Modeling the Transport Equation for Cosmic Strings

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Abstract

This documentation prescribes an algorithm for modeling the transport equation for cosmic strings as proposed by V. Vanchurin and D. Schubring in [3]. We use Lebedev Quadrature as our method of numerical integration.

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Introduction

We would like to study numerically how a distribution of strings with both longitudinal and transverse collisions goes to equilibrium under various expanding backgrounds. For an introduction to Cosmic Strings, see [7]. This document will be organized as follows. In part I, we introduce the Transport Equation for interacting Nambu-Goto strings, and prescribe an algorithm to model the collision terms. In Part II, we introduce the gravitational term, and a technique for calculating its components. In part III we introduce a method of loop removal and present results.

1 Transport Equation

$$\frac{df}{dt} = \left(\frac{df}{dt}\right)_{collision} + \left(\frac{df}{dt}\right)_{spatial} + \left(\frac{df}{dt}\right)_{qravitational} \tag{1}$$

The transport equation:

$$\left(\frac{df(\mathbf{A}, \mathbf{B})}{dt}\right)_{snatial} + \left(\frac{d}{dt} + \mathcal{H}\left(\partial_A + \partial_B - (1 + \mathbf{A} \cdot \mathbf{B}) - 4(\mathbf{A} \cdot \mathbf{B})\right)\right) f(\mathbf{A}, \mathbf{B}) =$$

$$\frac{1}{\rho} \int d\mathbf{A}' d\mathbf{B}' \, \Gamma\left(f(\mathbf{A}', \mathbf{B}) f(\mathbf{A}, \mathbf{B}') - f(\mathbf{A}, \mathbf{B}) f(\mathbf{A}', \mathbf{B}')\right) \tag{2}$$

More detail can be found on the spatial term in [Ref. 3, Eq. 5.5]. For the purposes of this paper, we will focus on the the collision and gravitational terms respectively. $\bf A$ and $\bf B$ are unit three-vectors on the sphere and correspond to tangent vectors of right and left moving waves. We can also define the quantities $\bf u$ and $\bf v$, which are also unit vectors that correspond to longitudinal and transverse velocities for string segments.

$$\mathbf{v} = \frac{\mathbf{A} + \mathbf{B}}{2}$$

$$\mathbf{u} = \frac{\mathbf{B} - \mathbf{A}}{2}$$

And since \mathbf{u} and \mathbf{v} can both be written in terms of \mathbf{A} and \mathbf{B} , this says that if $\mathbf{A}=-\mathbf{B}$, then the propagation is all along \mathbf{u} . Likewise, if $\mathbf{A}=\mathbf{B}$, then $\mathbf{u}=0$ and everything is along \mathbf{v} .

In the homogeneous limit, and ignoring gravitational effects, the localized transport equation reduces to just the right hand side, which is the collision term from (1):

$$\left(\frac{df}{dt}\right)_{collision} = \left(\frac{df}{dt}\right)_{transverse} + \left(\frac{df}{dt}\right)_{longitudinal}$$
(3)

$$\left(\frac{df}{dt}\right)_{collision} = \frac{1}{\rho} \int d\mathbf{A}' d\mathbf{B}' \, \Gamma\left(f(\mathbf{A}', \mathbf{B}) f(\mathbf{A}, \mathbf{B}') - f(\mathbf{A}, \mathbf{B}) f(\mathbf{A}', \mathbf{B}')\right) \quad (4)$$

So to start out, we are going to model the collision term on its own. As we can see from (4), we must integrate over \mathbf{A}' and \mathbf{B}' , which are unit vectors on the sphere and correspond to right and left moving tangent vectors. They depend on two coordinates. The azimuthal angle ϕ , and polar angle θ .

1.1 Lebedev Quadrature

Naively, solving (4) numerically, involves four integrals at each time step because A and B have two components each, which implies we have four nested loops (one for each component). But a numerical integration technique known as quadrature will help us to improve upon this. This is an important step, so some time will be spent ensuring you understand the technique and benefits of using it. Lebedev quadrature gives an approximation to the surface integral of a function over the sphere. When using Lebedev Quadrature, the distribution of points on the sphere (the points where your function is evaluated) have octahedral symmetry, which means the location of the points remain invariant under certain types of transformations. In addition, the points are relatively evenly distributed. Quadrature requires only one summation to perform a 2dimensional integral, although the number of iterations required would be the same as the naive approach. The main benefit is that the distribution of points does not bunch up near the poles, as in the naive approach. The technique also allows for exact integration of spherical harmonics, which will be extremely useful when evaluating the gravitational terms.

The core of this technique comes from a set of points on the sphere and corresponding weights for each point. These are known as "rules", and Vyacheslav Lebedev computed many of them using an algebraic method in the late seventies. So techniques exist for computing them on your own, but in the end vou will end up with a list of points and corresponding weights. John Burkardt from Florida State University has been so kind as to provide individual text files ranked in order of precision (the maximum order of the polynomial evaluated) referenced in [5]. My advice would be download them and use which ever order of precision you find necessary. A rule of precision p can be used to correctly integrate any polynomial for which the highest degree term $x^i y^j z^k$ satisfies $i+j+k \le p$. For example, a polynomial with i+j+k=3 has precision 3 and requires 6 points to correctly integrate. Higher precision requires a higher number of points, and in turn, requires more time to integrate. Thus the level of precision you choose is limited by the computational resources available. But the types of functions you wish to integrate may be sensitive to this precision as well. The level of precision is a side-note at this point, but will be discussed in more detail as we move on to discuss the gravitational terms in Part III.

When we integrate a function $f(\theta, \phi)$ over the surface of the unit sphere, we expect to get a number, a.

$$a = \int_{0}^{2\pi} \int_{0}^{\pi} f(\theta, \phi) \sin(\theta) d\theta d\phi$$

The naive approach would be to take interval of your coordinates and split them up into N pieces that correspond to the step-size, $\Delta x = 1/N$. You then make an array of your coordinates over which you are integrating and plug those into your function as you sum it up N times, multiplying by step size each iteration. The naive approach yields two summations for an integral in spherical coordinates on a unit sphere:

$$a = \sum_{i=0}^{N} \sum_{j=0}^{M} f(\theta_i, \phi_j) sin(\theta_i) \Delta \theta \Delta \phi$$

where

$$\Delta\theta = \frac{\pi}{N}$$

$$\Delta \phi = \frac{2\pi}{M}$$

The other facet of the naive approach is the fact that near the poles of the unit sphere, there are more "pieces" and hence more time is spent evaluating these parts of a function. Quadrature is a little different. We still require the list of coordinates (provided by the rule you choose), only now we multiply by the weight each iteration. These weights will be different depending on the location of the point, as opposed to the naive approach where Δx is constant. It allows us to give the same amount of computation time to points near the poles as we would of points around the azimuth. We can think of this as a way of making the points we evaluate the function at as being equidistant apart.

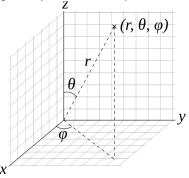
But before we get to the algorithm needed to perform Lebedev Quadrature, we need to develop a way to access the points and their corresponding weights. The first thing our algorithm requires is a "Point" object. This object has an important role to play. It will be a container for the file which contains the Lebedev points and their weights. Ideally, we would like to use an array of Point objects, each representing a specific point on the sphere. It should have a few basic functions built in: One for setting the coordinates of a particular point and its weight, and three for retrieving each individual component. If you have n points to store, then this should work:

Note that the above algorithm treats the first column as the θ -coordinate (i.e. the polar angle), and the second column as the ϕ -coordinate (i.e. the azimuthal angle). John Burkardt's rules treat these columns in the opposite way. Column one is labelled $\phi\epsilon[0,\pi]$ and column two is labelled $\theta\epsilon[-\pi,\pi]$ such that the traditional formulae used to convert between Spherical and Cartesian coordinate systems swap z=cos(theta) for z=cos(phi), as well as the coordinates

Algorithm 1 Read in weight and coordinate data from file

```
\begin{array}{ll} \textbf{for} & (i=0;\,i< N;\,i++) \ \textbf{do} \\ & infile(theta[i],phi[i],weight[i]) \ \{\text{fill arrays with} \theta_i,\phi_i,w_i \ \text{from 3-column} \\ & \text{data file} \} \\ & Point[i].SetTheta(theta[i]) \\ & Point[i].SetPhi(phi[i]) \\ & Point[i].SetWeight(weight[i]) \\ & \textbf{end for} \end{array}
```

in the formula for x and y. In this documentation, and the code referenced in [6], we will be treating column one as $\theta \epsilon [0, 2\pi]$, and column two as $\phi \epsilon [-\pi, \pi]$. Graphically this is what you would expect.



Where the Cartesian coordinates are given by,

 $x = sin(\theta)cos(\phi)$

 $y = sin(\theta)sin(\phi)$

 $z = cos(\theta)$

What you call theta and phi are determined only by preference, but care must be taken to be completely consistent in these preferences when defining your vector math, as well as the Spherical Harmonic functions used later.

Now, we are ready to integrate some functions. The format to integrate using the Lebedev Quadrature goes like,

$$a = \sum_{i=0}^{n} 4\pi f(\theta_i, \phi_i) w_i \tag{5}$$

Algorithm 2 General integration using Lebedev Quadrature

 $\begin{array}{ll} \mathbf{for} & (i=0;\, i < N;\, i++) & \mathbf{do} \\ & a = a + 4\pi f(Point[i].GetTheta())\, f(Point[i].GetPhi())\, Point[i].GetWeight() \end{array}$

end for

Where w_i is the weight corresponding to the two points. Notice there is no sine function here as would normally appear when integrating in spherical coordinates. We also have a factor of 4π out front. This implies that summing over the weights should sum to one, which they do. So that is a good first test. Adding the constant factor out front gives the correct surface area of a unit sphere. Now try integrating $f(\theta,\phi)=x^2y^2z^2$. This is a spherical harmonic. It should evaluate exactly. Recalling the rule for integration using the Lebedev Quadrature, $i+j+k \leq p$, p must be at least 6. Therefore the minimum number of points we can use for the function to evaluate exactly is 26, with a precision of 7. The function should come out to be $\frac{4\pi}{105}\approx 0.11968$. Algorithmically, we have:

$$a = \sum_{i=0}^{n} 4\pi \sin(\theta_i)^4 \cos(\theta_i)^2 \sin(\phi_i)^2 \cos(\phi_i)^2 w_i$$

Algorithm 3 Integrate $f(\theta, \phi) = x^2 y^2 z^2$

 $\begin{array}{ll} \textbf{for} & (i=0;\, i< N;\, i++) & \textbf{do} \\ & a=a+4\pi \sin(Point[i].GetTheta())^4 cos(Point[i].GetTheta())^2 \\ & sin(Point[i].GetPhi())^2 cos(Point[i].GetPhi())^2 Point[i].GetWeight() \end{array}$

end for

If you use the appropriate rule, the function will evaluate exactly as you would expect. However, what happens if you choose the prior set of points (p=5, with 14 points)? We get an answer over twice our expectation, $a \approx 0.279253$. Cleary taking care to use a precision high enough to deal with the polynomial evaluated is important.

Now let's try a function which is not a spherical harmonic, $f(\theta, \phi) = \cos(\theta)^4 \sin(\phi)^4$.

$$a = \sum_{i=0}^{n} 4\pi \cos(\theta)^4 \sin(\phi)^4 w_i$$

It should integrate to $\frac{3\pi}{10}$. Here you will notice a sensitivity to the number of points used because this function is not a spherical harmonic. When calculated using a rule of 11 (50 Points), we are within 92.9% of the correct value, but it's not exact. Using a rule with precision 17 (110 points) yields a result within 99.7%. Burkardt provides rules for precisions all the way up to 131 (5810 Points), but these will be outside the computational feasibility for our task. Most likely we will be operating between 26 and 110 points because most of the functions we will be dealing with will be spherical harmonics and therefore will be easy to evaluate using this method. Numerically this provides a good trade-off for speed while not sacrificing much accuracy. Now armed with our integration technique, we are ready to simulate the collision terms.

1.2 Numerical Transport Equation Collision Term

Recall that the collision terms evolve according to (4). Moving dt to the right hand side gives the rule for evolution at each time step $\triangle t$:

$$(df(\mathbf{A}, \mathbf{B}))_{col} = \frac{1}{\rho} \int d\mathbf{A}' d\mathbf{B}' \Gamma(f(\mathbf{A}', \mathbf{B}) f(\mathbf{A}, \mathbf{B}') - f(\mathbf{A}, \mathbf{B}) f(\mathbf{A}', \mathbf{B}')) dt$$
(6)

where

$$\Gamma(A, B, A', B') = \lambda(\frac{1}{\mu}) + \mu \rho p P(A, B, A', B')$$
 (7)

Both λ and p are probabilities. For now, we set both to 1, as well as the correlation length μ . Later on we will calculate μ dynamically. In terms of Lebedev Quadrature, we index over arrays labeled by the points A,B,A', and B' such that equation 9 becomes:

$$(df(A,B))_{col} = \sum_{A'=0}^{n} \sum_{B'=0}^{n} \frac{1}{\rho} w_{A'} w_{B'} \Gamma_{A,B,A',B'} \left(f(A',B) f(A,B') - f(A,B) f(A',B') \right) \Delta t$$
(8)

The first step is to create a time loop. The time loop is an iterative loop that goes from $t=t_0$ to $t=t_{max}$. Either of these constants are arbitrary, which is a benefit of the statistical approach. Defining $t_{max}\gg t_0$ so we have a long time to see if the system equilibrates. Then we also define the proper time, τ . This is a way of keeping track of the time according to your step size, as opposed to the iterative value of t.

$$T = t_0 + t \triangle t$$

The step size Δt will be somewhat arbitrary, although you will find that smaller step sizes allow you to probe finer details of the system as it equilibrates. This is something you can set at run-time. So your main loop has the form:

Everything we do from here on will take place within this loop.

Next we need to setup two arrays, one for $df(\mathbf{A}, \mathbf{B})$, and one for $f(\mathbf{A}, \mathbf{B})$.

Algorithm 4 Main time-loop

```
\begin{array}{ll} \mathbf{while} & t < t_{max} & \mathbf{do} \\ & \tau = t_0 + t \, \Delta t \\ & \{ \text{all calculations will go here} \} \\ & t++ \\ & \mathbf{end \ while} \end{array}
```

The first thing we need for this step is to setup a distribution function $f(\mathbf{A}, \mathbf{B})$. Luckily, the distribution function is just a 2-d matrix that is a place a holder for what the evolution does. It is indexed by the Lebedev points. So we simply need to define an empty 2-dimensional array. The same goes for $df(\mathbf{A}, \mathbf{B})$. The integration takes place within one time step Δt . We then update the matrix f[A][B], and repeat the operation for an arbitrary length of time τ . When the system reaches equilibrium, every component of df[A][B] should be zero (to a close numerical approximation).

Note that the iterators A, B, A', B' are simply integers that index our matrices. We use this convention just to keep our notation clear. The real coordinate values contained at a point come from our Point object and the corresponding weight. We then put the entire integration function inside the time loop.

Before we can model (8), we need to define a few more quantities. First The normalization term comes from the energy density, ρ . To calculate the energy density, simply integrate over the probability density function f(A,B).

$$\rho = \int f(\mathbf{A}, \mathbf{B}) \, d\mathbf{A} \, d\mathbf{B} \tag{9}$$

This is something that we now know how to do:

$$\rho = \sum_{A}^{n} \sum_{B}^{n} f(A, B) w_A w_B$$

Algorithm 5 Calculate the energy density using Lebedev Quadrature

The other term we need to define is from (7), $\Gamma(P,p)$. It depends on the cross-sectional volume element P, and the inter-commutation probability p. These terms tell us about the likelihood for strings to interact on their world sheets (see [4]). The volume element P contains wedge products (or a few dot and cross products) between points on the sphere. In general, Γ describes the rate

of interaction between string segments within the volume defined by P due to transverse collisions.

$$P = |A^{\hat{}}B^{\hat{}}A'^{\hat{}}B'|$$

$$P \propto |(v' - v) \cdot (u' \times u)| = \frac{1}{8} |(A' + B' - A - B) \cdot ((B' - A') \times (B - A))|$$

The 1 in (7) corresponds to the probability of longitudinal collisions. For now, this probability is unity, but it can be tweaked later on. You could calculate Γ directly in the inner-most loop using some vector math, but that turns out to be computationally expensive. Since the wedge product terms in P turn out to be a function of only the Lebedev points, we can calculate it one time before we even start the time loop, and then just index a 4-d array in which the values have been stored. In fact, a good rule of thumb is to keep the inner-loop as free of actual computation as possible. This means, do not call functions within the inner loops. Instead, try to do actual computation outside the loop and just store the values in an array to be iterated over. It is much more efficient to just look at memory locations rather than to call functions. This is true in C++ and likely the case in any other object-oriented programming language.

Algorithm 6 Store the wedge product terms to 4-d array

```
\begin{array}{l} \mbox{ for } (A=0;\,A< N;\,A++) \ \mbox{ do } \\ \mbox{ for } (B=0;\,B< N;\,B++) \ \mbox{ do } \\ \mbox{ for } (A=0;\,A< N;\,A++) \ \mbox{ do } \\ \mbox{ for } (B=0;\,B< N;\,B++) \ \mbox{ do } \\ \mbox{ } P[A][B][A'][B'] \ = \ (\frac{1}{8}) \, abs(\,(Point[A']+Point[B']-Point[A]-Point[A])) \, ) \\ \mbox{ end } \mbox{ for } \\ \mbox{ end for } \\ \mb
```

Here \circ and \times are taken to be the traditional dot and cross products for three-vectors. This brings us to an important aside. Your Point object should be capable of doing basic vector math. That is, you need to define an overloaded operator, or some function which computes cross and dot products by converting between spherical and Cartesian coordinates. You should also have a way to do vector addition and scalar multiplication. Later, we will also require that points go back and forth between spherical and Cartesian coordinate systems. So your Point object should have some additional functions, like GetX(), GetY(), GetZ(). Using overloaded operators, you can also define a wedge product such that the above code will be simplified further. The ability to do vector math in a compact and intuitive way is very helpful, but greatly depends on the language which you program in. In C++, operator overloading is by far the superior method due to its compactness. But one can use functions that perform the

above tasks just as quickly, or separate libraries like Boost, in which you can call predefined functions for most vector and matrix math.

Now that we have defined P, we can iterate over the stored values and set up our final integration step in modeling the collision terms.

$$(df(A,B))_{col} = \sum_{A'=0}^{n} \sum_{B'=0}^{n} \frac{1}{\rho} w_{A'} w_{B'} \left(1 + p\rho P(A,B,A',B')\right) \left(f(A',B)f(A,B') - f(A,B)f(A',B')\right) \Delta t$$

```
Algorithm 7 Calculate the collision term (df(A, B))_{col}
```

```
\begin{array}{l} \mbox{ for } (A=0;\,A< N;\,A++) \ \mbox{ do } \\ \mbox{ for } (B=0;\,B< N;\,B++) \ \mbox{ do } \\ \mbox{ for } (A=0;\,A< N;\,A++) \ \mbox{ do } \\ \mbox{ for } (B=0;\,B< N;\,B++) \ \mbox{ do } \\ \mbox{ } df[A][B]=df[A][B]+(\frac{1}{\rho})\,(1+\rho pP[A][B][A'][B'])(f[A'][B]f[A][B']-\\ \mbox{ } f[A][B]f[A'][B'])\,Point[A'].GetWeight()\,Point[B'].GetWeight()\Delta t \\ \mbox{ end for } \\ \mbox{ en
```

Then, simply add the change due to collisions back into the distribution function.

```
Algorithm 8 Update the distribution
```

```
for (A = 0; A < N; A + +) do
for (B = 0; B < N; B + +) do
f[A][B] = f[A][B] + df[A][B]
end for
end for
```

The time loop then starts over, and we repeat the operation.

1.3 Initial Conditions

Of course, the pseudo-code above will not do anything just yet because we have not filled the distribution function array with any values. We must fill f[A][B] with initial conditions from which the transport equation will determine the system's evolution. We need an initial distribution function on the sphere such that we can easily define a peak on the A and B spheres. This allows us to manipulate the initial average u and v with which the system starts out with.

In [4], it was thought that the distribution function need to be of a particular form. A probability distribution on the sphere is called a Von-Mis Fisher distribution. It is basically a Gaussian distribution peaked around some particular

 (θ, ϕ) on the unit sphere. However, you will find through numerical analysis that any non-factorisable distribution on the sphere eventually goes to equilibrium. Still the Von Mises-Fisher Distribution is extremely useful in setting initial conditions because it allows you to control the average direction velocities are peaked in. It is defined as:

$$VMF(A,B) = \frac{exp\left(\frac{a\cdot A}{\alpha} + \frac{b\cdot B}{\beta}\right) + \Gamma}{16\pi^2 \alpha \beta \sinh\left(\frac{1}{\alpha}\right) \sinh\left(\frac{1}{\beta}\right)}$$
(10)

This function is a non-factorisable normalized distribution on the unit 4-sphere. It is non-factorisable due to the gamma term, which was defined in equation 10 above. It contains the dot and cross product terms. The mean directions are determined by **a** and **b** on their respective spheres. For now, it suffices to say that non-factorisable initial distributions eventually equilibrate, and factorisable initial distributions are already in equilibrium. It's easiest to see what is meant by factorisable by example:

Factorisable: $e^{(x+y+z)} = f(x)f(y)f(z)$ Non-Factorisable: $e^{(xyz)} = f(x,y,z)$

In Statistical Mechanics, proving a system equilibrates requires we show that the distribution function (a distribution of velocities in a volume element) factorizes after enough time has passed. That is, we want to know whether a system that starts out as a big complicated mess, eventually settles down to something where the original parameters are no longer coupled. This obviously implies that systems in equilibrium must be factorisable. For a system of particles that means f(q,p) = f(q)f(p) in equilibrium. Intuitively, this just means that after a system has reached equilibrium, the velocities of particles are not correlated to their positions. There is an analogous conjecture for a distribution of strings with velocities $\mathbf{u}(\mathbf{A},\mathbf{B})$ and $\mathbf{v}(\mathbf{A},\mathbf{B})$. We will study this further in the next section.

1.4 H-Theorem

The first thing we can do once we have a distribution function that evolves according to a transport equation is prove an H-theorem for strings, which is analogous to Boltzmann's H-theorem for particles. This is the familiar notion that entropy of a system always increases. Because H is simply entropy without the minus sign, it should always decrease.

$$H(t) = \int d\mathbf{A} d\mathbf{B} f(\mathbf{A}, \mathbf{B}) \ln (f(\mathbf{A}, \mathbf{B}))$$

$$\frac{d}{dt}H \le 0$$

We see how H evolves numerically by evaluating the above integral at each time step. Algorithmically, this is the same approach as we took with the energy density integral:

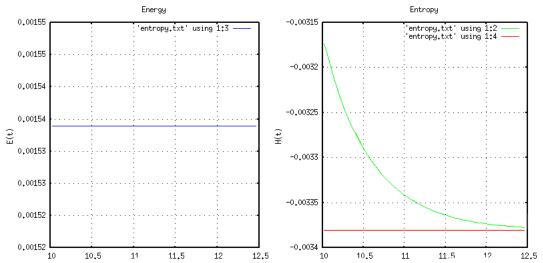
$$H = \sum_{A}^{n} \sum_{B}^{n} f(A, B) \ln(f(A, B)) w_A w_B$$

Algorithm 9 Calculate the entropy using Lebedev Quadrature

```
 \begin{array}{ll} \textbf{for} & (A=0;\ A< N;\ A++) & \textbf{do} \\ \textbf{for} & (B=0;\ B< N;\ B++) & \textbf{do} \\ & H=H+f[A][B]\log(f[A][B])\ Point[A].GetWeight()\ Point[B].GetWeight() \end{array}
```

end for end for

Boltzmann showed that H always decreases as long as the probability density function does not factorize. Thus the factorization of $f(\mathbf{A}, \mathbf{B})$ as $t \to \infty$ is a necessary condition for any equilibrium distribution to possess. Although Boltzmann's H-theorem was defined for particles in momentum space, it has been shown in [3] that indeed this condition is just as vital in showing a distribution of string segments moving with their corresponding velocities converges to an equilibrium distribution. So as the energy density ρ stays fixed, H should approach a limiting value determined by the entropy limit. If the entropy approaches this limit, then distribution function factorizes and the system is in equilibrium.



Our results here verify that the distribution converges to an equilibrium state which factorizes:

$$\lim_{t\to\infty}f(A,B,t)=\frac{1}{\rho}\int f(A,B')f(A',B)dA'dB'$$

And after integrating out A' and B', we have:

$$\lim_{t \to \infty} f(A, B, t) = f(A)f(B)$$

Which is exactly the requirement required by statistical mechanics proper for a probability density to equilibrate. The red line represents the entropy limit to which the entropy of the system will converge to at $t=\infty$. We are using sloppy language here because H is not really entropy, so the "entropy limit" is really the "H limit" but disregarding the minus sign, these are really the same quantities. It is calculated in the following way:

$$f(A) = \int \frac{f(\mathbf{A}, \mathbf{B})}{\rho} d\mathbf{B}$$

$$f(B) = \int \frac{f(\mathbf{A}, \mathbf{B})}{\rho} d\mathbf{A}$$

$$\mathcal{H}_{lim} = \int \rho f(\mathbf{A}) f(\mathbf{B}) ln(\rho f(\mathbf{A}) f(\mathbf{B}))$$

And in terms of the Lebedev Quadrature:

$$f(A) = \sum_{B}^{n} \frac{f(A, B)w_{B}}{\rho}$$

$$f(B) = \sum_{A}^{n} \frac{f(A, B)w_{A}}{\rho}$$

$$\mathcal{H}_{lim} = \sum_{A}^{n} \sum_{B}^{n} f(A) f(B) \ln(\rho f(A) f(B)) w_{A} w_{B}$$

1.5 Energy-Momentum Tensor

We can calculate the energy-momentum tensor by calculating the average x, y, and z values. This will allow us to calculate the pressure and the equation of state parameter p.

$$p = \rho w$$

We know how to calculate ρ , but the equation of state parameter is found through averaging over A and B, grabbing the Cartesian coordinates, then building a 3x3 matrix from the resulting quantities.

$$\langle A \rangle = \int Af(A,B)dB$$

$$\langle B \rangle = \int Bf(A,B)dA$$

Then the energy-momentum tensor is:

$$T_{ij} = \frac{< A_i > < B_j >}{\rho}$$

Thus,

$$w = \frac{Tr\left(F_{ij}\right)}{3\rho}$$

2 Adding the Gravitational Term

2.1 Introduction

In the previous section we determined that collisions between string segments could be modeled using (4). However, we made some assumptions in neglecting the other two terms in (1). In fact, ignoring the spatial and gravitational terms, the transport equation is valid in Minkowski space. But for a non trivial metric, such as one that includes expansion, we must add a new term which accounts for the effects. We'll still be ignoring the spatial term for now.

The actual terms for $\left(\frac{df}{dt}\right)_{gravitational}$ come from the left hand side of (2). Namely, the stuff with the Hubble parameter \mathcal{H} attached:

$$\left(\frac{df}{dt}\right)_{gravitational} = \mathcal{H}\left(\partial_A + \partial_B - (1 + A \cdot B) - 4(A \cdot B)\right) f(A, B) \tag{11}$$

The operators ∂_A and ∂_B can be reduced to theta derivatives:

$$\partial_A = sin(\theta_B) \frac{\partial}{\partial \theta_B}$$

$$\partial_B = sin(\theta_A) \frac{\partial}{\partial \theta_A}$$

We can access the components of each Point object, so we can actually represent these operators as something workable now:

$$\partial_A = -\sum_{i=1}^3 B_i sin(\theta_i) \frac{\partial}{\partial \theta_i}$$
 (12)

$$\partial_B = -\sum_{i=1}^3 A_i \sin(\theta_i) \frac{\partial}{\partial \theta_i}$$
 (13)

Here, i ranges over the Cartesian components of the Point A and B just like before, but the derivative term $\frac{d}{d\theta_i}$ is something new. These operators take the theta derivative in the i direction on the sphere. So we'd like a way to easily take derivatives of f(A,B) along x, y, and z with respect to theta. Then we act these operators on f(A,B) at every time step, and add this effect in as we update the distribution function. The first step is to create a new array that holds the values of $\left(\frac{df}{dt}\right)_{grav}$. So in the end, equation (21) is another 2-d array:

Algorithm 10 Calculate the gravitational term $(df(A, B))_{arav}$

```
\begin{array}{lll} \textbf{for} & (A=0;\, A< N;\, A++) & \textbf{do} \\ \textbf{for} & (B=0;\, B< N;\, B++) & \textbf{do} \\ & df_g[A][B] & = & \mathcal{H}\left(\partial_A[A][B] \ + \ \partial_B[A][B] \ - \ 1 \ - \ 5(Point[A] \ \circ \ Point[B]) \right) f[A][B] \Delta t \\ & \textbf{end for} \\ \textbf{end for} \end{array}
```

And then we update the distribution function f(A,B) like in Algorithm 8:

Algorithm 11 Update the distribution with the gravitational term

```
for (A = 0; A < N; A + +) do
for (B = 0; B < N; B + +) do
f[A][B] = f[A][B] + df[A][B] + df_g[A][B]
end for
end for
```

But how do we calculate the terms that go into $\left(\frac{df}{dt}\right)_{grav}$? We'll ignore the derivative terms for now (we'll deal with them in the next section). We know how to take the dot product between the two point objects **A** and **B**. Likewise, the Hubble parameter \mathcal{H} is a function of of the time τ , and is simple to calculate. This is the term that adds the expansion due to the metric. In particular, we'll be dealing with the Friedmann metric in conformally flat space-time:

$$ds^{2} = a^{2}(t)(t^{2} - x^{2} - y^{2} - z^{2})$$
$$\mathcal{H} = \left(\frac{\dot{a}}{a}\right)$$

$$a(t) \propto t^{\frac{2}{n}}$$

$$\rho \propto a^{-n} \propto t^{-\frac{2}{n}} \tag{14}$$

What we are interested in doing is having a function that accounts for expansion as a function of time. In Cosmology, this is the role that the Hubble parameter plays. We can find an expression for it by using the fact that the scale factor $a(\tau)$ is expressed as a function of time, and likewise for its derivative:

$$\dot{a}(t) \propto \left(\frac{2}{n}\right) t^{\left(\frac{2}{n}-1\right)}$$

$$\mathcal{H} = \left(\frac{\dot{a}}{a}\right) \propto \frac{\left(\frac{2}{n}\right) t^{\left(\frac{2}{n}-1\right)}}{t^{\left(\frac{2}{n}\right)}} \propto \frac{2}{nt} \text{ where n is an integer which takes on values of } 2.3, \text{ and } 4.$$

These n-values correspond to different eras in the expansion rate of the universe. When the universe was too hot for normal matter to form, n=4. This is referred to as a radiation dominated expansion rate. The Hubble parameter is $\mathcal{H} = \frac{1}{2t}$ for this era. Likewise, the matter dominated era refers to later times, and $\mathcal{H} = \frac{2}{3t}$. The quantity which we can probe comes from (12). It implies that when we include expansion in either of these two eras, we should find that the energy density falls off as $-\frac{2}{3}$ for matter dominated, and $-\frac{1}{2}$ for radiation. If we look at a log-log plot of energy density vs time, we will find that the slope of that line should match the predictions for the rate (either $-\frac{2}{3}$ or $-\frac{1}{2}$). This will be a powerful test to determine if the gravitational term is working. However, there is a caveat. This prediction for the energy density to fall off at a rate of $-\frac{2}{n}$ is only valid for particular initial conditions.

Recall from the introduction that we defined two quantities, u and v. These were unit vectors that describe the longitudinal and transverse velocities along strings. The predicted numerical values of the energy density decay's power are only valid in the case where $\langle v^2 \rangle = \frac{1}{2}$. Using the VMF distribution, we can choose initial conditions such that we have large peaks that point in the same direction on both the A and B spheres as discussed in section 1.3. By setting up the initial conditions correctly (a=b), we can set to start out near $\langle v^2 \rangle = \frac{1}{2}$ and watch as the system evolves to see how the energy density falls off.

So we need a way of calculating \mathbf{v} , such that we can check the decay rate of the energy density. Fortunately, this is easy. To calculate the expectation value of a quantity using a probability density, we simply integrate over the density function while multiplying by the quantity which we want averaged. Since \mathbf{u} and \mathbf{v} are just functions of \mathbf{A} and \mathbf{B} , we have:

$$< v^2 > = \int \frac{v^2 f(\mathbf{A}, \mathbf{B}) d\mathbf{A} d\mathbf{B}}{\rho}$$

where
$$\mathbf{v} = \frac{\mathbf{A} + \mathbf{B}}{2}$$

Then, we can also define $\langle v \rangle^2$, which we need $\langle \mathbf{v} \rangle$ to calculate:

$$<\mathbf{v}> = \int \frac{\mathbf{v} f(\mathbf{A}, \mathbf{B}) d\mathbf{A} d\mathbf{B}}{\rho}$$

Then,

$$< v >^2 = < \mathbf{v} > \circ < \mathbf{v} >$$

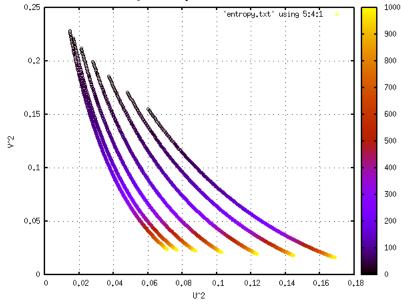
And likewise for **u**. The pseudo-code is what you'd expect:

```
Algorithm 12 Update the distribution with the gravitational term
```

```
\begin{array}{l} \textbf{for} \ \ (A=0;\,A<N;\,A++) \ \ \textbf{do} \\ \textbf{for} \ \ \ (B=0;\,B<N;\,B++) \ \ \textbf{do} \\ v=v+\big(\frac{Point[A]+Point[B]}{2}\big)\,f[A][B]\,Point[A].GetWeight()\,Point[B].GetWeight() \\ \left\{\text{recursive definition of } < v>\right\} \\ v^2=v^2+\big(\frac{Point[A]+Point[B]}{2}\big)\circ\big(\frac{Point[A]+Point[B]}{2}\big)\,f[A][B]\,Point[A].GetWeight()\,Point[B].GetWeight() \\ \left\{\text{recursive definition of } < v^2>\right\} \\ \textbf{end for} \\ \textbf{end for} \end{array}
```

Here $<\mathbf{v}>$ is a vector, while $< v^2>$ is a scalar. Then $<\mathbf{v}>^2$ is found by dotting $<\mathbf{v}>$ with itself, which also ends up being scalar.

We can do the same for the quantities $< \mathbf{u} >^2$ and $< u^2 >$. Outputting these quantities will help us later on to determine if the gravitational terms are being calculated correctly. Since \mathbf{v} and \mathbf{u} are vector fields, we can compute field lines by running the simulation with different initial conditions, and then plot $< v >^2$ and $< u >^2$ as the system equilibrates:



The above plots were made by running through the simulation for 1000 time steps (color map), and then changing the mean direction as determined by the VMF distribution function given in section 1.3. We varied the mean direction of the initial conditions (i.e. where the peak of the distribution was highest) by changing the constant vectors **a** and **b** for each run.

Now we are ready to move on to calculating the derivative terms.

2.2 Integral Transform and Kernels

We now want to numerically compute the derivative terms in (11). There are many ways to take derivatives numerically, but because of our Lebedev points, the method we'll be using involves Spherical Harmonics. The way we calculate derivatives on the sphere using spherical harmonics is rooted in an integral transform. From this, we find an operator known as a "Kernel".

To find the derivative of $f(\theta, \phi)$, we must use a kernel, which is obtained through the integral transform. The general integral transform is defined as:

$$(Tf)(u) = \int_{x_1}^{x_2} K(x, u) f(x) dt$$

Where K is the kernel of the function. The kernel is then an operator by which we multiply f(x) in order to obtain the transform. In our case, the input of the transform will be $f(\theta, \phi)$, and the output is another function $Tf = f(\theta', \phi')$. The Lebedev points serve as a way to guarantee that this condition is met for all points on the sphere over which we integrate (recall that the Lebedev points have octahedral symmetry).

For a polynomial on the sphere, $f(\theta, \phi) = P_m^l(\cos(\theta))e^{im\phi}C_m^l$; we can calculate the derivative using spherical harmonics and the integral transform. The general expression for a spherical harmonic is:

$$Y_{m}^{l} = \sqrt{\frac{2l+1}{4\pi} \frac{(l-m)!}{(l+m)!}} P_{m}^{l}(\cos(\theta)) e^{im\phi}$$

Using this method, we can construct the derivative of $f(\theta, \phi)$ using the kernel from the transform.

$$\frac{d}{d\theta}f(\theta',\phi') = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} C_m^l \frac{d}{d\theta} Y_m^l(\theta',\phi')$$

where

$$C_m^l = \int Y_m^l(\theta, \phi) * f(\theta, \phi) d\Omega$$

Thus,

$$\frac{d}{d\theta}f(\theta',\phi') = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \int Y_m^l * f(\theta,\phi) \, d\Omega_m^l \, \frac{d}{d\theta} Y_m^l(\theta',\phi')$$

Now, we can rearrange the integral into a more convenient form:

$$\frac{d}{d\theta}f(\theta',\phi') = \int f(\theta,\phi) \sum_{l=0}^{\infty} \sum_{m=-l}^{l} Y_m^l(\theta,\phi) * \frac{d}{d\theta} Y_m^l(\theta',\phi') d\Omega$$
 (15)

The summation within the integral is then the Kernel of this transform. Because it is independent of $f(\theta, \phi)$, can calculate it separately. This allows us to save a lot of computation time because we can calculate the kernel once, save it, and then iterate through the file to calculate the derivative. Thus,

$$K(\theta', \phi', \theta, \phi) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} Y_m^l(\theta, \phi) * \frac{d}{d\theta} Y_m^l(\theta', \phi')$$

where

$$\frac{d}{d\theta}Y_m^l(\theta',\phi') = m\cot(\theta')Y_m^l + \sqrt{(l-m)(l+m+1}e^{-i\phi}Y_{m+1}^l$$

Then, when we want the derivative we simply integrate:

$$\frac{d}{d\theta}f(\theta',\phi') = \int f(\theta,\phi) K d\Omega \tag{16}$$

Likewise, if we replace $\frac{d}{d\theta}Y_m^l(\theta',\phi')$ with $Y_m^l(\theta',\phi')$ in the kernel, we can use the same method to reconstruct the function as well. This has served as useful verification tool to show our method is working correctly because of the complicated functions required to build the kernel. For instance if we build two separate kernel files, one for the derivative and one for $\frac{d}{d\theta}Y_m^l(\theta',\phi')$ and one for $Y_m^l(\theta',\phi')$, we can test whether or not the method of building the kernel file is wrong, or if there is something in particular about the derivative of the spherical harmonic which is causing the kernel to reproduce the derivatives of known functions incorrectly.

2.3 Building the Kernel file

The code referenced in [6] is written in C++ and uses Boost libraries to calculate Spherical Harmonics. So depending on your language of choice, the following method may or may not work. Calculating the Spherical Harmonics manually is not so difficult, but special attention needs to be given to points at the poles on the sphere. As usual, m ranges from -l to l. The meaning integer l however corresponds to the order of accuracy to which we choose to estimate functions on the sphere. You will notice in the code given in [6] that l is defined from the Lebedev points. When you run the code, the first step you take will be to define the precision with which you'd like to run the model. This precision refers to the rule you are using to define your Lebedev points, and higher l requires more points to estimate, which in turn requires longer computations because the loop size increases. It's best to show you the algorithm for building the Kernel file and then explain what it is doing. Recall that the kernel function looks like:

$$K(\theta', \phi', \theta, \phi) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} Y_m^l(\theta, \phi) * \frac{d}{d\theta} Y_m^l(\theta', \phi')$$
 (17)

$$\frac{d}{d\theta}Y_m^l(\theta',\phi') = m\cot(\theta')Y_m^l + \sqrt{(l-m)(l+m+1}e^{-i\phi}Y_{m+1}^l$$
 (18)

This tells us that we need a four dimensional function that sums over all m for a given value of l. Using the Lebedev points, each function of θ, ϕ can be represented in one loop. Let's call our two spherical harmonic functions Y and Y' respectively. The Y' will be iterated over i in the outer loop as $Y'(\theta', \phi')$ and $\frac{d}{d\theta}Y'(\theta', \phi')$, and the inner loop will iterate over $Y(\theta, \phi)$. The derivative of Y will be referred to as dY'. Then we have the following loop to produce the Kernel file:

Algorithm 13 Generate the Kernel file

Require:

```
* GenerateKernel(N, L) {function call where L is the order of the polynomial,
and N is the number of points}
* array\ dkernel[n][n] {arrays to store kernel values}
* array fkernel[n][n]
* complex Y, Y', dY' {complex double variables for use with the spherical har-
monics}
  for (A = 0; A < N; A + +) do
     for (B = 0; B < N; B + +) do
       for (A = 0; A < N; A + +) do
          for (B = 0; B < N; B + +) do
            Y' = SphericalHarmonic(m, l, Point[i].GetTheta(), Point[j].GetPhi())
            Y = SphericalHarmonic(m, l, Point[j].GetTheta(), Point[j].GetPhi())
            if (m+1 \le l \text{ and } Point[i].GetTheta() \ne 0) then {prevent division
             by zero}
               \begin{array}{lll} dY' &= m \cot(Point[i].GetTheta()) \, Y' &+ \\ \sqrt{(l-m)(l+m+1)} e^{-\mathbf{i} \, Point[i].GetPhi()} Spherical Harmonic(m \, + \, \\ \end{array}
               dY'
               1, l, Point[i].GetTheta(), Point[i].GetPhi())
             end if \{i \text{ in boldface is } \sqrt{-1}\}
             fkern[i][j] = fkern[i][j] + Y^*Y' {where * is the complex conju-
            dkern[i][j] = dkern[i][j] + Y^*dY'
          end for
       end for
     end for
  end for
```

Let's unpack this. First, we declare some files in which to store the kernels. We want a kernel to reconstruct functions, and one to reconstruct derivatives. The one used to reconstruct functions is not necessary for the model, but it will

Algorithm 14 Update the distribution with the gravitational term

Require:

```
*makefile("DerivativeKernel.dat") dfile {a data file for derivative kernel} *makefile("FunctionKernel.txt") ffile {a data file for function kernel} for (i=0;\,i< N;\,i++) do for (j=0;\,j< N;\,j++) do dfile(dkern[i][j]Point[j].GetWeight()) ffile(fkern[i][j]Point[j].GetWeight()) {fill the data file with tabdelineated values, multiply by the weights} end for end for
```

allow you to trouble shoot any general problems with the construction of the kernels. Depending on how you calculate the spherical harmonics, you will likely end up with complex numbers which you can deal with as you choose. For a good introduction to coding Spherical Harmonics, see reference [8]. The code in [6] allows for complex math and the Boost libraries for C++ include a function for calculating spherical harmonics. However, the theta derivative of a spherical harmonic is not usually included, and one must use an explicit formula like the one given by (18). Notice the if condition in calculating dY'. We exclude the pole where θ is zero since the cotangent function blows up there. We've also been careful to exclude the case where we plug m+1>1 into the SphericalHarmonic() function because some libraries will not deal with this exception. The function should spit back zero, but if not, deal with the case like above and dY' will always be zero at the m+1>1 case.

We then sum over the l and m values as we load them into the kernel arrays. Finally, save the arrays to file as they are, but multiply by the weights so we don't have to map those as well. The weights can be safely absorbed into the Kernel. Now we can save Kernels for arbitrary numbers of Lebedev points and orders. You can produce some very big kernels and use these to quickly do take derivative at high order. This will allow us to compute the gravitational terms quickly in our main code. In C++, and using the Boost libraries as in [6], we can speed up the algorithm by filling an array with the Y value for each l and m. This reduces the heavy dependence on l from the inner-most loop, and also takes some pressure off the efficiency of the Spherical Harmonics algorithm contained within the Boost libraries.

2.4 Reconstruction of functions using a Kernel

We now have a way of estimating derivatives using the Kernel. The next step will be testing some functions with known derivatives and seeing how they reconstruct. During the tests, we'll be varying I and the number of points as we generate new kernels to explore how well (or how poorly) the functions and their derivatives reconstruct at low and high orders. For the file used in the distribution simulation, we will use a 2-dimensional array to find the derivative at each A, and B. The order of l need not be fixed for the derivative terms in the distribution function if we build the kernel to allow for access to each l. Of course this increases the size of your Kernel because the arrays used to store the kernels now include an extra dimension for l. The downfall of this approach is it increases the size of the file and the time it takes to put the new kernel into memory. But you should only need to do this once. The code in [6] is set to be calculated at fixed l. However, it can be easily modified by increasing the array size to allow for an extra dimension for l. It's important to understand how the order is related to number of points and the quality of the reconstructions we can obtain using this method. If we choose I wisely, we can build a kernel for a particular l value and certain number of points that runs in a timely way when we start doing the numerical approximation. And the benefit of using the kernel in this way is that we only need to construct it one time, and then we're free to use that kernel file in trial runs later on.

The nature of the Lebedev points requires that the order (l) not exceed the precision of a given set of weights and points. For instance, the precision of the 5810-point set is 131, thus I must be less than or equal to 131, or else even well-behaved functions (or derivatives) will not reconstruct at all. Choosing l < precision allows for successful reconstruction of well-behaved functions and their corresponding derivatives. However, for not-so-well-behaved functions, (i.e. functions with discontinuities or noise) high frequency oscillations occur throughout the reconstructed function, and it gets worse as I approaches the precision value for the set of points used.

The correlation between the number of Lebedev points and the order to which we solve spherical harmonics is analogous to the Nyquist Frequency, in which we must have some minimum number of sample points (the Lebedev points) in order to successfully reconstruct a function over which we're sampling at some frequency (the order l in our case).

First, load the kernel into a 2-d array. You'll need to be able to integrate over it using the quadrature method from (6), as well as locate particular elements, so an object that holds the array and has a function like GetKernelElement (i,j) would be preferred. In the code referenced in [6], the object that holds the Kernel in memory is referred to as Mapper. It contains a function for retrieving a particular kernel element from the data file saved as in Algorithm 13. Then, we can setup the equation (15) from the previous section. We'll also need an array that stores values from a function of the Lebedev points. To start, in spherical coordinates:

```
x = \sin(\theta)\cos(\phi)
y = \sin(\theta)\sin(\phi)
z = \cos(\theta)
\frac{d}{d\theta}x = \cos(\theta)\cos(\phi)
```

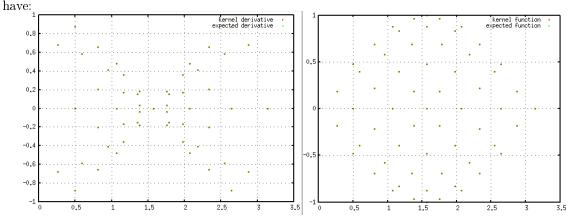
Combinations of these functions are Spherical Harmonics, so if your Kernel is

working, derivatives of them should reconstruct exactly if the order l is chosen correctly. Let's first differentiate x using the kernel. Evaluate $sin(\theta)cos(\phi)$ using the Lebedev points and load the results into an array, x[]. Well you are at it, load the derivative of that function into another array, dx[] as well so you can compare the results in the next step. Then we'll take that array and set it up like in (15). We've labeled the object which contains the Kernels and element retrieval functions as "Mapper", and the functions that return the Kernel elements as GetFKernel(i,j) and GetDKernel(i,j) for the function kernel and derivative kernel, respectively. Now we just integrate in the usual way, but leaving out the weights since we already absorbed them into the kernel file's elements (Algorithm 14):

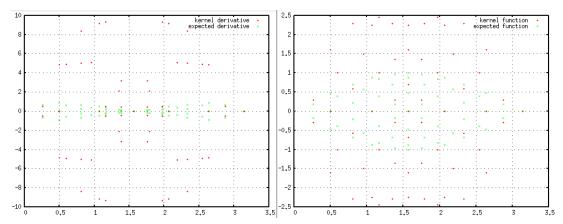
Algorithm 15 Evaluate a function x[] with the kernels. f[] is a reconstructed version of the function, and $\partial_f[]$ is the derivative of the function using the kernel files we constructed in Algorithm 13 & 14.

```
\begin{array}{l} \textbf{for} \ \ (i=0;\,i< N;\,i++) \ \ \textbf{do} \\ \textbf{for} \ \ (j=0;\,j< N;\,j++) \ \ \textbf{do} \\ \partial_f[i] = \partial_f[i] + x[j] \ Mapper.GetDKernel(i,j) \\ f[i] = f[i] + x[j] \ Mapper.GetFKernel(i,j) \\ \textbf{end for} \\ \textbf{end for} \end{array}
```

Now you have a reconstructed derivative ∂_f and a reconstructed function f using your two kernels developed in the last section. You should see numerical values that match every element in dx[] and x[] respectively. If f[] reconstructs correctly but ∂_f [] does not, your method of creating the kernel is functioning properly, but there is likely a problem with the formula used for the theta derivative of the spherical harmonic. With 110 points and an order l=12, we



But what happens if we choose l=17 (the limit for 110 points)? The estimate is no longer exact:



So the order at which we build the kernel files will greatly affect how accurate the derivative approximations are. We must choose l|precision of the Lebedev points or the method does not work.

2.5 Rotation using the Kernel

Recall that equations (12) and (13) require our operators for ∂_A and ∂_B to contain derivatives of the sphere in the x, y and z direction. By rotating the sphere by $\frac{\pi}{2}$ in both theta and phi, we can find the derivative with respect to theta along any axis using the same kernel we calculated above. But we need a method for rotating our Lebedev points to do so. Assuming the first derivative calculated was along the z-axis, we can find both the x-axis and y-axis derivatives by performing a rotation of the points and then integrating over the kernel as was shown in the last section.

The rotation is performed by converting the spherical coordinates to Cartesian, and swapping values such that the symmetry of the Lebedev points is maintained. Because the Lebedev points and their corresponding weights are produced with Octahedral symmetry, we can rotate the points in any way that would also preserve the symmetry of a cube. That is, if we rotate z by $\frac{\pi}{2}$ in the theta direction (holding phi at zero), our new point is at -y. As an example, let's rotate points about y (θ_y) :

```
\begin{array}{l} x \to -z \\ y \to y \\ z \to x \end{array} And likewise, about x (\theta_x):
 \begin{array}{l} x \to x \\ y \to z \\ z \to -y \end{array}
```

Recall in Section 1 that we said we'd need our Point object to have the capability to convert between Spherical and Cartesian coordinates. This will be an important function now. What we'd like to do is have a function that

takes in theta and phi components from the Lebedev files, then converts those components to Cartesian coordinates, and then allows us to access them through our old function GetX(), GetY(), and GetZ(). Then, we can do the following to create a list of rotated points. For the rotation about x, y and z, let's make arrays of point objects called ListX, ListY, and ListZ, and the original point object, Point. Then we can do the following:

Algorithm 16 Setup rotated lists of Lebedev points

```
 \begin{array}{ll} \textbf{for} & (i=0;\ i< N;\ i++)\ \textbf{do} \\ & ListX[i].SetCartesian(Point[i].GetX(),\ Point[i].GetZ(),\ -Point[i].GetY()) \\ & \{ rotation\ about\ X \} \\ & ListY[i].SetCartesian(Point[i].GetZ(),\ Point[i].GetY(),\ -Point[i].GetX()) \\ & \{ rotation\ about\ Y \} \\ & ListZ[i].SetCartesian(Point[i].GetX(),\ Point[i].GetY(),\ Point[i].GetZ()) \\ & \{ this\ list\ is\ redundant \} \\ & \textbf{end\ for} \\ \end{array}
```

With these three lists, we are set to evaluate the derivative along the X, Y, or Z axis of the sphere. But there is a catch. Our kernel was produced using the original Lebedev points, so calculating the derivative along another axis other than the original is not possible unless we can find the points in the kernel that correspond to the rotation. Of course, all of the points are present, just out of order. The next step involves a quick search algorithm to find the rotated points and build and iterator to find the Kernel. This will allow us to take derivatives with respect to theta along x, y, and z for (12) and (13).

Using a simple search algorithm we can find the rotated points within just one kernel file, and then save the location of the points to an iterator object and use that to evaluate the integral at the correct Lebedev points when we evaluate the derivative. This saves us a lot of memory because we only need one kernel. The idea is to apply the rotation to the iterators and use those to produce rotated kernel values that correspond to the rotated Lebedev points and weights. The algorithm goes as follows:

Algorithm 17 Create map to rotated points

```
\begin{array}{ll} {\bf for} & (i=0; \ i < N; \ i++) \ \ {\bf do} \\ & {\bf for} \ \ (j=0; \ j < N; \ j++) \ \ {\bf do} \\ & {\bf if} \ \ Point[i] = ListX[j] \ \ {\bf then} \\ & \ map[i] = j \\ & {\bf end} \ \ {\bf if} \\ & {\bf end} \ \ {\bf for} \end{array}
```

Now, we simply use the map array to find the rotated points in the kernel file. The kernel

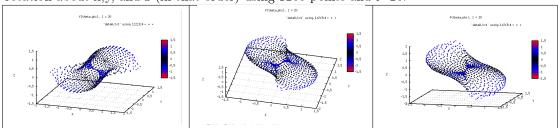
The object we called "Mapper" in the previous section was an object which contained functions like GetDkernel() and GetFKernel(). These functions should

Algorithm 18 Use map as iterator to find rotated points in kernel file

retrieve the elements of the $kernel_{map}[][]$ array which contains the rotated points.

The next step would be to define ListX[] a little more abstractly, such that when the function that calculates the gravitational terms needs a particular rotation, ListX[] changes to ListY[] or ListZ[]. The code in [6] does this in an object oriented way, by creating separate objects that correspond to each rotated kernel, and then uses these arrays to calculate the derivatives in the x, y, and z directions, as will be seen in the next section.

The iterator object, map[] just holds the index value of the point that was found. Then when we want to build the rotated map of the kernel, we simply fill the map array up with the values from the original file that correspond to the rotated index. Now, with this function we can specify the axis of rotation we'd like to have, and retrieve the associated kernel. Example plots of the function $f(\theta,\phi) = cos(\theta)cos(\phi)$ plotted using the above technique to determine the rotation about x,y, and z (in that order) using 1200 points and l=20:



In summary, we have a function that gives us a kernel file which acts as a derivative operator when integrated over. We found that we could take the derivative along different axis of the sphere by embedding it in \mathbb{R}^3 and performing rotations on the kernel file such that the theta derivative operator (the kernel) would be taken in different directions corresponding to rotations about the Cartesian coordinates. Now we can take derivatives of functions of A and B, which is exactly the distribution function f(A,B).

2.6 Calculating the Gravitational Term

Now we will put everything done in the last few sections together to calculate $\left(\frac{df}{dt}\right)_{gravitational}$. We now know how to take derivatives using the Kernel. We setup an object which contains the rules for rotating the kernel. This object is just like a Point object in that it contains functions like GetTheta(), and

GetPhi(), but the difference is that when you instantiate it, it calls GenerateK-ernel(), and in so doing prepares an accessor array that contains the rotated Lebedev points as well as as the Kernel itself. We make three of these objects using three different maps, one for each rotation, called RotatedAboutX, RotatedAboutY, and RotatedAboutZ. Each contains a map of the original kernel. Then, we take the derivatives just like we've done in the previous section. Recalling that the weights have been absorbed into the kernel, then our algorithm for ∂_A from (eq. 22) looks like:

$$\partial_A = -\sum_{i=1}^3 B_i sin(\theta_i) \frac{\partial}{\partial \theta_i}$$

```
Algorithm 19 Calculate \partial_A
```

And likewise for ∂_B , from (eq. 23) we have:

$$\partial_B = -\sum_{i=1}^3 A_i sin(\theta_i) \frac{\partial}{\partial \theta_i}$$

With these two arrays we are ready to calculate (9). Just organize the arrays as given in Algorithms 10 and 11 given at the beginning of section 2.1. Then add it back it back into f(A,B) like we did with the collision terms.

2.7 Effects of the Gravitational Term

The overall effect of adding in the Gravitational term is to balance the expansion due to the time-dependent scale factor $a(\tau)$ from the Friedmann metric. We included this term in the Hubble parameter from (11). The values of the \mathcal{H} were discussed in the Introduction of Part 2. By changing the values of the

Algorithm 20 Calculate ∂_B

Algorithm 21 Calculate the gravitational term $(df(A, B))_{grav}$

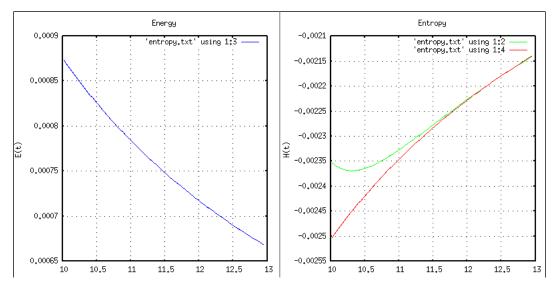
```
\begin{array}{lll} & \mbox{for} & (A=0;\, A < N;\, A++) & \mbox{do} \\ & \mbox{for} & (B=0;\, B < N;\, B++) & \mbox{do} \\ & df_g[A][B] & = & \mathcal{H}\left(\partial_A[A][B] & + & \partial_B[A][B] & - & 1 & - & 5(Point[A] & \circ \\ & & Point[B]) \, \right) f[A][B] \Delta t \\ & \mbox{end for} \\ & \mbox{end for} \end{array}
```

Algorithm 22 Update the distribution with the gravitational term

```
\begin{array}{ll} \textbf{for} & (A=0;\, A< N;\, A++) \  \, \textbf{do} \\ & \textbf{for} & (B=0;\, B< N;\, B++) \  \, \textbf{do} \\ & f[A][B]=f[A][B]+df[A][B]+df_g[A][B] \\ & \textbf{end for} \\ & \textbf{end for} \end{array}
```

parameter, we can easily change the era we'd like to probe from Cosmological constant dominated ($\mathcal{H}=constant$ (n=2)), to Radiation Dominated ($\mathcal{H}=\frac{1}{2t}$, n=4), or Matter Dominated ($\mathcal{H}=\frac{2}{3t}$, n=3). The time is numerically given in section 1.2 as the variable τ , which is a function of the step size and time iterator.

Looking at entropy when expansion is included, we see that the gravitational terms does not have an effect on the factorisability of the distribution function. The entropy should still approach the limit, but the expansion term will tend to pull both the limit and the entropy out of equilibrium at the same rate.



We would also like a good way to check the power with which the energy density is changing, because of equation 26. We know the energy density should fall off with a slope of $-\frac{2}{n}$ on a log-log plot. We can check what power the energy density slope falls off with by looking at the slope between two different points in time on a plot of $log(\rho) vs log(T)$. However, this requires us to store the data from previous time steps such that we can compare old energy densities with the most recent. The code in [6] requires that we initialize arrays of a size proportional to the total time the simulation will be run in order to store the energy values for the entirety. Then the values of the energy density and τ are stored in separate arrays, labeled as Energy[] and Time[] in the algorithm below. The slope of the line in the $log(\rho) vs log(T)$ plot is found by the classic formula

$$m_{\rho} = \frac{log(\rho_{old}) - log(\rho_{current})}{log(T_{old}) - log(T_{current})}$$

The subscript "old" and "current" refers to the iterative time step. This poses a problem because traditionally the iterators would be integers that increase by 1 every time step. If we set the old time step to a constant, we have to wait for the simulation to hit that time step to start to gain useful slope information, and then the estimate gets less and less accurate as $t\gg t_0$. Instead, we'd like to track the most recent slope. Again, we could use the current time-step plus or minus a constant, but the same problem arises at large t due to the logarithm. Instead, let's define a new quantity L, which will be a constant, and the current time step, t. The most recent slope can be tracked by taking L~1. If we increase L from 1.0 to 1.3, we've effectively changed the range of the most recent slope calculation. So this allows an easy way to adjust how far back we want to judge the slope. This becomes useful because the real-world time it takes for m_ρ to converge on $-\frac{2}{n}$ is proportional to the step size $\triangle t$. It is then useful to use only the most recent piece of the line from the log-log plot to determine the value of m_ρ .

Algorithm 23 Track recent slope on log-log plot

```
 \begin{array}{ll} \textbf{while} & (t < t_{max}) \ \ \textbf{do} \\ L = 1.1 \\ m_{\rho} = \frac{log(Energy[floor(\frac{t}{L})]) - log(Energy[t])}{log(Time[floor(\frac{t}{L})]) - log(Time[t])} \\ \textbf{end while} \end{array}
```

Notice the use of the floor() function in Algorithm 23. The floor(x) function returns the lowest integer for a given x. We could have just as easily used the ceil() function without effecting the outcome of the slope calculation.

Now probing different eras (n=2,3,4...etc) should result in log-log plots which are linear with a slope of $m_{\rho} = -\frac{2}{n}$. This will be a strong indication that the gravitational terms calculated in the previous sections are working correctly.

3 Loop Tracking and Removal

We would like to now understand how loop production affects the distribution. To do so, we will present a method of loop removal such that we can track how much energy density goes into large and small loops, respectively. begin, we assume that f(A,B) is a distribution of long strings. The long strings radiate loops due to self-intersecting wiggles and string inter-commutation. We will modify the transport equation (4) such that certain conditions will lead to the removal of string segments, which in turn removes energy density from the distribution. The removed energy density will be stored just like we did for the collision term, but we'll separate it into two new arrays, one for small loops, and one for large loops. Also, to keep the transport equation equivalent to what we did in Part 1 and 2, whenever we remove loops from the distribution, we'll also track what was removed and how much. Then we will add all of these back into the original distribution, effectively leaving the transport equation and distribution function unchanged. However, we will now be able to track the energy density present due to small, large, and red-shifted loops, as well as that due to long strings. Recall the original transport equation:

$$\left(\frac{df}{dt}\right)_{collision} = \frac{1}{\rho} \int d\mathbf{A}' d\mathbf{B}' \, \Gamma\left(f(\mathbf{A}',\mathbf{B})f(\mathbf{A},\mathbf{B}') - f(\mathbf{A},\mathbf{B})f(\mathbf{A}',\mathbf{B}')\right)$$

Or in terms of the Lebedev quadrature, with gamma expanded:

$$(df(A,B))_{col} = \sum_{A'=0}^{n} \sum_{B'=0}^{n} \frac{1}{\rho} w_{A'} w_{B'} \left(\lambda(\frac{1}{\mu}) + p\rho\mu P(A,B,A',B')\right) \left(f(A',B)f(A,B') - f(A,B)f(A',B')\right) \Delta t$$

We will now separate the above equation into two separate equations, one for small loops and one for large. Each of these will tell us about the change in energy density due to collisions among their corresponding types of string segments. The conditions for loop removal are two-fold. There are two different types of loops, small and large. Due to the Γ term, the equation is repeated twice and summed together. One is proportional to the probability λ , and the other is proportional to pP(A, B, A', B'), where p is the inter-commutation probability. These two parts of gamma correspond to small loop production and large loop production from inter-commutation. So only large loops depend on inter-commutation. In section 1.1 we set $\lambda = 1$. Now we will leave it as a tunable parameter. Then we can break up collision term into two separate terms.

$$(df(A,B))_{small} = \sum_{A'=0}^{n} \sum_{B'=0}^{n} \frac{1}{\rho} w_{A'} w_{B'} \left(\lambda(\frac{1}{\mu})\right) \left(f(A',B)f(A,B') - f(A,B)f(A',B')\right) \Delta t$$
(19)

$$(df(A,B))_{large} = \sum_{A'=0}^{n} \sum_{B'=0}^{n} w_{A'} w_{B'} \left(\mu p P(A,B,A',B') \right) \left(f(A',B) f(A,B') - f(A,B) f(A',B') \right) \Delta t$$
(20)

We will also need to track the changes in the distribution of long strings. This term will be modified in two parts as well, one for when small loops are removed, and one for when large loops are removed. These correspond (as in 38 and 39) to the side with λ dependence, and the side with P dependence.

$$(df(A,B))_{long} = (df(A,B))_{long (small)} + (df(A,B))_{long (large)}$$

Which splits up in terms of quadrature like:

$$(df(A,B))_{long\,(small)} = \sum_{A'=0}^{n} \sum_{B'=0}^{n} \frac{1}{\rho} w_{A'} w_{B'} \left(\lambda(\frac{1}{\mu})\right) \left(f(A',B)f(A,B')\right) \Delta t \quad (21)$$

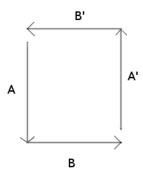
$$(df(A,B))_{long (large)} = \sum_{A'=0}^{n} \sum_{B'=0}^{n} w_{A'} w_{B'} (\mu p P(A,B,A',B')) (f(A',B)f(A,B')) \Delta t$$
(22)

3.1 Small Loop Production

Small loops are the smallest possible closed collection of unit vectors A, B, A' and B' that the system allows. This occurs when $\mathbf{u} = -\mathbf{u}'$. Because \mathbf{u} is defined in terms of \mathbf{A} and \mathbf{B} , and these vectors are perpendicular to one another, we can define a closed loop as follows.

$$B + B' - A - A' = 0 (23)$$

Graphically, we can think of these string segments as unit vectors connecting at their ends to form a loop.



The distribution of small loops is then comprised only of distributions of f(A,B) and f(A'B'). If we detect a loop, (e.g. equation 42 is true), we set f(A,B)f(A',B')=0, such that we have:

$$df(A,B)_{small} = \frac{1}{\rho} \int d\mathbf{A}' d\mathbf{B}' (0 - f(\mathbf{A}, \mathbf{B}) f(\mathbf{A}' \mathbf{B}')$$
 (24)

A simple if() statement can handle the small loops removal condition. We also track how much of the long string distribution we set to zero when the if() statement was true. The algorithm to remove loops then goes as follows.

```
Algorithm 24 Calculate the probability density of small loops (df(A, B))_{small}
```

Notice that the term CUTOFF is set at runtime, and the the quantity |(Point[B]+Point[B']-Point[A]-Point[A'])| represents the magnitude of the resulting vector. The amount of the distribution that is removed due to small

loops will obviously be sensitive to this parameter if it is set to high. It needs to be a good numerical approximation to zero on the machine which the code is run on. In our simulations from [6], $CUTOFF = 10^{-12}$.

3.2 Large Loop Production

In the same way we now want to remove any other segments that are loops, so long as they are greater than the small loops cutoff. These we call large loops. They again come from the term f(A,B)f(A',B'), so we want to set the term f(A',B)f(A,B') to zero if the condition is true. So we again have an if() statement that will determine whether or not a large loop is produced.

$$B + B' - A - A' > CUTOFF \tag{25}$$

If (46) is true, then our formula for the changes in the distribution due to interactions of large loops goes like:

$$df(A,B)_{large} = \int d\mathbf{A}' d\mathbf{B}' (0 - f(\mathbf{A}, \mathbf{B}) f(\mathbf{A}' \mathbf{B}')$$
 (26)

And at the same time, we calculate $df_{long(large)}$ to account for what we removed. Notice that the ρ cancels. Then the algorithm goes like one would expect:

$\overline{\textbf{Algorithm 25 Calculate the probability density of large loops } (df(A, B))_{large}$

```
for (A = 0; A < N; A + +) do
  for (B = 0; B < N; B + +) do
    for (A = 0; A < N; A + +) do
      for (B = 0; B < N; B + +) do
         F = f[A'][B]f[A][B']
         if (|(Point[B] + Point[B'] - Point[A] - Point[A'])| > CUTOFF)
         then
           F = 0
                                                    df_{long(large)}[A][B]
           df_{long(large)}[A][B]
           (pP[A][B][A'][B']) (f[A'][B]f[A][B']) Point[A']. GetWeight() Point[B']. GetWeight()\Delta t
         end if
         df_{large}[A][B]
                                                (pP[A][B][A'][B'])(F
         f[A][B]f[A'][B']) Point[A'].GetWeight() Point[B'].GetWeight() \Delta t
      end for
    end for
  end for
end for
```

The first thing you will notice is that these changes in the distributions are all negative, with the exception of $df(A,B)_{long}$. So adding the large and small loops terms removes energy density from the distribution and the long strings term adds energy back in. We can treat these terms as proper distribution functions all on their own, which obey all the familiar rules, such that we can still calculate energy density, pressure, and entropy.

Updating the distribution function as before will lead to the same results as we had in Section 1 and 2 because we've essentially just set up a means of tracking where energy goes. Add the removed probability density back into the distribution as always, but now replace $df_{coll}[A][B]$ with $df_{small}[A][B] + df_{large}[A][B] + df_{large}[A][B]$.

Algorithm 26 Track large and small loops in distribution function

```
\begin{array}{ll} {\bf for} & (A=0;\,A< N;\,A++) \  \, {\bf do} \\ & {\bf for} & (B=0;\,B< N;\,B++) \  \, {\bf do} \\ & f[A][B] &= f[A][B] + df_{small}[A][B] + df_{large}[A][B] + df_{long}[A][B] + \\ & df_g[A][B] \\ & {\bf end} \  \, {\bf for} \\ & {\bf end} \  \, {\bf for} \\ & {\bf end} \  \, {\bf for} \\ \end{array}
```

One can verify that the distribution function has not been changed by integrating over it and looking at a log-log plot of the energy density with time, as was shown in section 2.7. The same results should hold. The energy density falls off as $\rho \propto t^{-\frac{2}{n}}$, where n=2 for curvature, n=3 for matter, and n=4 for radiation

dominated universes. However, in the next section we will stop adding back the energy density due to long strings that is lost when loops are removed.

3.3 Ratio of Small to Large Loops

Now we would like to see how the distribution behaves when we actually remove large and small loops from the distribution. Simply remove the quantity $df_{long}[A][B]$ from the update function given in Algorithm 26. The slope of $log(\rho)$ vs log(t) should go to -2.

Algorithm 27 Remove large and small loops from the distribution function

```
for (A = 0; A < N; A + +) do
for (B = 0; B < N; B + +) do
f[A][B] = f[A][B] + df_{small}[A][B] + df_{large}[A][B] + df_g[A][B]
end for
end for
```

We are now set to define a few other quantities. The energy density which has been removed due to small loop production at each time step can be calculated like:

$$\rho_{small} = \int \left(df(A, B)_{small} \right) dA dB \tag{27}$$

And likewise for large loops:

$$\rho_{large} = \int (df(A, B)_{large}) dA dB$$
 (28)

As well as red-shifted loops:

$$\rho_{redshift} = \int (df(A, B)_g) dA dB \tag{29}$$

These can be calculated in the usual way with the Lebedev Quadrature according to equation 6. With these quantities we can construct the ratio between small and large loops, ℓ .

$$\ell = \frac{\rho_{small}}{\rho_{large}} \tag{30}$$

We must also define the correlation length μ , which we had set to 1 in the previous sections. We must calculate this quantity dynamically. The definition is recursive, so the current value μ is defined in terms of the value at the previous time step μ_0 :

$$\mu = \mu_0 \left(1 + x \left(\frac{\rho_{small}}{\rho}\right) + y \left(\frac{\rho_{large}}{\rho}\right) + z \left(\frac{\rho_{redshift}}{\rho}\right)\right)$$

We'll define the energy densities ρ_{small} , ρ_{large} and $\rho_{redshift}$ in section 3.3. The coefficients in front of these terms are constants which obey the following constraints.

$$x < -\frac{1}{2}$$

$$\gamma = \frac{\mathcal{H}}{\tau}$$

Then we can define predicted values for the energy densities ρ_{small} , ρ_{large} and $\rho_{redshift}$ in terms of x, y, and z. We call them A, B, and C respectively.

$$A + B + C = 1$$

Through numerical simulation, we have found that the ratio of small to large loops can be described in terms of x, y, and z in Minkowski space (i.e. z=0) as follows:

$$A = \frac{1+2y}{2y-2x}$$

$$B = \frac{1+2x}{2x-2y}$$

$$\ell = \frac{A}{B}$$

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