_{i'}(x)$ and $\phi_h(x,t)=\phi_{j'}(t)\varphi_{j'}(x)$, and obtain differential-algebraic system:

$$\frac{\mathrm{d}X_k}{\mathrm{d}t}=V_k \quad \& \quad \frac{\mathrm{d}V_k}{\mathrm{d}t}=-\,\phi_{j'}(\partial_x\varphi_{j'})|_{x=X_k} \tag{15a}$$

$$-S_{i'j'}\phi_{j'}=R_{i'}-M_{i'j'}\rho_{j'} \tag{15b}$$

$$M_{i'j'}\rho_{j'}=\sum_k \varphi_{i'}(X_k)\mathcal{D}_{0k}w_{0k}\Delta_k \tag{15c}$$

- vector $R_{i'}=\int\varphi_{i'}\mathrm{d}x$
- mass matrix $M_{i'j'}=\int\varphi_{i'}\varphi_{j'}\mathrm{d}x$
- "Laplace" matrix $S_{i'j'}=\int\partial_x\varphi_{i'}\partial_x\varphi_{j'}\mathrm{d}x$ ... also for splines!

Reformulation

Reformulated full HpFEM-system (drop primes)
$\phi_h = \phi_{i'}\varphi_{i'} = \phi_l\varphi_l + \phi_\alpha\tilde{\varphi}_\alpha$ (and likewise for ρ_h):

$$\frac{\mathrm{d}X_k}{\mathrm{d}t} = V_k \quad (16a)$$

$$\frac{\mathrm{d}V_k}{\mathrm{d}t} = -\phi_l(\partial_x\varphi_l)|_{x=X_k} - \phi_\alpha(\partial_x\tilde{\varphi}_\alpha)|_{x=X_k} \quad (16b)$$

$$-S_{lm}\phi_m - S_{l\beta}\phi_\beta = R_l - M_{lm}\rho_j - M_{l\beta}\rho_\beta \quad (16c)$$

$$-S_{\alpha m}\phi_m - S_{\alpha\beta}\phi_\beta = R_\alpha - M_{\alpha m}\rho_m - M_{\alpha\beta}\rho_\beta \quad (16d)$$

$$M_{lm}\rho_m + M_{l\beta}\rho_\beta = \sum_k \varphi_l(X_k)\mathcal{D}_{0k}w_{0k}\Delta_k \quad (16e)$$

$$M_{\alpha m}\rho_m + M_{\alpha\beta}\rho_\beta = \sum_k \tilde{\varphi}_\alpha(X_k)\mathcal{D}_{0k}w_{0k}\Delta_k \quad (16f)$$

Strategy

Exact, reformulated "coarse-scale" HpFEM-system:

$$\frac{\mathrm{d}X_k}{\mathrm{d}t} = V_k \tag{17a}$$

$$\begin{aligned}\frac{\mathrm{d}V_k}{\mathrm{d}t} &= -\phi_l \partial_x(\varphi_l - S^{-1}_{\alpha\gamma} S_{\gamma l} \tilde{\varphi}_\alpha)|_{x=X_k} \\ &\quad - \sum_{k'} S^{-1}_{\alpha\gamma} \tilde{\varphi}_\gamma(X_{k'}) D_{0k'} w_{0k'} \Delta_{k'} \partial_x \tilde{\varphi}_\alpha|_{X_k} + S^{-1}_{\alpha\gamma} R_\gamma \partial_x \tilde{\varphi}_\alpha|_{X_k}\end{aligned}$$

$$\begin{aligned}-\underline{(S_{lm} - S_{l\beta} S^{-1}_{\beta\alpha} S_{\alpha m})}\phi_m &= R_l - S_{l\beta} S^{-1}_{\beta\alpha} R_\alpha \\ &\quad - \sum_k (\varphi_l - S_{l\beta} S^{-1}_{\beta\alpha} \tilde{\varphi}_\alpha)(X_k) D_{0k} w_{0k} \Delta_k\end{aligned}$$

$$\underline{(M_{lm} - M_{l\beta} M^{-1}_{\beta\alpha} M_{\alpha m})}\rho_m = \sum_k (\varphi_l - M_{l\beta} M^{-1}_{\beta\alpha} \tilde{\varphi}_\alpha)(X_k) \mathcal{D}_{0k} w_{0k} \Delta_k$$

New Multi-Scale Basis Functions

- Multi-scale, new basis functions for ϕ and ρ

$$\Phi_l = (\varphi_l - S_{l\beta} S^{-1}_{\beta\alpha} \tilde{\varphi}_\alpha) \quad \text{and} \quad \tilde{\rho}_l = (\varphi_l - M_{l\beta} M^{-1}_{\beta\alpha} \tilde{\varphi}_\alpha) \tag{18}$$

but with additional terms in the momentum equation

- We define Schur complements:

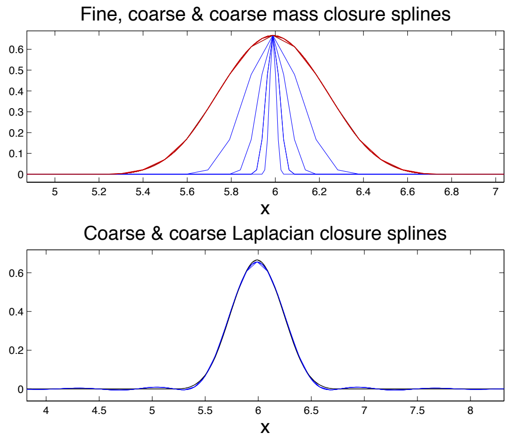
$$\tilde{S}_{lm} = \underline{S_{lm} - S_{l\beta} S^{-1}_{\beta\alpha} S_{\alpha m}} \tag{19}$$

$$\tilde{M}_{lm} = \underline{M_{lm} - M_{l\beta} M^{-1}_{\beta\alpha} M_{\alpha m}} \tag{20}$$

- Cf., variational multi-scale methods (Hughes 1995, E 2011).

Hierarchical Orthonormal Basis Functions

- Refined $(2\times, 4\times, 8\times, 16\times)$, fixed coarse, and closed mass and Laplace spline basis functions:



Exact coarse system

Exact "coarse-scale" HpFEM-system plus averaged terms:

$$\frac{\mathrm{d}X_k}{\mathrm{d}t} = V_k \tag{21}$$

$$\frac{\mathrm{d}V_k}{\mathrm{d}t} = -\phi_l \partial_x \Phi_l|_{x=X_k}$$

$$\underline{- \sum_{k'} S^{-1}_{\alpha\gamma} \tilde{\varphi}_\gamma(X_{k'}) D_{0k'} w_{0k'} \Delta_{k'} \partial_x \tilde{\varphi}_\alpha|_{X_k} + S^{-1}_{\alpha\gamma} R_\gamma \partial_x \tilde{\varphi}_\alpha|_{X_k}}$$

$$-\tilde{S}_{lm}\phi_m = \tilde{R}_l - \sum_k \Phi_l(X_k) D_{0k} w_{0k} \Delta_k$$

$$\tilde{M}_{lm}\rho_m = \sum_k \tilde{\rho}_l(X_k) \mathcal{D}_{0k} w_{0k} \Delta_k \tag{22}$$

6. Lagrangian Closure?

- The coarse-scale system is exact and thus Hamiltonian: find geometric formulation
- Linear algebra of new matrices $\tilde{S}$ and $\tilde{M}$ in fine-scale limits appears to converge numerically on a fixed coarse scale:

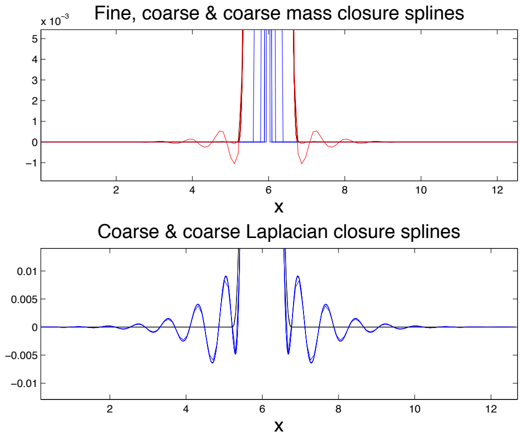
$$\tilde{M}_{lm} \rightarrow M_{lm}, \tag{23}$$

  and $\tilde{S}_{lm}$ is full, due to oscillatory tail, indicating its global elliptic nature.
- We must still approximate the fine-scale "new" terms

$$-S^{-1}_{\alpha\gamma} \sum_{k'} \tilde{\varphi}_\gamma(X_{k'}) D_{0l} w_{0k'} \Delta_{k'} \partial_x \tilde{\varphi}_\alpha |_{X_k} + S^{-1}_{\alpha\gamma} R_\gamma \partial_x \tilde{\varphi}_\alpha |_{X_k}$$

Lagrangian Closure?

- Oscillatory tails.
- Refined $(2\times, 4\times, 8\times, 16\times)$, fixed coarse, and closed mass and Laplace spline basis functions:



Exact Variational Principle Coarse System

- Coarse-scale system is exact and thus Hamiltonian.
- Find geometric formulation ito new basis functions plus potential:

$$0 = \int_0^T \sum_k \mathcal{D}_{0k} w_{0k} \Delta_k \big(V_k \frac{\mathrm{d}X_k}{\mathrm{d}t} - \frac{1}{2} V_k^2\big) + \frac{1}{2}\tilde{S}_{lm}\Phi_l\Phi_m + h_l\big(R_l - \sum_k \mathcal{D}_{0k} w_{0k}\Delta_k \tilde{\Phi}_l(X_k)\big) + P\mathrm{d}t \tag{24}$$

with fine-scale potential (incl. continuum limit)

$$P = -\sum_{k',k^*} \frac{1}{2}\underline{\tilde{\varphi}_\alpha(X_{k^*}) S^{-1}_{\alpha\gamma}\tilde{\varphi}_\gamma(X_{k'})}\mathcal{D}_{0k^*} w_{0k^*}\Delta_{k^*}\mathcal{D}_{0k'} w_{0k'}\Delta_{k'} + \sum_{k'} \underline{\tilde{\varphi}_\alpha(X_{k'}) S^{-1}_{\alpha\gamma}} R_\gamma \mathcal{D}_{0k'} w_{0k'}\Delta_{k'}. \tag{25}$$

Exact Variational Principle Coarse System

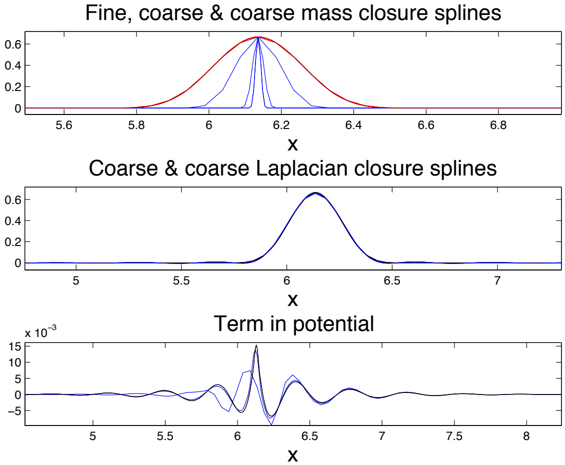
- Fine-scale potential (incl. continuum limit)

$$P = -\sum_{k',k^*} \underline{\frac{1}{2}\tilde{\varphi}_\alpha(X_{k^*}) S^{-1}_{\alpha\gamma} \varphi_\gamma(X_{k'})} \mathcal{D}_{0k^*} w_{0k^*} \Delta_{k^*} \mathcal{D}_{0k'} w_{0k'} \Delta_{k'}$$
$$+ \sum_{k'} \underline{\varphi_\alpha(X_{k'}) S^{-1}_{\alpha\gamma} R_\gamma} \mathcal{D}_{0k'} w_{0k'} \Delta_{k'} \qquad (26)$$
$$\Longrightarrow P_c = -\iint \underline{\frac{1}{2}\tilde{\varphi}_\alpha(X(x^*,\zeta^*,t)) S^{-1}_{\alpha\gamma} \tilde{\varphi}_\gamma(X(x',\zeta',t))}$$
$$\times \mathcal{D}_0(x',\zeta')\mathcal{D}_0(x^*,\zeta^*)\mathrm{d}x'\mathrm{d}\zeta'\mathrm{d}x^*\mathrm{d}\zeta^*$$
$$+ \int \underline{\tilde{\varphi}_\alpha(X(x',\zeta',t)) S^{-1}_{\alpha\gamma} R_\gamma} \mathcal{D}_0(x',\zeta')\mathrm{d}x'\mathrm{d}\zeta'$$

- We must approximate particles riding this smoothened fine-scale parcel potential P_c.
- Stochastic methods w. heavy/light particles ito PDF weights $\mathcal{D}_0$ (e.g, Frank & Gottwald 2013)?

Lagrangian Closure?

- For one γ, the potential term $\tilde{\varphi}_\alpha S^{-1}_{\alpha\gamma}\tilde{\varphi}_\gamma$ for refinements $(2\times, 8\times, 16\times)$:



7. Outlook

- Variational principle parcel Vlasov-Poisson system derived.
- Hamiltonian Particle Mesh method for Vlasov-Poisson system works: proper weak form.
- Hamiltonian Particle finite element method for Vlasov-Poisson system works; noisy density field with cubic Bernstein polynomials/splines.
- Established Eulerian closure by using coarse-fine hierarchical basis functions.
- Lagrangian closure is open. Link to a thermostat derivation? Use Mori-Zwanzig method (e.g., Bernstein 2007)?
- Extension to multi-dimensions and fluid systems? Noise reduction!

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