Asymptotic-preserving dynamical low-rank approximations to the Vlasov-Fokker-Planck system

Jack Coughlin, Jingwei Hu, (University of Washington)

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Outline

The Vlasov-Fokker-Planck system

First-principles model for plasma behavior:

$$\partial_t f_\alpha + \mathsf{v} \cdot \nabla_{\mathsf{x}} f_\alpha + \frac{q_\alpha}{m_\alpha} (\mathsf{E} + \mathsf{v} \times \mathsf{B}) \cdot \nabla_{\mathsf{v}} f_\alpha = \sum_\beta C[f_\alpha, f_\beta] = C_\alpha$$

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$$C[f_\alpha, f_\beta] = \nabla_{\mathsf{v}} \cdot [D_{\alpha\beta} \cdot \nabla_{\mathsf{v}} f_\alpha - U_{\alpha\beta} f_\alpha]$$

Many models of the drift and diffusion factors are possible:

- Rosenbluth potential formulation [14], [13]:

$$D_{\alpha\beta} = \nabla_{\mathsf{v}} \nabla_{\mathsf{v}} G_\beta, \quad U_{\alpha\beta} = \nabla_{\mathsf{v}} H_\beta$$

  The potentials G, H are found by inverting a Poisson operator.

- Single species Dougherty-Fokker-Planck operator [6]:

$$D_{\alpha\alpha} = v_{th}^2 \mathbb{I}, \quad U_{\alpha\alpha} = \mathsf{u}_\alpha = \langle \mathsf{v} f_\alpha \rangle_v$$

Asymptotic limits reduce computation

Normalization reveals parameters of interest [12]:

$$\partial_{\bar{t}} \bar{f}_\alpha + \bar{\mathsf{v}} \cdot \nabla_{\bar{\mathsf{x}}} \bar{f}_\alpha + (\omega_p \tau)^2 \frac{Z_\alpha}{A_\alpha} \bar{\mathsf{E}} \cdot \nabla_{\bar{\mathsf{v}}} \bar{f}_\alpha$$
$$+ (\omega_c \tau) \frac{Z_\alpha}{A_\alpha} (\bar{\mathsf{v}} \times \bar{\mathsf{B}}) \cdot \nabla_{\bar{\mathsf{v}}} \bar{f}_\alpha = (\nu_p \tau) \bar{C}_\alpha$$

Relative strength of collisions is $\nu_p \tau = \mathsf{Kn}^{-1}$: proton collision times per characteristic time τ.

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Relative strength of collisions is $\nu_p \tau = \mathrm{Kn}^{-1}$: proton collision times per characteristic time τ.

- $(\nu_p \tau) \gg 1$: Hydrodynamic limit. Fluid models are appropriate. $d = 3$
  - $13N$ and above moment models may push range of viability to moderate collisionalities, $(\nu_p \tau) \approx 10^2$ [12]
- $(\nu_p \tau) \ll 1$, $(\omega_c \tau) \gg 1$: Gyrokinetic models are possible in highly magnetized plasmas. $d = 5$
- $(\nu_p \tau) \ll 1$: in the absence of simplifying asymptotics, the full kinetic equation must be solved. $d = 6$

Low-rank approximation

Lesson from big data

- Almost all huge matrices are extremely (numerically) rank deficient.

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Meaning: a truncated SVD is a good approximation.

$$\mathsf{A} \in \mathbb{R}^{M\times N} \implies \mathsf{A} = \mathsf{U}\Sigma\mathsf{V}^T$$

$$\mathsf{A}_r \triangleq \mathsf{U}_{(,1:r)}\Sigma_{(1:r,1:r)}\mathsf{V}^T_{(1:r,)}$$

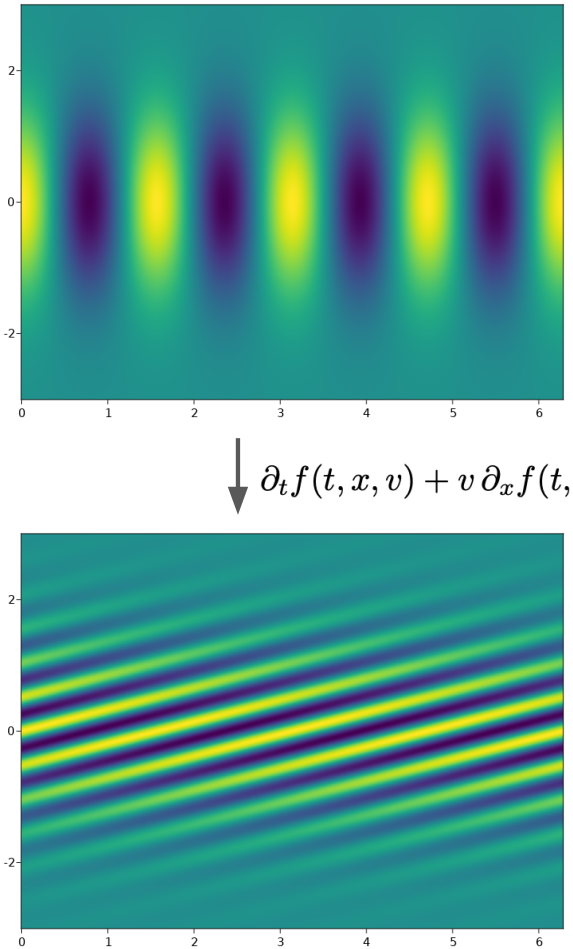
$$\sigma_r/\sigma_1 = \epsilon \implies \|\mathsf{A}-\mathsf{A}_r\|/\|\mathsf{A}\| = O(\epsilon)$$

Truncated SVD requires much less storage:

$$r \ll M, N \implies rM + r^2 + rN \ll MN$$

Low-rank approximation

Handles at least some numerical difficulties with ease [5]



$$f(\mathrm{x},\mathrm{v}) = \sum_{i,j}^{r} X_i(\mathrm{x}) S_{ij} V_j(\mathrm{v})$$

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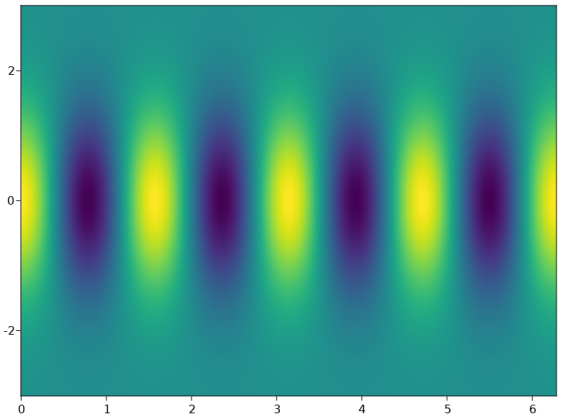
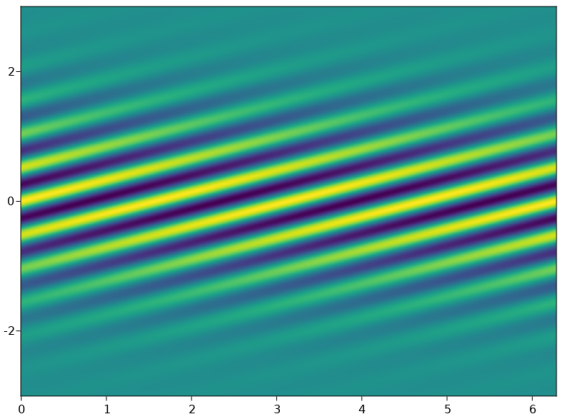


$$f(x, v) = \sum_{i,j}^{2} X_i(x) S_{ij} V_j(v)$$

$$\partial_t f(t,x,v) + v\,\partial_x f(t,x,v) = 0$$



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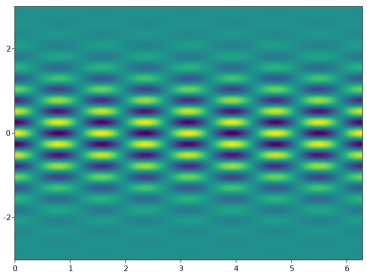

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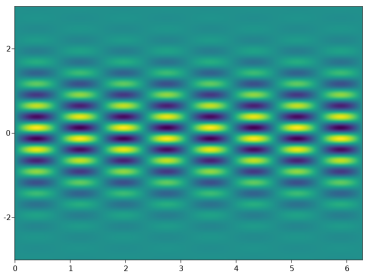

Outline

History of dynamical low-rank method

The dynamical low-rank method is a promising direction for reduced plasma models.

- Proposed by Koch and Lubich for ODEs (2007) [8]
- Extended to higher-order tensors in various formats [9], [11]
- Overapproximation-insensitive integrators developed [10], [1]
- Applied to kinetic equations (2018, 2021) [5], [3]

Example low-rank kinetic approximation

Consider an arbitrary equation of "kinetic type":

$$\partial_t f(x, v, t) = h$$

Look for approximate solutions of the form

$$\tilde{f} = \sum_{i,j=1}^{r} X_i(x, t) S_{ij}(t) V_j(v, t).$$

- The integer r is the rank
- Bases X and V are orthonormal:

$$\langle X_i, X_k \rangle_x = \delta_{ik}, \quad \langle V_j, V_l \rangle_v = \delta_{jl}$$

- Similar to the SVD, except that S is not necessarily diagonal.
  - $\implies$ the decomposition is not unique.

What makes it dynamical?

We impose a Galerkin condition on the time derivative of the system:

$$\langle h - \tilde{h}, \delta\tilde{f} \rangle = 0 \quad \text{for all} \quad \delta\tilde{f} \in \mathcal{T}_{\tilde{f}}\mathcal{M}_r.$$

- $\mathcal{M}_r$ is the manifold of low-rank functions
- $\mathcal{T}_{\tilde{f}}\mathcal{M}_r$ is the tangent space to the manifold at $\tilde{f}$.
- $\tilde{h}$ is our low-rank time derivative.

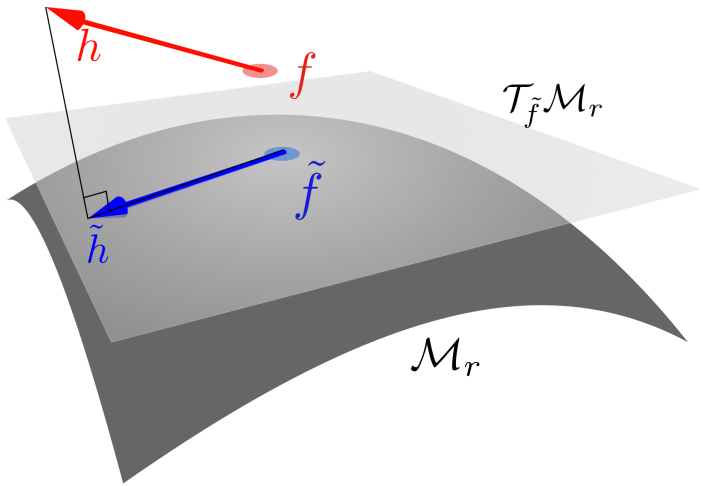

Figure: The method takes steps along the low-rank manifold's tangent space.

Projector-splitting integrator

Equivalently, $\tilde{h} = P(\tilde{f})h$ for an orthogonal projection $P(\tilde{f})$.
It turns out that P has the form

$$\tilde{h} = P(\tilde{f})h = X_i \langle X_i, h \rangle_x - X_i \langle X_i V_j, h \rangle_{xv} V_j + \langle V_j, h \rangle_v V_j.$$

An operator splitting of the projector leads to a simple first order time integration scheme:

$$\begin{aligned} \tilde{f}' &= \tilde{f}(t_0) + \Delta t (V_j \langle V_j, h \rangle_v) \\ \tilde{f}'' &= \tilde{f}' - \Delta t (X_i \langle X_i V_j, h \rangle_{xv} V_j) \\ \tilde{f}(t_1) &= \tilde{f}'' + \Delta t (\langle X_i, h \rangle_x X_i). \end{aligned}$$

The scheme is:

- Exact if f has rank r.
- Robust to overapproximation: S can have vanishing singular values!

Pros and Cons

Solving r equations of size N_x and r of size N_v is much cheaper than solving one equation of size $N_x N_v$.

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- Mass, momentum and energy conservation [a]
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- Mass, momentum and energy conservation [a]
  - The approximation can "leak" conserved quantities into the truncated ranks.
- Maxwellian asymptotic limit
  - A Maxwellian with spatially varying parameters is not low-rank.
  - Solution near fluid limit is just as costly as kinetic regime. We're leaving structure on the table! [b]

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[a] Einkemmer ([4]) presents a conservative low-rank scheme.

[b] Einkemmer, Hu et.al ([2], [3]) show that preserving the fluid limit is possible for BGK.

Outline

A simple collisional plasma model

Test case: high-field limit of the Vlasov-Ampere-Fokker-Planck system

$$\begin{cases} \partial_t f + v \cdot \nabla_x f + \frac{1}{\epsilon} E \cdot \nabla_v f = \frac{1}{\epsilon} \nabla_v \cdot (v f + \nabla_v f), \\ \partial_t E = -J \end{cases}$$

- The current density J is defined $J = \langle v f \rangle_v$.
- Physically, can describe high-frequency motion of electrons against a static ion background fluid.

Limiting distribution

Define the local "Maxwellian"

$$M(x, v, t) = e^{-\frac{|v-E(x,t)|^2}{2}}$$

Then our Vlasov-Fokker-Planck equation is

$$\partial_t f + v \cdot \nabla_x f = \frac{1}{\epsilon} \nabla_v \cdot [M \nabla_v (M^{-1} f)].$$

As $\epsilon \to 0$, f approaches

$$f^0 = \frac{\rho(x)}{(2\pi)^{d/2}} M,$$

for the density $\rho(x) = \langle f \rangle_v$.

Limiting fluid system

What is the governing equation for ρ in the $\epsilon \to 0$ limit?

- Multiply by 1 and v and integrate:

$$\partial_t \rho + \nabla_x \cdot J = 0$$
$$\partial_t J + \nabla_x \cdot \langle v \otimes vf \rangle_v = \frac{1}{\epsilon}(\rho E - J).$$

- Send $\epsilon \to 0$:

$$\rho E - J = 0 \quad \Longrightarrow \quad \begin{cases} \partial_t \rho + \nabla_x \cdot (\rho E) = 0, \\ \partial_t E = -\rho E. \end{cases}$$

The Asymptotic-preserving property

$$\begin{cases} C^{\text{kinetic}}: & \partial_t f + v \cdot \nabla_x f = \frac{1}{\epsilon} \nabla_v \cdot [M \nabla_v (M^{-1} f)], \\ C^{\text{fluid}}: & f = \frac{\rho}{(2\pi)^{d/2}} M, \text{ where } \partial_t \rho + \nabla_x \cdot (\rho E) = 0 \end{cases}$$

Both coupled with Ampere's equation.
We're looking for a kinetic discretization D^{kinetic} that makes this diagram commute:

$$\begin{array}{ccc} D^{\text{kinetic}} & \xrightarrow{\Delta t,x,v \to 0;\ r \to \infty} & C^{\text{kinetic}} \\ \Big\downarrow \epsilon \to 0 & & \Big\downarrow \epsilon \to 0 \\ D^{\text{fluid}} & \xrightarrow{\Delta t,x,v \to 0} & C^{\text{fluid}} \end{array}$$

Goal: the bottom path should hold for fixed r.

Low-rank algorithm

Key idea: evolve low-rank representation of $g = M^{-1}f$:

$$\epsilon \to 0 \implies f \to \frac{\rho(x)}{(2\pi)^{d/2}} M \implies g \to \frac{\rho(x)}{(2\pi)^{d/2}} \text{ (rank 1)}$$

Recall the low-rank ansatz is

$$g(x, v, t) = \sum_{i,j=1}^{r} X_i(x, t) S_{ij}(t) V_j(v, t).$$

Plug $f = gM$ into the Vlasov-Fokker-Planck equation:

$$h \triangleq \partial_t g = -v \cdot \nabla_x g - \underbrace{\frac{1}{M}(\partial_t M + v \cdot \nabla_x M) g}_{\mathcal{M}} + \frac{1}{\epsilon}[(\nabla_v - v + E) \cdot \nabla_v g].$$

Projector-splitting integration

Introduce auxiliary bases K and L:

$$K_j(x,t) = \sum_i X_i(x,t) S_{ij}(t), \quad L_i(v,t) = \sum_j S_{ij}(t) V_j(v,t).$$

$$\partial_t g = \sum_j \partial_t K_j V_j - \sum_{ij} X_i \partial_t S_{ij} V_j + \sum_i X_i \partial_t L_i$$

Projector-splitting integration: K step

$$\partial_t g = \sum_j \partial_t K_j V_j - \sum_{ij} X_i \partial_t S_{ij} V_j + \sum_i X_i \partial_t L_i$$

$$\partial_t K_j = -\sum_l (\nabla_x K_l) \cdot \langle v V_j, V_l \rangle_v - \sum_l K_l \langle V_j, V_l \mathcal{M} \rangle_v + \frac{1}{\epsilon} \sum_l K_l [\langle V_j (\nabla_v - v) \cdot \nabla_v V_l \rangle_v + E \cdot \langle V_j \nabla_v V_l \rangle_v]$$

1. Advance K_j^n to K_j^{n+1} via $\partial_t K_j = \langle V_j, h \rangle_v$.
2. Perform a QR decomposition of K_j^{n+1} to obtain X^{n+1}, S'.

Projector-splitting integration: S step

$$\partial_t g = \sum_j \partial_t K_j V_j - \sum_{ij} X_i \partial_t S_{ij} V_j + \sum_i X_i \partial_t L_i$$

$$\partial_t S_{ij} = \sum_{kl} S_{kl} \langle X_i \nabla_x X_k \rangle_x \cdot \langle v V_j V_l \rangle_v + \sum_{kl} S_{kl} \langle X_i X_k V_l V_j \mathcal{M} \rangle_{xv}$$

$$- \frac{1}{\epsilon} \left(\sum_{kl} S_{kl} \left[\langle X_i X_k \rangle_x \langle V_j (\nabla_v - v) \cdot \nabla_v V_l \rangle_v + \langle X_i X_k E \rangle_x \cdot \langle V_j \nabla_v V_l \rangle_v \right] \right).$$

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2. Perform a QR decomposition of K_j^{n+1} to obtain X^{n+1}, S'.
3. Advance S' to S'' via $\partial_t S_{ij} = -\langle X_i V_j, h \rangle_{xv}$.

Projector-splitting integration: L step

$$\partial_t g = \sum_j \partial_t K_j V_j - \sum_{ij} X_i \partial_t S_{ij} V_j + \sum_i X_i \partial_t L_i$$

$$\partial_t L_i = -\sum_k v \cdot \langle X_i (\nabla_x X_k) \rangle_x L_k - \sum_k \langle X_i X_k \mathcal{M} \rangle_x L_k + \frac{1}{\epsilon} \left(\sum_k [\langle X_i X_k \rangle_x (\nabla_v - v) + \langle X_i X_k E \rangle_x] \cdot \nabla_v L_k \right).$$

1. Advance K_j^n to K_j^{n+1} via $\partial_t K_j = \langle V_j, h \rangle_v$.
2. Perform a QR decomposition of K_j^{n+1} to obtain X^{n+1}, S'.
3. Advance S' to S'' via $\partial_t S_{ij} = -\langle X_i V_j, h \rangle_{xv}$.
4. Advance L_i^n to L_i^{n+1} via $\partial_t L_i = \langle X_i, h \rangle_x$.
5. Perform a QR decomposition of L_i^{n+1} to obtain V^{n+1}, S^{n+1}.

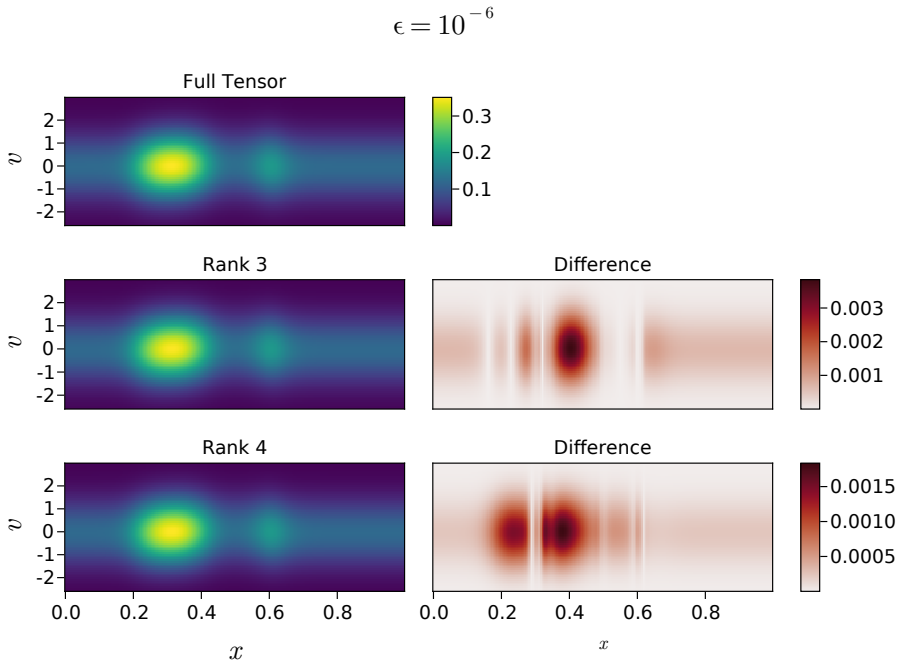
Discretization

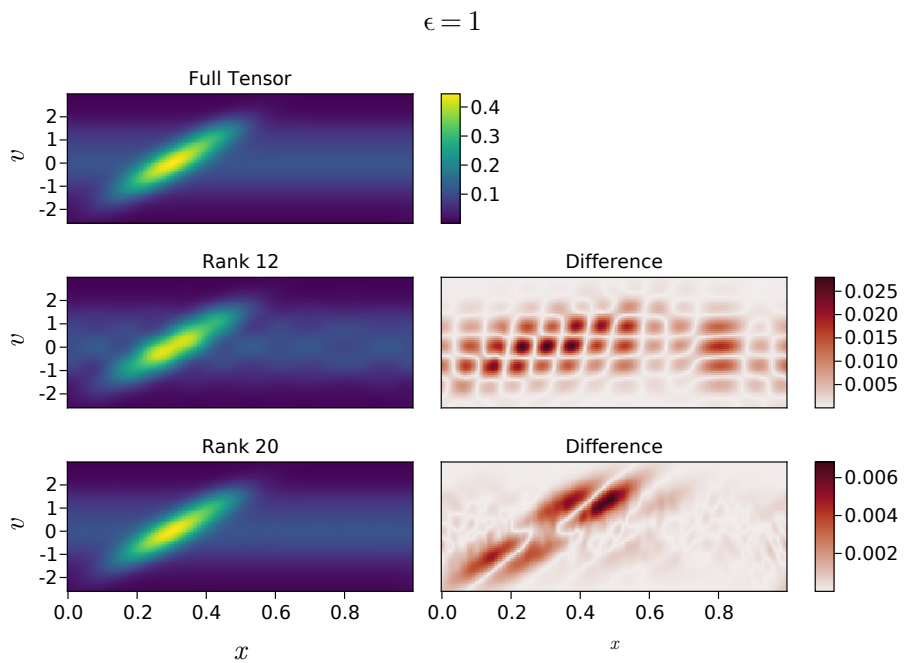
- Second-order central finite difference for diffusive part in v
- Flux-limited Lax-Wendroff scheme for hyperbolic advection in x
- First-order-in-time IMEX scheme to handle coupled advective-diffusive PDEs
- Care required for ill-posed ODE

$$\partial_t S_{ij} = -\langle X_i V_j h \rangle_{xv}.$$

Results

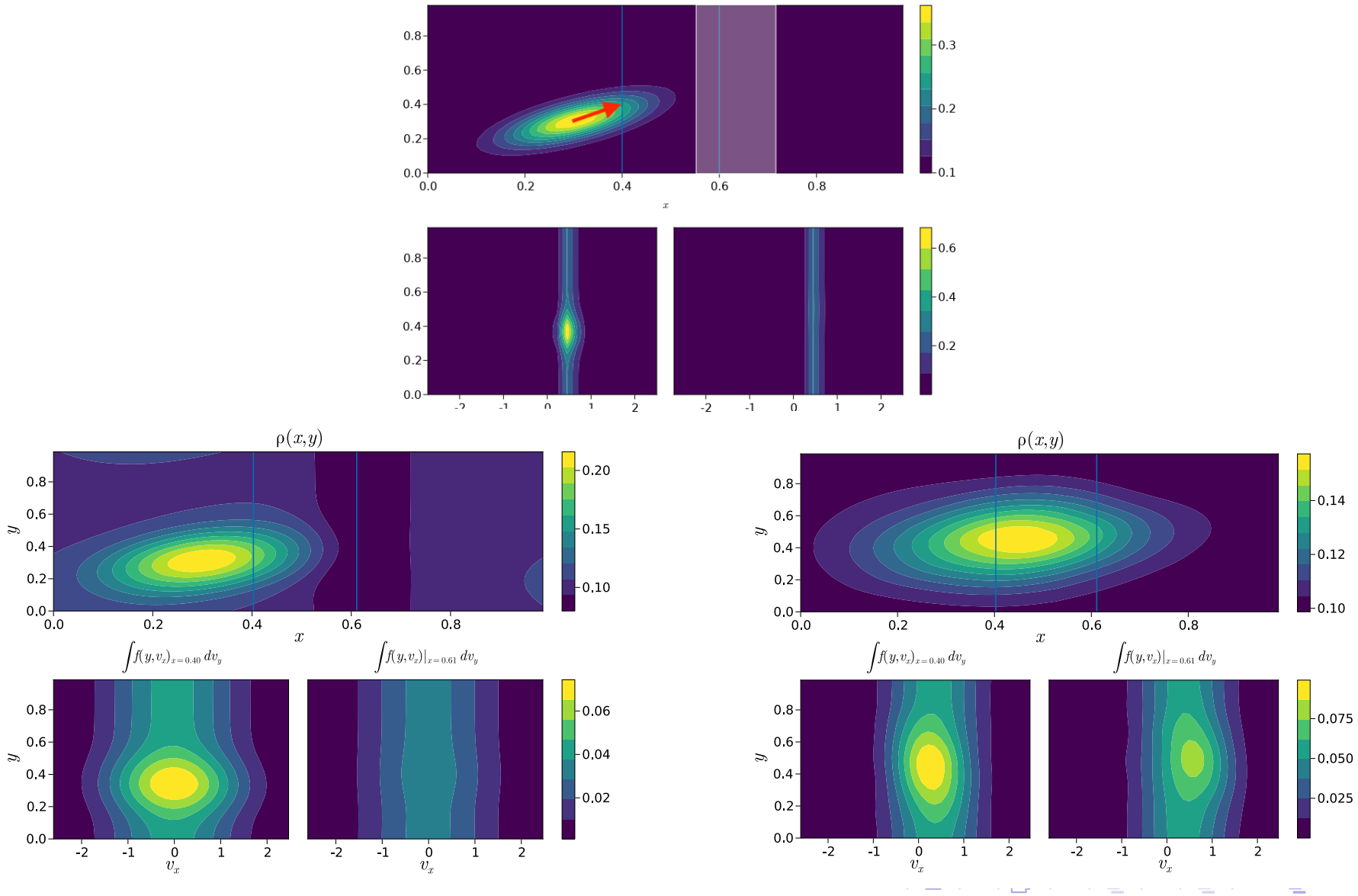
Small-ϵ dynamics are captured with very few ranks, while kinetic dynamics require higher rank:





Results

Our method reproduces dynamics through a range of regimes



Performance gains

We verify the expected $O(rN_x + rN_v)$ asymptotic complexity of our implementation:

N	Low Rank			Full Tensor
	$r = 5$	$r = 10$	$r = 15$	
24	1.00 / -	2.14 / -	3.89 / -	13.8 / -
48	3.21 / **1.7**	7.94 / **1.9**	14.4 / **1.9**	256 / **4.2**
72	10.5 / **2.1**	23.6 / **2.2**	46.7 / **2.3**	1.5e3 / **4.3**
96	18.6 / **2.1**	38.3 / **2.1**	54.7 / **1.9**	5.3e3 / **4.3**
120	29.2 / **2.1**	52.2 / **2.0**	88.9 / **1.9**	1.23e4 / **4.2**

Table: Computational runtime per time step of the 2D2V potential hill problem. Runtimes are normalized to the $r = 5, N = 24$ size. The bolded numbers are the empirical exponent of N. We see agreement with the expected asymptotic complexity of 2 for the low-rank case, compared with 4 for the full tensor solver.

Outline

Structure preservation remains a challenge

Projection of the collision operator disrupts its properties. We start with the well-behaved

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$$\delta_{ik} M_k^{-1}\nabla_v \cdot (M_k \nabla_v L_k) + e_{ik} \cdot \nabla_v L_k = 0$$

$$e_{ik} = \langle X_i, EX_k \rangle_x, \quad M_k = e^{-\frac{|v-e_{kk}|^2}{2}} \tag{1}$$

It's unclear how to prove the kernel of this operator.

Fast projection of the Maxwellian

A key step in this and similar schemes is computing projections of the Maxwellian. For example,

$$J = \sum_{ij}^{r} X_i S_{ij} \langle v V_j, M(x, v) \rangle_v .$$

Computing this integral costs $N_x N_v$ in a naive approach.
The situation is improved for an isothermal Maxwellian, where the integral has a convolution structure:

$$\langle v V_j M(x, v) \rangle_v = \int v V_j(v) e^{-\frac{|v-E|^2}{2}} \, dv$$

so may be computed with an FFT.

A couple extensions

- Rank adaptivity: It is possible to dynamically update the rank by monitoring the quality of the approximation σ_r/σ_1. (applied to nonlinear Boltzmann—Hu and Wang (2021) [7]).
- Tensor decomposition: Einkemmer (2018) [5] employs a hierarchical tensor decomposition to decompose the order-4 tensor $f(x_1, x_2, v_1, v_2)$ into 4 bases.

Conclusion

- The low-rank method is a promising approach to greatly accelerate the solution of kinetic equations.
- With no modifications, it is a bit of a sledgehammer.
  - But it is possible to help it preserve some structure.

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