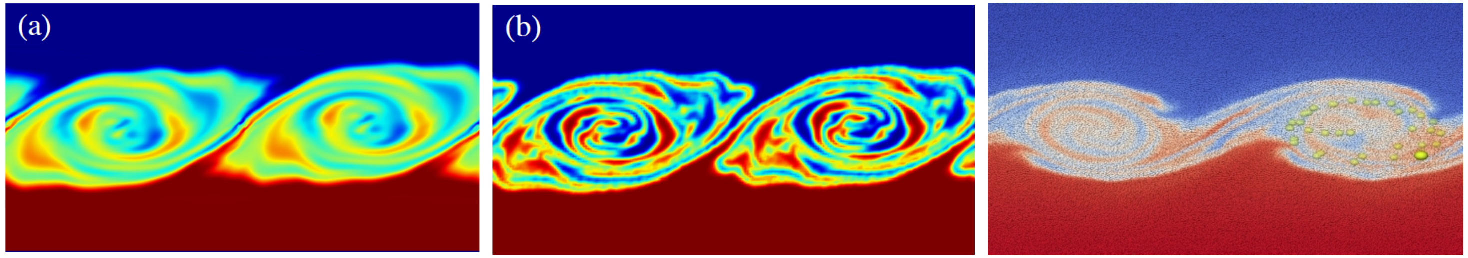
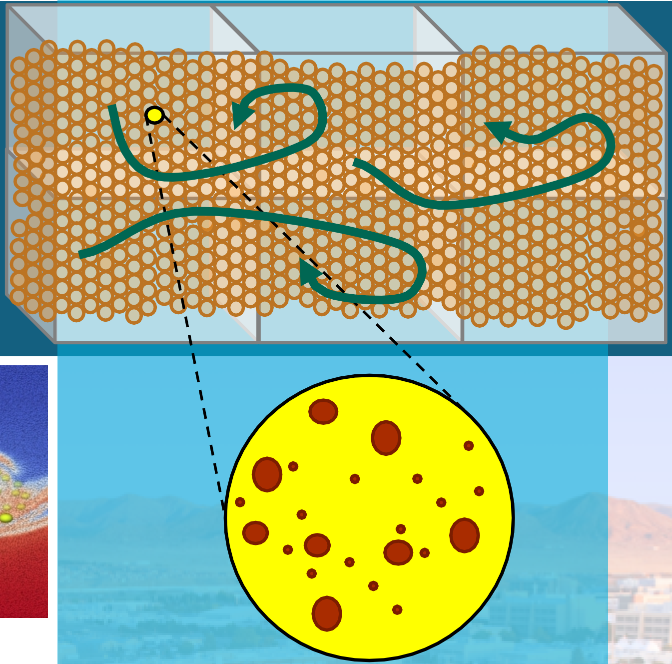
SAND2023-03018C

Application of the Eulerian-Lagrangian Point-Mass-Particle (ELPMP) Discretization to Bridge Regional to Global Impacts of Aerosols





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AMS 2023, Denver, CO

MOTIVATIONS FOR MODELING AEROSOL INJECTION?

Stratospheric aerosol injection (SAI) is the most cost effective means for climate intervention

- potential use for Earth-wide cooling to offset global warming

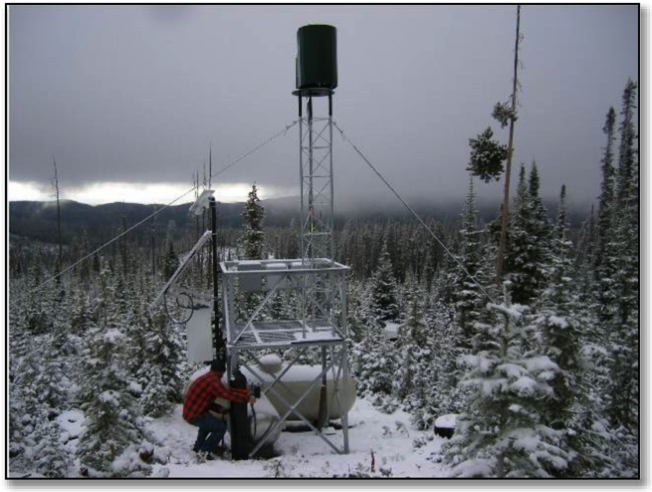
Unilateral cloud seeding likely to continue increasing

- used currently to increase arable lands by inducing precipitation

Widespread impacts of aerosol injection poorly understood

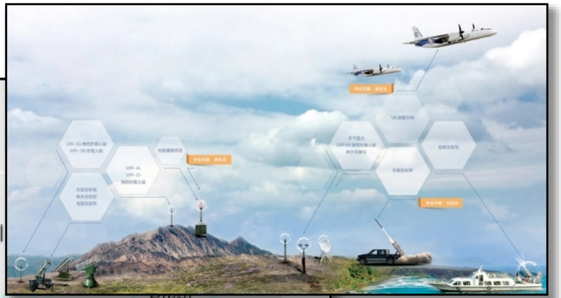
- geopolitical and climate impacts will be complex
  - neighboring country weather patterns may be altered
- long-term effects and aerosol lifetimes are poorly understood

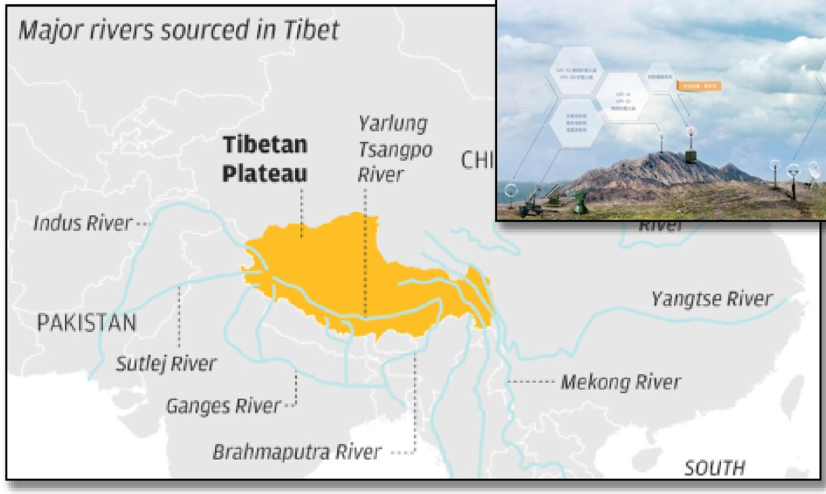
American Meteorological Society official policy statement begins: "Reflecting sunlight would likely reduce Earth's average temperature but could also change global circulation patterns with potentially serious consequences such as changing storm tracks and precipitation patterns."



Silver iodide ground generator
photo credit: North American Weather Modification Council

reproduced from Hunchuck, Ferrari & Cheng, Prologue to the Sky River, *The Avery Review*.

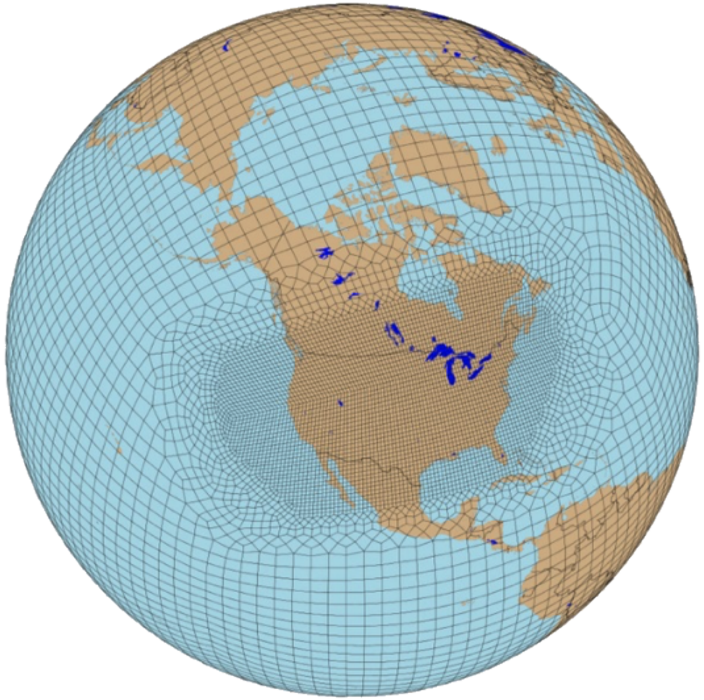




South China Morning Post.

WHY IS IT DIFFICULT TO PREDICT AEROSOL EFFECTS?

- Earth-scale models use kilometer-scale (or 10s of km) mesh resolutions
  - existing methods introduce numerical diffusion error, effectively blending any information on the sub-kilometer scale
- Aerosol injection (SAI or cloud seeding) occurs on the length-scale of meters
  - aerosol development depends strongly on time-temperature-concentration history



E3SM mixed resolution mesh (100 km standard, 25 km high res, O(10 km) regionally refined

Wing-tip seeding generator

End-burning flares

photo credit: North American Weather Modification Council

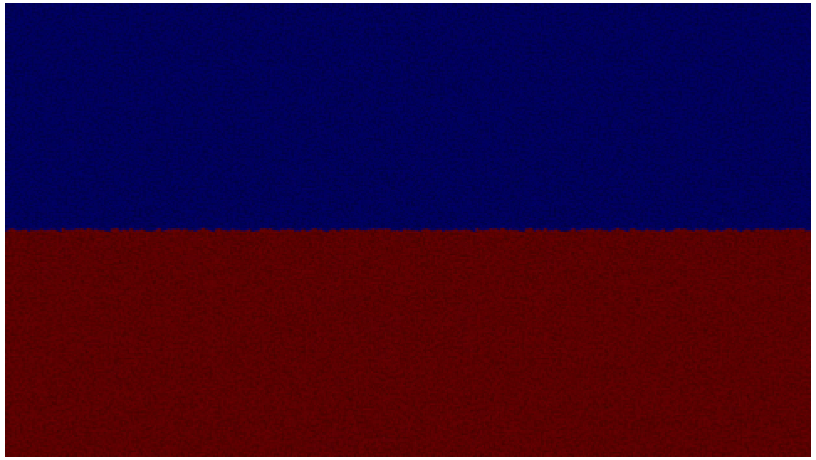
CHALLENGE OF MULTI-SCALE TRANSPORT OF AEROSOLS

Disparity of scales between Earth-models and aerosol injection must be bridged with negligible numerical dissipation and long-time, accurate time-temperature-chemistry information.

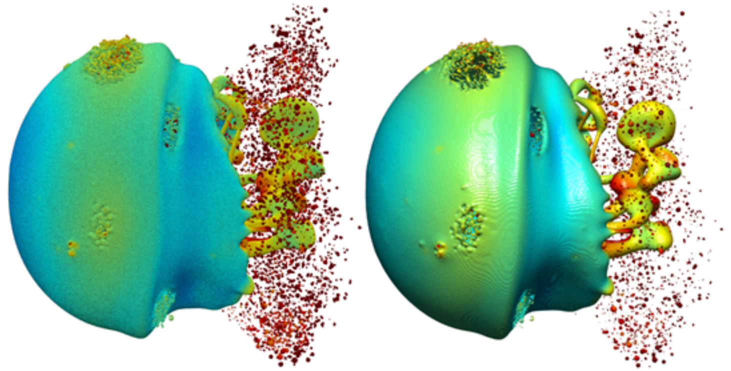
A new approach is required to describe these processes.

- **The Eulerian-Lagrangian Point Mass Particle method is a new multi-physics, multi-scale discretization paradigm that is consistent, conservative, bounded, multi-scale, and free of numerical diffusion errors. It couples with an existing mesh-based solution, such as E3SM, to bridge scales from meter to km.**
    - method has been verified in the context of phase tracking[1] and the advection/diffusion of scalars, and is a major focus of an active ONR Multi-University Research Initiative[2] addressing hypersonic shock/drop interactions.

(a)



(b)



ELPMP applied to: (a) a large-scale Kelvin-Helmholtz instability between hot and cold gas; (b) an atomizing liquid droplet heated by hot gas [1]

1. Wenzel, E.A., and Garrick, S.C., "A point-mass particle method for the simulation of multiphase flows on an Eulerian grid." J. Comput. Phys. 397 (2019) 108835
2. MURI title: Particulate and Precipitation effects on High-speed Flight Vehicles, Prof. Schwartzentruber, PI, FY20-25.

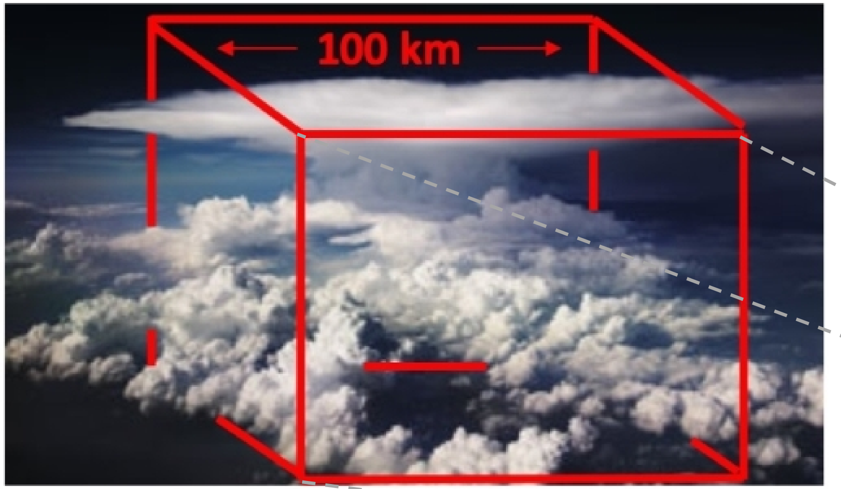
KEY QUESTION

Can the ELPMP method model the seeding, transport, and evolution of aerosols at resolutions far below the Earth-model mesh resolution, enabling the prediction of Earth-scale impacts of atmospheric aerosol injection or cloud seeding in established Earth-system models (here E3SM)?

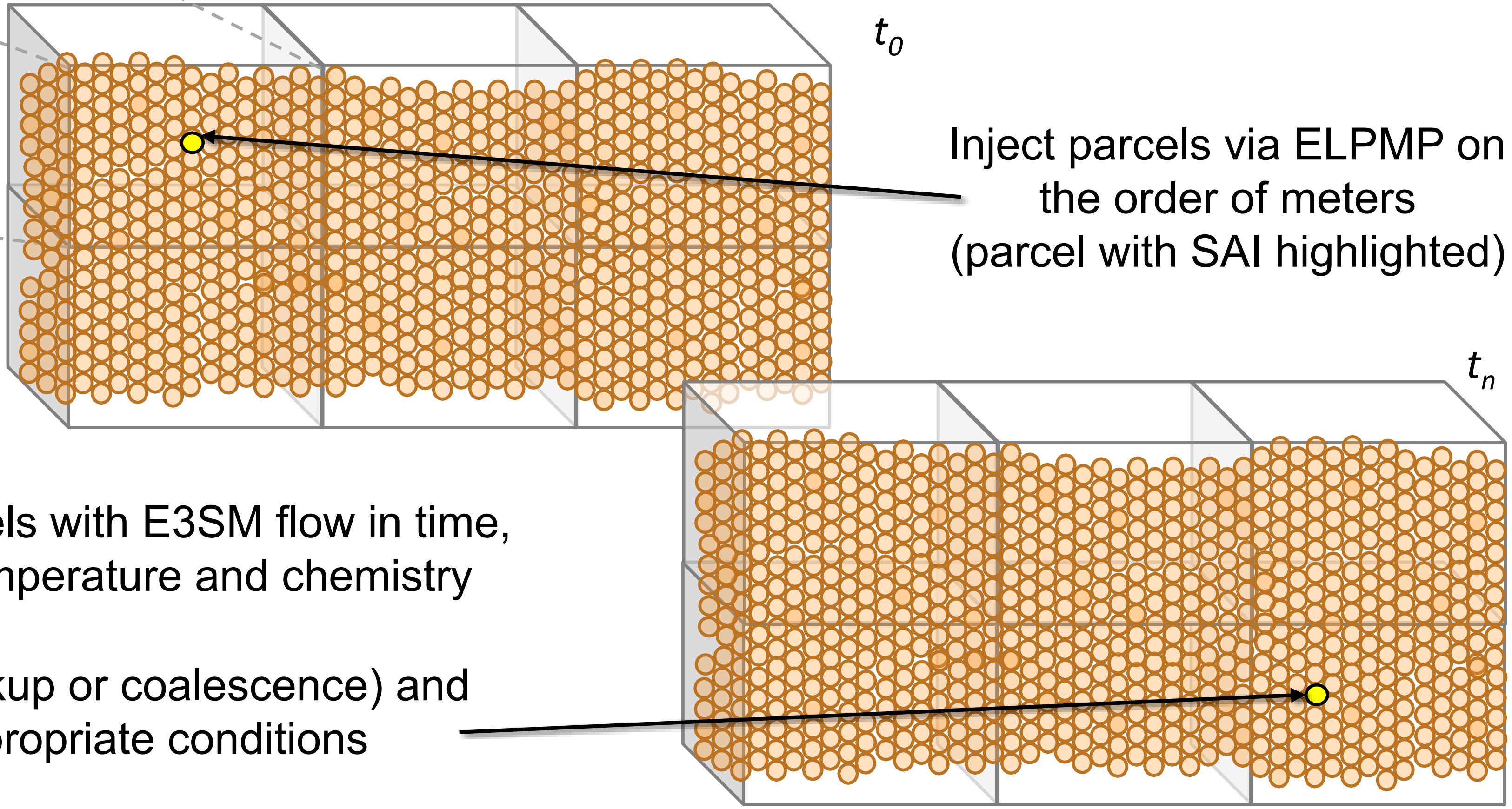
Yes! Coupling of solution has been demonstrated.

PROPOSED SOLUTION - ELPMP + E3SM OVERVIEW

https://e3sm.org/the-e3sm-nonhydrostatic-dynamical-core/



partial E3SM domain with existing flow / temperature solution in time



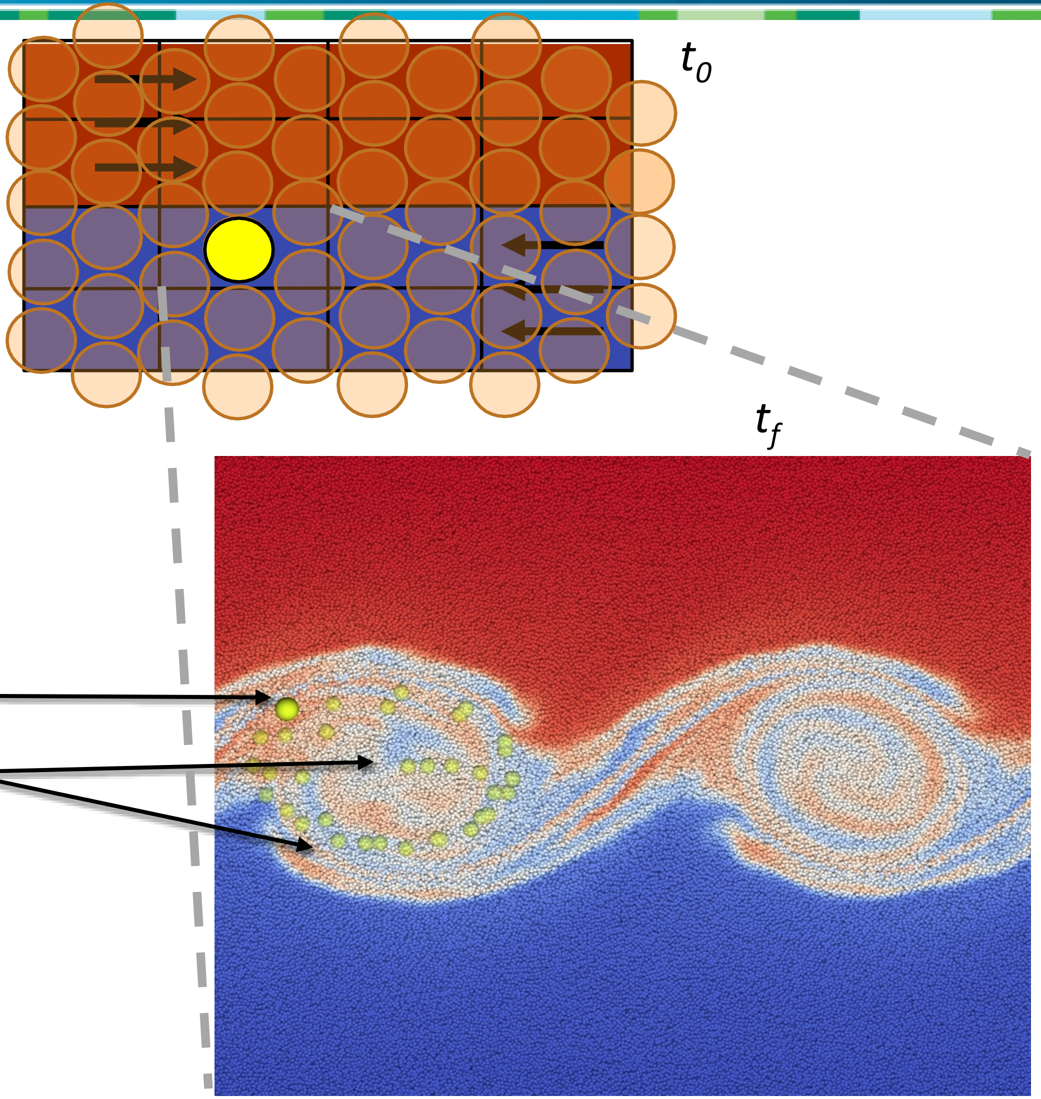
Inject parcels via ELPMP on the order of meters (parcel with SAI highlighted)

Advect ELPMP parcels with E3SM flow in time, conserving mass, temperature and chemistry

calculate physical processes (breakup or coalescence) and chemistry when parcel reaches appropriate conditions

HOW ELPMP ALLOWS DIFFUSION-FREE TRANSPORT

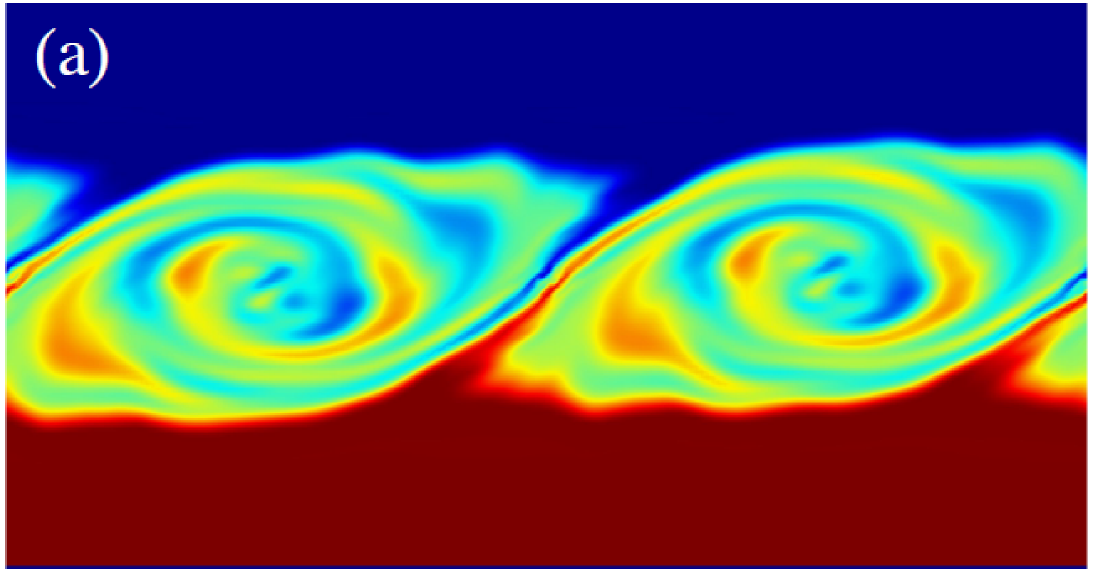
- Consider large-scale mixing of warm air (top) and cool air (bottom)
- Simulation domain is discretized by
  - an Eulerian mesh (equivalent to E3SM)
  - simultaneously by ELPMP parcels responsible for transporting scalars
- At the initial time t_0
  - single fluid parcel (a region) undergoes an aerosol seeding event
  - now carries scalar representations
- Solution at time t_f, after significant mixing and transport
  - the special aerosol-rich particle is enlarged
  - the position of this fluid region at various earlier times is indicated by smaller, translucent spheres
- Scalar carried by the particle suffers zero numerical diffusion and preserves the Lagrangian statistics required to evolve an aerosol.



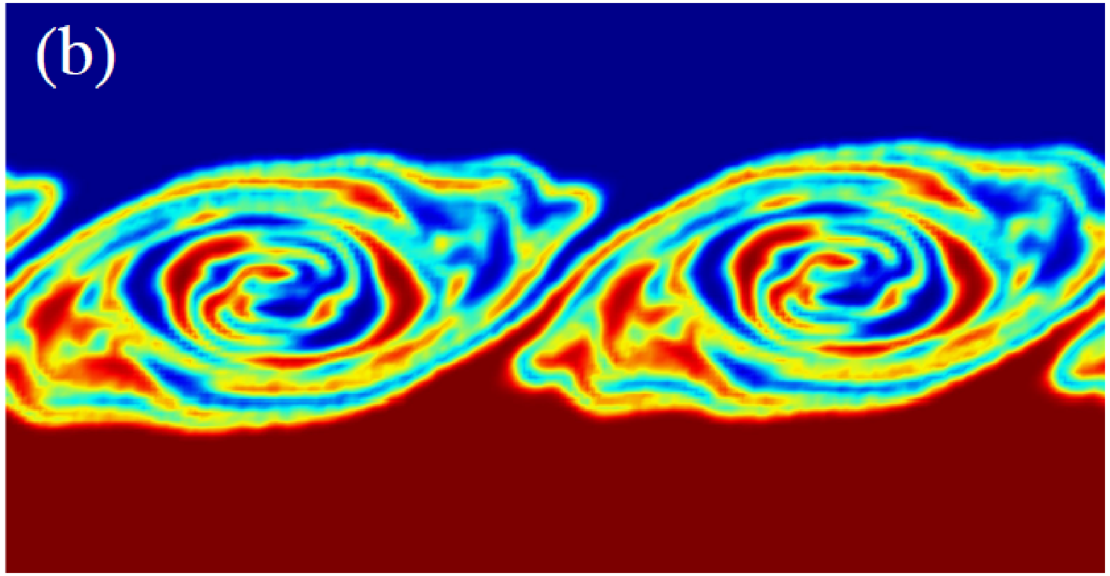
Yellow parcel carries important information, such as the total aerosol mass, the type of aerosol, the initial and current size distribution of aerosol, when and where the aerosol seeding occurred. This is enabled by ELPMP discretization, which allows parcels to never require re-seeding, re-meshing, or re-initialization.

ELPMP VS. EXISTING LOW NUMERICAL DIFFUSION SCHEMES

Existing low diffusion scheme



ELPMP scheme



ELPMP maintains much sharper gradients required to predict physical and chemical processes

- consistent discretization approach guarantees no additional uncertainty due to numerical discretization
  - eliminates a source of mesh-dependent uncertainty that exists with other discretization methods

COMPARISON TO EXISTING TRACER METHODS IN E3SM

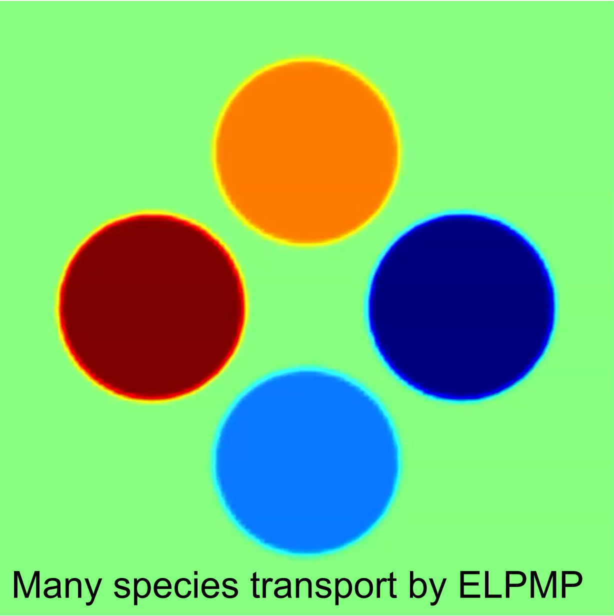
- Semi-Lagrangian advection provides high-fidelity, low-dissipation transport on the mesh scale, but cannot maintain features on the length scales of SAI
- Unique set of properties allow ELPMP to provide a physically consistent bridge connecting seeding events and large-scale transport

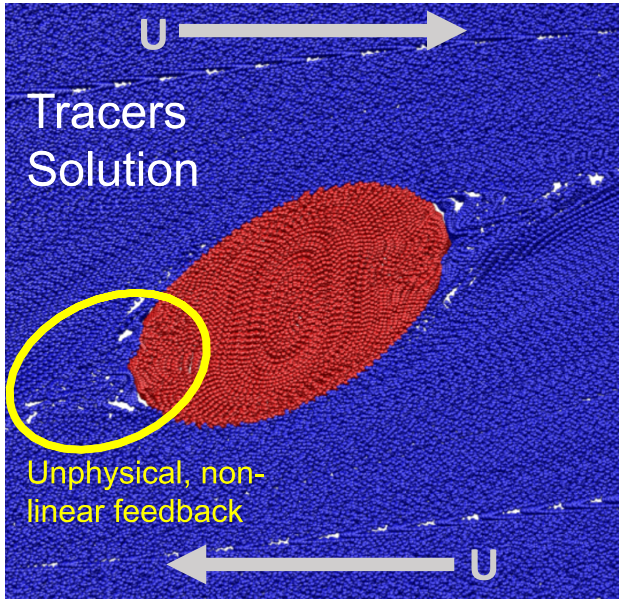
Required mesh-independent properties

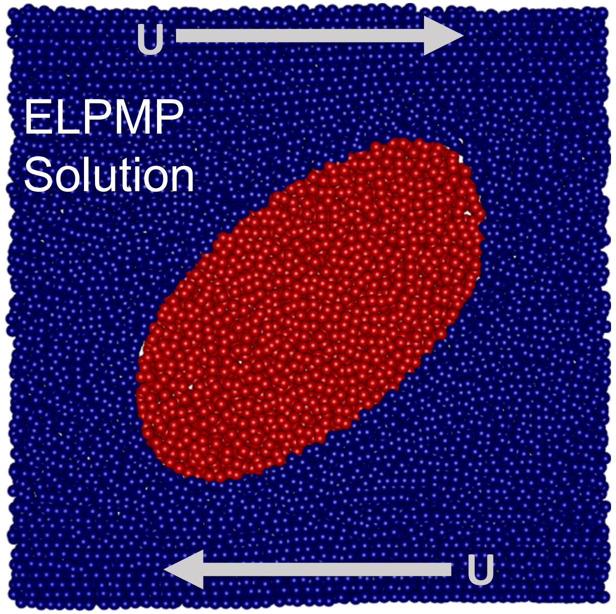
- *Conservation and Scalar boundedness without limiters*
- *"Zero numerical diffusion"*
- *Transport of Lagrangian quantities (general size distributions, discretized size classes, chemistry, etc.)*

Why not classical tracer particles?

- *The goal is to produce physically meaningful coupling across scales*
- *Tracer particles are not a discretization – their evolution is not constrained to satisfy physics*
- *Consider corruption of tracers due to merging/diverging characteristics in shear flow around a droplet, shown below*







ELPMP AEROSOL SEEDING AND EVOLUTION

ELPMP and code coupling:

- New capability allows seeding and evolution of aerosol particle size distribution (PSD) on individual ELPMP parcels
  - function of local conditions
- Spatial transport of aerosol PSD by established ELPMP methodology

Aerosol evolution:

- Aerosol evolution model currently implemented is a nodal approximation to the general dynamic equation
  - more general than what is typically used in an ESM, but may be necessary to describe the complicated SAI process.
  - If appropriate, a simpler phenomenological model can be implemented
- Here physical processes implemented are described by the equations shown to the right for each particle size *k*

In general, ELPMP is agnostic to aerosol modeling strategy (can be incorporated with any existing scheme to increase fidelity of aerosol physics)

Coagulation rate

generation of size k — *destruction of size k*

$$\omega_c^k = \underbrace{\frac{1}{2}\sum_{i=2}^{N_s}\sum_{j=2}^{N_s}\chi_{ijk}\beta_{ij}Q_iQ_j}_{\text{generation of size } k} - \underbrace{Q_k\sum_{i=2}^{N_s}\beta_{ik}Q_i}_{\text{destruction of size } k}$$

collision frequency fcn. (β), *Size-splitting fcn.* (χ), *# density of size i* (Q_i)

Condensation rate

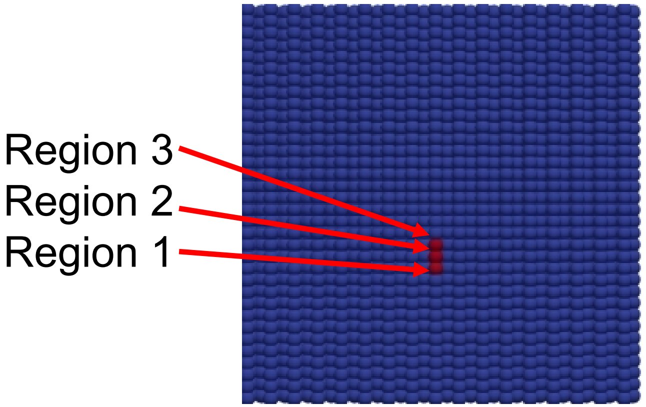
saturation monomer # density ($Q^s_{1,k}$), *saturation pressure* (P_s)

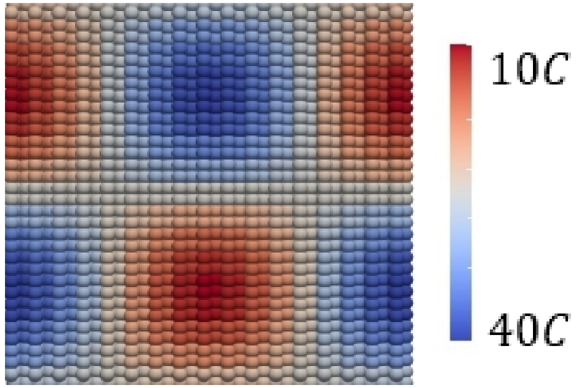
$$Q^s_{1,k} = \frac{P_s}{k_bT}\exp\left(\frac{4\sigma \mathrm{MW}}{RT\rho_c d_k}\right)$$

$$\omega_s^k = \begin{cases} \frac{v_m}{v_k - v_{k-1}}\beta_{1,k-1}\left(Q_1 - Q^s_{1,k-1}\right)Q_{k-1} & \text{if } Q_1 > Q^s_{1,k-1} \\ -\frac{v_m}{v_{k+1} - v_k}\beta_{1,k+1}\left(Q_1 - Q^s_{1,k+1}\right)Q_{k+1} & \text{if } Q_1 < Q^s_{1,k+1} \\ -\frac{v_m}{v_{k+1} - v_k}\beta_{1,k}\left(Q_1 - Q^s_{1,k}\right)Q_k & \text{if } Q_1 > Q^s_{1,k} \\ \frac{v_m}{v_k - v_{k-1}}\beta_{1,k}\left(Q_1 - Q^s_{1,k}\right)Q_k & \text{if } Q_1 < Q^s_{1,k} \end{cases}$$

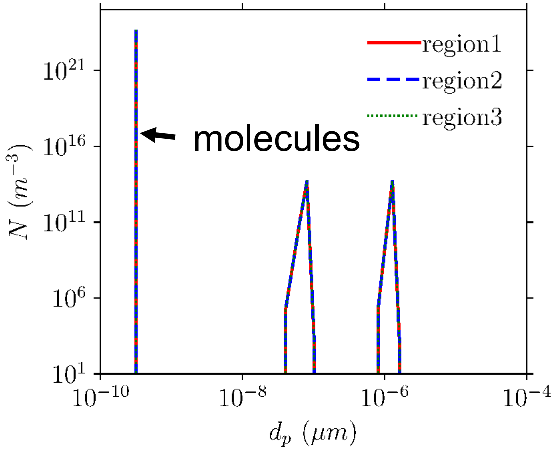
RESULTS: TIME EVOLVED AEROSOL EVAPORATION

- Particles are seeded across an isolated region. The seeded aerosol is bi-modal.
- Decompose the seeding event into three sub-regions (1, 2, and 3)
- As time progresses, slightly different conditions result in divergence of the PSDs
  - here observe primarily evaporation in region 1

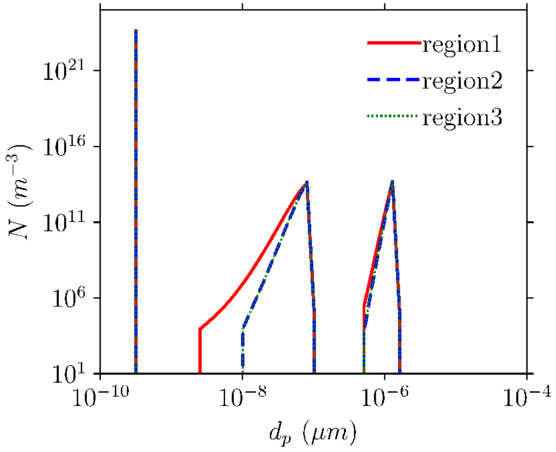




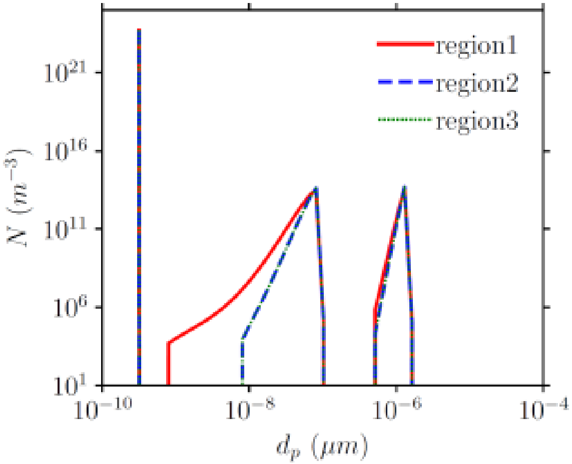
Temperature at time of seeding



Initial particle size distribution (seeded aerosol)

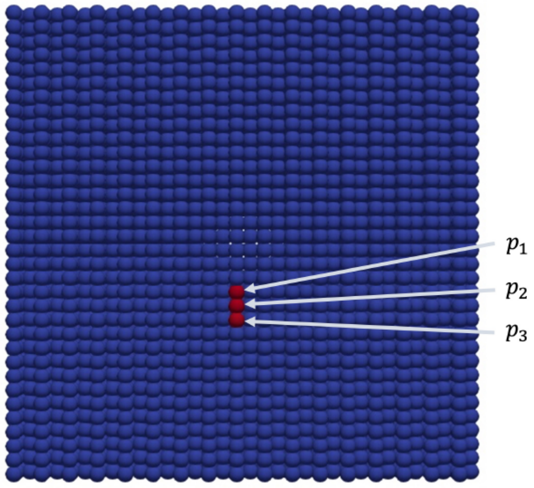


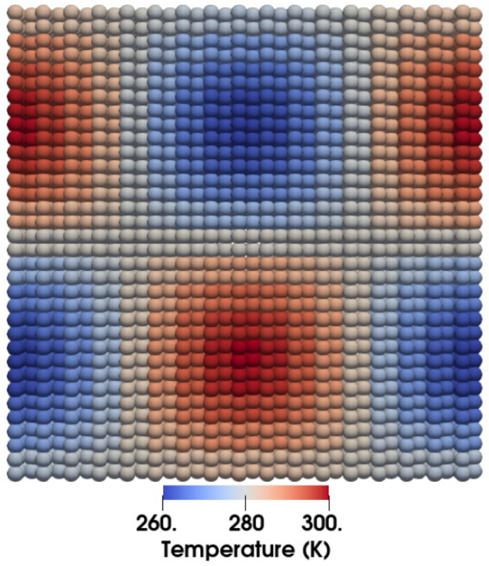
Time-evolved aerosol:
Warmer region 1 evaporating more quickly



+ Δt

RESULTS: INERT TRANSLATED AEROSOLS

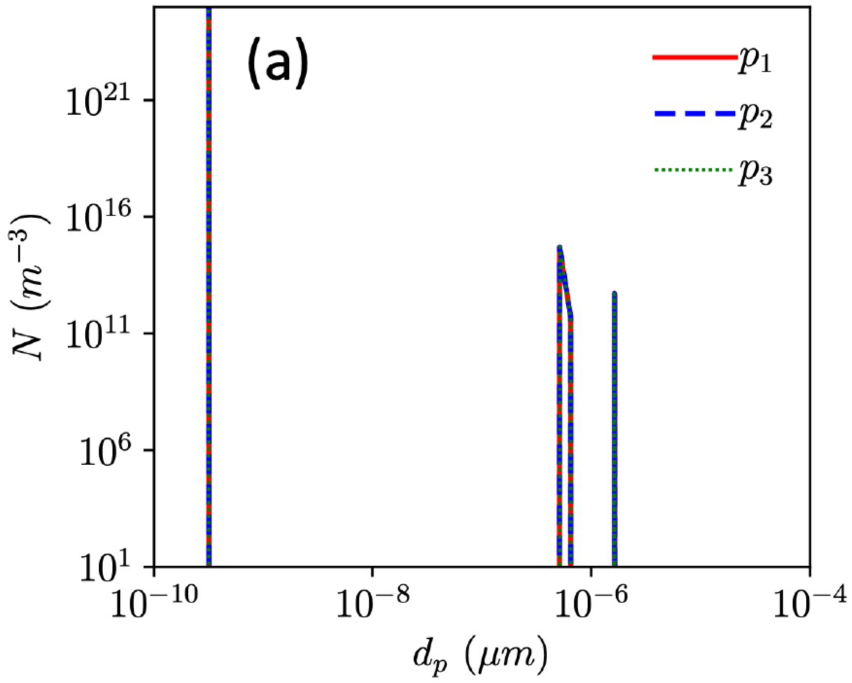


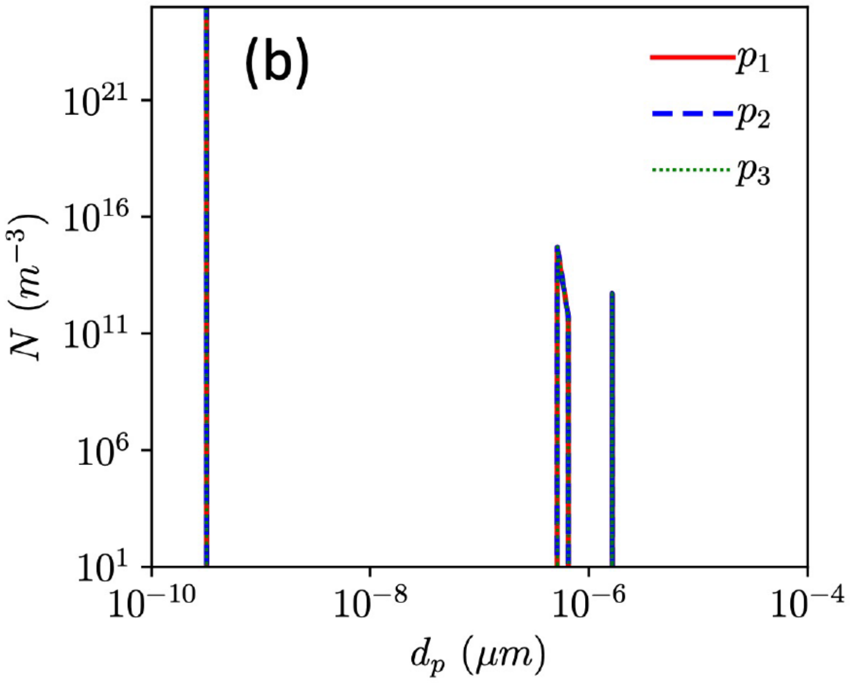


Temperature at time of seeding

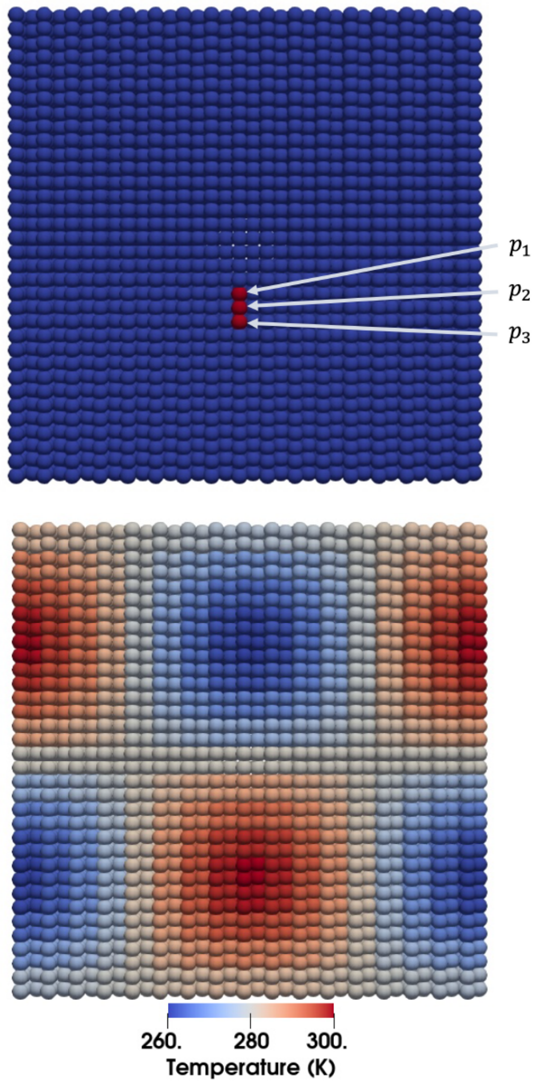
Inert translation verification test:

- particle size distribution unmodified after complete translation across domain
  - bounded and conservative due to ELPMP transport without remeshing





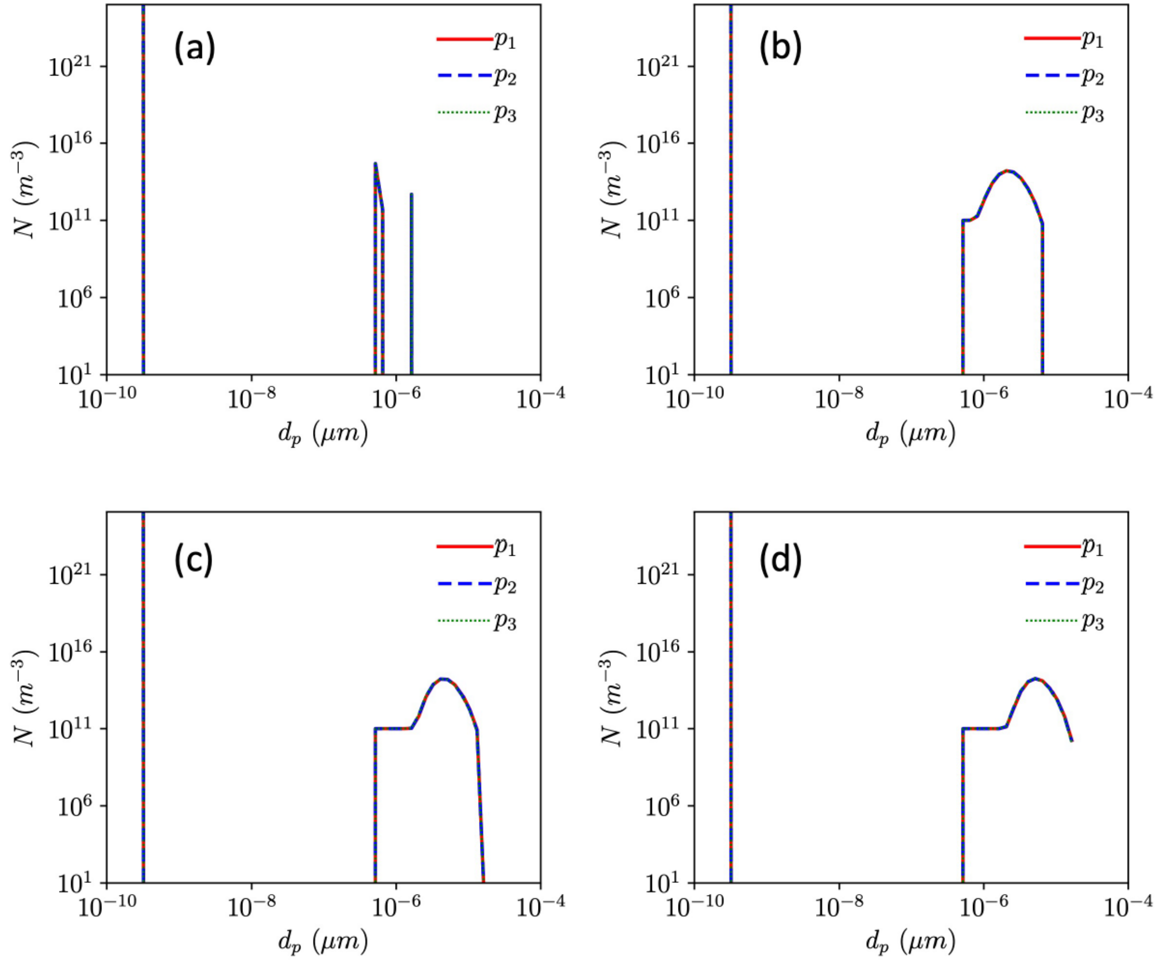
RESULTS: ACTIVE TRANSLATED AEROSOLS



Temperature at time of seeding

Active translation test:

- with aerosol dynamics active, particles grow in time
  - primarily condensation
  - some coagulation



CONCLUSIONS & FUTURE WORK

ELPMP demonstrated for prototypical SAI problem

- long-timescale climate implications can be investigated as particles are free of numerical diffusion
- because particle history is known, attribution is possible

Next step is to implement in a larger problem to determine computational cost at Earth scale

Future includes wide applicability to any problem where particle-scale information must be preserved over disparate length- and time-scales to capture the physics

- algae blooms from river runoff into the sea
- dispersion of toxins (chemical, biological or radioactive)
- targeted drug delivery with minimized dilution and impact to healthy cells

Acknowledgements

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