Optical Properties of Nonspherical Particles: Physical Models and Machine Learning

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Acknowledgment: Funding support from CMA, NSF. Contributions from postdocs and graduate students: Wushao Lin, Zheng Wang, Meng Li, Hejun Xie, Lanhui Sun, Jinhe Yu, Senyi Kong.

Zhejiang University (1897-)

“Seeking Truth, Pursuing Innovation”.

Atmospheric Sciences (1936-)

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INTERNATIONAL RADIATION SYMPOSIUM

JUNE 2024, HANGZHOU, CHINA

Zhejiang University

Lei Bi (local host, IRC commissioner)

Celebrate the 20-year Anniversary in Asia!

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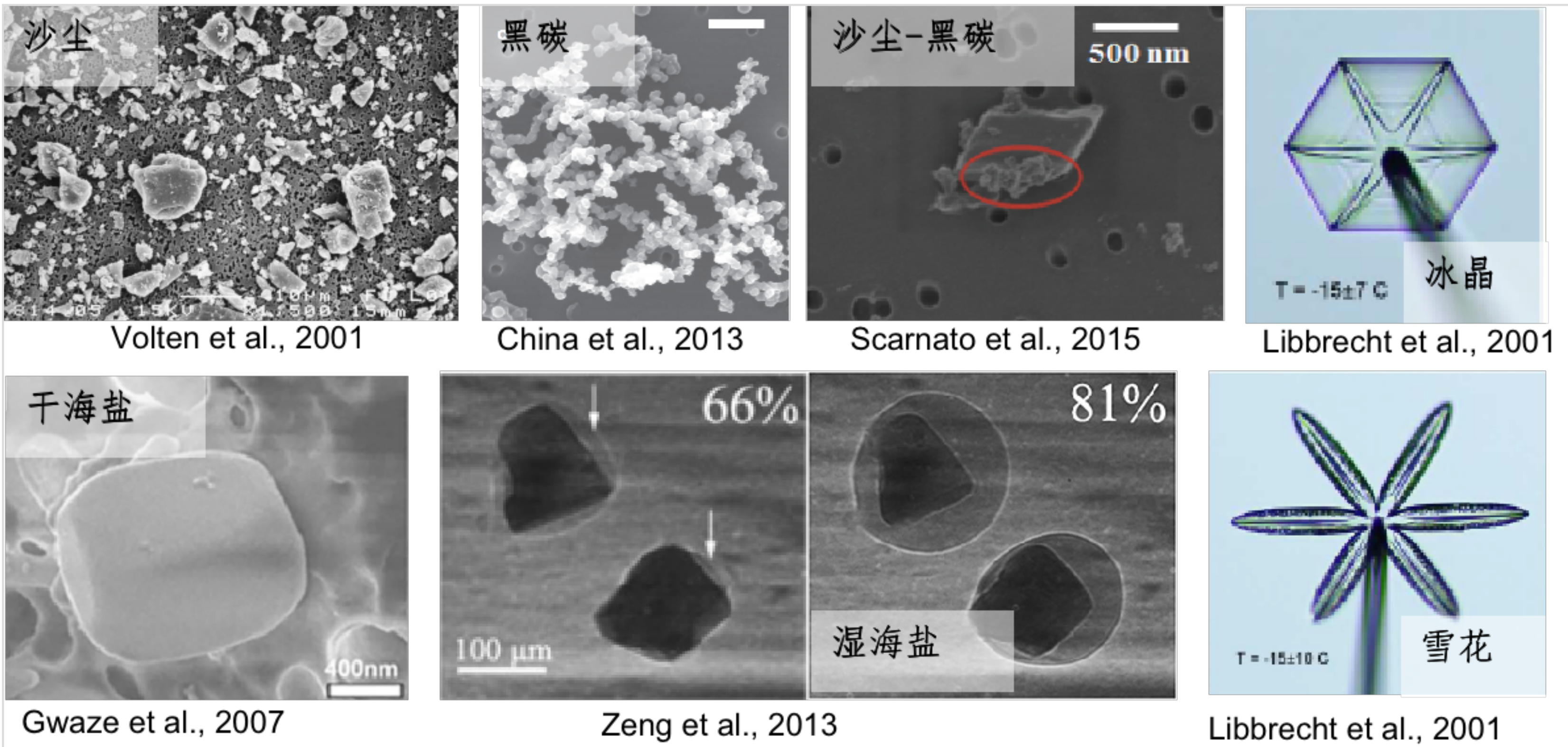
Cloud, Aerosol and Precipitation Particles



Volten et al., 2001 | China et al., 2013 | Scarnato et al., 2015 | Libbrecht et al., 2001

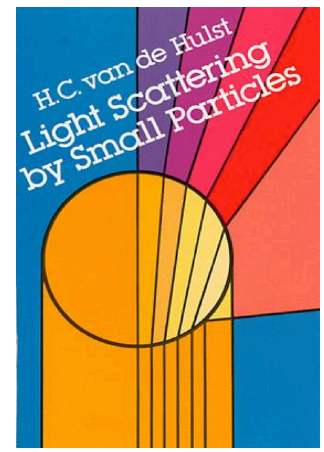
Gwaze et al., 2007 | Zeng et al., 2013 | Libbrecht et al., 2001

We hope that all particles are spheres, but they are not.

Van de Hulst: A long way …

PREFACE

The scattering of electromagnetic waves by a homogeneous sphere is a problem with a known solution. I first met this problem when I needed some numbers and curves in an astrophysical investigation. I soon learned that it is a long way from the formulae containing the solution to reliable numbers and curves. Subsequent conversations and correspondence with other research workers, notably in chemistry, showed that the same difficulty was felt in other fields.



Light Scattering by Small Particles
(A "bible" of light scattering)

The story is also very true for nonspherical particles.

Problems and Challenges

- Efficient and accurate computational methods

  arbitrary shapes, inhomogeneities and sizes

- Flexible particle representations (aerosols, hydrometeors)

  shapes, refractive indices , size distributions

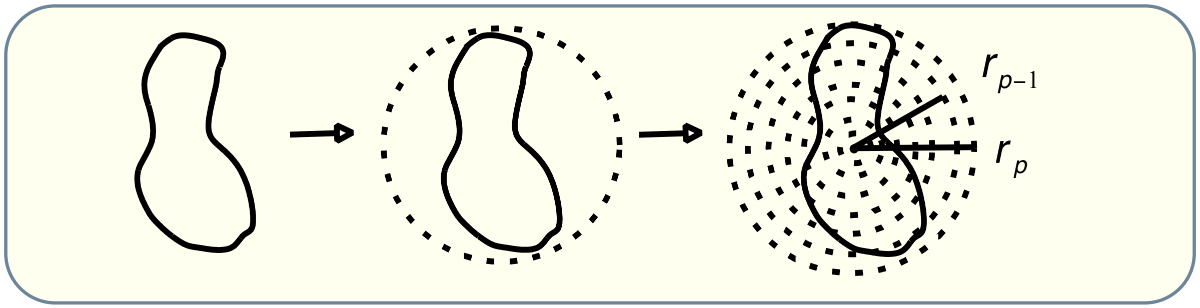
- Datasets, parameterization, validation …

  tremendous efforts

Progresses

- **T-matrix, Super-formula, Machine Learning**

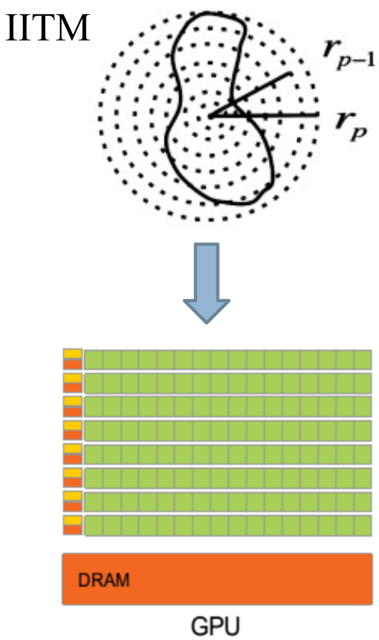
Invariant Imbedding T-matrix

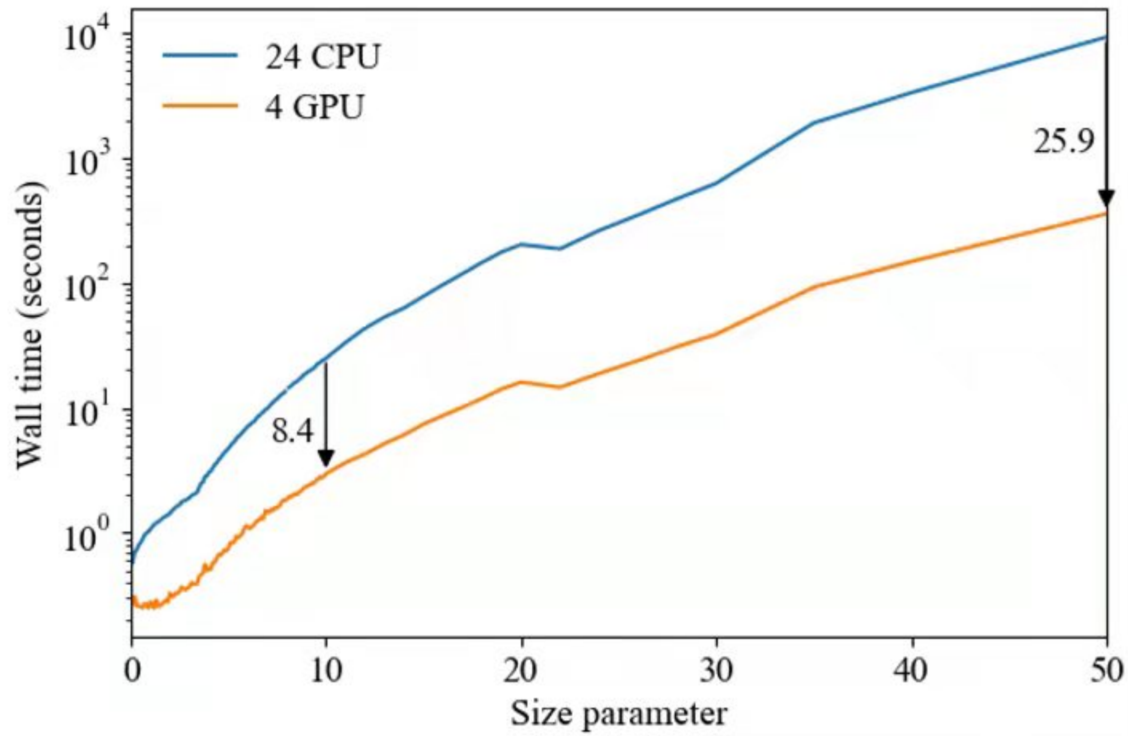


$$T_{mnmn'}(r+dr) = Q_{11}^{m}(r+dr) + \left[\mathbf{I} + Q_{12}^{m}(r+dr)\right]\left[\mathbf{I} - T_{mnmn'}(r) Q_{22}^{m}(r+dr)\right]^{-1} T_{mnmn'}(r)\left[\mathbf{I} + \tilde{Q}_{12}^{m}(r+dr)\right]$$

(Johnson, 1988; Bi et al., 2013;Bi and Yang, 2014; Bi et a., 2018; Bi et al., 2022)

G-IITM: A GPU Implementation

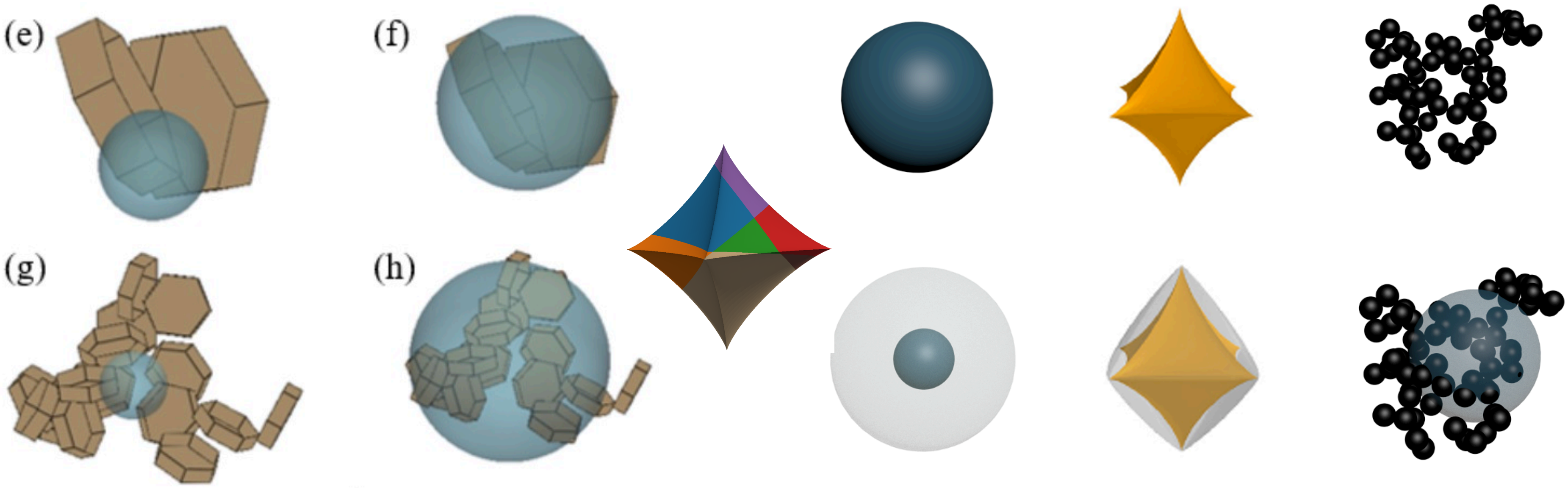




The computation speed increases by 10~20 times.

Lei Bi, Zheng Wang , Wei Han, Weijun Li, Xiaoye Zhang, 2022: ***Frontiers in Remote Sensing***, 3:903312.

Level of particle complexity is significantly improved.



IITM T-matrix Features

- Arbitrary shaped and inhomogeneous particles (flexibility)
- Analytical random orientation average (accuracy and efficiency)
- Particle size parameter up to geometric-optics domains (applicability)

Conventional EBCM T-matrix: homogeneous axially symmetric particles.

Progresses

- T-matrix, Super-formula, Machine Learning

Freedom

Sphere: No shape freedom

Spheroid: one

Tri-axial ellipsoids: two

Super-formula: more freedom

Atmospheric particles: infinite, optimized freedom?

Why more freedom is useful?

Drawing an elephant with four complex parameters

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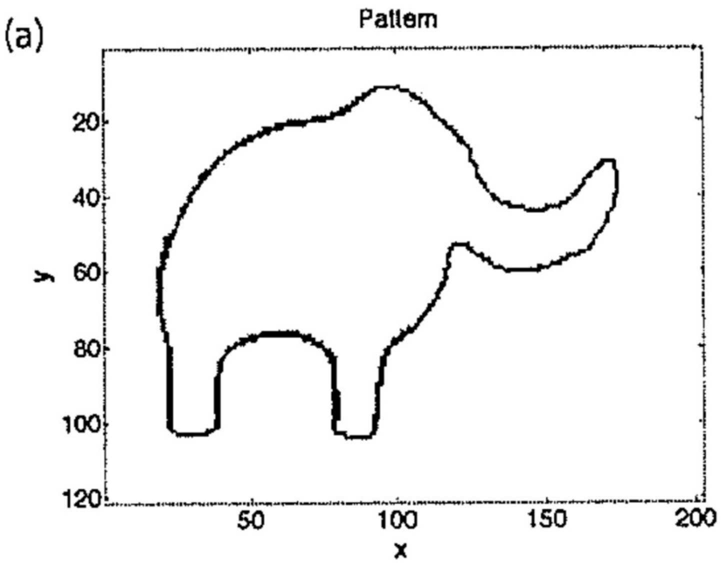
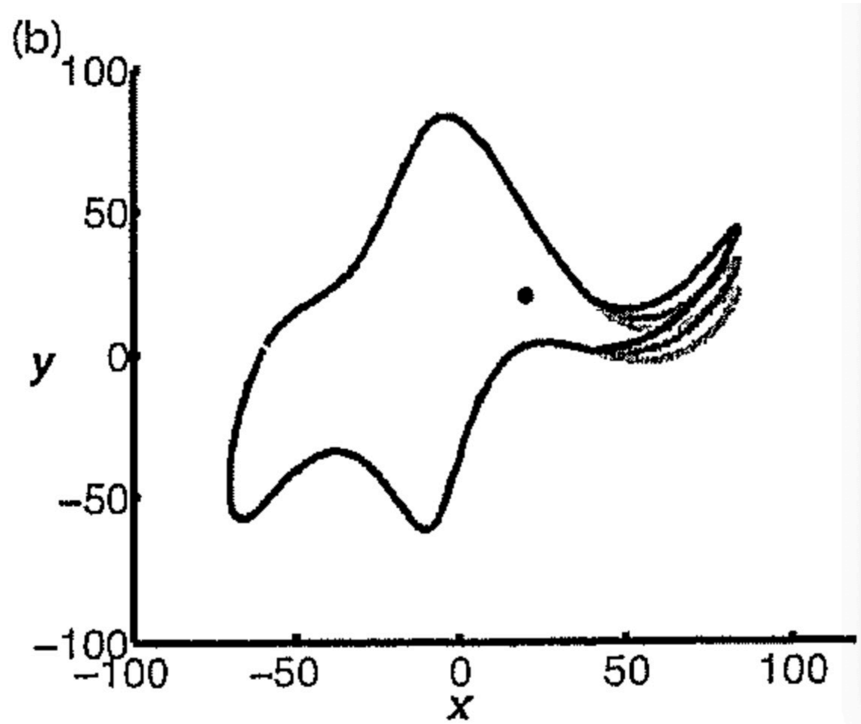
(Received 20 August 2008; accepted 5 October 2009)

We define four complex numbers representing the parameters needed to specify an elephantine shape. The real and imaginary parts of these complex numbers are the coefficients of a Fourier coordinate expansion, a powerful tool for reducing the data required to define shapes. © *2010 American Association of Physics Teachers.*

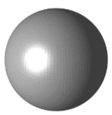
[DOI: 10.1119/1.3254017]



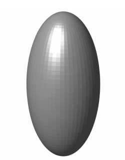


Wiggling Trunk

Super-spheroid model



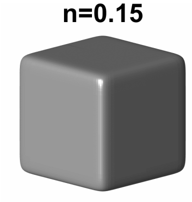
sphere $$\left(\frac{x}{a}\right)^2+\left(\frac{y}{a}\right)^2+\left(\frac{z}{a}\right)^2=1$$



spheroid $$\left(\frac{x}{a}\right)^2+\left(\frac{y}{a}\right)^2+\left(\frac{z}{c}\right)^2=1$$

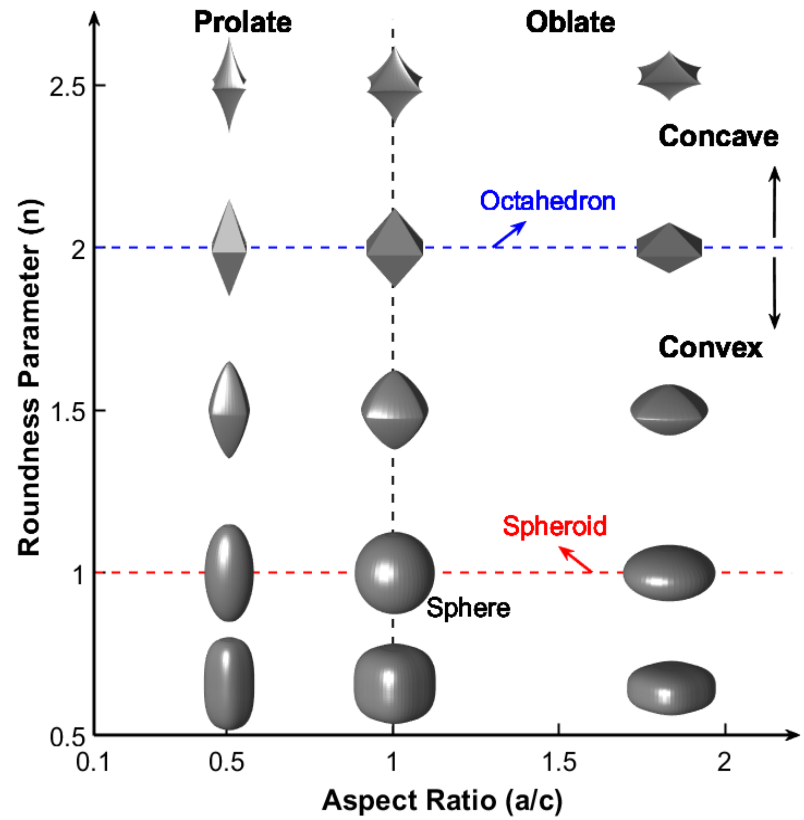
super-spheroid $$\left(\frac{x}{a}\right)^{2/n}+\left(\frac{y}{a}\right)^{2/n}+\left(\frac{z}{c}\right)^{2/n}=1$$

n=0.15



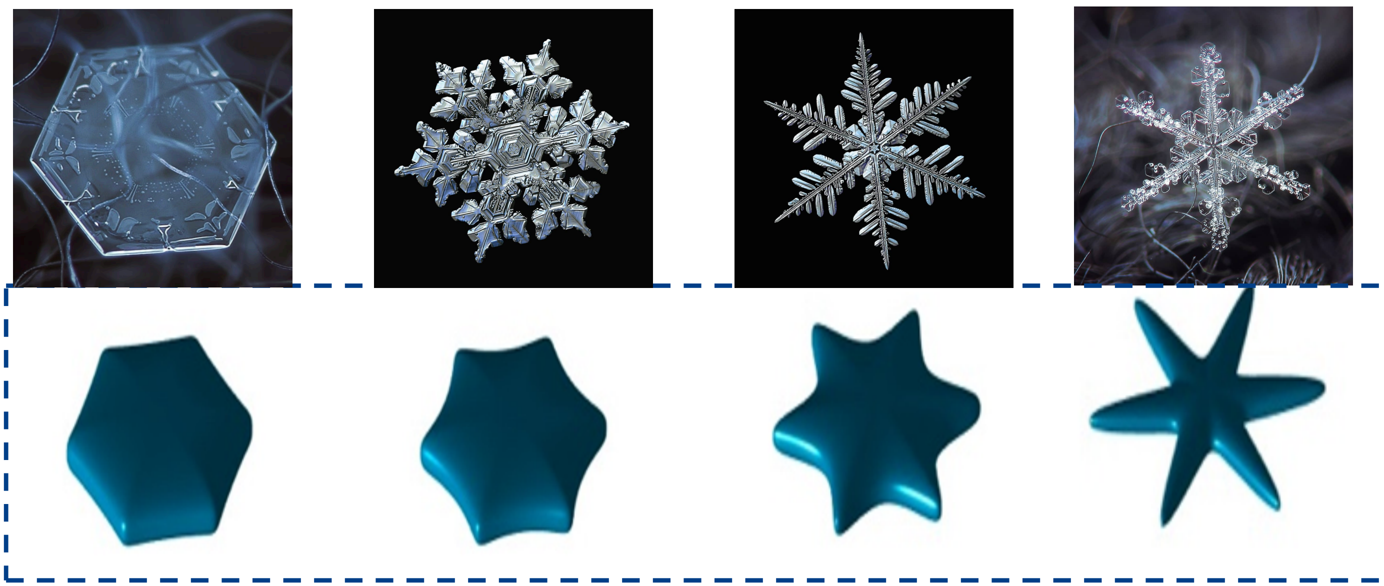
aspect ratio: ***a/c***

roundness parameter: ***n***



Continuous Parameter Snowflake Model

Picture from
alexey_kljatov



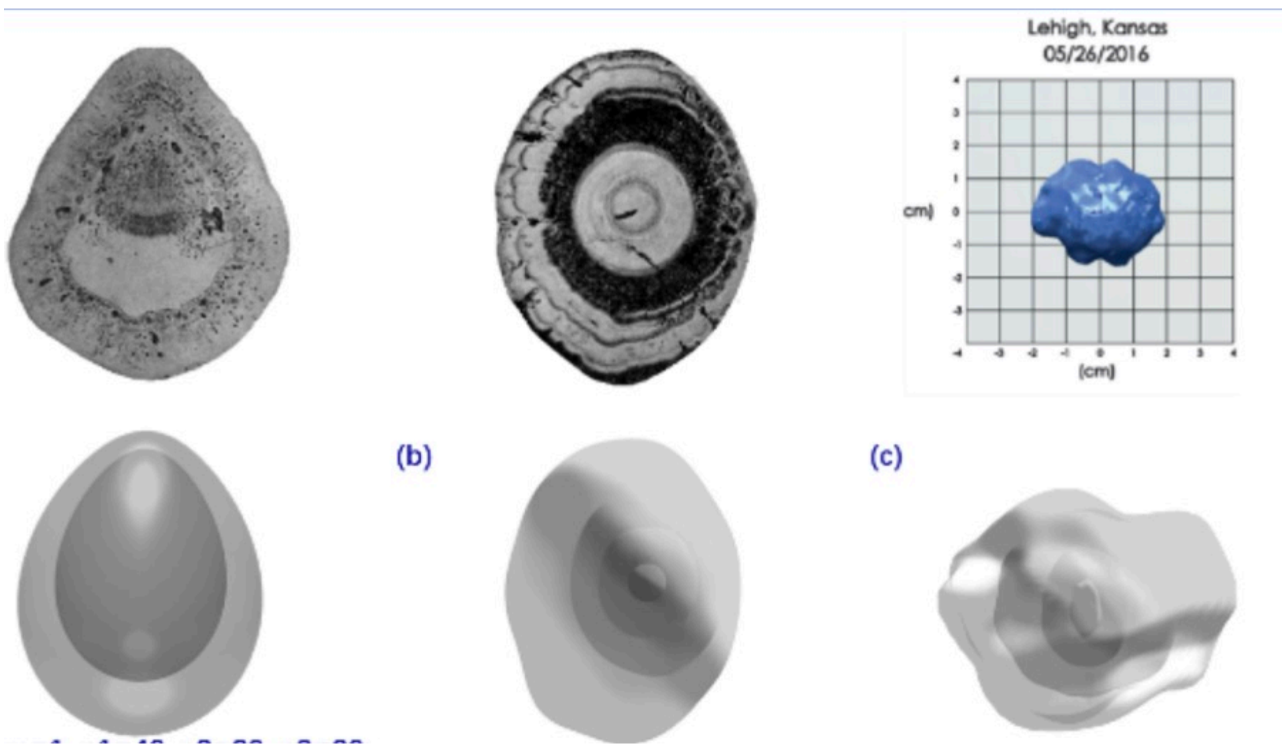
Superformula $$r(\phi) = a\left[2^{\frac{n_2}{2}-1}\left(\left|\cos(1.5\phi)\right|^{n_2} + \left|\sin(1.5\phi)\right|^{n_2}\right)\right]^{-\frac{1}{2n_1}}$$

- ➢ Shape parameter n_1、 n_2 controls continuous change of snowflake shape

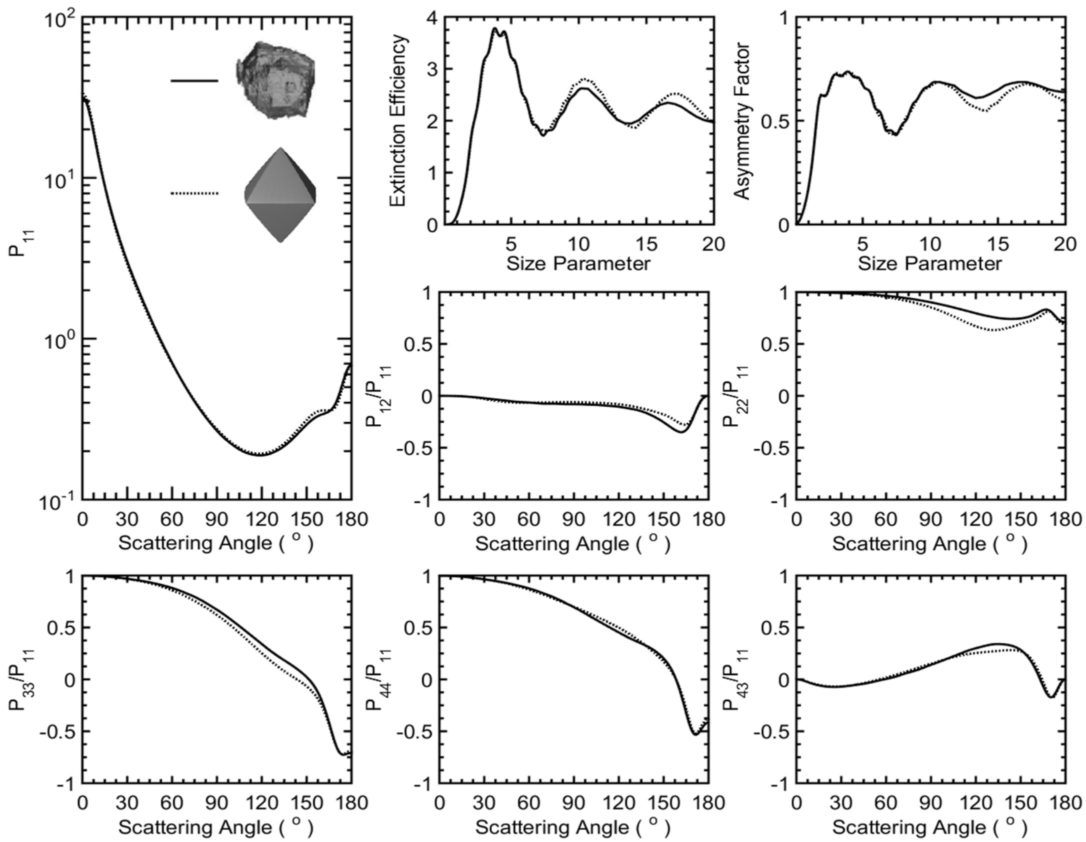
Graupel

Observations

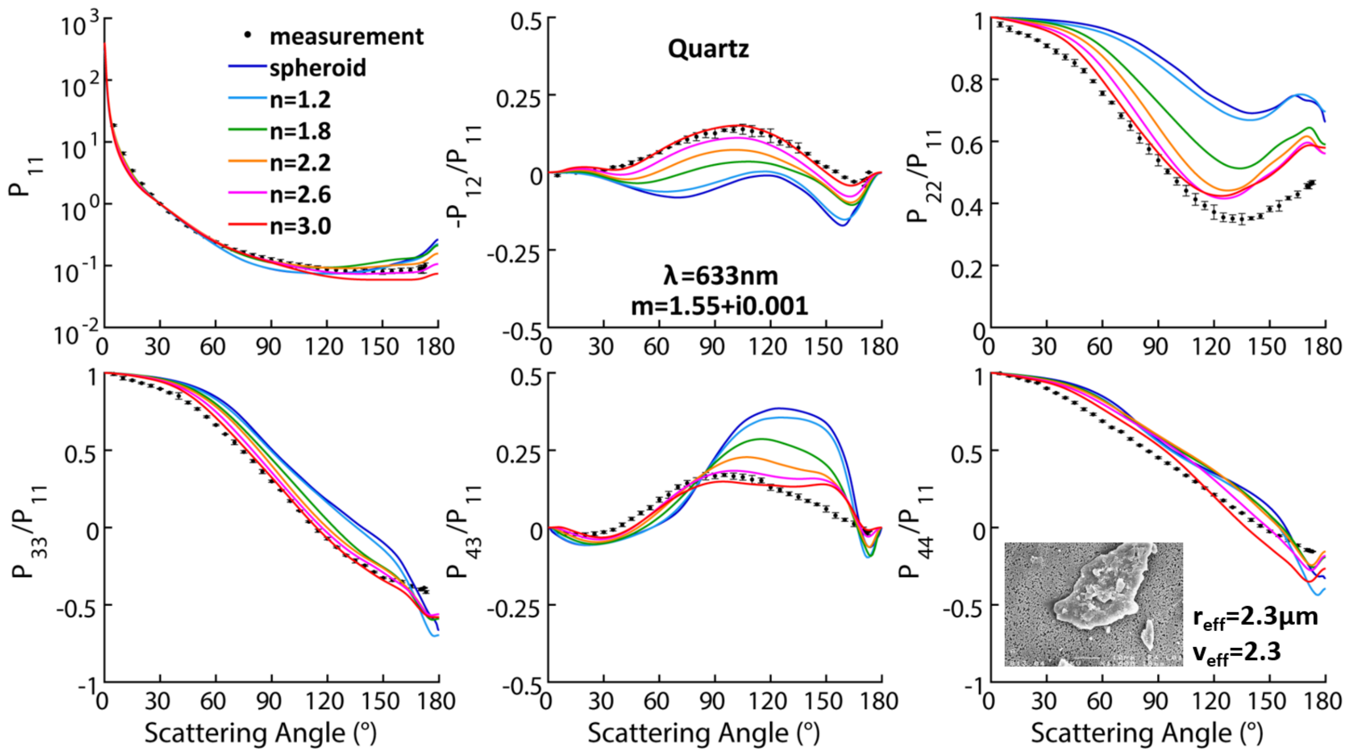
Formula



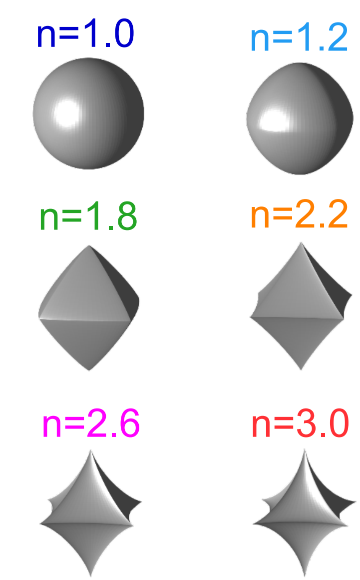
Optical “equivalence”



Modeling scattering matrices of dust aerosols



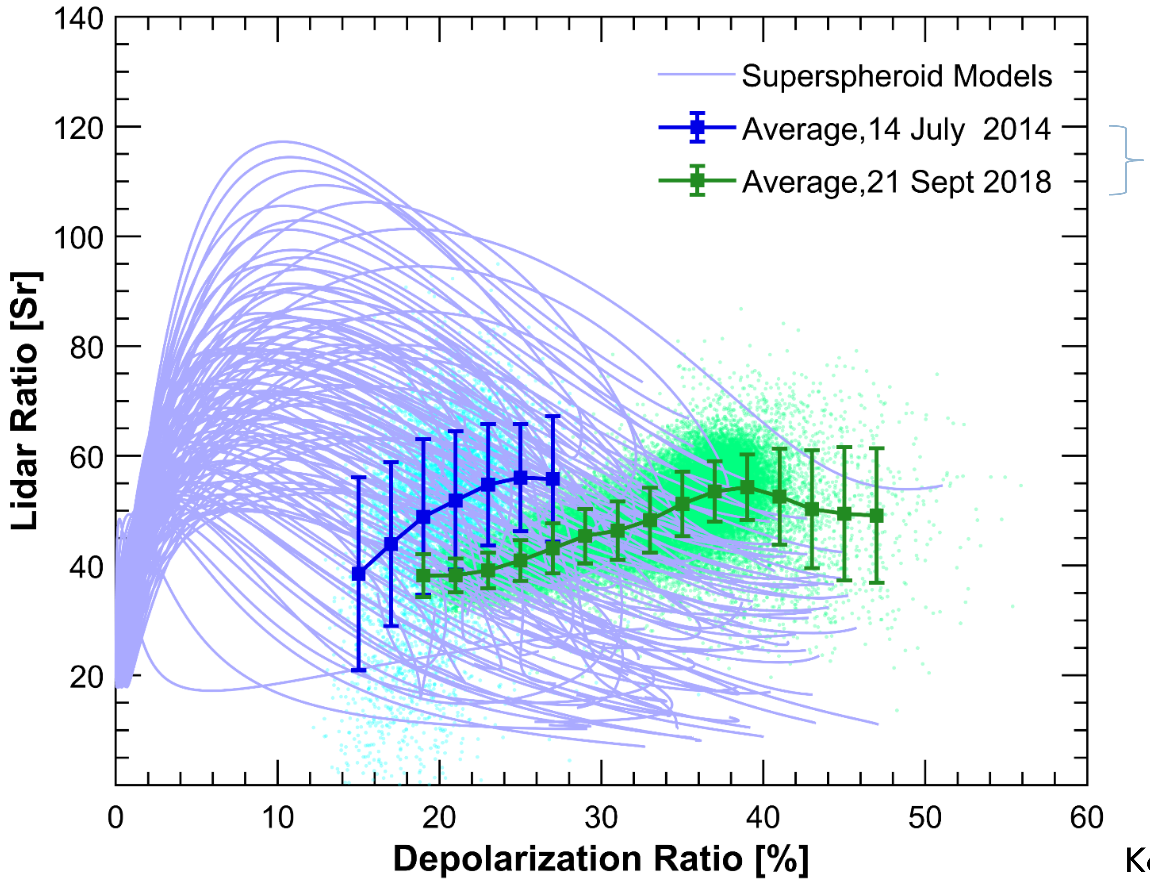
Equi-probable aspect ratio distribution



Lin et al., *JGR*, 2018

- Concave super-spheroids can reproduce the scattering matrices of dust samples from the Amsterdam-Granada Light Scattering Database.

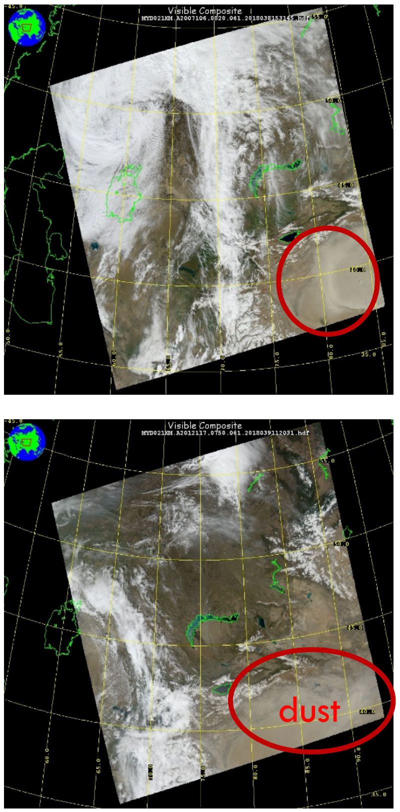
Modeling the depolarization ratio and lidar ratio of dust



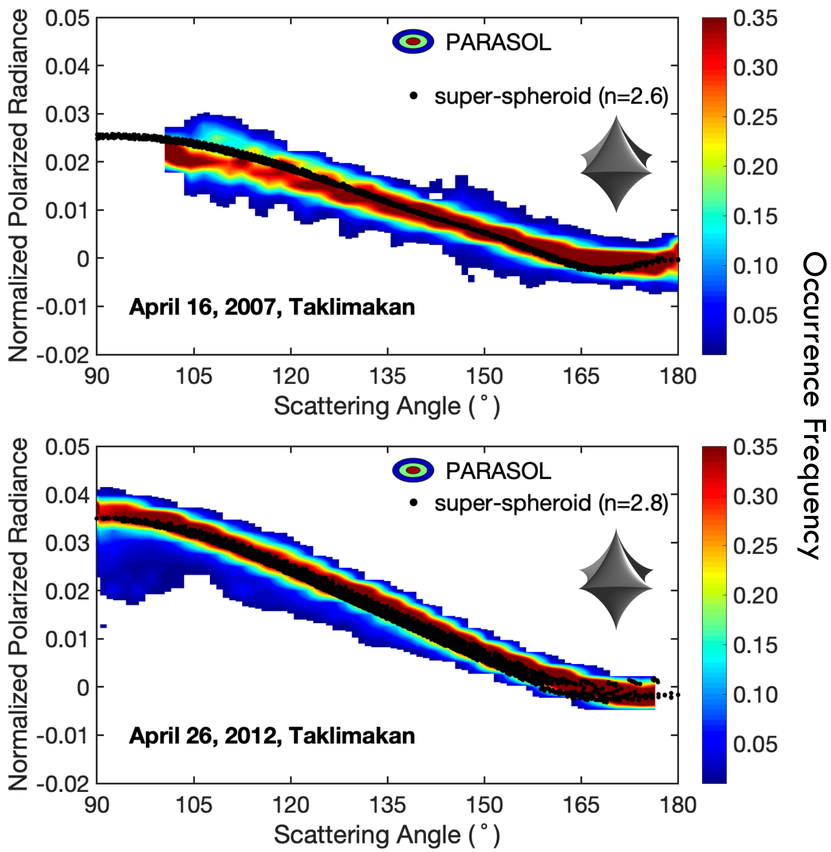
The superspheroid models were capable of simulating the entire lidar ratio-depolarization ratio range of atmospheric dust obtained from the HSRL measurement at 355 nm.

Kong et al., JGR, 2022

Modeling PARASOL observations under dusty-sky conditions



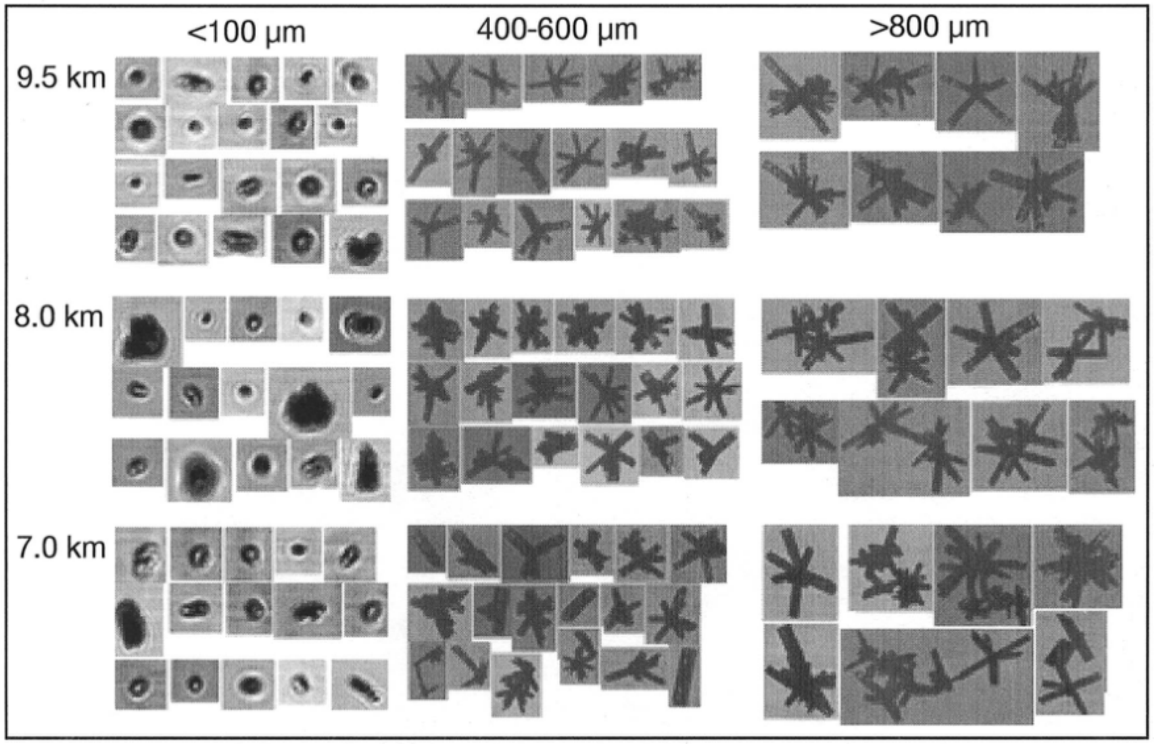
From MODIS



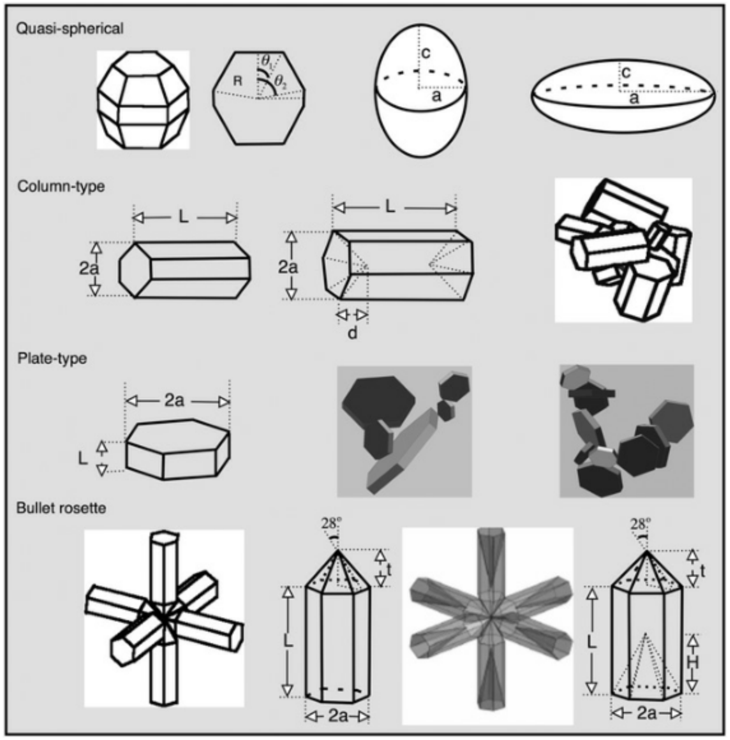
- Concave super-spheroids successfully reproduce the angular distribution of the observed TOA polarized radiance under dusty-sky conditions.

Lin et al., JGR, 2021

Different shapes and physical models of ice crystal



Heymsfield, et al., 2003

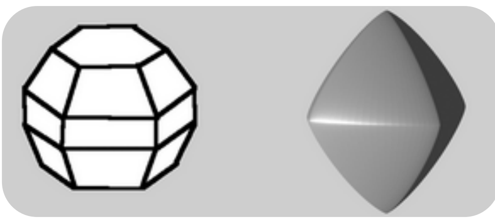


Yang, Bi, et al., 2013

- Electromagnetic wave scattering by ice particles is commonly modeled by defining representative habits, including droxtals, columns, plates, and aggregates, although actual particles in the atmosphere can be even much more complex.

The use of super-spheroids as surrogates for ice crystal

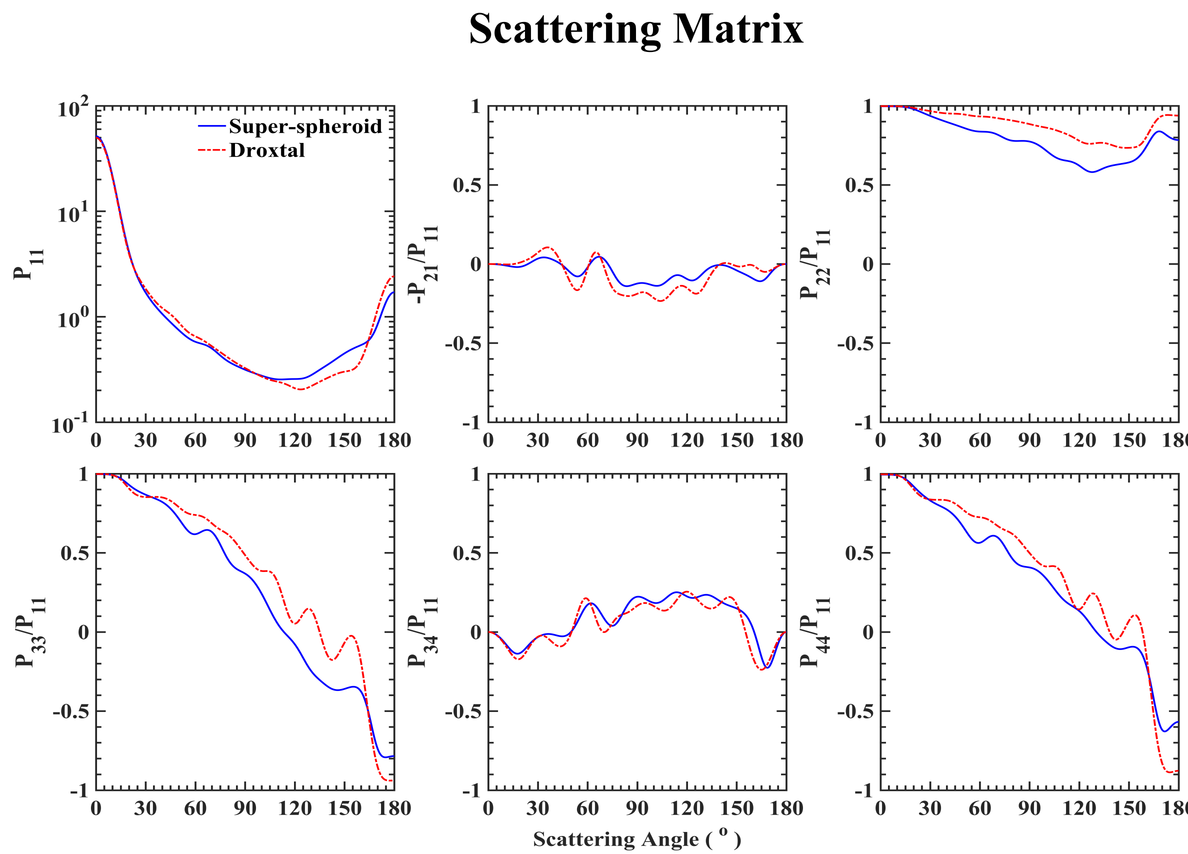
Droxtal **Super-spheroid**



Optical "equivalence"

$$SI = \frac{3V}{4\pi S/\pi^{3/2}}$$

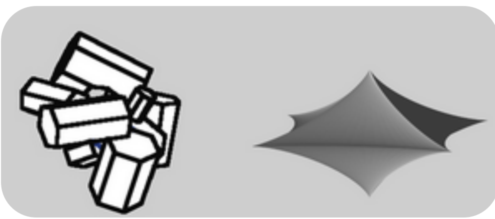
V = Volume
S = Average projected area



Sun et al., Remote Sensing, 2021

The use of super-spheroids as surrogates for ice crystal

Aggregate **Super-spheroid**

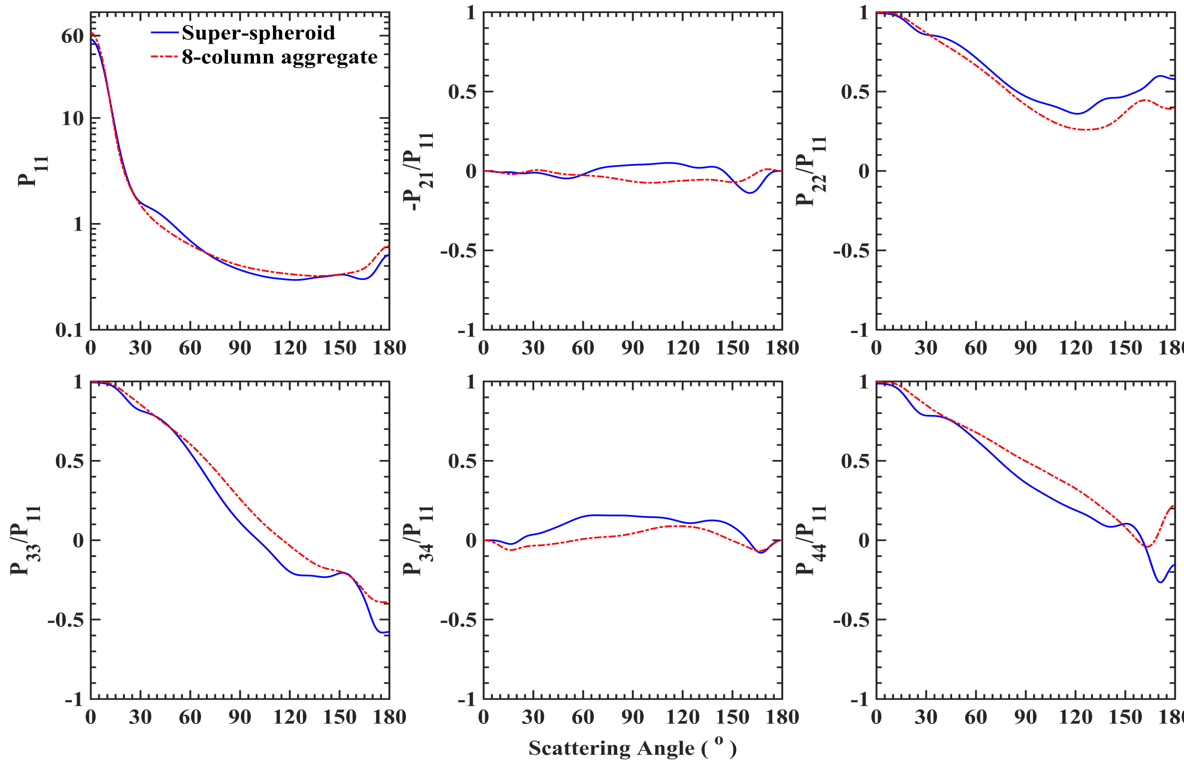


Optical "equivalence"

$$SI = \frac{3V}{4\pi S/\pi^{3/2}}$$

V = Volume
S = Average projected area

Scattering Matrix



Sun et al., Remote Sensing, 2021

Progresses

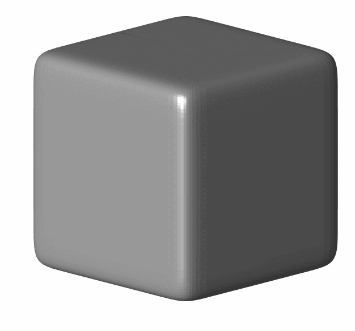
- T-matrix, Super-formula, Machine Learning

Super-spheroids Scattering Database

Super-spheroid

$$\left(\frac{x}{a}\right)^{2/n} + \left(\frac{y}{a}\right)^{2/n} + \left(\frac{z}{c}\right)^{2/n} = 1$$

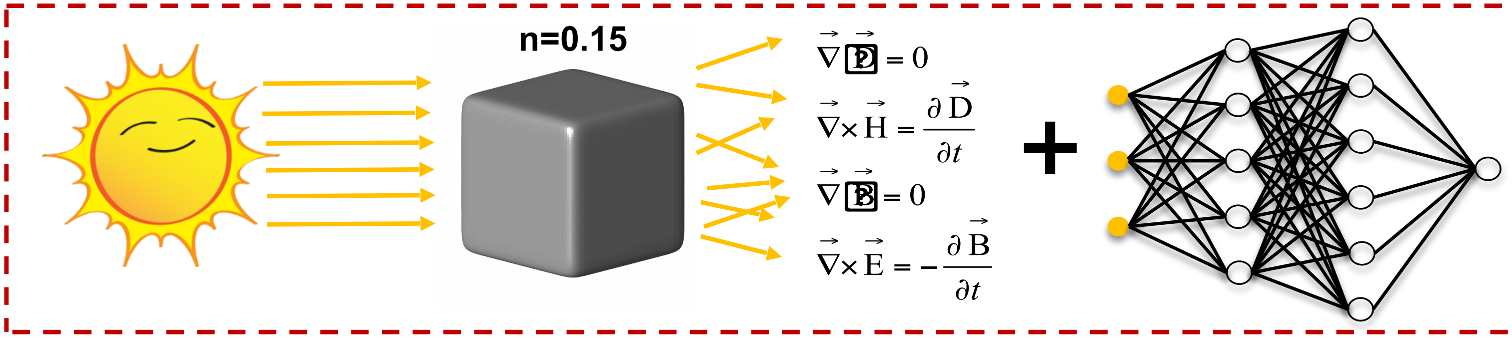
n=0.15



Aspect ratio	Roundness	Refractive index Real part	+ Imag. part	Size parameter	Scattering angle (°)
0.5	1.2	1.30	10^{-7}	0.1	0
0.6	1.4	1.35	10^{-6}	0.2	0.25
0.7	1.6	1.40	10^{-5}	......	0.5
0.8	1.8	1.45	10^{-4}	9.9	0.75
0.9	2.0	1.50	0.001	10	1
1.0	2.2	1.55	0.005	10.2	......
1.2	2.4	1.60	0.01	......	179
1.4	2.6	1.65	0.05	19.8	179.25
1.6	2.8	1.70	0.1	20	179.5
1.8	3.0	1.75		21	179.75
2.0		1.80		......	180
				49	
				50	

- The database is too **huge(~127GB)** to share and apply

Deep learning on the Super-spheroids Scattering Database



Input → **DNN model** ↔ **Output**

Input: super-spheroids particle parameters

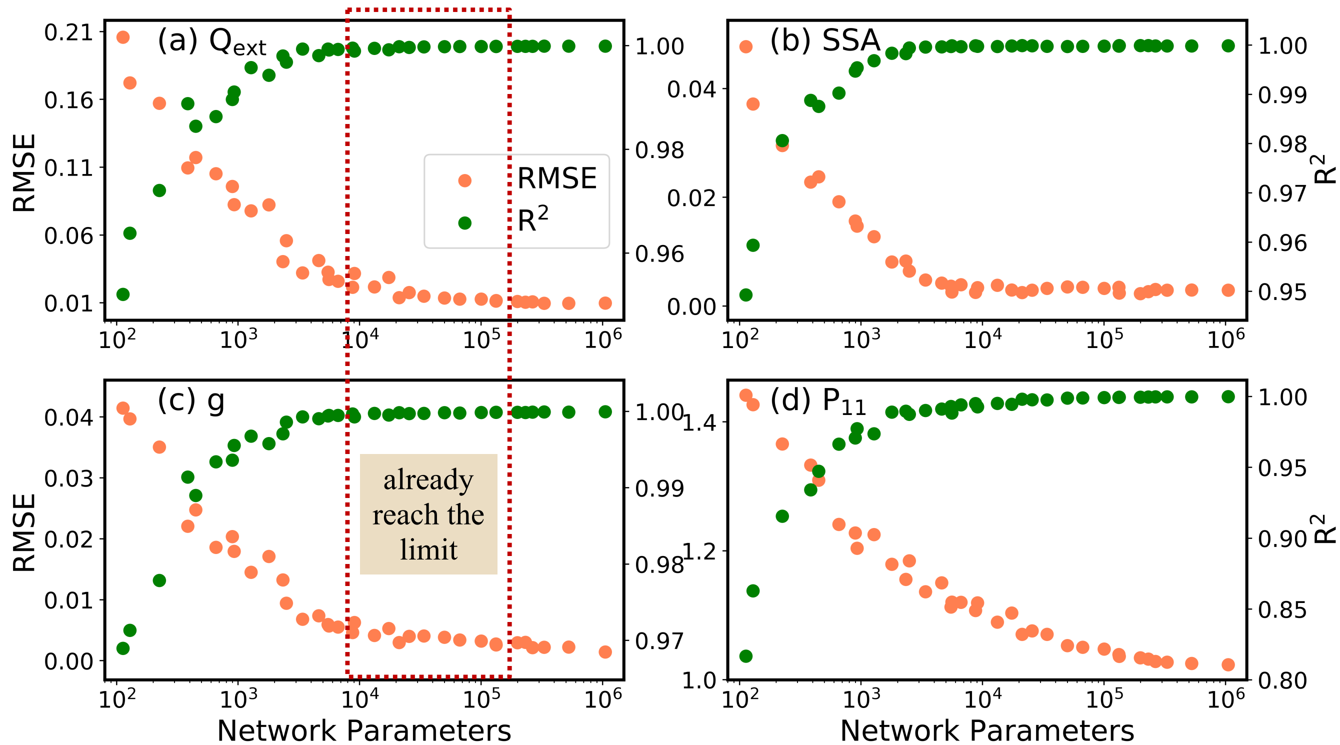
- Aspect ratio
- Roundness
- Ref. index Real part
- Ref. index Imag. part
- Size parameter
- Scattering angle

Output: optical properties

- Extinction efficiency factor
- Single scattering albedo
- Asymmetry factor
- Phase matrix elements

- **Note: Shapes are training parameters.**

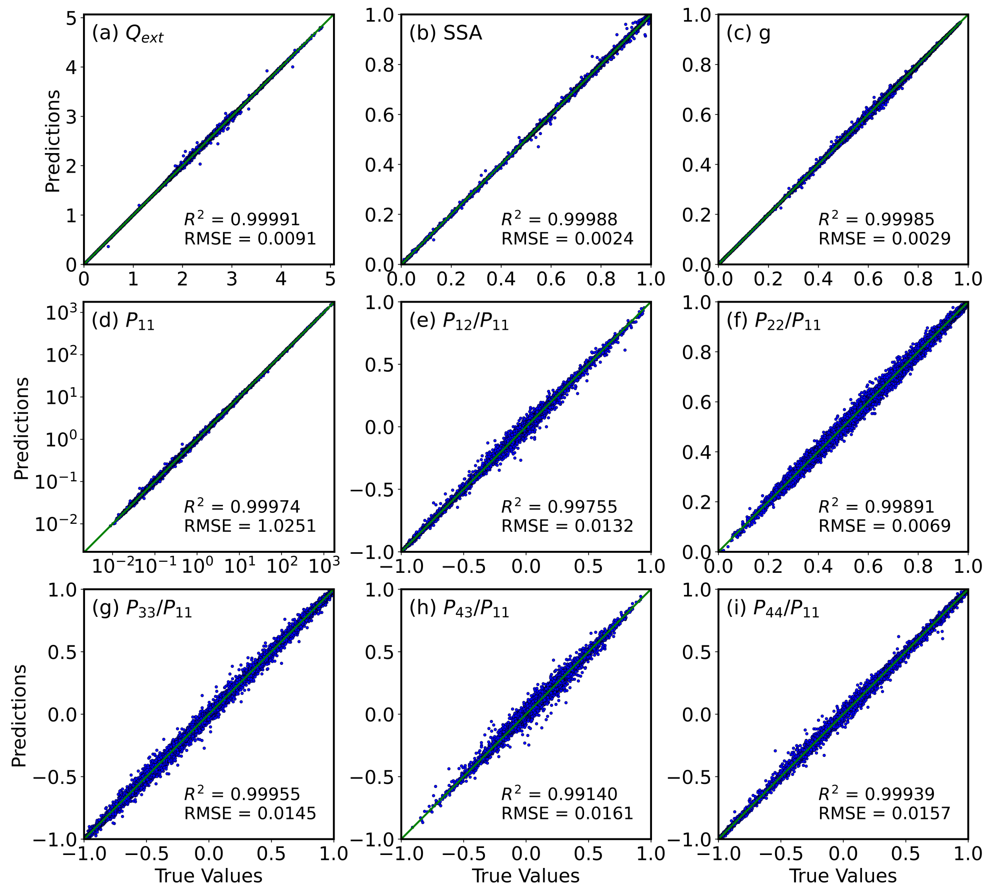
Choose appropriate models via RMSE-R2-Network parameters



Small size (~10^4 parameters inside) DNN models can gain low error and good performance, **replace the big database by ~6800 compression ratio.**

J. Yu, Lei Bi, Wei Han, Xiaoye Zhang, Advances in Atmospheric Sciences, 2022

Performance of the optimal models



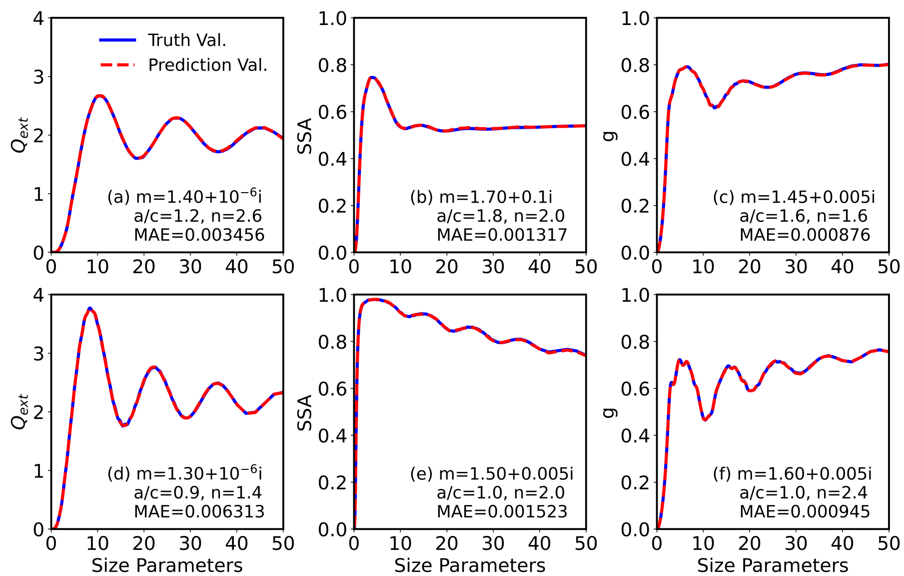
Yu et al., Advances in Atmospheric Sciences, 2022

- Performance on the test set (including 100,000 samples)

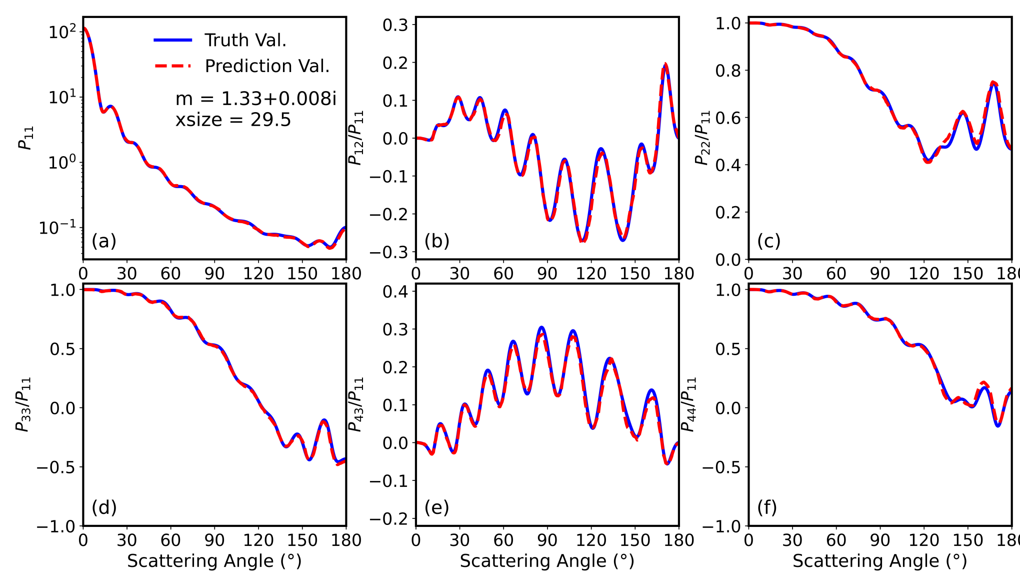
$R^2 > 0.99$

Deep learning on the Super-spheroids Scattering Database

Test on specific known particles



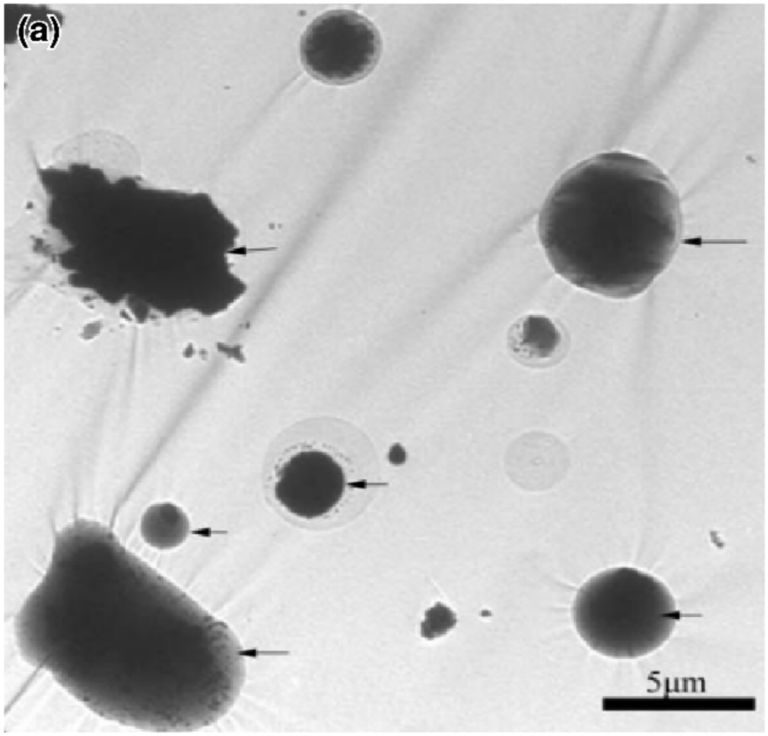
Test on specific known particles

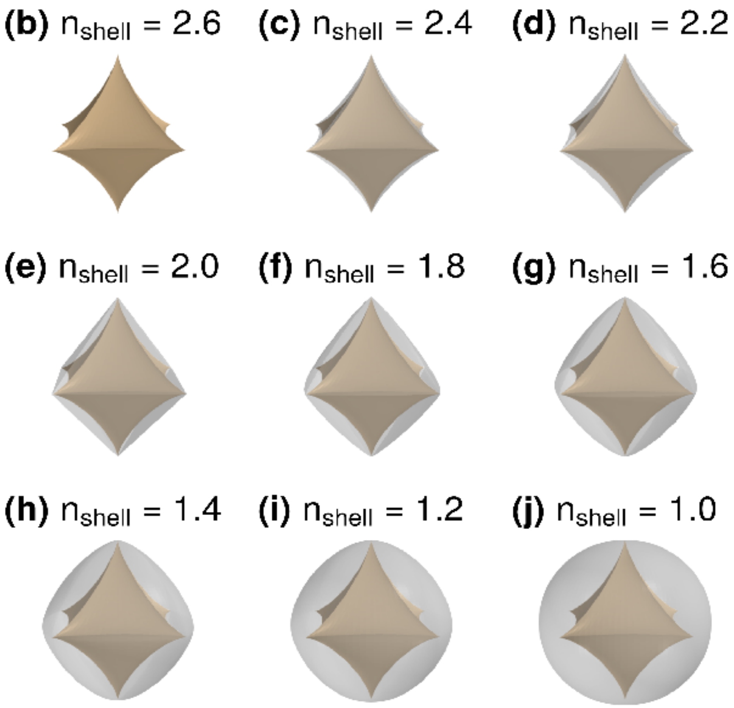


- **The DNN models can accurately predict the optical properties of specific particles which are already existed in the database or unknown before.**

Yu et al., Advances in Atmospheric Sciences, 2022

A new optical scheme for inhomogeneous particles

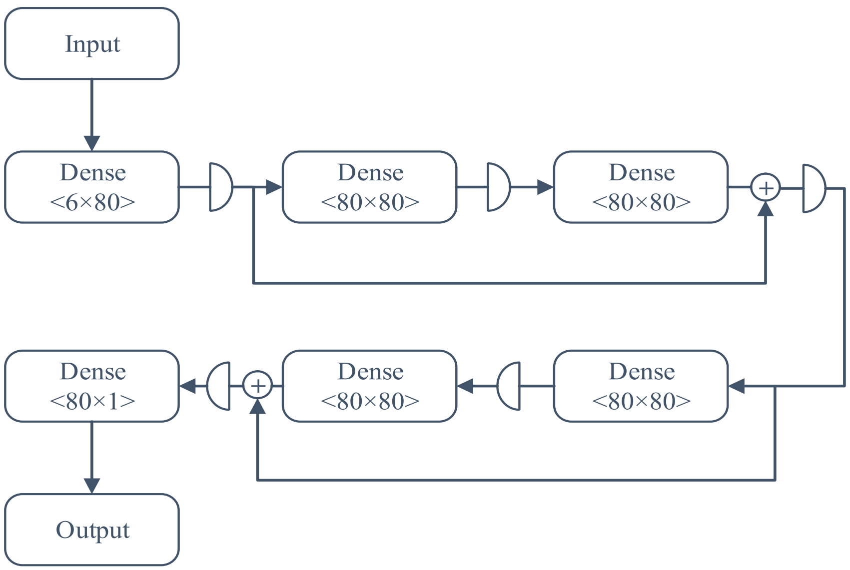




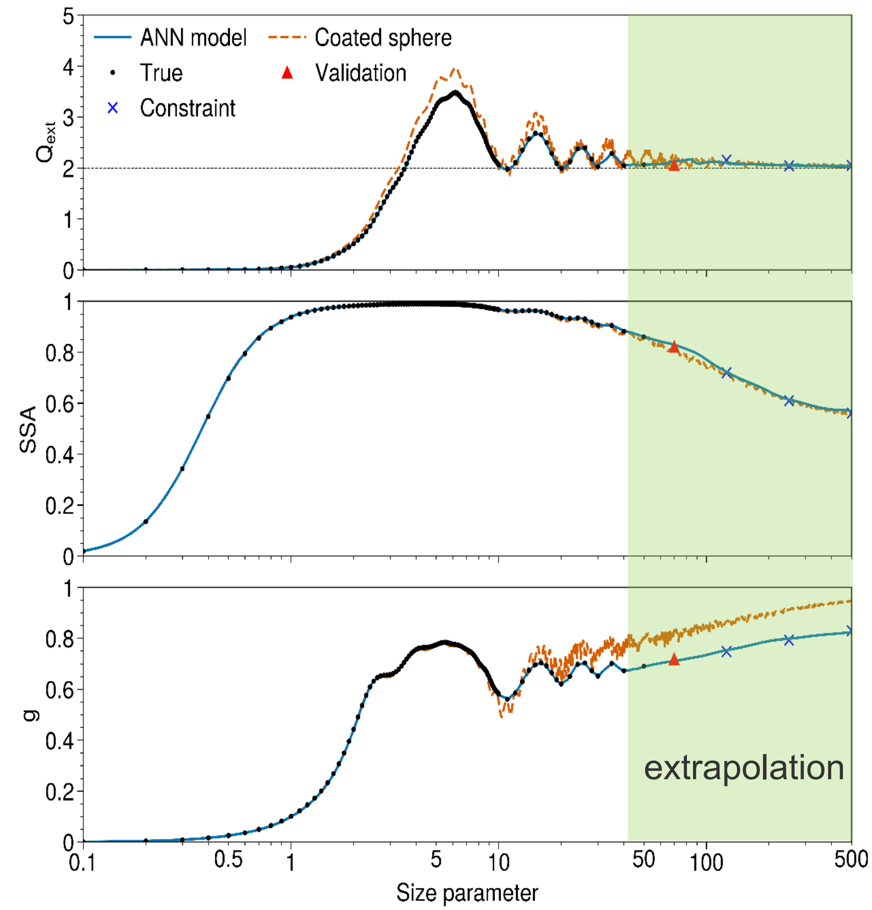
(Li and Shao, 2009)

(Wang et al., JQSRT, 2022)

Use of residual networks



Design of the ResNet



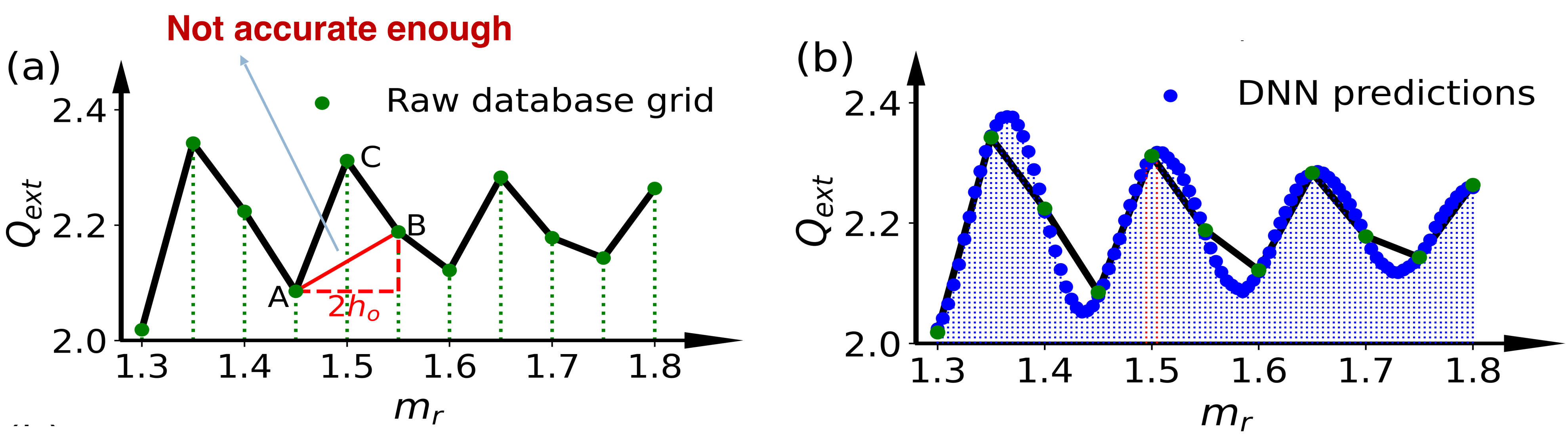
The ResNet is used to predict the optical properties of large-size particles.

Optical property Jacobians

- Derivatives of extinction efficiency, single scattering albedos, scattering phase matrix respect to shape parameters, refractive indices (real and imaginary part), and size parameters.

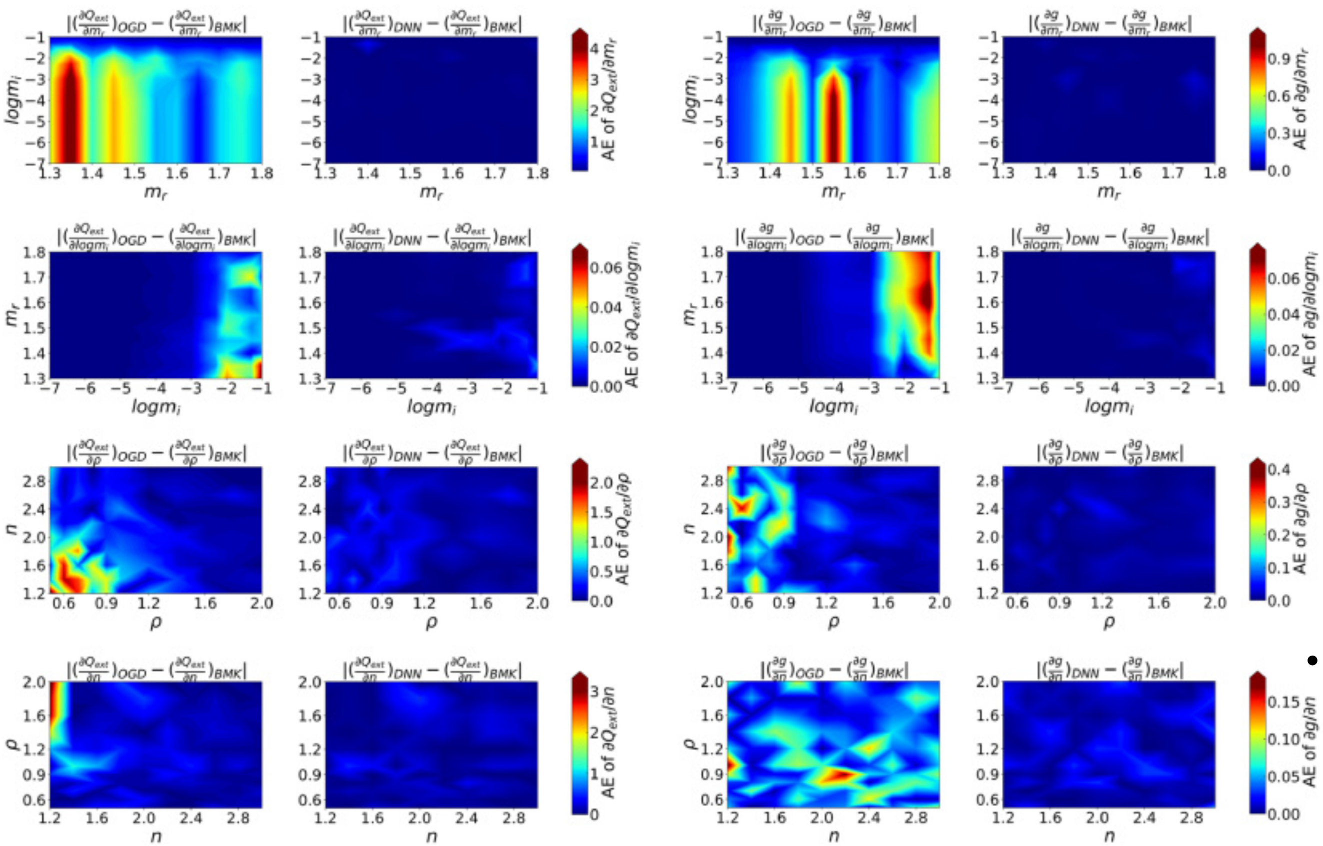
Jacobians of optical properties computed using neural networks

Finite Difference Method (FDM)



- **The neural networks provide a large number of grid points, so that the FDM grid interval becomes denser and more accurate partial derivatives are calculated.**

Comparison of with Benchmarks



Compare the absolute error of the raw grid point and NN scheme with the benchmark

The mean absolute errors are **reduced by more than 60%.**

- Yu et al., Optics Express, 2022

Benefits of machine learning

- No repeat light scattering calculations when particle models, refractive indices and size parameters are updated.
- Significantly compress the original optical property database.
- Look-up tables can be conveniently replaced with neural networks.

Applications +++

Geophysical Research Letters

Research Letter | Open Access

More or Less: How Do Inhomogeneous Sea-Salt Aerosols Affect the Precipitation of Landfalling Tropical Cyclones?

Limin Zhu, Shoujuan Shu, Zheng Wang, Lei Bi

First published: 28 January 2022 | https://doi.org/10.1029/2021GL097023

The inhomogeneity of sea salt further suppresses the rainfall.

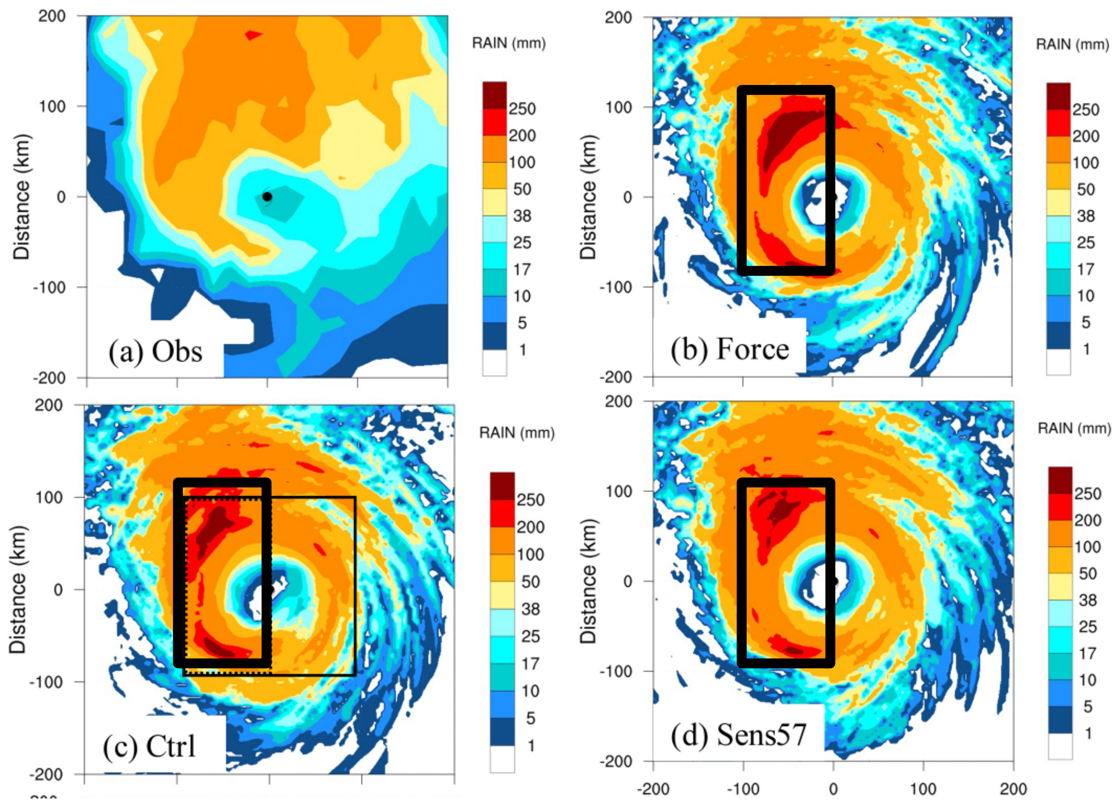
Observation and simulation of rainfall of Fitow

Observation

Without sea slat

Homogeneous

Inhomogeneous✔



- The inhomogeneity of sea salt suppresses the rainfall.

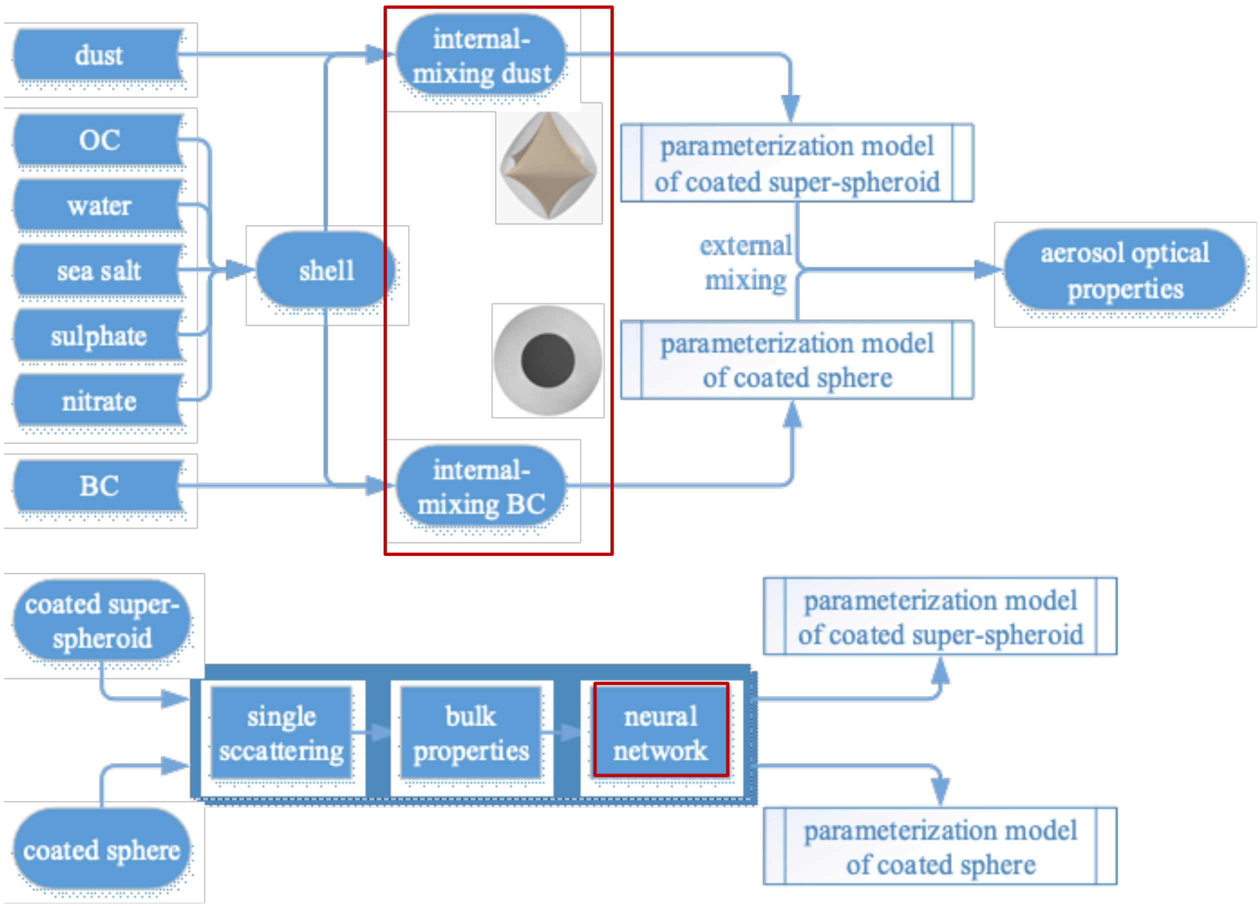
Zhu et al., GRL, 2022

Journal of Quantitative Spectroscopy and Radiative Transfer
Volume 283, June 2022, 108147

Evaluation of a new internally-mixed aerosol optics scheme in the weather research and forecasting model

Zheng Wang [a], Lei Bi [a], Hong Wang [b], Yaqiang Wang [b], Wei Han [c], Xiaoye Zhang [b]

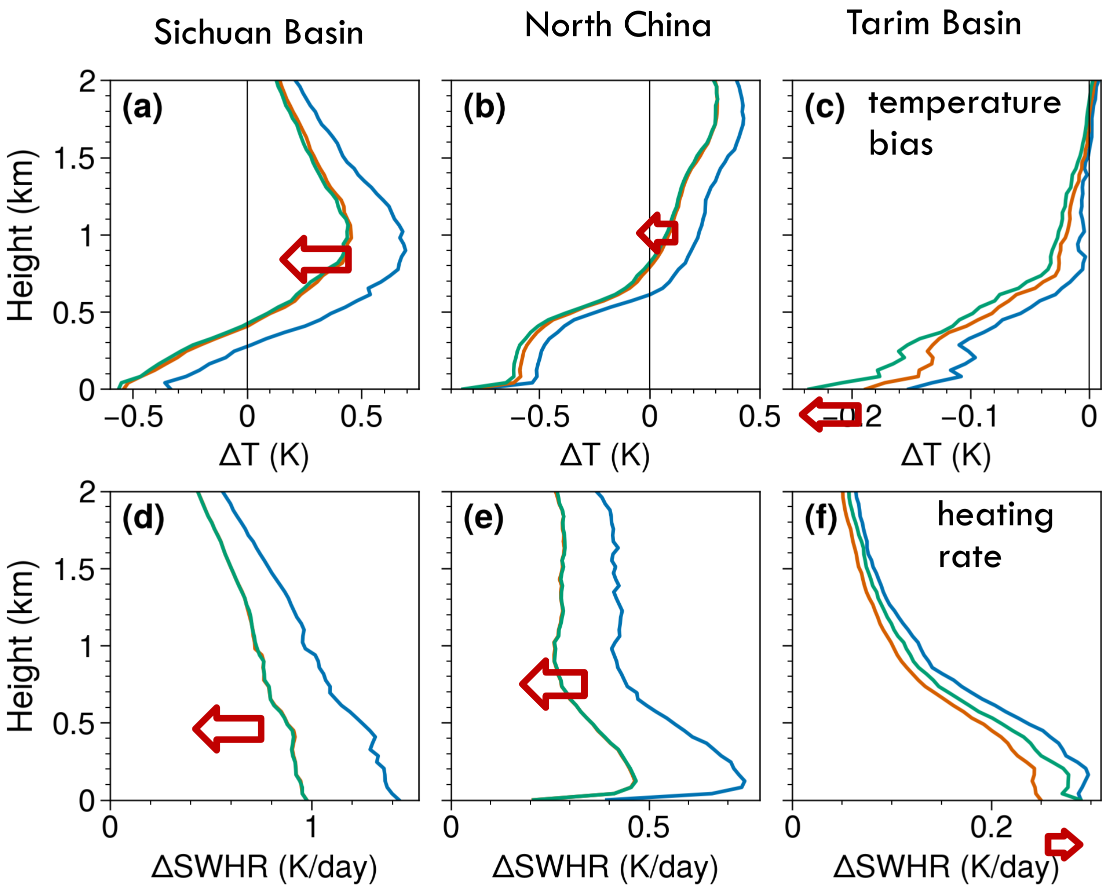
A new internally-mixed aerosol optical scheme



- **Inhomogeneity of the internal mixing**
- **Non-sphericity of dust-containing particles**
- **Parameterization by neural network**

Wang et al., JQSRT, 2022

Implemented in the weather research and forecasting model



Effect of nonsphericity and inhomogeneity on the boundary layer

- The inhomogeneity of aerosols reduces the solar heating effect.
- The nonsphericity of aerosols enhances the surface dimming effect.

Wang et al., JQSRT, 2022

Summary

Key words: T-matrix, Super-formula, Machine Learning

We DONOT hope that all particles are spheres, because nonspherical particles are so fun.

Hangzhou, China

- **"the most graceful and splendid city of the world"**(Italian traveler Marco Polo).
- 1/52 **most desirable places to go** (The New York Times, 2016)
- 3rd among the **Top 10 most attractive Chinese cities for foreigners** (Conference on International Exchange of Professionals, 2017)

浙江大學
ZHEJIANG UNIVERSITY

THANKS!