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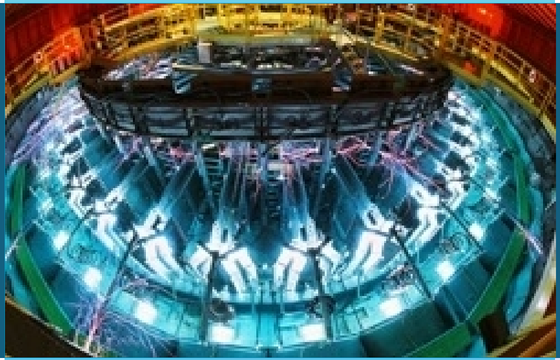
Sandia National Laboratories

Relativistic DSMC Collisions in EMPIRE



EMPIRE

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Motivation

- With EMPIRE, we care about high energy plasmas involving electrons in strong EM fields.

- Charged particles can attain relativistic speeds, but they still collide with slow neutrals.

- Where standard DSMC works at lower energies, we need a relativistic algorithm (that still works for non-relativistic cases).

- Also relevant for astrophysical flows, like galaxy collisions.

Why Is This Hard?

- Numerical issues arise that aren't a problem for analytic physics, especially when we want to be accurate for both v ~ c and v ~ 0.
- Non-obvious "gotchas" can trip up a DSMC expert who isn't very familiar with special relativity.
- There's no "cookbook" for implementing relativistic DSMC, although several people have shown results.

Special Relativity

- SR says light moves at speed c (~3e8 m/s) in every reference frame.

- Everything else pretty much follows from that.

- Under SR we have to modify our understanding of kinetic theory, and the algorithms we use to model it – DSMC as usually implemented is going to have no problem allowing speeds >c.

Notation

We want to think in terms of the Lorentz factor:

$$\gamma = \frac{1}{\sqrt{1 - v^2/c^2}}$$

This lets us define a proper velocity: $\boldsymbol{u} = \gamma \boldsymbol{v}$

...and we can write:

$$\gamma = \sqrt{1 + u^2/c^2}$$

Numerical Issues

Let's say that we want to compute the kinetic energy of a slow object (m=1, v=10) with a relativistic-safe algorithm.

Remember: $\gamma = \frac{1}{\sqrt{1-v^2/c^2}}$, $E_k = (\gamma - 1)mc^2$

In python I get γ=1.0000000000000007, E_k = 59.95204332975845

This isn't just $\frac{1}{2}mv^2 = 50$

The problem is that the computer does finite precision arithmetic and so my $\gamma - 1$ only has one significant figure.

Numerical Issues

We have to rewrite:

$$E_k = (\gamma - 1)mc^2 = \left(\frac{1}{\sqrt{1 - v^2/c^2}} - 1\right)mc^2 = \left(\frac{v^2}{1 - \frac{v^2}{c^2} + \sqrt{1 - v^2/c^2}}\right)m$$

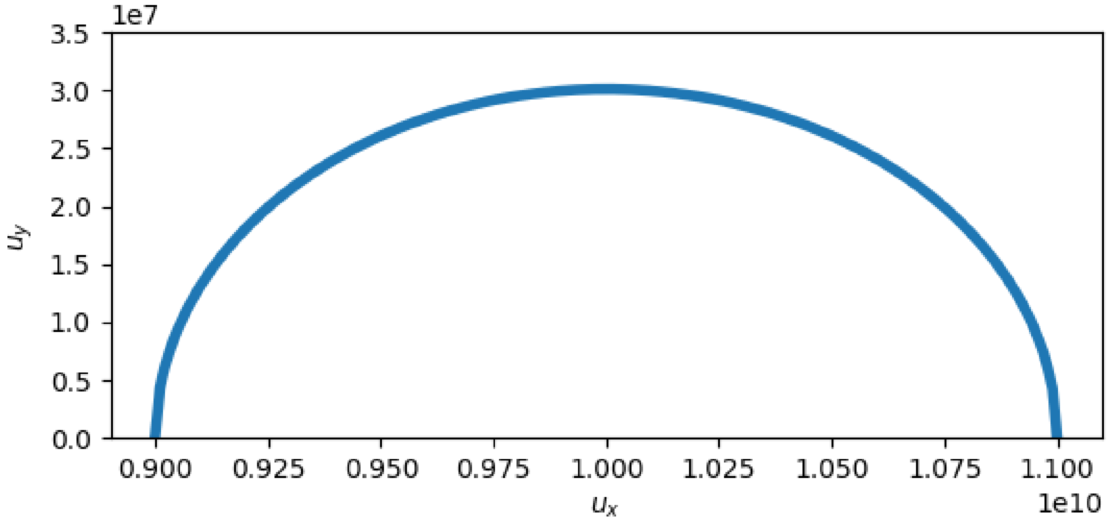
Now python gives $E_k = 50.00000000000004$

We can also see from this how it reduces to the classical expression at low speeds.

A Relativistic Collision

Classically, we perform a collision by finding $\boldsymbol{v}_{CM}$ and $\boldsymbol{v}_r$ and rotating $\boldsymbol{v}_r$ about $\boldsymbol{v}_{CM}$ according to a scattering probability distribution.

In principle we can still do this, but it's awkward. When we collide two particles with proper velocities $\mathbf{u} = (1\text{e}10 \pm 1\text{e}9{,}0{,}0)$ they can scatter like this while conserving momentum and energy:



Not spherical!

A Relativistic Collision

The most convenient way to do this is to find $\mathbf{u}_{\mathrm{CM}}$ and then shift the particle velocities to that frame.

$$\boldsymbol{v}_{\mathrm{CM}} = \frac{m_1 \boldsymbol{u}_1 + m_2 \boldsymbol{u}_2}{\gamma_1 m_1 + \gamma_2 m_2}$$

$$\boldsymbol{u}_{\mathrm{CM}} = \frac{m_1 \boldsymbol{u}_1 + m_2 \boldsymbol{u}_2}{E_{CM}/c^2}$$

We can shift a proper velocity **u** by a proper velocity **w** like this:

$$\boldsymbol{u} \oplus \boldsymbol{w} = \boldsymbol{u} + \boldsymbol{w}\left(\frac{\gamma_w - 1}{w^2}(\boldsymbol{u} \cdot \boldsymbol{w}) - \gamma_u\right)$$

Collision Rate

$$n_1 n_2 \boldsymbol{v_r} \sigma$$

We're going to keep σ as-is, as a function of E_{CM} (though you still need to be using the right cross-section!)

$n_1 n_2 \boldsymbol{v_r}$ is tricky. We know that SR does weird things with clocks and distances, but can't we just do this from our perspective in the lab?

We need a quantity that is Lorentz invariant. It turns out (Moller 1945) that if you use:

$$\boldsymbol{v}_r = \sqrt{(\boldsymbol{v}_1 - \boldsymbol{v}_2)^2 - (\boldsymbol{v}_1 \times \boldsymbol{v}_2)^2 / c^2}$$

you get the correct Lorentz-invariant collision rate.

Relativistic DSMC

- Get a number of selections from the density and $(\boldsymbol{v}_r\sigma)_{max}$
- Pick two random particles.

$$\boldsymbol{v}_r = \sqrt{(\boldsymbol{v}_1 - \boldsymbol{v}_2)^2 - (\boldsymbol{v}_1 \times \boldsymbol{v}_2)^2 / c^2}$$

$$\sigma = \sigma(E)$$

- The probability that they collide is $\boldsymbol{v}_r\sigma/(\boldsymbol{v}_r\sigma)_{max}$

If they collide:

- Transform to the CM frame
- Randomly rotate $\boldsymbol{u}_r$ and then apply it back to the particles
- Transform back to the lab frame

Relativistic Equilibrium

Maxwell-Jüttner is the relativistic equivalent of the Maxwell-Boltzmann distribution:

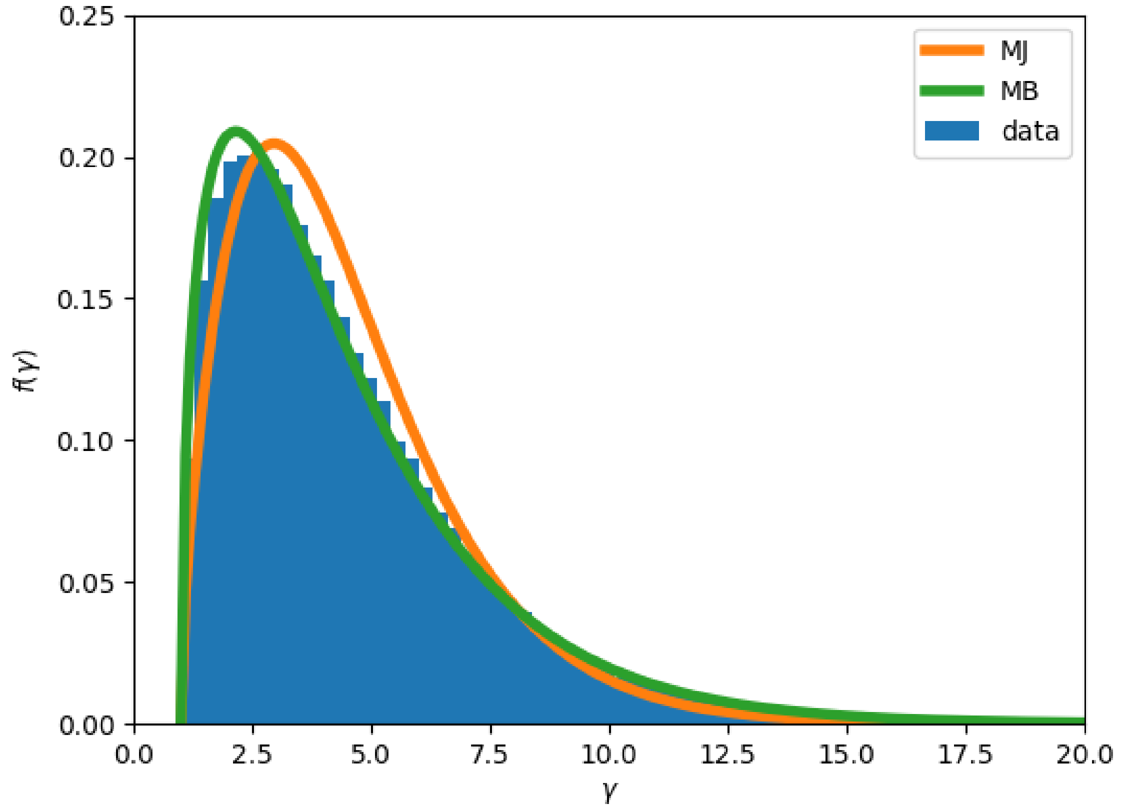
$$f(\mathbf{p}) = \frac{1}{4\pi m^3 c^3 \theta K_2(1/\theta)} \exp\left(-\frac{\gamma(p)}{\theta}\right) \qquad \text{, where } \theta = \frac{kT}{mc^2}$$

As before, this should be the distribution that yields detailed balance for any reasonable collision model.

Because $E = \gamma mc^2$, it has the same property as Maxwell-Boltzmann that $f(\boldsymbol{u}_1)f(\boldsymbol{u}_2) = h(E)$

Maxwell Molecules

Because these 3D velocity distributions are spherically symmetric, it's convenient to instead look at distributions of energy or speed.



For a long time I couldn't get the right equilibrium distribution and my answer was closer to a M-B energy distribution.

Maxwell Molecules

To make things easy on myself, I said that every pair of particles was equally likely to collide.

These are Maxwell molecules, $\sigma = \frac{\sigma_{ref}}{v_r}$, so that $\mathrm{v_r}\sigma = \sigma_{ref}$.

The problem was that there's no $\sigma(E_{CM})$ that can do this relativistically. Classically it's possible because $E_{CM} = \frac{1}{2}\mu v_r^2$.

Instead define a Maxwell-like cross-section as:

$$\sigma = \frac{\sigma_{ref}}{\sqrt{\frac{2}{\mu}E_{CM}}}$$

Detailed Balance

There are a few ways to think about what's going wrong here.

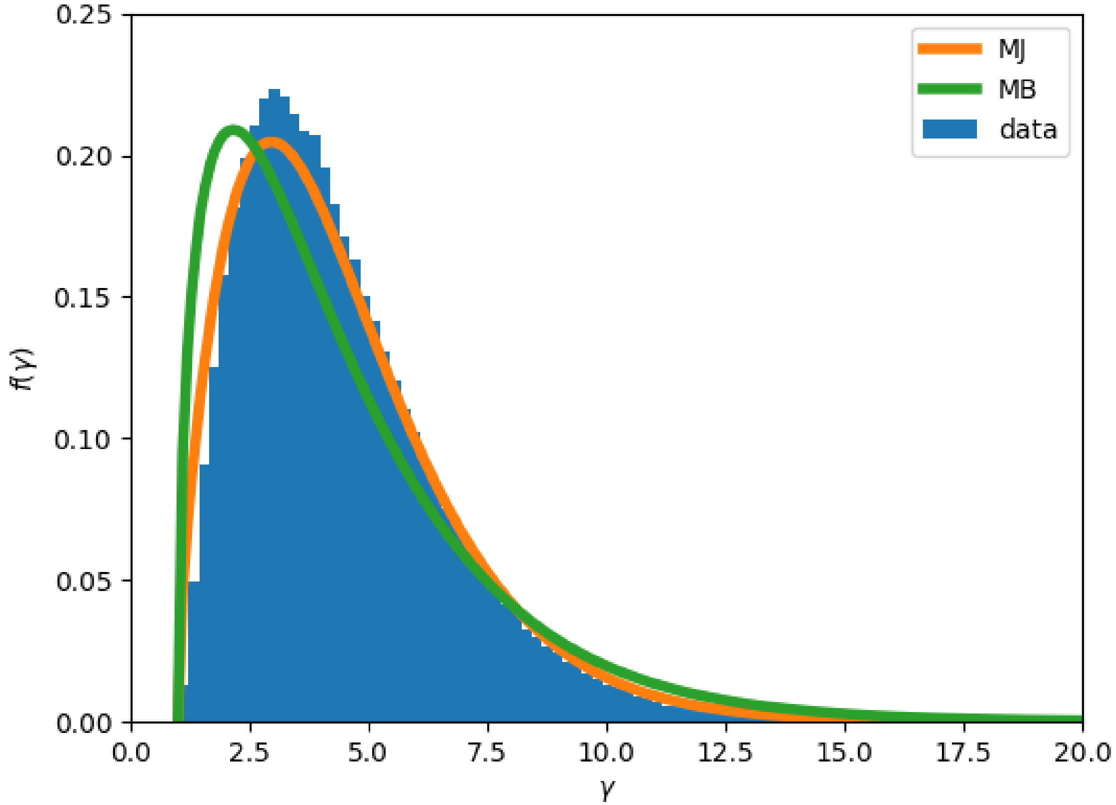
Peano et al. (2009) encountered a similar issue and ascribed it to the need for the collision rate to be a Lorentz invariant.

But also we are restricted to functional forms for the cross-section that can possibly satisfy detailed balance at equilibrium.

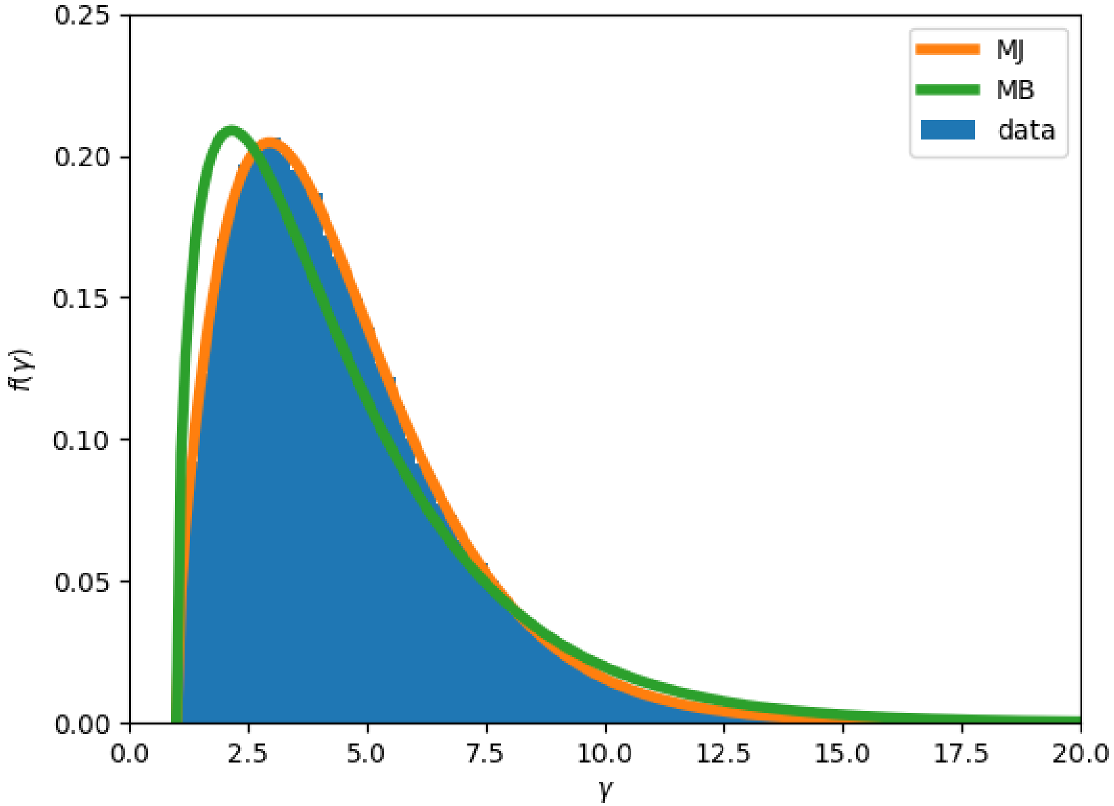
Under SR an iso-energy contour is an ellipsoid, not a sphere. This implies that $v_r\sigma$ *cannot* be equal for pre-collision and post-collision velocities. And so a constant value can't give detailed balance.

Relativistic Equilibrium

When my collision probability was wrong, I didn't get the right equilibrium because I didn't have detailed balance in an M-J distribution.



Initial condition



Equilibrium

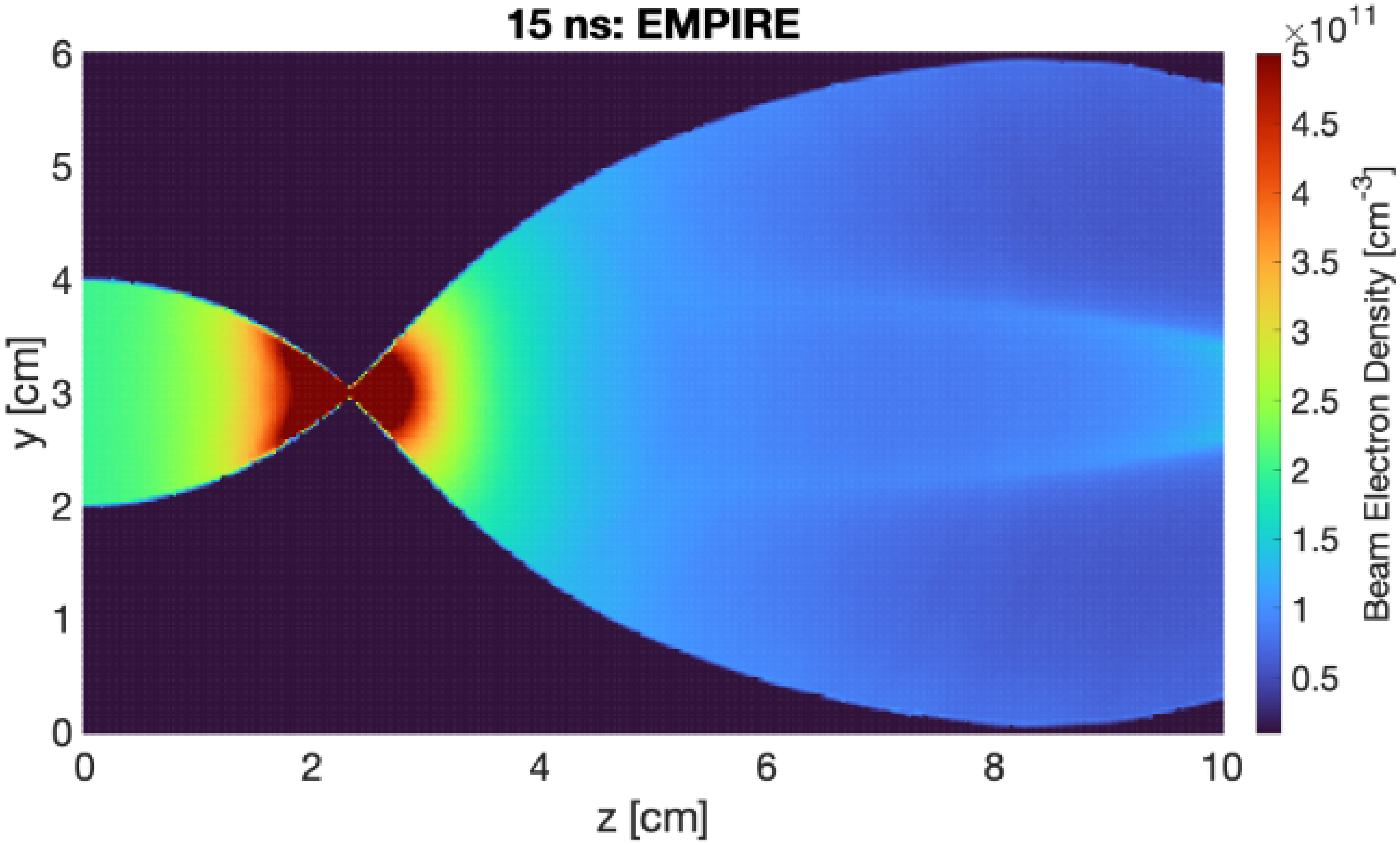
Beam Simulations

We use this algorithm in all of our collisional simulations now.

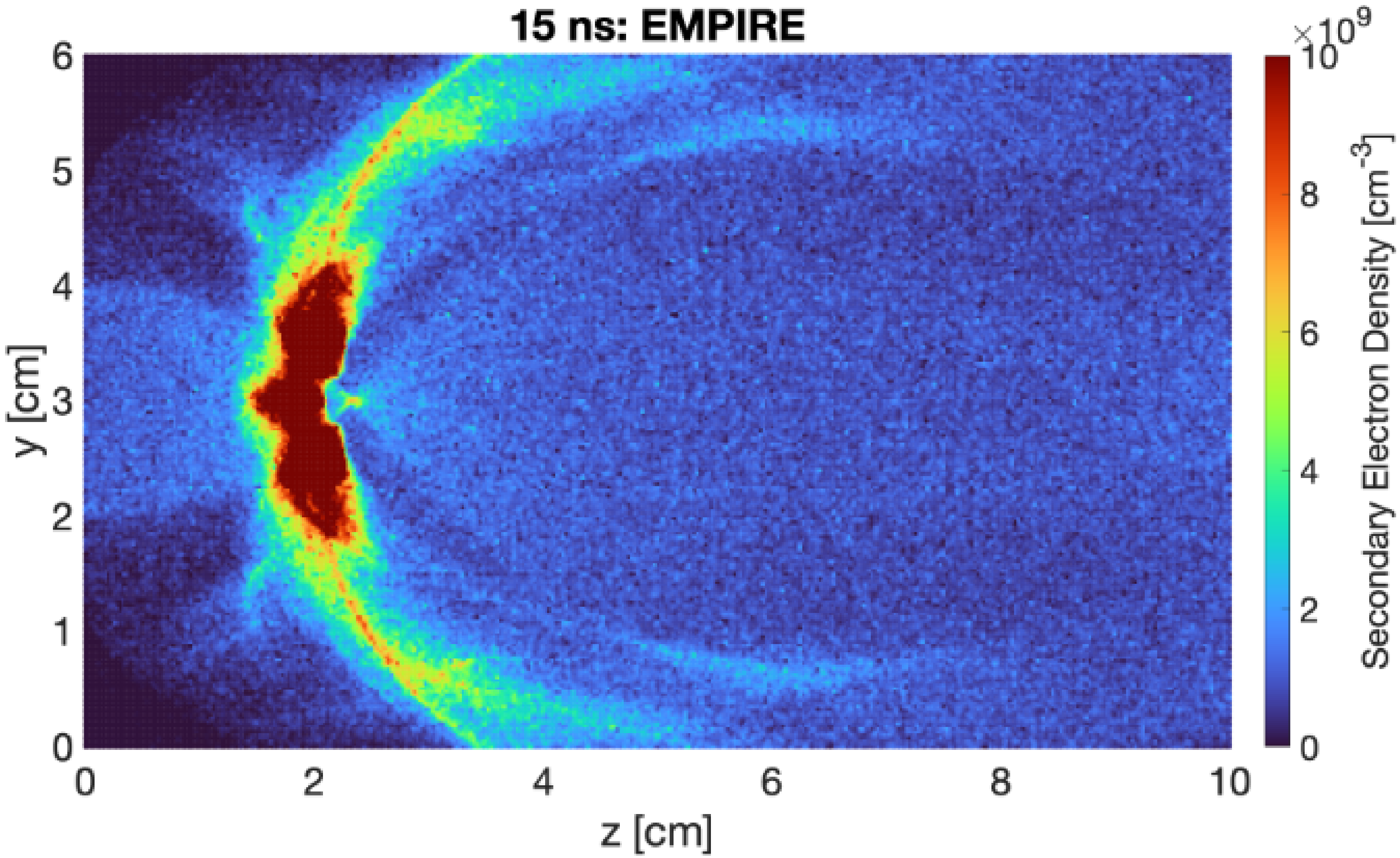
We've been comparing and getting good agreement with Cesta's hybrid GAZEL code (see forthcoming paper from Brandon Medina).

One case Brandon has run is a 0.5 MeV electron beam into 0.1 mbar argon. These electrons are relativistic – about 2.5×10^8 m/s. If interpreted classically this energy would give a speed > c.

0.5 MeV electron beam into 0.1 mbar Ar



0.5 MeV electron beam into 0.1 mbar Ar



Conclusion

- EMPIRE has a single code path that efficiently performs collisions from low to relativistic energies.

- There are a number of “gotchas” to watch out for when implementing such a scheme.

- The conference paper will aim to be a cookbook for implementing the algorithm.

Questions
?

Temperature

Classically, you can get temperature from particle kinetic energy as:

$$T = \frac{m\overline{v^2}}{3k_B}$$

There's not one uncontroversial way to get a relativistic temperature, but with the definition of temperature from the Hamiltonian you can get:

$$T = \frac{m\overline{\gamma v^2}}{3k_B}$$

This works well to parameterize the M-J distribution, but note that it's not proportional to kinetic energy and can change as a distribution changes shape.

Equilibrium

If there are no/weak external forces, if you let a cloud of particles collide with itself long enough, you get a Maxwell-Boltzmann distribution:

$$f(v)\, d^3v = \left(\frac{m}{2\pi kT}\right)^{3/2} e^{-\frac{mv^2}{2kT}}\, d^3v,$$

This the distribution that yields detailed balance for collisions where $\sigma(E)$ and scattering is symmetric, where $N(\boldsymbol{v}_1, \boldsymbol{v}_2 \rightarrow \boldsymbol{v}_3, \boldsymbol{v}_4) = N(\boldsymbol{v}_3, \boldsymbol{v}_4 \rightarrow \boldsymbol{v}_1, \boldsymbol{v}_2)$

The joint pdf of a pair of velocities is just a function of the total kinetic energy:

$f(\boldsymbol{v}_1) f(\boldsymbol{v}_2) = h(v_1^2 + v_2^2)$

Detailed Balance

For elastic collisions we can write $f(\boldsymbol{u}_1)f(\boldsymbol{u}_2) = f(\boldsymbol{u'}_1)f(\boldsymbol{u'}_2)$

Detailed balance requires:

$$f(\boldsymbol{u}_1)f(\boldsymbol{u}_2)(v_r\sigma)d\boldsymbol{u} \;= f(\boldsymbol{u'}_1)f(\boldsymbol{u'}_2)(v_r\sigma)'d\boldsymbol{u}'$$

When velocities scatter about a sphere, we don't have to worry about the stretching of $d\boldsymbol{u}$. But under SR velocities scatter on an ellipsoid.

$f(\boldsymbol{u}_1)f(\boldsymbol{u}_2) = f(\boldsymbol{u'}_1)f(\boldsymbol{u'}_2)$, so $v_r\sigma$ can't be constant. The Moller flux factor in v_r suffices to account for the stretching of velocity space, so σ rather than $v_r\sigma$ should be constant for collisions at some energy.

That is, $\sigma = \sigma(E)$, where E is not a function of v_r