Emulating Aerosol Optical Properties Using Machine Learning

International Aerosol Modeling Algorithms Conference

Session 1: Machine Learning and Data Science

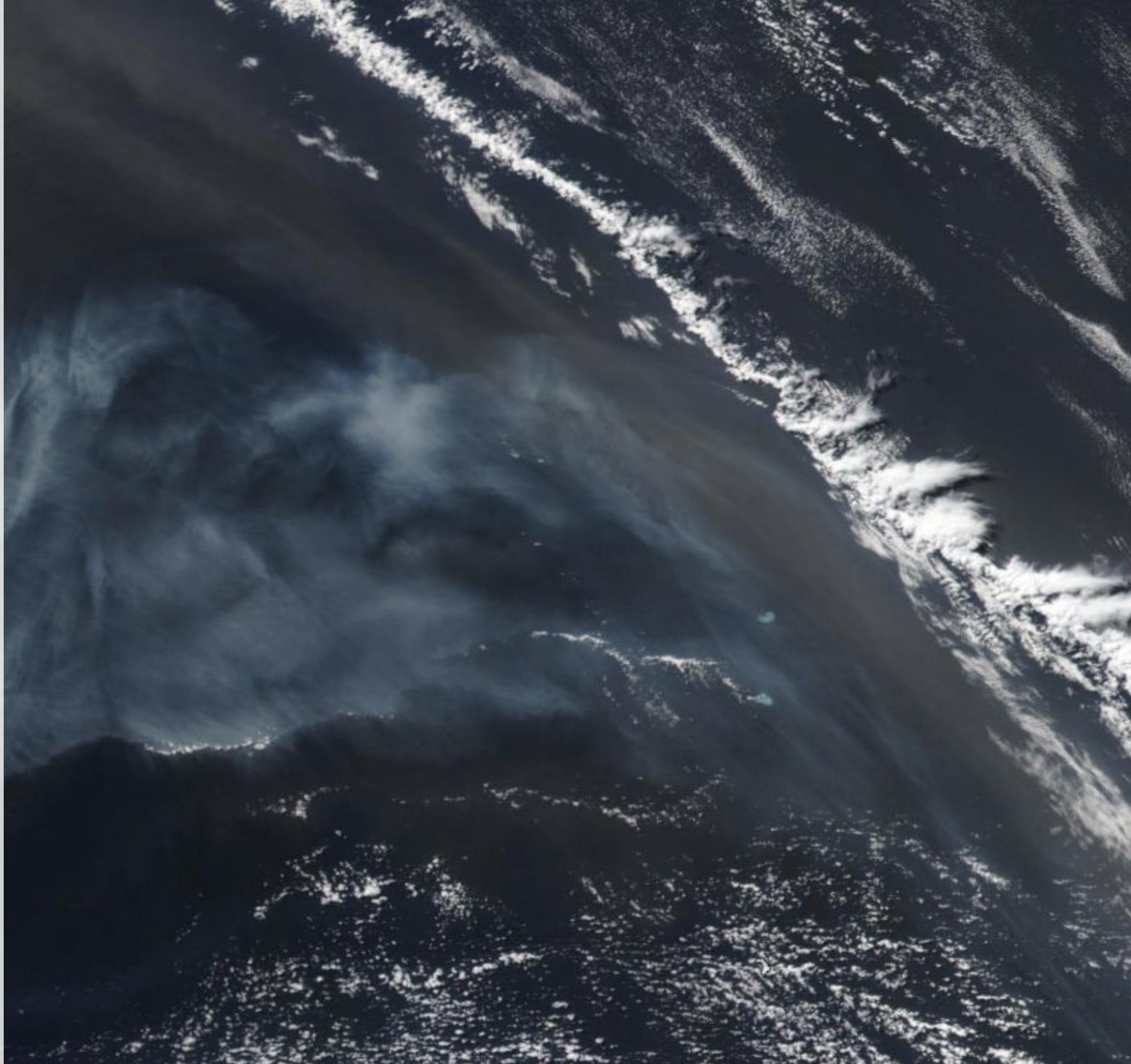
6th Dec 2023

Andrew Geiss, Po-Lun Ma, Balwinder Singh, and Joseph C. Hardin

Pacific Northwest National Laboratory

Enabling Aerosol-cloud interactions at GLobal convection-permitting scalES (EAGLES)

Contact: andrew.geiss@pnnl.gov



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Overview

- Aerosols have a substantial direct and indirect impact on Earth's radiative budget and adequately modeling aerosol radiative effects is critical for accurate climate prediction
- Calculating the optical properties of aerosol populations is too computationally expensive to be done on the fly in climate models, so it is parameterized
- Here we develop a machine learning based parameterization for aerosol optical properties for use in E3SM that is significantly more accurate than the existing parameterization
- We leverage a random neural architecture search strategy to find a light-weight neural network

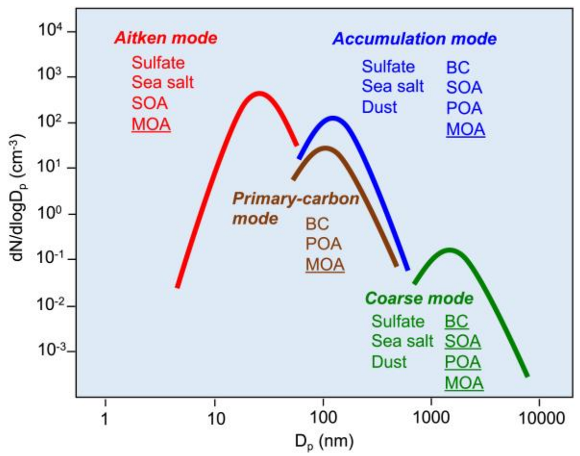
Background: Aerosol Direct Effects in E3SM

Energy Exascale Earth System Model (E3SM)

DOE climate model, simulates Earth's atmosphere, land, ocean, ice etc.

Aerosol Model (MAM4)

Represents many aerosol types in 4-"modes" with assumed log-normal size distributions

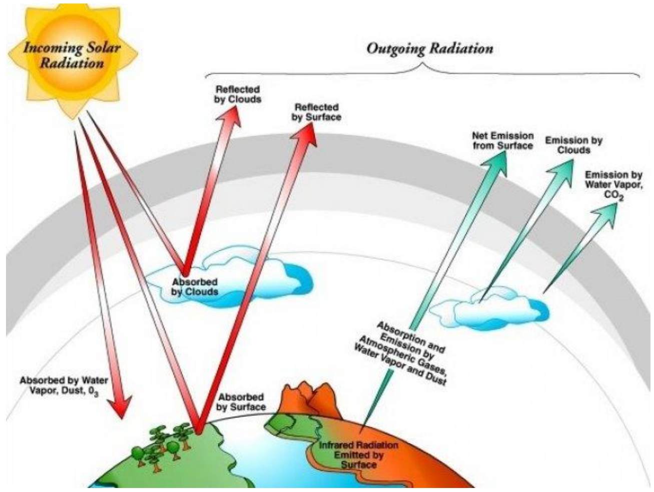


(MAM4 and RRTMG are components of E3SM's atmosphere model)

Parameterized bulk aerosol optical properties

Radiation Code (RRTMG)

Models how radiation propagates through the atmosphere, calculates resulting heating rates



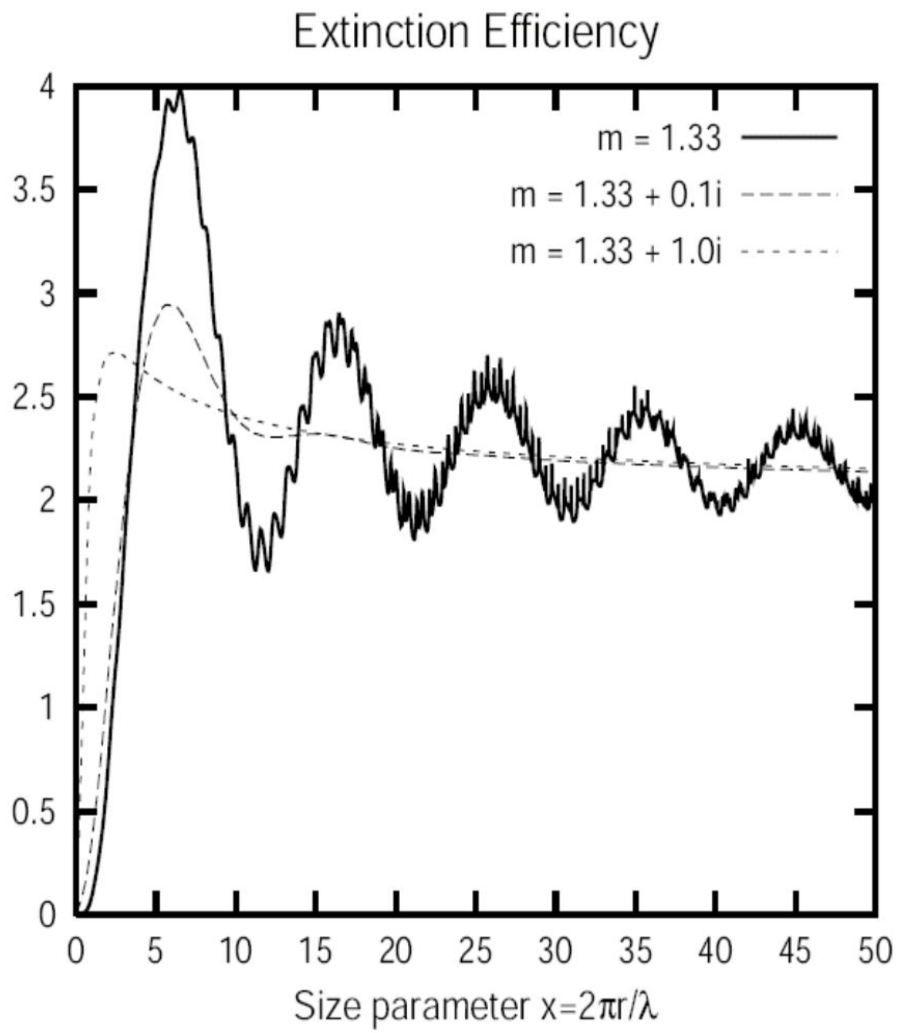
Why Parameterize Aerosol Optics?

A substantial fraction of atmospheric aerosols scatter in the Mie regime (particle diameter ~ wavelength), where optical properties vary wildly as a function of particle size

To find an individual particle's optical properties (extinction, absorption, and scattering efficiencies) requires a Mie solver. These codes are relatively slow. (solutions are infinite series that might require 10s-100s of terms for sufficient accuracy)

To find a population's optical properties we need to numerically integrate particle optical properties over the population's size distribution, which requires 100's of calls to Mie code to do accurately

…and this needs to be repeated for each aerosol mode/wavelength combination



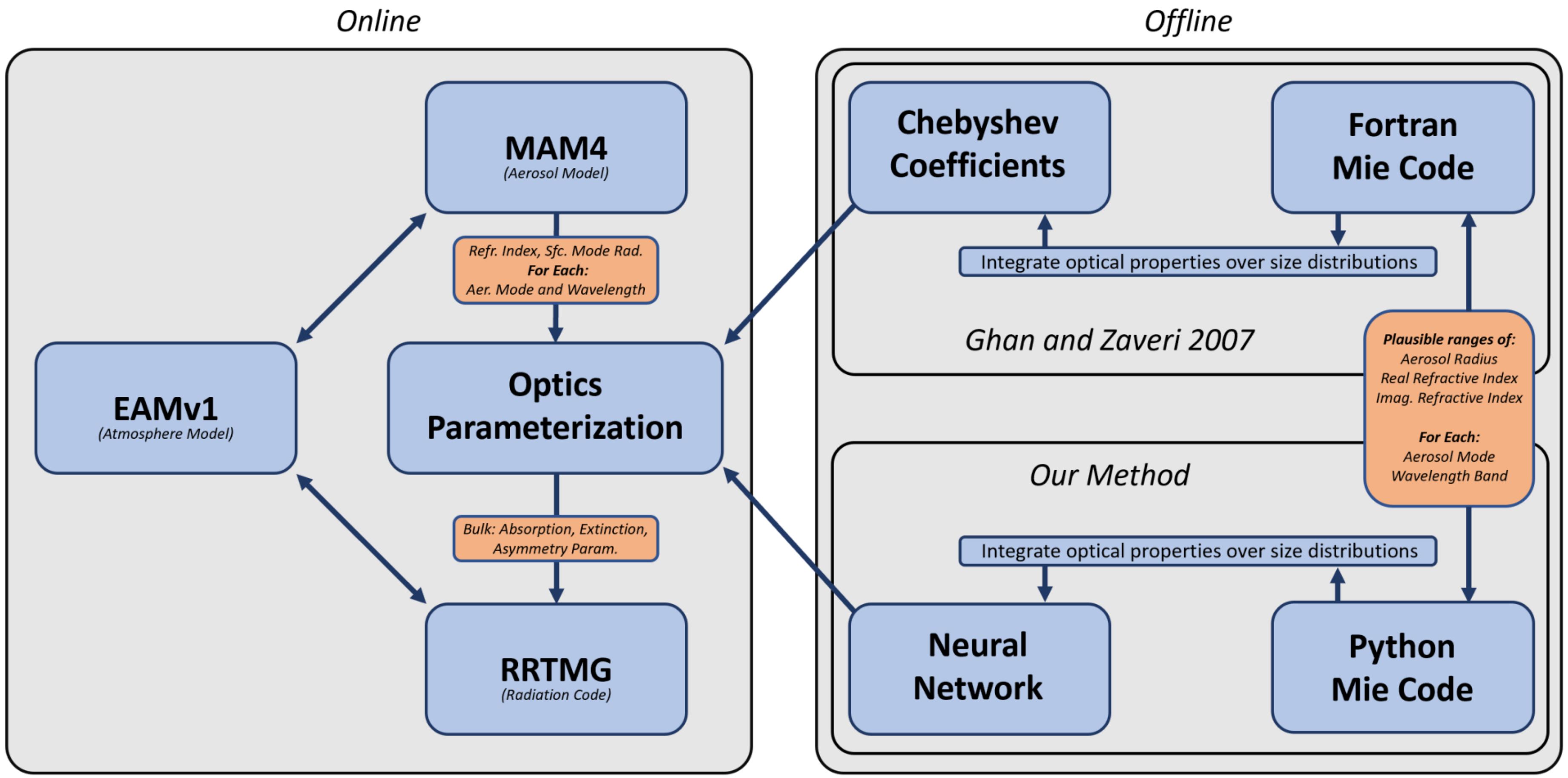
$$\overline{Q} = \frac{1}{\log\sigma\sqrt{2\pi}} \int_0^\infty Q(r,\lambda,m) e^{\left(-0.5\left(\frac{\log(r/\mu)}{\log\sigma}\right)^2\right)} \frac{1}{r} dr$$

How are Aerosol Optics Parameterized?

Approach: Pre-compute bulk optical properties for different aerosol populations, look up at run time

Current method stores this information in a look-up table of Chebyshev coefficients

We will use a neural network



Inputs:	
Real refractive index	*(within-mode mixing)*
Imaginary refractive index	*(within-mode mixing)*
Wavelength	*(14-SW, 16-LW)*
Aerosol Mode	
Mode radius	*(estimated from MAM, defines size distribution)*

Outputs:

Bulk absorption, extinction, and asymmetry parameter for SW.

Bulk absorption only for LW

Neural Network Based Parameterization

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Approach:

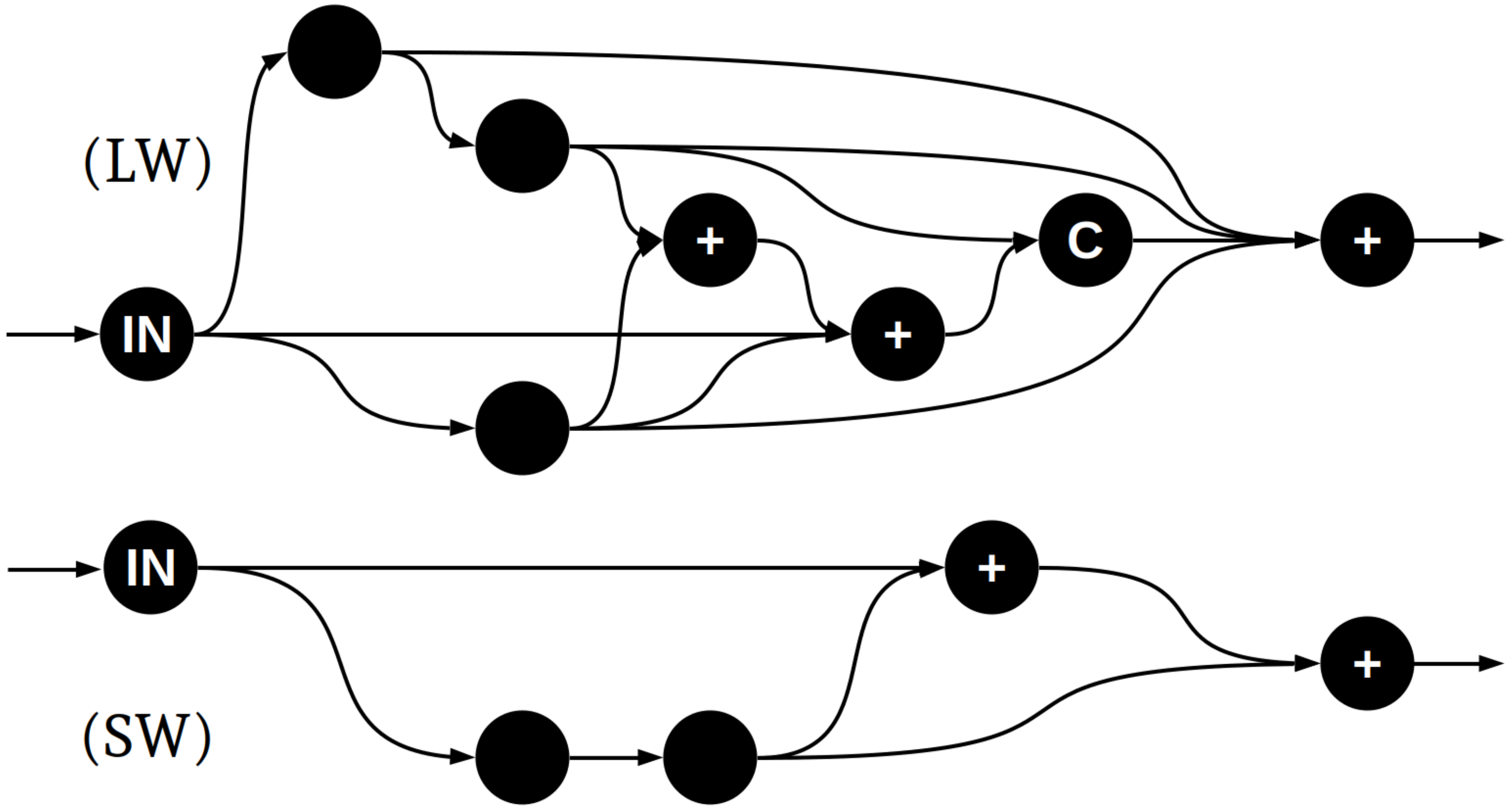
- Replace the parameterization with an ANN
- Use Mie code to pre-compute exact solutions for possible inputs and create a training set

This problem is ideal for neural architecture search:

- We can generate unlimited training data
- The ANN needs to be as lightweight as possible
- Relatively small ANNs can train very quickly on CPU

Random Neural Networks:

- *Random network graph*
- Transfer functions
- Tensor merging operators
- Layer sizes
- Number of layers
- Based on concepts from Xie et al. 2019: *"Exploring randomly wired neural networks for image recognition"*

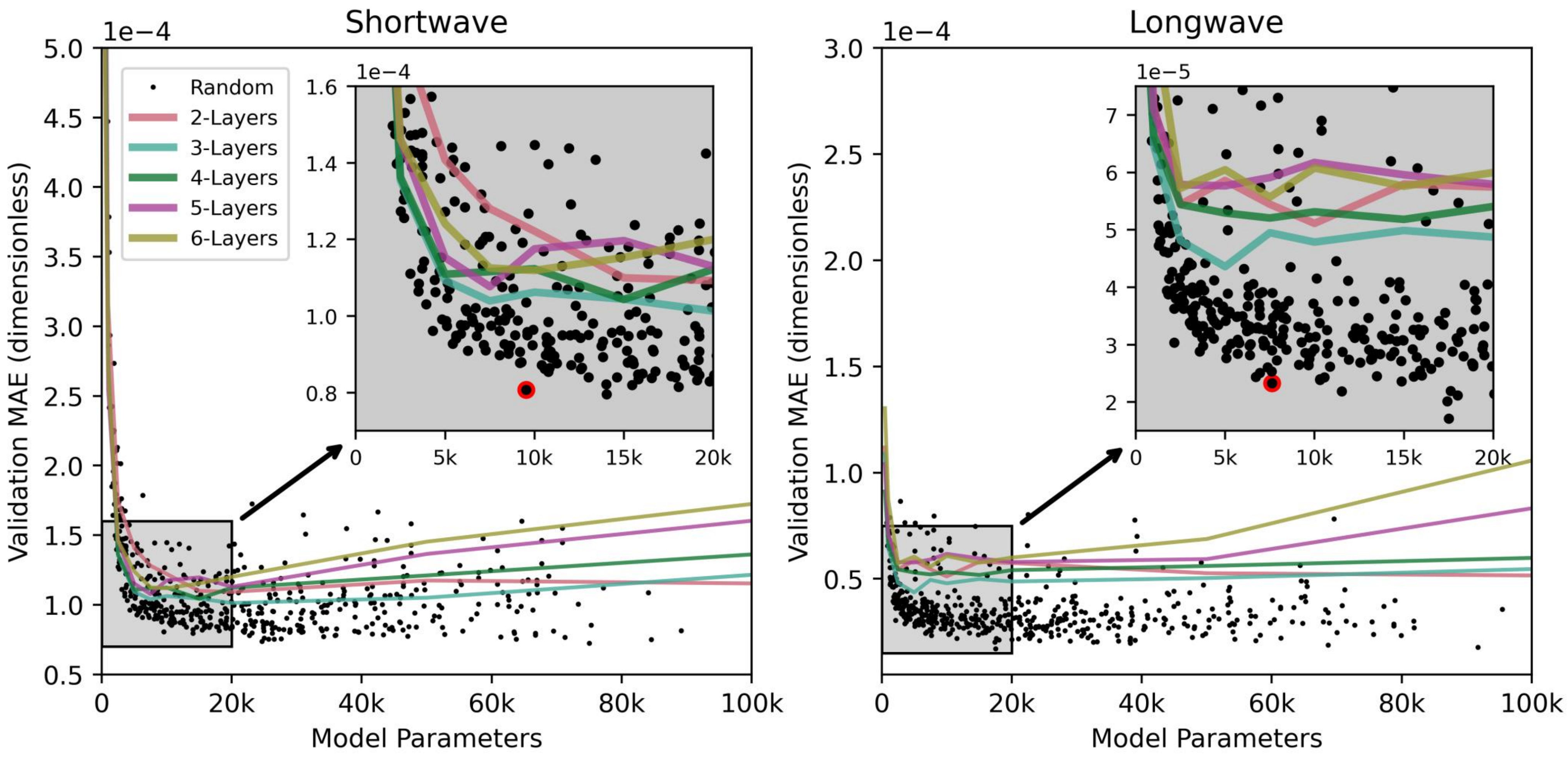


Evaluating Random Networks

Want to find skillful neural networks with as few parameters as possible, this shows validation scores versus model size.

Points are random ANNs (trained 500 each for LW and SW)

Lines show performance of conventional ANNs trained between 2-6 layers, 10-different parameter counts, 5-trials for each (reporting the best) (250 total)



The best random ANNs get a ~20%-50% improvement over their conventional counterparts.

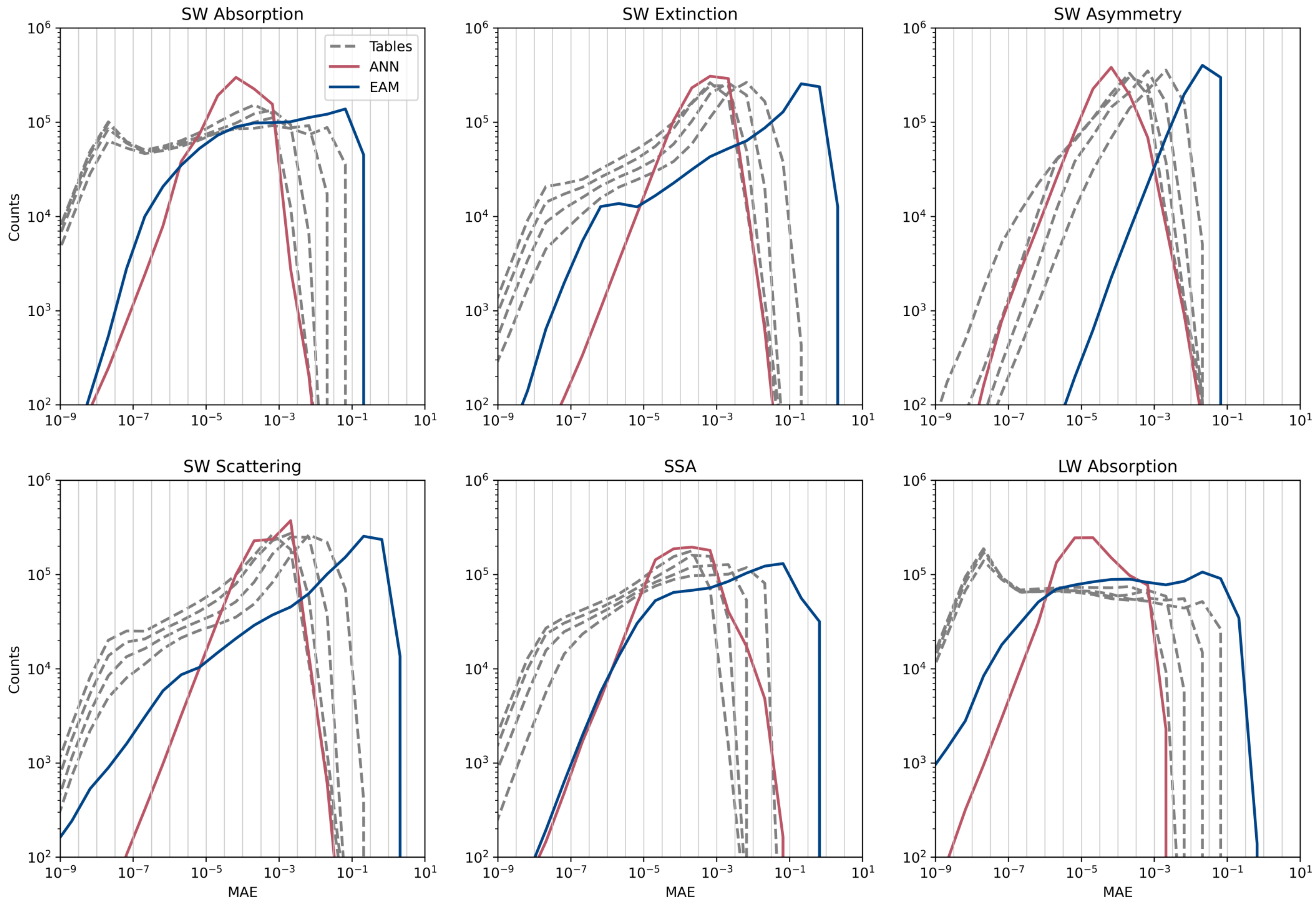
Most of the randomly wired ANNs performed better (skip connections must be important for performance)

Evaluating Random Networks

Test set: gridded over input domain, 2x size of training set

Even worst-case errors are small

Note:
SSA = Scat./Ext.
Abs. = Ext.-Scat.



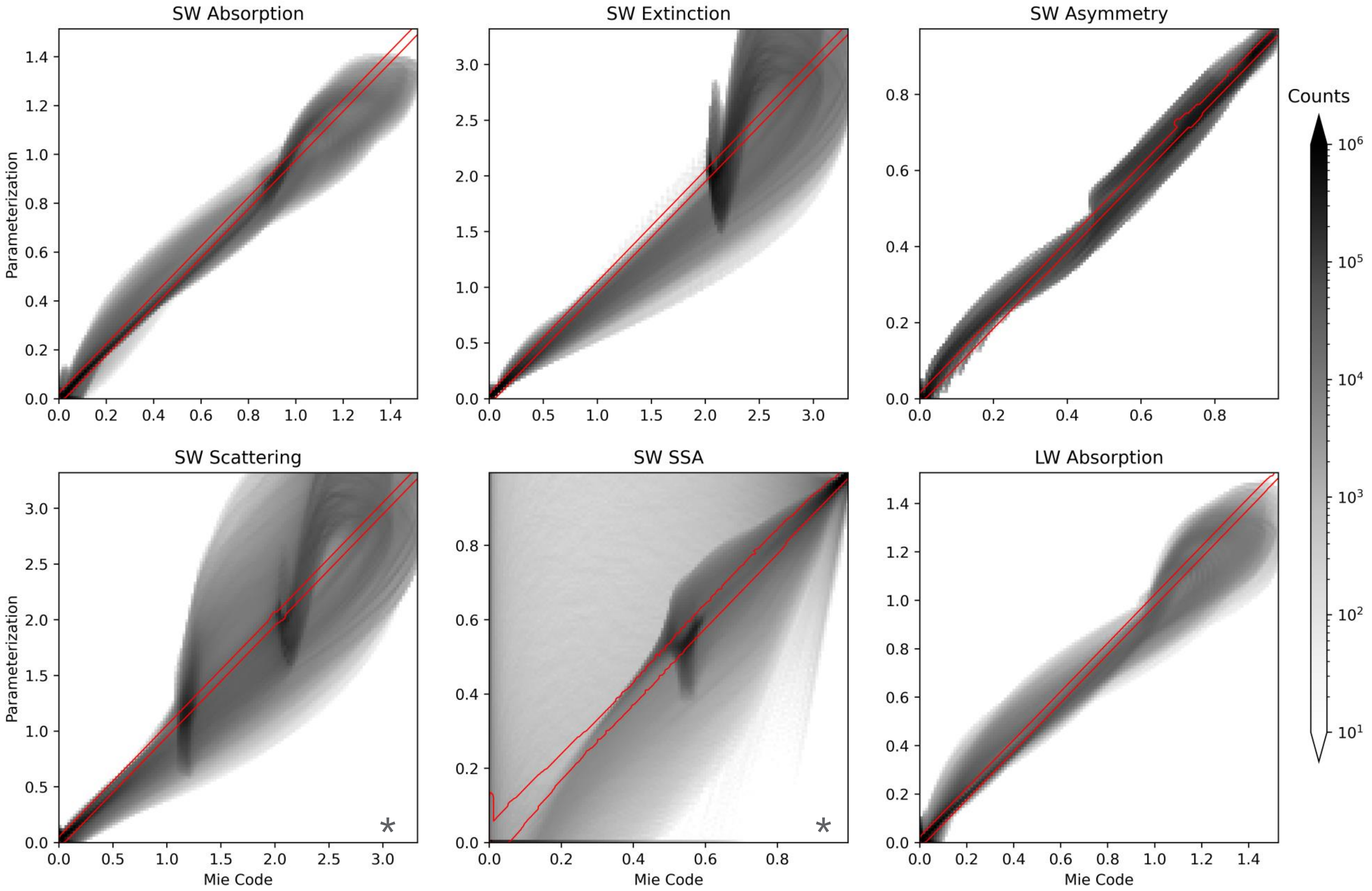
Parameterization Skill

Comparison of Mie code optical properties to parameterization on test dataset

Gray = joint histogram of existing parameterization

Red contour contains all ANN samples

Below: MAE comparison between ANNs and lookup table and interpolation based approach



Method	N-Params.	$\overline{Q}_{\text{Abs.}}$ (SW)	$\overline{Q}_{\text{Ext.}}$ (SW)	$\overline{g}$ (SW)	$\overline{Q}_{\text{Sca.}}$ (SW)	$\overline{SSA}$ (SW)	$\overline{Q}_{\text{Abs.}}$ (LW)
Random ANN:	10^4	8.6×10^{-5}	3.6×10^{-4}	1.1×10^{-4}	3.5×10^{-4}	3.2×10^{-4}	3.7×10^{-5}
Serial ANN:	10^4	1.1×10^{-4}	4.2×10^{-4}	1.2×10^{-4}	4.1×10^{-4}	4.3×10^{-4}	7.3×10^{-5}
Ghan and Zaveri (2007):	10^5	1.8×10^{-2}	2.0×10^{-1}	2.5×10^{-2}	2.0×10^{-1}	5.2×10^{-2}	1.4×10^{-2}

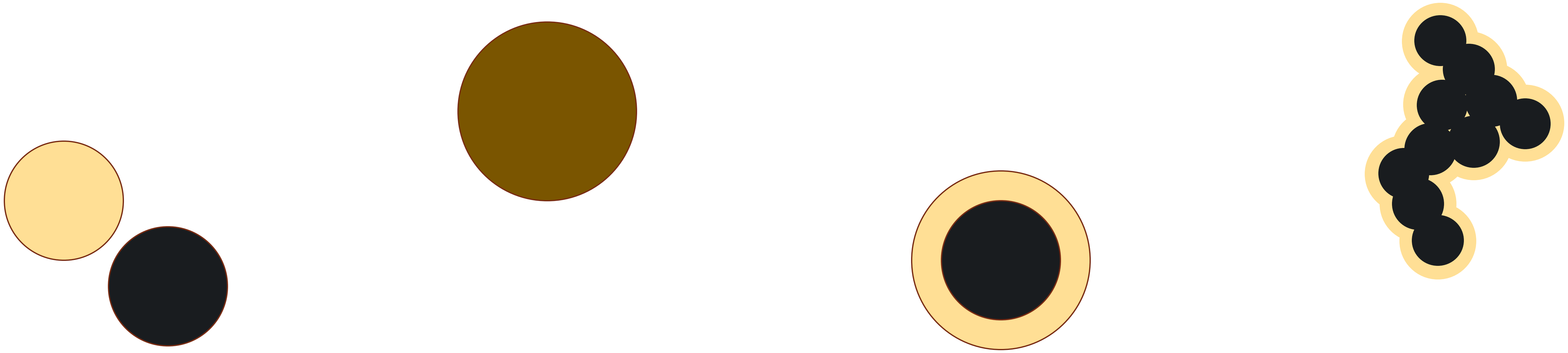
Adding core-shell optics

Geiss, A., Ma, P.-L., Singh, B., and Hardin, J. C.: Emulating aerosol optics with randomly generated neural networks, Geosci. Model Dev., 16, 2355–2370, https://doi.org/10.5194/gmd-16-2355-2023, 2023.

Existing parameterization assumes aerosol species are mixed within modes

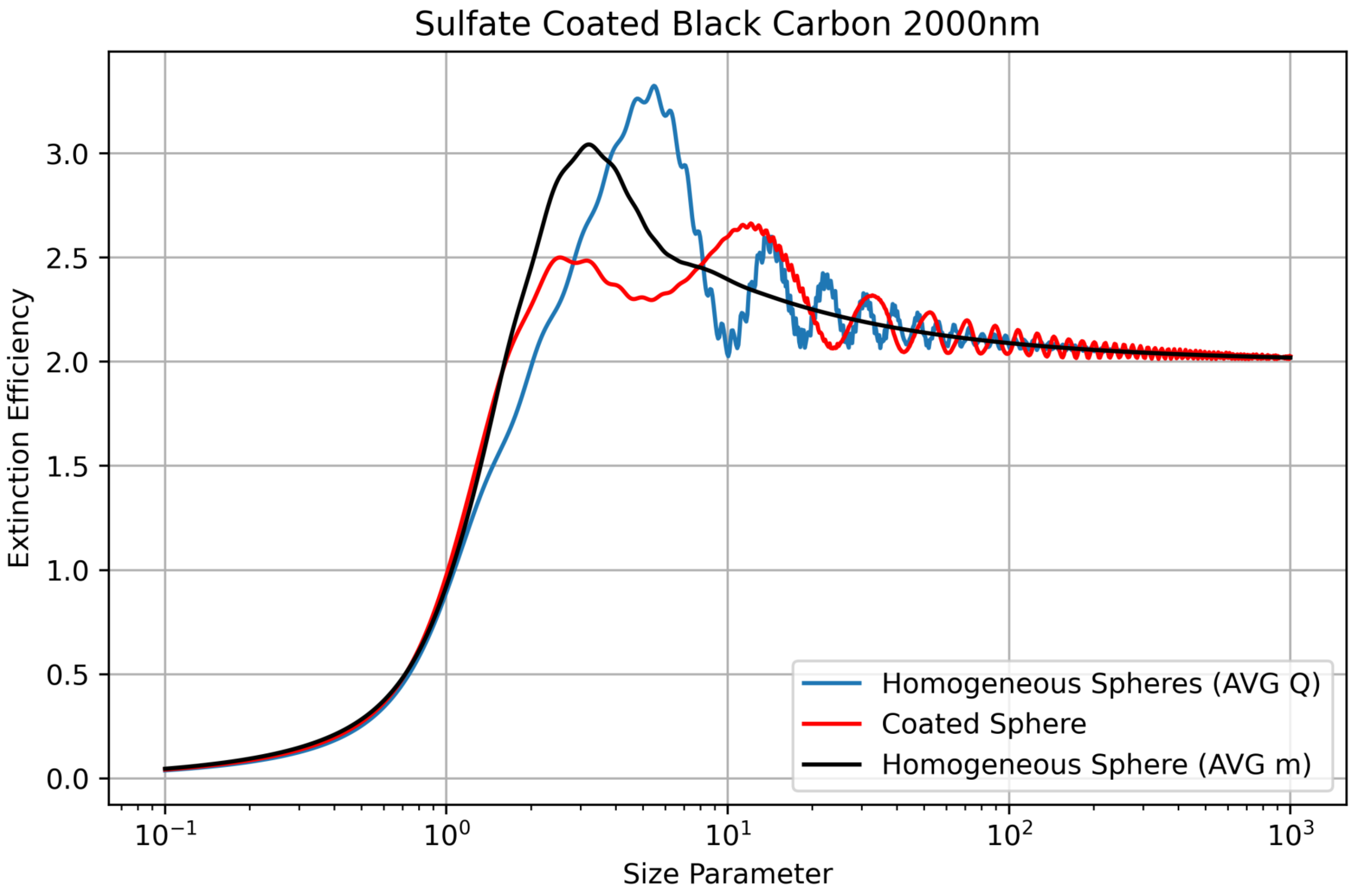
Uses volume-weighted mixing of refractive indices

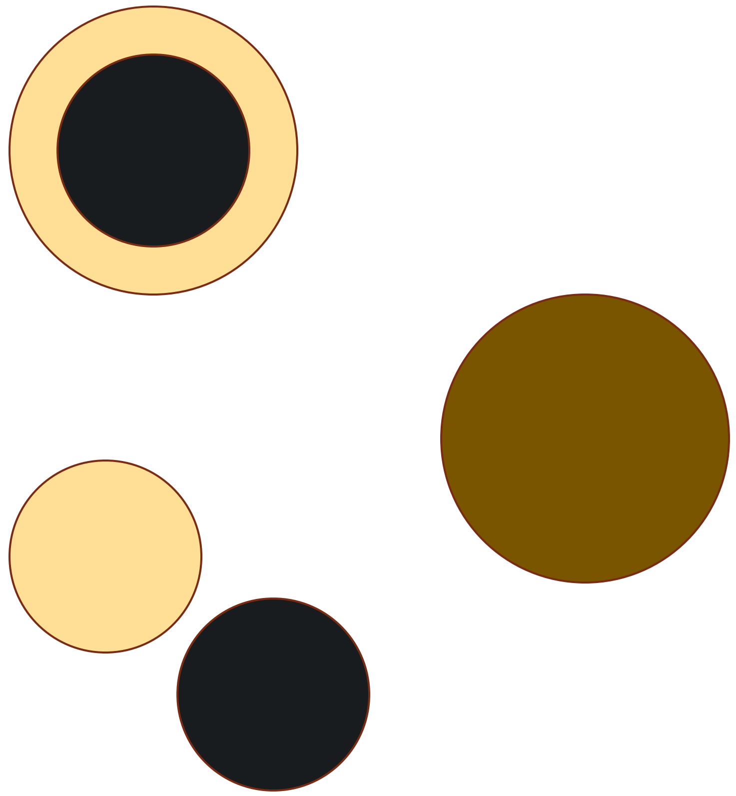
This is not always realistic – black carbon, for instance, can be coated by sulfate and a core-shell model is more reasonable than mixing:



Adding core-shell optics

Mixing assumptions can significantly alter the optical properties of a particle:





(This involved creating a Python core-shell Mie solver based on algorithms from Toon and Ackerman 1981, and Shiloah 2018)

Improving generalizability

$$k_e = \frac{3\int_0^\infty p(r)Q_e(r,\lambda,m)r^2dr}{4\rho\int_0^\infty p(r)r^3dr} \qquad p(r) = \frac{1}{r\sigma\sqrt{2\pi}}e^{-\frac{\log(r/\mu)^2}{2\sigma^2}}$$

A general-purpose parameterization that works alongside other aerosol models and other choices of wavelength is preferable (not specific to MAM4), if model complexity isn't increased too much

Mie calculations have a symmetry, they only depend on the size parameter $x=2\pi r/\lambda$, I can re-formulate the above eqn and predict λk_e instead as a function of σ (distribution width), $m=n+ik$ (complex refractive index), and $\mu_x=2\pi\mu/\lambda$ to eliminate an input variable

For large and small size parameters we can directly calculate Rayleigh and Geometric approximations and have support for all wavelengths and particle sizes

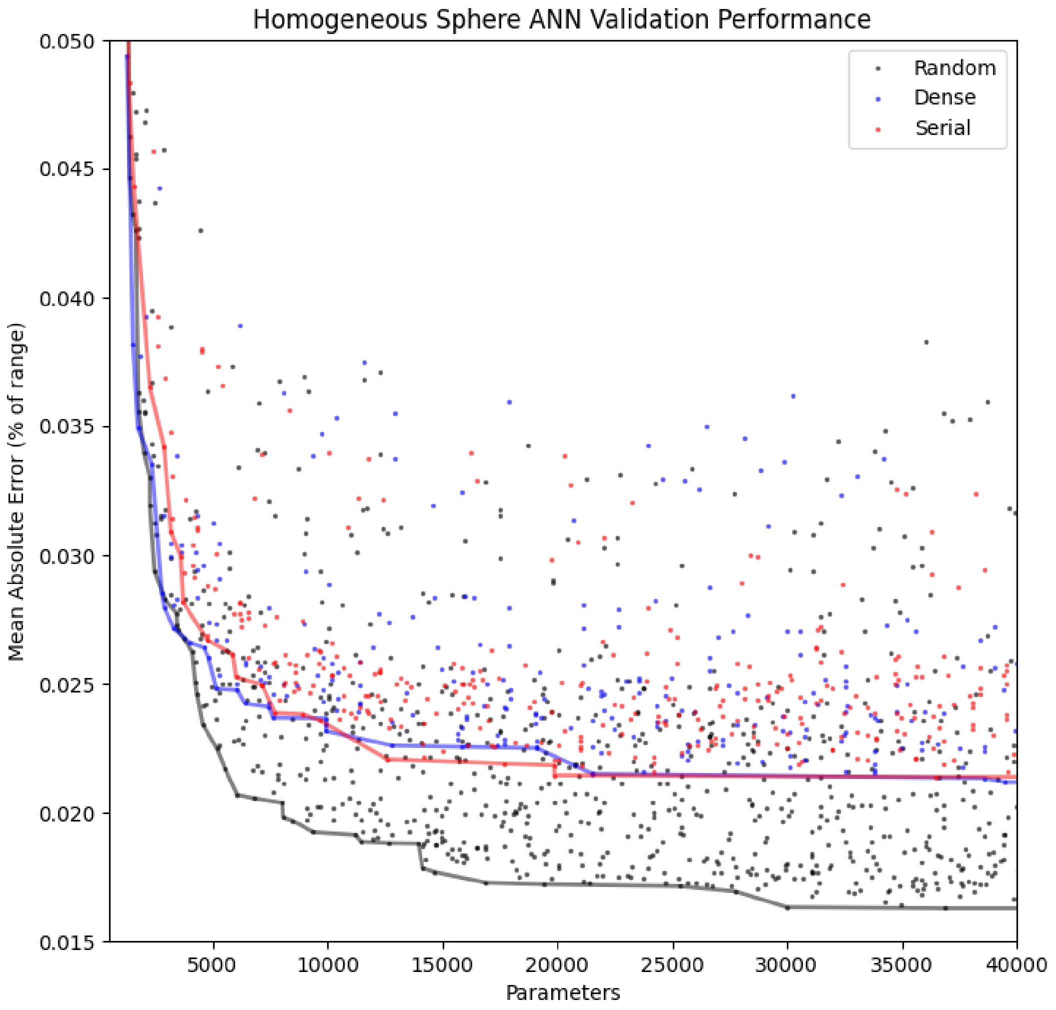
$$r = \frac{\lambda x}{2\pi} \qquad \mu = \frac{\lambda \mu_x}{2\pi}$$

$$\lambda\rho k_e = \frac{3\pi\int_0^\infty e^{-\frac{1}{2}\left(\frac{\log(x/\mu_x)}{\sigma}\right)^2}Q_e(x,m)x\,dx}{2\int_0^\infty e^{-\frac{1}{2}\left(\frac{\log(x/\mu_x)}{\sigma}\right)^2}x^2dx}$$

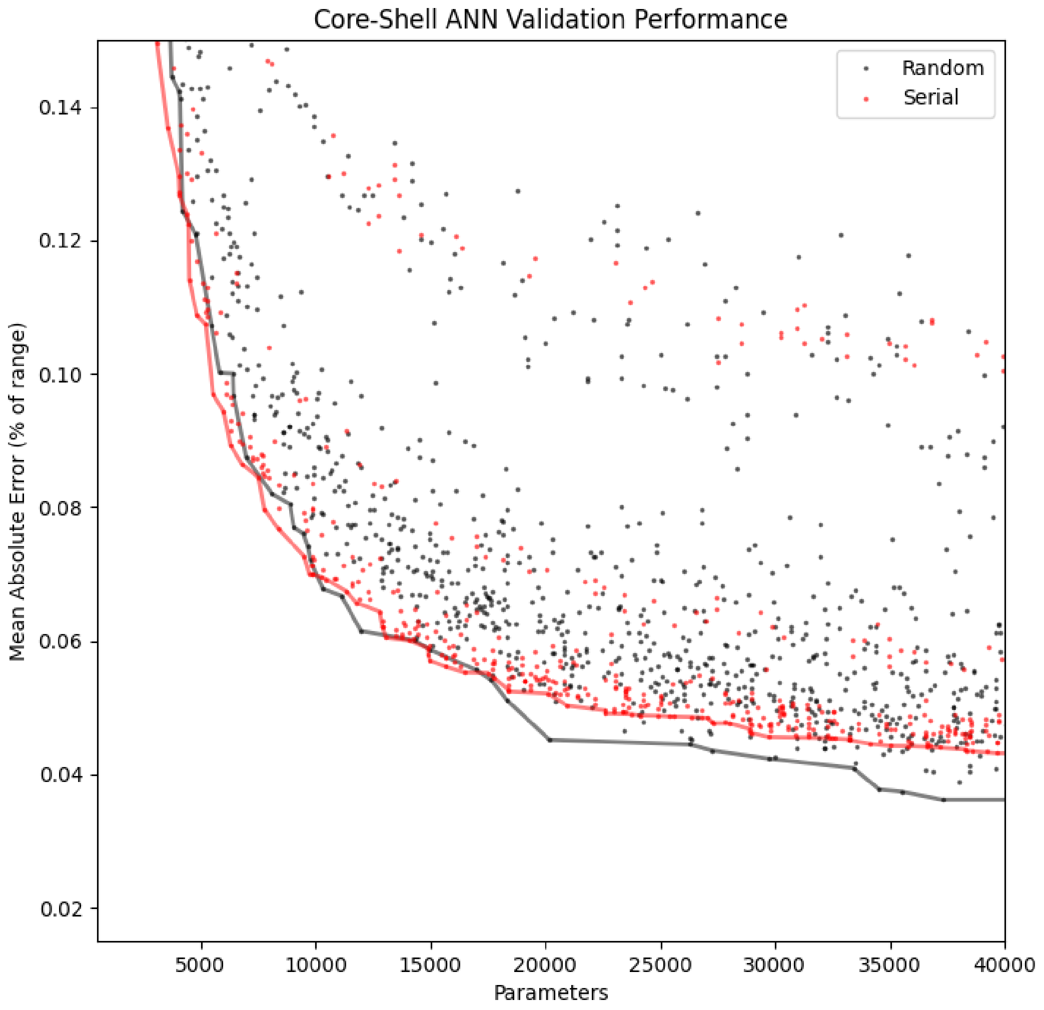
Evaluating core-shell optics

After training new neural networks using the random wiring method and the lower dimensional formulation of the problem, the test error remains negligible.

Sphere Test Error %: 0.018



Core-Shell Test Error %: 0.045



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Summary:

- The optical properties of aerosol populations can be very accurately represented by a neural network for use in an ESM
- Neural architecture search including wiring can find better performing ANNs
- We have developed ANNs that can solve a more generalized problem than the MAM4 parameterization (SW and LW, range of PSDs) and represent core-shell optics

Ongoing Work:

- Currently working on integration into E3SM
- Collaboration with Laura Fierce, Peyton Beeler, and Rahul Zaveri to represent non-spherical black carbon

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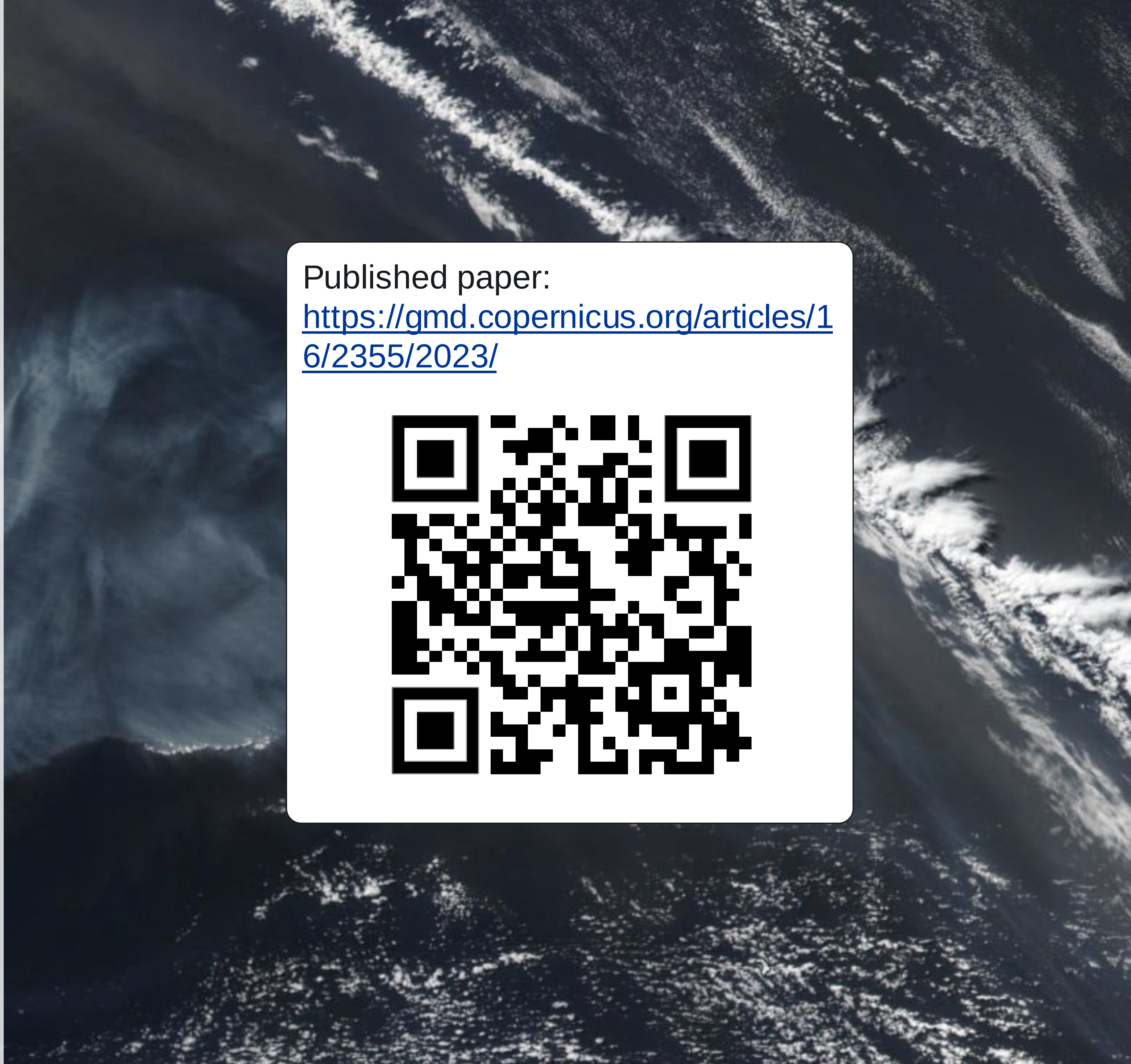

Published paper:
https://gmd.copernicus.org/articles/16/2355/2023/