Karlsruhe Institute of Technology

CONSORTIUM FOR SMALL SCALE MODELING

COSMO

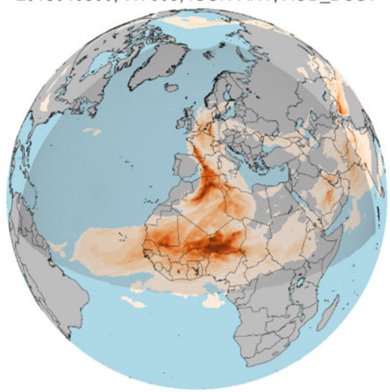
WG3 Meeting, Gdańsk, September 2023

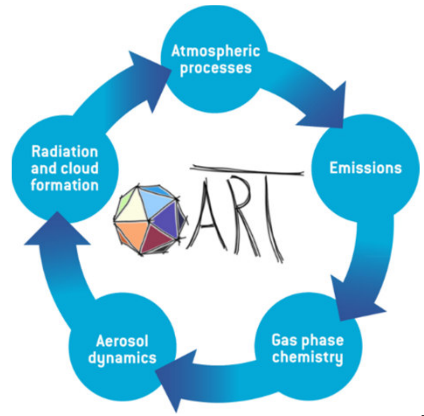
ICON-ART

Aerosol-radiation interactions

Ali Hoshyaripour and the ARTists

2018040800, vv: 003, ICON-ART, AOD_DUST





Aerosol optical properties in models

- **Extinction Coefficient (k_e)**
- **Single Scattering Albedo (ω_o)**
- **Asymmetry Parameter (g)**

These parameters change with:

- Wavelength (λ)
- Particle shape (sphere, ellipsoid, monomer aggregate)
- Composition (refractive index)
- Particle size distribution (PSD)
- Mixing state (externally and internally mixed)

Variable during atmospheric transport

Aerosol optics in ICON-ART

- **Externally mixed**
  - Dust → 3 modes (non-spherical particles with variable D)
  - Sea Salt → 3 modes
  - Volcanic ash → 3 modes
  - Smoke aerosols → 1 mode

Hard-coded as look-up tables and XMLs → transferring to netCDF kernels

- **Internally mixed**
  - Volcanic aerosols → flexible

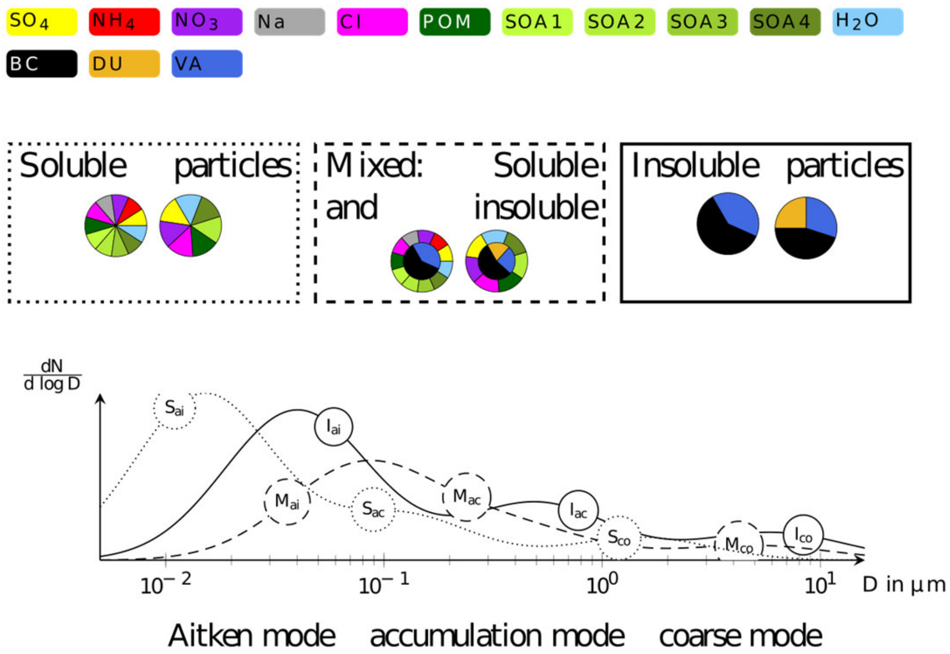
Large variability → how to proceed?

Aerosol Dynamics (AERODYN) in ICON-ART

- Flexible number of log-normal modes
- For each mode, prognostic equations for the number density and the mass concentration are solved:

$$\frac{\partial}{\partial t} M_{0,i} = -\mathrm{Ca}_{0,ii} - \mathrm{Ca}_{0,ij} + \mathrm{Nu}_0,$$
$$\frac{\partial}{\partial t} M_{3,i} = -\mathrm{Ca}_{3,ij} + \mathrm{Co}_{3,i} + \mathrm{Nu}_3,$$

- the ISORROPIA II for gas–aerosol partitioning



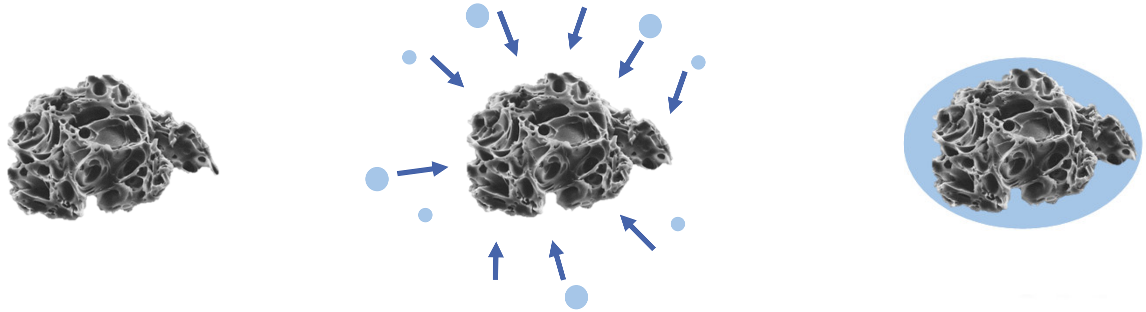
 Muser et al. (2020); Vogel et al. (2009); Fountoukis and Nenes (2007)

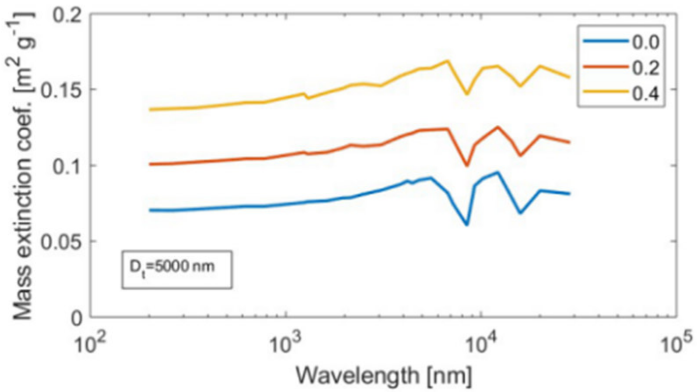
Aerosol dynamics and optics

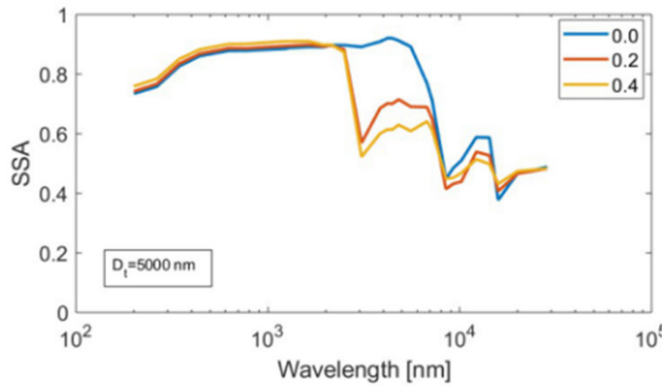
1) Fresh emitted particles

2) Condensation and coagulation

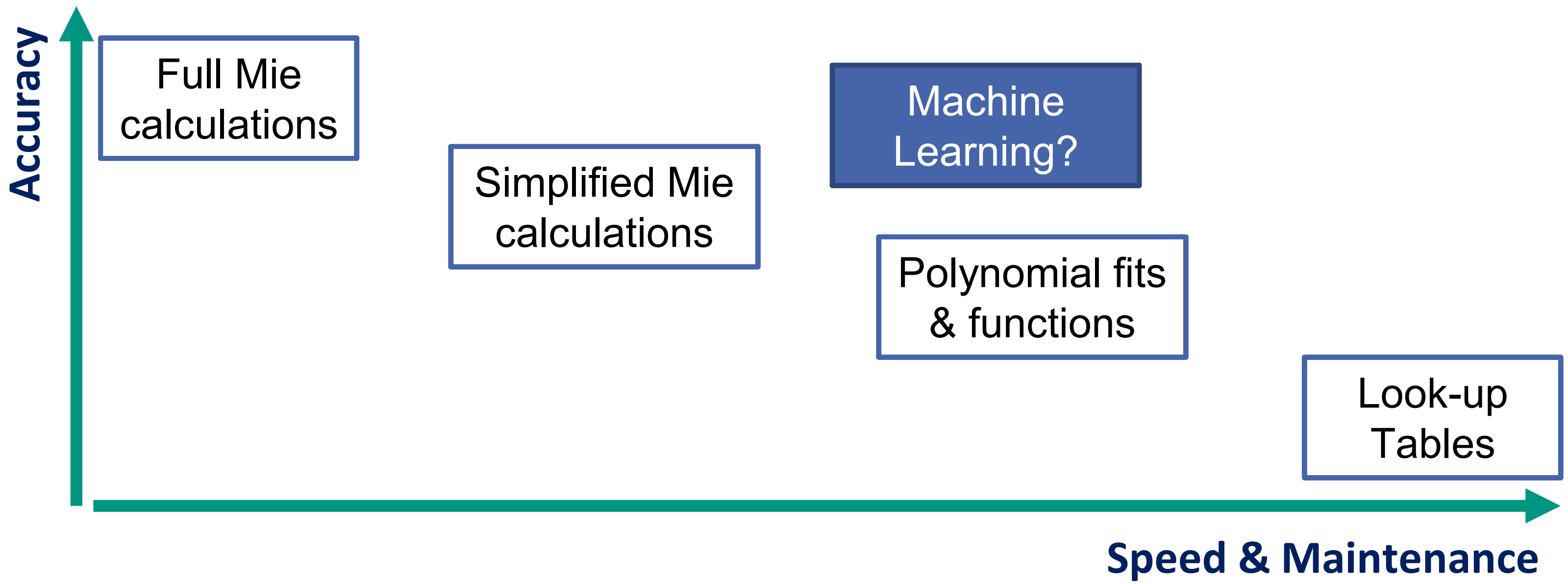
3) Coated/aged particles



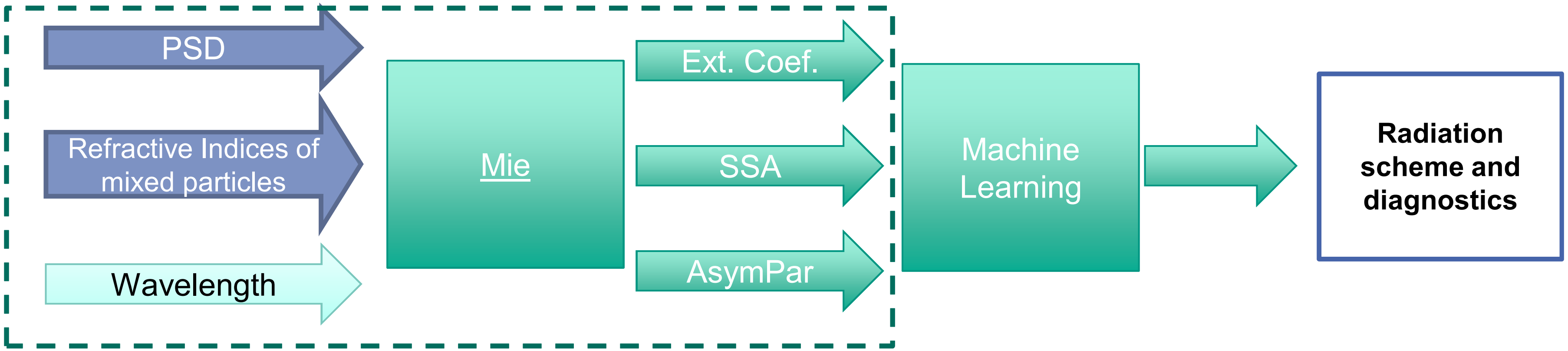




Aerosol optics in models



Online aerosol optics: ML Approach

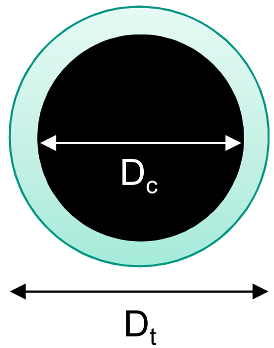


- How good (in terms of accuracy and speed) can a ML model emulate the Mie calculations for internally mixed aerosols?

Training data set

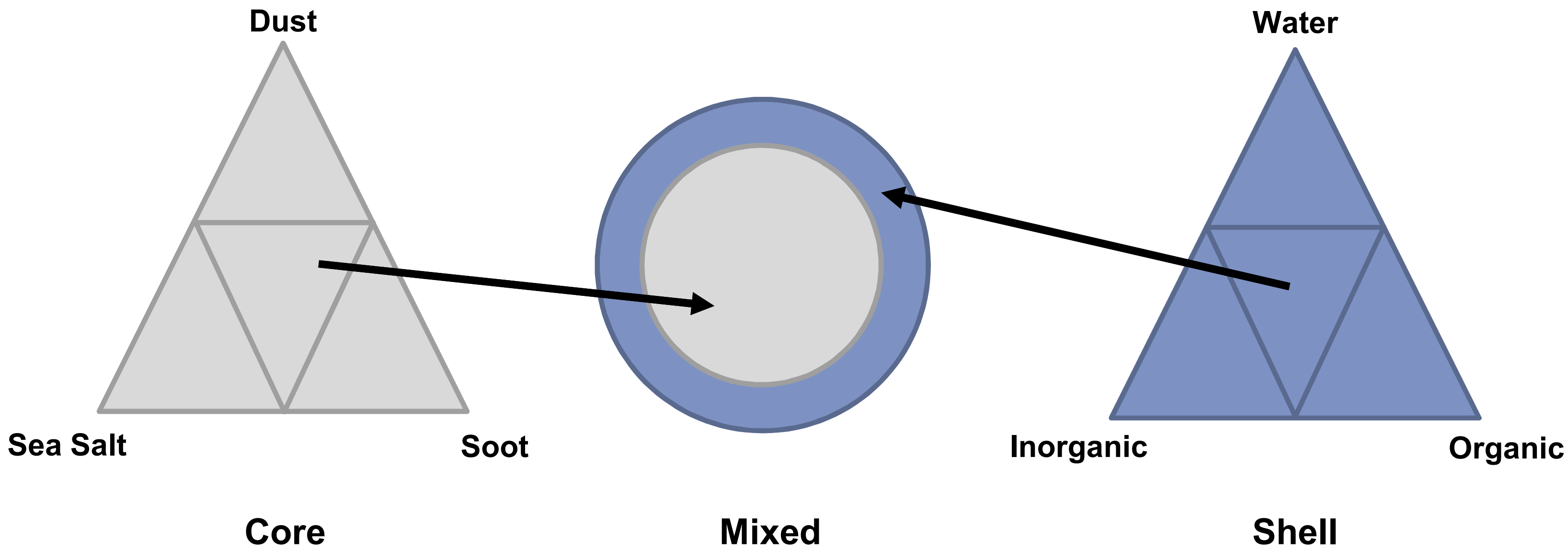
- To be generic enough, we need to consider all possible combinations of

• λ	66	0.2 to 100 µm
• f	41	Shell thickness (0-0.4D_t)
• Core diam	31	Core diameter
• Shell com	30	Chemical composition of shell
• Core com	30	Chemical composition of shell

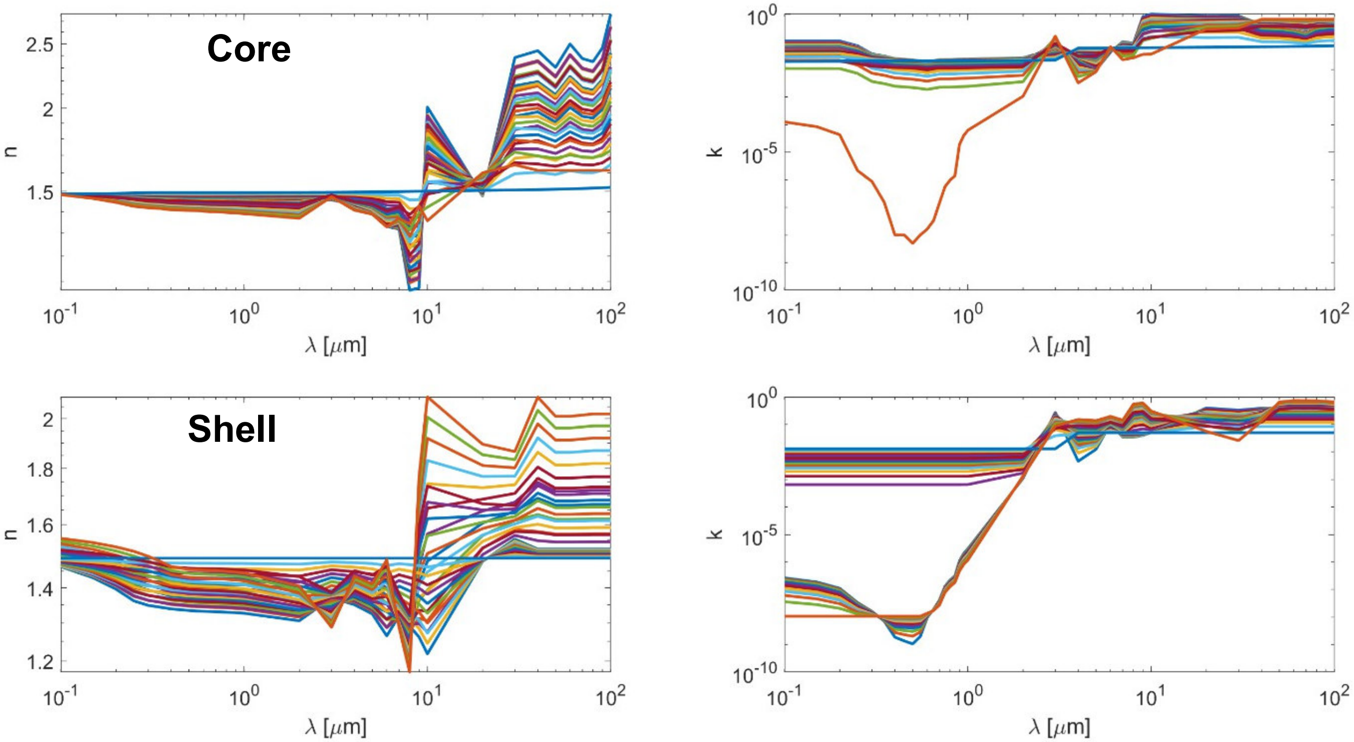


This means 75 million Mie calculations !

Ternary systems to estimate *n* and *k*

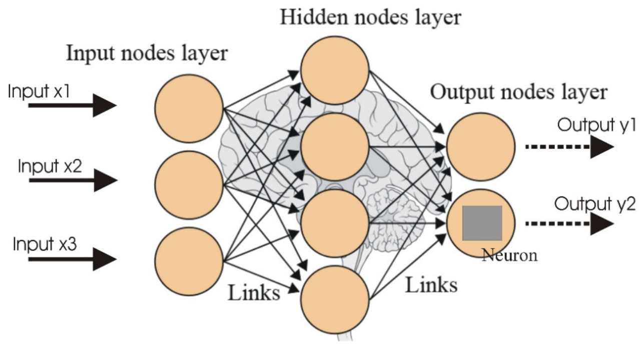


Refractive index of mixed components



Machine learning: artificial neural network

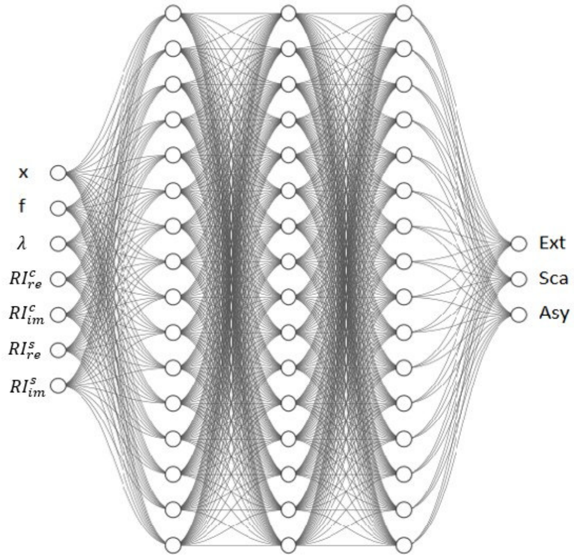
- From simple linear regression to complex neural network approaches
- Chosen based on the system complexity, performance and computational cost
- **Artificial Neural Network (ANN)**: “the most recommended AI technique” as it satisfactorily learns the associations, functional dependencies and patterns with excellent prediction skill



Source: https://www.analyticsvidhya.com

ANN development

- **Network architecture**
  - 3-layers MLP and ReLU activation in Tensorflow

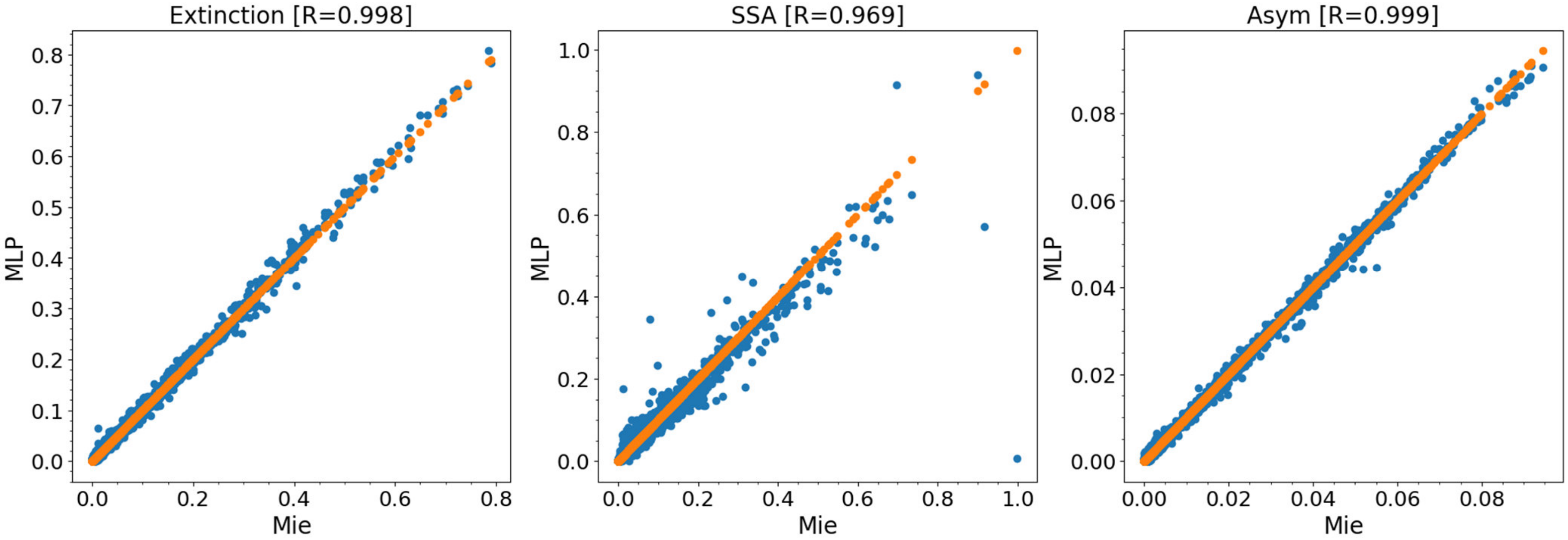


- **Training algorithm:**
  - Data division: 20000 Random samples
  - 70% for Training,15% for validation, 15% for testing
  - Optimizer: ADAM, Loss Function: MSE
  - Two networks are trained: one for x <= 0.5 and one for x > 0.5
  - Hyperparameter optimization using random search

$$x = \frac{2\,\pi\,r}{\lambda}$$

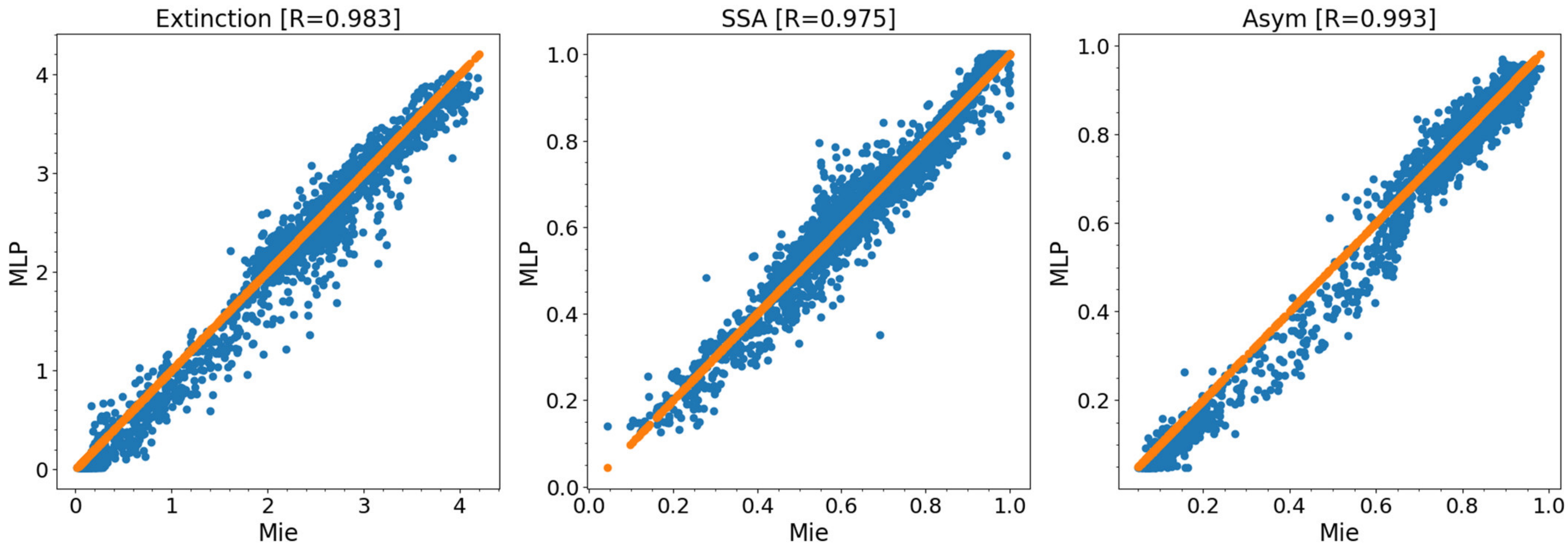
Results of the training

X<=0.5



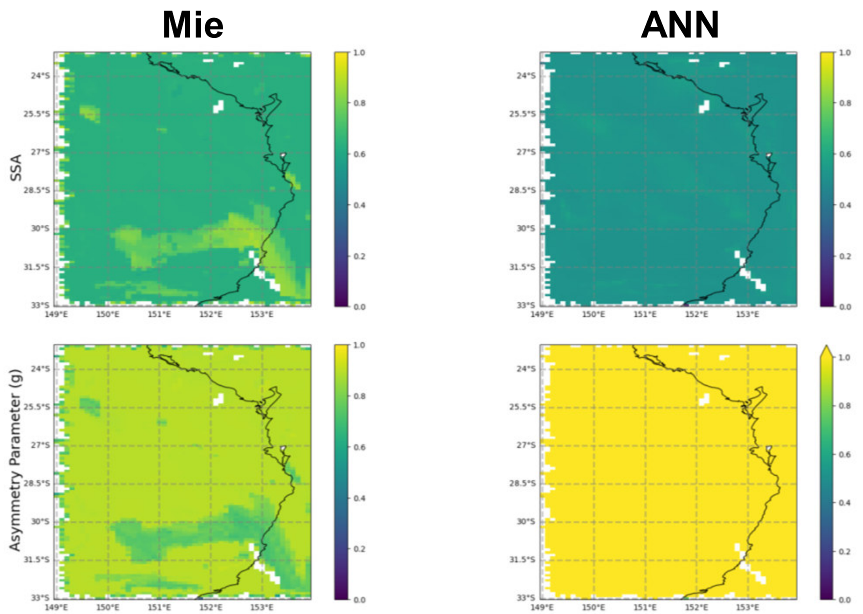
Results of the training

X>0.5



Pre-implementation 1

- We applied the Mie code and ANN model to the outputs of three ICON-ART simulations:
    - Saharan dust outbreak June 2019
    - La Soufrière eruption April 2021
    - Australian bushfires 2019-20

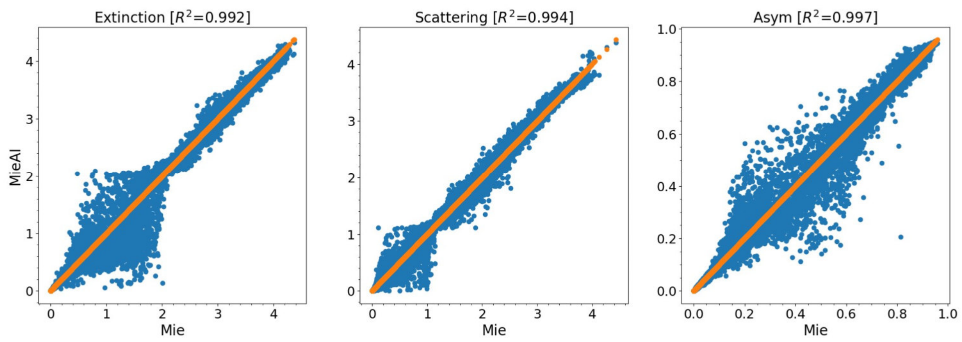


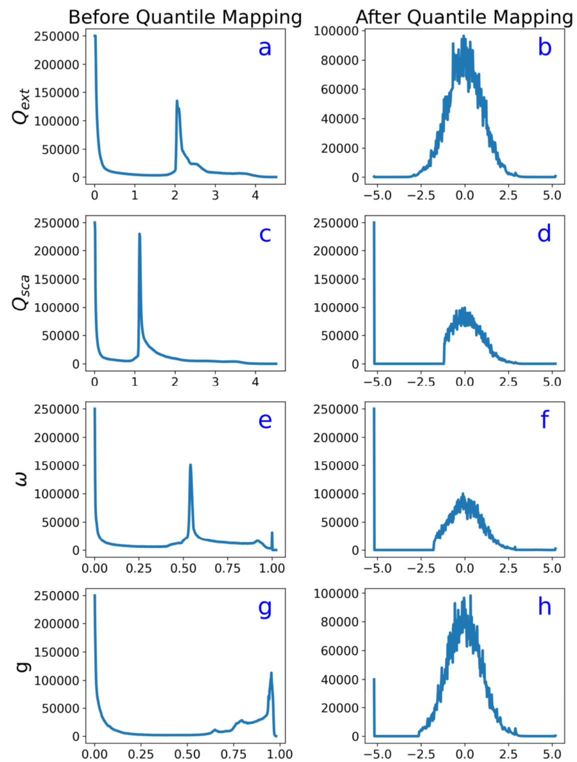
The ANN model fails to predict SSA and Asym!

ANNs learn the variability!

- The target parameters in the training dataset are not normally distributed.

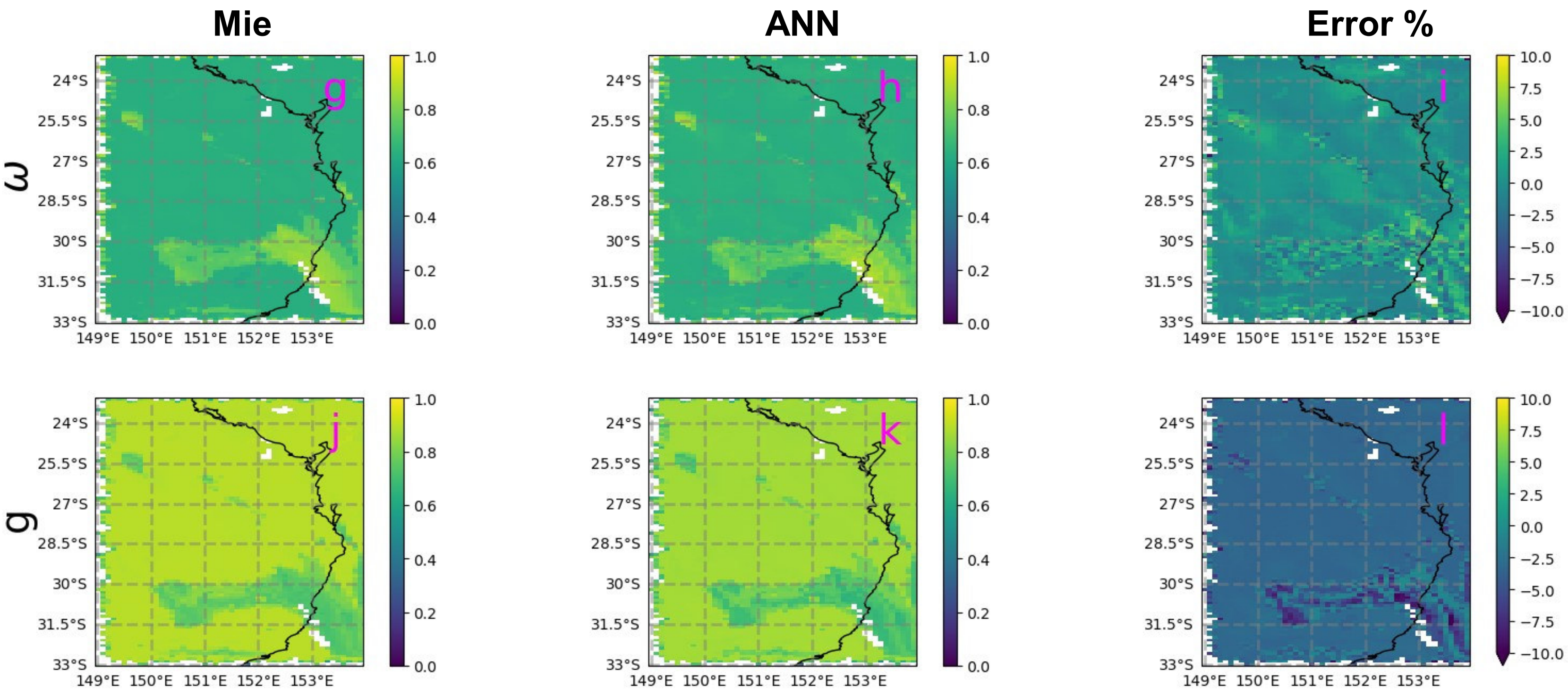
- We apply quantile mapping to transform target features to a Gaussian distribution with mean 0 and standard deviation 1.





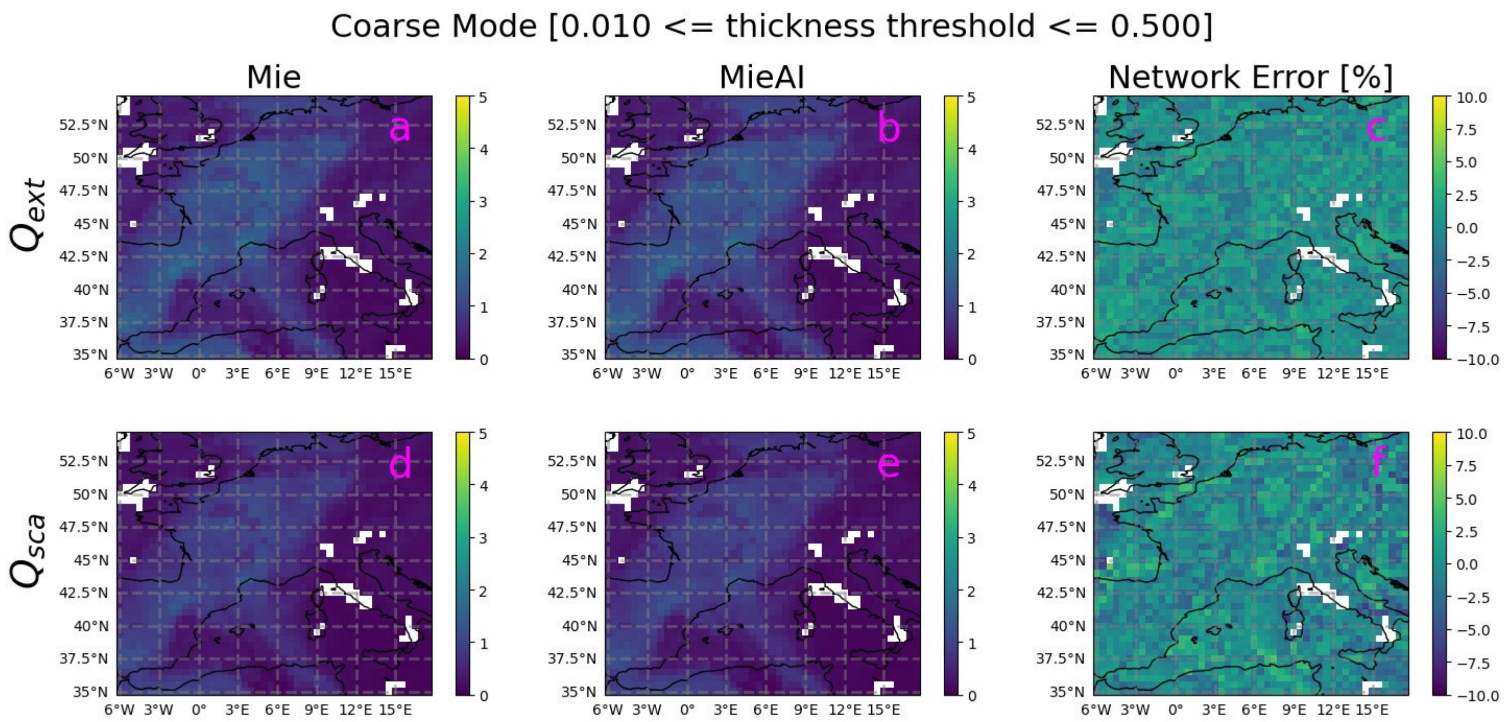
 Kumar et al. 2023 (in prep)

Pre-implementation 2

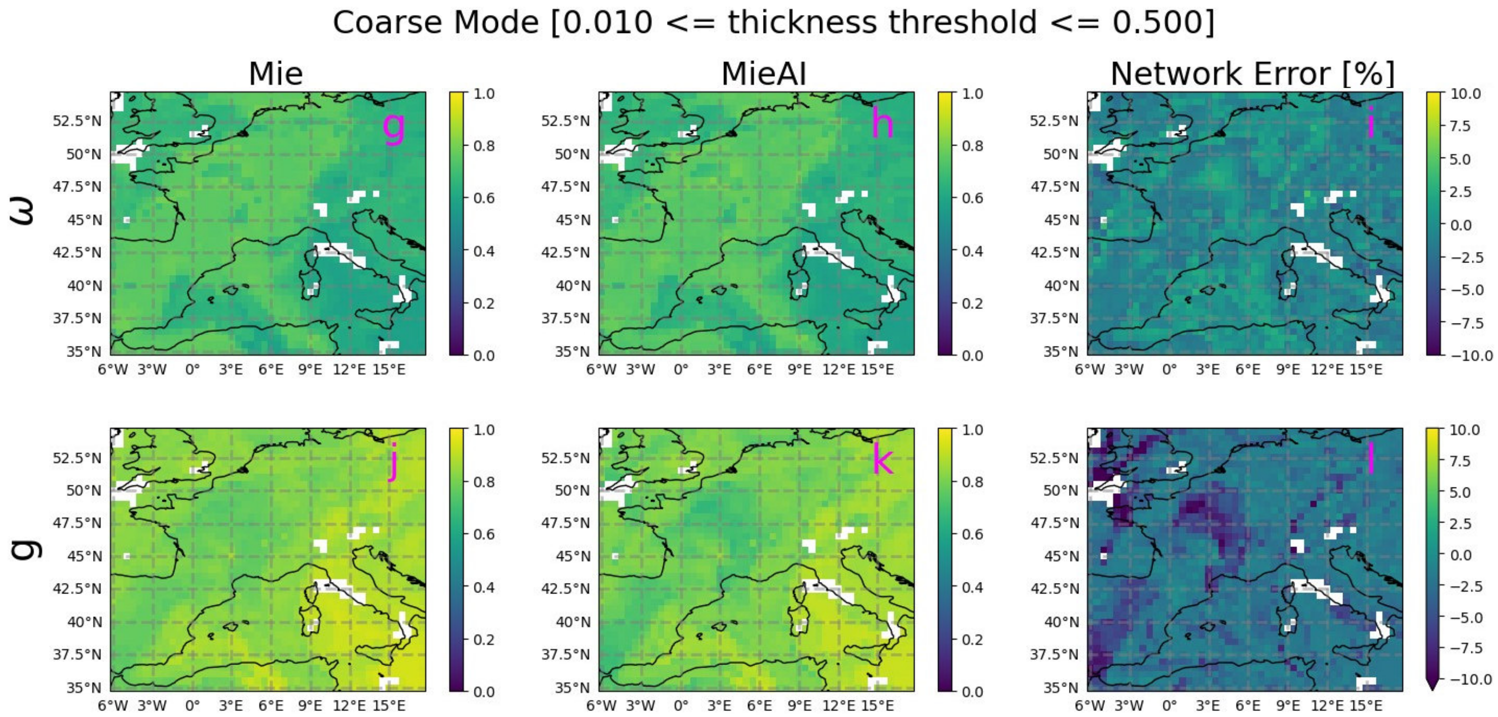


Kumar et al. 2023 (in prep)

Saharan dust outbreak June 2019



Saharan dust outbreak June 2019



 Kumar et al. 2023 (in prep)

Ideas for ICON-ML Coupling

- Mapping modes to bins and composition to RI
- Ongoing collaboration with DKRZ to use Fortran-Keras Bridge (FKB), YAC or CFFI (C Foreign Function Interface)
- Performance of the MieAI in the online setting

Summary

- Flexible, generic and computationally affordable tool for calculation of aerosol optical properties
- One ANN for all optical parameters
- ANN leads to R^2>0.95 for all parameters
- $O(10^3)$ faster than Mie code