Fast and spectrally accurate evaluation of gyroaverages for nonperiodic simulations

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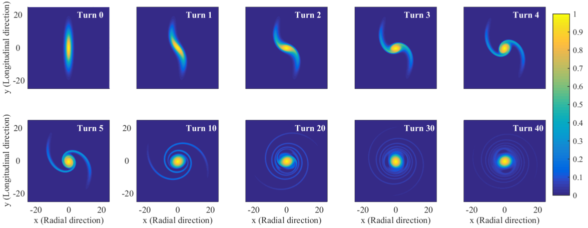
Motivation – Abstract

- In many situations in plasma physics, gyrokinetics needs to be applied to problems with non-periodic boundary conditions
- Physical quantitites cannot be expanded as Fourier series
  $\Rightarrow$ Numerical evaluation of their gyroaverages challenging, and in practice often not very accurate
- We propose a new method for gyroaveraging based on the combination of Fourier transforms and a Hankel transform

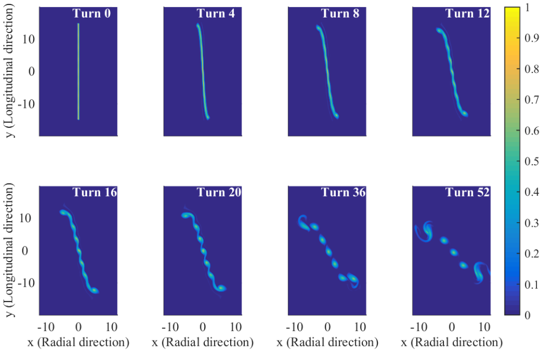
  Our numerical scheme relies on fast and high order accurate algorithms
- Focusing on the gyrokinetic-Poisson system, we demonstrate geometric convergence for a near-optimal computational complexity $(N + \hat{N}) \log(N + \hat{N})$

  N: # of grid points in real space; $\hat{N}$: # of grid points in Fourier space

NONPERIODIC GYROKINETICS: EXAMPLE



Beam spiraling in cyclotrons



Beam breakup in cyclotrons

SIMPLE TEST BED

- Gyrokinetic-Poisson system in uniform magnetic field $\mathbf{B} = \mathbf{e}_z$
  Let $\mathbf{r} = \mathbf{R} + \boldsymbol{\rho} = \langle X, Y \rangle + \langle -\rho \sin\gamma, \rho\cos\gamma \rangle$

  $\mathbf{R}$: guiding center position; ρ: Larmor radius; γ: gyrophase

$$\frac{\partial f}{\partial t} + \boldsymbol{e}_z \times \langle \boldsymbol{\nabla}_{\boldsymbol{r}} \Phi \rangle_{\boldsymbol{R}} \cdot \boldsymbol{\nabla}_{\boldsymbol{R}} f = 0$$

$$\begin{aligned}\nabla^2_{\boldsymbol{r}} \Phi(\boldsymbol{r}, t) &= -\int_0^{+\infty} \int_0^{2\pi} f(x + \rho\sin\gamma, y - \rho\cos\gamma, \rho, t)\, \rho \, \mathrm{d}\rho \mathrm{d}\gamma \\ &\equiv -2\pi \tilde{f}(x, y, t)\end{aligned}$$

$\langle \cdot \rangle_{\mathbf{R}}$: gyroaverage at fixed guiding centre position $\mathbf{R}$:

$$\langle \Phi \rangle_{\boldsymbol{R}} = \frac{1}{2\pi} \int_0^{2\pi} \Phi(X - \rho\sin\gamma, Y + \rho\cos\gamma, t)\, \mathrm{d}\gamma \qquad (1)$$

where X and Y fixed are held fixed.

Difficulties with gyroaverage potential

- In Fourier space, gyroaveraging is just multiplication by $J_0(k_\perp \rho)$ – GOOD
- Difficulty: Φ not necessarily periodic, and may be unbounded or very slowly decaying
- Well-known efficient Fourier methods not applicable – BAD
- Two methods typically used to address this difficulty:
  - Direct numerical quadrature (e.g. Using cubic basis)
  - Replace multiplication by J_0 with Padé approximant, so that gyroaveraging in real space tantamount to solving tractable PDE
- All methods typically low order accurate

Reformulating the equations

- Reformulate gyrokinetic - Poisson system as

$$\frac{\partial f}{\partial t} + \boldsymbol{e}_z \times \boldsymbol{\nabla}\chi \cdot \boldsymbol{\nabla} f = 0$$
$$\nabla^2 \chi = -2\pi \langle \tilde{f} \rangle$$

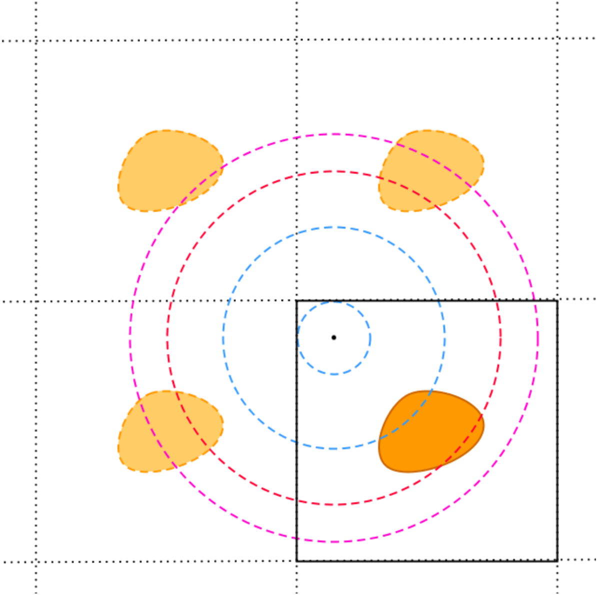
with

$$-2\pi\langle\tilde{f}\rangle \equiv \frac{1}{2\pi}\int_0^{2\pi} \tilde{f}(X + \rho \sin\gamma, Y - \rho\cos\gamma, t)\,\mathrm{d}\gamma$$

- Function to gyroaverage is now compactly supported
- Its Fourier transform is numerically well defined
- Drawback: χ depends on $\rho \Rightarrow$ Poisson's equation needs to be solved several times

  Acceptable drawback with existence of very efficient Fast Poisson solvers

WHY FOURIER SERIES DO NOT WORK FOR $\langle \tilde{f} \rangle$



Incorrect contributions to desired integral

Fourier and Hankel transforms

Fourier transform

$$\hat{u}(\boldsymbol{\xi}, \rho) \equiv (\mathcal{F}_{\boldsymbol{x}} u)(\boldsymbol{\xi}, \rho) = \int_{\mathbb{R}^2} u(\boldsymbol{x}, \rho) \mathrm{e}^{-\mathrm{i}\boldsymbol{\xi}\cdot\boldsymbol{x}} \, \mathrm{d}\boldsymbol{x}$$

Inverse Fourier transform:

$$\check{u}(\boldsymbol{x}, \rho) \equiv (\mathcal{F}_{\boldsymbol{\xi}}^{-1} u)(\boldsymbol{x}, \rho) = \frac{1}{4\pi^2} \int_{\mathbb{R}^2} u(\boldsymbol{\xi}, \rho) \mathrm{e}^{\mathrm{i}\boldsymbol{\xi}\cdot\boldsymbol{x}} \, \mathrm{d}\boldsymbol{x}$$

Hankel transform

$$(\mathcal{H}_0 u)(s) = \int_0^\infty u(\rho) J_0(\rho s) \, \rho \, \mathrm{d}\rho$$

We have the identity:

$$\begin{aligned}(\mathcal{F}\tilde{f})(\boldsymbol{\xi}, t) &= \int_0^\infty (\mathcal{F}\langle f \rangle)(\boldsymbol{\xi}, \rho, t) \, \rho \, \mathrm{d}\rho \\ &= \int_0^\infty J_0(\rho\xi)(\mathcal{F}f)(\boldsymbol{\xi}, \rho, t) \, \rho \, \mathrm{d}\rho = (\mathcal{H}_0 \mathcal{F} f)(\boldsymbol{\xi}, t)\end{aligned}$$

Fourier and Hankel transforms

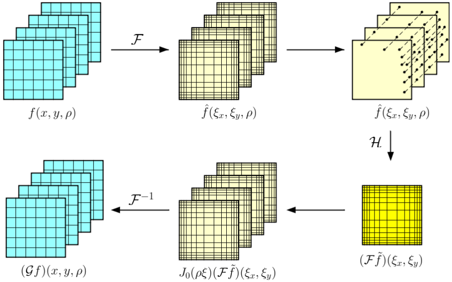
Likewise,

$$(\mathcal{F}\langle\tilde{f}\rangle)(\boldsymbol{\xi},\rho,t) = J_0(\rho\xi)(\mathcal{F}\tilde{f})(\boldsymbol{\xi},t) = J_0(\rho\xi)(\mathcal{H}_0\mathcal{F}f)(\boldsymbol{\xi},t)$$

Hence,

$$\langle\tilde{f}\rangle(\mathbf{x},\rho,t) = \mathcal{F}^{-1}\left(J_0(\rho\xi)\mathcal{H}_0\mathcal{F}f\right)(\boldsymbol{x},\rho,t) \equiv \mathcal{G}f(\boldsymbol{x},\rho,t)$$

which leads to the following numerical scheme for $\langle\tilde{f}\rangle$:



PART I: EVALUATING $\mathcal{F}f$ (I)

- Focus on 1-variable case for the simplicity of the notation:

$$\hat{u}(\xi) = \int_{-\infty}^{\infty} u(x) \mathrm{e}^{-\mathrm{i}\xi x} \, \mathrm{d}x$$

  u is compactly supported on the domain $I = [-\frac{a}{2}, \frac{a}{2}]$

- Write u as the *exact* series

$$u(x) = \left(\sum_{k=-\infty}^{\infty} c_k \mathrm{e}^{2\pi \mathrm{i} k x / a} \right) \mathbf{1}_I(x) \quad , \quad c_k = \frac{1}{a} \int_{-a/2}^{a/2} u(x) \mathrm{e}^{-2\pi \mathrm{i} k x / a} \, \mathrm{d}x$$

  Compute the c_k with the FFT

- Exact expression for the Fourier transform of u:

$$\hat{u}(\xi) = a \sum_{k=-\infty}^{\infty} c_k \, \mathrm{sinc} \left(k - \frac{a\xi}{2\pi} \right)$$

PART II: EVALUATING $\mathcal{F}f$ (I)

- Fast and spectrally accurate evaluation of sum with the Fast Sinc Transform[1]

- Method allows ξ grid in Fourier space to be arbitrary

  Choose Chebyshev grid for spectrally accurate operations in Fourier space

  Choose # of grid points $\hat{N}$ to efficiently resolve function in Fourier space

- Run time complexity of the FST: $O(N + \hat{N}) \log(N + \hat{N})$

[1] L. Greengard, L., J.-Y. Lee and S. Inati *CAMCoS*, **1**, 121 (2006)

Part II: Evaluating $\mathcal{H}_0\mathcal{F}f$

$$H(\xi) = \int_0^\infty h(\rho) J_0(\rho\xi)\,\rho\,\mathrm{d}\rho$$

$h = 0$ outside the interval $I_\rho = [0, \overline{\rho}]$.

- Evaluate integral with Clenshaw-Curtis quadrature, with a Chebyshev grid for I_ρ:

$$H(\xi) \approx \sum_{k=1}^{N_\rho} w_k h(\rho_k) J_0(\rho_k \xi)\rho_k \tag{2}$$

- For fixed computational ρ- and ξ- grids, $w_k J_0(\rho_k\xi)\rho_k$ can be precomputed.
- Each Hankel integral is inner product of a time-dependent data vector and a vector of fixed kernel weights.
- Time spent computing $\mathcal{H}_0\mathcal{F}f$ negligible compared to time spent computing $\mathcal{F}f$.

Part III: Evaluating $\mathcal{G}f = \mathcal{F}^{-1}(\mathcal{H}_0\mathcal{F}f)$

$$u(x) = \frac{1}{2\pi}\int_{-\hat{a}}^{\hat{a}} \hat{u}(\xi)\mathrm{e}^{\mathrm{i}\xi x}\,\mathrm{d}\xi$$

- Use ξ Chebyshev grid chosen for that purpose, and write

$$u(x_j) \approx \frac{1}{2\pi}\sum_{k=1}^{\hat{N}} w_k \hat{u}(\xi_k)\mathrm{e}^{\mathrm{i}\xi_k x_j}$$

  with w_k the Clenshaw-Curtis weights

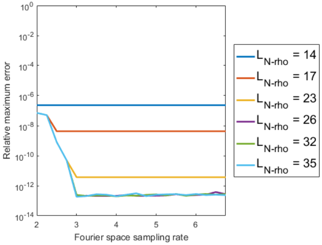
- Compute this sum in near-optimal run time $O(N+\hat{N})\log(N+\hat{N})$ with the Non Uniform Fast Fourier Transform (NUFFT)[2,3]

[2] A. Dutt and V. Rokhlin *SIAM J. Sci. Comput.*, **1**, 121 (1993)
[3] J.-Y. Lee and L. Greengard *J. Comp. Phys* **206**, 1 (2005)

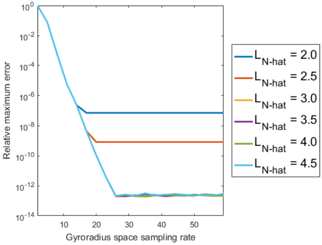
NUMERICAL RESULTS: TEST CASE

- Take f as
$$f(x, y, \rho) = e^{-A(x^2+y^2)} e^{-B\rho^2}$$
where $A = B = 15$
- One can calculate $\mathcal{G}f$ analytically:
$$\mathcal{G}f(x, y, \rho) = \frac{1}{2(A+B)} e^{-\alpha(x^2+y^2+\rho^2)} I_0\left(2\alpha\rho\sqrt{x^2+y^2}\right)$$
where $\frac{1}{\alpha} = \frac{1}{A} + \frac{1}{B}$ and $I_0(z)$ is the modified Bessel function of the first kind of order 0.
- Interval sizes
$$\begin{aligned} \text{Real space}: &\quad (x, y) \in [-3, 3] \\ \text{Fourier space}: &\quad (\xi_x, \xi_y) \in [-66, 66] \\ \text{gyroradius}: &\quad \rho \in [0, 1.55] \end{aligned}$$

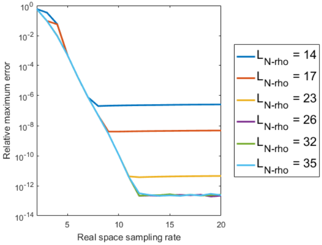
NUMERICAL RESULTS



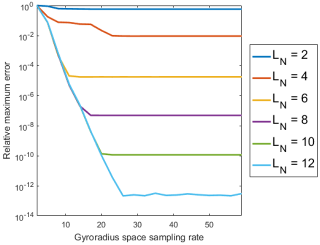
$L_N = 12$



$L_N = 12$

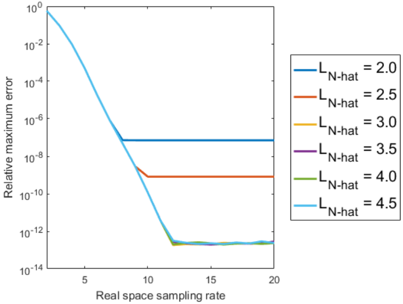


$L_{\hat{N}} = 4.5$

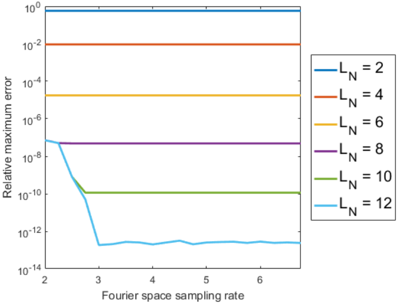


$L_{\hat{N}} = 4.5$

Numerical results



$L_{N_\rho} = 35$



$L_{N_\rho} = 35$

- Exponential decrease of the error as we increase all three sampling rates uniformly
- For $L_N = 12$, $L_{\hat{N}} = 4.5$, and $L_{N_\rho} = 35$, the error is on the order of 10^{-13}

Summary

- We presented a fast, spectrally accurate numerical scheme for the evaluation of the gyroaveraged electrostatic potential in gyrokinetic Poisson simulations

- We successfully applied our method to simulate the dynamics of intense beams in cyclotrons

Future work

- Extend formulation to more general gyrokinetic equation
  - Spatial dependence of the magnetic field
  - Electromagnetic effects

- Application to nonperiodic simulations of turbulent transport in fusion devices