Development and applications of benchmarking aerosol models on the regional scale using a stochastic particle-resolved approach

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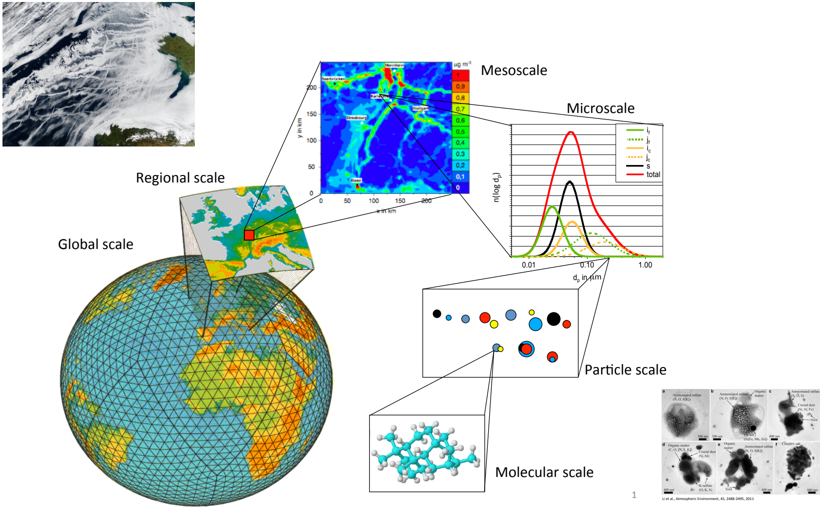
Atmospheric modeling: A multiscale challenge



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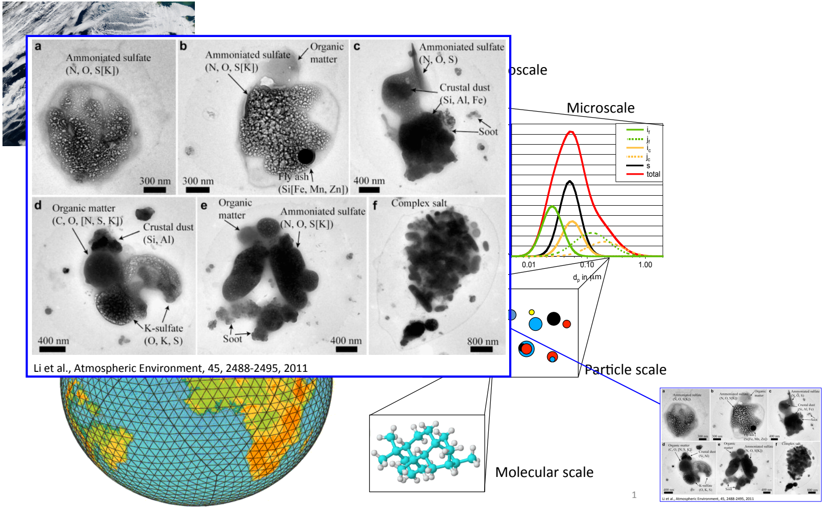
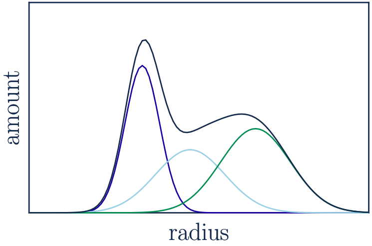
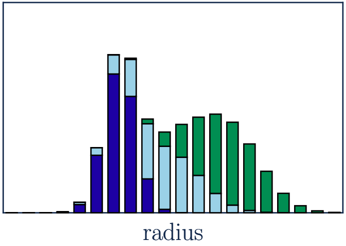


How do models represent aerosol composition?



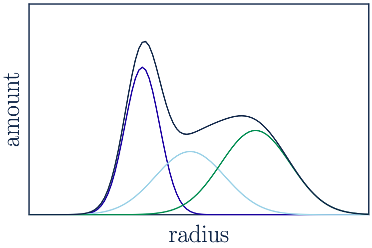
Modal



Sectional

- Simplifying assumptions regarding the aerosol composition
  - Sectional model: aerosols in a bin are fully internally mixed.
  - Modal model: aerosols in a mode are fully internally mixed.

How do models represent aerosol composition?



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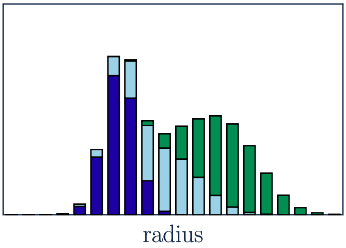

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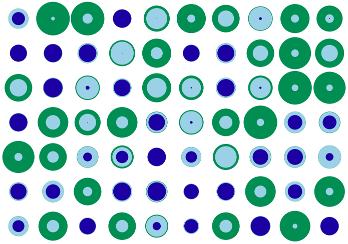
Alternative representation: Particle-resolved



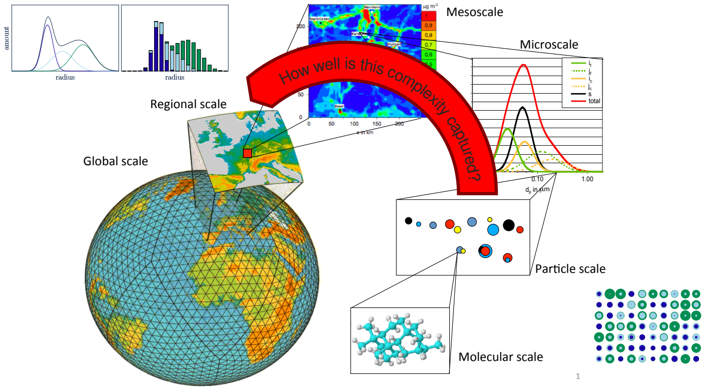
Particle-resolved

- Use a discrete representation of particles
- Representation of processes are straight-forward to model
- No bins or modes
- No assumption made regarding how particles are mixed

N. Riemer, M. West, R. A. Zaveri, and R. C. Easter, *Journal of Geophysical Research*, 2009

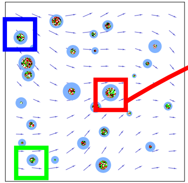
Model verification of aerosol representation

We need approximations at the regional and global scales.
But approximations cause error and uncertainties.



Particle-resolved modeling technique

What is composition space? Each particle is uniquely represented as an A-dimensional vector with mass composition components $\{\mu_1^i, \mu_2^i, \ldots, \mu_A^i\}$



	Particle 1	Particle 2	Particle 3
BC	3	10	1
SO_4	12	3	4
OC	5	8	2

N. Riemer, M. West, R. A. Zaveri, and R. C. Easter, *Journal of Geophysical Research*, 2009

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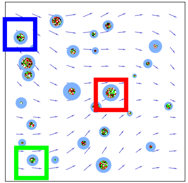

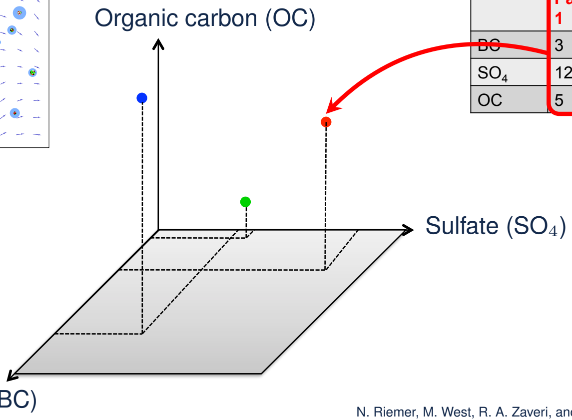

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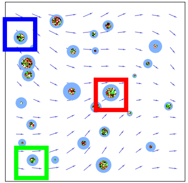

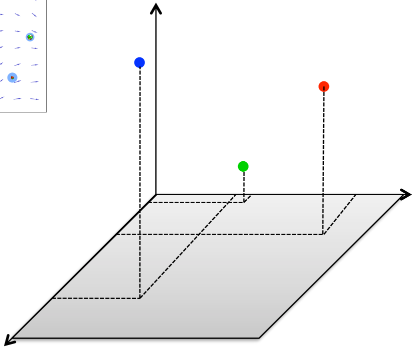

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Composition space $A \approx 20$

N. Riemer, M. West, R. A. Zaveri, and R. C. Easter, *Journal of Geophysical Research*, 2009

Benefits of particle-resolved models

- No approximation need for representing mixing state
  - Coarse graining tool: deriving parameters for more approximate models
  - Benchmark and error quantification for more approximate models
  - Detailed studies on the particle scale and experimental intercomparison.
- Scales efficiently for high-dimensional data (number of aerosol species)
  - Avoids curse of dimensionality
- Efficient algorithms make particle-resolved modeling feasible
  - Accelerated binned coagulation (Riemer et al. 2009, Michelotti et al. 2013)
  - Particle weighting methods to reduce statistical error (DeVille et al. 2011, 2019)
  - Accelerated particle removal algorithms (Curtis et al. 2016)

Benchmarking approximate models

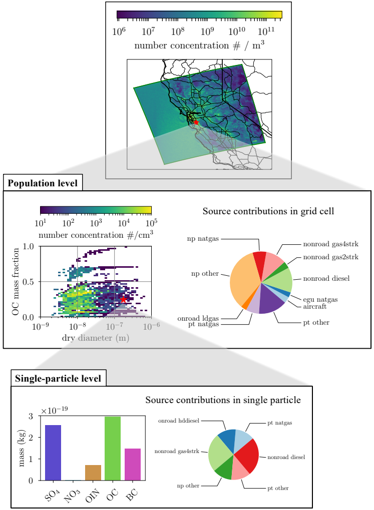
Simulation inputs and processes should be as similar as possible

- Same meteorological model
- Same chemical mechanisms
- Consistency in emissions
- Identical particle removal processes
- Identical transport algorithms

Only change the aerosol microphysics

Particle-resolved modeling on the regional scale

- PartMC coupled with WRF allows regional simulations with highly-detailed mixing state.
- Each grid cell simulates 10 000 computational particles - billions of particles for the domain.
- Many levels of detail from the large-scale to population level to single-particle details of composition and emission source.
- Computational expense: 300 000 core hours for 2 day simulation from the domain to right

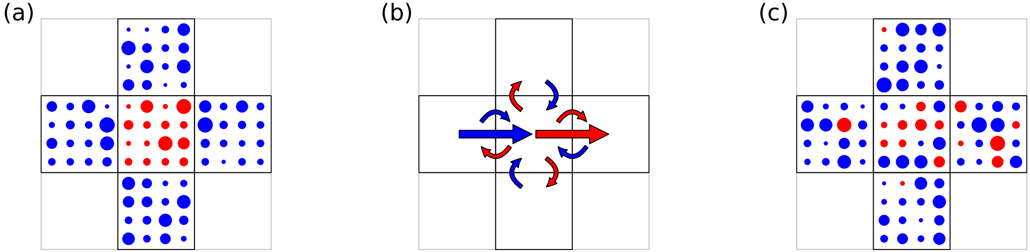


Curtis, Riemer and West, *Geoscientific Model Development*, 2017

How do we move vectors of particle composition?

Transport PDE $\rightarrow$ Discretize in space, time, and particles $\rightarrow$ Determine probabilities $\rightarrow$ Sample particle sets

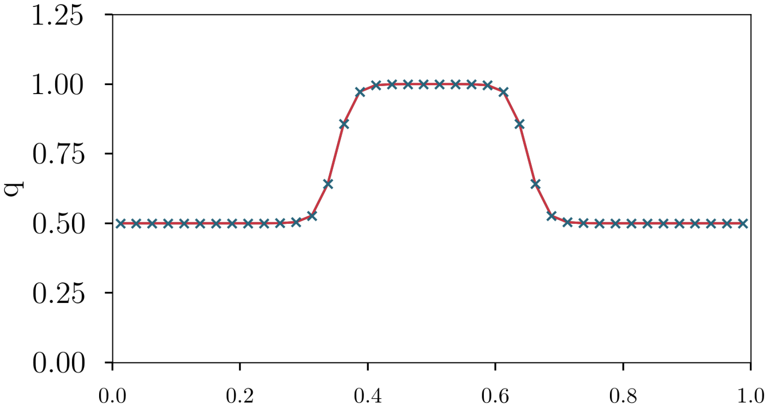
$$q^{t+1}_{i,j} - q^{t}_{i,j} = \Delta t \frac{F^{t}_{i+1/2,j} - F^{t}_{i-1/2,j}}{\Delta x} + \Delta t \frac{F^{t}_{i,j+1/2} - F^{t}_{i,j-1/2}}{\Delta y}$$



Replicates deterministic finite volume method to isolate importance of representation

Simulating stochastic aerosol transport

Testcase: 1D constant positive u advection (third order)



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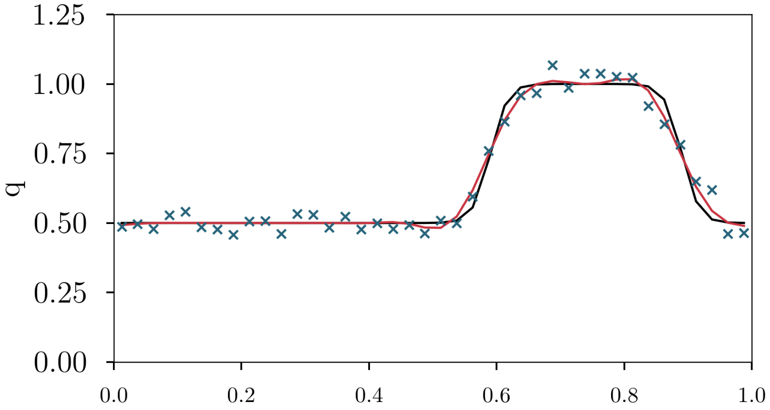

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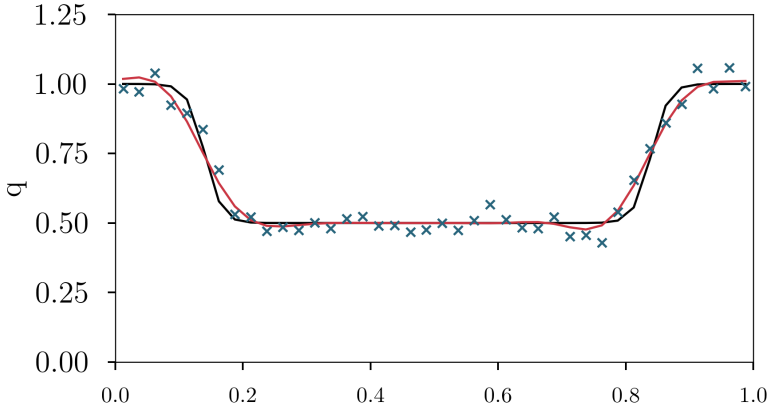

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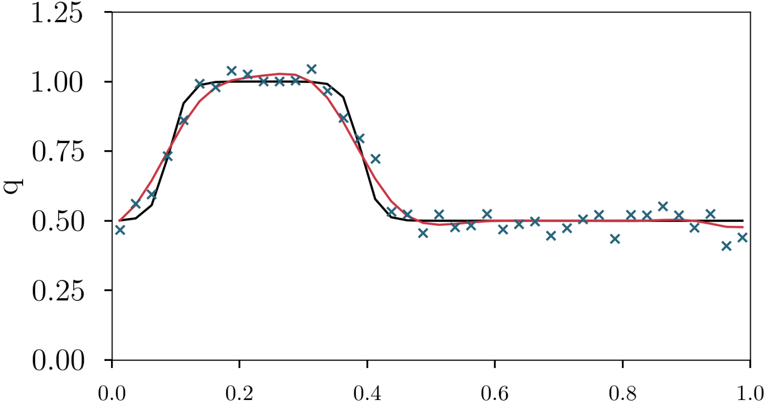

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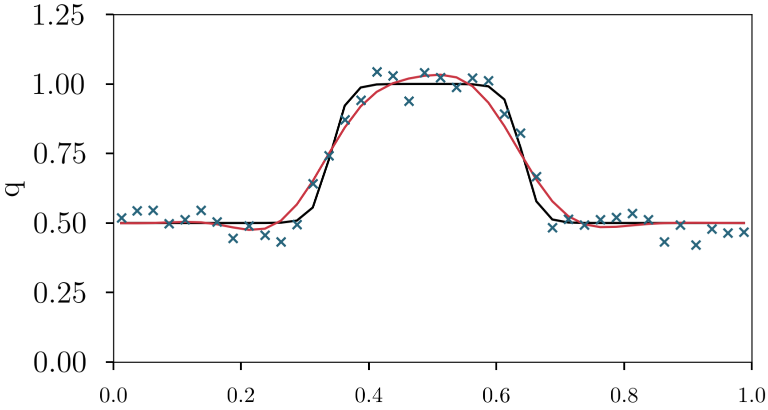

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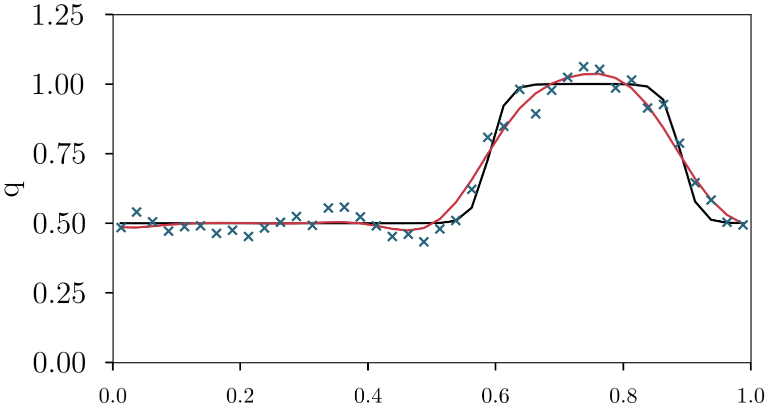

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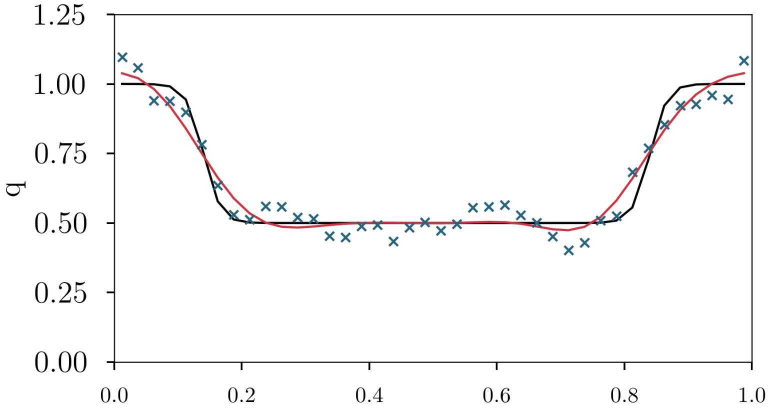

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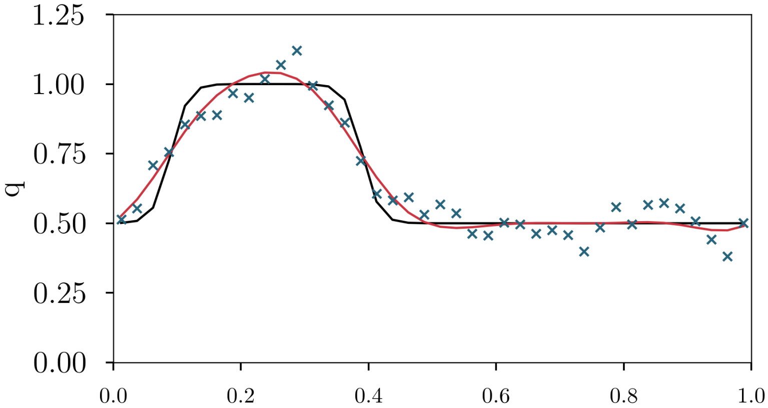

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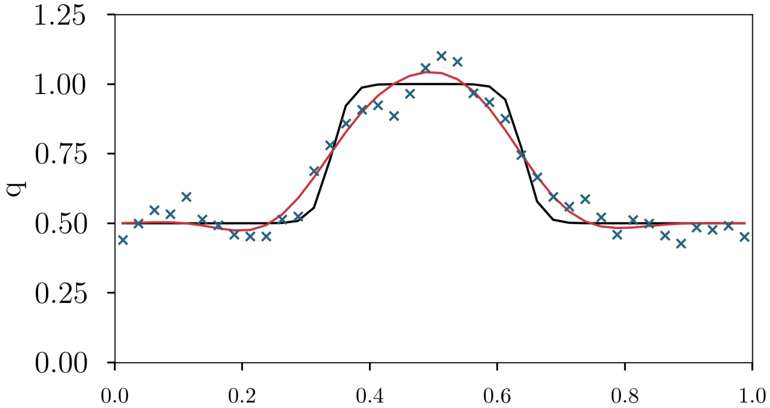
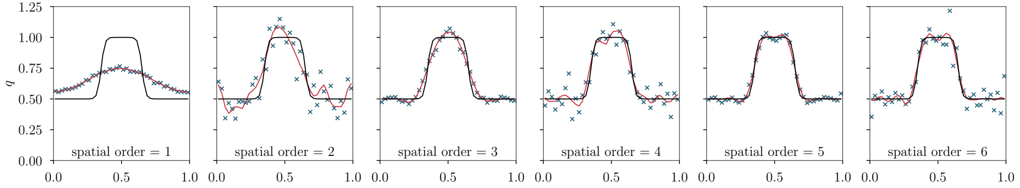
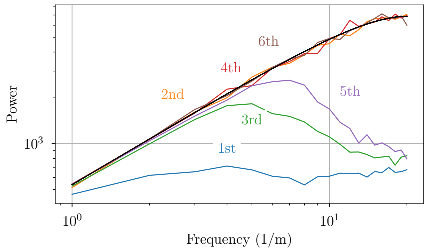
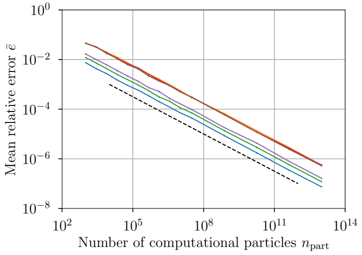


Results: Simulating stochastic aerosol transport







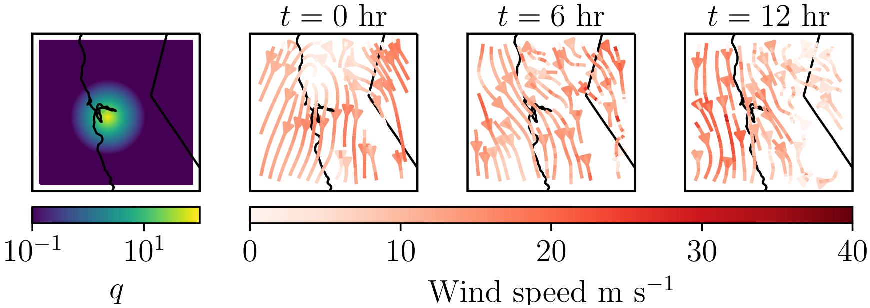
Odd orders perform better (implicit diffusion)

Converges to FV method in particle number

Curtis, Riemer and West, *Geoscientific Model Development* (in prep)

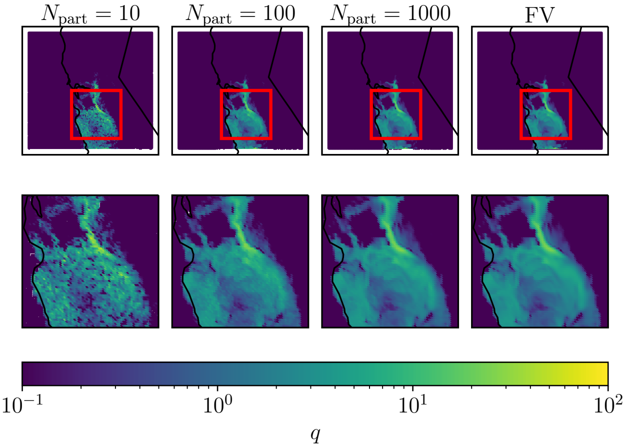
Transport performance in real-world case

Complex terrain, complex and evolving wind field



Transport performance in real-world case

Stochastic algorithm applied to third order monotonic advection scheme in WRF



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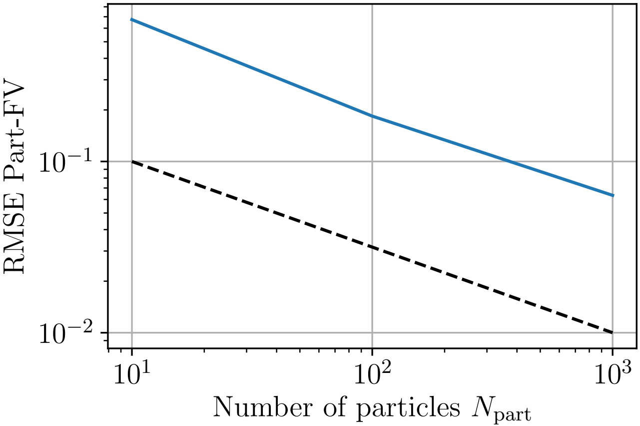
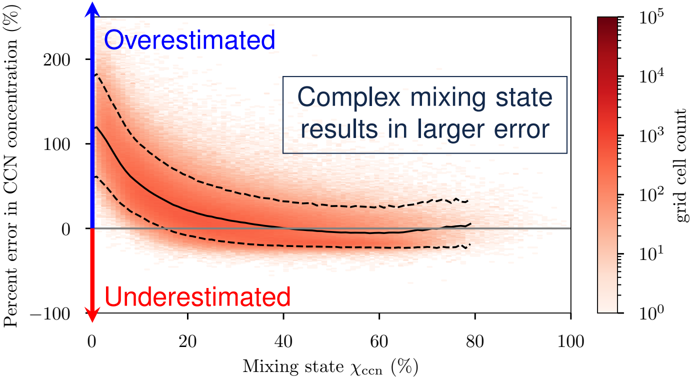
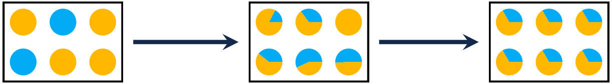


First step: CCN error quantification for a sectional projection



Externally mixed

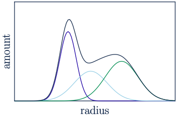


Internally mixed

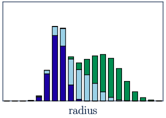
Concluding thoughts

Future work: Model benchmarking

Use particle-resolved modeling and mixing state metrics to benchmark aerosol models that use varying levels of mixing state



Modal



Sectional

Code availability

https://github.com/compdyn/partmc

GitHub docker Travis CI

Funding

ASR Atmospheric System Research

DE-SC0011771
DE-SC0019192

BLUE WATERS