LEM/ODT Multiphase Applications

Alan Kerstein
Consultant
Danville CA, USA

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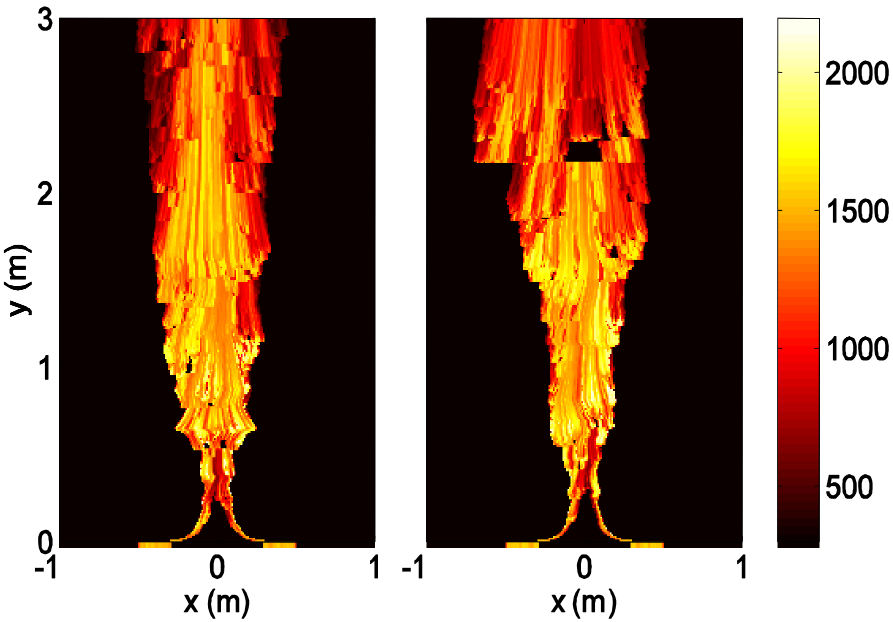
MetStröm Short Course at BTU

Outline of presentation

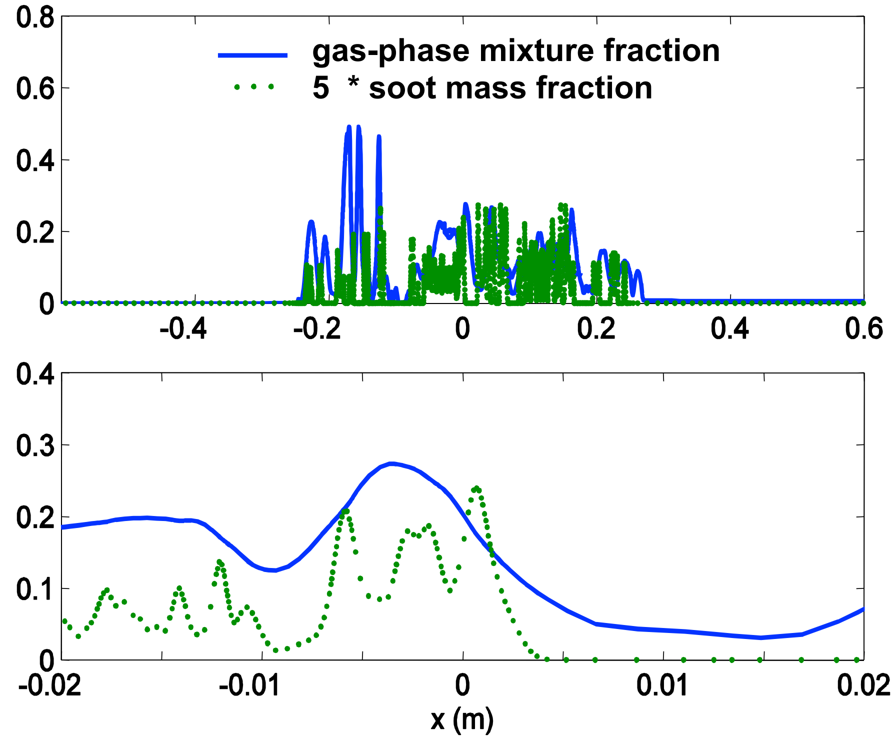
- Sooting plume
- Wall deposition
- Clustering

Adaptive-mesh ODT was used to simulate an ethylene-air sooting plume



An effect captured by spatial advancement:

The spatial continuity equation induces narrowing of temperature fields above the inlet due to lateral inflow balancing vertical buoyant acceleration



The adaptive mesh efficiently resolves small features – the new code allows different meshes for different properties, e.g., high-Sc scalars, enabling a big time-step increase

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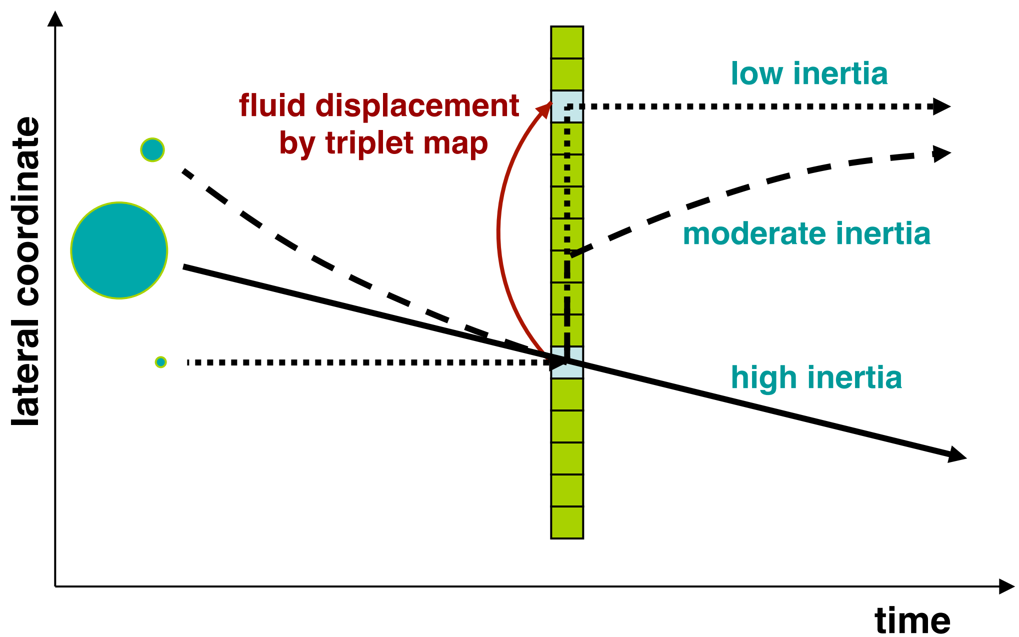
A particle-eddy interaction couples entrained particles to fluid motion (one-way coupling)

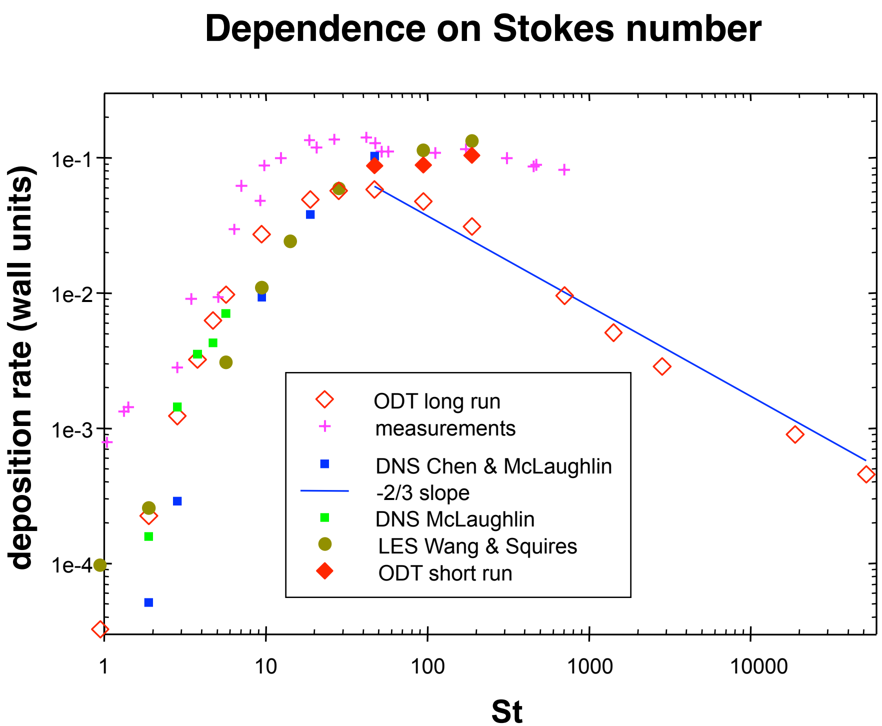
- In ODT, motion and velocity are distinct, though dynamically consistent
- Particles respond, via drag law, to motion (in ODT, eddy events)
- Because ODT eddies are instantaneous
  - an internal (eddy) time coordinate for particle-eddy interaction is introduced
  - this involves another free parameter, relating the interaction time to t

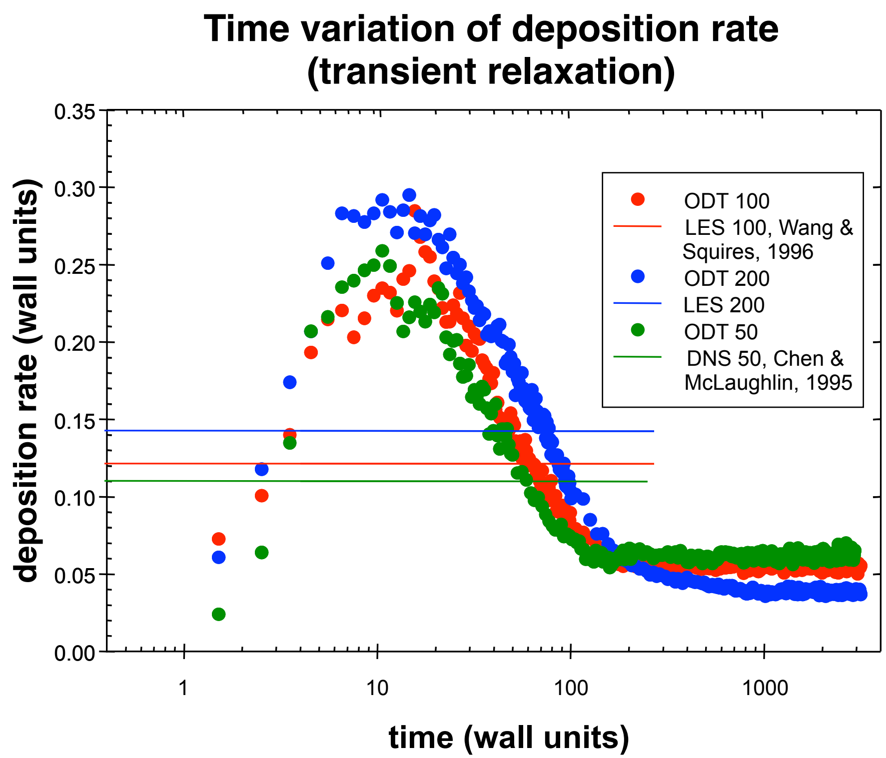


- **Eddy-time integration determines a trajectory 'jump condition' representing the eddy-induced trajectory change, adjusted so future motion is not double-counted**
- **Ballistic motion remains linear**
- **Zero-inertia (no-slip) particles follow the fluid**
- **Particle-fluid relative motion is realistic, though absolute motion is discontinuous**

Measured and 3D-simulated wall deposition is reproduced, and a new regime is found

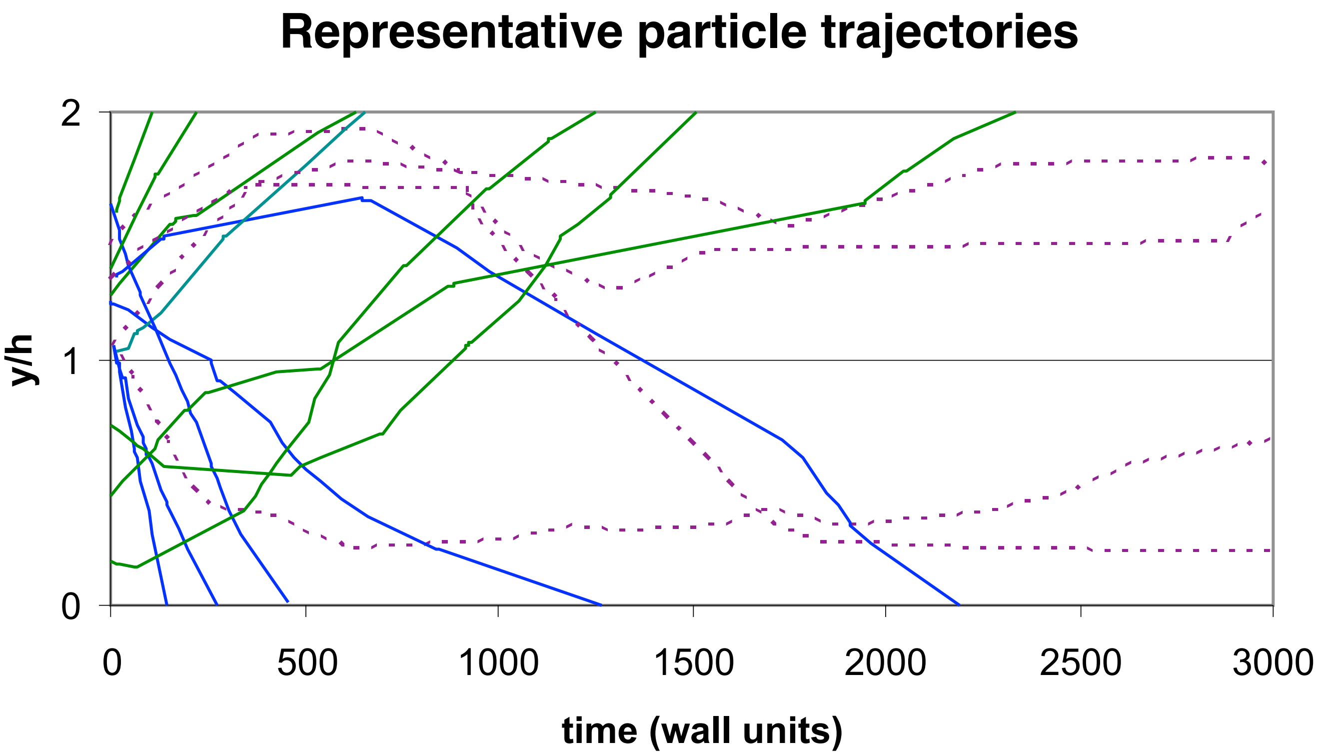
Wall deposition in *turbulent channel flow* (the ODT domain is wall-normal)





Comparisons suggest that measurements and 3D simulations are seeing initial transients rather than the late-time regime indicated by ODT

Early deposition is ballistic, late deposition is Stokes-number dependent



The -2/3 power dependence on St is explained by a simple scaling analysis. Closure analysis gives a much milder decline – and is 'validated' by data that mainly reflects initial conditions!

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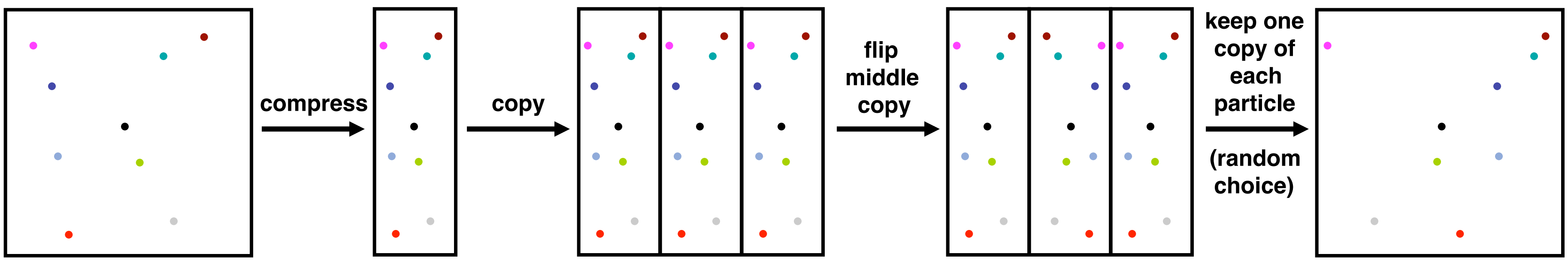
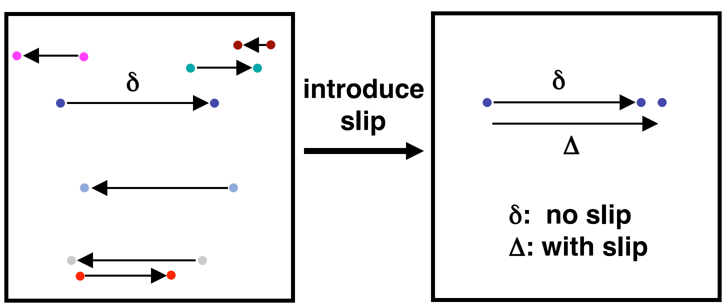
Using map-based advection, a 3D Lagrangian (grid-free) low-inertia particle advancement model is formulated

Displacement of slip-free (zero-inertia) particles by a 3D triplet map:



Fluid displacements δ are multiplicatively incremented to represent particle inertia:



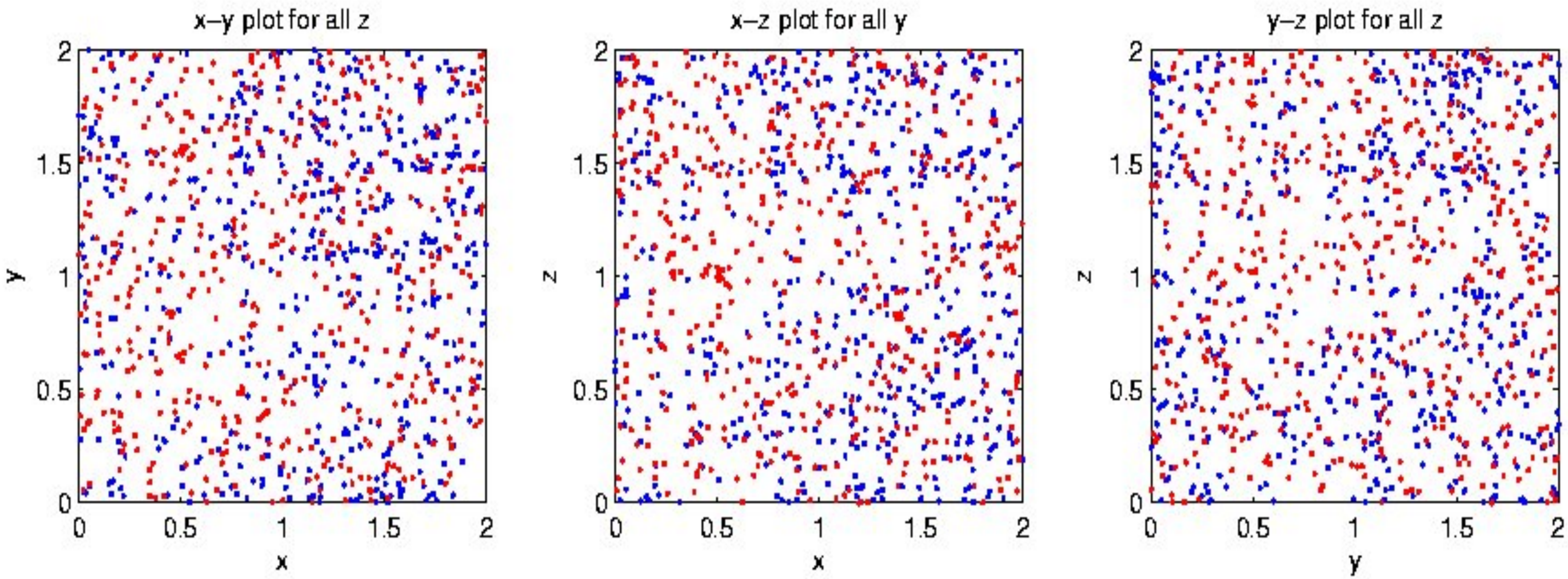
<u>Inertia model</u>:

$$\Delta = (1+S)\,\delta$$

S<<1 is the model analog of Stokes number,
St = [particle response time] / [flow time]

If polydisperse, S can be different for each particle

For nonzero S, clustering is observed

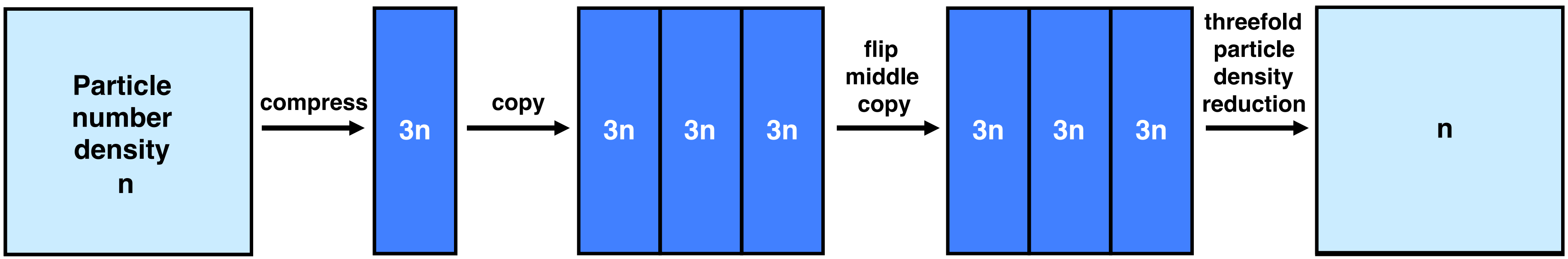


Simulation:

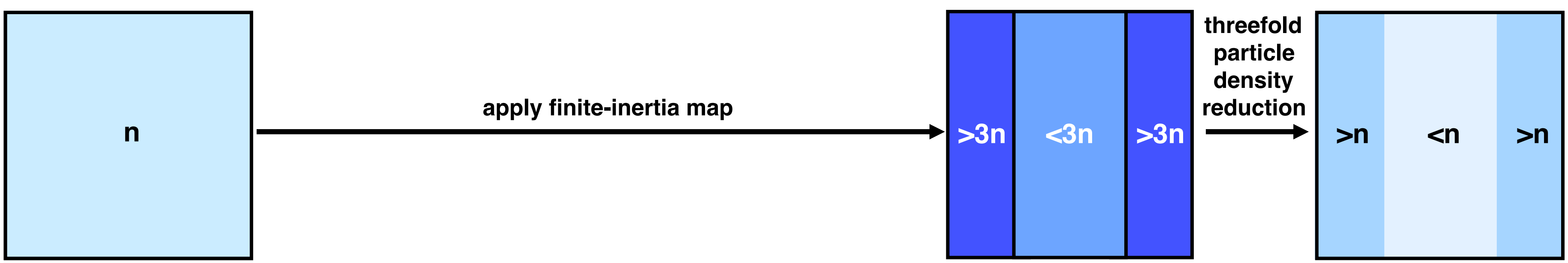
- Cubic domain, map size = domain size
- Maps in x, y and z directions, randomly positioned
- Periodic boundary conditions
- Iterated to statistical steady state
- Red, S = 0; blue, S = 0.1

Continuum interpretation: slip induces fluctuations in an initially uniform particle-density field

Zero inertia: uniform multiplicative compression, compensated by number reduction



Non-zero inertia: non-uniform compression, inducing particle-density fluctuations



Exact analysis yields parameter dependence of a clustering metric

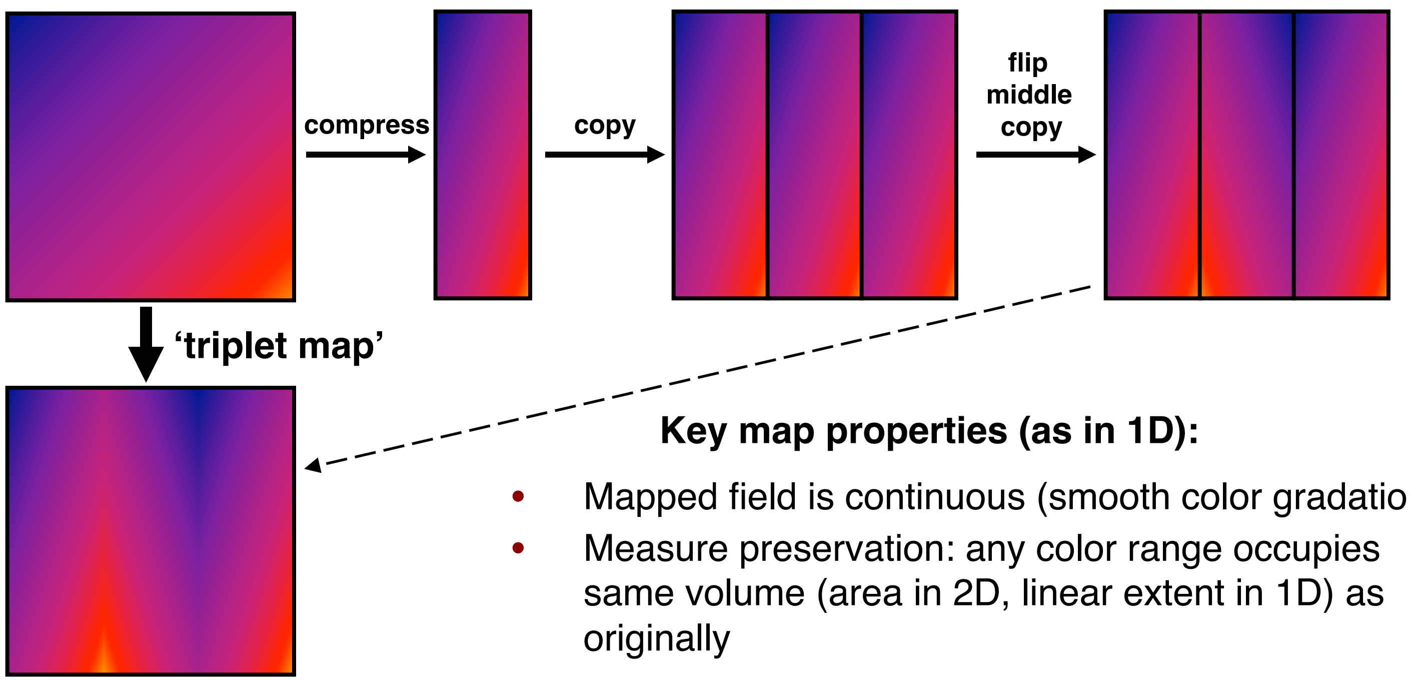
- Radial distribution function (RDF) g(r):
  - Likelihood of finding a particle at a distance r from a given particle
  - Normalized so g=1 for statistically independent particles

- Prediction:
  - $g \sim r^{-cS_1 S_2}$ for particles, labeled 1 and 2, with different S values
  - Valid for a restricted r range dependent on $|S_1 - S_2|$ and flow structure
  - Previously obtained heuristically and with DNS (e.g., Chun et al. 2005)

Significance (1): the analysis elucidates the geometrical basis of clustering

- Slip proportionality to displacement leads to the power-law r dependence of g
- Clustering is a second-order effect (bilinear in S) for <u>continuous</u> maps

Application of the advective map to an arbitrary continuous field:



Key map properties (as in 1D):

- Mapped field is continuous (smooth color gradation)
- Measure preservation: any color range occupies same volume (area in 2D, linear extent in 1D) as originally

Significance (2): model properties suggest an efficient algorithm for simulation of particle motion

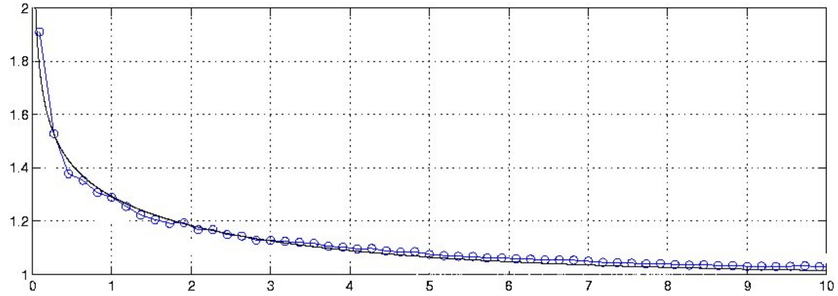
- Motivation: turbulence enhancement of droplet coalescence
  - Collision rates are proportional to n^2 locally, hence greater if n fluctuates
  - Gillespie's (1975) Stochastic Simulation Algorithm (SSA) captures collision randomness but not clustering effects
  - Map method captures both at no greater cost

- Application in progress (with Steve Krueger, U. of Utah): rain formation
  - Each raindrop that falls gathers a million others (snowball effect)
  - The one per million droplet that grows big enough to fall is rate controlling
  - Rare events (rapid coalescence) dominate, so need detailed simulations

- Future work: Embed this model in a simulation of larger-scale processes (explained shortly)

Benchmarked the 3D model using DNS data, will imbed it in a multi-process cloud representation

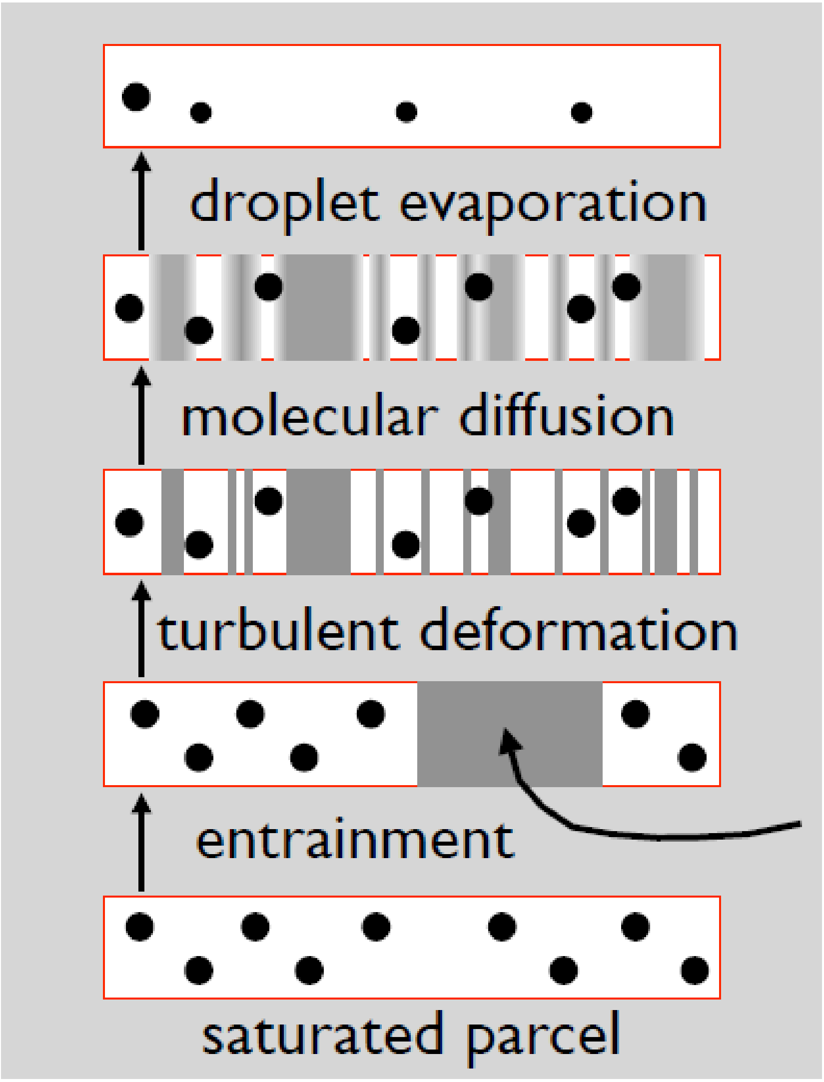
- Benchmarking:
  - Have tuned to match monodisperse (below) and bidisperse RDFs.
- Cloud application: simulate small scales in a 1D map-based scheme
  - Krueger's 1D EMPM captures condensational growth in fluctuating humidity
  - Coalescence variability is important at smaller scales
  - Therefore structure the 1D scheme as a stack of cubes; 3D evolution in each
  - Sedimentation and droplet collision phenomenology have been incorporated



g vs. r/[Kolmogorov microscale] for St=0.136.
Symbols, model; smooth curve, functional fit to DNS (Reade and Collins, 2000).

The 1D Explicit Mixing Parcel Model (EMPM) incorporates entrainment and phase change into LEM

LEM: 'turbulent deformation' consists of triplet maps, randomly placed, with sizes sampled from a distribution that idealizes the energy spectrum of turbulence



EMPM includes all the indicated processes, but needs subgrid 3D Lagrangian droplet advancement to capture droplet clustering and coalescence at scales not resolved by LEM

EMPM flow states resemble (and help interpret) measured data traces

EMPM water vapor and temperature fields