MANTA-Ray: AEROSOLS ARE NOT SPHERICAL COWS

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SUPER-CHARGING CALCULATION SPEEDS IN THE RAYLEIGH REGIME

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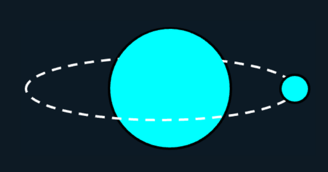
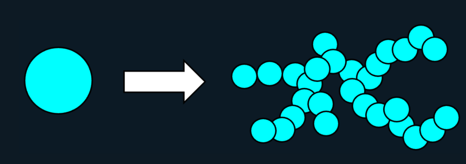
CONTEXT

Atmospheric aerosols have been discovered on almost every major body in the solar system, and are expected to exist in most exoplanet and brown dwarf environments.[1-5]



Radiative transfer codes and retrievals require **accurate** absorption and scattering **cross-sections;** without them, the entire energy balance of the planet might be misunderstood.[6-10]

As a first-order estimate, many choose to model the particles as spherical. However, TEM (Transmission Electron Microscope) images of aerosols on Earth show that this is often a **significant** simplification.[11,12]



We recently demonstrated[13] (Lodge et al., 2023) the differences obtained from spherical/non-spherical models. However, despite the speed increase obtained from using low-resolution Discrete Dipole Approximation (DDA), it is still **computationally intensive** to calculate optical properties for the large range of particle sizes and wavelengths required in models.

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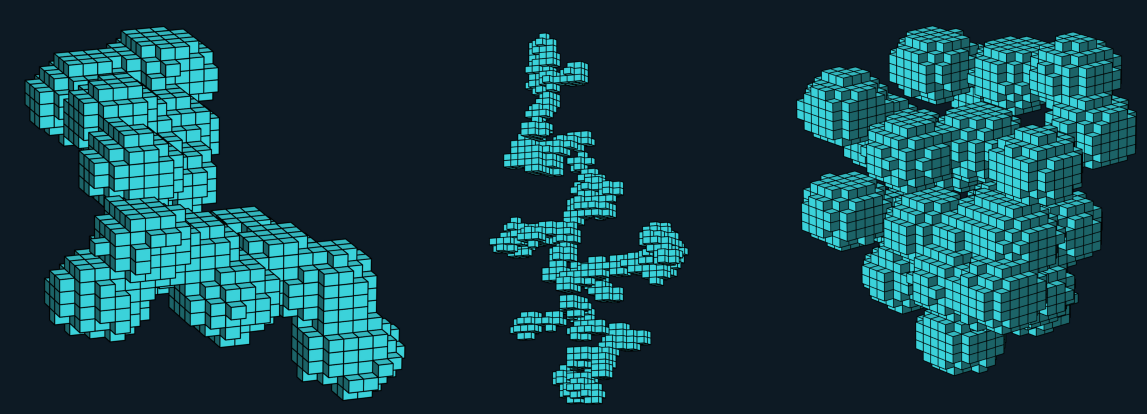
THE RAYLEIGH REGIME

When the **wavelength** is much larger than the **particle diameter**, the mathematics for spherical particles is greatly **simplified**.

We have found that by adding modification term *X* to the equation for spheres, we can **successfully calculate** the properties of complex, non-spherical particles:

$$C_{abs} = \chi \frac{8\pi^2 R^3}{\lambda} \mathrm{Im}\left(\frac{m^2-1}{m^2+2}\right). \quad (1)$$

Our **MANTA-Ray** model (**M**odified **A**bsorption for **N**onspherical **T**iny **A**ggregates in the **Ray**leigh regime) predicts how *X* changes as a function of particle shape. We determined this by exploring a range of 'fractal aggregates' (clusters of particles) with very different geometrical properties.



Scan to view 3D fractals!

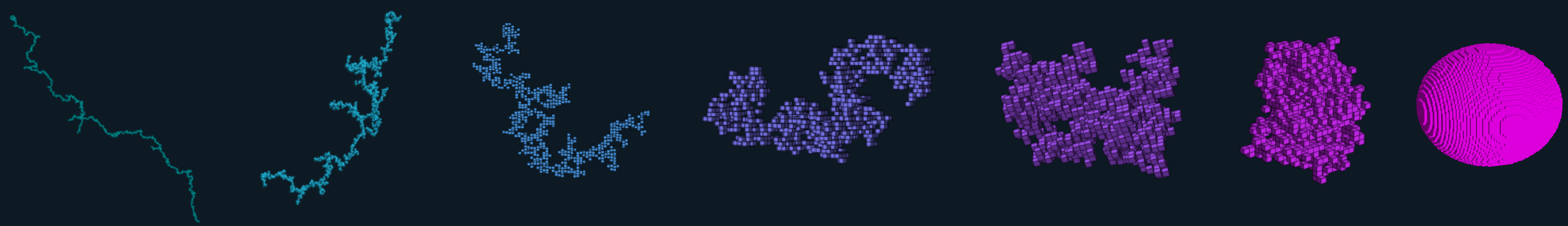


Fig 1: A range of fractal aggregate shape-types were studied, with fractal dimensions (d_f) ranging from 1.2 to 2.7 (left to right), plus a sphere for reference. From this, we systematically determined how much the absorption cross-section in each case deviates from the original equation that was designed for perfect spheres (see Fig 2).

RESULTS

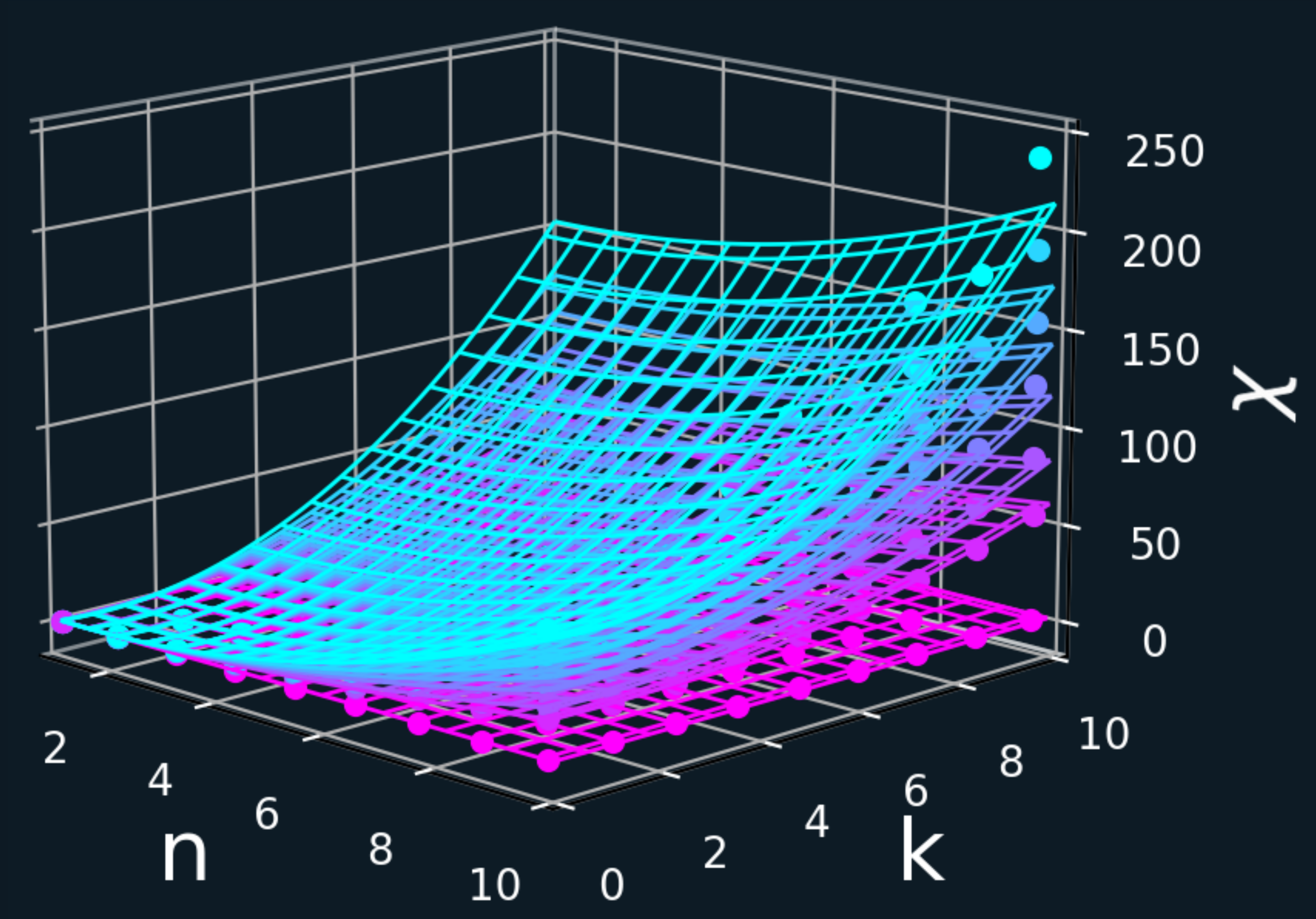


Fig 2: Modification factor plotted as a function of refractive index components (n,k) for a variety of shapes between compact (pink) and linear (light blue) aggegates, matching the colours in Fig 1.

We have found that the modification factor *X* is strongly-dependent on shape type (d_f), and refractive index (***m***). The dependance for a particular shape can be well-described by a multivariate quadratic polynomial of the real (***n***) and imaginary (***k***) components of ***m***:

$$\chi(n, k, d_f) = a_0 + a_1 n + a_2 k + a_3 n^2 + a_4 nk + a_5 k^2. \quad (2)$$

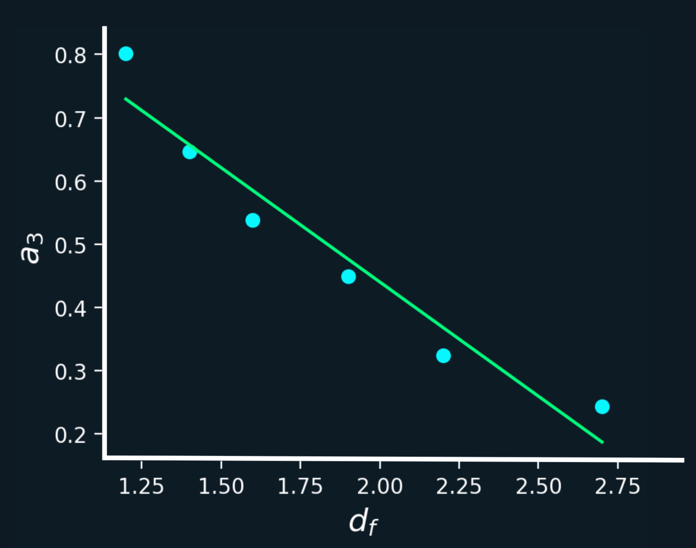
This polynomial fits each shape within an average error of 10% or better across the (*n*, *k*) parameter space studied (0 to 11 in both *n* and *k*), for all shapes.

The coefficients of these polynomials have been found to depend on specific shape type (e.g. compact, linear/branched etc -- see below). By calculating *X* and using Eq. (2) in (1), we can obtain accurate absorption cross-sections much faster than usual for non-spherical particles.

We have demonstrated that the original spherical model can significantly underestimate absorption, by orders of magnitude for high refractive indices. The **MANTA-Ray** model correctly predicts this absorption, and the computation time is **10^9 times faster** than full, rigorous DDA analysis.

SHAPE TYPE

We have discovered that different shape types have different coefficients (a_0, a_1 etc...) for *X*. By tracking how these coefficients change as a function of fractal dimension, we have created a simple predictive formula that works for any **particle geometry** and **any chemical composition** -- covering all possibilities of physical and chemical aerosol compositions within the Rayleigh regime.



CONCLUSION / KEY MESSAGE

1) For cases where the **wavelength** is much larger than the **particle size**, we can combine Eq. (1) and (2) to very quickly calculate the **optical** properties of **fractal aggregates**.

2) This modification **significantly improves the accuracy** versus the spherical model. MANTA-Ray decreases an **average error** of **>10,000%** to **<10%,** and it remains incredibly fast (**10^9 times faster** than a full, rigorous DDA analysis).

CONTACT

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