Map-Based Advection, Low-Dimensional Simulation, and Superparameterization

Alan Kerstein
Combustion Research Facility
Sandia National Laboratories
Livermore, CA

Multiple Scales in Fluid Dynamics and Meteorology
International MetStröm Conference, Berlin, Germany

June 8, 2011

The U.S. Department of Energy Laboratory Directed Research and Development Program at Sandia National Laboratories supported this work. Sandia is a multi-program laboratory operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

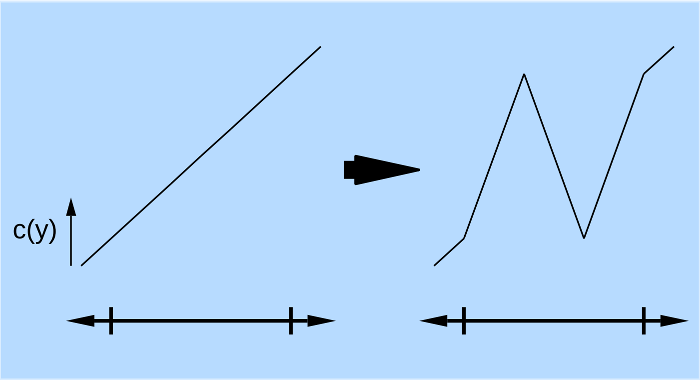
Outline of Presentation

- Turbulence simulation using map-based advection
- A simple case with surprising behavior
- Multi-scale modeling of cloud droplet evolution mechanisms
- 1D simulation of turbulent flow
- Cloud modeling applications
- Superparameterization using map-based advection
- Concluding remarks

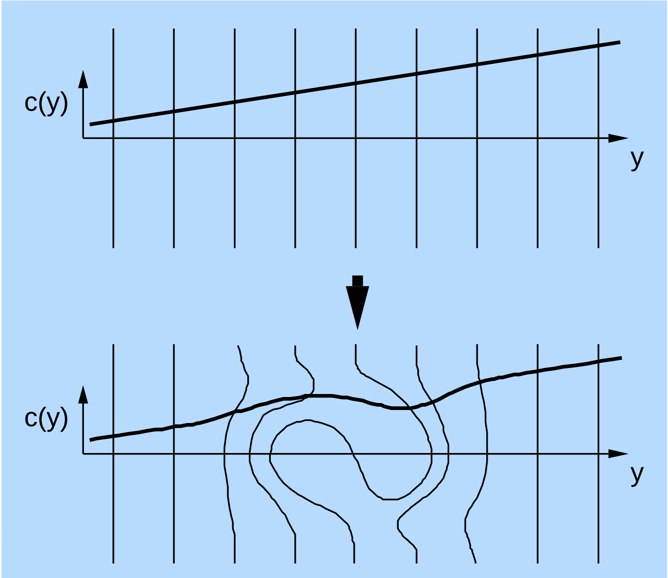
What is map-based advection?

- In Lagrangian numerical schemes, it is flow advancement by v Δt displacement of mesh cell boundaries
- Here, it is a physical modeling construct for reduced representation of turbulent flow that is useful for
  - Low-dimensional flow simulation
  - Cost-effective 3D flow simulation in some cases
  - Substructure simulation within superparameterization frameworks

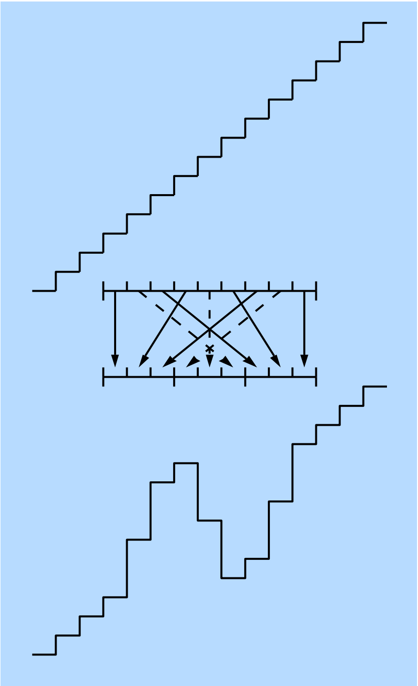
Advection is modeled as a sequence of *triplet maps* that preserve desired advection properties, even in 1D



The triplet map captures compressive strain and rotational folding effects, and causes no property discontinuities



This procedure imitates the effect of a 3D eddy on property profiles along a line of sight



The triplet map is implemented numerically as a permutation of fluid cells (or on an adaptive mesh)

The triplet map (1D eddy)

- moves fluid parcels without intermixing their contents
- conserves energy, momentum, mass, species, etc.
- reduces fluid separations by at most a factor of 3
- Conjecture: It is optimal in this respect

There are different ways to specify the map sequence during a simulation

- Linear-Eddy Model (LEM): Eddy occurrences and properties (size, location) are sampled from fixed distributions
  - Predicts turbulent mixing based on specified turbulence
  - Evolves scalar profiles but not velocity

- One-Dimensional Turbulence (ODT): Eddy sampling is based on the flow state evolved by the model
  - Predicts turbulence evolution after setting sampling parameters
  - Input is the flow configuration (ICs, BCs)

- In either model, the eddies (instantaneous maps) punctuate continuous-in-time advancement of molecular-diffusive transport, chemistry, etc. For example (temporal advancement):

$$\theta_t = \kappa\theta_{yy} + \text{'eddies'} \qquad\qquad u_t = \nu u_{yy} + \text{'eddies'}$$

scalar **velocity component (ODT only)**

Outline of Presentation

- Turbulence simulation using map-based advection
- A simple case with surprising behavior
- Multi-scale modeling of cloud droplet evolution mechanisms
- 1D simulation of turbulent flow
- Cloud modeling applications
- Superparameterization using map-based advection
- Concluding remarks

Sandia National Laboratories

CRF

Simple configuration: one eddy size, sinusoidal initial scalar – what happens?

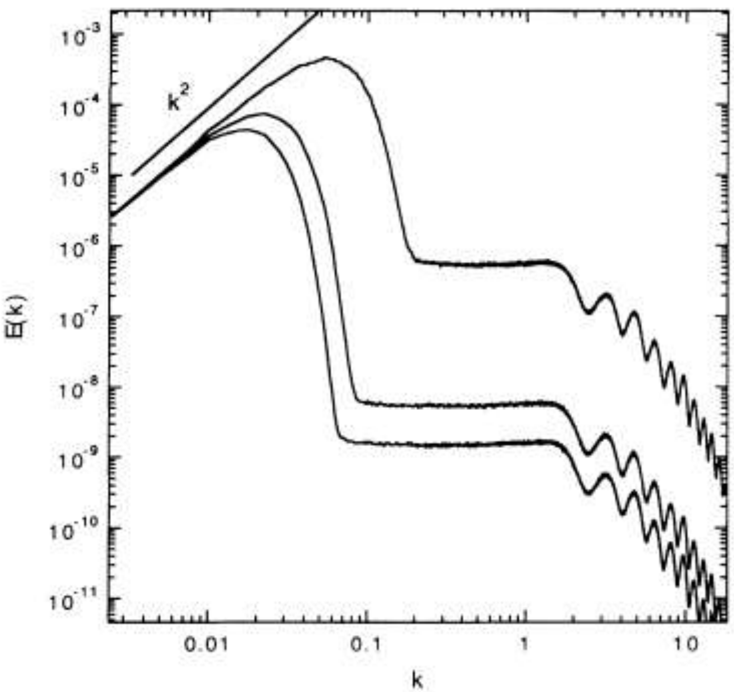
Evolve $\theta_t = \kappa\theta_{yy}$ + ‘eddies’ with

- $\theta(y,0) = \sin(2\pi y/L)$
- Randomly placed triplet maps, all size L
- High map frequency (eddy transport >> κ)
- Domain size >> L, periodic boundary conditions

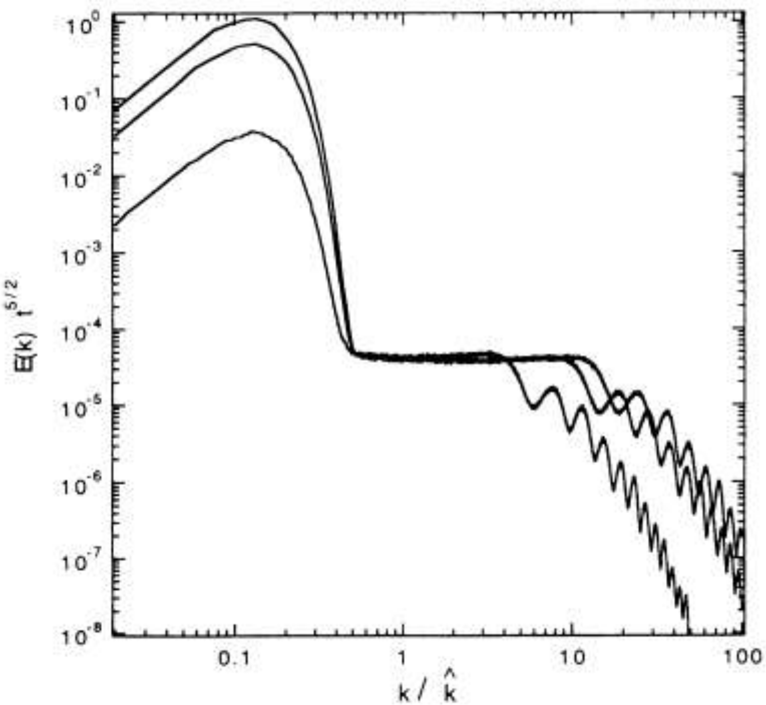
What is the time evolution of

- Scalar variance?
- Scalar power spectra?

The result was surprising (amazing!) – then an explanation was found



top to bottom: increasing t



analysis predicts the collapse
seen in this scaled plot

Pipe flow measurements motivated by these results illustrate the cause of this behavior

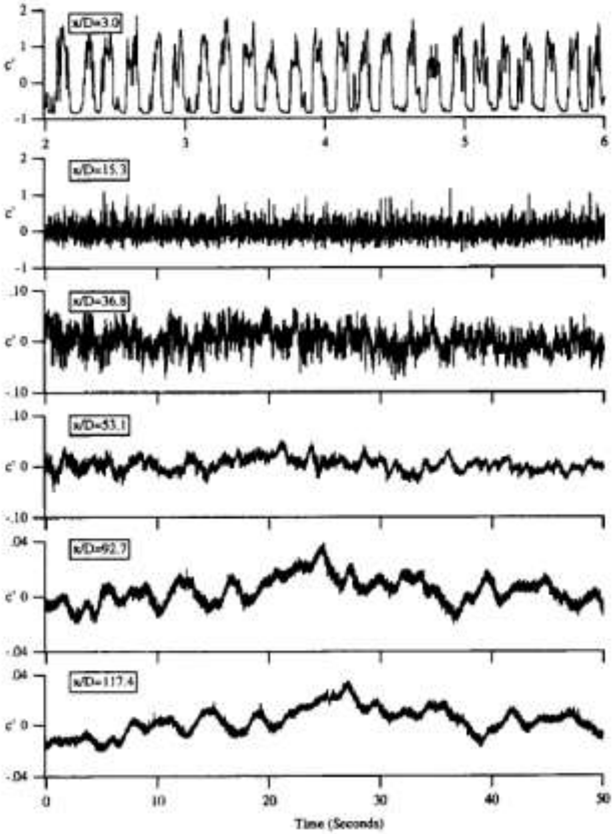
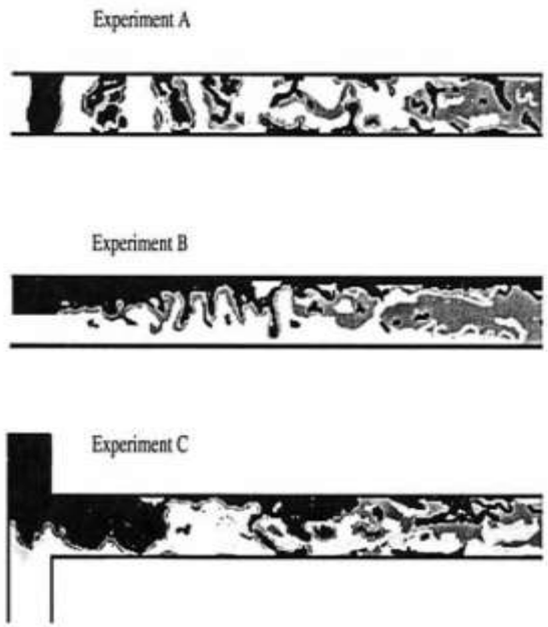


Figure 3. Time series of measured scalar field at the center of the pipe for experiment A.

A 4-s period is shown for $x/D = 3.0$ to show the idealized inlet condition achieved. At all other locations a 50-s time series is shown.



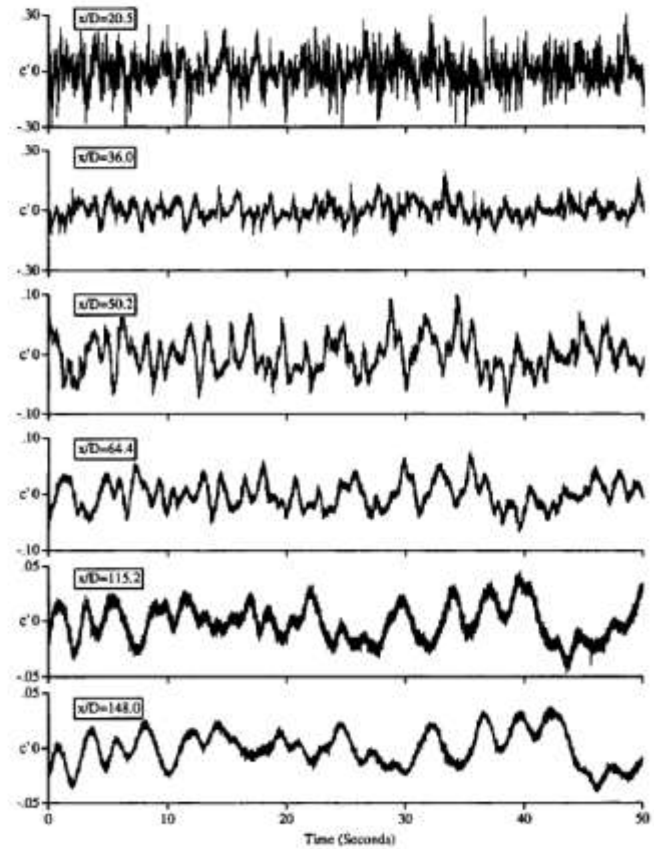
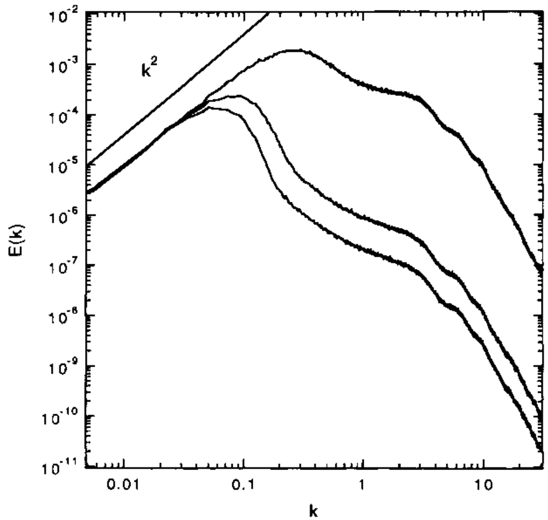
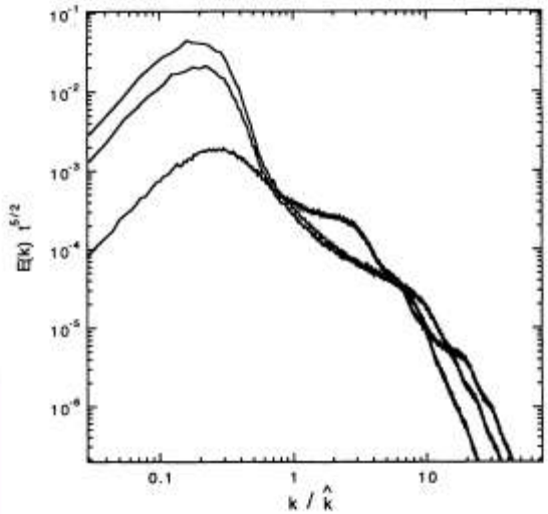


Figure 11. Time series of measured scalar field at the center of the pipe for experiment C.

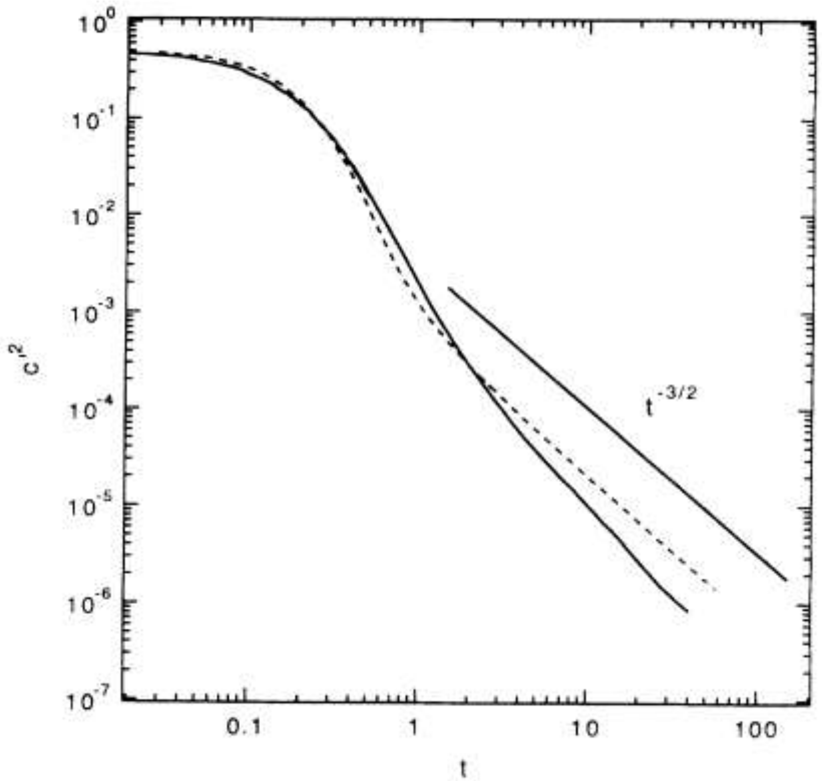
Guilkey, McMurtry, and Klewicki, 1997

Simulations were performed for a ‘pipe-like’ map-size distribution





Analysis predicts $t^{-3/2}$ scalar-variance decay



— — one map size
—— pipe-like size distribution

Scalar power-spectrum measurements exhibit the predicted features

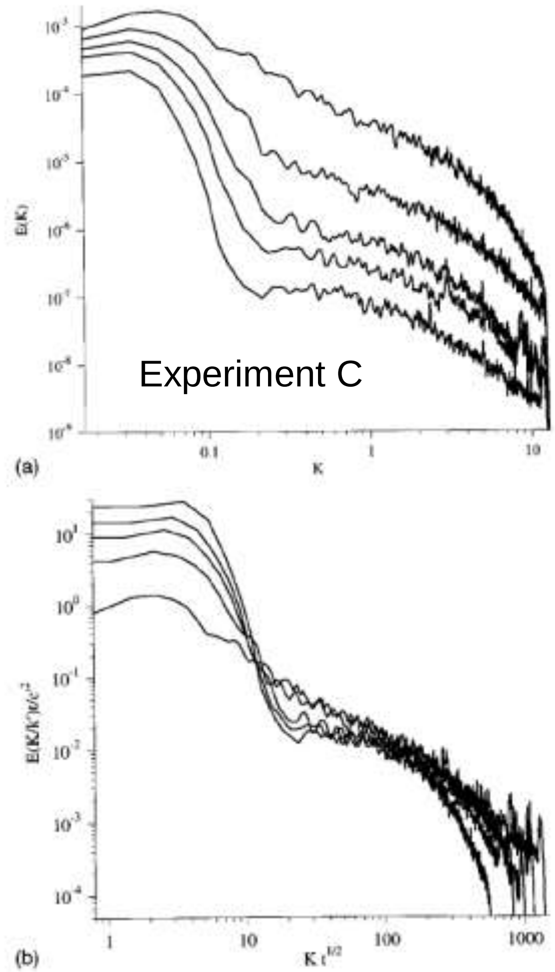


FIG. 5. (a) Power spectral densities of scalar fluctuations, experiment 2. Axial locations (from top to bottom) are $x/D=20.5$, 36.0, 50.2, 64.4, and 90.3. (b) Spectra subject to "equilibrium" range scalings, indicating self-preserving behavior.

Pipe measurements show a transition from exponential to power-law variance decay

Brodkey, 1966, ‘confirmed’ exponential decay (Corrsin’s batch-reactor analysis) to x/D = 30

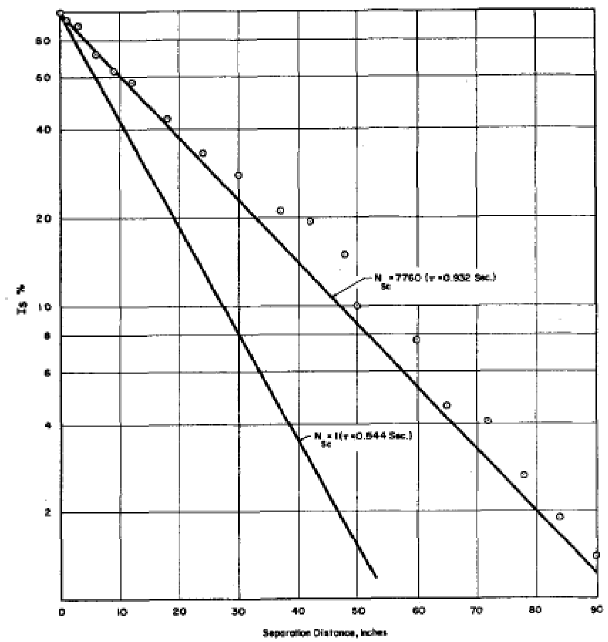
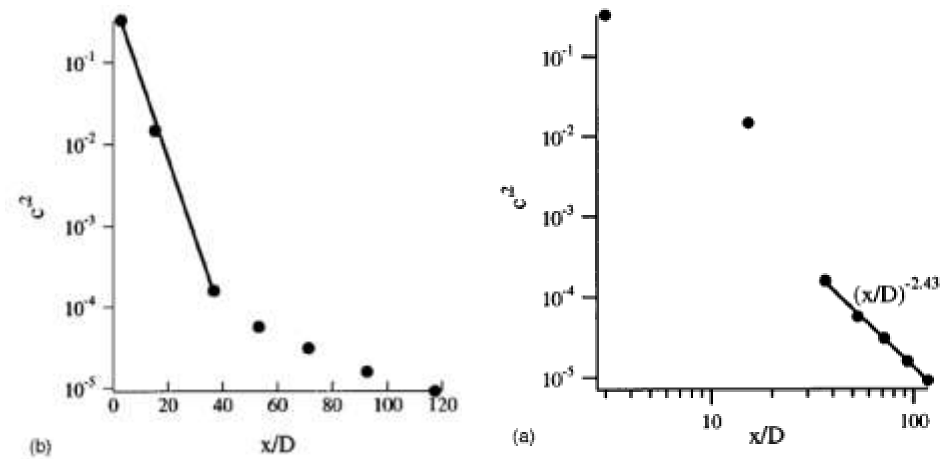
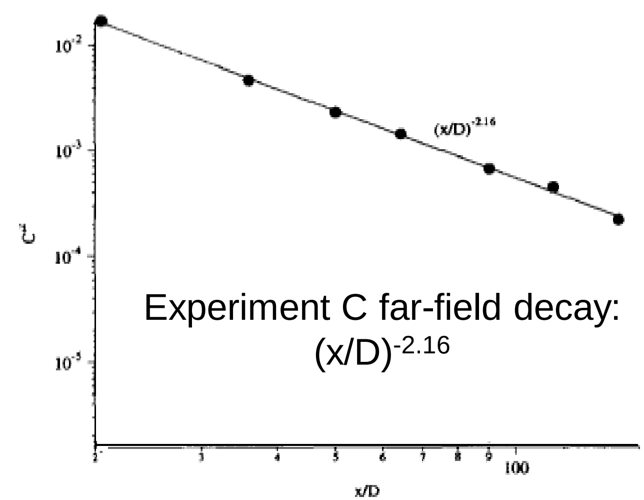


Fig. 1. Intensity of segregation.

Experiment A: near-field exponential, far-field $(x/D)^{-2.43}$





Experiment C far-field decay: $(x/D)^{-2.16}$

Near-field decay depends on initialization – <u>the only robust result is the far-field power law</u> (with a non-universal exponent)

Don’t trust your intuition about turbulent mixing!

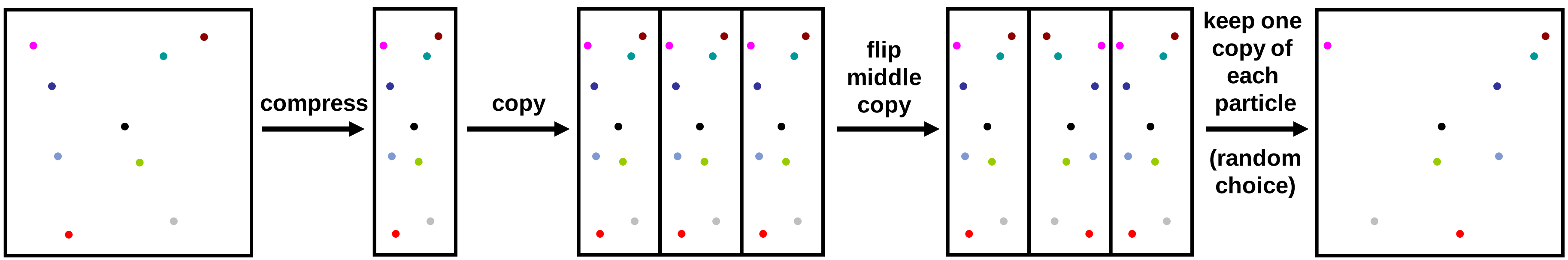
- There are other counterintuitive examples
- Even a minimal advection-diffusion model (with good physics) can reveal unexpected behavior

Outline of Presentation

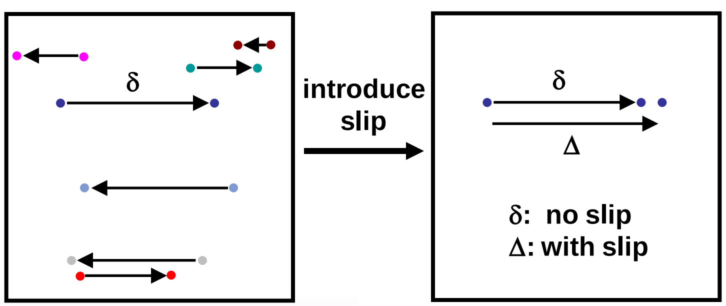
- Turbulence simulation using map-based advection
- A simple case with surprising behavior
- Multi-scale modeling of cloud droplet evolution mechanisms
- 1D simulation of turbulent flow
- Cloud modeling applications
- Superparameterization using map-based advection
- Concluding remarks

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:



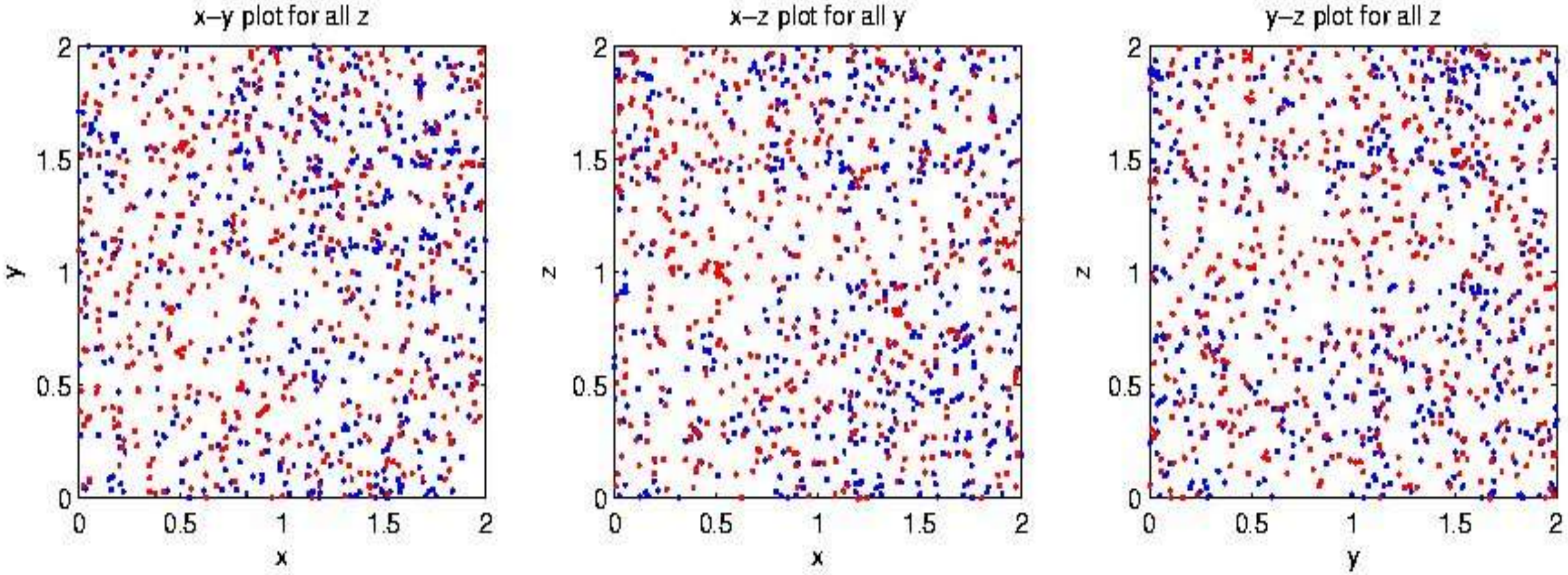
<u>Inertia model</u>:

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

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:

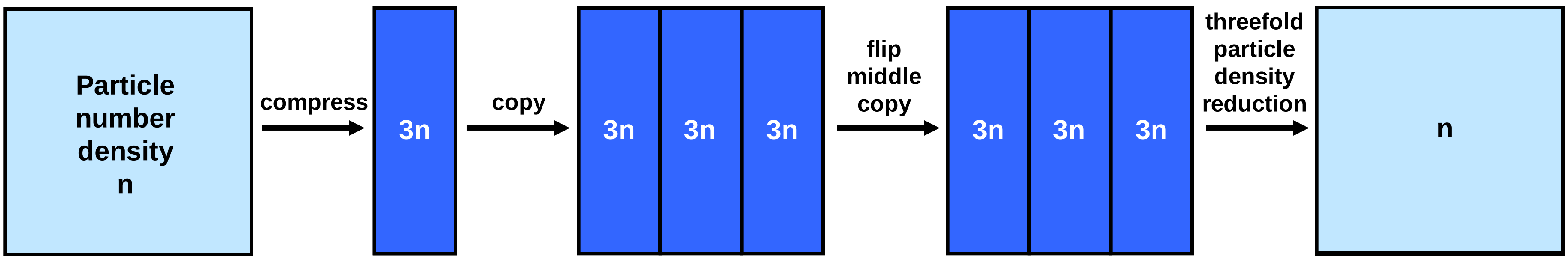
- Cubic domain, map size = domain size
- Maps in x, y and z directions, randomly positioned
- Periodic boundary conditions
- Iterated to statistical steady state
- Red, S = 0; blue, S = 0.1

Sandia National Laboratories

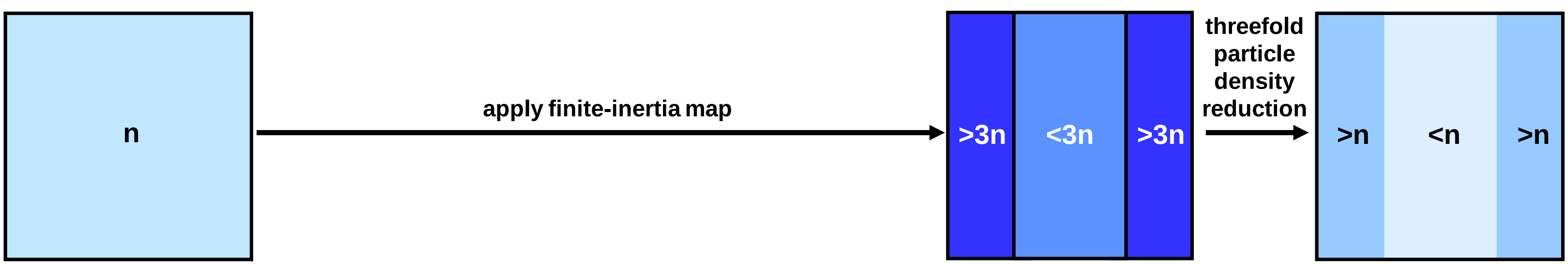
CRF

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



Sandia National Laboratories

CRF

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)

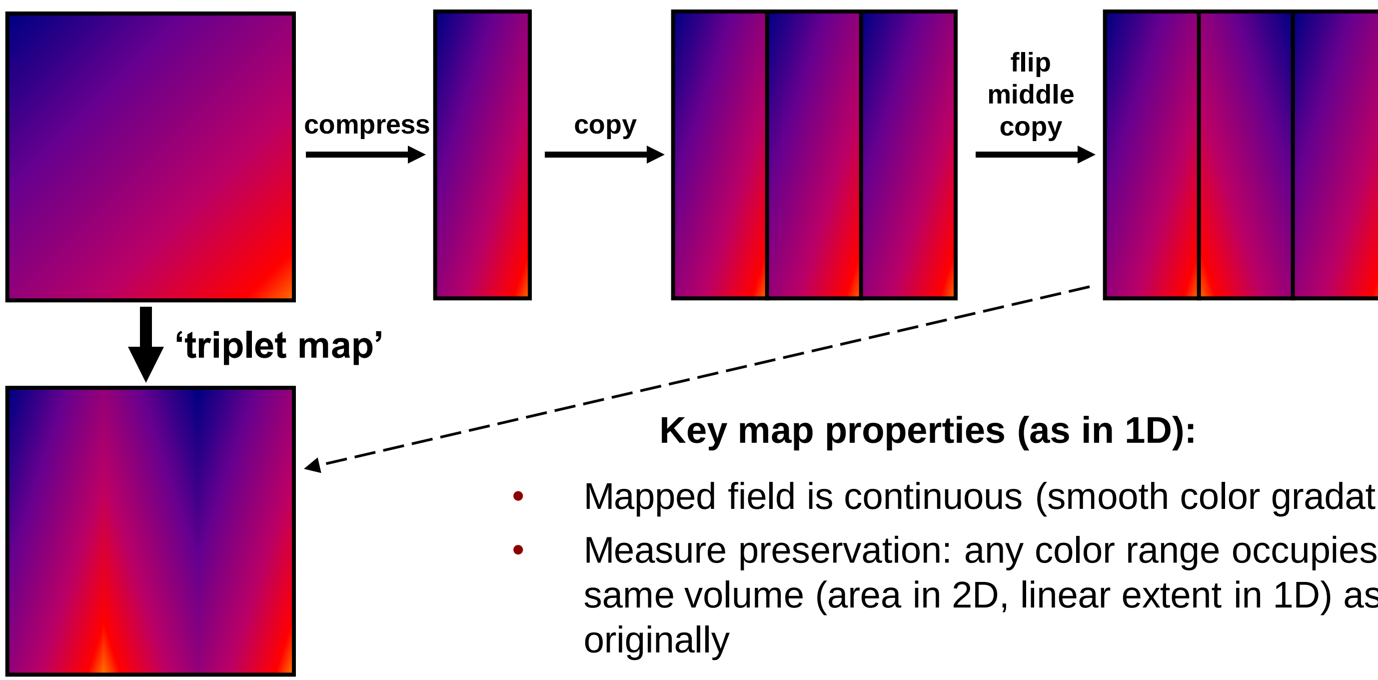
Sandia National Laboratories

CRF

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):

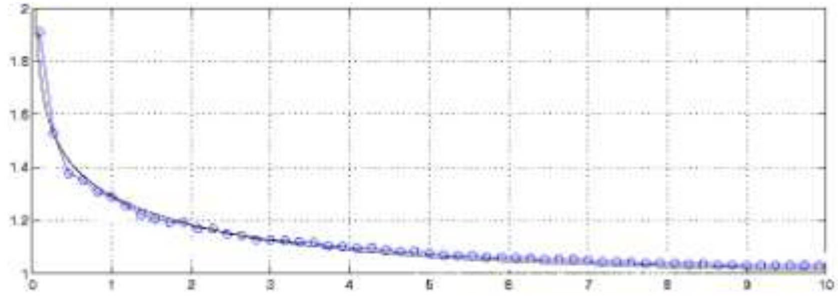
- Mapped field is continuous (smooth color gradation)
- Measure preservation: any color range occupies same volume (area in 2D, linear extent in 1D) as originally

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

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

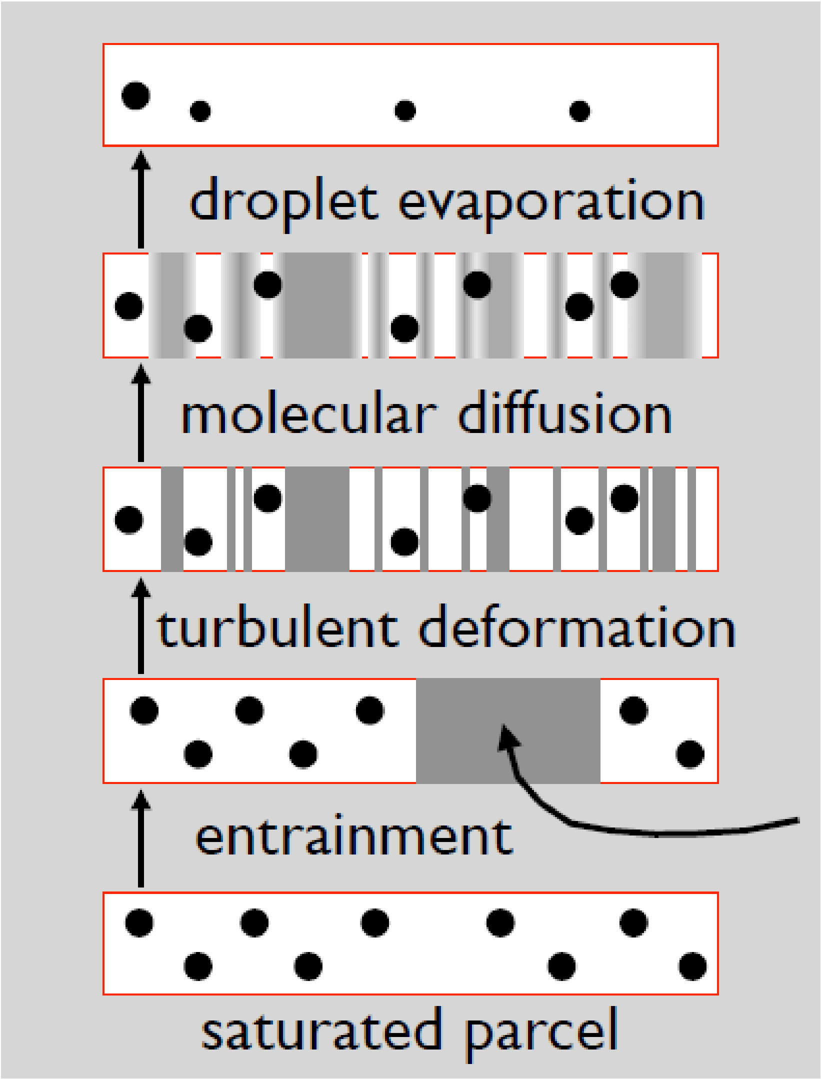
- Benchmarking:
  - Have tuned to match monodisperse (below) and bidisperse RDFs.
- Cloud application: simulate small scales in a 1D map-based scheme
  - Krueger's 1D EMPM captures condensational growth in fluctuating humidity
  - Coalescence variability is important at smaller scales
  - Therefore structure 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

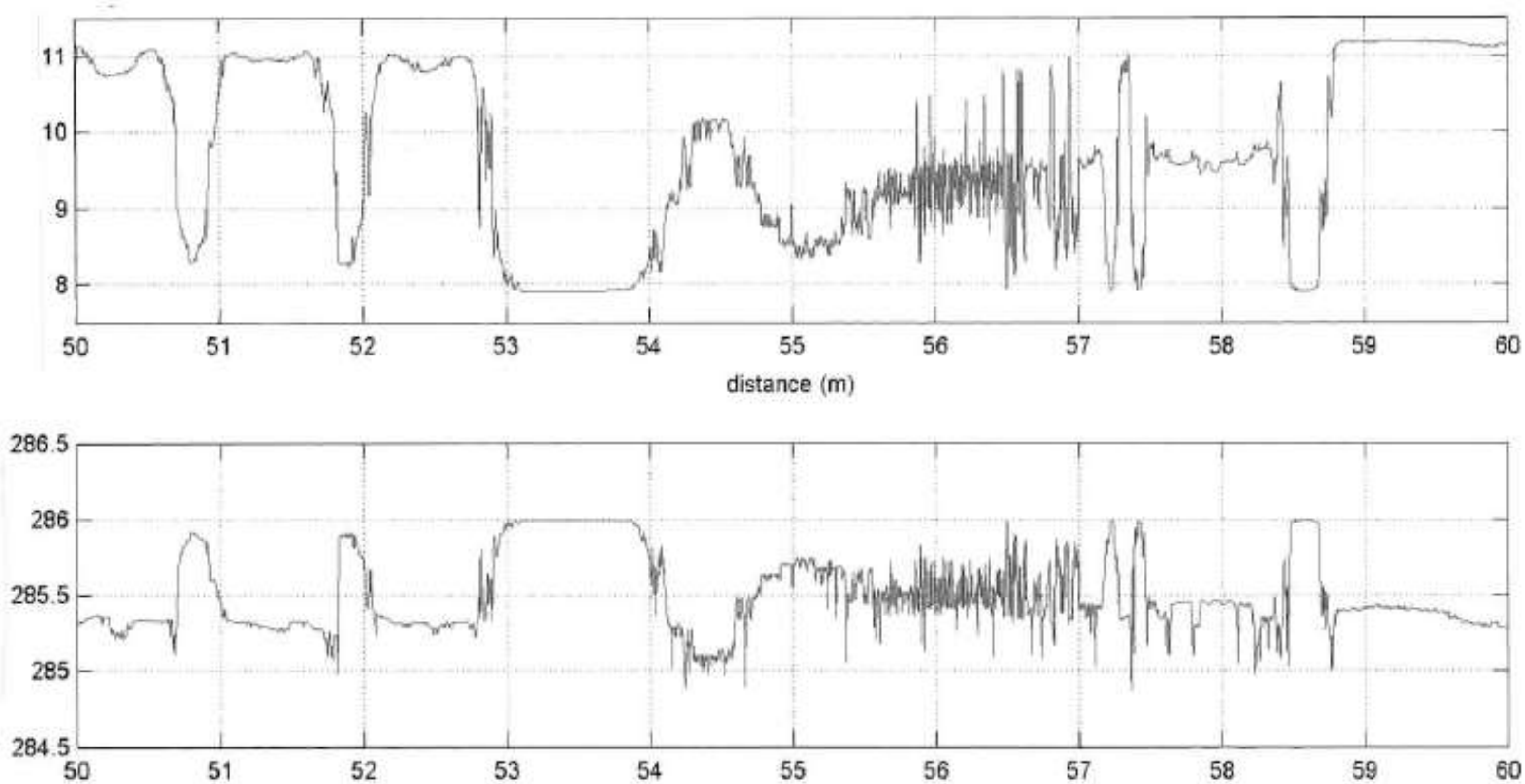
LEM: ‘turbulent deformation’ consists of triplet maps, randomly placed, with sizes sampled from a distribution that idealizes the energy spectrum of turbulence



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

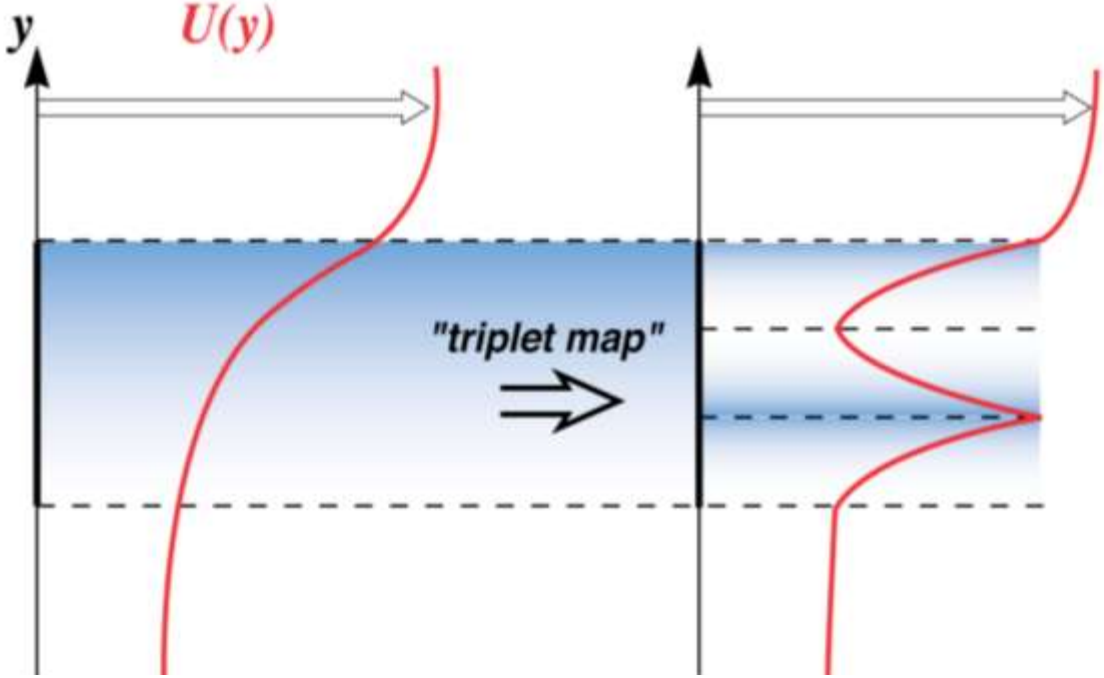


Outline of Presentation

- Turbulence simulation using map-based advection
- A simple case with surprising behavior
- Multi-scale modeling of cloud droplet evolution mechanisms
- 1D simulation of turbulent flow
- Cloud modeling applications
- Superparameterization using map-based advection
- Concluding remarks

In ODT, the triplet map amplifies shear, inducing an *eddy cascade* (feedback mechanism)

- **The key to model performance is the eddy selection procedure**
- Eddy likelihood, in a random sampling procedure, is governed by local shear
- When an eddy occurs, the local shear is amplified, which modifies eddy likelihoods



High shear at small scales drives small eddies, leading to an eddy cascade

(In LEM, inertial-range-cascade scaling is hard-wired)

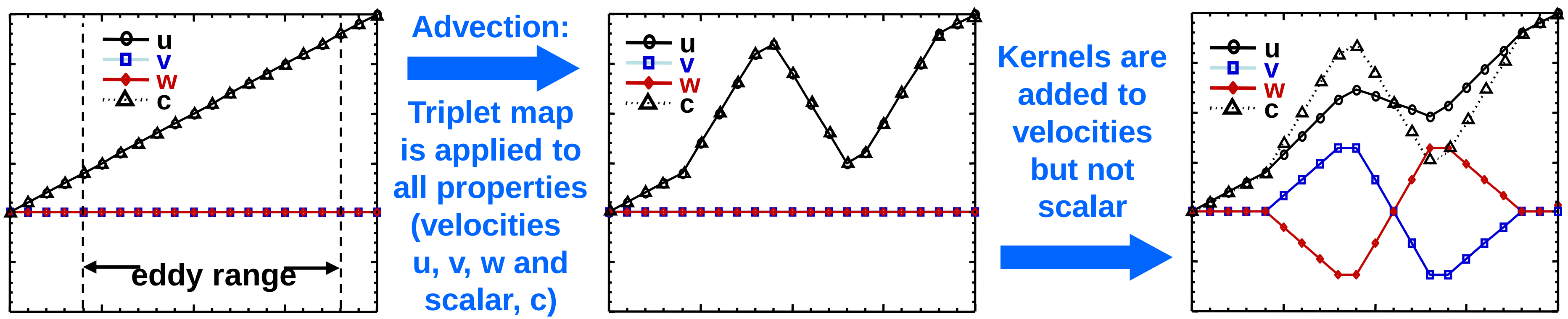
ODT eddy selection is based on the mixing-length concept, applied locally

- Each possible eddy, defined by eddy spatial location and size (S), is assigned a time scale τ based on the current flow state
- This defines an eddy velocity S/τ and energy density $E = \rho\,(S/\tau)^2$
- The set of τ values determines an eddy rate distribution from which eddies are sampled
- Whenever the flow state changes, the eddy rate distribution changes
- Unlike conventional mixing-length theory, this procedure is local in space and time (no averaging) and is applied to all eddy sizes S (multi-scale) rather than a single selected S value (‘mixing length’)

To capture energy transfers (e.g., buoyancy-induced), the ODT eddy time scale is based on an energy balance

- Energy balance (schematic): S E = C (K – P – Z V)
- S E = ρ S (S/τ)^2 is the eddy kinetic energy based on S and τ
- Right-hand side: functionals of the evolving property profiles
  - K: ‘available’ kinetic energy of velocity profiles within the eddy
  - P: gravitational potential energy change caused by the eddy
  - V: ‘viscous penalty’ (imposes a threshold eddy Reynolds number)
  - C, Z: free parameters (Z is optional, but is empirically useful)
- For a given eddy at a given instant, this determines τ
- The approach is reminiscent of CAPE and of Stull’s transilient flux parameterization, but in an unsteady simulation framework

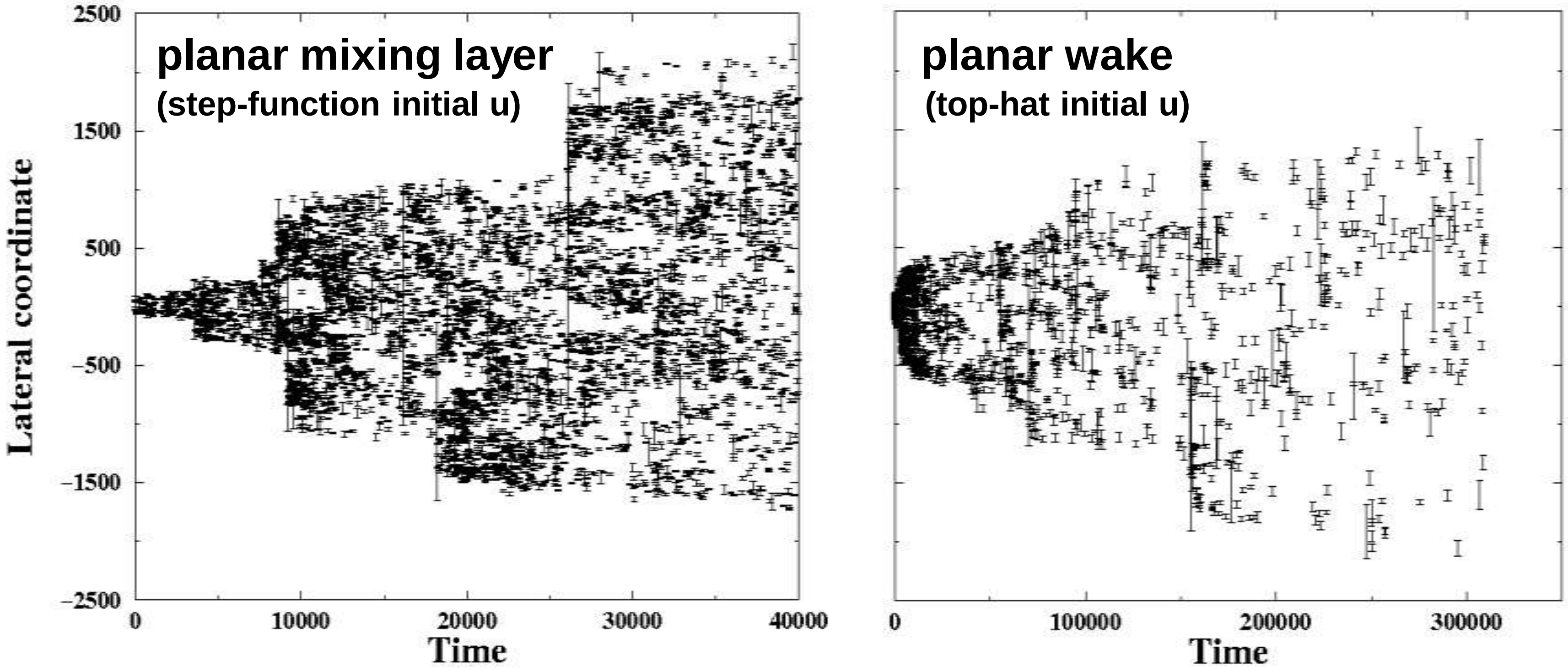
Energy couplings require an additional eddy operation



- Eddy-induced energy couplings imply kinetic-energy changes
- ‘Kernels’ (wavelets) added to velocity profiles implement these changes
- Kernels are also used to measure ‘available’ kinetic energy

ODT simulations provide detailed flow-specific representations of turbulence

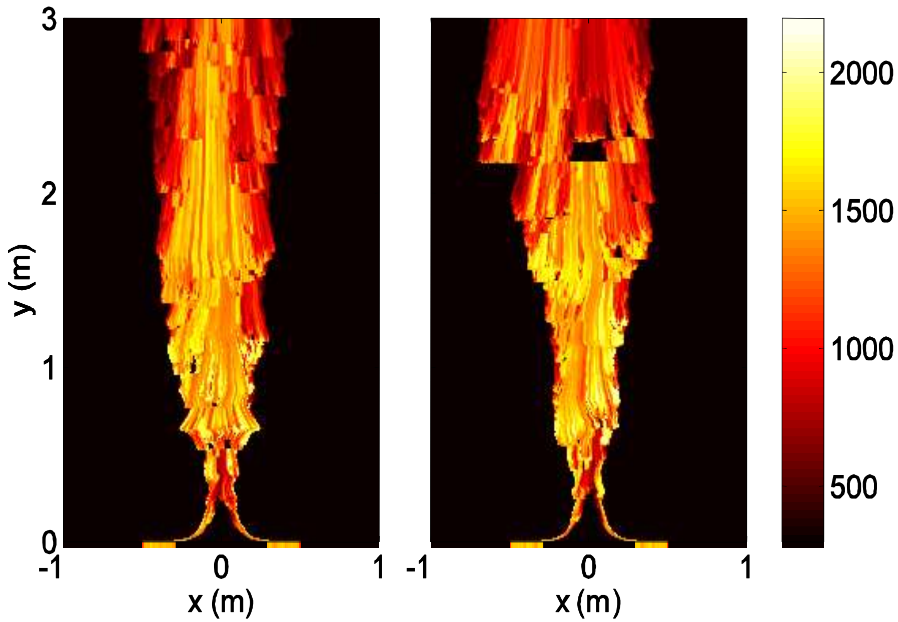
These simulations are based on time advancement of $u_t = \nu u_{yy}$ with flow-specific initial u profiles (see below), plus eddies

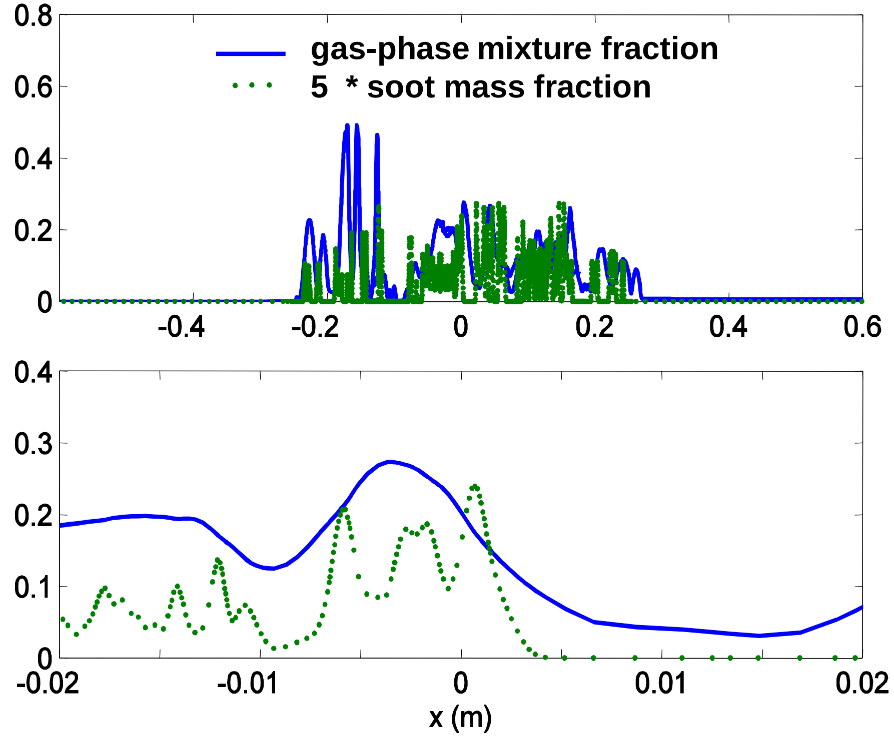


- **Each vertical line shows the spatial extent of an eddy**
- **Horizontal location is its time of occurrence**
- **Units are arbitrary**

Spatially advancing ODT captures the structure of an ethylene-air sooting plume

Instantaneous temperature field





An effect captured by spatial advancement:

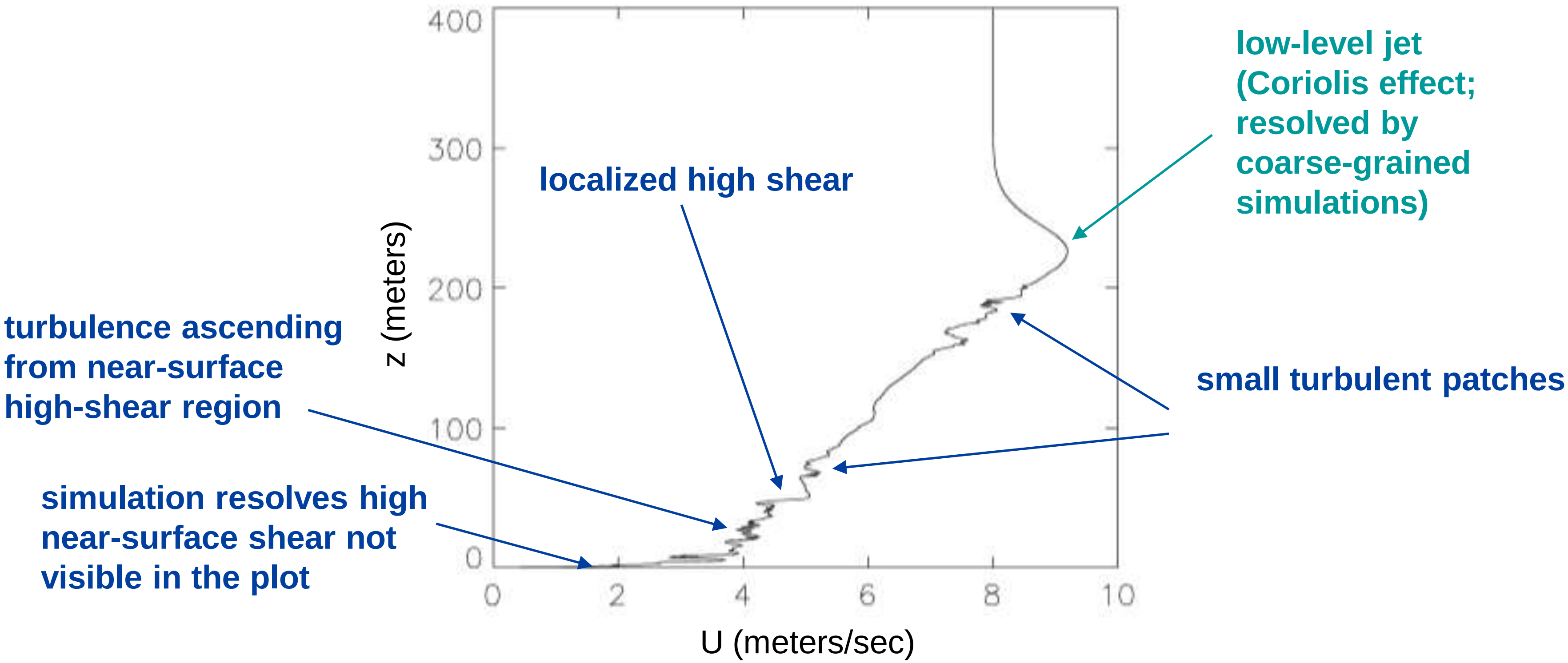
The spatial continuity equation induces narrowing of temperature fields above the inlet due to lateral inflow balancing vertical buoyant acceleration

An adaptive mesh efficiently resolves small features

Outline of Presentation

- Turbulence simulation using map-based advection
- A simple case with surprising behavior
- Multi-scale modeling of cloud droplet evolution mechanisms
- 1D simulation of turbulent flow
- Cloud modeling applications
- Superparameterization using map-based advection
- Concluding remarks

Eddy-viscosity closure within ODT enables atmospheric flow simulations



- An instantaneous vertical (z) profile of horizontal velocity (U) is shown
- Simulation corresponds to stably stratified conditions (surface cooling: GABLS inter-comparison case)
- 16000 computational cells, resolving 2.5 cm
- Roughly 100 eddy events / sec

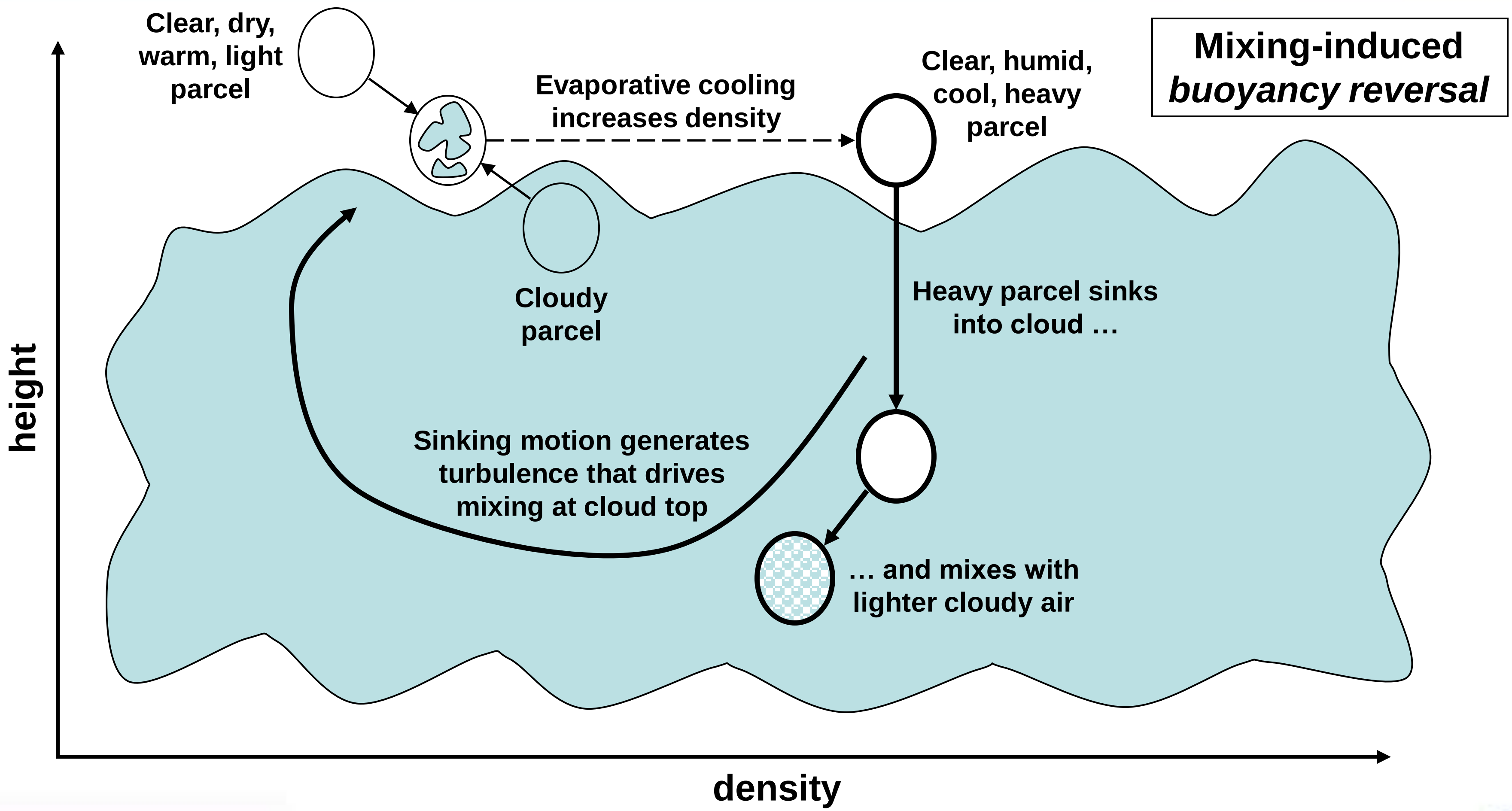
ODT is being used to simulate multiple mechanisms governing cloud dynamics

- Incorporating
  - CAPE-like eddy-rate determination based on moist thermodynamics
  - Cloud-top radiative cooling
  - Surface sources of heat and moisture
  - Precipitation

- Coupling ODT to LES to capture 3D effects
  - LES tracks the clear-cloudy interface with coarse resolution
  - Interface-following ODT captures cloud-top subgrid-scale details
  - Previous use of this approach: combustion with subgrid-scale LEM

(with Heiko Schmidt and Bjorn Stevens)

One mechanism of entrainment of overlying clear air into clouds is mixing-driven



S. Wunsch (2003) showed that ODT captures this feedback loop and reproduces laboratory-scale observations

Sandia National Laboratories

CRF

This approach links atmospheric and laboratory conditions

Dependences of buoyant stratified flow phenomena on Sc and Re are key science questions that ODT has addressed by:

- **Validation against laboratory data**
- **Extrapolation (parameter studies)**
- **Construction of new mathematical models by physical reasoning applied to the simulation results**

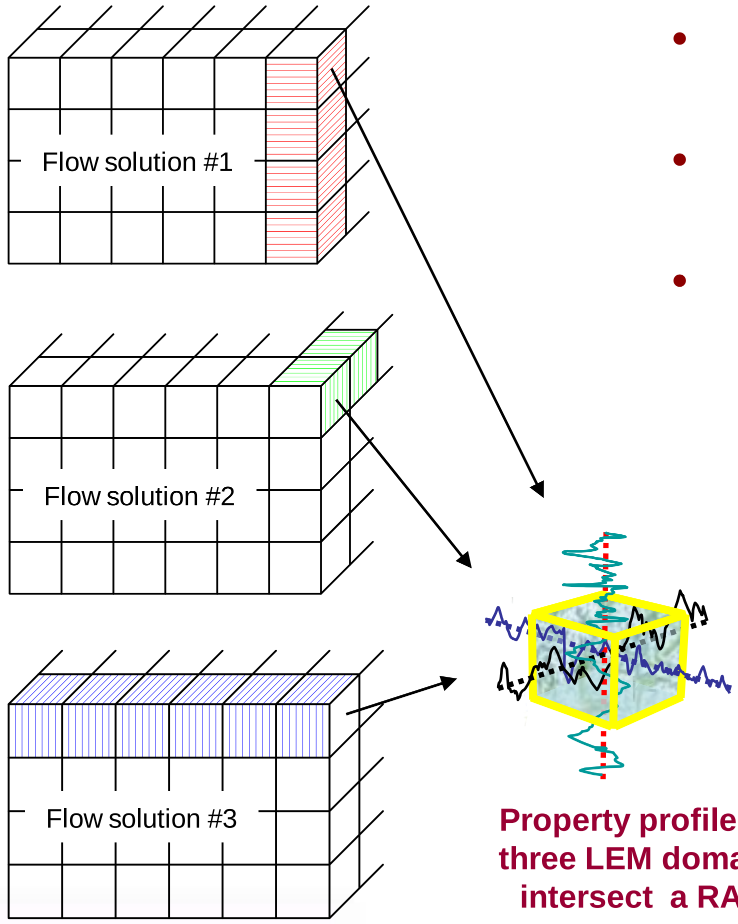
Sc is a fluid property:
[molecular diffusivity]/[kinematic viscosity]
Re measures turbulence intensity:
[turbulent diffusivity]/[kinematic viscosity]

ODT is uniquely applicable over wide ranges of Sc and Re values, allowing <u>validation at high Sc and moderate Re</u> (liquid-phase laboratory experiments) and subsequent <u>application at Sc ≈1 and high Re</u> (atmospheric flow)

Outline of Presentation

- Turbulence simulation using map-based advection
- A simple case with surprising behavior
- Multi-scale modeling of cloud droplet evolution mechanisms
- 1D simulation of turbulent flow
- Cloud modeling applications
- Superparameterization using map-based advection
- Concluding remarks

Time advancement of a 3D lattice-work of coupled LEM domains can be driven by RANS input: 'LEM3D'

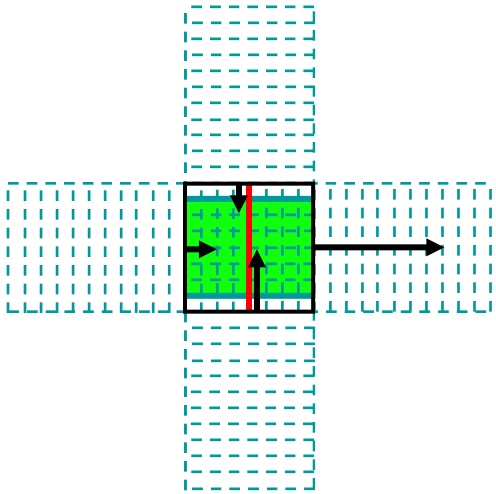


Property profiles on the three LEM domains that intersect a RANS CV

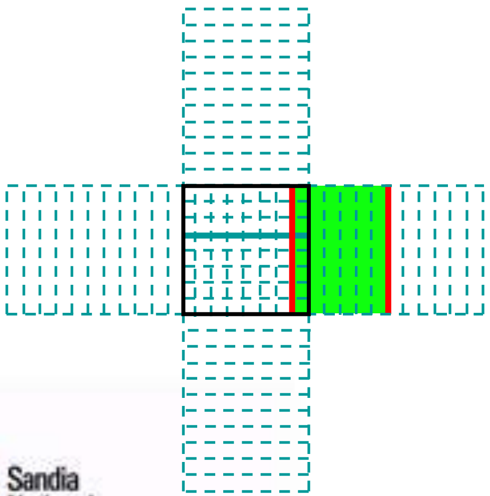
- Each LEM domain spatially refines RANS control volumes (CVs) in one coordinate direction
- Each CV is thus contained within three orthogonal LEM domains, each within a different flow solution
- Time-advancement cycle:
  - **Advancement on individual LEM domains**
    - **1D representation of small-scale motions**
    - **Requires <u>RANS eddy diffusivities</u> to determine local eddy frequencies**
  - **Cell transfers (conservative mapping) couple domains**
    - **3D representation of large-scale motions**
    - **Transfers implement displacements prescribed by <u>RANS mean velocities</u>**

RANS: Reynolds-Averaged Navier-Stokes (steady-state flow model)

A 2D example illustrates the domain-coupling procedure



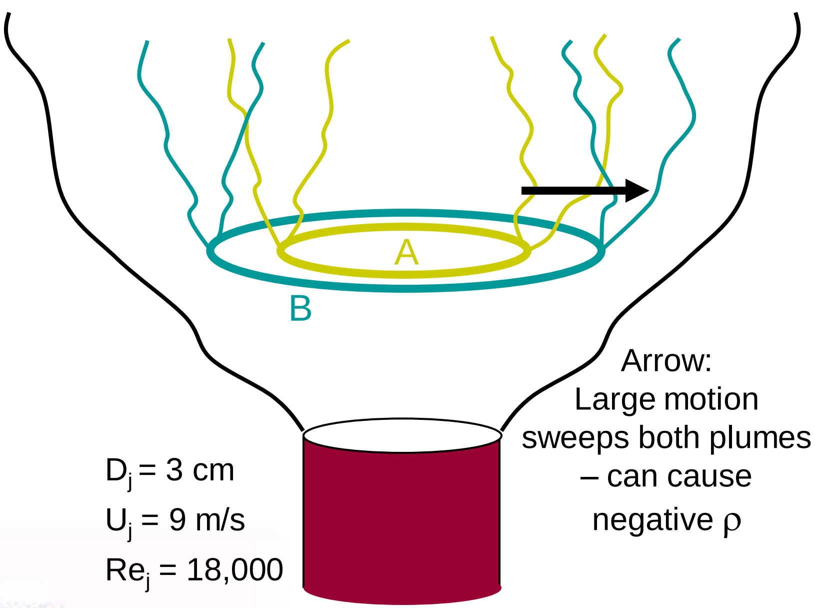
- **Arrows are RANS CV face-normal displacements (velocities × time step)**
- **In this example, there is net vertical inflow and net horizontal outflow through CV faces (box)**
- **Horizontal LEM domain: cut at red line and displace uniformly on either side, <u>leaving a gap</u>**
- **Vertical LEM domain: remove green region and insert it into the gap on the horizontal domain (between the red lines), then displace uniformly above and below the green region, causing the solid blue lines to meet**



- Advantage: Displaces fluid advectively (no mixing)
- Issue: Brings dissimilar fluid states into contact
- Remedy: Use coarse CVs to minimize the artifact

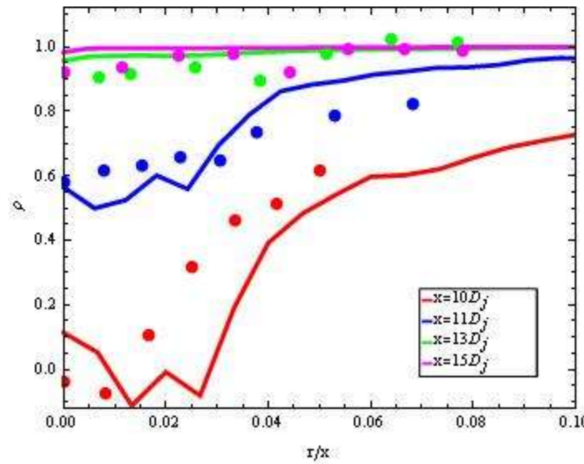
Using measured properties (surrogate RANS), LEM3D captures the mixing of scalars released within a jet

- Two ring sources (various diameter combinations) at $x/D_j = 9$ release scalars A and B, respectively
- A-B cross-correlation, ρ, is measured at various downstream locations (Tong & Warhaft, 1995)
- This configuration has not previously been modeled

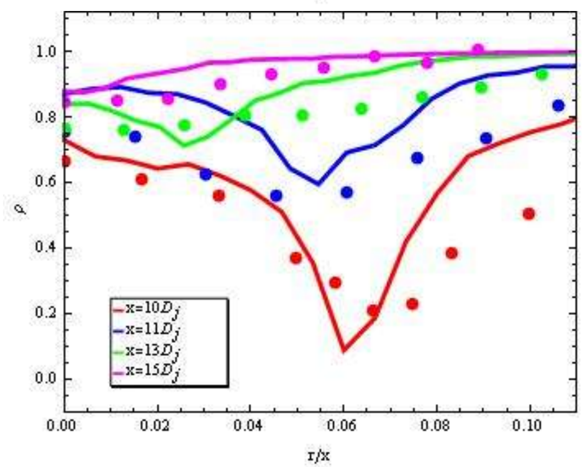


Radial profiles of ρ
(measurements: •, model: —)

Ring diameters



10 and 15 mm



35 and 40 mm

ODT domains can be coupled to obtain a 3D flow simulation (ODT3D)

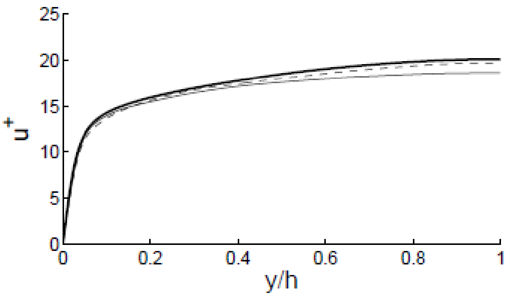
- Same mesh geometry as LEM3D
- Different domain coupling because
  - for momentum, adjacent dissimilar states should be avoided
  - for momentum (but not species), some under-resolved mixing is acceptable
- Advection feedbacks between LEM3D and ODT3D:
  - LEM3D gets eddy events and CV face-normal mass fluxes from ODT3D
  - ODT3D gets thermal expansion from LEM3D

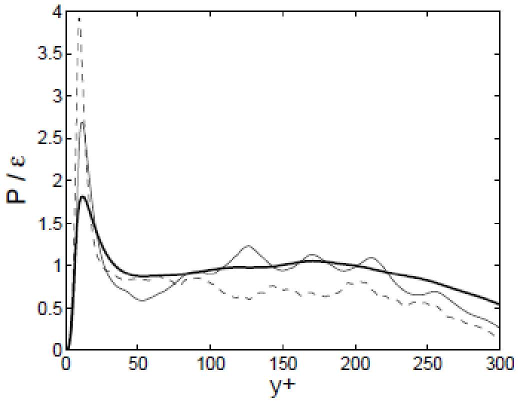
Treatment of 3D pressure-velocity coupling distinguishes two ODT3D formulations

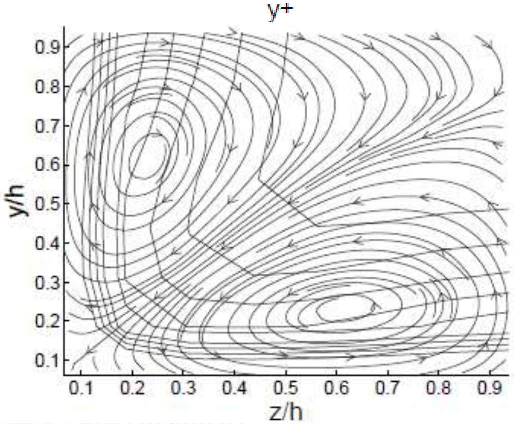
- Incompressible formulation:
  - Continuity enforced using coarse-grained (CV scale) 3D pressure projection
  - ODT-resolved flow field is modified accordingly, a downscale coupling
  - Status: Captures 3D effects while fully resolving wall layers in
    - Channel flow
    - Open channel (with a free-slip surface)
    - Square duct
    - Lid-driven cavity

- Pseudo-compressible formulation:
  - Enables domain coupling with no coarse-graining or downscale coupling
  - Hence termed 'Autonomous Microscale Evolution' (AME)
  - Status: under development

ODT3D captures 3D flow effects while fully resolving wall layers

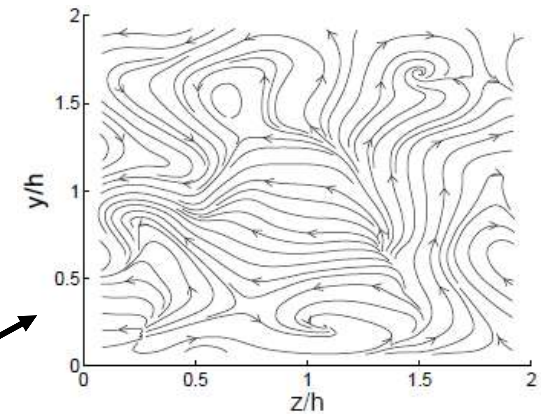


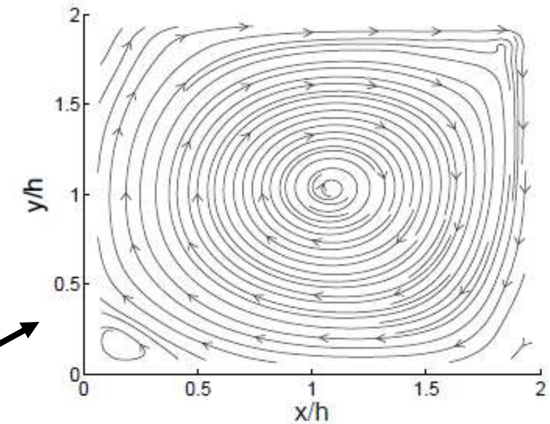




Validation cases:

- **Channel flow**: ODT3D performance is comparable to ODT, indicating that ODT3D domain coupling causes no significant loss of fidelity
- **Open channel** (no-slip wall and free-slip surface): Captures free-surface upwelling/downwelling
- **Square duct**: Captures secondary recirculation (spontaneous symmetry breaking)
- **Lid-driven cavity**: Captures wall-layer distortions induced by the primary recirculation



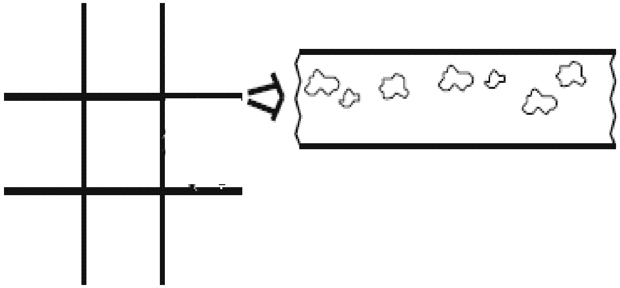


ODT3D resembles ‘superparameterization’ (SP) closure of atmospheric flow simulations

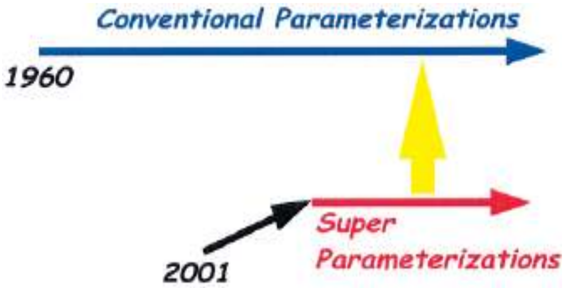
- SP: small scales resolved in 2D (vs. 1D in LEM and ODT)
- Needed despite high cost due to the ‘cloud parameterization deadlock’
- As with ODT3D, there are several SP implementation strategies

top view of a lattice-work of coupled vertical planar domains

side view of one domain (2D cloud simulation)



this approach is viewed as a climate modeling paradigm shift (Randall et al. 2003)



Outline of Presentation

- Turbulence simulation using map-based advection
- A simple case with surprising behavior
- Multi-scale modeling of cloud droplet evolution mechanisms
- 1D simulation of turbulent flow
- Cloud modeling applications
- Superparameterization using map-based advection
- Concluding remarks

LEM and ODT are being applied to diverse geophysical and environmental problems

Ongoing and planned efforts:

- Cloud droplet growth mechanisms
  - with Steve Krueger
- Ocean transport
  - with Esteban Gonzalez
- Cloud-top entrainment
  - with Heiko Schmidt
- Pollutant mixing and photochemistry (planned)
  - with Heiko Schmidt
- Turbulence scalings in the stable troposphere (planned)
  - with Zbigniew Sorbjan

Resolving local couplings is crucial for difficult regimes, so efficient resolution is vital for affordable prediction

- Map-based advection is an advantageous strategy for cost-effective simulation of turbulence-microphysics couplings in diverse geophysical flows

- Its uses include
  - Fundamental studies
  - Input to other modeling approaches
  - Building block for 3D simulation