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Trying to solve the Faint Young Sun Paradox: Computing fractal atmospheric haze aerosol cluster structures and light scattering by these clusters

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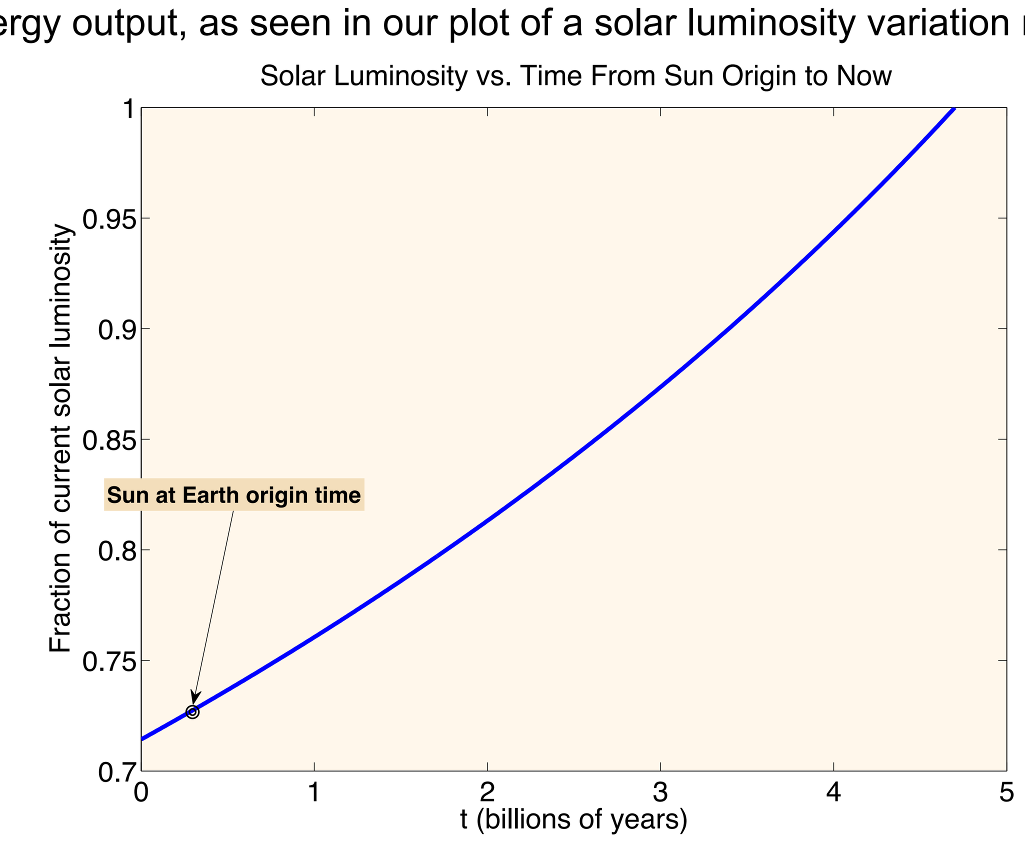
Abstract

About four billion years ago when the Sun and the Earth were young, the Sun's radiant energy output was about 25% less than it is today because the young Sun had little helium in its core to fuse (Gough, 1981). Yet geological evidence shows that the Earth was warm enough in its first billion years to have liquid water, a prerequisite for life to evolve. This mystery is called the "Faint Young Sun Paradox" (Sagan and Mullen, 1972). Greenhouse gases in the early Earth atmosphere have been invoked to resolve the paradox, with CO_2 being most mentioned. Yet ancient rocks have minerals inconsistent with there having been much CO_2 then (Rosing *et al*., 2010) and fossil raindrop splashes now prove that CO_2 concentration could not have been extremely high (Som *et al*, 2012). Another recent suggestion is that photochemical haze, composed of fractal aggregate aerosols, blocked the UV light that would destroy other greenhouse gases yet let in enough visible light to keep the Earth from freezing over (Wolf and Toon, 2010). To test this hypothesis we are writing computer programs using the physics of cluster-cluster aggregation (CCA) to generate fractal haze aggregates, and then we are using a large light scattering T-matrix code to investigate the scattering of sunlight by these aggregates.

Motivation for this Study, and Background

It has been well-known since the pioneering work by the British physicist John Tyndall in the mid-19th century that CO_2 has infrared absorption bands and so must act as a greenhouse gas in limiting the escape of Earth thermal radiation, thereby raising the mean temperature of Earth or planetary atmospheres where CO_2 is present. But atmospheric aerosols, much bigger than molecules, also play a (complicated) role in affecting climate. Two types of aerosol that have similar structures are carbonaceous soot (see Liu and Mishchenko, 2007) and some high-altitude hydrocarbon haze aggregates. Each of these has a non-integer fractal structure with a dimension more than 1 and less than 3, and with the fractal aggregate composed of many small (radii from 20 to 50 nm) spherical monomers that aggregate through a diffusional process in the air.

Planetary scientists studying Saturn's moon Titan are very interested in understanding the optical effects of the Titan high-altitude organic haze, made of fractal aggregates. The early Earth, after the deadly time of bombardment from large asteroids and small planetary bodies, had an atmosphere with little oxygen and abundant organic haze. Geologic evidence shows that there has been liquid water for 4 billion years, and life first evolved perhaps as early as 3.8 billion years ago. But the young Sun had less energy output, as seen in our plot of a solar luminosity variation model (Gough, 1981):



The recent *Science* paper by Wolf and Toon (2010) claims to "solve" the Faint Young Sun Paradox without invoking substantial early Earth atmospheric CO_2 by arguing that the early Earth had a photochemical haze composed of fractal hydrocarbon aerosols, and they claim that these fractal haze aerosols were optically thick in the UV range (protecting reduced gases from photolysis) while allowing enough visible solar radiation to reach Earth's young surface to allow liquid water, and hence life, in spite of the early Sun's lesser luminosity. We wanted to test their conclusions by using more accurate and sophisticated fractal aggregate light scattering computations than they report.

Methods

We use the T-matrix technique first developed by Waterman (1971) and reviewed for EM wave scattering by nonspherical aerosols by Liou (2002). The code is from Dan Mackowski (Mackowski and Mishchenko, 1996), and was updated to Fortran 95 in 2011. The fractal aerosol particles (early-Earth haze) used in our calculation consist of spherical Rayleigh-scatterer (radius of 50 nm) monomers aggregated into a larger (non-Rayleigh) fractal particle (fractal dimension D_f between 1.2 and 2.4), consistent with electron micrograph and optical scattering experiments on real aerosol aggregates, and analogous to expected early Earth haze.

The T-matrix method begins with Maxwell's equations and the Lorenz-Mie theory (see Born and Wolf, 1999; Van der Hulst, 1957; Bohren and Huffman, 1983) for a single scattering sphere. To calculate the scattering of a nonspherical particle made of smaller spheres, the Lorenz-Mie relations are extended by superposition of electric fields:

$$\mathbf{E}_s = \sum_{i=1}^{N} \mathbf{E}_{s,i}$$

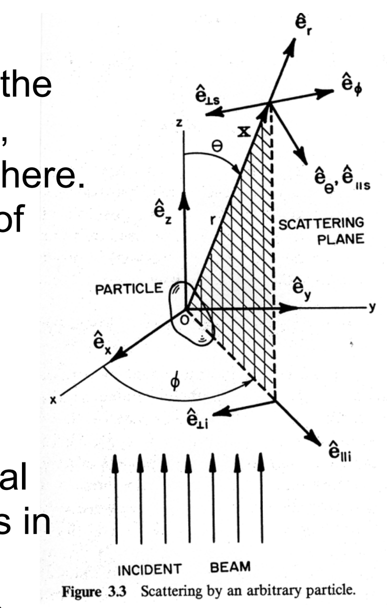


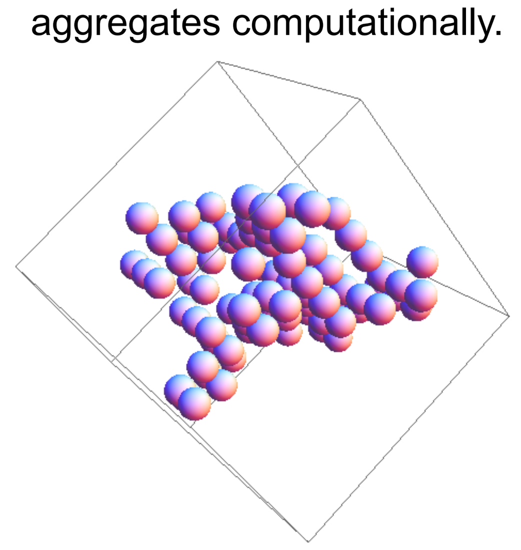
Figure from Bohren and Huffman (1983) showing the scattering geometry used in our calculations. The incoming light is plane, linearly polarized, with scattering angles $\varphi=\alpha$ and $\theta=\beta$ in Mackowski's T-matrix code.

Here the sum is over the *N* spherical monomers of the fractal aggregate. The T-matrix method represents the partial fields in the sum, for each individual sphere, as a vector spherical harmonic expansion (VSH), centered about the origin of the sphere. For further details, see Mackowski and Mishchenko (1996) or Liou (2002).

But before any systematic light scattering calculations can be done, realistic fractal aggregate clusters must be generated by computer programs. This is much more challenging than it may seem. In the early to mid-1980s there were many published papers in physics journals about generating 2-dimensional on-lattice versions of clusters using diffusion-limited aggregation (DLA), and studying the statistical physics of these simple clusters. But for realistic atmospheric aerosol soot or haze clusters, we need to use a much more difficult concept: cluster-cluster aggregation (CCA), and in 3 dimensions, and off lattice. Implementing this has been very challenging because the positions of the monomers are not constrained on a lattice, and there are 3 dimensions, and each growing cluster moves until it hits another cluster, so the program must keep track of many large boundaries in 3-D space.

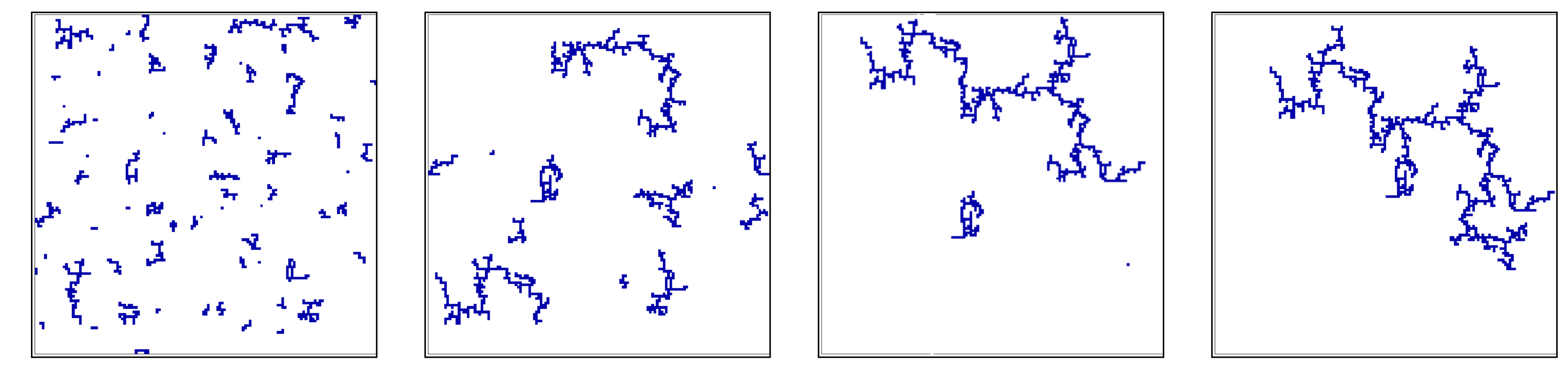
Results

As input for the T-matrix code, we need to calculate positions of the individual monomer spheres in fractal aggregates. Some other research groups have used diffusion limited aggregation (DLA) to generate aerosol fractal morphologies. However, DLA due to its single-cluster growth leads to 3-D fractal structures of the wrong fractal dimension and with an overly radial structure (compared to real soot or haze aggregates). Because real soot or haze aggregates vary in size (from several to 500 monomers) and fractal dimension (*D*=1.8 is typical for new aggregates and *D*>2 for older, more spherical aggregates), we have used the more physically-realistic cluster-cluster aggregation (CCA) to generate aerosol aggregates computationally.



CCA cluster calculated in MATLAB by having new monomers randomly walk (diffusion) until they hit any growing cluster. This new 3-D on-lattice program was developed by Trevor Simpkin, based on 2-D CCA discussion in Gould and Tobotchnik (1996).

3-D off-lattice atmospheric haze cluster with N = 300 monomers, generated by Trevor Simpkin using FracMAP (program courtesy of Dr. Rajan Chakrabarty). The fractal dimension is 1.82.



2-D on-lattice Cluster-cluster aggregation (CCA) calculated in 2010 by SU physics major Bernice Terrell-Martinez using an algorithm by Gould and Tobochnik (1996). Note that because the individual aggregates are all separately growing while diffusing according to a mass-dependent diffusion coefficient, the resulting fractal aerosol haze aggregate is much more like real haze aerosol aggregates than the DLA method usually employed. Lattice linear dimension L=500 and released monomer number N=1000.

Future Work

These results will also have relevance to optical haze scattering in Titan's current atmosphere. For current Earth atmosphere carbonaceous fractal soot aerosol comparisons between theory and experiment, we plan to write better directionally-biased cluster-cluster aggregate (CCA) program to generate even more realistic fractal clusters, simulating aggregate growth under electrostatic force alignment. After running the T-matrix scattering code for many angles, cluster sizes, refractive indices, and fractal dimensions, we will compare our results with related results of Liu and Mishchenko (2007) in the context of the IPCC climate change report (IPCC, 2007). In 2011, Dan Mackowski of Auburn University re-wrote his light scattering program in Fortran 95, so we are implementing that new code now.

Acknowledgements

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References

Bohren, C. F., and Huffman, D. R. (1983). *Absorption and Scattering of Light by Small Particles*. New York: Wiley.

Born, M., and Wolf, E. (1999). *Principles of Optics, 7th ed.* Cambridge: Cambridge University Press.

Gough, D. O. (1981). Solar interior structure and luminosity variations. *Solar Physics* 74: 21-34.

Gould, H., and Tobotchnik, J. (1996). *An Introduction to Computer Simulation Methods: Applications to Physical Systems*, 2nd ed. (Addison-Wesley, Reading, Massachusetts).

IPCC. (2007): *Climate Change 2007: The Physical Science Basis. Contribution of Working Group I to the Fourth Assessment Report of the Intergovernmental Panel on Climate Change* [Solomon, S., D. Qin, M. Manning, Z. Chen, M. Marquis, K.B. Averyt, M.Tignor and H.L. Miller (eds.)]. Cambridge, UK, and New York, NY, USA: Cambridge University Press.

Liou, K. N. (2002). *An Introduction to Atmospheric Radiation*, 2nd ed. Amsterdam: Academic Press.

Liu, L., and Mishchenko, M. I. (2007). Scattering and radiative properties of complex soot and soot-containing aggregate particles. *J. Quant. Spectrosc. Radiat. Transfer* 106: 262-273.

Mackowski, D. W., and Mishchenko, M. I. (1996). Calculation of the T matrix and the scattering matrix for ensembles of spheres. *J. Opt. Soc. Am. A* 13: 2266-2278.

Rosing, M. T, *et al.* (2010). No climate paradox under the faint early Sun. *Nature* 464: 744-747.

Sagan, C., and Mullen, G. (1972). Earth and Mars: Evolution of atmospheres and surface temperatures. *Science* 177: 52-56.

Som, S. M., *et al.* (2012). Air density 2.7 billion years ago limited to less than twice modern levels by fossil raindrop imprints. *Nature* 484: 359-362.

Sorensen, C. M. (2001). Light scattering by fractal aggregates: A review. *Aerosol Sci. Tech.* 35: 648-687.

Van de Hulst, H. C. (1957). *Light Scattering by Small Particles*. New York: Wiley.

Waterman, P. C. (1971). Symmetry, unitarity, and geometry in electromagnetic scattering. *Phys. Rev. D* 3: 825-839.

Wolf, E. T., and Toon, O. B. (2010). Fractal Organic Hazes Provided an Ultraviolet Shield for Early Earth. *Science* 328: 1266-1268.