Effects of artificial collisions, filtering, and nonlocal closure approaches on collisionless kinetic simulations[1]

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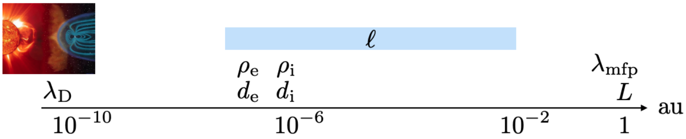
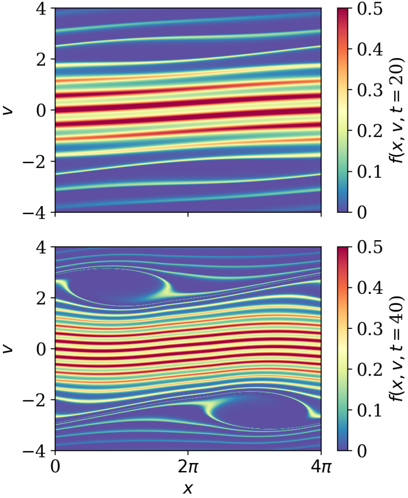
Computational challenges in collisionless kinetic simulations

- **High-dimensional 3D3V**: Discretizing each direction in phase space via 10^3 grid points results in 10^{18} degrees of freedom $\Rightarrow$ **8 exabytes of memory in double precision for each timestep**. Frontier supercomputer has 0.0092 exabytes of memory.

- **Rich geometric structure**: Infinitely many invariants (*Casimirs*) and non-canonical Poisson bracket of the Hamiltonian system $\Rightarrow$ filamentation and echos.

- **Large spatial and temporal scale separation**: Solar corona Debye length $\lambda_D \approx 10$m, whereas the system length scale is $L \approx 10^{11}$m.





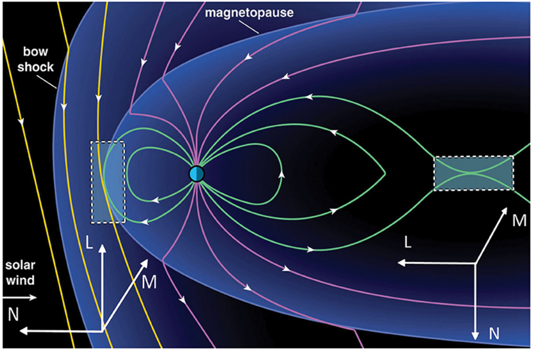
Earth's magnetosphere global modeling requires kinetic physics

Global magnetospheric models either lack kinetic physics or incorporate it in an *ad hoc* manner. Kinetic physics is essential for

- **Magnetic reconnection** in the magnetopause and in the magnetotail
- **Foreshock dynamics** driven by ions reflected back upstream, which generate beam instabilities
- **Gyroresonant wave-particle interaction** in the radiation belt leading to whistler-mode pitch angle scattering

There is a need to account for **kinetic physics (non-Maxwellian distributions) in global simulations**!

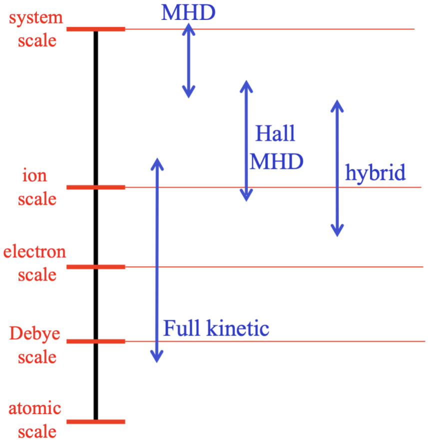
⇒ **GEM 2022 Dayside Kinetic Challenge**



Credit: [Burch et al., 2016].

Beyond MHD approaches and challenges

1. **Hybrid models**
   [von Alfthan et al., 2014]
   - Kinetic ion + fluid electron
   - Neglect electron kinetic physics
2. **Embedded PIC in MHD models**
   [Walker et al., 2019, Makwana et al., 2018]
   - Sharp interface
3. **Spectral Methods ⇒ focus of this talk!**
   [Grad, 1949, Schumer and Holloway, 1998, Delzanno, 2015, Koshkarov et al., 2021]
   - Adapt spectral terms in space and time
   - Smooth transition from fluid to kinetic region



$N_v = 3$ $\qquad$ $N_v \to \infty$

MHD $\qquad$ Hermite Solver $\qquad$ Fully Kinetic

Let us start simple $\Rightarrow$ 1D1V Vlasov-Poisson equations

1D1V quasi-neutral collisionless plasma composed of electrons and immobile background ions:

$$\left(\frac{\partial}{\partial t} + v\frac{\partial}{\partial x} + \frac{\partial \phi(x,t)}{\partial x}\frac{\partial}{\partial v}\right) f(x,v,t) = 0$$

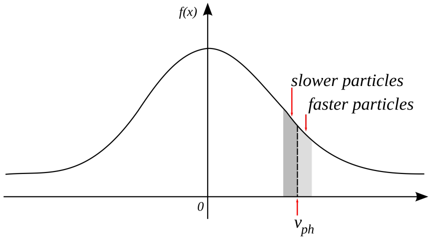
$$-\frac{\partial^2 \phi(x,t)}{\partial x^2} = 1 - \int f(x,v,t)\mathrm{d}v$$

All quantities above are normalized as follows:

$$t := t_d \omega_{pe} \qquad x := \frac{x_d}{\lambda_D} \qquad v := \frac{v_d}{v_{te}}$$

$$f := f_d \frac{v_{te}}{n_e} \qquad \phi := \phi_d \frac{e\lambda_D^2}{T_e}$$

$\omega_{pe} := \sqrt{4\pi e^2 n_e / m_e} \Rightarrow$ electron plasma frequency
$\lambda_D := \sqrt{T_e / 4\pi e^2 n_e} \Rightarrow$ electron Debye length
$v_{te} := \sqrt{T_e / m_e} \Rightarrow$ electron thermal velocity



Landau damping schematic [Landau, 1946] $\Rightarrow$ *socialist redistribution!*

Boundary conditions

$$f(x=0,v,t) = f(x=\ell,v,t)$$

$$\lim_{v\to\pm\infty} f(x,v,t) = 0$$

Linear electrostatic theory

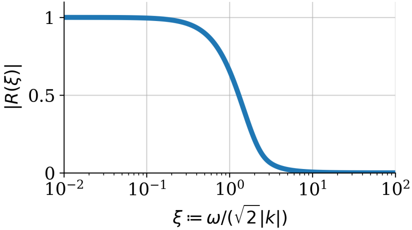
$$f(x,v,t) = f_0(v) + \tilde{f}(x,v,t) \quad \text{s.t.} \quad \tilde{f} \ll f_0 \quad \tilde{f}(x,v,t) = \exp(-i\omega t + ikx)\hat{f}(v)$$

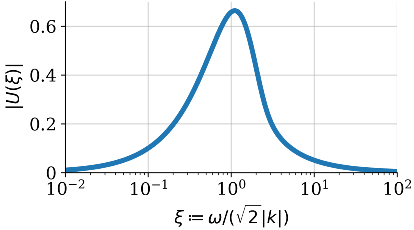
$$\phi(x,t) = \phi_0(x) + \tilde{\phi}(x,t) \quad \text{s.t.} \quad \phi_0(x) = 0 \quad \tilde{\phi}(x,t) = \exp(-i\omega t + ikx)\hat{\phi}$$

For a Maxwellian equilibrium $f_0(v) = \exp\left(-v^2/2\right)/\sqrt{2\pi}$:

$$\hat{n} := \int \hat{f}(v)\mathrm{d}v = k\hat{\phi}\int \frac{\mathrm{d}f_0/\mathrm{d}v}{\omega - kv}\mathrm{d}v = \hat{\phi}R(\xi) \quad \text{s.t.} \quad R(\xi) := 1+\xi Z(\xi) \quad \text{and} \quad \xi := \frac{\omega}{\sqrt{2}|k|}$$

where $Z(\xi)$ is the plasma dispersion function [Fried and Conte, 1961].
The velocity response function is $U(\xi) := \hat{u}/\hat{\phi} = -\text{sign}(k)\xi R(\xi)$.





The response function captures key microscopic dynamics, such as electrostatic wave-particle resonance.

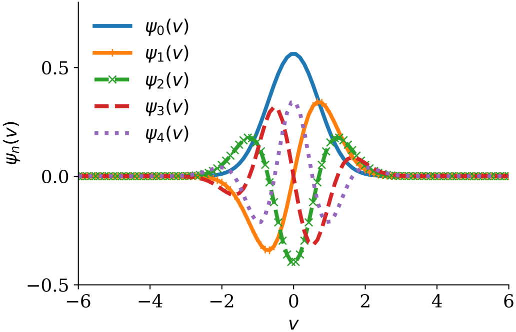
Hermite discretization

$$\hat{f}(v) \approx \sum_{n=0}^{N_v-1} \hat{C}_n \psi_n(v)$$

$$f_0(v) = \frac{1}{\sqrt{2}}\psi_0(v)$$

$$\psi_n(v) := \frac{1}{\sqrt{\pi 2^n n!}} \mathcal{H}_n\left(\frac{v}{\sqrt{2}}\right) \exp\left(-\frac{v^2}{2}\right)$$

$$\mathcal{H}_n(v) := (-1)^n \exp\left(v^2\right) \frac{\mathrm{d}^n}{\mathrm{d}v^n} \exp\left(v^2\right)$$



After Galerkin projection, we get

$$-i\omega \hat{C}_n + \underbrace{ik\left(\sqrt{n+1}\hat{C}_{n+1} + \sqrt{n}\hat{C}_{n-1}\right)}_{\text{advection}} - \underbrace{\frac{ik\hat{\phi}}{\sqrt{2}}\delta_{n,1}}_{\text{acceleration}} = 0 \qquad \text{and impose} \qquad \hat{C}_{N_v} = 0$$

Linear kinetic response function of the discretized system

$$R_3(\xi) = \frac{-1}{2\xi^2 - 3} \qquad R_4(\xi) = \frac{3 - 2\xi^2}{4\xi^4 - 12\xi^2 + 3} \qquad R_5(\xi) = \frac{7 - 2\xi^2}{4\xi^4 - 20\xi^2 + 15}$$

The asymptotic results for $|\xi| \ll 1$:

$$R_3(\xi) = \frac{1}{3} + \frac{2\xi^2}{9} + \dots \qquad R_4(\xi) = \boxed{1} + \frac{10\xi^2}{3} + \dots \qquad R_5(\xi) = \frac{7}{15} + \frac{22\xi^2}{45} + \dots$$

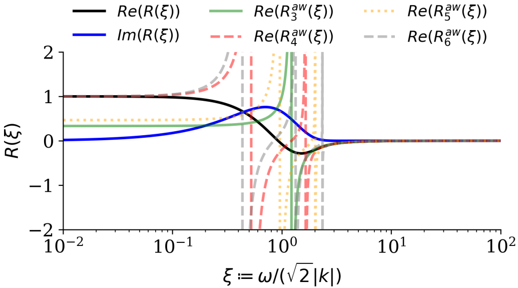
and for $|\xi| \gg 1$:

$$R_3(\xi) = \boxed{-\frac{1}{2\xi^2} - \frac{3}{4\xi^4}} - \frac{9}{8\xi^6} + \dots$$

$$R_4(\xi) = \boxed{-\frac{1}{2\xi^2} - \frac{3}{4\xi^4} - \frac{15}{8\xi^6}} - \frac{81}{16\xi^8} + \dots$$

$$R_5(\xi) = \boxed{-\frac{1}{2\xi^2} - \frac{3}{4\xi^4} - \frac{15}{8\xi^6} - \frac{105}{16\xi^8}} - \frac{825}{32\xi^{10}} + \dots$$

- Fictitious real poles $\Rightarrow$ numerical instability
- Even N_v is more accurate at $\xi \ll 1$



What is filamentation?

Consider the 1D linear Vlasov equation (with periodic

$$\left(\frac{\partial}{\partial t} + v\frac{\partial}{\partial x}\right) f(x,v,t) = 0$$

$$f(x,v,t) = f(x - vt, v, t = 0)$$

Let's set the initial condition to a perturbed Maxwelliian distribution

$$f(x,v,t=0) = \cos(x) f_M(v)$$

Then

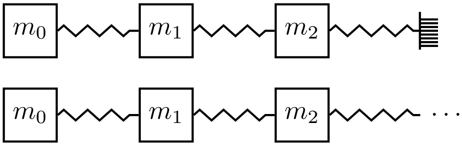
$$\begin{aligned} f(x,v,t) &= \cos(x - vt) f_M(v) \\ &= \underbrace{\left[\cos(x)\cos(vt) + \sin(x)\sin(vt)\right]}_{\text{fine scale in velocity!}} f_M(v) \end{aligned}$$

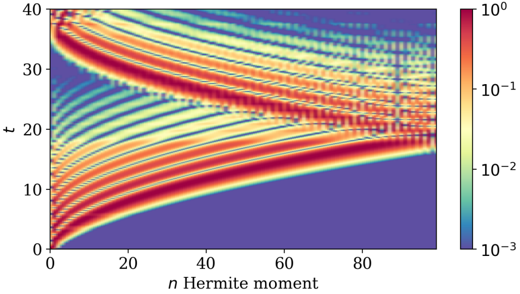
such that as $t \uparrow \Delta v \downarrow$!

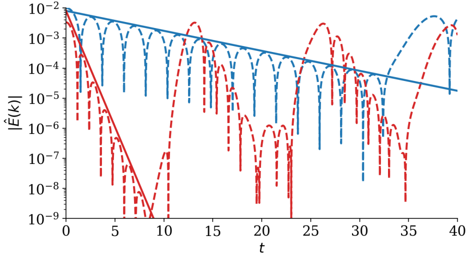
Credit: Vincent Ledvina, also known as *The Aurora Guy*

Filamentation leads to numerical recurrence

- Filamentation ⇒ microstructures in velocity
- In nature, there is a cutoff scale where diffusive scattering effects become important [Pezzi et al., 2019]
  - Slow solar wind $N_v \sim$ 1,800
  - Inter-stellar medium $N_v \sim$ 19,000
- The semi-infinite spring-mass system is analogous to the spectral moment system [Smith, 1997]







Artificial collisions and filtering–they are fundamentally alike!

Artificial collisions [Joyce et al., 1971]

Powers of the [Lenard and Bernstein, 1958] collisional operator:

$$\mathcal{C}_{\text{hyper}}(f) := \nu \mathcal{D}^{2\alpha-1}\tilde{\mathcal{D}}^{2\alpha-1} f \qquad \mathcal{D} := \frac{\partial}{\partial v} \qquad \tilde{\mathcal{D}} := \left(\frac{\partial}{\partial v} + v\right)$$

$$\mathcal{C}_{\text{hyper}}(\hat{C}_n) = -\nu \frac{n!(N_v - 2\alpha)!}{(n-2\alpha+1)!(N_v-1)!}\hat{C}_n$$

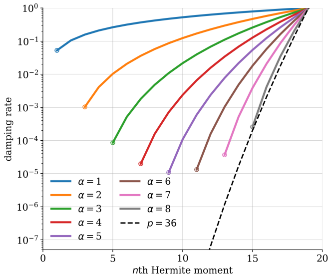
Filtering [Hou and Li, 2007, Cai and Wang, 2018]

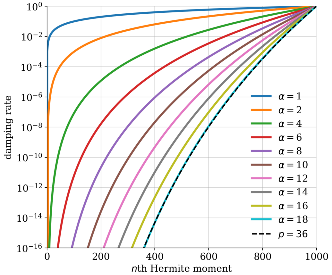
Low-pass exponential filter:

$$\mathcal{C}_{\text{filter}}(f) = \chi \frac{(-1)^{p+1}}{\Delta t (N_v - 1)^p}\hat{\mathcal{D}}^p f$$

$$\hat{\mathcal{D}} f := \frac{\partial}{\partial v}\left[\exp\left(-\frac{v^2}{2}\right)\frac{\partial}{\partial v}\left(\exp\left(\frac{v^2}{2}\right) f\right)\right]$$

$$\mathcal{C}_{\text{filter}}(\hat{C}_n) = -\frac{\chi}{\Delta t}\left(\frac{n}{N_v - 1}\right)^p \hat{C}_n$$





Hermite nonlocal closures

The transformation from fluid to Hermite moments is **nonlinear and invertible**

$$\hat{n} := \int \hat{f}(v)\mathrm{d}v \qquad \hat{n}\hat{u} := \int v\hat{f}(v)\mathrm{d}v \qquad \hat{p} := \int (v-\hat{u})^2\hat{f}(v)\mathrm{d}v \qquad \hat{q} := \int (v-\hat{u})^3\hat{f}(v)\mathrm{d}v$$

$$\hat{n} = \sqrt{2}\hat{C}_0 \qquad \hat{u} = \frac{\hat{C}_1}{\hat{C}_0} \qquad \hat{p} = \sqrt{2}\left(\sqrt{2}\hat{C}_2 + \hat{C}_0 - \frac{\hat{C}_1^2}{\hat{C}_0}\right) \qquad \dots$$

[Hammett and Perkins, 1990] derived a closure for four-dimensional fluid models

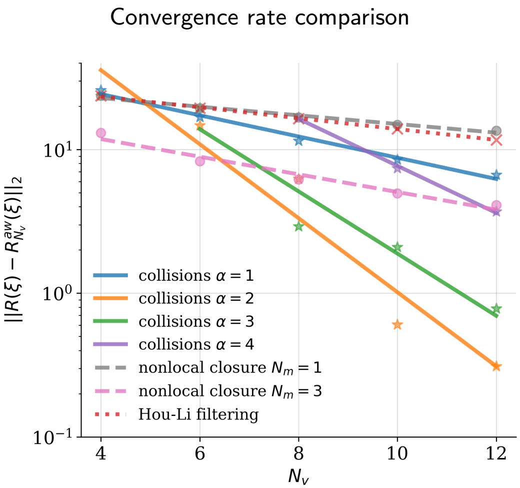
$$\hat{q} = -i\frac{2\sqrt{2}}{\sqrt{\pi}}\frac{k}{|k|}(\hat{p}-\hat{n}) \propto \frac{k}{|k|}\hat{T} \qquad \xRightarrow[\text{real space}]{} \qquad q(x) \propto \int_0^{\ell} \frac{T(x+\tilde{x}) - T(x-\tilde{x})}{\tilde{x}}\mathrm{d}\tilde{x}$$

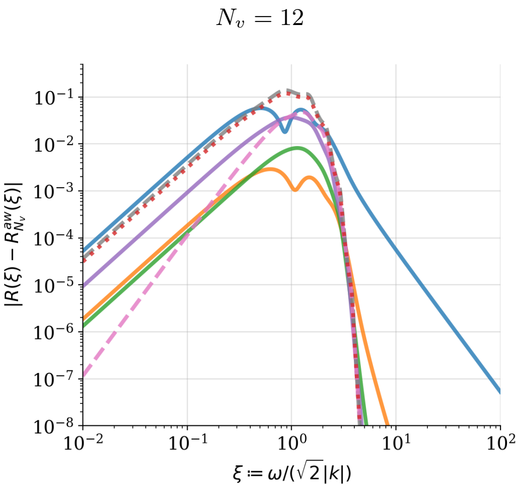
$$\xRightarrow[\text{Hermite space}]{} \qquad \hat{C}_3 = -i\frac{2\sqrt{2}}{\sqrt{3\pi}}\frac{k}{|k|}\hat{C}_2$$

Hermite nonlocal closure [Smith, 1997]

$$\hat{C}_{N_v} = \sum_{n=N_v-N_m}^{N_v-1} i\mu_n \frac{k}{|k|}\hat{C}_n.$$

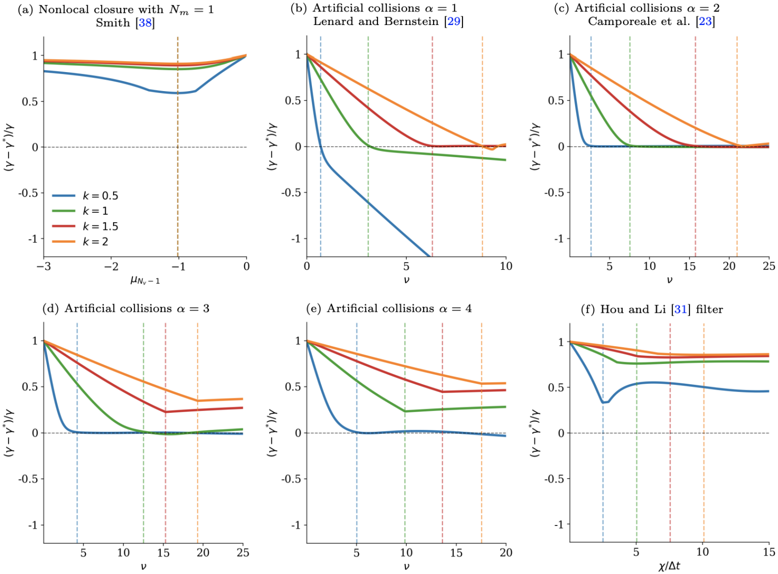
Density response function approximation





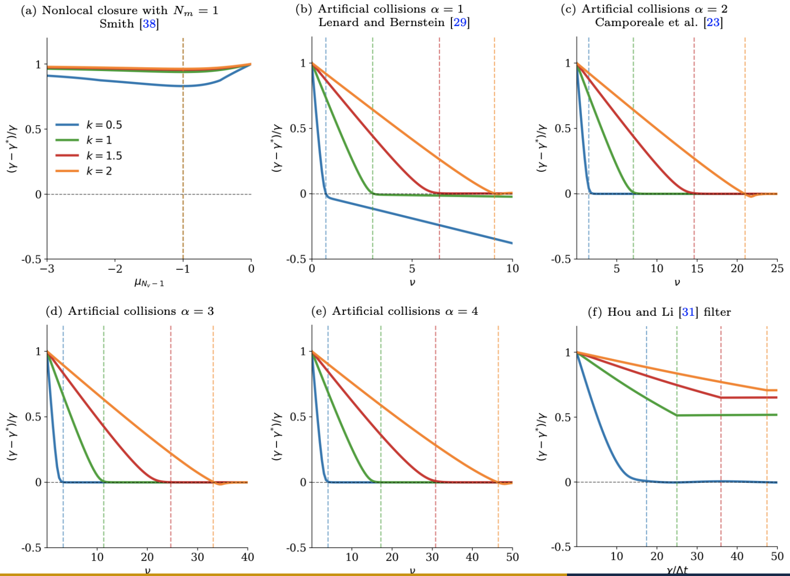
Artificial collisions with $\alpha = 2$ and $\alpha = 3$ provide the highest accuracy and converge the fastest to the analytic response function.

Discrete system eigenvalue analysis $N_v = 20$



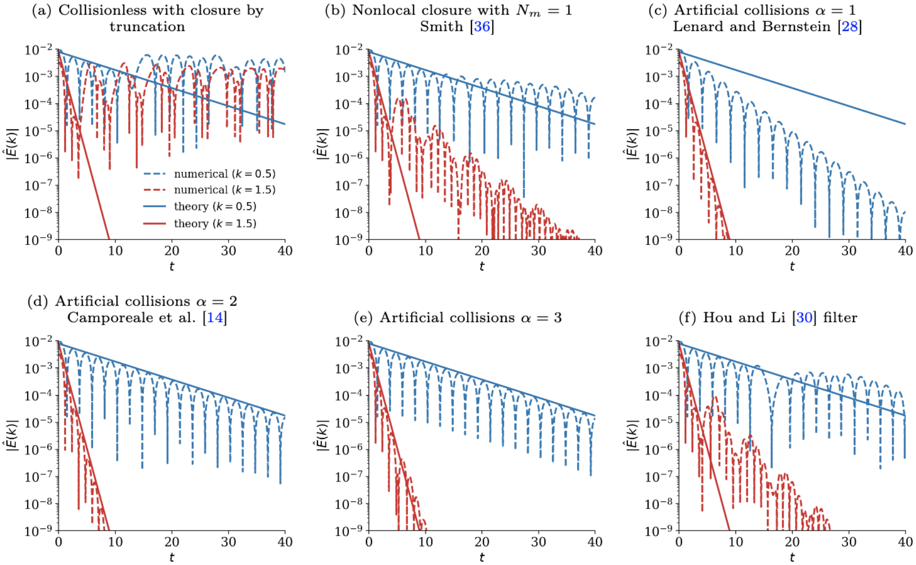
- Nonlocal closure, filtering, and artificial collisions with $\alpha \geq 3$ approaches under-damp higher order wavenumber modes.
- LB collisions overdamp higher order wavenumbers.
- Only artificial collisions with $\alpha = 2$ can recover the Landau root for a range of wavenumbers.

Discrete system eigenvalue analysis $N_v = 100$

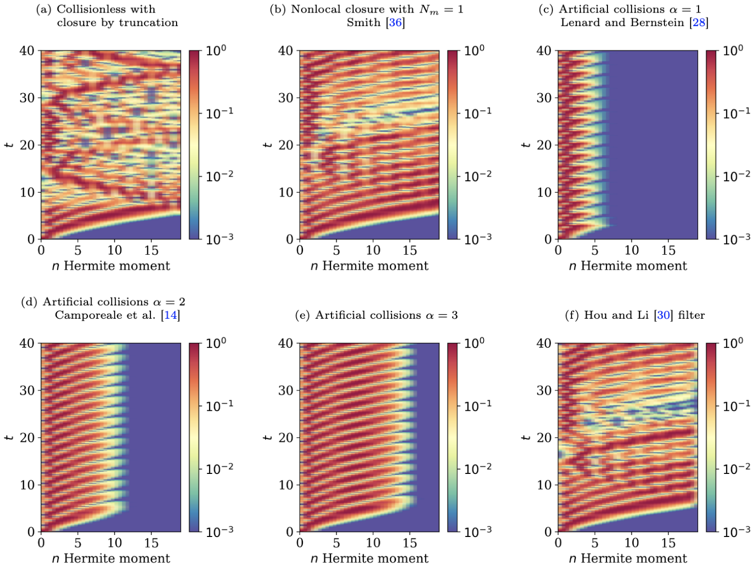


- Nonlocal closure and filtering approaches still under-damp higher order wavenumber modes.
- All artificial collision orders can recover the Landau root for a range of wavenumbers.

Linear Landau damping electric field $N_v = 20$

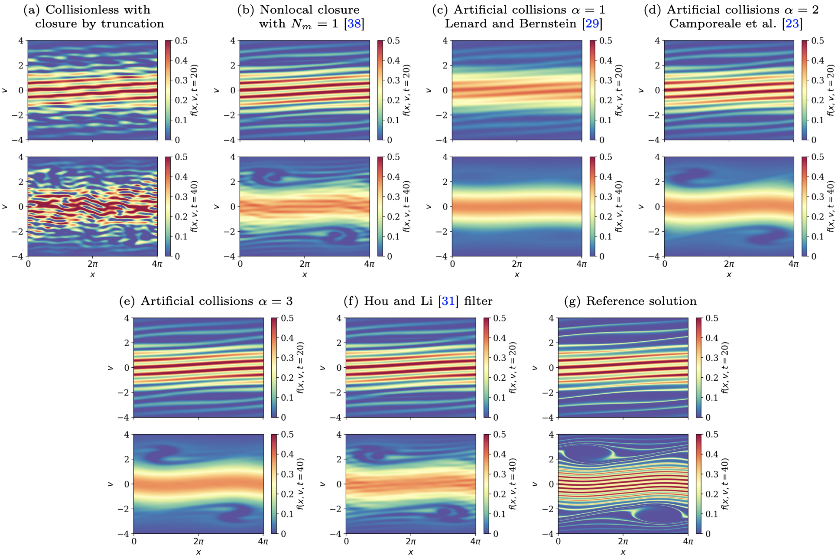


Linear Landau damping Hermite cascade $N_v = 20$



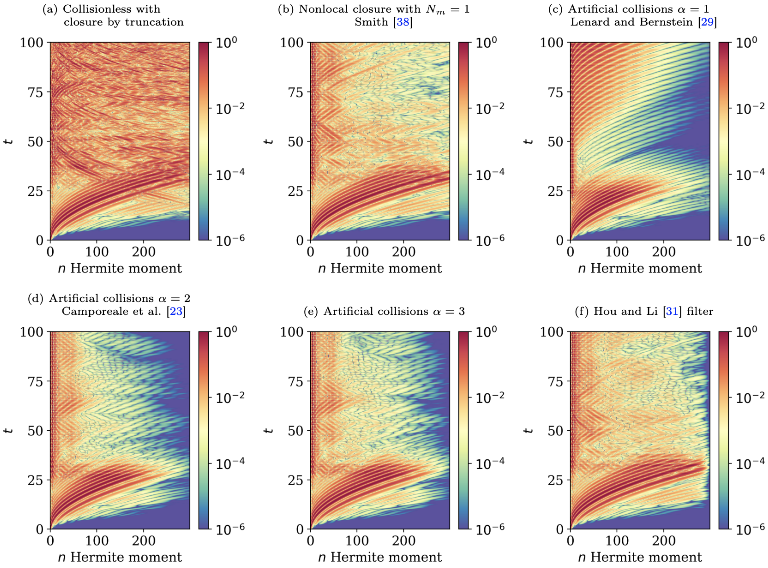
- Only artificial collisions suppress incorrect backward propagating Hermite flux caused by the finite truncation.
- LB collisions severely damp the higher Hermite modes.

Nonlinear Landau damping $N_v = 300$

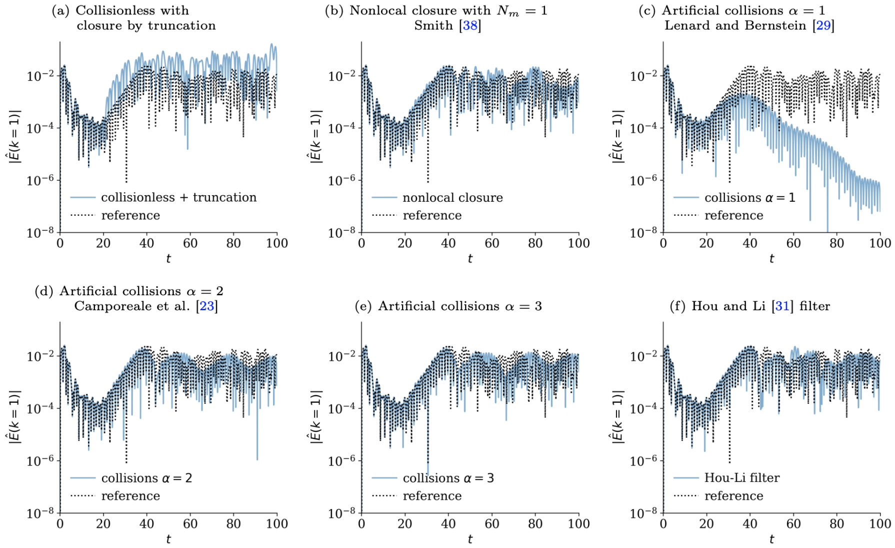


"Blowup of an aliased, non-energy-conserving model is God's way of protecting you from believing a bad simulation." [Boyd, 2001]

Nonlinear Landau damping Hermite cascade $N_v = 300$



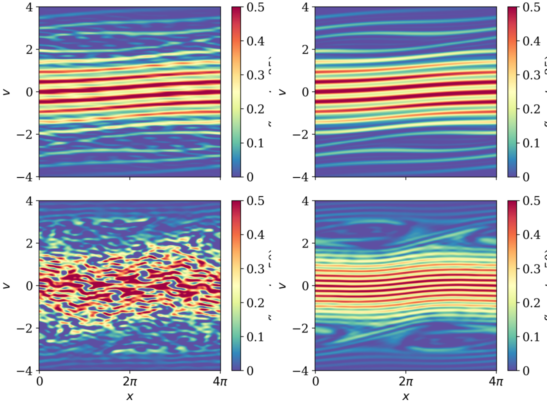
Nonlinear Landau damping electric field $N_v = 300$



Conclusions and future work

- Hypercollisions are a promising approach to mitigate recurrence and filamentation numerical artifacts in limited velocity resolution.
- Filtering and nonlocal closures are also effective in nonlinear simulations, yet underdamp Landau modes in the linear setting.
- LB collisions overdamp the linear and nonlinear evolution [Pezzi et al., 2016].
- **Future work** regarding Hermite closures
  1. What about a general framework for non-Maxwellian distributions, e.g., super-Maxwellian or cutoff Maxwellian [Fan et al., 2022]?
  2. What about incorporating cyclotron resonance effects [Jikei and Amano, 2021]?

  $\Rightarrow$ nonlocal operators in local methods (e.g., finite difference) are very expensive; however, approximations exist [Dimits et al., 2014]



Collisionless & truncation $N_v = 1024$

Artificial collisions $\alpha = 5$ $N_v = 1024$

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