A structure preserving, conservative, low-rank tensor scheme for solving the 1D2V Vlasov-Fokker-Planck equation

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Kinetic models to describe plasmas

Why should we care?

- Plasmas compose 99% of visible matter in the universe.
- Space plasmas (space weather, astrophysical systems, solar physics), laboratory fusion plasmas (magnetic confinement, inertial confinement), electric propulsion systems, etc...
- Designing next-generation high-powered systems.
- Experimental iterations are expensive and time consuming.
- Numerical simulations can accelerate the design iteration procedure.

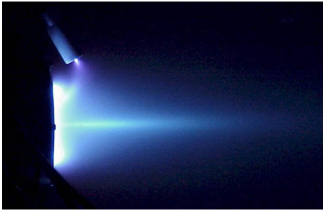


Figure: AFRL Hall effect thruster, taken from AFRL website.

Kinetic models to describe plasmas

- Plasma is a gas containing ionized atoms and/or free electrons.
- Hybrid fluid electron – kinetic ion model.
- Single ion species α.
- Distribution function $f_\alpha(\mathbf{x}, \mathbf{v}; t)$, $\mathbf{x} \in \mathbb{R}^3$, $\mathbf{v} \in \mathbb{R}^3$, $t \in \mathbb{R}_+$.

Algorithmic challenges:

- High-dimensional simulations (e.g., 3D3V) are expensive in computation and storage
- Respect the physics: conservation, positivity preservation, equilibrium preservation, relative entropy dissipation, etc...

Tensor decompositions and the CP format

A tensor $\mathscr{X}$ can be thought of as a multi-index array, e.g., $\mathscr{X}_{i,j,k} \approx f(x_i, y_j, z_k)$.

$$\text{(CP format)} \qquad \mathscr{X} \approx \sum_{r=1}^{R} \mathbf{a}_r^{(1)} \circ \ldots \circ \mathbf{a}_r^{(d)} \equiv \sum_{r=1}^{R} \left(\bigotimes_{n=1}^{d} \mathbf{a}_r^{(n)} \right)$$

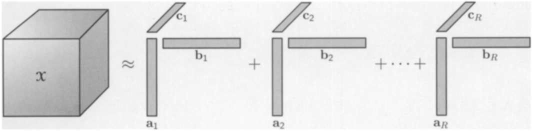
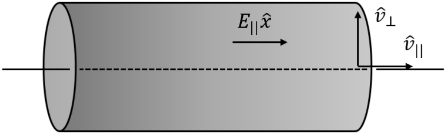


Fig. 3.1 *CP decomposition of a three-way array.*

(Kolda and Bader [5], pp. 463)

- Discretize each dimension with N grid points.
- Store $\{\mathbf{a}_r^{(n)} \in \mathbb{R}^N : r = 1, \ldots, R\}$ in frames $\mathbf{A}^{(n)} \in \mathbb{R}^{N \times R}$ for $n = 1, \ldots, d$.
- Storage complexity is dRN; much less than N^d if naturally low rank.

The 1D2V Vlasov-Leonard-Bernstein-Fokker-Planck equation



$$\frac{\partial f_\alpha}{\partial t} + v_{||}\frac{\partial f_\alpha}{\partial x} + \frac{q_\alpha}{m_\alpha}E_{||}\frac{\partial f_\alpha}{\partial v_{||}} = C_{\alpha\alpha} + C_{\alpha e}, \tag{1a}$$

$$C_{\alpha\alpha} = \nu_{\alpha\alpha}\nabla_{\mathbf{v}} \cdot \left(\frac{T_\alpha}{m_\alpha}\nabla_{\mathbf{v}} f_\alpha + (\mathbf{v} - \mathbf{u}_\alpha) f_\alpha\right), \tag{1b}$$

$$C_{\alpha e} = \nu_{\alpha e}\nabla_{\mathbf{v}} \cdot \left(\frac{T_e}{m_\alpha}\nabla_{\mathbf{v}} f_\alpha + (\mathbf{v} - \mathbf{u}_e) f_\alpha\right), \tag{1c}$$

where f_α is the distribution function for the single ion species α, and the charge, mass, temperature, drift velocity, and collision frequencies for the ion species and electron are respectively denoted by q, m, T, $\mathbf{u}$, and ν.

The fluid electron model

Assumptions: Quasi-neutrality ($n_\alpha = n_e$), ambipolarity ($\mathbf{u}_\alpha = \mathbf{u}_e$), and Ohm's law ($E_{||} = \frac{1}{q_e n_e}\frac{\partial p_e}{\partial x}$).

$$\frac{3}{2}\frac{\partial p_e}{\partial t} + \frac{5}{2}\frac{\partial}{\partial x}\left(u_{e,||}p_e\right) - u_{e,||}\frac{\partial p_e}{\partial x} - \frac{\partial}{\partial x}\left(\kappa_{e,||}\frac{\partial T_e}{\partial x}\right) = W_{e\alpha}, \tag{2a}$$

$$W_{e\alpha} = -\left\langle \frac{m_\alpha |\mathbf{v}|^2}{2}, C_{\alpha e}\right\rangle = 3\nu_{\alpha e} n_\alpha \left(T_\alpha - T_e\right), \tag{2b}$$

where $p_e = n_e T_e$ is the electron pressure, $\kappa_{e,||}$ is the thermal conductivity, and the velocity space L^2 inner product is defined as

$$\langle F(\mathbf{v}), G(\mathbf{v})\rangle \doteq 2\pi \int_{-\infty}^{\infty}\int_0^{\infty} F(\mathbf{v})G(\mathbf{v}) v_\perp dv_\perp dv_{||}. \tag{3}$$

Goal: Solve the nonlinear coupled system for $f_\alpha(x, v_\perp, v_{||}, t)$.

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The semi-discrete kinetic model

Full rank in space and low rank in velocity.

Letting $[a, b]$ be the spatial domain in x, we assume a uniform grid

$$a = x_1 < x_2 < ... < x_{N_x} = b,$$

where $\Delta x = x_{i+1} - x_i$, for all $i = 1, 2, ..., N_x - 1$.

First-order implicit-explicit (IMEX) scheme,

$$f_{\alpha,i}^{k+1} - \Delta t C_{\alpha\alpha,i}^{k+1} - \Delta t C_{\alpha e,i}^{k+1} + \frac{q_\alpha}{m_\alpha} \Delta t E_{||,i}^{k+1} \frac{\partial f_{\alpha,i}^{k+1}}{\partial v_{||}} = f_{\alpha,i}^{k} - v_{||} \frac{\Delta t}{\Delta x} \left(\hat{f}_{\alpha,i+\frac{1}{2}}^{k} - \hat{f}_{\alpha,i-\frac{1}{2}}^{k} \right), \tag{4}$$

where k is the time step index, $\hat{f}_{\alpha,i+\frac{1}{2}}^{k}$ are the numerical fluxes at the cell boundaries, and the collision operators are dependent on n_i^{k+1}, $u_{||,i}^{k+1}$, $T_{\alpha,i}^{k+1}$, $T_{e,i}^{k+1}$.

Outline of the scheme

$$f_{\alpha,i}^{k+1} - \Delta t C_{\alpha\alpha,i}^{k+1} - \Delta t C_{\alpha e,i}^{k+1} + \frac{q_\alpha}{m_\alpha} \Delta t E_{||,i}^{k+1} \frac{\partial f_{\alpha,i}^{k+1}}{\partial v_{||}} = f_{\alpha,i}^{k} - v_{||} \frac{\Delta t}{\Delta x} \left(\hat{f}_{\alpha,i+\frac{1}{2}}^{k} - \hat{f}_{\alpha,i-\frac{1}{2}}^{k} \right)$$

1. Solve for n_i^{k+1}, $u_{||,i}^{k+1}$, $T_{\alpha,i}^{k+1}$, $T_{e,i}^{k+1}$ for LHS.
2. Discretize $C_{\alpha\alpha,i}^{k+1}$ and $C_{\alpha e,i}^{k+1}$ using the robust structure preserving Chang-Cooper (SPCC) method [7].
3. Discretize in velocity space, $\mathbf{f}_{\alpha,i}^{k+1,\star} \in \mathbb{R}^{N_{||} \times N_{\perp}}$, in tensorized CP format.
4. Solve the linear system of tensor product structure for $\mathbf{f}_{\alpha,i}^{k+1,\star}$.
5. Perform a conservative truncation for the low rank solution $\mathbf{f}_{\alpha,i}^{k+1}$.

Outline of the scheme

$$f_{\alpha,i}^{k+1} - \Delta t C_{\alpha\alpha,i}^{k+1} - \Delta t C_{\alpha e,i}^{k+1} + \frac{q_\alpha}{m_\alpha} \Delta t E_{||,i}^{k+1} \frac{\partial f_{\alpha,i}^{k+1}}{\partial v_{||}} = f_{\alpha,i}^{k} - v_{||} \frac{\Delta t}{\Delta x} \left(\hat{f}_{\alpha,i+\frac{1}{2}}^{k} - \hat{f}_{\alpha,i-\frac{1}{2}}^{k} \right)$$

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Step 1. Zeroth, first, and second order moments of the semi-discrete kinetic ion model + semi-discrete fluid electron model. Use a quasi-Newton solver.

Step 2. Proven positivity preserving, equilibrium preserving, and relative entropy dissipative for the full rank solution.

Step 3. CP format in 2V cylindrical coordinates

Letting $[c_{||}, d_{||}]$ and $[c_\perp, d_\perp]$ be the domains for the cylindrical velocity coordinates, we assume uniform grids

$$c_{||} = v_{||,1} < v_{||,2} < \ldots < v_{||,N_{||}} = d_{||}, \tag{5a}$$

$$c_\perp = v_{\perp,1} < v_{\perp,2} < \ldots < v_{\perp,N_\perp} = d_\perp, \tag{5b}$$

where $\Delta v_{||} = v_{||,j_1+1} - v_{||,j_1}$ and $\Delta v_\perp = v_{\perp,j_2+1} - v_{\perp,j_2}$, for all j_1, j_2.

For each spatial node x_i and time t^k,

$$\mathbf{f}^{k,\star}_{\alpha,i} = \sum_{r=1}^{R_i^k} c^k_{i,r} \mathbf{U}^{(1),k}_{i,r} \otimes \mathbf{U}^{(2),k}_{i,r}. \tag{6}$$

$$\Updownarrow$$

$$\mathbf{f}^{k,\star}_{\alpha,i} = \sum_{r=1}^{R_i^k} \left(\mathrm{sgn}(c^k_{i,r}) \sqrt{|c^k_{i,r}|} \mathbf{1}_{v_{||}} * \mathbf{U}^{(1),k}_{i,r} \right) \otimes \left(\sqrt{|c^k_{i,r}|} \mathbf{1}_{v_\perp} * \mathbf{U}^{(2),k}_{i,r} \right). \tag{7}$$

The fully discrete kinetic formulation

$$f_{\alpha,i}^{k+1} - \Delta t C_{\alpha\alpha,i}^{k+1} - \Delta t C_{\alpha e,i}^{k+1} + \frac{q_\alpha}{m_\alpha} \Delta t E_{||,i}^{k+1} \frac{\partial f_{\alpha,i}^{k+1}}{\partial v_{||}} = f_{\alpha,i}^{k} - v_{||} \frac{\Delta t}{\Delta x} \left(\hat{f}_{\alpha,i+\frac{1}{2}}^{k} - \hat{f}_{\alpha,i-\frac{1}{2}}^{k} \right)$$

$$\mathbf{f}_{\alpha,i}^{k,\star} = \sum_{r=1}^{R_i^k} c_{i,r}^k \mathbf{U}_{i,r}^{(1),k} \otimes \mathbf{U}_{i,r}^{(2),k}$$

$$(\mathbf{A}_{1,i} \otimes \mathbf{I}_{N_\perp \times N_\perp} + \mathbf{I}_{N_{||} \times N_{||}} \otimes \mathbf{A}_{2,i}) \text{vec} \left(\mathbf{f}_{\alpha,i}^{k+1,\star} \right) = \mathbf{b}_i \tag{8}$$

Solve to get $\mathbf{f}_{\alpha,i}^{k+1,\star}$.

Step 4. An implicit solver for linear systems of tensor product structure by Grasedyck [2]

The general solution to

$$(A_1 \otimes I + I \otimes A_2)x = \sum_{k=1}^{m} b_1^k \otimes b_2^k \tag{9}$$

can be approximated by

$$x \approx -\sum_{k=1}^{m} \left(\sum_{j=-K}^{K} \frac{2w_j}{\lambda_{min}} \bigotimes_{i=1}^{2} \left(\exp\left(\frac{2t_j}{\lambda_{min}} A_i \right) b_i^k \right) \right), \tag{10}$$

where (t_j, w_j) are the Stenger nodes and weights, $\lambda_{min} = \min(\Lambda(A_1 \otimes I + I \otimes A_2))$.

- Extends Stenger quadrature for scalar exponentials to matrix exponential.
- Rank is $m(2K+1)$.

Step 5. A Local Macroscopic Conservative (LoMaC) low rank tensor method [3]

Motivation: SVD destroys the conservation.

Idea: Define the subspace that preserves the zeroth, first, and second order moments,

$$\mathcal{N} \doteq \mathrm{span}\{1, v_{||}, v_{||}^2 + v_{\perp}^2\}. \tag{11}$$

$$\mathbf{f}^{\star} = \mathbf{f}^{(M)} + \mathbf{f}^{(2),\star} \tag{12}$$

$\mathbf{f}^{(M)}$ carries all the mass, momentum, and energy.
$\mathbf{f}^{(2),\star}$ carries zero mass, momentum, and energy.
Truncate $\mathbf{f}^{(2),\star}$ using an SVD-type truncation algorithm [4].

Weighted inner product space for projection

Consider the weighted L^2 inner products

$$\langle F(\mathbf{v}), G(\mathbf{v})\rangle_w \doteq \int_{-\infty}^{\infty}\int_0^{\infty} F(\mathbf{v})G(\mathbf{v})w(\mathbf{v})v_\perp dv_\perp dv_{||}, \tag{13a}$$

$$\langle F(v_{||}), G(v_{||})\rangle_{w_1} \doteq \int_{-\infty}^{\infty} F(v_{||})G(v_{||})w_1(v_{||})dv_{||}, \tag{13b}$$

$$\langle F(v_\perp), G(v_\perp)\rangle_{w_2} \doteq \int_0^{\infty} F(v_\perp)G(v_\perp)w_2(v_\perp)v_\perp dv_\perp, \tag{13c}$$

where the weight functions are defined as

$$w(\mathbf{v}) = w_1(v_{||})w_2(v_\perp), \tag{14a}$$

$$w_1(v_{||}) = \frac{\exp(-v_{||}^2)v_{||}^2}{2}, \tag{14b}$$

$$w_2(v_\perp) = \exp(-v_\perp^2)v_\perp. \tag{14c}$$

Discrete orthonormal basis

Discrete tensor-product orthonormal basis for $\mathcal{N}$, $\{\mathbf{V}_1, \mathbf{V}_2, \mathbf{V}_3\}$ given by

$$\left\{ \mathbf{V}_1 = \mathbf{X}_1^{(1)} \otimes \mathbf{X}_1^{(2)}, \mathbf{V}_2 = \mathbf{X}_2^{(1)} \otimes \mathbf{X}_1^{(2)}, \mathbf{V}_3 = \frac{\left(\mathbf{X}_3^{(1)} \otimes \mathbf{X}_1^{(2)} + \mathbf{X}_1^{(1)} \otimes \mathbf{X}_2^{(2)} \right)}{\sqrt{2}} \right\}, \tag{15}$$

where

$$\left\{ \mathbf{X}_1^{(1)} = \frac{\mathbf{1}_{v_{||}}}{\left\| \mathbf{1}_{v_{||}} \right\|_{w_1}}, \quad \mathbf{X}_2^{(1)} = \frac{\mathbf{v}_{||}}{\left\| \mathbf{v}_{||} \right\|_{w_1}}, \quad \mathbf{X}_3^{(1)} = \frac{\mathbf{v}_{||}^2 - c_1 \mathbf{1}_{v_{||}}}{\left\| \mathbf{v}_{||}^2 - c_1 \mathbf{1}_{v_{||}} \right\|_{w_1}} \right\}, \tag{16a}$$

$$\left\{ \mathbf{X}_1^{(2)} = \frac{\mathbf{1}_{v_\perp}}{\left\| \mathbf{1}_{v_\perp} \right\|_{w_2}}, \quad \mathbf{X}_2^{(2)} = \frac{\mathbf{v}_\perp^2 - c_2 \mathbf{1}_{v_\perp}}{\left\| \mathbf{v}_\perp^2 - c_2 \mathbf{1}_{v_\perp} \right\|_{w_2}} \right\} \tag{16b}$$

are orthonormal bases with respect to the inner products $\langle \cdot, \cdot \rangle_{w_1}$ and $\langle \cdot, \cdot \rangle_{w_2}$, respectively.

Projecting the solution

Given the weights we defined, $c_1 = c_2$ and $\left\| v_{||}^2 - c_1 \right\|_{w_1} = \left\| v_{\perp}^2 - c_2 \right\|_{w_2} \doteq \gamma$.

$$\begin{aligned} \mathbf{f}^{(M)} \doteq \frac{1}{2\pi} \Bigg(& \frac{n}{\|1\|_w} \mathbf{X}_1^{(1)} \otimes \mathbf{X}_1^{(2)} + \frac{n u_{||}}{\left\| v_{||} \right\|_w} \mathbf{X}_2^{(1)} \otimes \mathbf{X}_1^{(2)} \\ & + \frac{(2(nU) - (c_1 + c_2) n)}{2\gamma} \left(\mathbf{X}_3^{(1)} \otimes \mathbf{X}_1^{(2)} + \mathbf{X}_1^{(1)} \otimes \mathbf{X}_2^{(2)} \right) \Bigg), \end{aligned} \tag{17}$$

where n, $nu_{||}$, and nU are the ion mass, momentum, and energy.

$$\boxed{\mathbf{f} = \mathbf{f}^{(M)} + (I - P_{\mathcal{N}}) \left(T_\epsilon \left((I - P_{\mathcal{N}})(\mathbf{f}^\star) \right) \right) \qquad (18)}$$

Outline of the scheme

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Standing shock problem

Simulation of a Mach-5 steady-state shock.

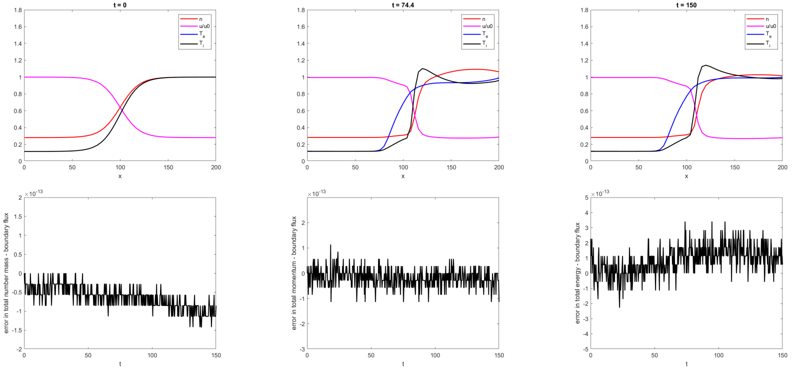

Figure: Top row (a,b,c): evolution of the number density, drift velocity, ion temperature, and electron temperature. Bottom row (d,e,f): conservation of mass, momentum, and energy. Spatial mesh $N_x = 51$. Velocity domain $[0, 8] \times [-8, 10]$ with mesh $N_{v_\perp} = 121$, $N_{v_{||}} = 121$. Stenger quadrature $K = 15$. Singular value tolerance $\epsilon = 1.0e - 05$. Time-stepping size $\Delta t = 0.3$.

cont...

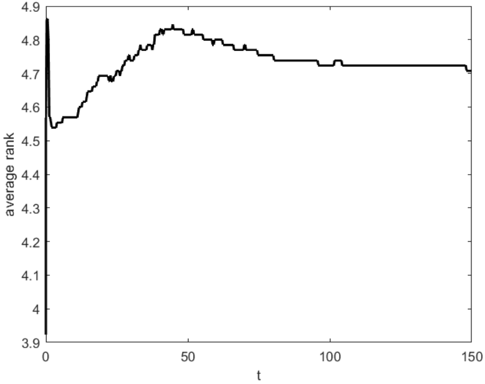

Figure: Average rank $\frac{1}{N_x}\sum_{i=1}^{N_x} J_i^k$, where $J_i^k < R_i^k$.

Single ion species relaxation

$$\frac{\partial f_\alpha}{\partial t} = \nu_{\alpha\alpha} \nabla_{\mathbf{v}} \cdot \left(\frac{T_\alpha}{m_\alpha} \nabla_{\mathbf{v}} f_\alpha + (\mathbf{v} - \mathbf{u}_\alpha) f_\alpha \right) \tag{19}$$

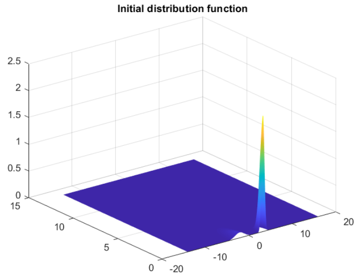

Figure: Velocity domain $[0, 14] \times [-14, 16]$ with mesh $N_{v_\perp} = 301$, $N_{v_{||}} = 301$. Stenger quadrature $K = 150$. Singular value tolerance $\epsilon = 1.0e - 05$. Time-stepping size $\Delta t = 0.3$.

cont...

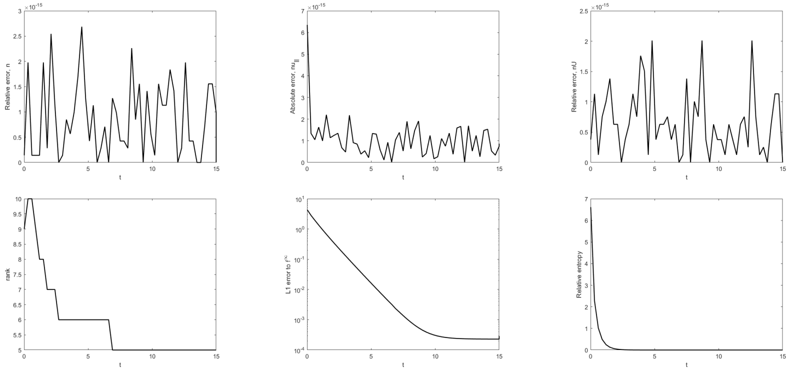

Figure: Top row (a,b,c): conservation of mass, momentum, and energy. Bottom row (d,e,f): rank, L^1 decay, relative entropy dissipation.

Convergence study with mesh refinement

$$\frac{\partial f_\alpha}{\partial t} = \nu_{\alpha\alpha} \nabla_{\mathbf{v}} \cdot \left(\frac{T_\alpha}{m_\alpha} \nabla_{\mathbf{v}} f_\alpha + (\mathbf{v} - \mathbf{u}_\alpha) f_\alpha \right) \tag{20}$$

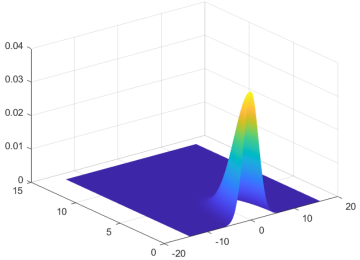

Table: Time-stepping with backward Euler.

Strang splitting		
$N_{\|\|} = N_\perp$	L^1 Error	Order
41	1.17E-02	-
81	2.99E-03	1.97
161	8.19E-04	1.87
321	1.77E-04	2.21

Figure: Velocity domain $[0, 14] \times [-14, 16]$. Stenger quadrature $K = 150$. Singular value tolerance $\epsilon = 1.0e-05$. Time-stepping size $\Delta t = 0.3$. Final time $T_f = 1$.

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What's next?

Take-home messages: conservative truncation in cylindrical coordinates, low rank tensor scheme for kinetic models.

- Model two or more ion species.
- Modify algorithm to avoid Grasedyck's method.
  - Matrix exponentials make up nearly 90% of run time.
  - Several quadrature nodes are required ($\sim$100 nodes for three digits of accuracy).
  - But, highly parallelizable.
  - Switching to a preconditioned tensorized Krylov method [6].
  - Dynamical low rank algorithm similar to [1].
- Extend to 2D2V.

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Thank you.

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