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

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International Aerosol Modeling Algorithms Conference
December 5, 2019
Atmospheric modeling: A multiscale challenge

Global scale
Regional scale
Global scale

Mesoscale
Microscale
Particle scale
Molecular scale

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Atmospheric modeling: A multiscale challenge

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

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How do models represent aerosol composition?

- 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?

- 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**.
Alternative representation: 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

Model verification of aerosol representation

We need approximations at the regional and global scales. But approximations cause error and uncertainties.
**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-resolved modeling technique

What is composition space? Each particle is uniquely represented as an $A$-dimensional vector with mass composition components $\{\mu^i_1, \mu^i_2, \ldots, \mu^i_A\}$

![Diagram showing composition space with particles and mass composition components]

<table>
<thead>
<tr>
<th></th>
<th>Particle 1</th>
<th>Particle 2</th>
<th>Particle 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>BC</td>
<td>3</td>
<td>10</td>
<td>1</td>
</tr>
<tr>
<td>SO$_4$</td>
<td>12</td>
<td>3</td>
<td>4</td>
</tr>
<tr>
<td>OC</td>
<td>5</td>
<td>8</td>
<td>2</td>
</tr>
</tbody>
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Sulfate (SO$_4$)  Organic carbon (OC)  Black carbon (BC)

Particle-resolved modeling technique

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Composition space \(A \approx 20\)

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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
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.
How do we move vectors of particle composition?

Transport PDE → Discretize in space, time, and particles → Determine probabilities → Sample particle sets

\[ q_{i,j}^{t+1} - q_{i,j}^t = \Delta t \left( \frac{F_{i+1/2,j}^t - F_{i-1/2,j}^t}{\Delta x} + \frac{F_{i,j+1/2}^t - F_{i,j-1/2}^t}{\Delta y} \right) \]

(a) (b) (c)

Replicates deterministic finite volume method to isolate importance of representation
Simulating stochastic aerosol transport

Testcase: 1D constant positive $u$ advection (third order)
Simulating stochastic aerosol transport

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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

$\frac{q}{10^1} \sim 10^{10}$

$t = 0 \text{ hr}$
$t = 6 \text{ hr}$
$t = 12 \text{ hr}$

Wind speed $\text{m s}^{-1}$

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Transport performance in real-world case

Stochastic algorithm applied to third order monotonic advection scheme in WRF

$N_{\text{part}} = 10 \quad N_{\text{part}} = 100 \quad N_{\text{part}} = 1000 \quad \text{FV}$

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Transport performance in real-world case

Stochastic algorithm applied to third order monotonic advection scheme in WRF

![Graph showing RMSE Part-FV versus Number of particles N_{part}](image)

Number of particles

RMSE Part-FV

$10^{-1}$

$10^{-2}$

$10^1$  $10^2$  $10^3$

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First step: CCN error quantification for a sectional projection

The diagram shows a graph with the mixing state \( \chi_{ccn} \) on the x-axis and the percent error in CCN concentration on the y-axis. The graph illustrates the impact of complex mixing states on error predictions.

- **Overestimated** regions indicate higher error predictions than actual values.
- **Underestimated** regions indicate lower error predictions than actual values.

Complex mixing states result in larger errors, as shown by the deviation from the ideal mixing states (Externally and Internally mixed).

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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.

Code availability

https://github.com/compdyn/partmc

Funding

DE-SC0011771
DE-SC0019192