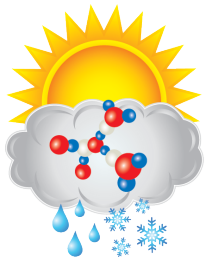
Quantifying structural uncertainty in the aerosol modeling hierarchy: particle-resolved modeling on LES scales

Matt West

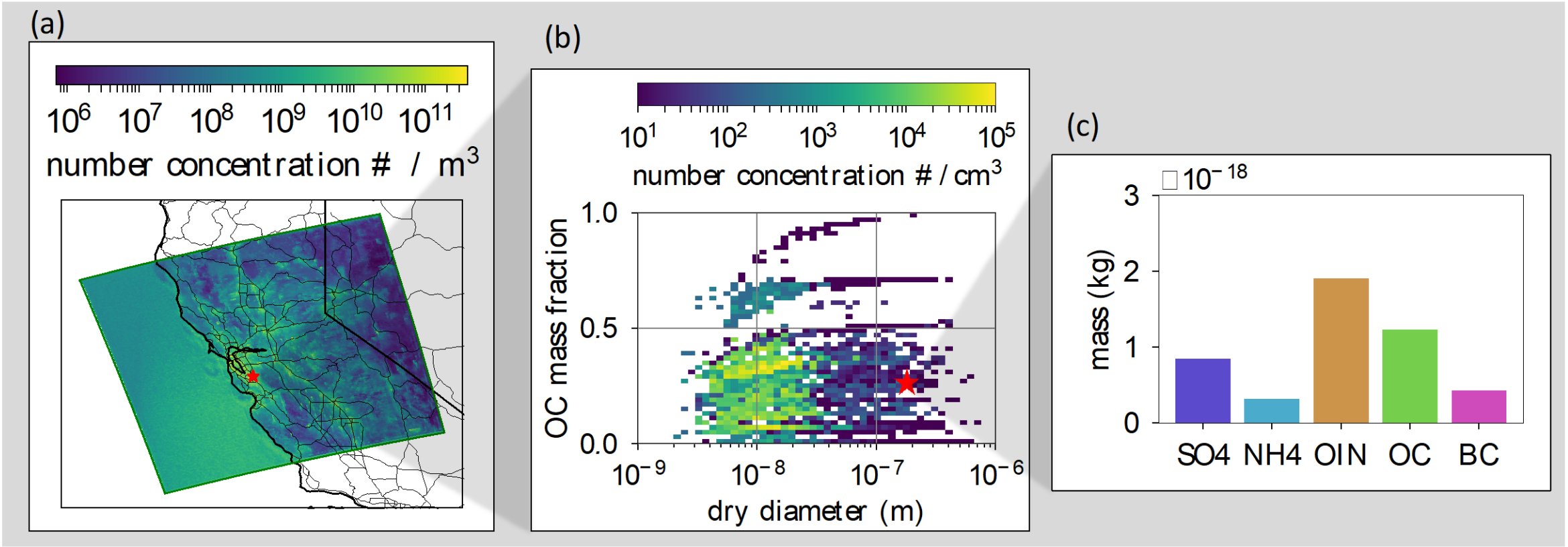
2023 Joint ARM User Facility and
ASR PI Meeting, Aug 9, 2023



ASR
Atmospheric System Research

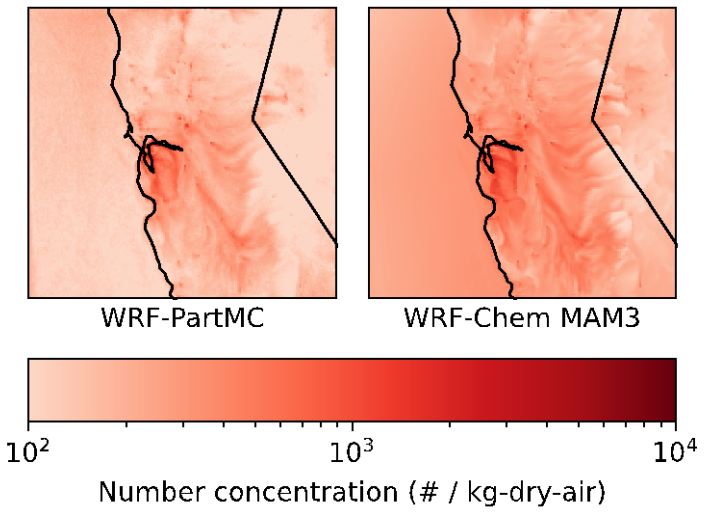
Joint work with Jeff Curtis, Sam Frederick, Zach D'Aquino, Matin Mohebalhojeh, and Nicole Riemer

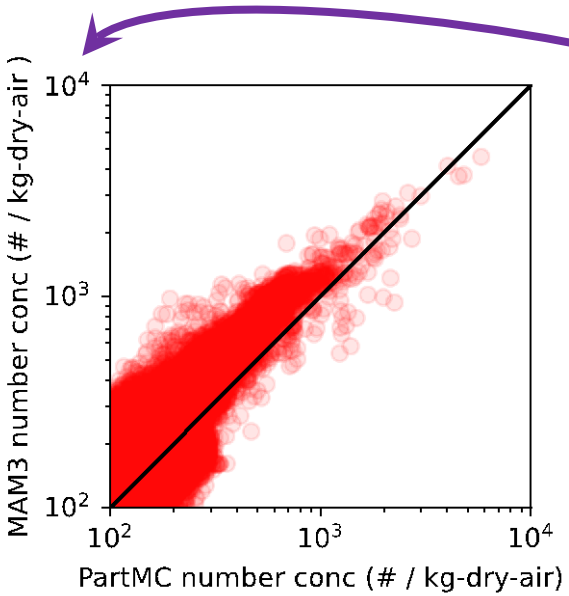
Particle-resolved aerosol model: PartMC

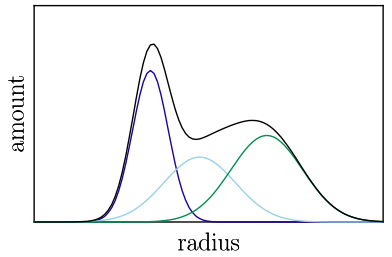


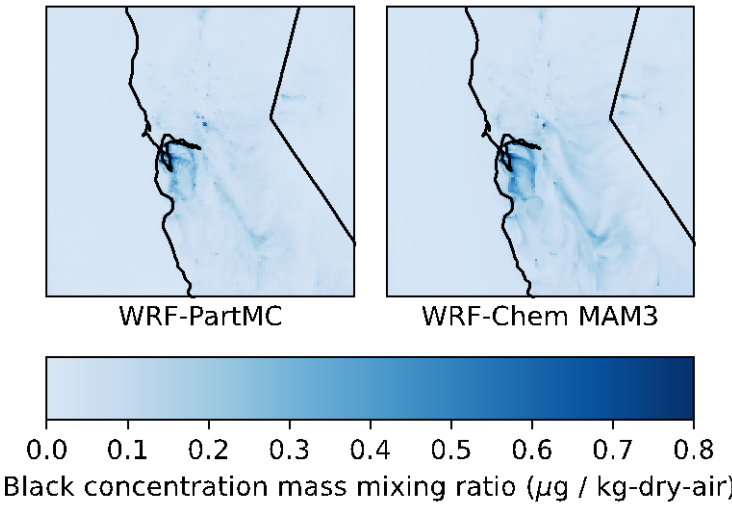
170 x 160 x 40 domain
10 billion particles computational particles
10,000 cores on Bridges2

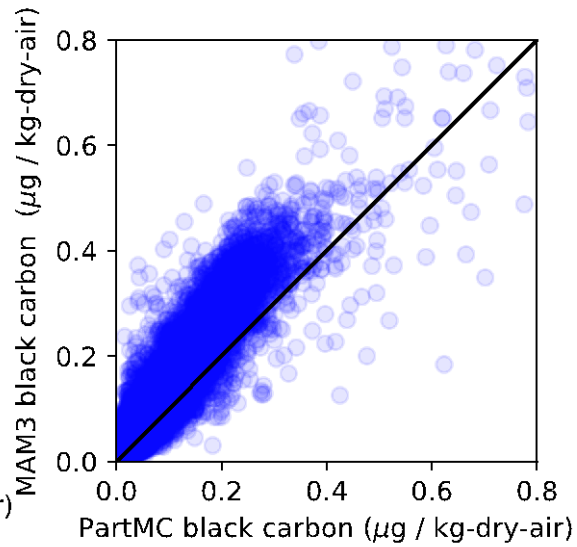
CARES: Comparison with WRF-Chem (MAM3)

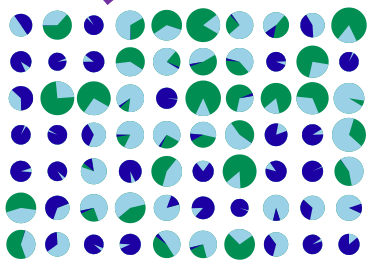


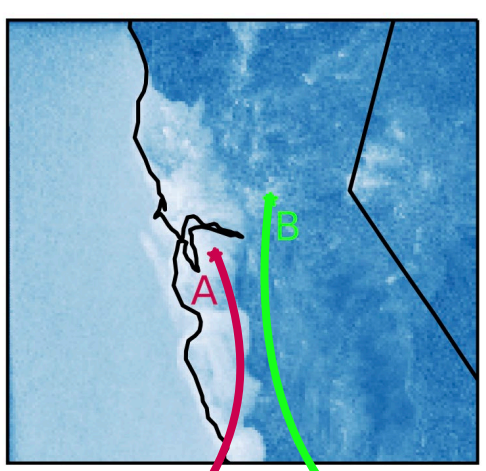


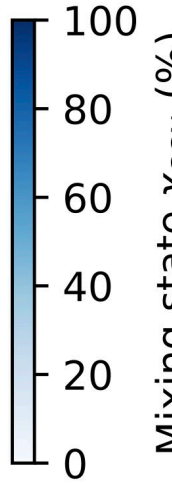


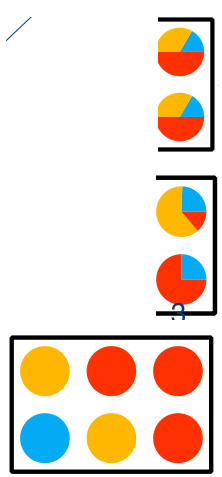








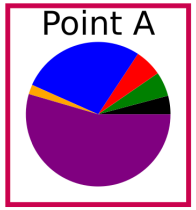


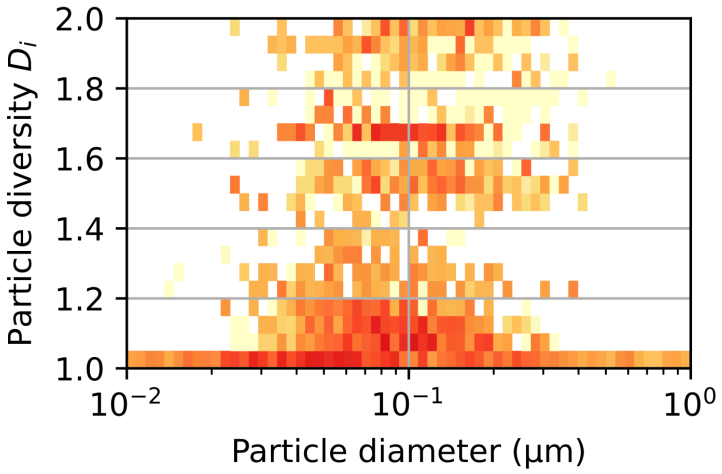


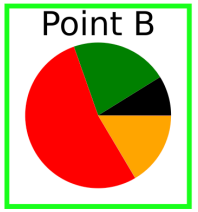
Internally mixed aerosol: χ = 100%

Externally mixed aerosol: χ = 0%

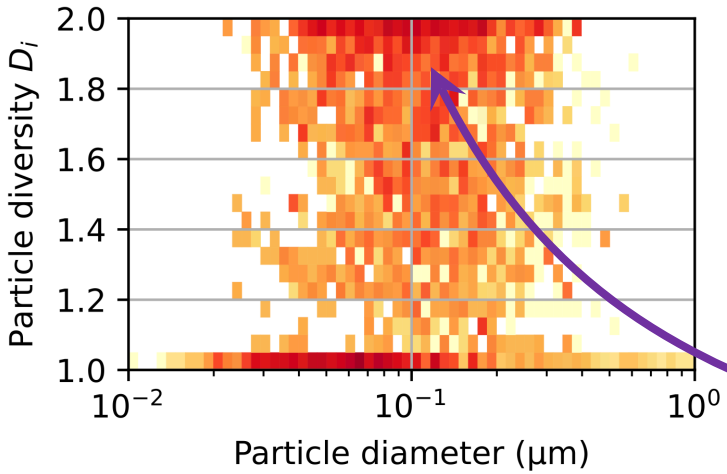
Externally mixed
χ = 17%

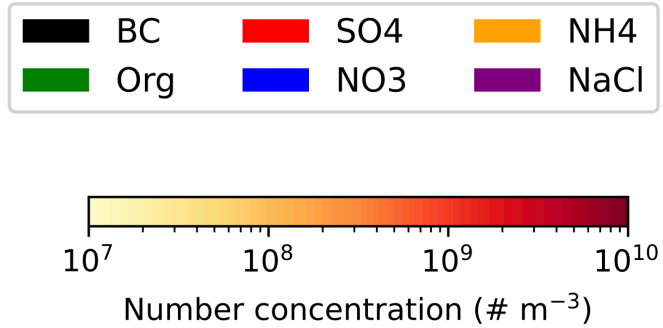






Internally mixed
χ = 43%

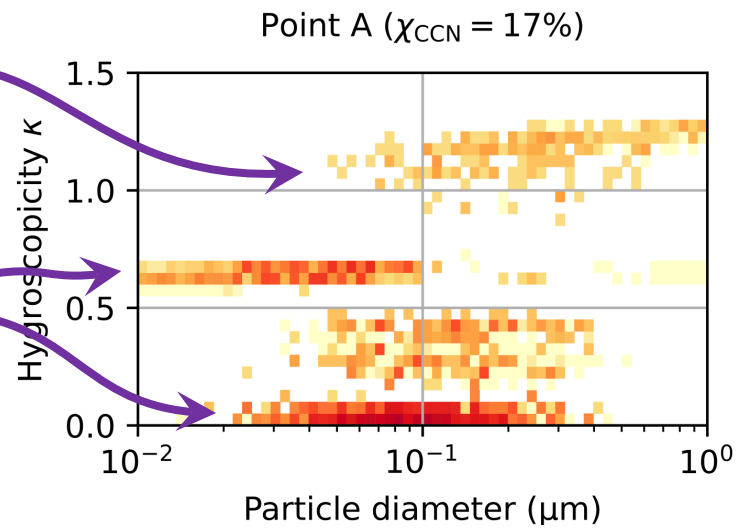


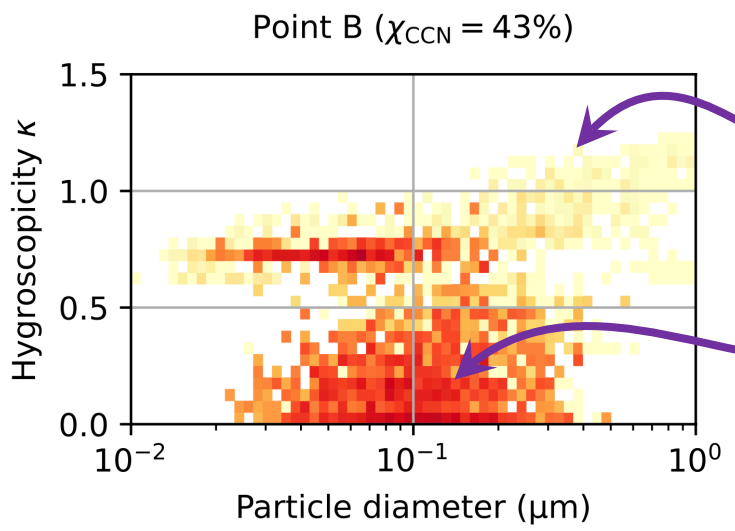


High diversity particles

Externally mixed

Internally mixed



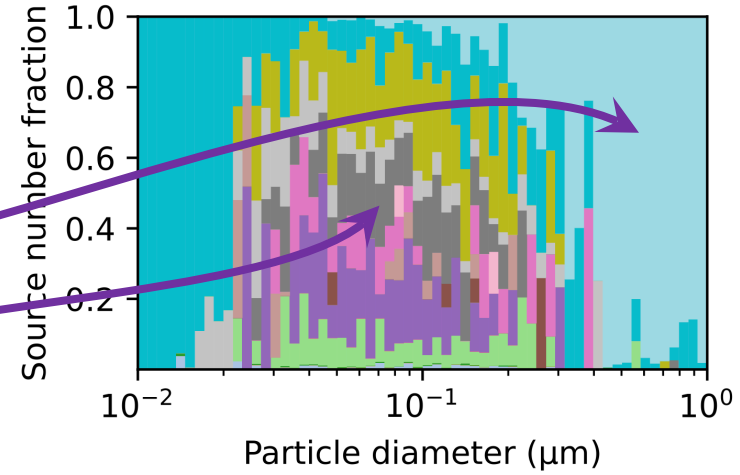


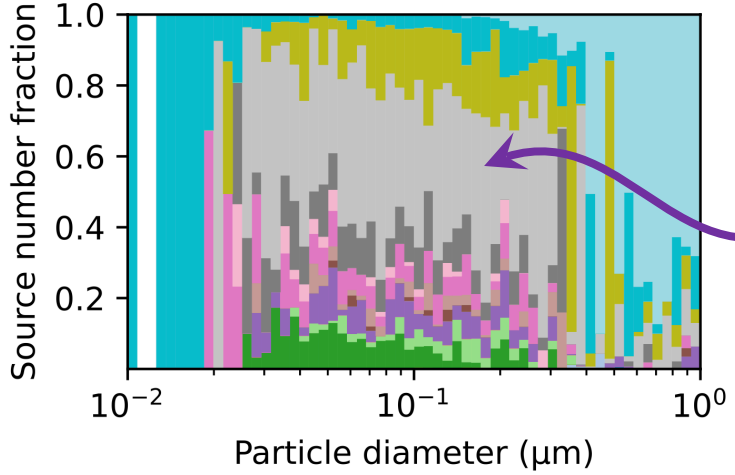
Sea salt

Narrow bands of kappa (inorganics and combustion)

Coagulated sea salt

Continuous range of kappa (aged combustion)





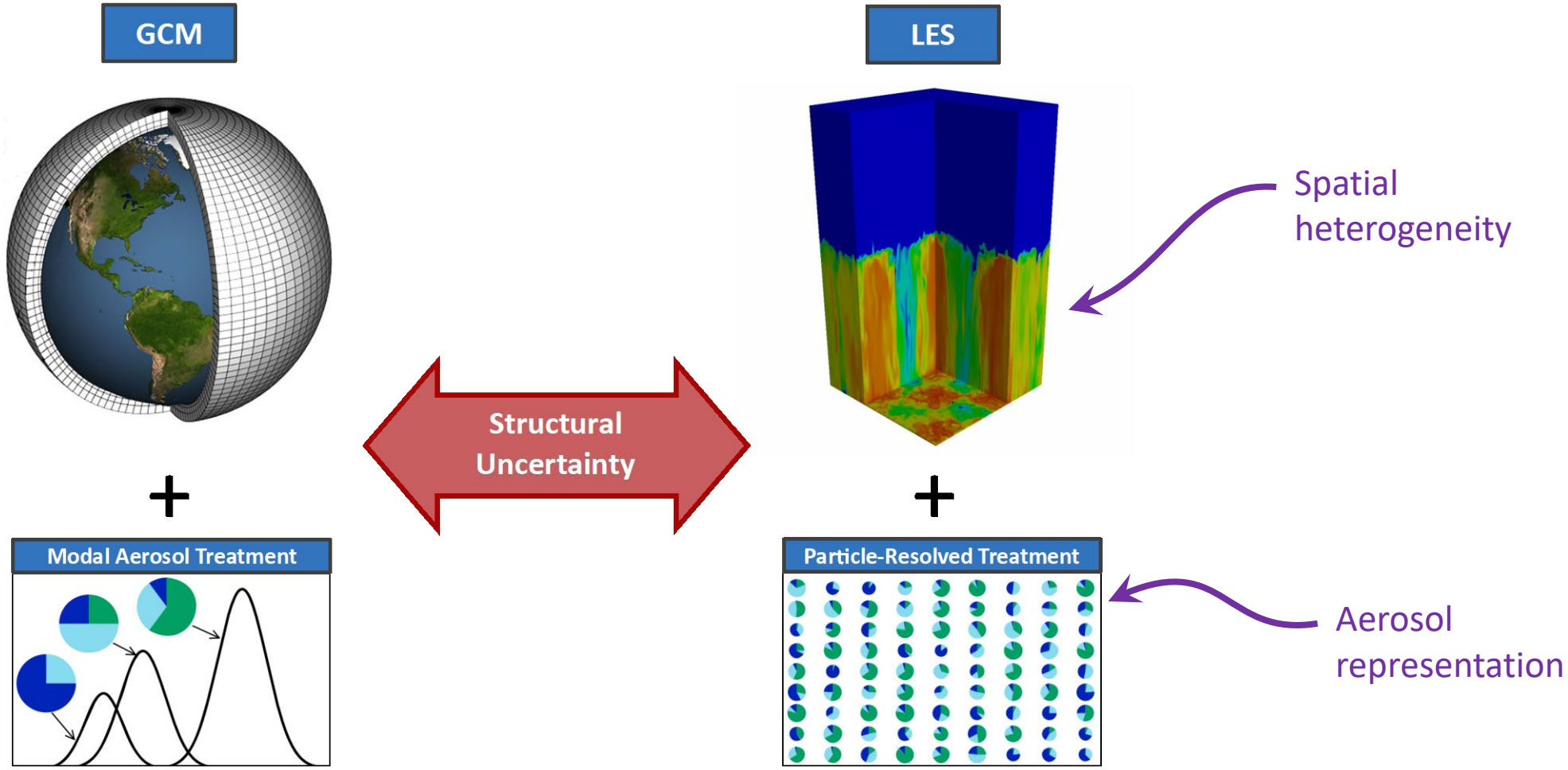
Sea salt

Fresh anthropogenics

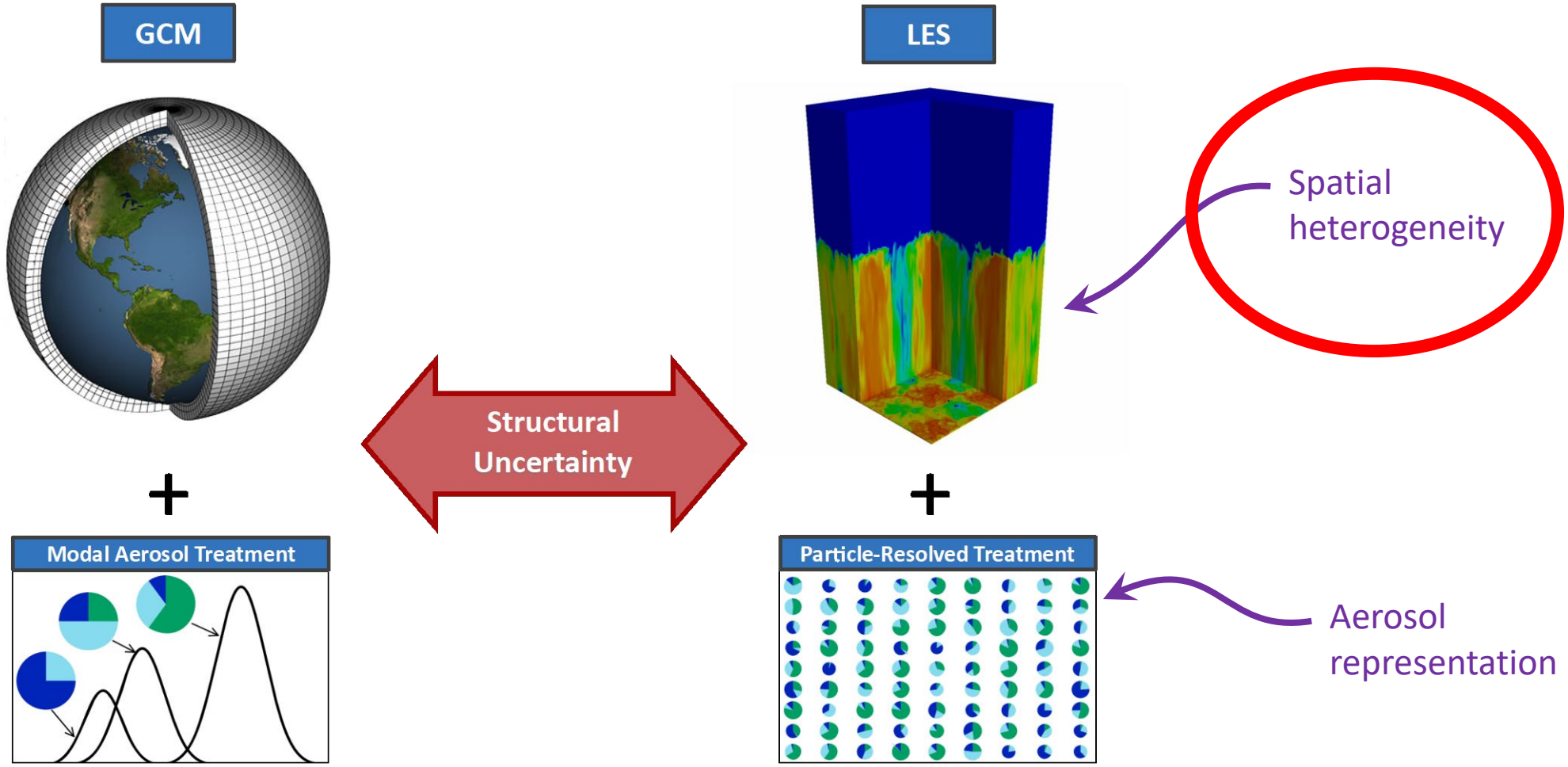
Point combustion

Init. cond.
Aircraft
Biogenic
Cooking
EGU
Nonroad
Non-point Ag.
Non-point Coal
Non-point Fug dust
Non-point Gas Ops
Non-point Indus.
Non-point Gas
Non-point Other
Non-point Rail
Onroad
Point combustion
Res Heating
Shipping
Boundary cond.
Sea salt

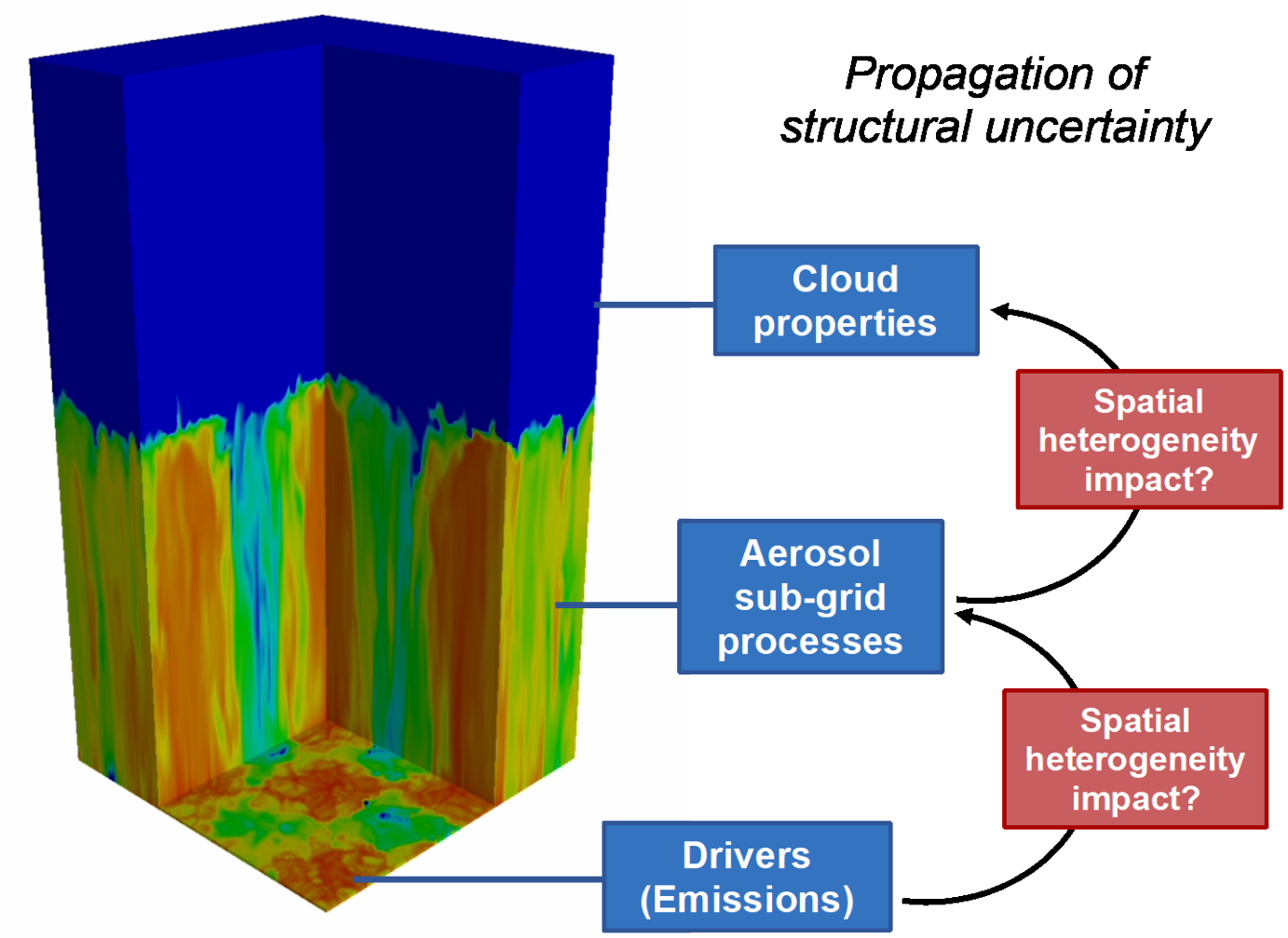
Structural uncertainty



Structural uncertainty



Focus on LES with checkerboard emissions



Quantifying heterogeneity

Decreasing heterogeneity
Increasing homogeneity

SH = 0.25 SH = 0.13 SH = 0.05

Spatial heterogeneity metric

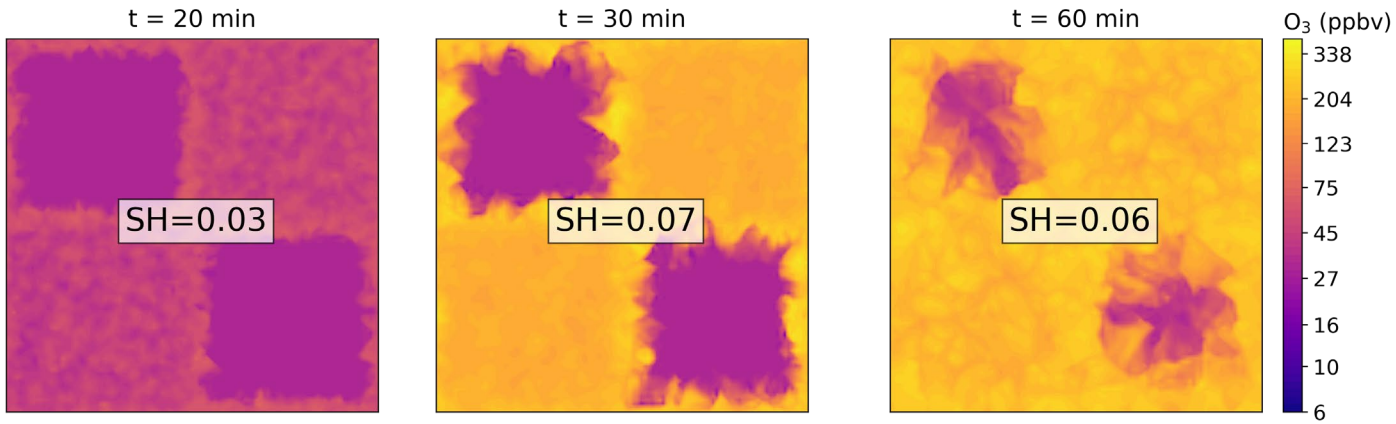
$$\mathrm{SH} = E\left[\left|\bar{f}(\tilde{S}) - \bar{f}(S)\right|\right]$$

$$= \int \left|\bar{f}(\tilde{S}) - \bar{f}(S)\right| p(\tilde{S}) d\tilde{S}$$

All three emission patterns have the same standard deviation

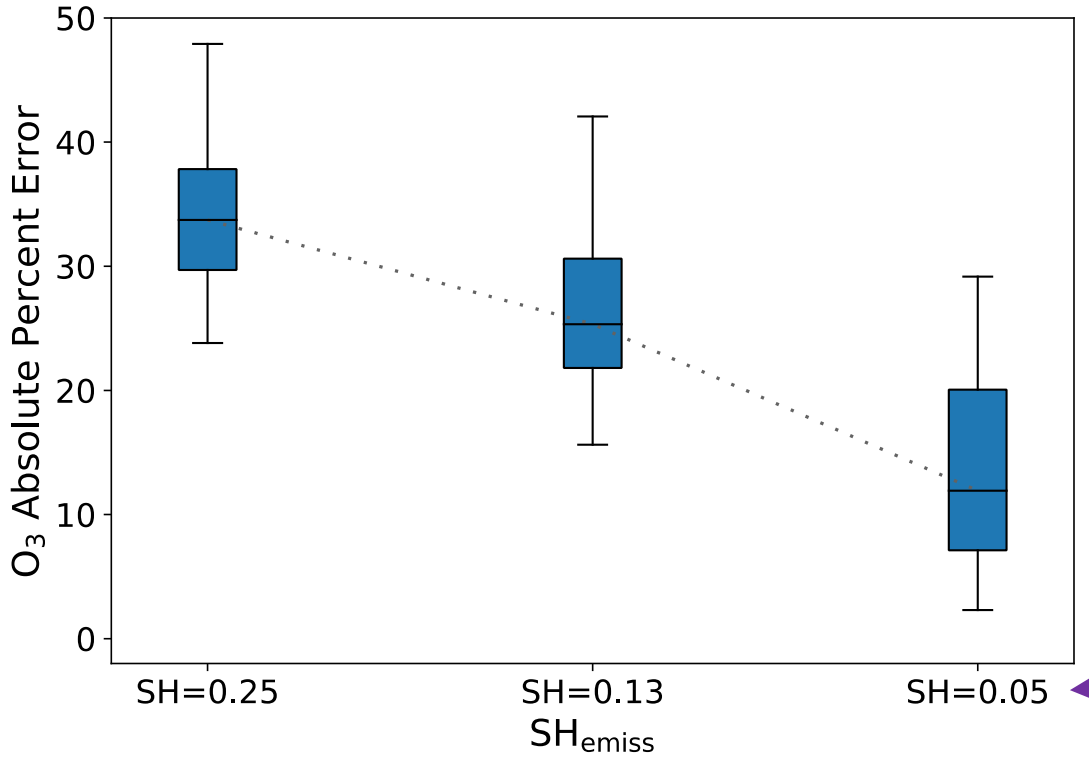
Cloud-base fields evolve in time

Overlapping Precursors



Spatial heterogeneity causes error

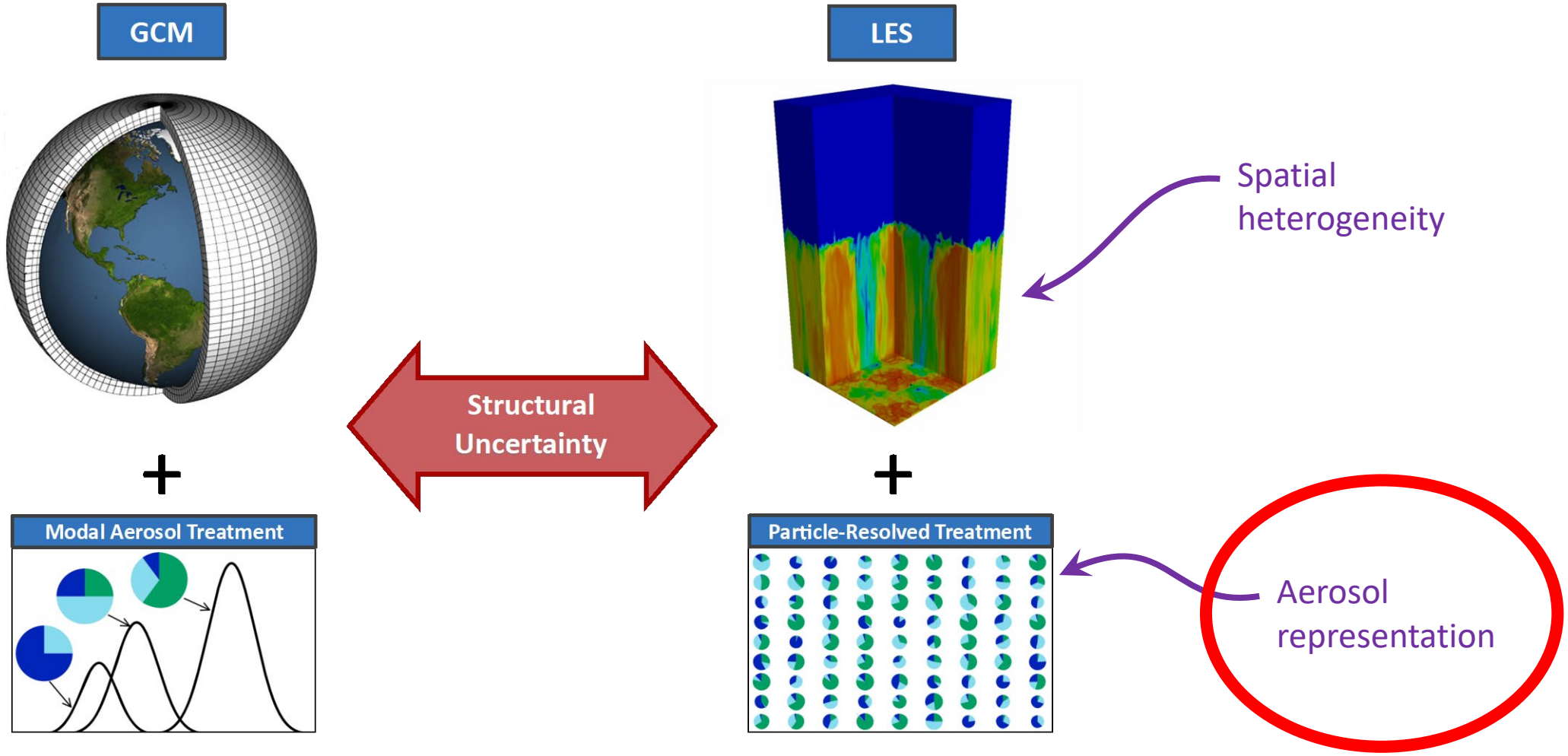
Increasing error in cloud base fields
Compared to uniform emissions



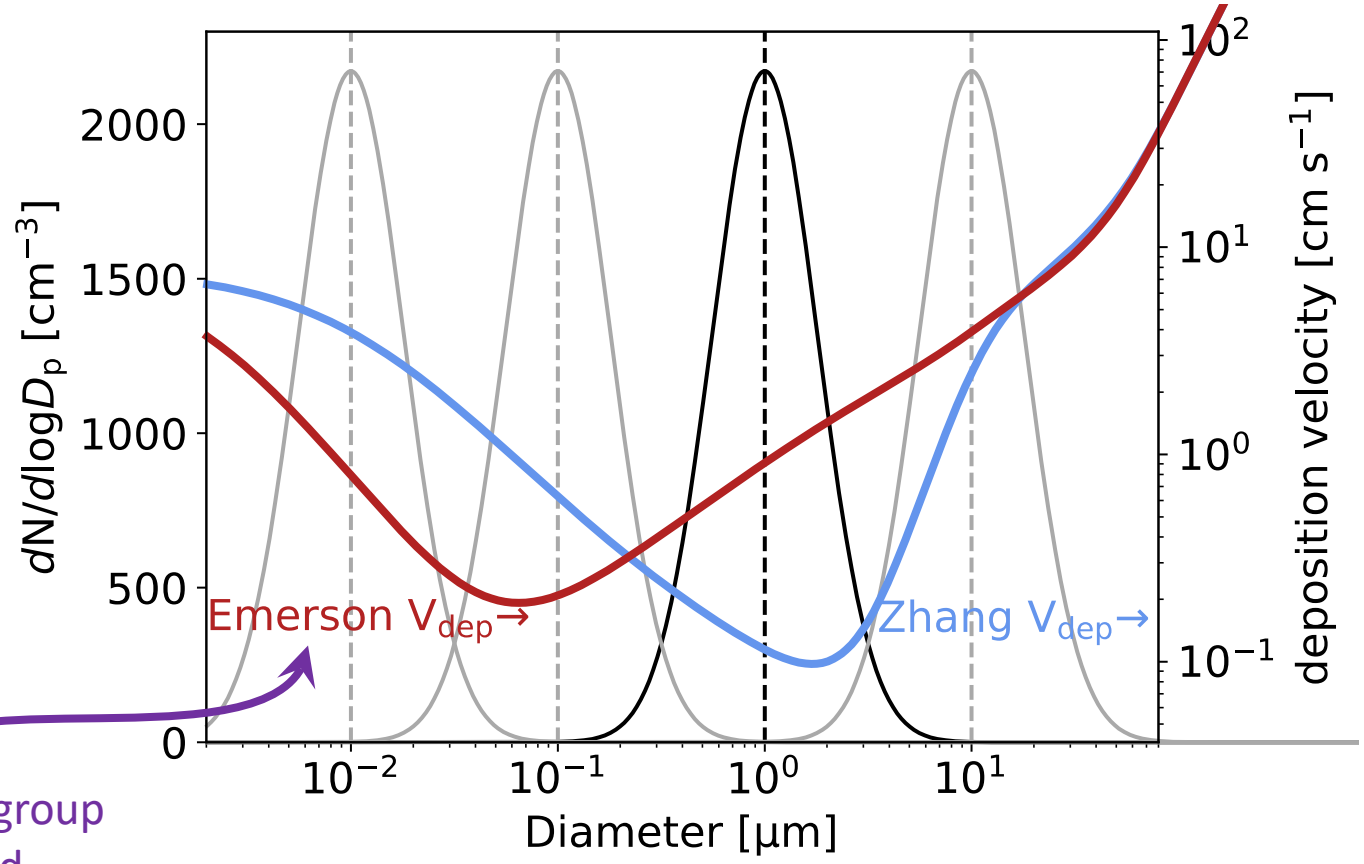
Quantitative!

Increasing homogeneity of emissions

Structural uncertainty

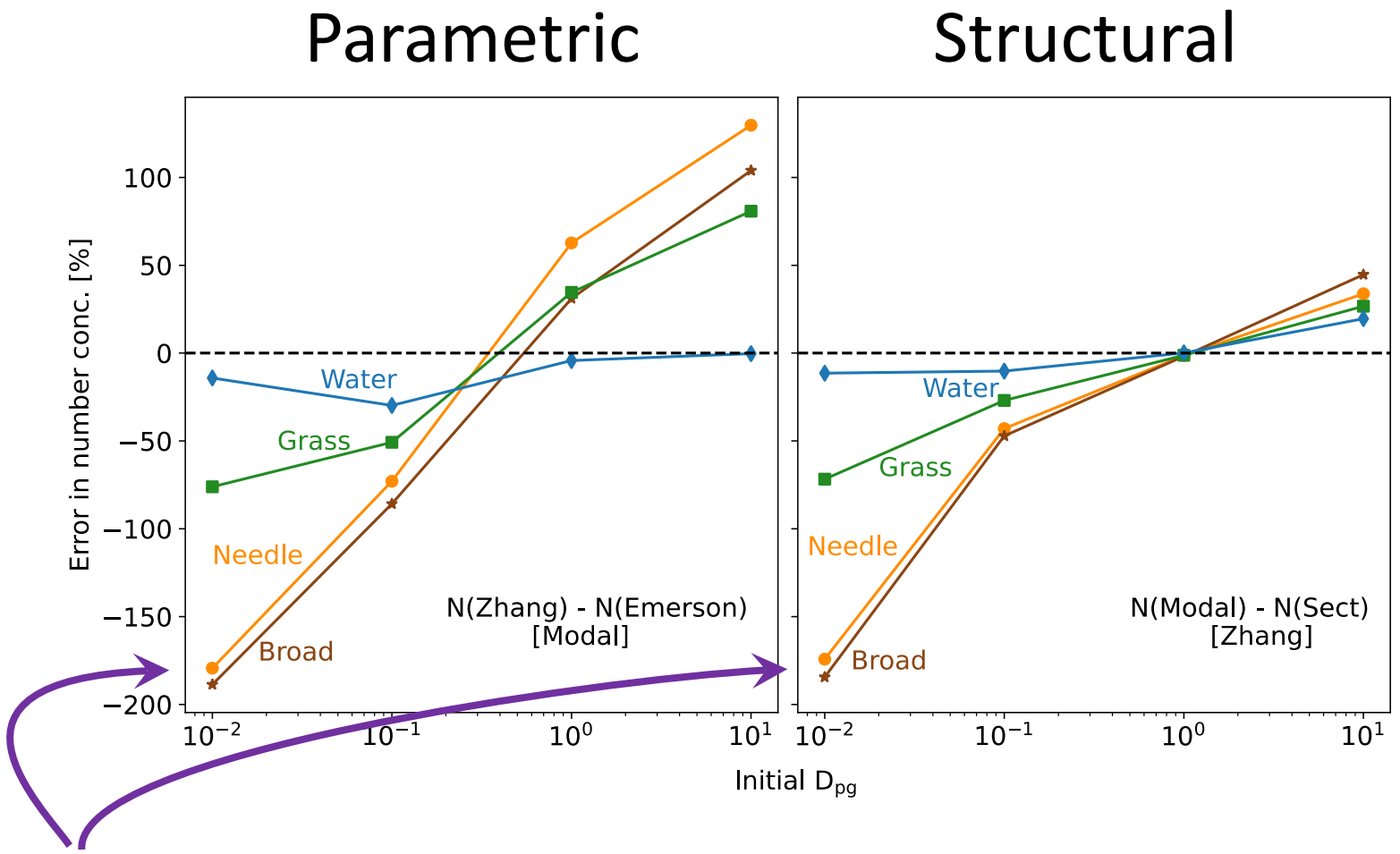


Case study: Dry deposition



Delphine Farmer's group
ASR/ARM supported

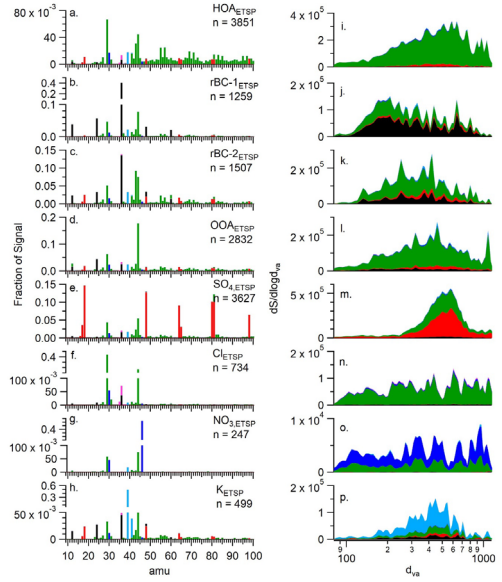
Comparing types of uncertainty (dry dep.)

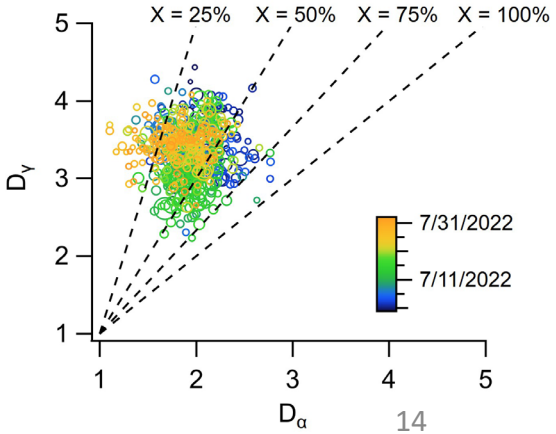


Same order of magnitude

AMF3 BNF: Aerosol structural uncertainty

- Spatial heterogeneity
  - Well-quantified emission data
  - 3D sampling: gasses + aerosol size + aerosol composition
- Aerosol composition heterogeneity
  - SP-AMS *in event-trigger mode*
  - Quantitative single-particle data (with uncertainty)
- Emulators for data coverage
  - Need training data (single particle) at some locations and times
  - Sample representative aerosol populations over space and time





TRACER data from Ryan Farley & Qi Zhang, UC Davis