LIGHTNINGBOLTZ: A fast spectral solver for the nonlinear Boltzmann equation

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Outline

- Solving the Boltzmann equation
- Applications
  - Neutrals in divertors
  - Electron runaway
  - Discharges and more . . .
The Boltzmann equation can be extended to inelastic collisions

Total change of energy is still known, even if non-zero. Express as a velocity-dependent *restitution coefficient* $\alpha_k$.

$$\frac{df_s(v)}{dt} = \sum_{s',k} \int \int |v-w| \sigma_k(v,w) \left[ \frac{1}{\alpha_k^2} f_s(v') f_s'(w') - f_s(v) f_s'(w) \right] d^2\Omega d^3w$$

$$v' = v'(v, w, \Omega, \alpha_k) \quad w' = w'(v, w, \Omega, \alpha_k)$$

$$\alpha_k = \sqrt{\frac{KE_{tot} - \frac{1}{2}KE_{cm}}{KE_{tot} - \frac{1}{2}KE_{cm} + E_{loss}}}$$

Challenges to direct solution:

- Nonlinear integral equation
- Nonlocal
- High dimensionality
General features of numerical solution to Boltzmann equation

Choose a discretization: \( f \) represented with \( N \) degrees of freedom: \( f_i \) (values on a 3D mesh, spectral coefficients, etc.).
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Because the Boltzmann equation is \textbf{quadratically nonlinear}, we can write a discretization scheme for the collision operator as:

$$
\frac{\partial}{\partial t} f = f \cdot \mathbb{C} \cdot f ; \quad \frac{\partial}{\partial t} f_p = \sum_{q=1}^{N} \sum_{r=1}^{N} f_q f_r C_{pqr}
$$

where $\mathbb{C}$ is a $N \times N \times N$ \textbf{collision hypermatrix}, which is \textit{independent} of the distribution function.
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Suppose we attempt to solve on a finite-difference velocity space grid and trapezoidal quadratures with \( N = 30^3 \) grid points.

- \( \sim 10^{18} \) operations to calculate the \( \sim 4 \) TB collision matrix.
Expand distribution function in an orthonormal basis:

\[ f(v) \approx \sum_{k,l,m} f_{klm} \phi_{klm}(v) \]

\[ = \sum_{k,l,m} f_{klm} \sqrt{\frac{2k!}{\Gamma(k + l + 3/2)}} e^{-v^2/2} v^l L^{l+1/2}_k (v^2) Y_{lm}(\theta, \phi) \]

Gamba & Rjasanow. JCP, 2018
Galerkin-Petrov method

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2. Solve the weak form of the Boltzmann equation.

Multiply through by a test function:

\[ \psi_{klm}(v) \equiv v^l L_k^{l+1/2} Y_{lm} (\theta, \phi) \]

and integrate over all \( v \).

Now \( C \) relates the spectral coefficients \( f_{klm} \). Storage still scales like \( N^3 \), but one gets away with much fewer degrees of freedom . . .
Time-advancing the spectral coefficients

\[
\frac{\partial}{\partial t} f_p = M^{-1} \sum_{p=1}^{N} \sum_{q=1}^{N} C_{pqr} f_q f_r
\]

\[
M_{ij} = \int \phi_i (v) \psi_j (v) d^3v
\]

\[
C_{pqr} = \int \int \int |v - w| \sigma (v, w) \phi_q (v) \phi_r (w)

[\psi_p (v') + \psi_p (w') - \psi_p (v) - \psi_p (w)] d^2\Omega d^3w d^3v
\]

For each triplet of \(N\) spectral coefficients \(f_p\), an **8-dimensional** integral needs to be performed: two in speed and three in solid-angle. Need to be as efficient as possible.
Gaussian quadrature provides spectral accuracy and is extended to arbitrary weightings.

**Gaussian quadrature:**

- Approximate an integral:
  \[ I = \int g(x) \omega(x) \, dx \approx \sum_{i} w_i g(x_i) \]

- With the right weights \( w_i \) and co-location points \( x_i \), **spectral accuracy** is achieved.

- Integrates exactly if \( g \) is a polynomial of degree \((2N_g - 1)\) or less.

- Makes use of orthogonal polynomials with respect to the function \( \omega(x) \) (nominally Maxwellian).
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Can be extended to 2D integrals over solid angle:

(Lebedev. USSR Comp. Math. 1976)
An implementation of the Gamba-Rjasanow scheme has been developed

- Extends the Galerkin-Petrov algorithm for:
  - Inelastic collisions.
  - Improved Gaussian quadrature.
- Optimized, parallelized, and rigorously benchmarked.
- Written in the Julia programming language (for now).
- Reads from online database of pre-computed collision matrices.
Analytic benchmark of LightningBoltz

Benchmark: Maxwell molecules \((\sigma \propto |\mathbf{v} - \mathbf{w}|^{-1})\) with \(N = 27\). Initialize with a two-stream dual-Maxwellian and relax under self-collisions.
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![Graphs showing analytical vs numerical solutions for Boltzmann equation](image-url)
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Precomputation of collision matrix takes about 60 seconds.
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Divertors limit exposure of the plasma to solid material

- **Advantage**: low plasma impurity contamination
- **Disadvantage**: escaping hot plasma strikes a limited surface area

There is concern that the scrape-off layer (SOL) width scales unfavorably with plasma current.

Heuristic (but experimentally verified) model predicts $\lambda_{SOL}^{(ITER)} \sim 2\,\text{mm}$, compared to about 5 mm in JET (which has much less outgoing heat flux)

For burning reactors, the situation is even more dire. A solution is needed...

_Eich, et al. PRL 2011_  
_Goldston. NF 2012_
A “detached divertor” will be necessary for a burning reactor

- A regime of operation exists where the plasma recombines before reaching the solid wall.
- The gas radiates energy, protecting the wall from bombardment of a narrow plasma.
- Situation is unstable and difficult to control: ionization front tends to either falls back to the wall or the plasma.
- Dynamics of neutrals and the gas-plasma transition are important for predictive control methods.


(from Krasheninnikov, et al. J. PoP 2016:)

G. Wilkie
Progress toward a fully kinetic neutral model for divertor detachment

LightningBoltz appears to be a good candidate for a comprehensive Boltzmann solver for neutrals.

\[
\frac{\partial f_n}{\partial t} = n_e \alpha_{\text{recom}} f_i - n_e \langle v \sigma_{\text{ion}} \rangle_e f_n + C_{\text{el}} [f_n, f_n] + C_{\text{inel}} [f_n, f_n]
\]

“Proof of principle” model

- \( C_{\text{el}} [f_n, f_n] \approx \) Elastic collisions
- \( C_{\text{inel}} [f_n, f_n] \approx \) Impact excitation
- \( \alpha_{\text{recom}} = \) Radiative recombination
- \( \sigma_{\text{ion}} = \) Electron-impact ionization

\[\text{Cross section (cm}^{-1}\text{)}\]

\[E (\text{eV})\]

\(\sigma_{\text{ex}}, \sigma_{\text{exc}}, \sigma_{\text{ion}}\)

Without a source of neutrals, distribution collapses as it radiates all energy away

Evolution of density and temperature:

Collisions only
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With sources and sinks
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Runaway electrons threaten fusion experiments

- Tokamaks are liable to sudden drops in thermal energy known as *disruptions*.
- Most of the plasma current can be converted into a *super-relativistic electron beam*.
- These *runaway electrons* threaten the structural integrity of the tokamak hardware.

Tore Supra ($I = 1.7$ MA):

KSTAR ($I = 2.0$ MA):

JET ($I = 5.0$ MA):

ITER ($I = 17$ MA):

kstarmovie
Avalanche multiplies the runaway population exponentially

- Friction *decreases* at high energy for Coulomb collisions.
- For particles faster than a *critical speed* $v_c$ (a function of electric field strength), *runaway acceleration* results.

\[
|F_{\|}| = eE_{sa} \\
eE = eE_c \\
eE_c \\
v_{th} < v_c < c
\]

Net acceleration $F_e - F_c > 0$
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A large angle collision between a relativistic electron and a thermal electron results in a multiplication of the runaway population

\[
\frac{\partial n_r}{\partial t} = \Gamma_{av}(E)n_r
\]

Even when large angle collisions are rare, their effect is substantial!
New basis is needed to apply spectral methods for runaway dynamics

Runaway electron distributions are highly anisotropic with a long tail. Simplified analytic theories result in a distribution with a known angular dependence:

\[ f(p, \xi) = G(p) \exp [A\xi] \]

Define a new set of polynomials in \( \xi \equiv p_\parallel / p \) that obey the orthogonality relation:

\[ \int_{-1}^{1} e^{A\xi} \Pi_n(\xi) \Pi_m(\xi) \, d\xi = \delta_{nm} \]

An example anisotropic basis function:

\[ \Upsilon_{lm} (\theta, \phi) = \Pi_l (\cos \theta) e^{im\phi} \]

A generalized Laguerre basis is not appropriate.

Embreus model for relativistic large-angle collisions

Account for both small angle and large angle collisions in linearized collision operator, where \( f = f_{Maxw} + f_r \):

\[
C [f_r, f_{Maxw}] = C_{FP}^- + C_{Boltz}^-
\]

\[
C [f_{Maxw}, f_r] = C_{FP}^+ + C_{Boltz}^+
\]

- Approximate \( f_{Maxw} \propto \delta(p) \) compared to the energetic population \( f_r \).
- To avoid double-counting collisions, adjust the cutoff in the Fokker-Planck operator.
- Results in an energy-dependent Coulomb logarithm:

\[
\ln \Lambda^* = \ln \Lambda - \ln \left( \cot \frac{\theta_c(p)}{2} \right)
\]

Form of the field particle operator (source of knock-ons):

Chiu-Harvey model

\( Chiu, et al. \ NF 1998 \)

Embreus model

- Avoids double-counting
- Includes full pitch-angle dependence of energetic distribution
- Conserves particles and energy
- Transferred energy independent of choice of cutoff \( \theta_c \)

\( Embreus, et al. \ JPP 2018 \)
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**Lightning**

Seed of energetic electrons
Study of weakly ionized plasma has a wide variety of applications

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**Atmospheric reentry**
Plasma layer surrounding spacecraft blocks communications.
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**Disassociation of carbon dioxide**
Vibrationally-excited CO$_2$ more efficient to break apart.

Many other possible applications for directly solving the Boltzmann equation

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  *(Pierrard, AIP Conf. Proc. 2003)*
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- **Economics**  
Conclusion

- Numerical solution of the Boltzmann equation is feasible and efficient with modern techniques.

  **LightningBoltz** aims to bring direct solution of the Boltzmann equation “to the masses”. Collision matrices pre-computed, perhaps on clusters; time-advance performed on local workstations.

- **Ongoing work:**
  - Populate database with many physically-relevant cross sections.
  - Add spatial dependence. *(Keßler & Rjasanow. Preprint, 2018)*
  - Generalize basis and quadrature for strong anisotropy.

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