Enhancing aerosol predictions on the global scale with particle-resolved modeling and machine learning
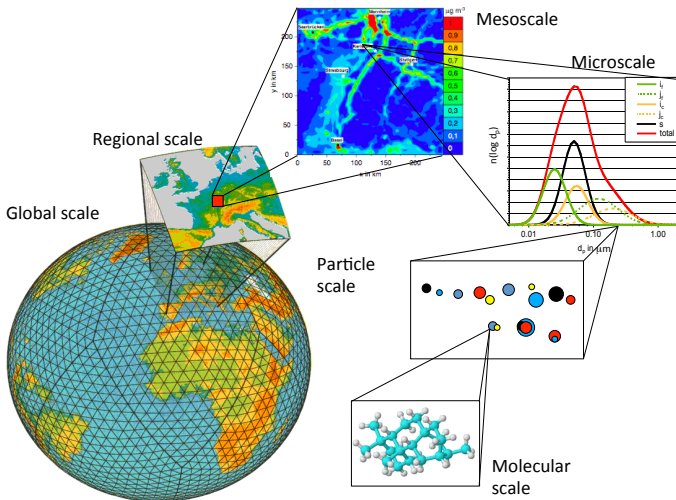
Nicole Riemer

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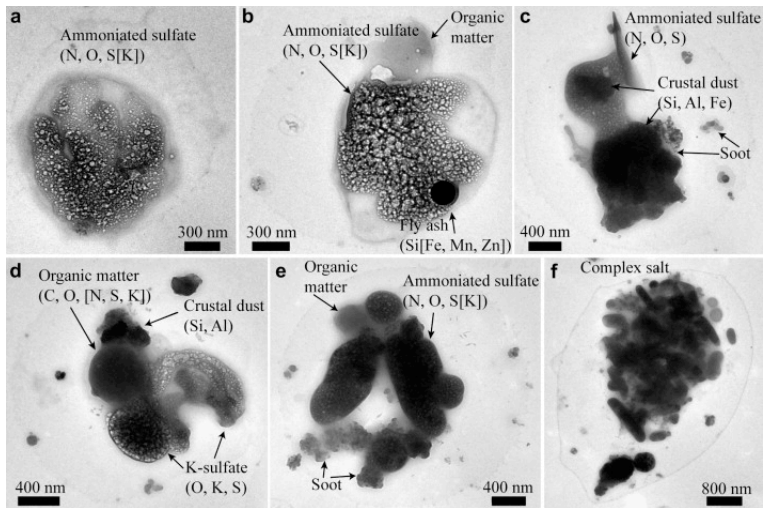with Zhonghua Zheng, Jeff Curtis and Matthew West

October 29, 2020
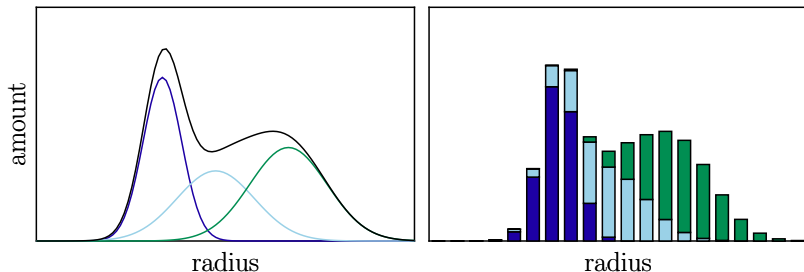
Aerosol science — a multiscale problem

# Real particles in the ambient atmosphere

Li et al., Atmospheric Environment, 45, 2488-2495, 2011

Traditional aerosol representations in models

- Modal and sectional models are distribution-based.
- Inherent assumption: All particles in one mode/bin have the same composition.
- Mixing state is an "unknown unknown" — structural uncertainty of the model.
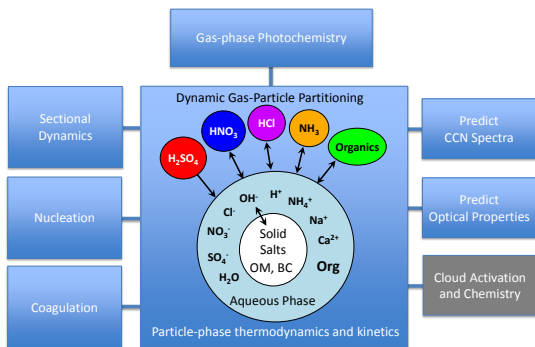
Could we do this instead?
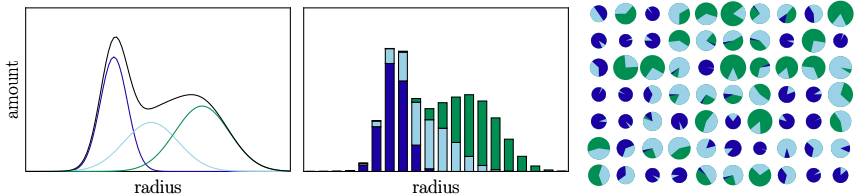
- PartMC-MOSAIC:
    - No modes or bins.
    - Instead: discrete particles — Particle-resolved modeling
    - Evolution of mixing state is straight-forward to represent.
   - Computationally expensive.

Stochastic aerosol model PartMC-MOSAIC

Figure courtesy of R. Zaveri, PartMC is open source, http://lagrange.mechse.illinois.edu/partmc/

- PartMC: simulates coagulation, particle emissions, dilution, nucleation stochastically.
- MOSAIC: simulates gas phase chemistry, aerosol thermodynamics deterministically (Zaveri et al., 2008)
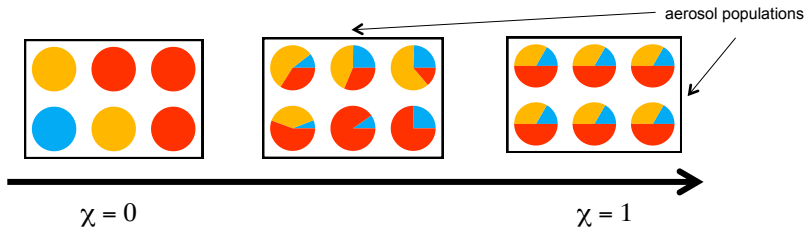
Role of PartMC in the model hierachy
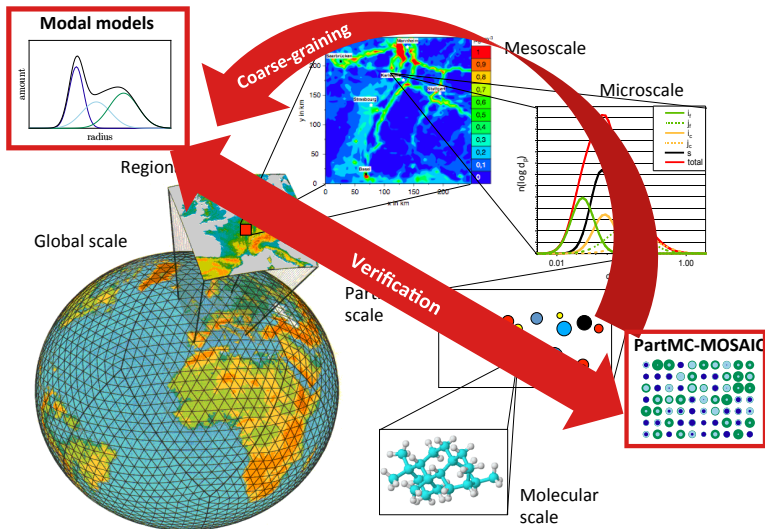
- "The same net composition of an aerosol can be caused by an infinite variety of different internal distributions of the various compounds." (Winkler, 1973)
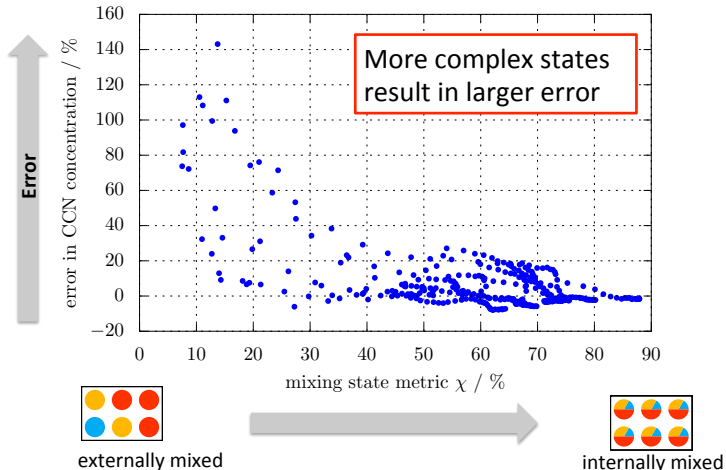

aerosol populations

$\chi = 0$ $\chi = 1$

- Metric: Mixing state index $\chi = \frac{D_\alpha - 1}{D_\gamma - 1}$

Riemer & West, ACP, 2013

Error quantification: Does it matter?

Error in CCN concentration when assuming average composition

More complex states result in larger error

externally mixed → internally mixed

Ching et al., ACP, 2017

How does mixing state vary globally?
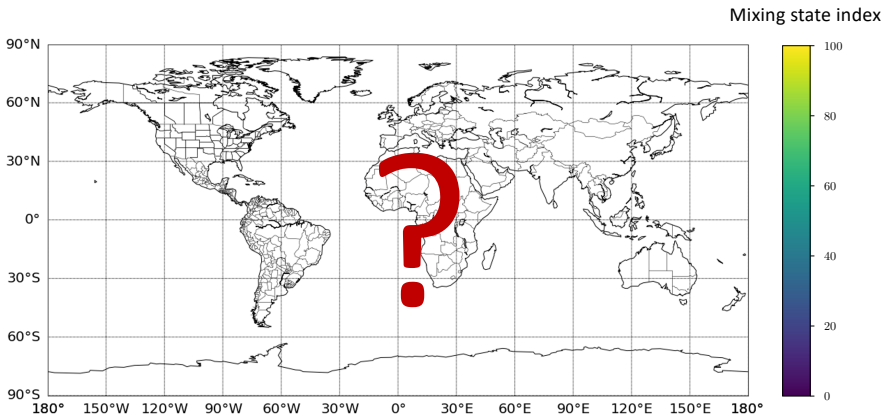
Particle-resolved modeling on the regional scale with WRF-PartMC
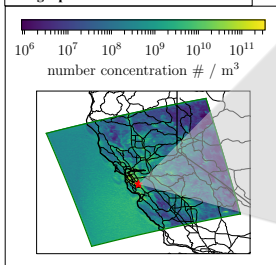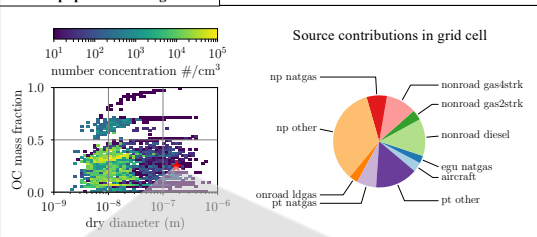
- 170 x 160 x 40 domain
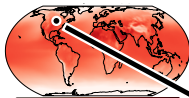- 6,656 cores on Blue Waters
- 10 billion computational particles
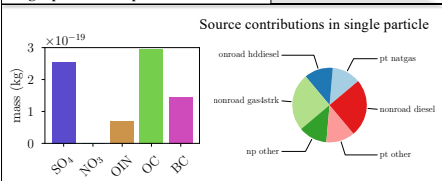
Curtis et al., GMD, 2017; Curtis et al., in preparation for GMD

What we want:

Global model outputs
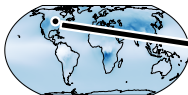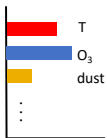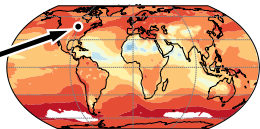
PartMC box model outputs

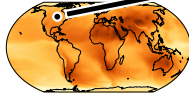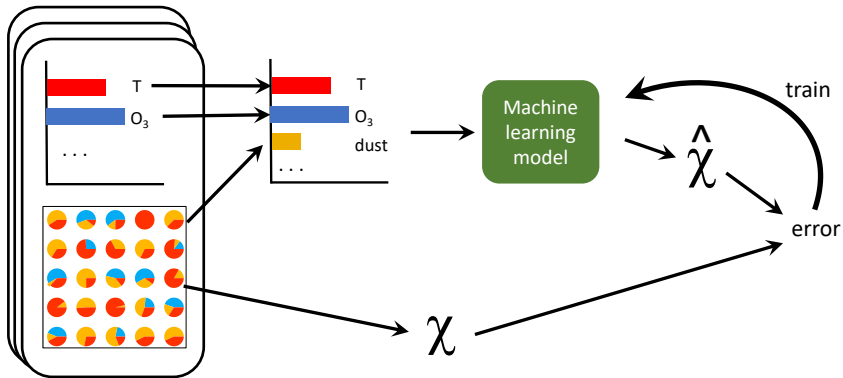# Global distribution of mixing state

(a) DJF   (b) JJA

mixing state index χ_a (%)
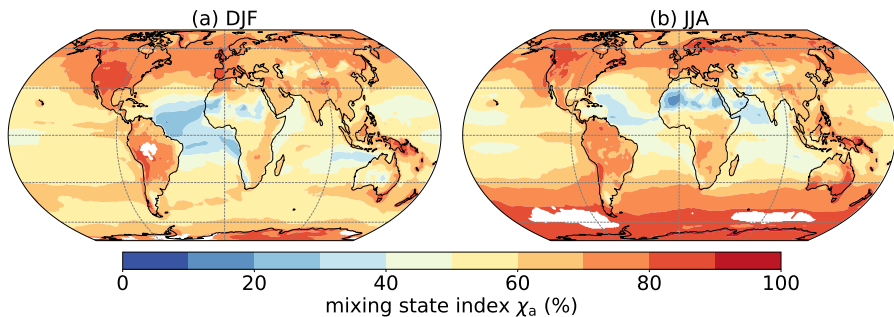
- Used CESM/MAM4 as GCM
- XGBoost to train emulator that predicts χ.
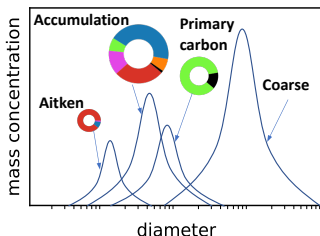- Uses bulk aerosol concentrations, gas phase concentrations, meteorological variables that are available in CESM.

Zheng et al., *Earth and Space Science, under review*

Next steps

- Aerosol module MAM4 represents mixing state to some extent.
    - Two distinct accumulation modes, fresh and aged carbonacous aerosol

- How does MAM4 mixing state differ from PartMC-emulated mixing state?