# closures-2d

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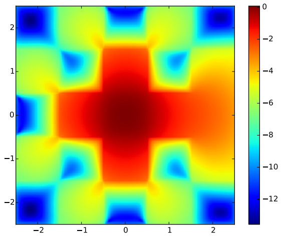
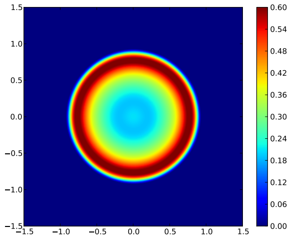
## Goals

We are releasing software that tests angular approximations in kinetic transport simulations

- Based on code used for a previous publication (Garrett and Hauck 2013)
- Open source so that others can use/collaborate
- Modular, making it easy to implement new features
- Implements $S_N$, $P_N$, $FP_N$, $M_N$, $PP_N$, $D_N$ (experimental)



$P_N$ Order 3



$FP_N$ (sspline) Order 3

## Improvements

Algorithmic changes:

- Added experimental Lebedev quadrature
- Removed $\gamma$ factor for ansatz correction in `momopt`
- Changed `momopt`'s regularization in case of bad condition number

Software-related improvements:

- Cross-platform build system
- Automated testing
- Better MPI communication
- Improved documentation
- Improved interface
- Bugfixes
- Profiling and optimization

## Release

We are releasing this code as open source software.

Now uses SCons, a Python-based build system, rather than Makefiles

- Cross platform
- Sets up library search paths
- Intelligent compilation

Depends on:

- GSL
- BLAS
- LAPACK
- OpenMP (optional)
- MPI (optional)
- PAPI (optional)

## What Are Kinetic Equations?

**Macroscopic**

- $\rho(x, t)$ – Density
- $u(x, t)$ – Velocity
- $E(x, t)$ – Kinetic Energy

Discretize $x$, $t$ into 100 values: 4GB memory requirement

**Mesoscopic**

- $f(x, v, t)$ – Density with respect to space *and velocity*

Discretize $x$, $v$, $t$ into 100 pieces: 800TB memory requirement

Macroscopic can be derived from mesoscopic

- $\rho(x, t) = \int_{\mathbb{R}^3} f \, \mathrm{d}v$
- $u(x, t) = \frac{1}{\rho} \int_{\mathbb{R}^3} vf \, \mathrm{d}v$
- $E(x, t) = \frac{1}{2} \int_{\mathbb{R}^3} \|v - u\|^2 \, \mathrm{d}v$

## What Are Kinetic Equations?

First used for rarefied gas dynamics (e.g. high altitude gases where collisions do not dominate the physics)

$$\partial_t f + v \cdot \nabla_x = C(f)$$

where $\int C(f)\,\mathrm{d}v = 0$.

Integrate against $v$ to get First Euler/Navier-Stokes equation

$$\partial_t \rho + \nabla_x \cdot (\rho u) = 0$$

Other areas:

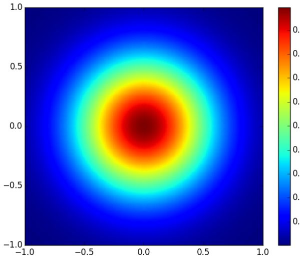
- Radiation transport
- Plasma simulations

# Kinetic Problem

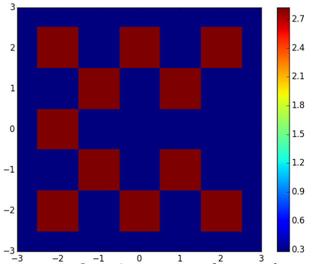
## Unit Speed, Isotropic Scattering

$$\partial_t f + \Omega \cdot \nabla_x = \frac{\sigma_s}{4\pi} \int_{S^2} f \, d\Omega - \sigma_t f$$

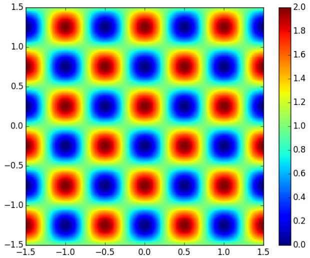
where $x \in \mathbb{R}^3$, $\Omega \in S^2$, and $\sigma_s$,$\sigma_t$ are the scattering and transmission cross sections.



Gaussian Initial Condition



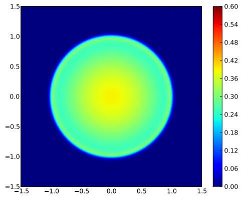
$\sigma_T$ for Lattice Initial Condition

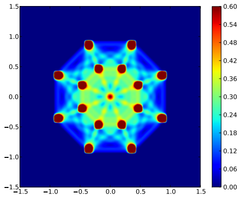


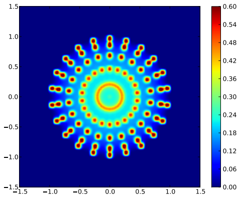
Smooth Initial Condition

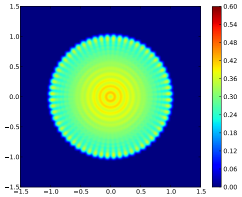
## kinetic

- Implements $S_N$
- Easy to compute
- Permits negative densities
- Suffers from ray effects at low order


Analytic Solution

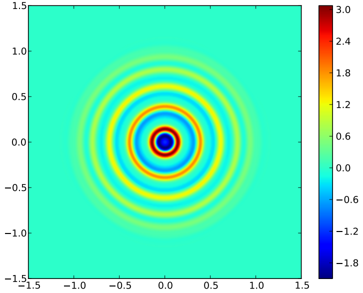

$S_N$ Order 4


$S_N$ Order 11

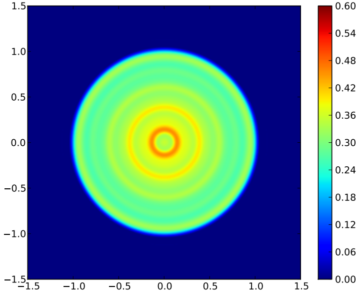

$S_N$ Order 30

## moment

- Implements $P_N$, $FP_N$
- Somewhat easy to compute
- Permits negative densities
- Suffers from oscillatory artifacts
- Filters can improve performance



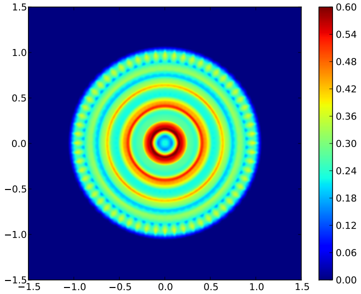
$P_N$ Order 11



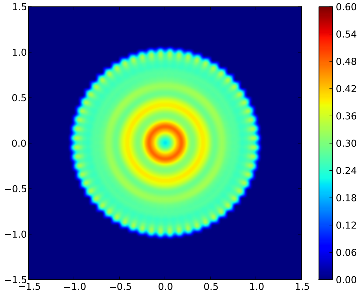
$FP_N$ (Lanczos) Order 11

## momopt

- Implements $M_N$ and $PP_N$
- Difficult to compute
- Ensures positivity
- Requires additional optimization procedure



$PP_N$ Order 11



$M_N$ Order 11

## Testing

We implemented several automated tests for the software. The testing code is written in Python and integrated with the build system.
The testing code carries out

- Regression tests – compare output to reference data included with the software
- Mass Conservation tests – check that total density remains the same
- Convergence tests – measure the effect of decreasing the cell size on the precision of the output

### Convergence: `moment (sspline)`

| Cell size | Error | Order |
|---|---|---|
| $\Delta x/1$ | 8.075049 | 1.954163 |
| $\Delta x/2$ | 2.083932 | 2.082828 |
| $\Delta x/4$ | 0.491915 | 2.340759 |
| $\Delta x/8$ | 0.097107 | — |

## Performance

Added timing and profiling-related measurement capabilities

Tested additional optimizations

- Spatial blocking (reduce scheduling overhead, cache misses)
- CPU pinning (ccNUMA)
- Memory alignment

## Caching Example: Matrix Multiplication

```
for(int i = 0; i < N; i++) {
for(int j = 0; j < N; j++) {
for(int k = 0; k < N; k++) {
    result[i][j] += left[i][k] * right[k][j]
}}}
```

## Caching Example: Matrix Multiplication

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}}}
```

## Caching Example: Matrix Multiplication

| Loop order | Time |
|---|---|
| ijk | 8.139175 |
| ikj | 5.316213 |
| jik | 6.160773 |
| jki | 19.494467 |
| kij | 5.406215 |
| kji | 19.666042 |

Factor of 4 difference

## Blocking

Cache utilization:

- Using a simple loop: move over each row and column, fetching values from main memory on *every iteration*
- Using a block-oriented loop: compute one section, fetching most nearby values from a CPU cache

OpenMP Scheduling:

- Using a simple loop: dispatch each cell to a (possibly different) core
- Using a block-oriented loop: dispatch an entire block to core, improving cache utilization and reducing scheduling overhead

## Quadratures

Currently uses Chebyshev-Legendre quadrature.

- Product quadrature on the sphere

$$\int_{S^2} \cdot \, \mathrm{d}\Omega = \int_{\mu=-1}^{1} \int_{\phi=0}^{2\pi} \cdot \, \mathrm{d}\phi \, \mathrm{d}\mu$$

- $n$ Gauss-Legendre points on $\mu$
- $2n$ equally spaced points on $\phi$
- Exactly integrates to degree $2n - 1$ moments
- Easily optimized for symmetry

## Quadratures

Added (experimental) Lebedev quadrature

- Constructed based on octahedral symmetry group
- Asymptotically optimal with respect to number of points (2/3 that of Chebyshev-Legendre)
- Structure does not lend itself to symmetry optimizations
- Negative weights break positivity

## Optimization Problem

`momopt` uses nonlinear spectral methods, so updates entail solving an optimiztion problem for a given constant vector $u$ and moments $m(\Omega)$.

$$\min_{\alpha} \int_{S^2} \exp(\alpha^{\mathsf{T}} m)\, \mathrm{d}\Omega - \alpha^{\mathsf{T}} u$$

To use a Newton solver, we need

$$\begin{aligned}
\text{Objective funtion } F(\alpha) &= \int_{S^2} \exp(\alpha m^{\mathsf{T}})\, \mathrm{d}\Omega - \alpha^{\mathsf{T}} u \\
\text{Gradient } g(\alpha) &= \int_{S^2} m \exp(\alpha^{\mathsf{T}} m)\, \mathrm{d}\Omega - u \\
\text{Hessian } H(\alpha) &= \int_{S^2} m u^{\mathsf{T}} \exp(\alpha^{\mathsf{T}} m)\, \mathrm{d}\Omega
\end{aligned}$$

Now the estimated $\alpha_{i+1} = \alpha_i + td$ where $d = -H(\alpha)^{-1} g(\alpha)$.

## $\gamma$ factor

In `momopt`'s optimization steps, we compute an approximate $\alpha$ for a given $u$ such that $u \approx \int_{S^2} m \exp(\alpha^\mathsf{T} m) \, d\Omega$.

- Needed to estimate error and try to correct via $\gamma = \frac{\exp(\bar{\alpha}^\mathsf{T} m)}{\exp(\hat{\alpha}^\mathsf{T} m)}$. Here, the numerator of $\gamma$ is our approximation, and the denominatior is exact.
- Required fine mesh and low tolerance on optimization to prevent non-realizability.

Instead, compute $\hat{u}$ such that $\hat{u} = \int_{S^2} m \exp(\hat{\alpha}^\mathsf{T} m) \, d\Omega$

- Adjust scaling to conserve mass
- Exact equality ensures positivity

## Fixed regularization

If cond($H(\alpha)$) is too large

- $H(\alpha)$ is difficult to invert
- Can't find the direction $d = -H(\alpha)^{-1} g(\alpha)$

Need to adjust the problem to make it more tractable

- Set isotropic initial guess
  $\alpha = (2\sqrt{\pi} \log \frac{1}{2\sqrt{\pi}}, 0, 0, \ldots, 0)$ for $\mathrm{M_N}$,
  $\alpha = (1 - 4\pi\delta, 0, 0, \ldots, 0)$ for $\mathrm{PP_N}$, where $\delta$ is a parameter of $\mathrm{PP_N}$
- For $i = 2, \ldots$, multiply each $u_i$ by $1 - r$, where $r$ is a regularization constant with $0 < r < 1$

## Source Code

The source code is available on Github
`https://github.com/ckrisgarrett/closures-2d`

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