Equal Complexity Configurations of the N-body System

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Abstract

The shape space of systems with high numbers of particles is extremely difficult to explore as it is a 3N-7 dimensional manifold (N being the number of particles). By generating and analyzing equal complexity configurations it is possible to develop more understanding the equi-potential curves in higher dimensional shape space. This document focuses on the creation of said equal complexity configurations, and discusses the mathematics behind the numerical methods. In addition, the same principles are applied to finding central configurations of N-body systems, which have many applications in shape dynamics.

1 Introduction

The Complexity is a collective variable defined for each N-body configuration. It is a measure of clustering or collinearity, as both of those properties correlate strongly with high complexities. This will be discussed in more detail later in this document. The Complexity is defined in terms of the Newtonian potential, V_{New} and I_{cm} , as

$$C = \frac{1}{m_{tot}^3} |V_{New}| \sqrt{I_{cm}} \tag{1}$$

This quantity is dependent on all of the inter-particle distances, and it is worthy to note that the inverse cube of the total mass is canceled out when all particles have an equal mass. This document will focus heavily on equal mass systems, so as not to complicate calculations and so that the images make more sense to the viewer.

2 The Numerical Method

2.1 The Gradient

Multiple methods were discussed in order to numerically find configurations of a given complexity. The most prominent were the ideas that relied on evolution, or "stepping" the system towards a higher or lower complexity until reaching the desired value. The first method was to evolve the system gravitationally, as it has been shown that the complexity will generally increase in both directions away from a minimum in a gravitational system. The second method was to determine the gradient of the complexity for a given system, and step in that direction (or opposite direction), as the gradient provides the direction steepest ascent for a function.

Due to the computational requirements of the gravitational evolution, the gradient ascent method was chosen to reach configurations of a given complexity. In order to do this, the gradient must first be analytically derived, in order to save much computing power.

2.2 Analytic Derivation of the Gradient

As stated above, the complexity of the system is defined as the product of the Newtonian potential and the square root of the center-of-mass moment of inertia. These two values can also be called the inverse mean-harmonic-length and the root-mean-squared-length. Using (1), and r_i as the set of particle positions, we can determine a function for the gradient of the N-body complexity.

$$\nabla C = \frac{\partial}{\partial r_i} C = \sqrt{I_{cm}} \frac{\partial}{\partial r_i} |V_{New}| + \frac{|V_{New}|}{2\sqrt{I_{cm}}} \frac{\partial}{\partial r_i} I_{cm}$$
 (2)

It is also helpful to view the equations for the I_{cm} ,

$$I_{cm} = \sum_{a < b} m_a m_b r_{ab}^2 \tag{3}$$

and the Newtonian potential,

$$|V_{New}| = \sum_{a < b} \frac{m_a m_b}{r_{ab}} \tag{4}$$

It also becomes useful to split these equations into the parts that specifically contain r_i .

$$I_{cm} = \sum_{a < b \neq i} m_a m_b r_{ab}^2 + \sum_{a \neq i}^N m_a m_i ||r_i - r_a||^2$$
(5)

$$|V_{New}| = \sum_{a < b \neq i} \frac{m_a m_b}{r_{ab}} + \sum_{a \neq i}^{N} \frac{m_a m_i}{||r_i - r_a||}$$
(6)

These are more computationally oriented forms of the equations, which clearly show a major part of each value that will vanish when the partial derivative is applied. This then allows us to use the equation

$$\frac{\partial}{\partial r_i} I_{cm} = \left\langle \frac{\partial}{\partial r_{ix}}, \frac{\partial}{\partial r_{iy}}, \frac{\partial}{\partial r_{iz}} \right\rangle \sum_{a \neq i}^{N} m_a m_i [(r_{ix} - r_{ax})^2 + (r_{iy} - r_{ay})^2 + (r_{iz} - r_{az})^2]$$
(7)

which yields

$$\frac{\partial}{\partial r_i} I_{cm} = \left\langle \sum_{a \neq i}^{N} 2m_a m_i (r_{ix} - r_{ax}), \sum_{a \neq i}^{N} 2m_a m_i (r_{iy} - r_{ay}), \sum_{a \neq i}^{N} 2m_a m_i (r_{iz} - r_{az}) \right\rangle = 2 \sum_{a \neq i}^{N} m_a m_i (r_i - r_a)$$
(8)

A similar process can be taken with the Newtonian potential, V_{New} , and can be used to obtain the final gradient. The components of each differential can be placed in a larger vector in order to evolve the system. Note that this vector will contain 3N elements, one for each component of each position vector.

$$\nabla C = \frac{\partial}{\partial r_i} C = -\sqrt{I_{cm}} \sum_{a \neq i}^N \frac{m_a m_i (r_i - r_a)}{r_{ia}^3} + \frac{|V_{New}|}{\sqrt{I_{cm}}} \sum_{a \neq i}^N m_a m_i (r_i - r_a)$$

$$\tag{9}$$

The above equation represents the direction of steepest ascent for the complexity, allowing us to easily increase or decrease the complexity of a system as we desire. This will form the foundation for the numerical algorithm.

2.3 Algorithms to Step the Complexity

The main premise of the algorithm we will use to generate these equal complexity configurations involves "stepping" the system in the direction of steepest ascent or descent. However, due to the complex structure of shape space, simply using the full gradient vector will not be enough to create a sample with statistical significance.

The solution to this is to change the number of particles being moved in each step. The original method was to move every single particle in one step. However, moving different numbers of particles each step is analogous to evolving in a different direction in shape space, meaning the final outcome will likely be different than others. To explore this, we show samples of different equal complexity configurations that all started with the same initial conditions, but evolved in different directions through shape space.

The algorithm itself is quite simple. The current gradient is computed every step, and then added to the positional data in order to evolve the system. Then the new complexity is calculated, and the program moves on to the next step. There are a few interesting quirks to take note of. First, the complexity will never be exactly the desired value, as that is computationally impossible to guarantee, but there is an error variable that allows the user to choose how close the computer should get before

halting the program. We believe that as long as the complexity of the system is very close to the desired complexity, we can treat it as the same. I feel this might become less and less true as the number of particles increases, and shape space becomes much more sensitive and complex. A second quirk of the program is that the randomly generated initial conditions tend to have lower complexities. This creates some imbalances computationally, as it takes much longer to generate a high complexity configuration, but it also may provide some insight into what low complexity truly means.

2.4 Central Configurations

Another use for this algorithm presented itself in the form of central configurations. These are very interesting systems of particles, where the points are arranged in such a way that each acceleration vector is proportional to the corresponding positional vector, each with the same constant of proportionality. In mathematical terms, if γ_i is the acceleration vector of the particle, and r_i is the position, then a central configuration possesses the property that

$$\gamma_i = \lambda r_i \tag{10}$$

where λ is a constant. Another interesting property is that each acceleration vector points towards the center of mass. As one will see, they create very interesting images, especially in two dimensions. A common way to generate these configurations is to solve the system of nonlinear equations defined by the above equation. However, another way is to determine when the gradient of the complexity is equal to zero. Using the algorithm above, we can then minimize the complexity in order to find the zero gradient, essentially locating the nearest critical point of the complexity function.

3 Results and Visual Analysis

In this section I would like to present some of generated configurations created using the algorithms discussed above. I would also like to present pictures of these configurations and discuss some interesting visual features of the shapes.

3.1 Low Complexity Configurations

Albeit slightly less interesting than high complexity, lower complexity configurations are still important to understand how complexity changes. Below are three pictures of different configurations, all with complexities of 0.5, a lower value for that number of particles.



Figure 1: Three Configurations of 0.5 Complexity in 3 dimensions (50 particles)

A detail to note is that all of these seem to be hollow in the center, meaning there are no particles in the center of the configuration. The particles appear to form some sort of shell around the center of mass. It is yet to be determined if this physically significant or simply a result of the computational method.

3.2 High Complexity Configurations

The higher complexity configurations have much more distinct features that include high amounts of clustering and collinearity. Below are three pictures of different configurations, all with complexity of



Figure 2: Three Configurations of 40 Complexity in 3 dimensions (50 particles)

Notice how the picture in the center is very close to being completely collinear, corresponding with our previous ideas that collinear configurations correspond to higher values of complexity. These images also show how complexity can be considered a measure of clustering, as many small clusters formed in higher complexity configurations.

3.3 Central Configurations

Multiple different central configurations, in both two and three dimensions, were generated to explore their structure and patterns. The left image is a low complexity, two dimensional central configuration, and the right image is a low complexity three dimensional central configuration. Notice how the

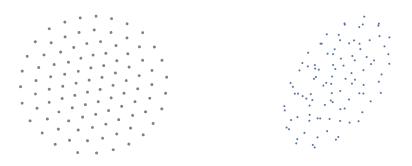


Figure 3: Two Central Configurations (100 particles)

lower complexity configuration is very evenly distributed. It might not be apparent, but the three dimensional version is the same way, except in three dimensions, of course.

4 Conclusion

While the ability to generate configurations of a desired complexity and find central configurations is incredibly useful, there is a large limiting factor in the computing power required. Since the complexity, and therefore the gradient, requires the computation of all of the inter-particle distances, the amount of calculations scales with n^2 (where n is the number of particles). However, the insight these configurations could give to the structure of shape space could be very important to the development of shape dynamics and shape statistics. There are still many upgrades and features to add to the program to allow for more experimentation and data collection, hopefully all of which will be implemented in the future.