A Method-of-Lines Low Rank Tensor Approach for Nonlinear Kinetic Simulations

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Supported by AFOSR, DOE(CHaRMNET) and NSF

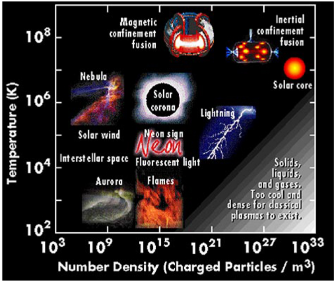
Workshop on Sparse Tensor Computations,
October 18-19, 2023

Outline

- Plasma physics and fusion energy
- **Method-of-lines low rank tensor approach** for multi-scale kinetic models
  - Explicit time stepping schemes: Vlasov model (this talk)
  - Implicit time stepping schemes: heat equation and Fokker-Planck model (poster by J. Nakao)
  - Implicit-explicit time stepping schemes for multi-scale kinetic models. (poster by J. Nakao)
- **Locally Macroscopic Conservative (LoMaC) projection** on preservation of macroscopic conservation laws
- Summary and outlook for future.

What is plasma?

- Plasma is known as the fourth state of matter after solid, liquid and gas, containing interacting free electrons and ions.
- It compose 99% of visible matter in the universe, being mostly associated with stars, including the sun.
- Applications include fusion reactors, plasma assisted combustion, spacecraft charging in the ionosphere, semi-conductor devices.



A fundamental model for plasma

- Boltzmann equation for f_s:

$$\frac{\partial f_s}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f_s + \frac{q_s}{m_s}(\mathbf{E} + \mathbf{v} \times \boldsymbol{B}) \cdot \nabla_{\mathbf{v}} f_s = \sum_i Q(f_i, f_s).$$

- Maxwell equations for the electromagnetic fields $\mathbf{E}$ and $\boldsymbol{B}$:

$$\frac{\partial \boldsymbol{B}}{\partial t} = -\nabla \times \mathbf{E}, \quad \frac{\partial \mathbf{E}}{\partial t} = \nabla \times \boldsymbol{B} - \mathbf{J},$$

$$\nabla \cdot \mathbf{E} = \rho, \quad \nabla \cdot \boldsymbol{B} = 0,$$

with the charge density $\rho = \sum_s q_s \int f_s d\mathbf{v}$, and the current density $\mathbf{J} = \sum_s q_s \int f_s \mathbf{v} d\mathbf{v}$.

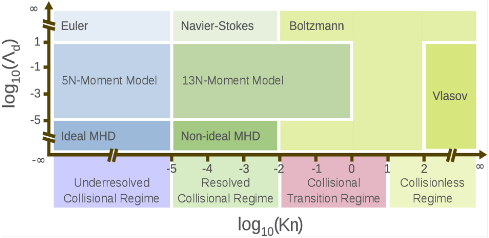
- $f_s(t, v, x)$ is the distribution function of particle of species s.
- 6D + time nonlinear dynamical systems.

Computational Challenges

- Curse of Dimensionality (CoD): 6D+time.
- Vastly spanned temporal and spatial scales
  - Temporal scale 10^{14}

    From 10^{-10} for electron gyrofrequency
    To 10^{4} for the time scale to run ITER
  - Spatial scale 10^{8}

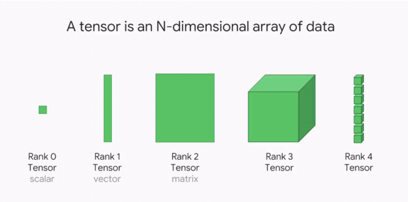
    From 10^{-6} for electron gyroradius
    To 10^{2} for system size

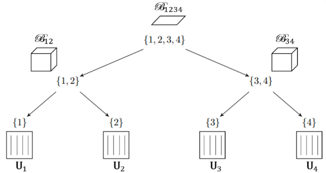


Credit: Uri Shumlak, University of Washington

Tame the CoD for multi-scale kinetic modeling of plasmas

- Reduced representation via low rank hierarchical Tucker format
- Structure preservation with reduced presentation
  - local conservation laws for mass, momentum and energy
  - Asymptotic preservation of multi-scale model hierarchies





Complexity for 4D tensors: $\mathcal{O}(N^d)$ vs $\mathcal{O}(dNr + dr^3)$

Existing computational approaches

- Particle methods, e.g., the Particle-In-Cell method
  - $+$: efficient for qualitative Vlasov simulations in high D
  - $-$: suffer from the statistical noise
- Sparse grid methods
  - $+$: mesh-based high order methods with significantly reduced computational cost
  - $-$: yet CoD is not well-tamed
- Reduced order modeling (ROM)
  - $+$: consider low rank structure in time and in parameter spaces
  - $-$: low rank structure in phase space remains unexplored.
- Low-rank approach for kinetic solutions.
  - Dynamical low-rank approach: Einkemmer & Lubich (2018), Venturi (2018).
  - Low rank tensor approach: low rank truncation of a full rank high order solution with modern tool of hierarchical Tucker tensor representation.

Method-of-lines low rank tensor approach:

Explicit time stepping for a simple 1D1V nonlinear Vlasov Dynamics

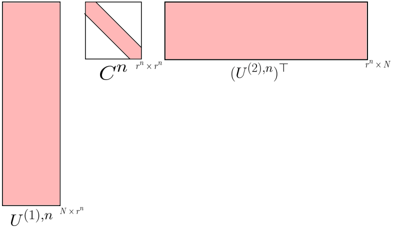
1D1V Vlasov-Poisson system for electrons,

$$f_t + v \cdot \nabla_x f + E(x,t) \cdot \nabla_v f = 0, \tag{1}$$

$$E(x,t) = -\nabla_x \phi(x,t), \quad -\triangle_x \phi(x,t) = \rho(x,t) = \int f dv - 1. \tag{2}$$

A low rank idea for 1D1V Vlasov-Poisson system

- At the discrete level: SVD of A with $A_{ij} = f(x_i, v_j)$.



  - Frames in x and v-directions as orthogonal global basis.
  - Storage: $\mathcal{O}(Nr)$. Low rank if $r^n \ll N$.
- At the continuous level: Schmidt decomposition.

$$f^n(x,v) = \sum_{j=1}^{r^n} \left(C_j^n \quad U_j^{(1),n}(x) U_j^{(2),n}(v) \right), \tag{3}$$

  - $U_j^{(1),n}(x)$ and $U_j^{(2),n}(v)$ are problem-dependent global orthonormal basis in x- and v-directions.

At the continuous level

1D1V VP system

$$f_t + v \cdot f_x + E \cdot f_v = 0.$$

Keep the phase space continuous, a low rank representation of function f at t^n

$$f^n(x,v) = \sum_j c_j^n U_j^{(1),n}(x) U_j^{(2),n}(v)$$

A forward Euler discretization of the VP system gives

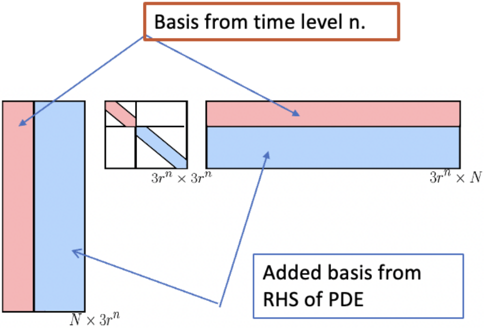
$$f^{n+1}(x,v) = \sum_{j=1}^{r^n} C_j^n \left[U_j^{(1),n}(x) U_j^{(2),n}(v) - \Delta t \right.$$
$$\left. \left(\frac{\partial}{\partial x} U_j^{(1),n}(x)(v U_j^{(2),n}(v)) + (E^n(x) U_j^{(1),n}) \frac{\partial}{\partial v} U_j^{(2),n}(v) \right) \right],$$

Dynamically and adaptively update basis and solutions

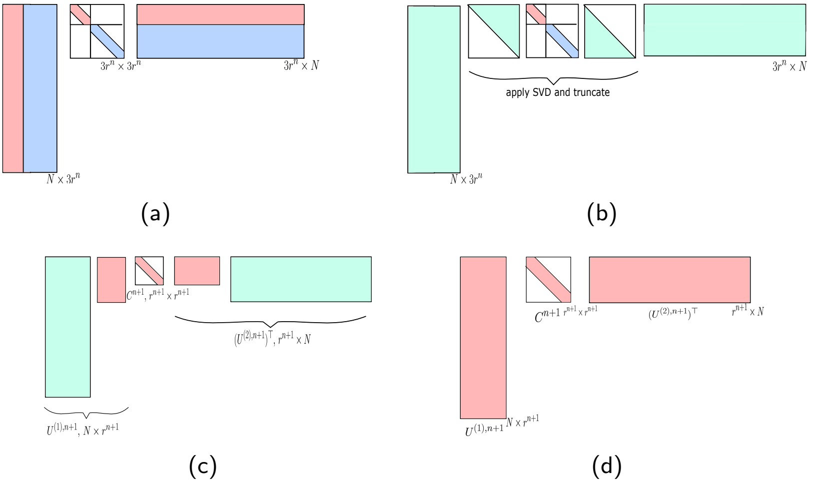
1 Add basis. Take the forward Euler method for example,

$$f^{n+1,*} = \sum_{j=1}^{r^n} C_j^n \left[\left(U_j^{(1),n} \otimes U_j^{(2),n} \right) \right.$$
$$\left. -\Delta t \left(D_x U_j^{(1),n} \otimes v \star U_j^{(2),n} + E^n \star U_j^{(1),n} \otimes D_v U_j^{(2),n} \right) \right],$$

Here D_x and D_v represent a differentiation matrix, e.g. from finite difference scheme, spectral method or high order DG discretization with upwind principle.

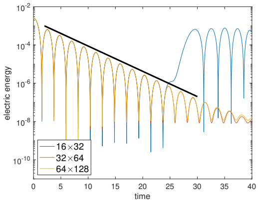


2 SVD Truncation.

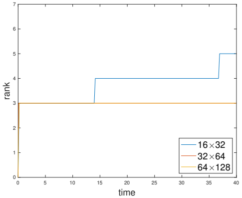


(a)→(b): perform Gram-Schmidt to obtain orthonormal basis;
(b)→(c): perform SVD on and truncate small singular values;
(c)→(d) update low rank form of solution at t^{n+1}.

Nonlinear Vlasov Poisson: weak Landau damping



(a)

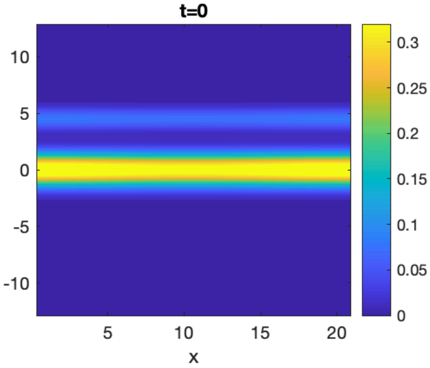


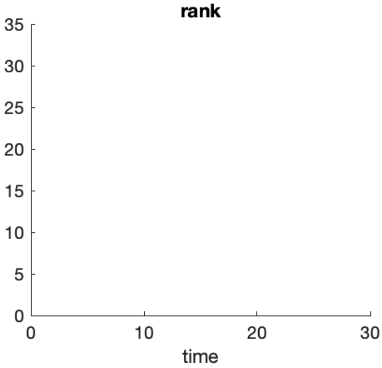
(b)

For $N_x \times N_v = 16 \times 32$, 32×64 and 64×128, the CPU times are 15.5s, 32.1s, and 59.0s. $\varepsilon = 10^{-5}$ for truncation. The time evolution of the rank, the electric energy.

Bump-on-tail instability

Truncation threshold $\varepsilon = 10^{-4}$. $N_x \times N_v = 64 \times 128$.





Low rank approach for 1D1V Vlasov system

- Low rank and rank adaptive.
- Mitigating the curse of dimensionality: CPU time only doubled with mesh refinement, but not 2^{d+1}.
- High order in spatial and temporal accuracy.
- Flow map approach: mitigate rank increase by following the flow map (in the spirit of coordinate transform) *
- Conservative in the "add basis step"; but conservation is destroyed in the truncation step.

*Guo and Qiu, JCP, 2022

Preserving conservation via an orthogonal decomposition

$\mathbf{f}$: the pre-compressed solution from the adding basis step.

$$\mathbf{f} = \mathbf{f}_1 + \mathbf{f}_2,$$

- $\mathbf{f}_1 = P_W(\mathbf{f})$: the orthogonal projection of $\mathbf{f}$ onto the subspace $W = span(\mathbf{1}_v,\ \boldsymbol{v},\ \boldsymbol{v}^2)$ †, preserving the mass, momentum and kinetic energy of $\mathbf{f}$.
- $\mathbf{f}_2 = (I - P_W)(\mathbf{f})$: the orthogonal remainder with zero mass, momentum and kinetic energy,
- The compressed low-rank solution:

$$\mathbf{f} = \mathbf{f}_1 + \mathcal{T}(\mathbf{f}_2),$$

  preserving the mass, momentum and kinetic energy of $\mathbf{f}$.

† in a weighted inner product space with a Maxwellian weight w

Construction of $\mathbf{f}_1$

- Scale: $\tilde{\mathbf{f}} = \frac{1}{\mathbf{w}} \star \mathbf{f}^{n+1,*}$.
- Perform the orthogonal projection $P_W(\tilde{\mathbf{f}})$ onto subspace W:

$$\langle P_W(\tilde{\mathbf{f}}), \mathbf{g} \rangle_w = \langle \tilde{\mathbf{f}}, \mathbf{g} \rangle_w, \quad \forall \mathbf{g} \in W.$$

- Rescale back: $\mathbf{f}_1 = \mathbf{w} \star P_W(\tilde{\mathbf{f}})$.

Proposition. $\mathbf{f}_1$ admits an explicit low-rank representation:

$$\mathbf{f}_1 = \mathbf{w} \star \left(c_1 \otimes \mathbf{1}_v + c_2 \otimes \mathbf{v} + c_3 \otimes (\boldsymbol{v}^2 - c) \right),$$

with $c = \frac{\langle \mathbf{1}_v, \boldsymbol{v}^2 \rangle_w}{\|\mathbf{1}_v\|_w^2}$, $c_1 = \frac{\boldsymbol{\rho}}{\|\mathbf{1}_v\|_w^2}$, $c_2 = \frac{\mathbf{J}}{\|\boldsymbol{v}\|_w^2}$, and $c_3 = \frac{2\kappa - \boldsymbol{\rho} c}{\|\boldsymbol{v}^2 - c\|_w^2}$. $\boldsymbol{\rho}$, $\mathbf{J}$ and $\boldsymbol{\kappa} \in \mathbb{R}^{N_x}$ are macroscopic charge, current and kinetic energy densities of $\mathbf{f}^{n+1,*}$. $\mathbf{f}_1$ preserves the mass, momentum and kinetic energy of $\mathbf{f}^{n+1,*}$.

Weighted truncation of $\mathbf{f}_2$

Let $\mathbf{f}_2 = \mathbf{f}^{n+1,*} - \mathbf{f}_1$.

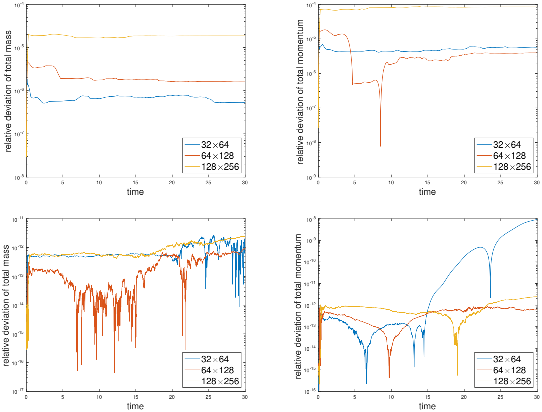
- $\mathbf{f}_2$ is orthogonal to W in $l^2_w(\Omega_v)$.
- A weighted SVD truncation for $\mathcal{T}_w(\mathbf{f}_2)$

$$\mathbf{f}_2 \overset{rescaling}{\rightarrow} \tilde{\mathbf{f}}_2 = \mathbf{f}_2 \star \frac{1}{\sqrt{\mathbf{w}}} \overset{truncation}{\rightarrow} \mathcal{T}(\tilde{\mathbf{f}}_2) \overset{rescaling}{\rightarrow} \sqrt{\mathbf{w}} \star \mathcal{T}(\tilde{\mathbf{f}}_2)$$

  Then, $\mathcal{T}_w(\mathbf{f}_2)$ is still orthogonal to W in $l^2_w(\Omega_v)$.
- Update the solution $\mathbf{f}^{n+1} = \mathbf{f}_1 + \mathcal{T}_w(\mathbf{f}_2)$.

Proposition. $\mathcal{T}_w(\mathbf{f}_2)$ has zero density, zero current density, and zero kinetic energy. Hence, ρ^{n+1}, J^{n+1}, κ^{n+1} are preserved for f^{n+1} after the truncation. The method is locally conservative with mass and momentum, as with the associated full rank high order method.

Bump-on-tail instability



Non-conservative (upper panels) and conservative (lower panels) methods. $\varepsilon = 10^{-4}$.

Yet, the energy is not conserved, as the full rank method is not energy conserving.

- Conservation of energy is of paramount importance to avoid unphysical plasma self-heating or cooling.
- Existing full-rank methods with energy conservation require implicit symplectic time integrators.
- Our work: an explicit **Lo**cally **Ma**croscopic **C**onservative (LoMaC) method by working alongside with macroscopic conservation laws and a construction of low rank $\mathbf{f}_1$.

Macroscopic conservation

The VP system satisfies the macroscopic moment equations

$$\rho_t + \nabla_{\mathbf{x}} \cdot \mathbf{J} = 0$$
$$\partial_t \mathbf{J} + \nabla_{\mathbf{x}} \cdot \sigma = -\rho \mathbf{E}$$
$$\partial_t e + \nabla_{\mathbf{x}} \cdot \mathbf{Q} = 0.$$

- particle density: $\rho(\mathbf{x}, t) = \int_{\Omega_{\boldsymbol{v}}} f(\mathbf{x}, \boldsymbol{v}, t) d\boldsymbol{v}$
- current density: $\mathbf{J}(\mathbf{x}, t) = \int_{\Omega_{\boldsymbol{v}}} \boldsymbol{v} f(\mathbf{x}, \boldsymbol{v}, t) d\boldsymbol{v}$
- kinetic energy density: $\kappa(\mathbf{x}, t) = \frac{1}{2} \int_{\Omega_{\boldsymbol{v}}} \boldsymbol{v}^2 f(\mathbf{x}, \boldsymbol{v}, t) d\boldsymbol{v}$
- energy density: $e(\mathbf{x}, t) = \kappa(\mathbf{x}, t) + \frac{1}{2} \mathbf{E}^2$
- fluxes:
  - $\sigma(\mathbf{x}, t) = \int_{\Omega_{\boldsymbol{v}}} (\boldsymbol{v} \otimes \boldsymbol{v}) f(\mathbf{x}, \boldsymbol{v}, t) d\boldsymbol{v}$,
  - $\mathbf{Q}(\mathbf{x}, t) = \frac{1}{2} \int_{\Omega_{\boldsymbol{v}}} \boldsymbol{v}\boldsymbol{v}^2 f(\mathbf{x}, \boldsymbol{v}, t) d\boldsymbol{v}$.

$$
\partial_t f + \mathbf{v}\cdot\nabla_{\mathbf{x}} f + \mathbf{E}\cdot\nabla_{\mathbf{v}} f = 0
\quad
\begin{array}{c}
\xrightarrow{\text{Kinetic flux}} \\[2em]
\xleftarrow[\text{Macroscopic densities}]{}
\end{array}
\quad
\begin{aligned}
\rho_t + \nabla_{\mathbf{x}}\cdot\mathbf{J} &= 0\\
\partial_t\mathbf{J} + \nabla_{\mathbf{x}}\cdot\sigma &= \rho\mathbf{E}\\
\partial_t e + \nabla_{\mathbf{x}}\cdot\mathbf{Q} &= 0.
\end{aligned}
$$

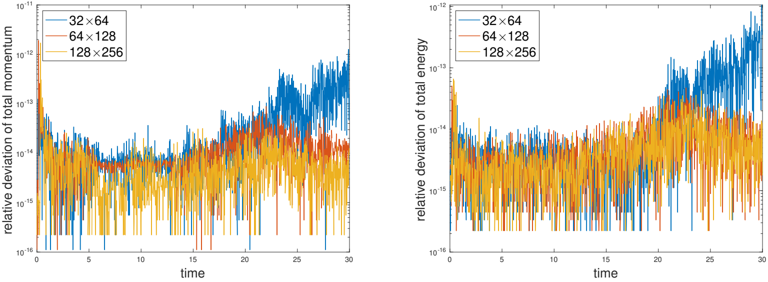
1. Employ a conservative method for the macroscopic model with kinetic flux vector splitting (KFVS) computed from $\mathbf{f}$:

$$
\nabla_x\cdot\begin{pmatrix}\mathbf{J}\\ \sigma\\ \mathbf{Q}\end{pmatrix} = \nabla_x\cdot\left[\int fv\begin{pmatrix}1\\ v\\ \frac{1}{2}v^2\end{pmatrix}dv\right]
$$

2. Replace the macroscopic charge, current and kinetic energy densities in $\mathbf{f}_1$ by the ones from the macroscopic model.

$$
\mathbf{f}_1 = \mathbf{w}\star\left(c_1\otimes\mathbf{1}_v + c_2\otimes\mathbf{v} + c_3\otimes(\boldsymbol{v}^2 - c)\right),
$$

with $c = \frac{\langle\mathbf{1}_v,\boldsymbol{v}^2\rangle_w}{\|\mathbf{1}_v\|_w^2}$, $c_1 = \frac{\boldsymbol{\rho}}{\|\mathbf{1}_v\|_w^2}$, $c_2 = \frac{\mathbf{J}}{\|\boldsymbol{v}\|_w^2}$, and $c_3 = \frac{2\kappa-\boldsymbol{\rho}c}{\|\boldsymbol{v}^2-c\|_w^2}$. $\boldsymbol{\rho}$, $\mathbf{J}$ and $\boldsymbol{\kappa}$ are macroscopic charge, current and kinetic energy densities.



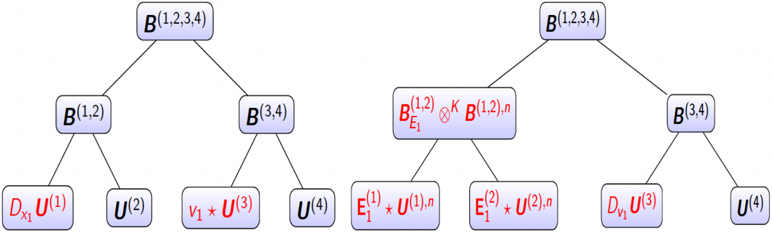
Bump-on-tail instabilities. The time evolution of relative deviation of total momentum and total energy from the energy conserving method. Mesh $N_x \times N_v = 128 \times 256$. $\varepsilon = 10^{-4}$.

Hierarchical Tucker (HT) approximations

High dimensional Vlasov solutions with explicit time stepping with high order discretizations

$$f_t + v_1 f_{x_1} + v_2 f_{x_2} + E_1 f_{v_1} + E_2 f_{v_2} = 0.$$

- Adding basis:



- Removing basis: hierarchical high order SVD, cost $\mathcal{O}\left(dNr^2 + (d-2)r^4\right)$.
- LoMaC projections for preservation of macroscopic conservation laws.

Linear advection equation

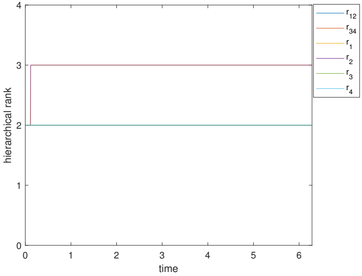
$$u_t + \sum_{m=1}^{d} u_{x_i} = 0, \quad \mathbf{x} \in [-\pi, \pi]^d$$

with periodic conditions and a smooth initial condition with $d = 4$

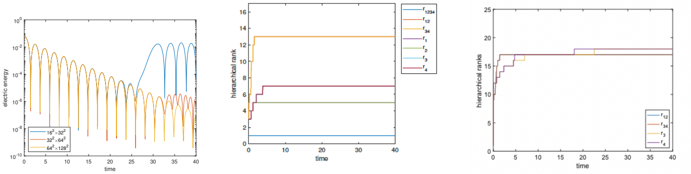
$$u(\mathbf{x}, t = 0) = \exp\left(-2(x_1^2 + x_2^2)\right)\sin(x_3 + x_4), \tag{4}$$

$T = 2\pi$, $\varepsilon = 10^{-6}$. CPU time is 4.2s, 7.8s, 14.2, 30.1s, 65.3s, respectively.

N	L^2 error	order
16	2.56E-02	
32	5.76E-03	2.15
64	1.41E-03	2.04
128	3.52E-04	2.00
256	8.09E-05	2.12



Nonlinear Vlasov-Poisson: weak Landau damping

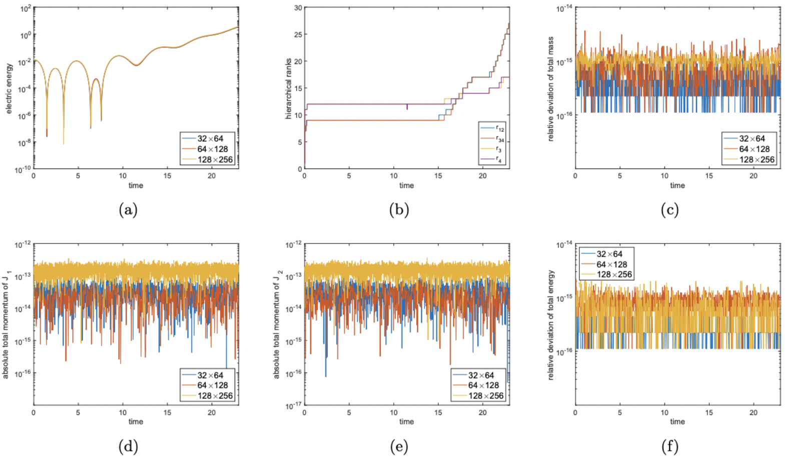


(a) (b) (c)

Weak Landau damping 2D2V. Truncation threshold in SVD is $\epsilon = 1.e-6$. $N_x \times N_v = 16^2 \times 32^2$, $32^2 \times 64^2$ and $64^2 \times 128^2$. The time evolution of the electric energy (left), the rank of non-LoMaC vs. LoMaC low rank tensor method for $64^2 \times 128^2$ (middle and left).

CPU time is $76s$, $117s$, and $265s$ for three sets of the mesh respectively for low rank scheme wo/ conservation. CPU time is $377s$, $670s$, and $1177s$ for the scheme with LoMaC property.

LoMaC low rank method for 2D2V two stream instability. $\varepsilon = 10^{-5}$.



Two stream instability 2D2V. LoMaC low-rank tensor method.

Summary

- Low rank tensor representation of high dimensional kinetic solutions.
- LoMaC projection: ensures consistency between model hierarchy and preservation of conservation laws.

Ongoing work: method-of-lines implicit and implicit-explicit methods

1. Prediction and correction of basis functions in each dimension (w/J. Nakao and L. Einkemmer, Poster)
2. Extended Krylov subspaces and residual evaluations (w/ H. Kahza, L. Chacon and W. Taitano)

Future pursuits: tensor approach for multi-scale kinetic models in CHaRMNET.

- Software development of tensor simulations of high dimensional PDE solutions.
- Hardware acceleration of tensor PDE computations.

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