EFFICIENT NON-FOURIER IMPLEMENTATION
OF LANDAU-FLUID OPERATORS
IN THE BOUT++ CODE

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Motivation and Introduction

- Effective phase-mixing damping rate in Landau-fluid closure

\[ \gamma \propto -|k_{||}| v_{th} \]

- Specific example, with collisions

\[ \nabla_{||} Q_{||}(z) \approx -8n_0 v_{th}^2 \int dk_{||} e^{ik_{||}z} \frac{k_{||}^2 \tilde{T}_{||}}{\sqrt{8\pi} |k_{||}| v_{th} + (3\pi - 8) \nu_s} \]

- Such operators are easy to represent and efficient to calculate in Fourier (\(k_{||}\)) space.

- When large (including background) spatial inhomogeneities are present in the phase-mixing operators, evaluation using Fourier methods becomes inefficient.
With mesh-based schemes (finite difference, volume, element, etc.), it is straightforward to construct approximations to $(\nabla_{||})^n \leftrightarrow (ik_{||})^n$, but harder for, e.g., $|k_{||}| \times k_{||}^n = \text{sgn} (k_{||}) \times k_{||}^{n+1}$.

- not local in configuration space

Direct use of the corresponding discretized configuration space kernel by convolution or matrix multiplication is potentially expensive.

- $N_g^2$ scaling vs. $N_g \log (N_g)$ of computational expense

**ACCURATE APPROXIMATIONS ARE POSSIBLE THAT CAN BE IMPLEMENTED WITH FOURIER-LIKE SCALING.**
Basic idea

- Approximate $1/|k|$ as a sum of suitably scaled Lorentzians
  \[
  \frac{1}{|k|} \approx \sum_{n=0}^{N} \frac{\alpha^n}{k^2 + \alpha^{2n}}
  \]

- Each individual component of the sum has the correct parity, but asymptotic dependence $1/k^2$ for large $k$.
- With the above scaling of the height and width, successive terms approximately “fill in” successively higher parts of the $1/|k|$ curve.
- The sum provides a quite good fit over some spectral range, which increases with $N$.
- Lorentzians in $k$ space are inverses of Helmholtz operators in real space.
Approximate calculation

- Discretize the Helmholtz equations
- Solve via a tridiagonal (for 2-point differences) or banded (for higher-order differences) matrix solution
- Direct solvers should work well
  - the matrices are well conditioned
  - parallelizeable along direction of solve
- Sum the results of the matrix solves
Accuracy of the basic approximation

- Look at how close to $\text{sgn}(k) = k/|k|$ is

$$\psi(k; \alpha, \beta, N) = \beta k \sum_{n=0}^{N-1} \frac{\alpha^n}{k^2 + \alpha^{2n}}$$

- $\alpha = 5, \beta = 1.04, N = 7$
Accuracy of the basic approximation

\[ \alpha = 5, \beta = 1.04, N = 7 \]

\[ \alpha = 6, \beta = 1.16, N = 5 \]

\[ \frac{k_{\text{min}}}{k_{\text{max}}} = 400 \]

\[ \frac{k_{\text{min}}}{k_{\text{max}}} = 50 \]
Finite-grid effects

Compare exact, 3-point and 5-point approximations to $k^2$

\[ K_2^2(k\Delta) = \left[\frac{2 \sin(k\Delta/2)}{\Delta}\right]^2 \]

\[ K_4^2(k\Delta) = \frac{4}{3} \left[\frac{2 \sin(k\Delta/2)}{\Delta}\right]^2 - \frac{1}{3} \left[\frac{\sin(k\Delta)}{\Delta}\right]^2 \]
Finite-grid effects

- Finite differences good to some \( k_d = \hat{k}_d / \Delta \); \( k_d \approx 0.8 \) for 3-point; \( k_d \approx 1.6 \) for 5-point

- Given \( \psi (\hat{k}) \) which fits the desired operator well for \( \hat{k}_{\text{min}} \lesssim \hat{k} \lesssim \hat{k}_{\text{max}} \), scale \( \hat{k} \) by factor \( \lambda \) so that \( \lambda \hat{k}_{\text{max}} = \hat{k}_d / \Delta \), i.e., \( \lambda = \hat{k}_d / (\hat{k}_{\text{max}} \Delta) \).

- Then \( \psi (k / \lambda) = \psi \left( k \Delta \hat{k}_{\text{max}} / \hat{k}_d \right) \) gives a good fit for

\[
\hat{k}_d \hat{k}_{\text{min}} / \hat{k}_{\text{max}} \lesssim k \Delta \lesssim \hat{k}_d, \text{ i.e., for all modes in system for } L \lesssim 2\Delta \hat{k}_{\text{max}} / \hat{k}_{\text{min}}.
\]
Include collisions

- Can scale operator fit problem to obtaining a fit to $k/(|k| + 1)$
- Can obtain reasonable fit by adjusting coefficient of first Lorentzian

$$\psi (k; \alpha, \beta, N) = \beta k \left[ \frac{\eta}{k^2 + 1} + \sum_{n=1}^{N} \frac{\alpha^n}{k^2 + \alpha^{2n}} \right]$$

- $\alpha = 6, \beta = 1.15, N = 5, \eta = 0.5$

comparison

relative error
Implementation

- Non-Fourier approximation to $1/|k|$ and $-|k|$ operator.

\[1/|k| \approx \beta \sum_{n=0}^{N} \frac{\alpha^n}{k^2 + (\alpha^n k_0)^2}\]

\[-|k| = -\frac{k^2}{|k|} \approx -\beta \sum_{n=0}^{N} \alpha^n + \beta \sum_{n=0}^{N} \frac{\alpha^{3n} k_0^2}{k^2 + (\alpha^n k_0)^2}\]

- Use 3-point second difference for second derivative

\[\frac{\partial^2 \psi}{\partial z^2} \rightarrow \frac{1}{\Delta^2} (\psi_{i+1} + \psi_{i-1} - 2\psi_i)\]

\[\therefore k^2 \rightarrow K_2^2(k\Delta) = [2 \sin(k\Delta/2)/\Delta]^2\]

- Periodic domain; "periodic tridiagonal" routine.
Spatial Oscillations (Gibbs Phenomenon) for $|k|$ Operator

- $\alpha = 5$, $N = 7$, $\beta = 1.04$.
- System length = $2\pi$; 16 grid cells

Real Space

![Graph](image-url)
Spatial Oscillations (Gibbs Phenomenon) for $-|k|$ Operator

- $\alpha = 5, N = 7, \beta = 1.04$.
- System length $= 2\pi$; 16 grid cells

**Fourier Space**

![Graph showing $-|k|f_k$ in Fourier space]

- **Fourier**
- **non-Fourier**
- **Analytical**
- **Fourier - 3-pt**
- **Fourier - 5-pt**

System length $= 2\pi$; 16 grid cells
Spatial Oscillations (Gibbs Phenomenon) for $-|k|$ Operator

- $\alpha = 5, N = 7, \beta = 1.04$.
- System length = $2\pi$; 16 grid cells

Real Space
Spatial Oscillations (Gibbs Phenomenon) for \( |k| \) Operator

- \( \alpha = 5, \ N = 7, \ \beta = 1.04. \)
- System length = \( 2\pi \); 64 grid cells

**Real Space**

![Graphs showing spatial oscillations](image-url)
Non-Fourier has similar computational scaling to Fourier

- Non-Fourier, with fixed $N$, scales as $N_z$, c.f. $N_z^2$ for direct convolution
- Crossover point is at $N_z \approx 128 \Rightarrow$ advantage for $N_z \gtrsim 200$.

Timings

![Timings graph](image)
Collocation solution for Laplace inversion ansatz: \( \eta_j(k) = b^j / (k^2 + b^{2j}) \)

- Collocation at uniformly spaced points \( b^i \), for \( i = -N, \ldots, N \) lead to the symmetric linear problem \( Ma = 1 \) where
  \[
  M^s_r = b^r b^s / (b^{2r} + b^{2s})
  \]

- For \( b = e \) the solutions are

<table>
<thead>
<tr>
<th>( N )</th>
<th>( 2N + 1 )</th>
<th>([a^r])</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>3</td>
<td>[1.84807, 1.68115, 1.84807]</td>
</tr>
<tr>
<td>2</td>
<td>5</td>
<td>[1.54322, 0.866876, 1.04278, 0.866876, 1.54322]</td>
</tr>
<tr>
<td>3</td>
<td>7</td>
<td>[1.53232, 0.300129, 0.811828, 0.575391, 0.811828, 0.300129, 1.53232]</td>
</tr>
<tr>
<td>4</td>
<td>9</td>
<td>[1.70273, -0.263771, 0.885701, 0.293448, 0.656293, \ldots]</td>
</tr>
<tr>
<td>5</td>
<td>11</td>
<td>[2.01764, -0.999102, 1.27026, -0.110205, 0.727017, 0.127763, \ldots]</td>
</tr>
</tbody>
</table>

- However, error grows at edges of logarithmic interval

\[
k f_N(k)
\]

\[
|k f_N(k) - 1|
\]
Uniform accuracy can be obtained with Chebyshev collocation points

- Chebyshev polynomial approximation can generate uniform error convergence over the logarithmic interval
  - For exponential interval $b^N$, first renormalize by taking the logarithm $\beta = \beta_0 \log b$
  - The Chebyshev collocation points $\beta_s$ with $2N + 1$ polynomials, $s = -N, \ldots, N$, are
    \[ \beta_s = \cos \left( (s - N) \frac{\pi}{2N} \right) \rightarrow b_s = \exp \left( \beta_0 \cos \left( (s - N) \frac{\pi}{2N} \right) \right) \]

- Chebyshev solution for $\beta_0 = 1$:

<table>
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<tr>
<th>$N$</th>
<th>$2N + 1$</th>
<th>$[a_j]$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>3</td>
<td>[1.6529, -0.142332, 1.6529]</td>
</tr>
<tr>
<td>2</td>
<td>5</td>
<td>[4.06838, -3.65237, 2.52162, -3.65237, 4.06838]</td>
</tr>
<tr>
<td>4</td>
<td>9</td>
<td>[82.5576, -124.155, 62.226, -30.1305, 22.6809, ...]</td>
</tr>
<tr>
<td>5</td>
<td>11</td>
<td>[445.908, -720.514, 409.297, -199.35, 110., -86.8668, ...]</td>
</tr>
</tbody>
</table>

- Maximum error is similar, but now more uniform over logarithmic interval

\[ k f_N(k) \]

\[ |k f_N(k) - 1| \]
Systematic collocation analysis \(\rightarrow\) improved fits: collisionless

- Collisionless - good (near best) fit is of the form

\[
\frac{1}{|k|} \approx \beta \sum_{n=1}^{N} \frac{\zeta_n}{k^2 + (\alpha^{n-1} \kappa_0)^2},
\]

- Match exact and approximate forms at collocation points \(k = k_n, k_n = \alpha^{n-1} \kappa_0, n = 2, 3, \ldots, N - 1, \kappa_0 = \kappa_0/\eta, k_N = \eta \alpha^{N-1} \kappa_0\).
- \(\rightarrow\) matrix problem that can be handled e.g., by Mathematica
- Extends spectral range of good fit by \(\sim 10\text{-}100\) for given \(N, \alpha\).

Improved fits vs. original fit

![Graph showing improved fits vs. original fit.](image-url)
Collisional case introduces a scale length, the mean-free path: $\lambda$

- **Key dimensionless parameter:** $b = k_{\text{max}} \lambda$
- **Now, collocation at points** $k\lambda = b^s$ **for** $s = -N, \ldots N$ **generates the equation**

$$M_s a^r = b^s / (i + b^s)$$

- **For** $b = e$ **the solutions are**

<table>
<thead>
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<th>$2N + 1$</th>
<th>$[a^j]$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>3</td>
<td>[0.19703, -0.0711661, 1.45587]</td>
</tr>
<tr>
<td>2</td>
<td>5</td>
<td>[0.0280711, 0.0210288, 0.470837, 0.155383, 1.53263]</td>
</tr>
<tr>
<td>3</td>
<td>7</td>
<td>[0.00382669, 0.00401212, 0.0966353, 0.261622, 0.714043, 0.219054, 1.5438]</td>
</tr>
</tbody>
</table>

- **Again, error grows for the limit** $k\lambda \gg 1$

$$(k + 1) f_N(k)$$

$$|(k + 1) f_N(k) - 1|$$
Chebyshev collocation reduces error at large $k \sim k_{\text{max}}$

- **Perform collocation at points** $k\lambda = \exp(s\beta_s)$
  where $\beta_s = \cos((s - N)\pi/2N)$ and $s = -N, \ldots, N$

- **For** $b = e$ **the solutions are**

  \[
  N \quad | \quad 2N + 1 \quad | \quad \begin{bmatrix} a_j \end{bmatrix}
  \]

  \[
  \begin{array}{c|c|c}
  N & 2N + 1 & \begin{bmatrix} a_j \end{bmatrix} \\
  \hline
  1 & 3 & [0.19703, -0.0711661, 1.45587] \\
  2 & 5 & [0.0308817, -0.00571965, 0.590679, -0.0967698, 1.68609] \\
  3 & 7 & [0.00571954, -0.00531807, 0.0514562, 0.451945, 1.03353, -0.960316, 2.30743] \\
  \end{array}
  \]

- **Still may want to reduce error in middle of domain further ...**

\[
(k + 1) f_N(k)
\]

\[
|(k + 1) f_N(k) - 1|
\]
Systematic collocation analysis $\rightarrow$ improved fits: collisional

- Good (near best) fit is of the form

$$\frac{1}{1 + |k|} \approx \beta \sum_{n=-N}^{N} \frac{\zeta_n}{k^2 + \alpha^2 n},$$

- collocation points: $k_n = \alpha^n, n = -N, \ldots, N - 1, k_N = \eta \alpha^N$.

- $\alpha = 3, 4; N = 3, 4; \eta = 0.5, 0.6, 1.$

Various fits
Effect of using sum of Lorentzians on the response functions

- We have implemented a set of Mathematica scripts, which reproduce the HP90 analytic calculations, and also modified them to give the effect of using the sum of Lorentzians for $k/|k|$.

Using exact $k/|k|$ reproduces the HP90 3-field model.

FIG. 1. The real and imaginary parts of the normalized response function $R(\zeta) = -\bar{n}T_0/n_0 e\phi$ vs the normalized frequency $\zeta$. The solid lines are the exact kinetic result for a Maxwellian, $R(\zeta) = 1 + \zeta Z(\zeta)$. The dashed lines are from the three-moment fluid model with $\Gamma = 3$, $\mu_1 = 0$, and $\chi_1 = 2/\sqrt{\pi}$. The dotted lines are from the four-moment model.
Replacing $k/|k|$ by the sum of Lorentzians approximation yields good fits to the Landau-fluid response functions.

Effect of replacing $k/|k|$ by sum of Lorentzians

3-fluid

\[ R = R_3 \left( \frac{k}{k_0} \right), \text{ for } k_0 = 1, 10, 100. \]

4-fluid

\[ R = R_4 \left( \frac{k}{k_0} \right) \text{ for } k_0 = 1, 100. \]
Replacing $k/|k|$ by the sum of Lorentzians approximation yields good fits to the Landau-fluid response functions.

- considered local ($q=-\chi \text{ grad}T$) and nonlocal ($qk=-ik/\text{abs}(k) \ Tk$) models for the spectral response function.
- The calculation is done by fourier and non-Fourier methods, for comparison.
- Local non-Fourier means finite-difference, and nonlocal non-Fourier means the Lorentzian method (our main interest).
- Naming convention is: local/nonlocal $\iff$ local=1/0, and similar for Fourier and non-Fourier.
Finite-difference and Fourier implementations of local (diffusive) heat flux in time evolution give response function in agreement with theoretical spectral analysis.
Finite-difference and Fourier implementations of nonlocal heat flux in time evolution give response function in agreement with theoretical spectral analysis.
Normalizing wavenumber $k_{z0}$ must be chosen to have region of good fit overlap with resolved modes

- $k_0 = K_0 \times z_{\text{period}}$, where $K_0$ is an $O(1)$ multiplier
- e.g., for parallel case, $\nabla_\parallel = (1/h_y) \partial_y$, so $k_{||0} = K_{y0}/\sqrt{g_{yy}(y_0)}$.
  - $\sqrt{g_{yy}(y_0)} = h_y(y_0)$ is a measure of the parallel connection length
BOUT++ tests: Parallel advection across parallel boundary

- Gaussian source pulse initialized away from parallel boundary advects across boundary with correct shift
BOUT++ tests: Parallel Laplace Solver

- Parallel (direction) Laplace solver gives sensible solutions with twist-shift boundary condition
- Reconstructed source function is consistent with original source function

---

**Single Helmholtz inversion**

```
phi vs. (z,y)
```

```
0.000 0.008
```

**reconstructed source**

```
deriv vs. (z,y)
```

```
0.000 0.095
```
BOUT++ tests: Implementation of non-Fourier sum-of-Lorentzians for parallel Landau-fluid operator

- Non-Fourier LF operator gives sensible solutions with twist-shift boundary condition

Source function

**LF flux**

qvar nl vs. (z,y)


*also, School of Physics, Peking University Work performed for U.S. DOE by LLNL under Contract DE-AC52-07NA27344)
Toroidal Landau-fluid ($|\omega_d|$) closure

- Example from Beer ‘96 - 3+1 equations:

\[
\begin{align*}
\frac{du_{||}}{dt} &= \text{stuff} - 4i\omega_d u_{||} - 2|\omega_d| \nu_5 u_{||} \\
\frac{dp_{||}}{dt} &= \text{stuff} - i\omega_d (7p_{||} + p_{\perp} - 4n) - 2|\omega_d| (\nu_1 T_{||} + \nu_2 T_{\perp}) \\
\frac{dp_{\perp}}{dt} &= \text{stuff} - i\omega_d (5p_{\perp} + p_{||} - 3n) - 2|\omega_d| (\nu_3 T_{||} + \nu_4 T_{\perp})
\end{align*}
\]
Toroidal Landau-fluid ($|\omega_d|$) closure

- Linear forms for $i\omega_d$

\[
  i\omega_d \Phi = i V_d \cdot k_\perp \Phi = \frac{1}{2(T_{\text{norm}} B_0)} \left[ \frac{T_{\perp 0}}{B_0} \hat{b} \times \nabla B_0 \cdot \nabla + T_{\parallel 0} \hat{b} \times (\hat{b} \cdot \nabla \hat{b}) \cdot \nabla \right] \Phi
\]

- Need to add correct combination and generalize $T_0$ to finite amplitude

- To get coefficients for modified version of invert_laplace, decompose $V_d$ and $\nabla \Phi$ into components

\[
  V_d = V_d^i e_i \\
  \nabla \Phi = e^i \partial_i \Phi \\
  V_d \cdot \nabla \Phi = V_d^i \partial_i \Phi
\]
BOUT++ implementation

- Components $V_d^1$, $V_d^3$ easily calculated with existing routines in BOUT++
- Basic Helmholtz equation can be solved using a modified version of existing perpendicular Laplace solver
  - Current equation is of the form
    \[
    (c_1 k_z^2 - c_2 \partial^2_\psi + c_3) \Phi = S
    \]
  - Modify to solve
    \[
    \left\{ \left[ (V_d^z)^2 k_z^2 - \left( V_d^\psi \right)^2 \partial^2_\psi - 2i V_d^\psi V_d^z k_z \partial_\psi \right] + \alpha^2 (V_d^z)^2 k_z^2 \right\} \Phi = S
    \]
BOUT++ tests: Perpendicular Laplace solver for $|\omega_d|$ terms

- Perpendicular (direction) Laplace solver gives sensible solutions
- Spreading by Helmholtz inversion is in the same direction as advection

(solutions with periodic radial BC’s)
Conclusions

- We have developed a new non-Fourier method for the calculation of Landau-fluid operators.
- Useful for situations with large (including background) spatial inhomogeneities.
- Good accuracy (relative error $\lesssim 1\%$ over wide spectral range) is readily achievable.
- Computational cost has value and scaling similar to Fourier method.
- Considerable advantage over direct convolution or matrix multiplication for $N_g \gtrsim 200$.
- Readily applied to toroidal phase-mixing operators ($|\omega_d|$).
- Method is also useful for capturing correct asymptotic form of gyrofluid operators.