EFFICIENT NON-FOURIER IMPLEMENTATION OF LANDAU-FLUID CLOSURE OPERATORS FOR EDGE PLASMA SIMULATION*

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Simulations of tokamak (and other MFE) edge plasmas need to go beyond collisional (Braginskii) models

- Kinetic effects are important in the tokamak edge
- Gyro-Landau-fluid (GLF) approach is a way to incorporate some kinetic effects into fluid simulation codes such as BOUT++
- Radial inhomogeneities and large relative perturbation amplitudes necessitate a non-Fourier implementation of the Landau-fluid (LF) closure operators

- Related work at this meeting:
  - Higher-order (profile and nl) effects: I. Joseph, PS II, #19
  - Plasma response & transport with collisions: M. Umansky, PS III, #20
  - GLF effects on ELMs: C. Ma, PS II; #25, P. Xi, previous talk

The Landau-fluid (LF) closure operators are highly nonlocal in configuration space

- 1D (e.g., parallel) collisionless closure phase-mixing:
  - $\gamma \propto -|k|\, v_{\rm th}$
  - e.g., 3-moment model (collisionless: Hammett-Perkins, PRL '90):

$$\tilde{Q}_k \approx -\alpha n_0 v_{\rm th} \frac{1}{|k|}\left(ik\tilde{T}_k\right) \quad \Longleftrightarrow \quad \tilde{Q}\left(z\right) \approx \int_{-\infty}^{\infty} dz' G(z-z')\tilde{T}\left(z'\right)$$

$$G(z) \quad = \quad \frac{\alpha}{\pi} n_0 v_{\rm th} \frac{1}{z}$$

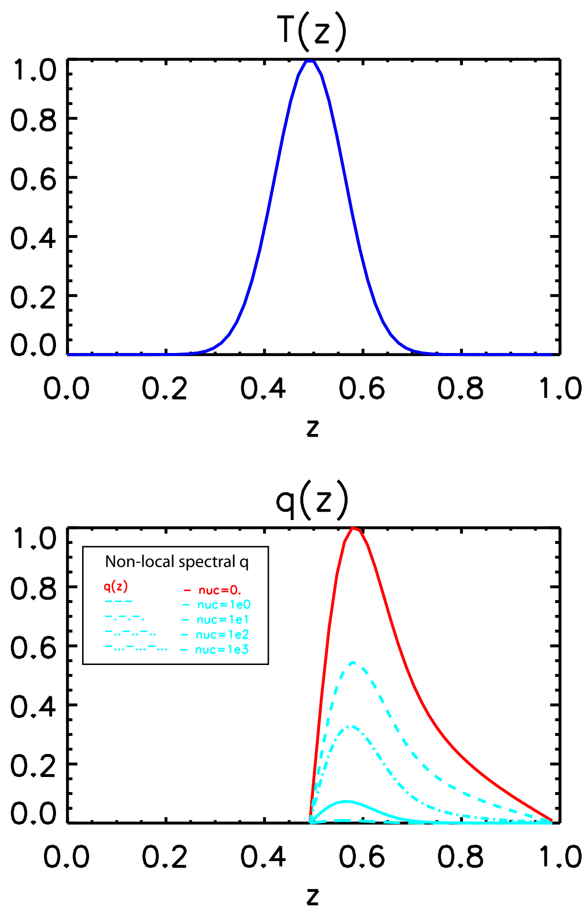
  - with collisions (Beer-Hammett, Phys. Plasmas '96):

$$\tilde{Q}_k \approx -\frac{8 n_0 v_{\rm th}^2 ik\tilde{T}_k}{\sqrt{8\pi}\,|k|\,v_{\rm th} + (3\pi - 8)\,\nu_s}$$

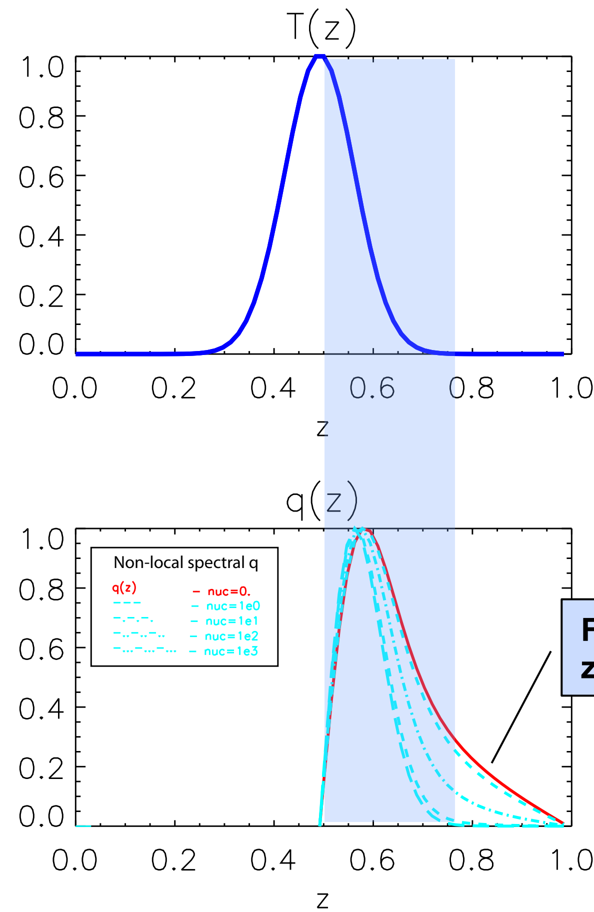
- If spatially homogeneous closure model can be used, the LF operators are easy to represent and efficient to calculate in Fourier ($k_{||}$) space.

Landau-fluid non-local heat flux w/ collisions shows correct trend to approximate local diffusive heat flux

Non-normalized



Normalized



Finite q for zero gradT

The LF closure operators for edge must deal with spatial inhomogeneities

- Example: toroidal Landau-fluid ($|\omega_d|$) closure:
- e.g., Beer-Hammett '96, 3+1 equations:

$$\frac{dp_{\shortparallel}}{dt} = \text{stuff} - i\omega_d\,(7p_{\shortparallel} + p_\perp - 4n) - 2\,|\omega_d|\,(\nu_1 T_{\shortparallel} + \nu_2 T_\perp)$$

- ω_d defined by

$$\begin{aligned} i\omega_d \Psi &= v_d \hat{\mathbf{V}}_d \cdot \nabla_\perp \Psi \\ &= \frac{1}{2(T_{\mathrm{norm}} B_0)} \left[\frac{T_\perp}{B_0} \hat{\mathbf{b}} \times \nabla B_0 \cdot \nabla + T_{\shortparallel} \hat{\mathbf{b}} \times \left(\hat{\mathbf{b}} \cdot \nabla \hat{\mathbf{b}} \right) \cdot \nabla \right] \Psi \end{aligned}$$

  - In the edge, $T_\perp$ and $T_{\shortparallel}$ have significant spatial variations due to
    - equilibrium profile variation
    - finite amplitude perturbations

Computation of the LF operators becomes challenging when significant spatial inhomogeneities are present

- Operators are no longer local in k space
  - Fourier-based computation inefficient
- LF operators intrinsically nonlocal in configuration space $\rightarrow$ mesh-based discretization schemes used for derivatives (finite difference, volume, element, etc.) are no longer applicable.
- Straightforward direct approach:
  - discretize configuration-space kernel
  - aplply by direct convolution or matrix multiplication
  - computationally expensive; N_g^2 scaling [vs. $N_g \log(N_g)$ for local-k Fourier]
- ACCURATE APPROXIMATIONS ARE POSSIBLE THAT CAN BE IMPLEMENTED WITH FOURIER-LIKE SCALING.

Approximation by a sum of Lorentzians allows for computation using efficient sparse linear solvers

- Lorentzians in k space are inverses of Helmholtz operators in real space
- Could provide very efficient way to implement nonlocality

- Consider

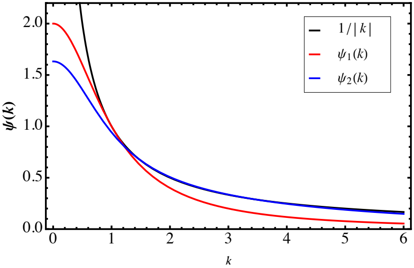
$$\frac{1}{|k|^{\gamma}} \approx \psi_{\infty}(k, \alpha, \gamma) \approx \sum_{n=-\infty}^{\infty} \frac{\alpha^{\gamma n}}{k^2 + \alpha^{2\gamma n}}, \ 0 < \gamma < 2$$

- Converges pointwise; satisfies $\psi_{\infty}(\alpha k, \alpha) = \alpha^{-\gamma} \psi_{\infty}(k, \alpha)$
- Each individual component of the sum has the correct parity.
- With the above scaling of the height and width, different terms approximately "fill in" different parts of the $1/|k|$ curve
- Suggests an approximation by a simple truncation.

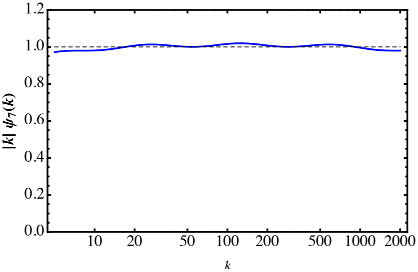
Simple truncated sum of Lorentzians is very accurate, even with few terms

$$\frac{1}{|k|} \approx \psi_N\left(k, \alpha, \beta, k_0\right) \approx \beta \sum_{n=0}^{N-1} \frac{\alpha^n k_0}{k^2 + \left(\alpha^n k_0\right)^2}$$

$\psi_N\left(k\right)$ - 1 and 2 terms



$|k|\,\psi_7\left(k\right)$ - 7 terms



Systematic collocation analysis → improved fits: collisionless

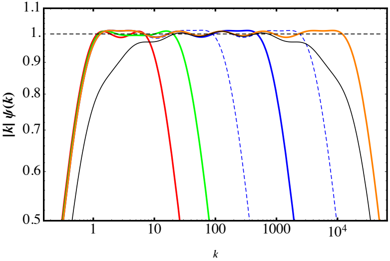
- Collisionless - good (near best) fit is of the form

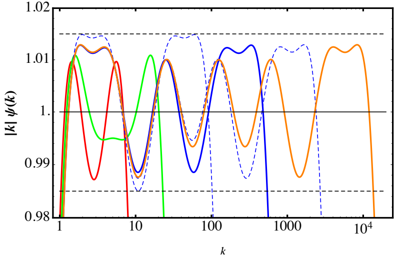
$$1/|k| \approx \sum_{n=0}^{N-1} \frac{\zeta_n \alpha^n \kappa_0}{k^2 + (\alpha^n \kappa_0)^2},$$

- Match exact and approximate forms at collocation points
  - $k = k_n$, $k_n = \alpha^{n-1}\kappa_0$, $n = 1, 3, \ldots, N-2$
  - shift end collocation points: $k_0 = \kappa_0/\eta$, $k_N = \eta\alpha^{N-1}\kappa_0$.
- → matrix problem that can be handled e.g., by Mathematica

Systematic collocation analysis → improved fits: collisionless

- Extends spectral range of good fit by ~10-100 for given N, α.
- Improved fits vs. original fit
- Spectral range of good fit: 7, 20, 80, 400, 2000, 10000

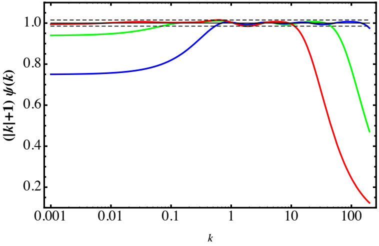


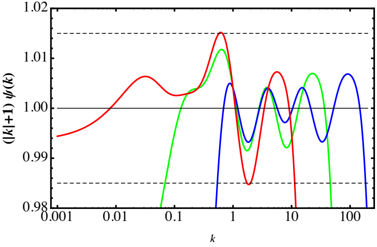


Systematic collocation analysis → improved fits: collisional

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

- Collocation points: $k_n = \alpha^n$, $n = -M, \ldots, N-1$, $k_N = \eta\alpha^N$.
- 5 terms → good fit over spectral range ≈ 400, $\forall\, k\lambda_{\mathrm{mfp}}$.
- $\alpha = 3;\ N + M + 1 = 5,$





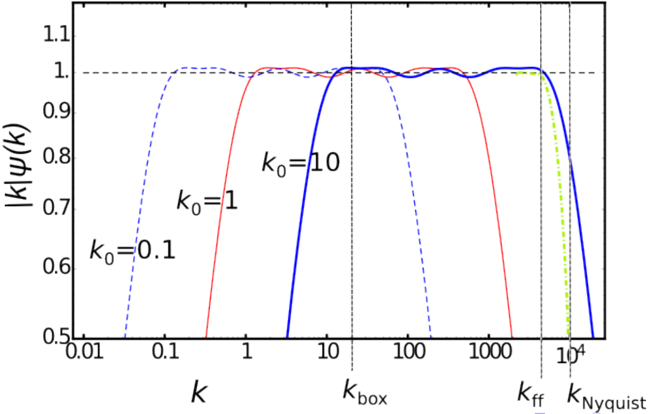
Implementation is by replacement of Lorentzians in wavenumber space by Helmholtz-equation solves

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

$$\Psi(z) \approx \sum_n \zeta_n \alpha^n \kappa_0 \left[(\alpha^n \kappa_0)^2 - \frac{\partial^2}{\partial z^2} \right]^{-1} S(z)$$

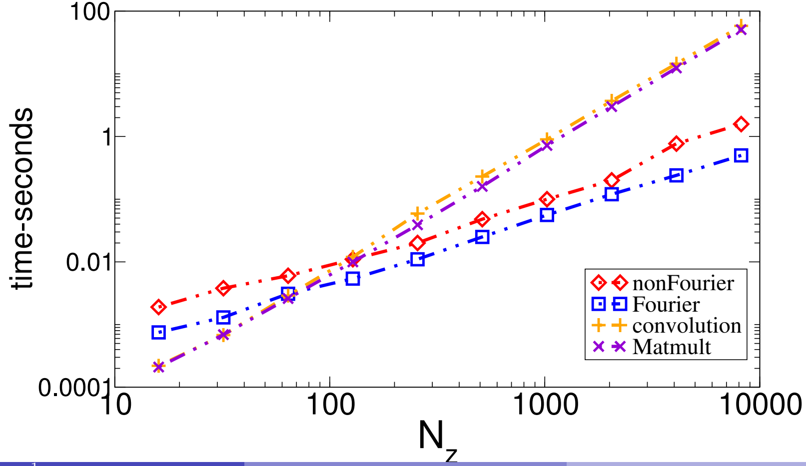
Normalizing wavenumber k_0 must be chosen to have region of good fit overlap with resolved modes

- Choose k_0 so that
  - $k_{\rm box}$ is to right of left boundary of good fit
  - $k_{\rm ff}$ is to left of right boundary of good fit



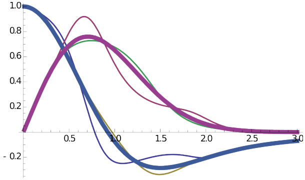
Sum-of-Lorentzians method has similar computational scaling to Fourier

- Scales as $N_z \log(N_z)$, c.f. N_z^2 for direct convolution or matrix multiplication.
- Crossover point is at $N_z \approx 128 \Rightarrow$ advantage for $N_z \gtrsim 200$.



Using sum of Lorentzians approximation preserves Hammett-Perkins '90 LF response functions

- Implemented Mathematica scripts; reproduced HP90 calculations,
- modified to also use sum of Lorentzians for $1/|k|$.



$$R = R_4\,(k/k_0),$$
$$k_0 = 1,\ 10,\ 100.$$

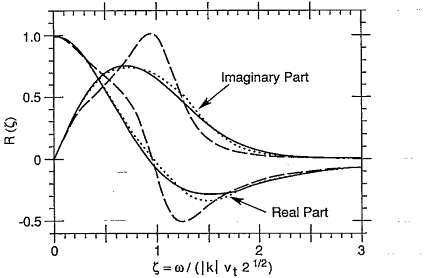


FIG. 1. The real and imaginary parts of the normalized response function $R(\zeta) = -\tilde{n}T_0/n_0e\tilde{\phi}$ vs the normalized frequency ζ. The solid lines are the exact kinetic result for a Maxwellian, $R(\zeta) = 1 + \zeta Z(\zeta)$. The dashed lines are from the three-moment fluid model with $\Gamma = 3$, $\mu_1 = 0$, and $\chi_1 = 2/\sqrt{\pi}$. The dotted lines are from the four-moment model.

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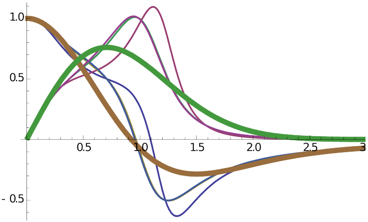
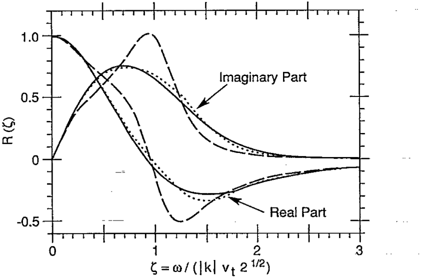


$$R = R_3\,(k/k_0),$$
$$k_0 = 1,\ 10,\ 100.$$



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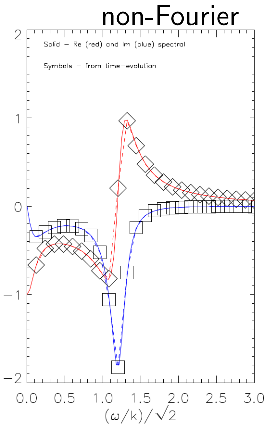
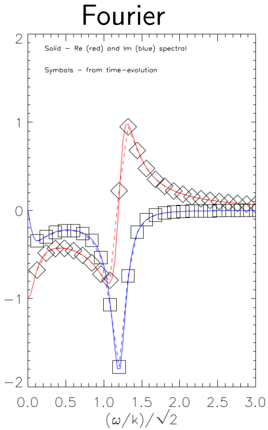
Using sum of Lorentzians approximation preserves collisional LF response functions

collisional response Functions





Toroidal Landau-fluid ($|\omega_d|$) closure

- Linear forms for $i\omega_d$

$$
\begin{aligned}
i\omega_d\Psi &= i\mathbf{V}_d\cdot\mathbf{k}_\perp\Psi \\
&= \frac{1}{2(T_{\rm norm}B_0)}\left[\frac{T_{\perp 0}}{B_0}\hat{\mathbf{b}}\times\nabla B_0\cdot\nabla + T_{\parallel 0}\hat{\mathbf{b}}\times\left(\hat{\mathbf{b}}\cdot\nabla\hat{\mathbf{b}}\right)\cdot\nabla\right]\Psi
\end{aligned}
$$

- $T_{\perp 0} = T_{\perp 0}(\psi)$, $T_{\parallel 0} = T_{\parallel 0}(\psi)$; - eventually will need to generalize to finite amplitude
- Decompose $\mathbf{V}_d$ and $\nabla\Psi$ into components

$$
\begin{aligned}
\mathbf{V}_d &= V_d^i\mathbf{e}_i \\
\nabla\Psi &= \mathbf{e}^i\partial_i\Psi \\
\mathbf{V}_d\cdot\nabla\Psi &= V_d^i\partial_i\Psi
\end{aligned}
$$

The LF terms have been implemented in BOUT++

- $|k_{\shortparallel}|$ terms implemented using existing parallel "Laplace" solver
  - Has correct offset periodic parallel boundary conditions
- $|\omega_d|$ terms implemented using modification of existing perpendicular Laplace solver(s)
  - Existing solver solves

$$\left(c_1 k_\phi^2 - c_2 \partial_\psi^2 + c_3\right)\Psi = S$$

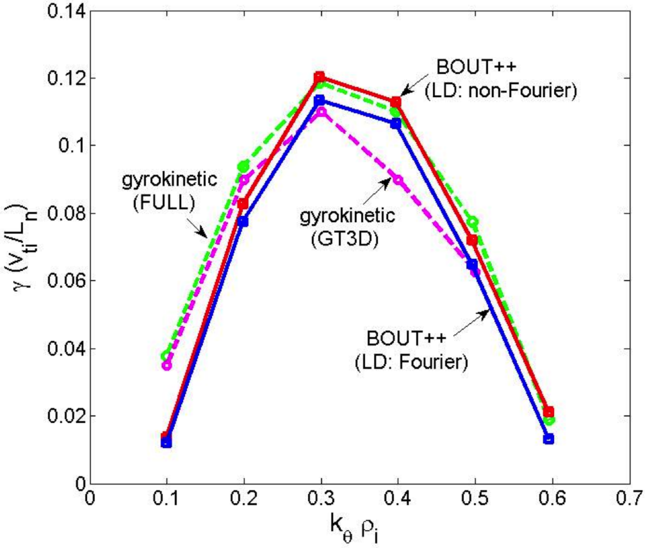
  - Modify to solve

$$\left\{\left[\left(V_d^\phi\right)^2 k_\phi^2 - \left(V_d^\psi\right)^2 \partial_\psi^2 - 2iV_d^\psi V_d^\phi k_\phi \partial_\psi\right] + \alpha^2\left(V_d^z\right)^2 k_{\phi 0}^2\right\}\Psi = S$$

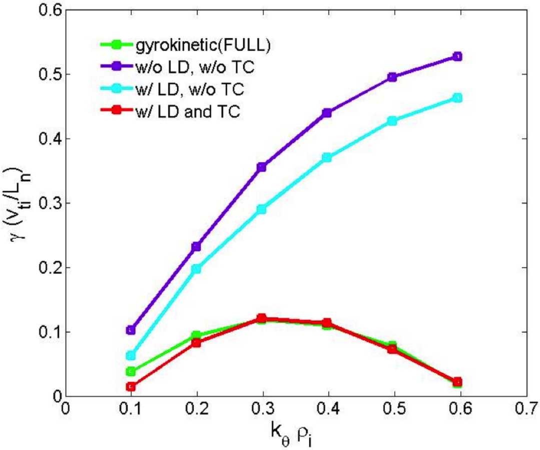
- Radial inhomogeneities in ∇B and curvature drifts can be included via the manifestly conservative dissipative form:

$$|\mathbf{k}.\mathbf{v_d}(x)|\,\Psi = \nabla \cdot \left[\hat{\mathbf{v}}_\mathbf{d}\sqrt{\mathrm{v}_\mathbf{d}}\frac{1}{|\mathbf{k}.\hat{\mathbf{v}}_\mathbf{d}|}\sqrt{\mathrm{v}_\mathbf{d}}\left(\hat{\mathbf{v}}_\mathbf{d}\cdot\nabla\Psi\right)\right]$$

Good agreement is achieved with previous calculations for ITG instability frequencies and growth rates



The Landau-Fluid terms are essential for agreement of the GLF toroidal ITG linear growth rates with gyrokinetic results



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 $\lesssim 1.5\%$ over wide spectral range) is readily achievable with 5 terms for all $k\lambda_{\rm mfp}$.
- Computational cost has value and scaling similar to Fourier method.
- Considerable advantage over direct convolution or matrix multiplication for $N_g \gtrsim 200$.
- Implemented for parallel ($|k_{\shortparallel}|$) and toroidal ($|\omega_{\rm d}|$) LF operators in BOUT++
- Good agreement is achieved with previous calculations for ITG instability frequencies and growth rates.

BOUT++ 2013 Workshop

September 3rd - 6th 2013

https://bout2013.llnl.gov

T. Y. Xia, X. Q. Xu, Z. X. Liu, *et al*, 24th IAEA FEC, 8-13 Oct 2012 San Diego, CA, USA.

Workshop Theme

BOUT++ is a collaboration between the LLNL, University of York, and a growing number of other institutions around the world. The mission of the 2013 BOUT++ Workshop is (1) to provide a forum for the discussion of key physics and computational issues as well as innovative concepts of direct relevance to fluid and gyro-fluid plasma simulations; (2) to prepare researchers to use and further develop the BOUT++ code for simulations of edge turbulence, transport and ELMs in magnetic fusion devices; and (3) to promote effective collaboration within the BOUT community and beyond.

Workshop Format

This 4 day workshop, held at Lawrence Livermore National Laboratory (LLNL) California, USA; covers tutorial lectures on the basics of the BOUT++ code and tools used by BOUT++, special lectures on plasma/material-surface interactions, integrated modeling, synthetic diagnostics for validating simulations, and on innovative numerical schemes and preconditioners, plus talks and posters in topical applications by present BOUT++ users/developers. Some sessions will include hands-on exercises using Linux machines.

Abstract Deadline: June 30, 2013 (see below)

Instructions for preparing and submitting abstracts are found on the workshop web site.

Registration Deadlines:

June 30, 2013 – Non-US citizens
July 31, 2013 – US citizens

Instructions for workshop registration are found on the web site. Due to access restrictions and badging requirements at LLNL, participants are required to register by the dates noted.

As the program is interactive and seats are limited, the number of participants is limited to 55. Pre-registration will be required.

Visas:

It is recommended that participants requiring U.S. visas should submit their visa applications as soon as possible. Participants requiring an invitation letter for their visa should request it by an email sent to **massiatt1@llnl.gov**.

Past BOUT++ Workshop:

https://bout.llnl.gov/html/workshops/2011/bout2011.html

Accommodation:

Accommodation suggestions available on the web site.

Organizing Committee:

Xueqiao Xu (Chair, LLNL, USA)
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Francois Waelbroeck (IFS, U Texas, USA)
Howard Wilson (University of York, UK)
Xueqiao Xu (Lawrence Livermore National Laboratory, USA)

National Ignition Facility (NIF) Tour:

The workshop will include a NIF tour on September 6 for all interested participants. The NIF web site:

https://lasers.llnl.gov

BOUT++ 2011 workshop participants on NIF tour.

Lawrence Livermore National Laboratory

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