

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

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May 3, 2010



The U.S. Department of Energy, Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences, and Energy Biosciences 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.

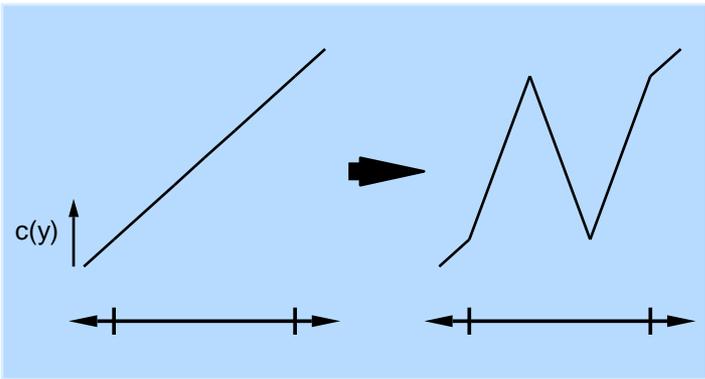
Outline of Presentation

- 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

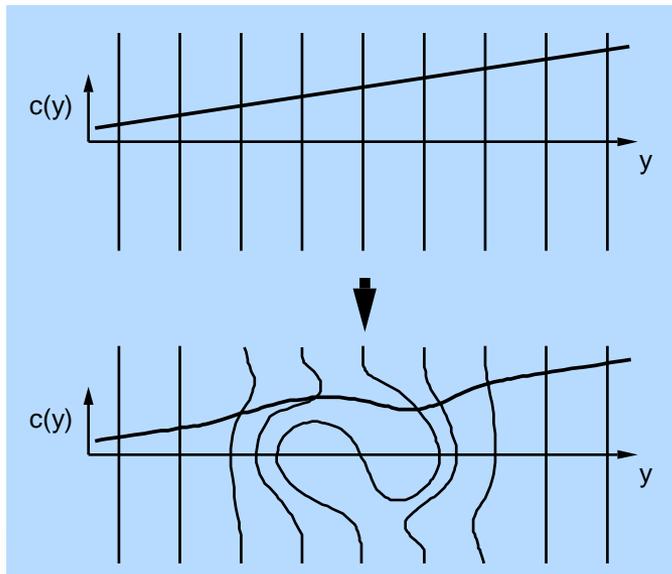
What is map-based advection?

- In Lagrangian numerical schemes, it is flow advancement by $v \Delta t$ 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

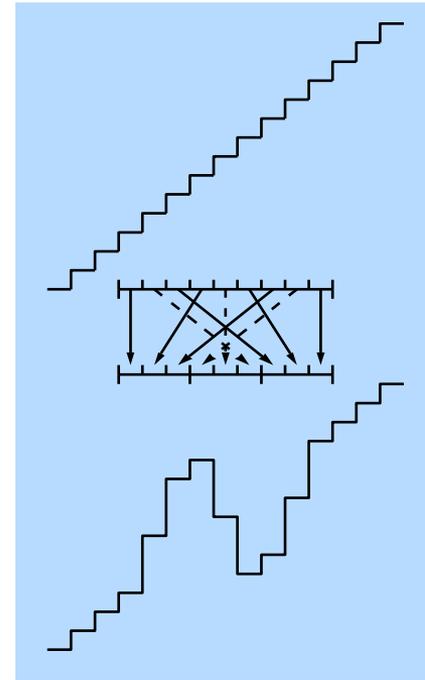
Advection is modeled as a sequence of *triplet maps* that preserve desired advection properties, even in 1D



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 (mathematicians please help!): 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):

$$\theta_t = \kappa\theta_{yy} + \text{'eddies'}$$

scalar

$$u_t = \nu u_{yy} + \text{'eddies'}$$

velocity component (ODT only)

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

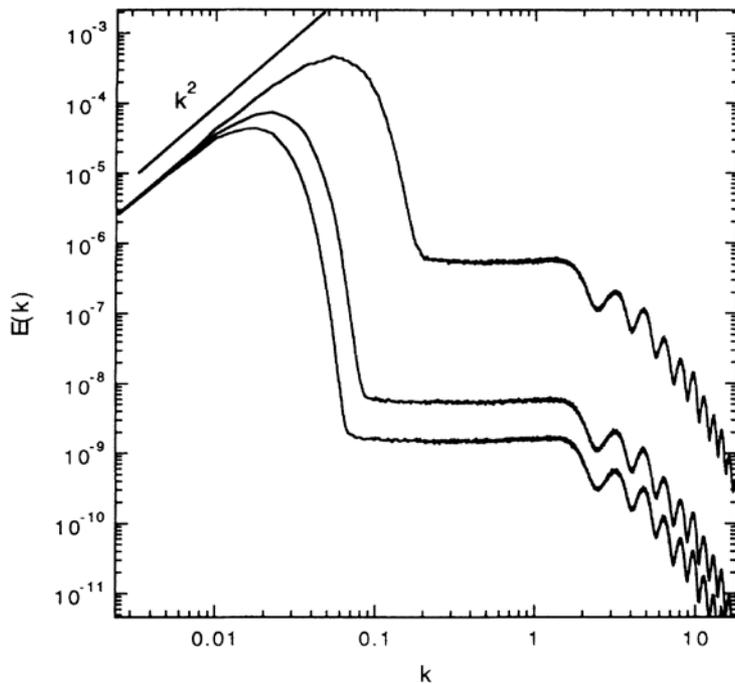
Evolve $\theta_t = \kappa \theta_{yy} + \text{'eddies'}$ with

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

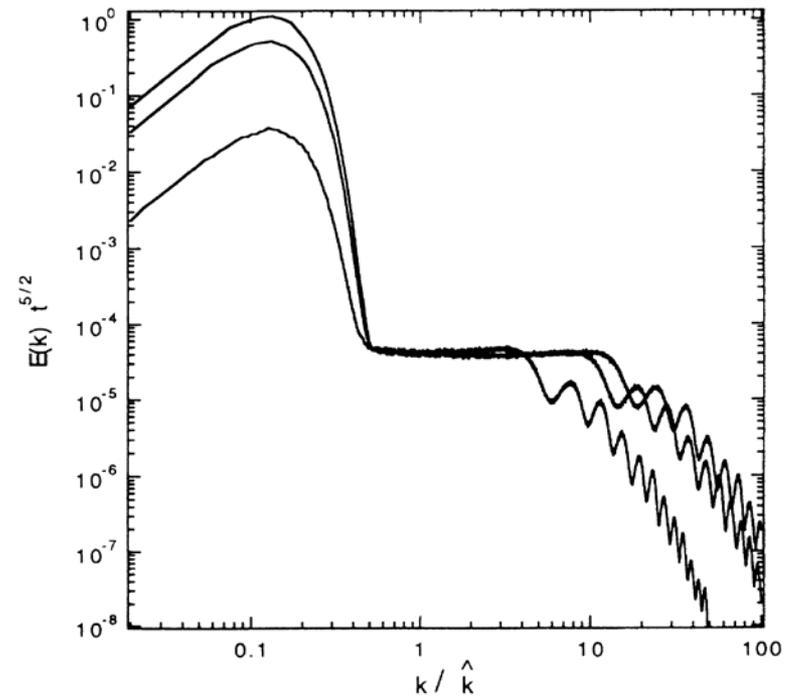
What is the time evolution of

- 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

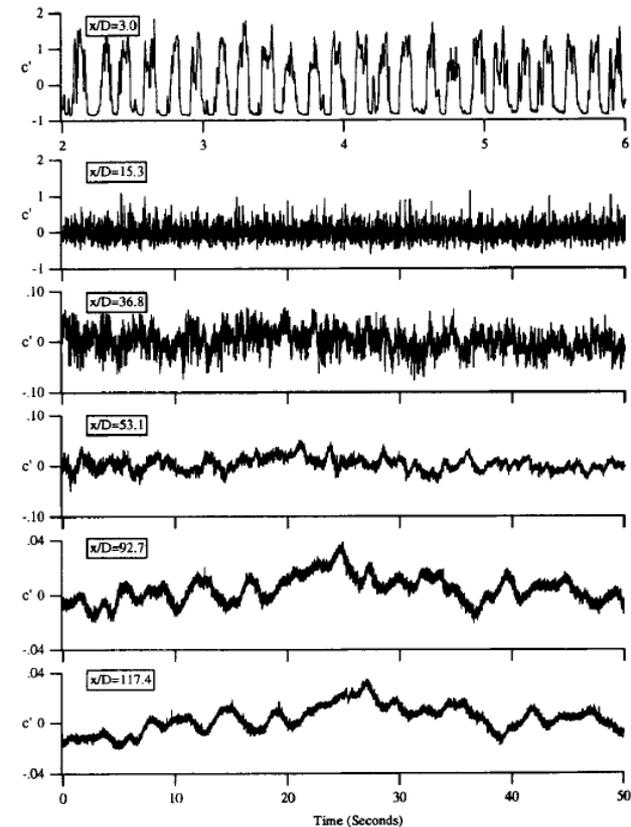


Figure 3. Time series of measured scalar field at the center of the pipe for experiment A.

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.

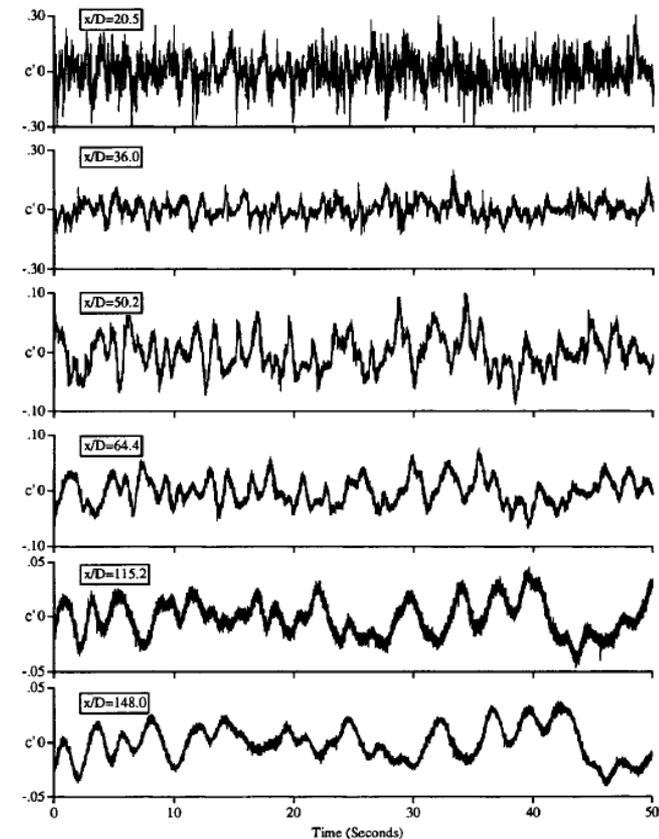
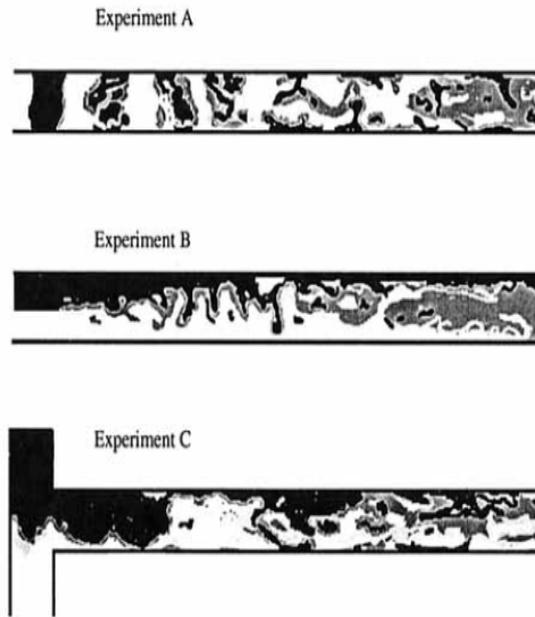
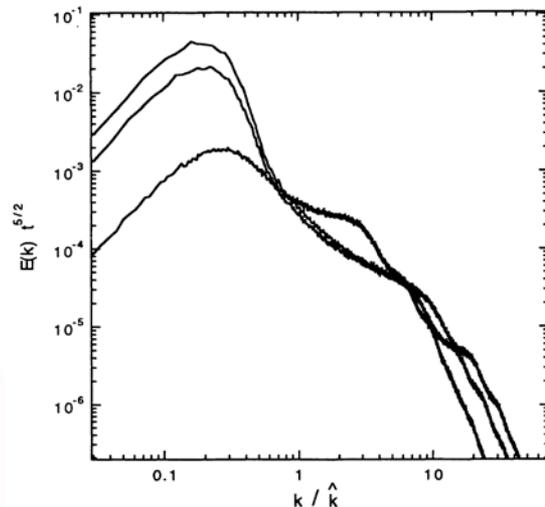
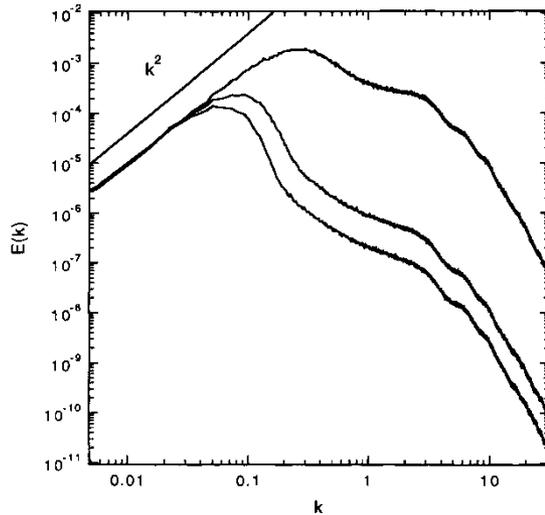


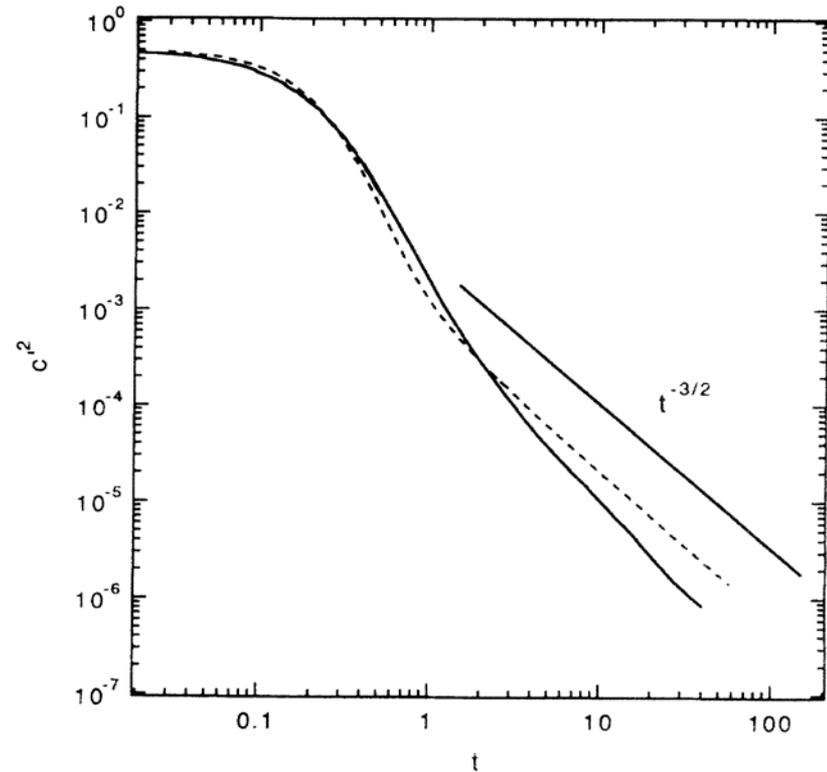
Figure 11. Time series of measured scalar field at the center of the pipe for experiment C.

Guilkey, McMurtry, and Klewicki, 1997

Simulations were performed for a 'pipe-like' map-size distribution

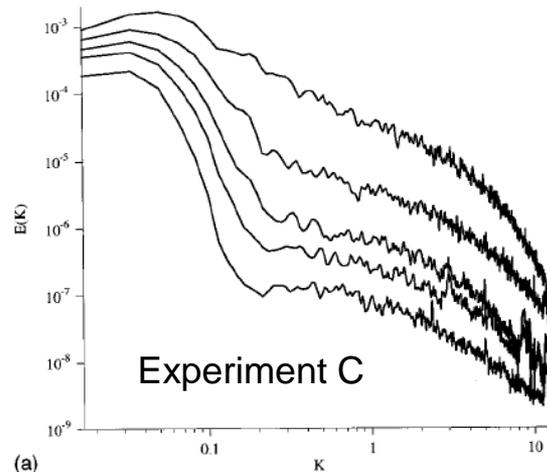


Analysis predicts $t^{-3/2}$ scalar-variance decay

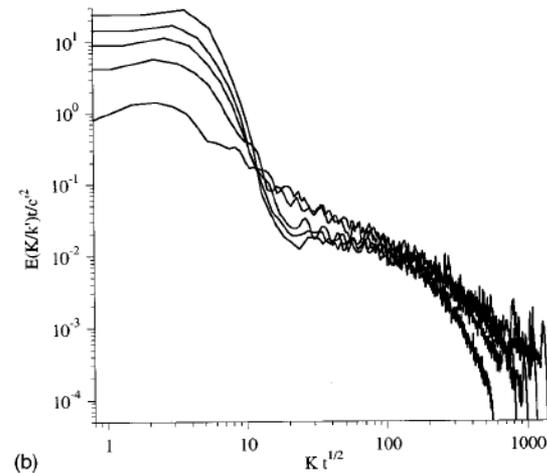


--- one map size
— pipe-like size distribution

Scalar power-spectrum measurements exhibit the predicted features



(a)



(b)

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 $x/D = 30$

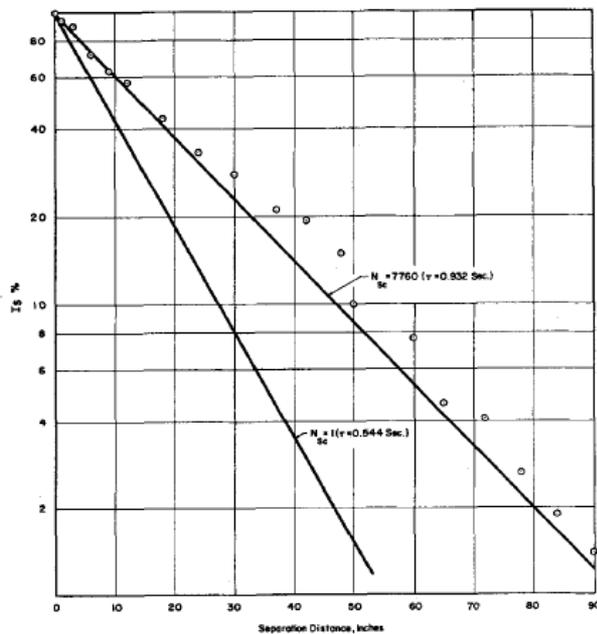
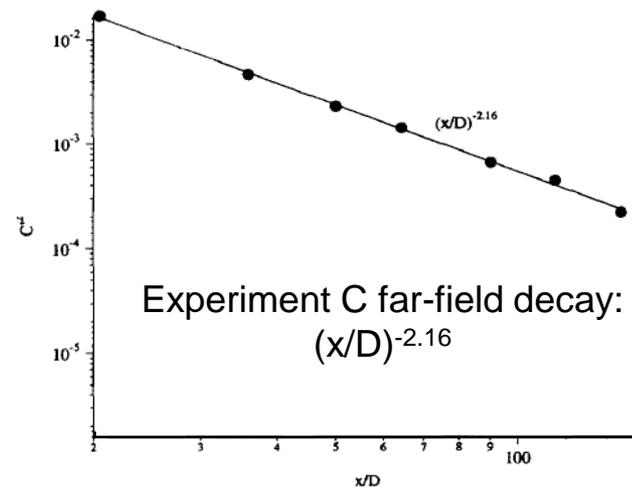
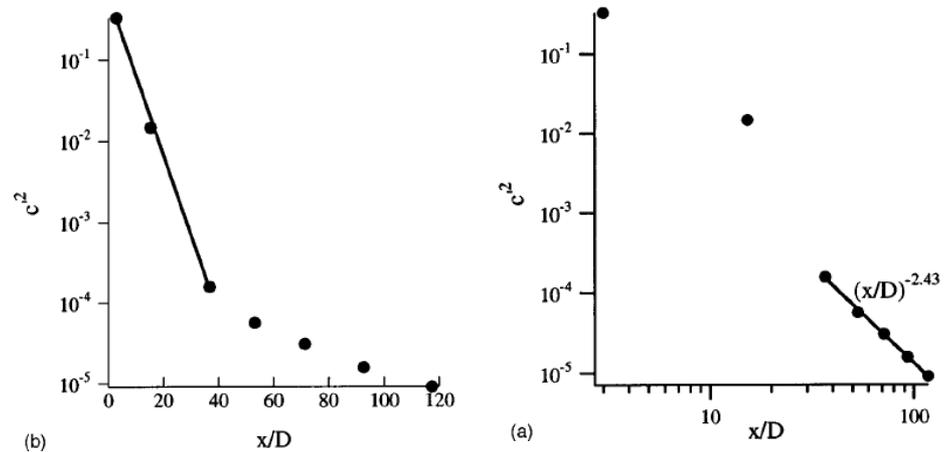


Fig. 1. Intensity of segregation.

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

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



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

Don't trust your intuition about turbulent mixing!

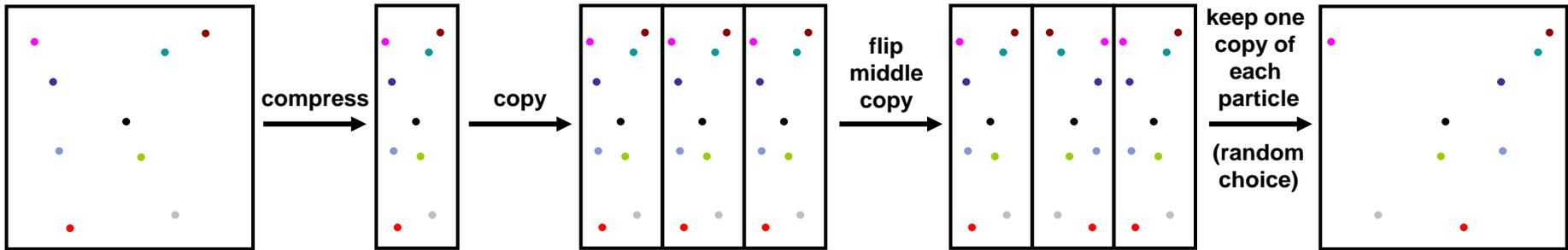
- There are other counterintuitive examples
- Even a minimal advection-diffusion model (with good physics) can reveal unexpected behavior

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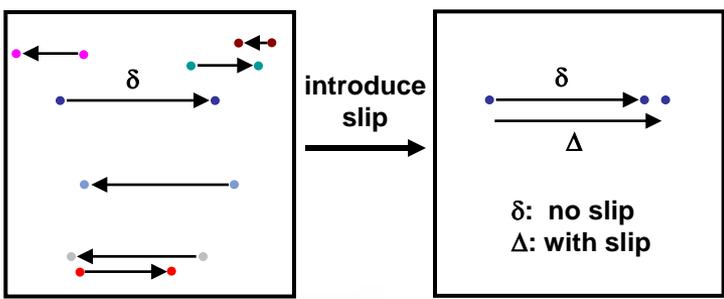
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Using map-based advection, a 3D Lagrangian (grid-free) low-inertia particle advancement model is formulated

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



Fluid displacements δ are multiplicatively incremented to represent particle inertia:



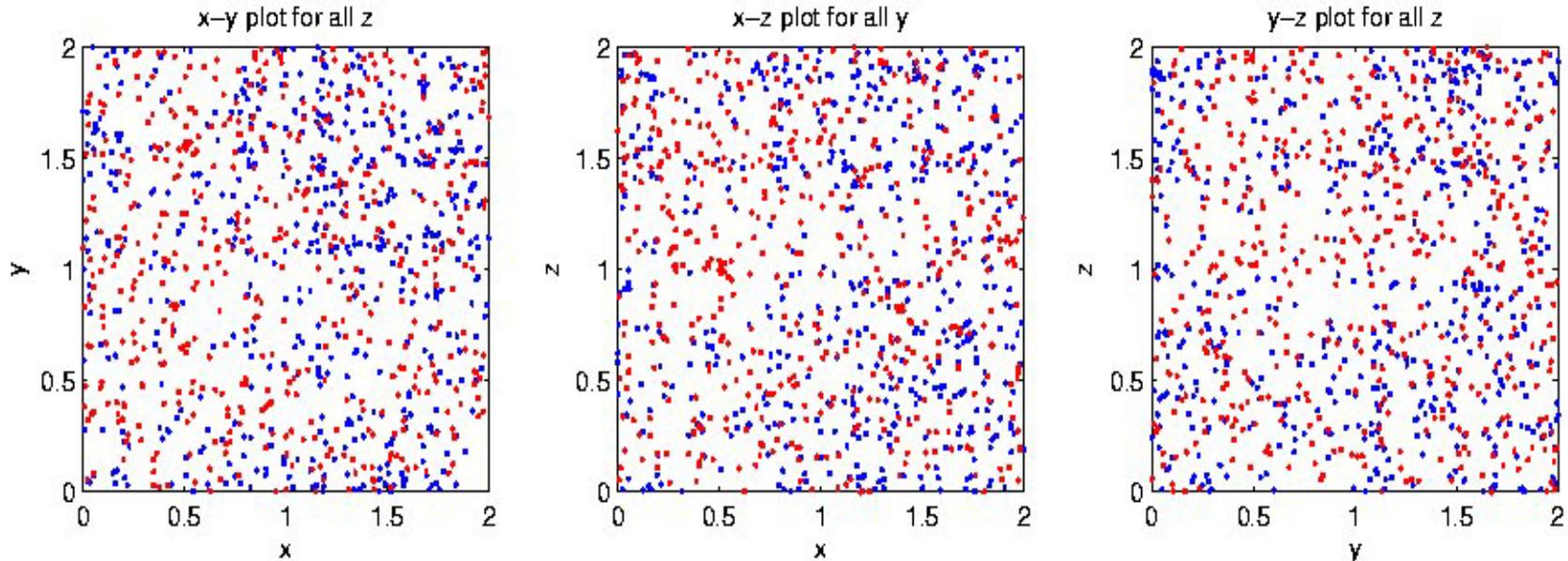
Inertia model:

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

$S \ll 1$ is the model analog of Stokes number,
 $St = [\text{particle response time}] / [\text{flow time}]$

If polydisperse, S can be different for each particle

For nonzero S , clustering is observed

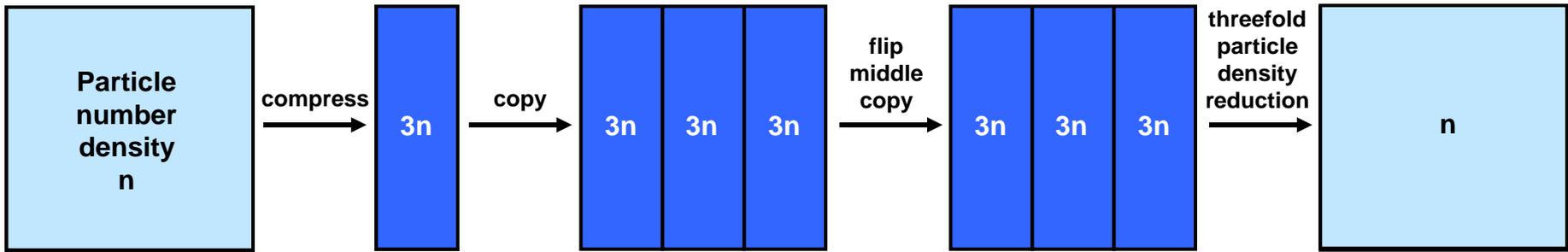


Simulation:

- 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



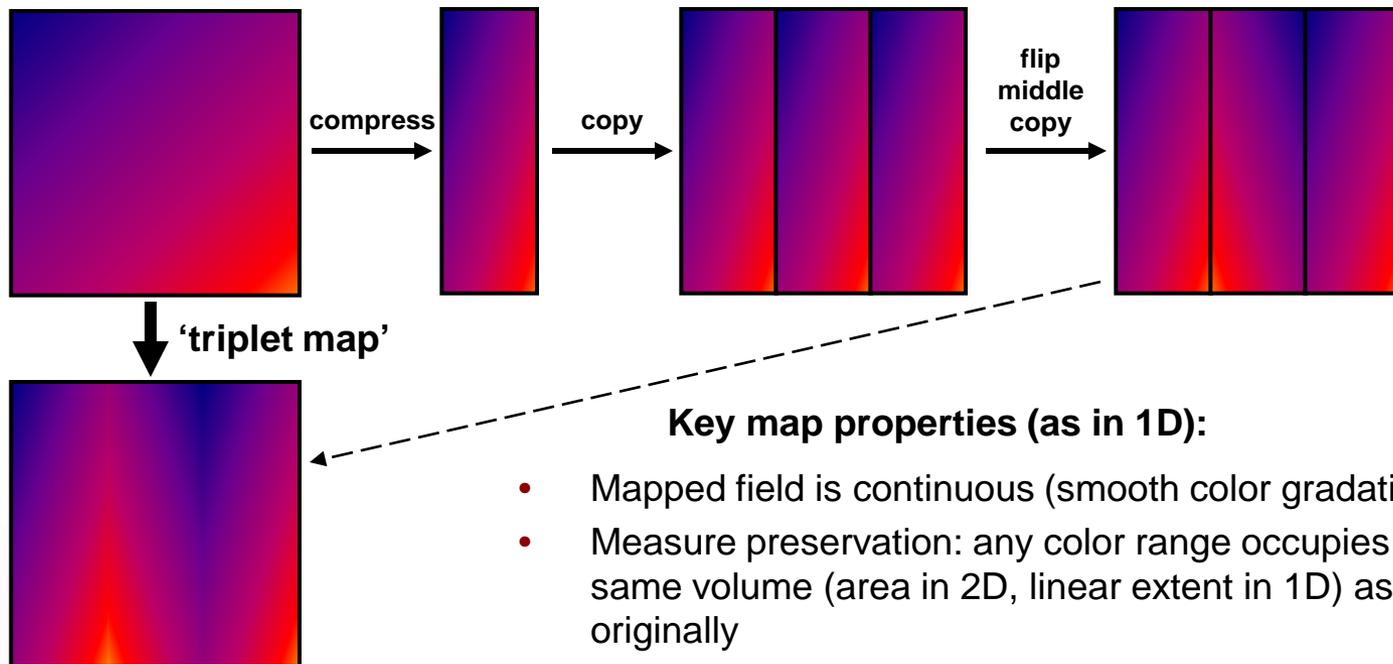
Exact analysis yields parameter dependence of a clustering metric

- 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:
 - $g \sim r^{-cS_1S_2}$ 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 continuous maps

Application of the advective map to an arbitrary continuous field:

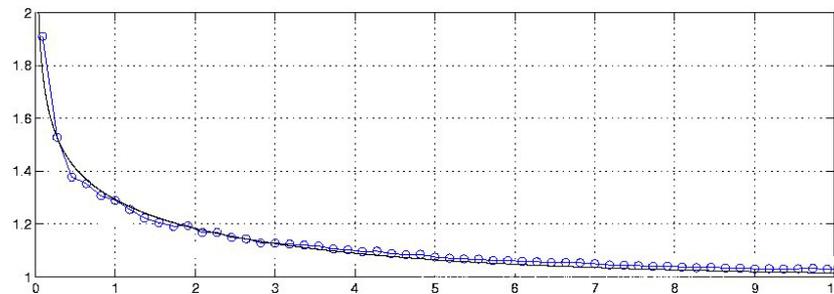


Significance (2): model properties suggest an efficient algorithm for simulation of particle motion

- 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 embed 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 EPM captures condensational growth in fluctuating humidity
 - Coalescence variability is important at smaller (sub-Kolmogorov) scales
 - Therefore structure the 1D scheme as a stack of cubes; 3D evolution in each
 - Sedimentation and droplet collision phenomenology have been incorporated

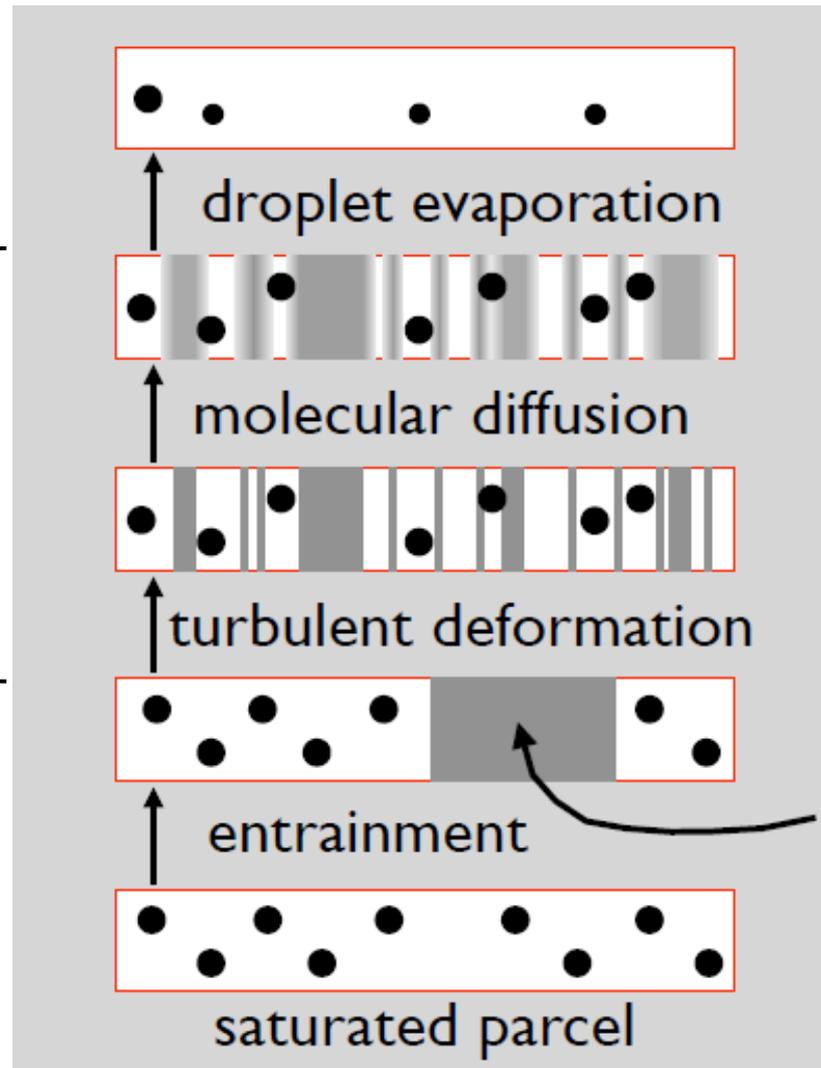


g vs. r /[Kolmogorov microscale] for $St=0.136$.

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

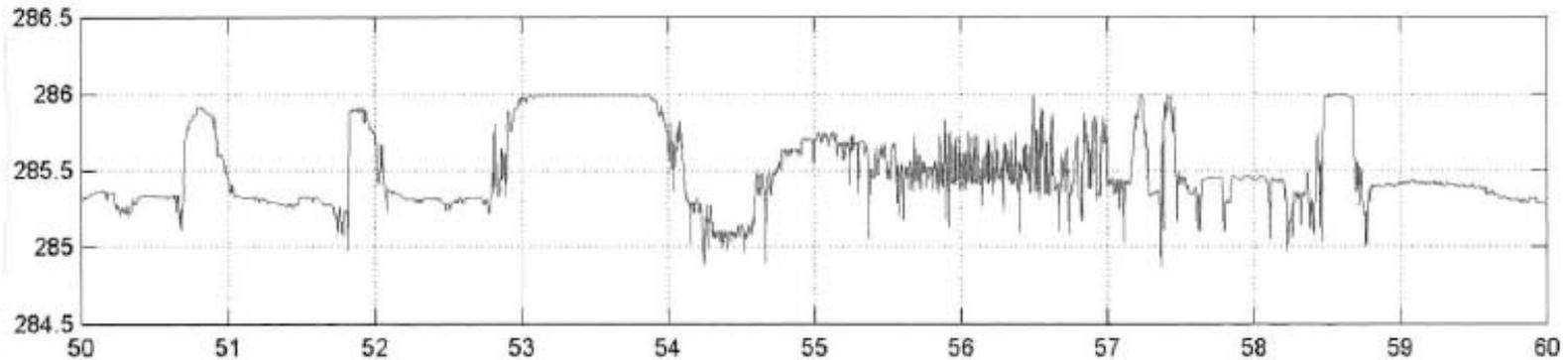
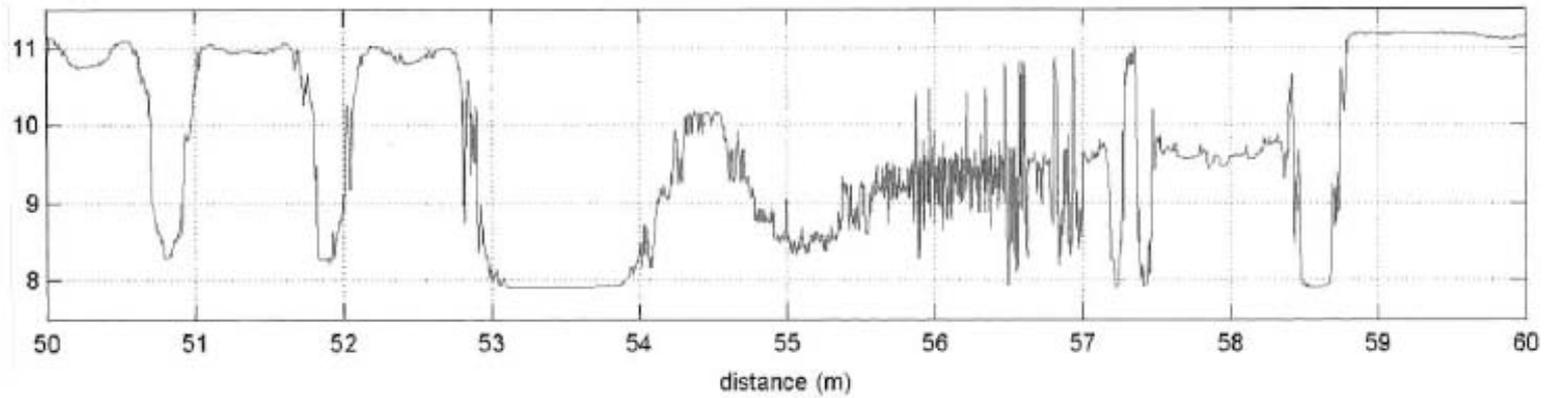
LEM: 'turbulent deformation' consists of triplet maps, randomly placed, with sizes sampled from a distribution that idealizes the energy spectrum of turbulence



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

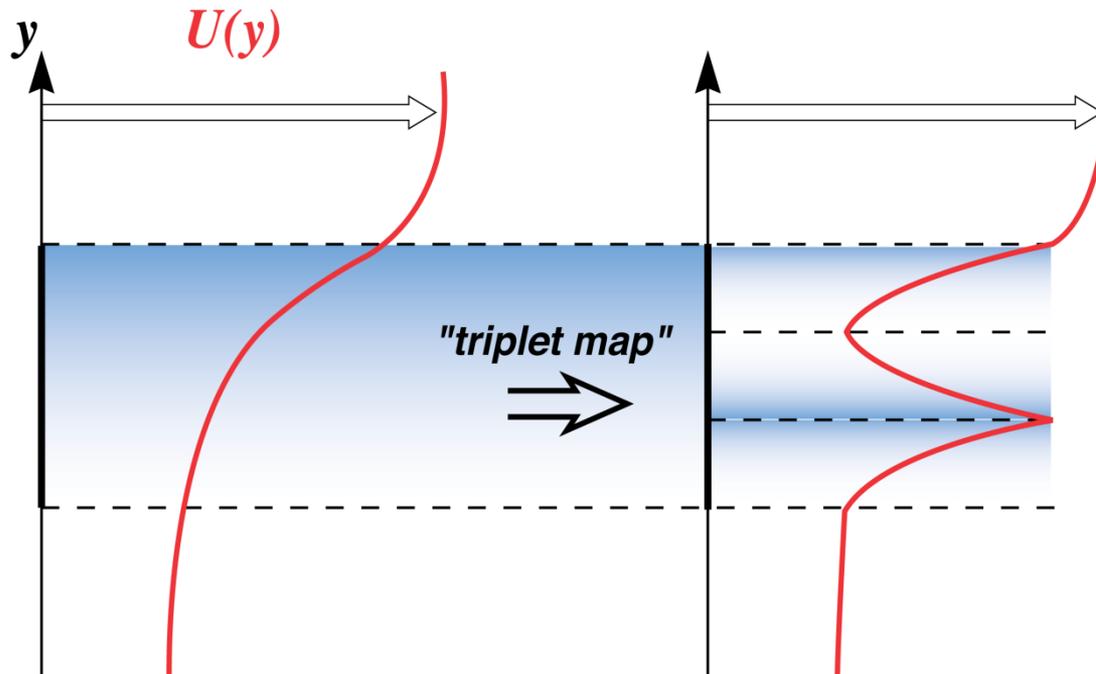


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In ODT, the triplet map amplifies shear, inducing an *eddy cascade* (feedback mechanism)

- **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)

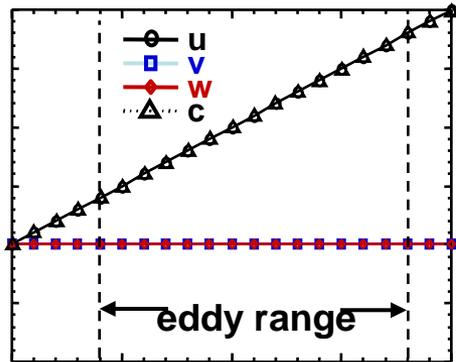
ODT eddy selection is based on the mixing-length concept, applied locally

- 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')

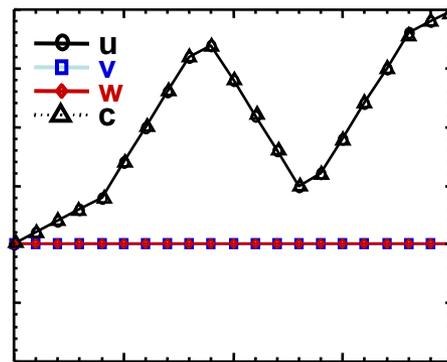
To capture energy transfers (e.g., buoyancy-induced), the ODT eddy time scale is based on an energy balance

- Energy balance (schematic): $S E = C (K - P - Z V)$
- $S E = \rho S (S/\tau)^2$ 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 transient flux parameterization, but in an unsteady simulation framework

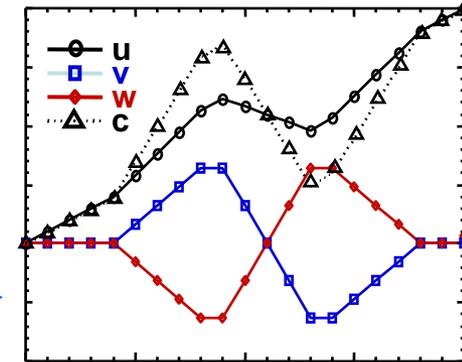
Energy couplings require an additional eddy operation



Advection:
Triplet map
is applied to
all properties
(velocities
u, v, w and
scalar, c)



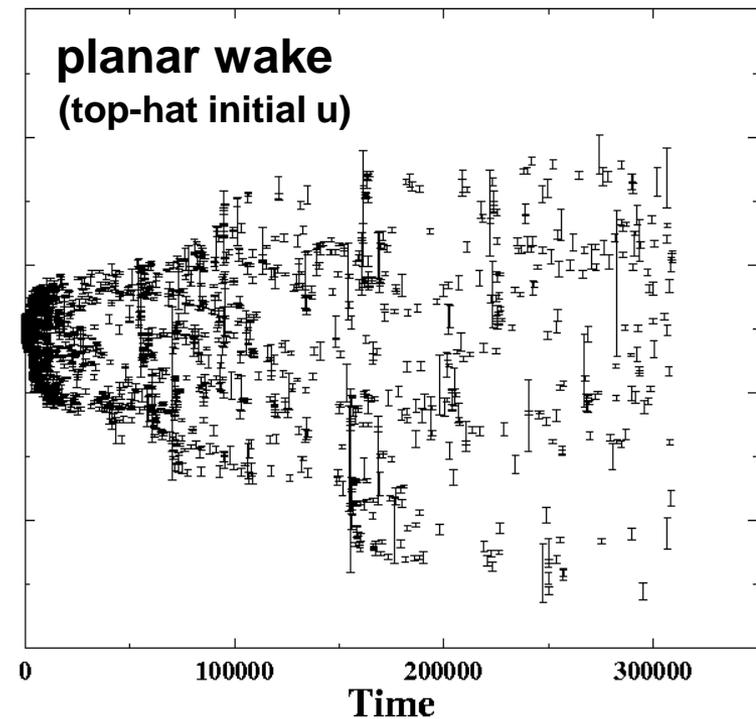
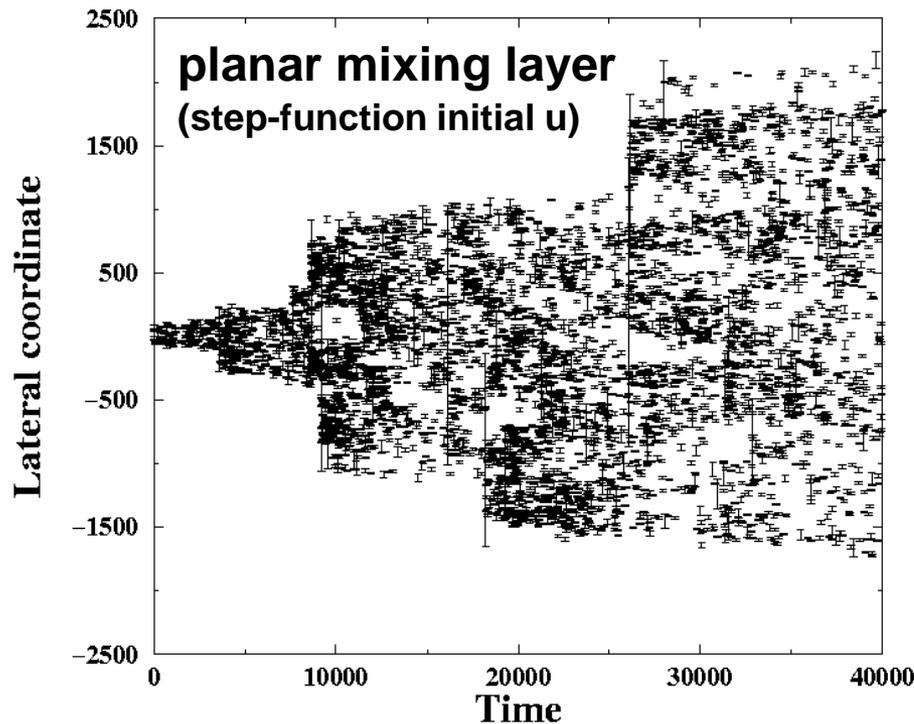
**Kernels are
added to
velocities
but not
scalar**



- 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

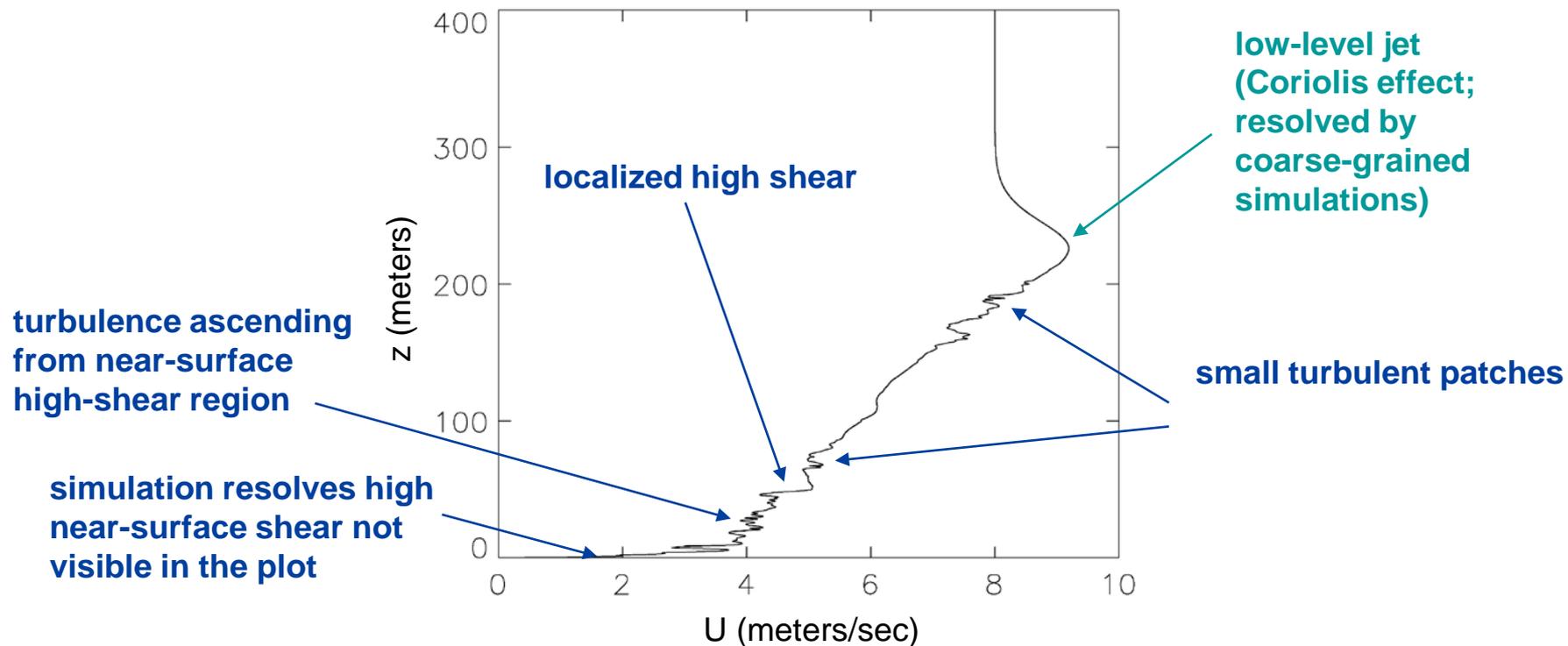


- Each vertical line shows the spatial extent of an eddy
- Horizontal location is its time of occurrence
- Units are arbitrary

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Eddy-viscosity closure within ODT enables atmospheric flow simulations



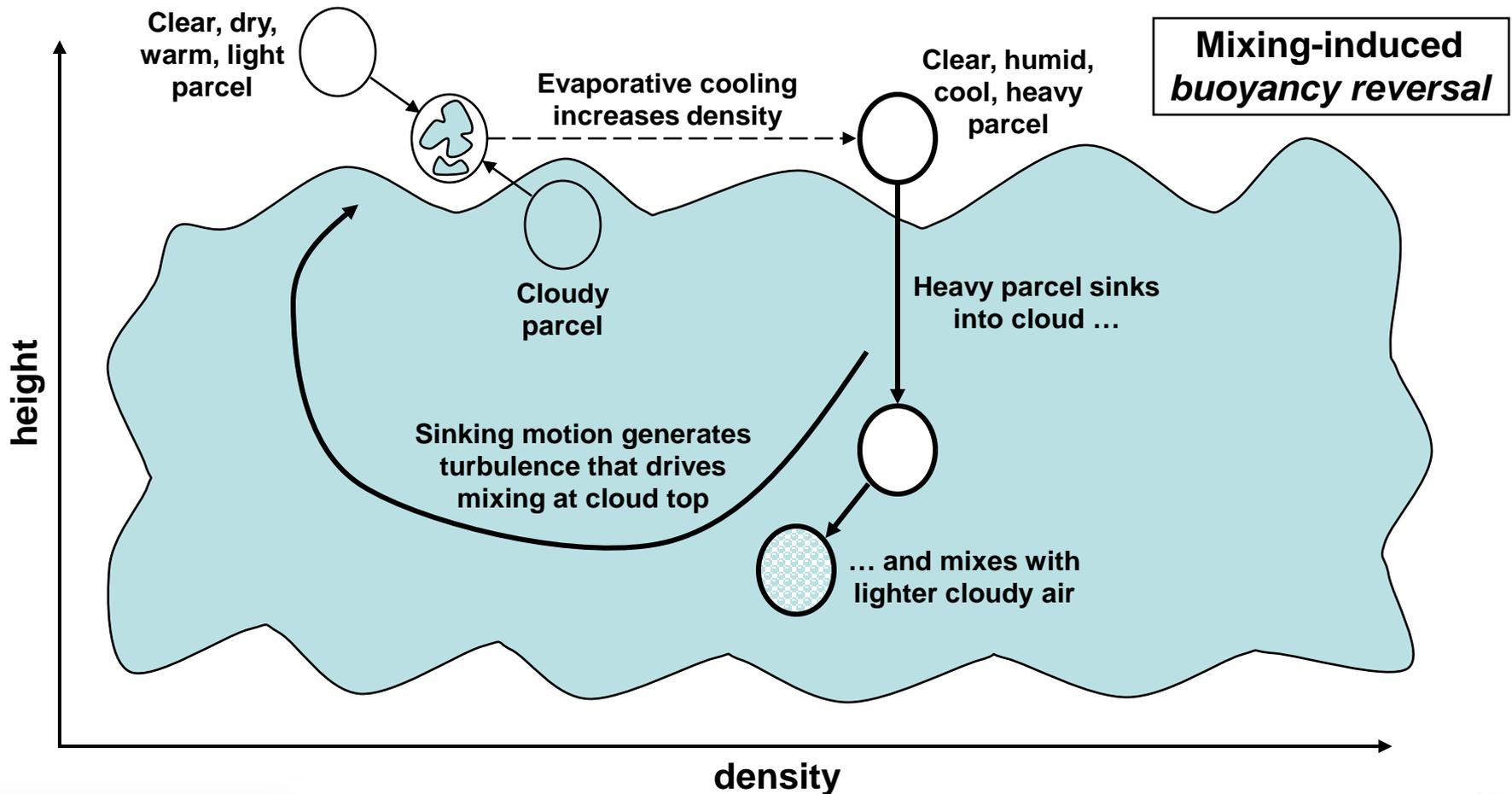
- An instantaneous vertical (z) profile of horizontal velocity (U) is shown
- Simulation corresponds to clear, stably stratified conditions (surface cooling: GABLS inter-comparison case)
- 16000 computational cells, resolving 2.5 cm
- Roughly 100 eddy events / sec

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

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:

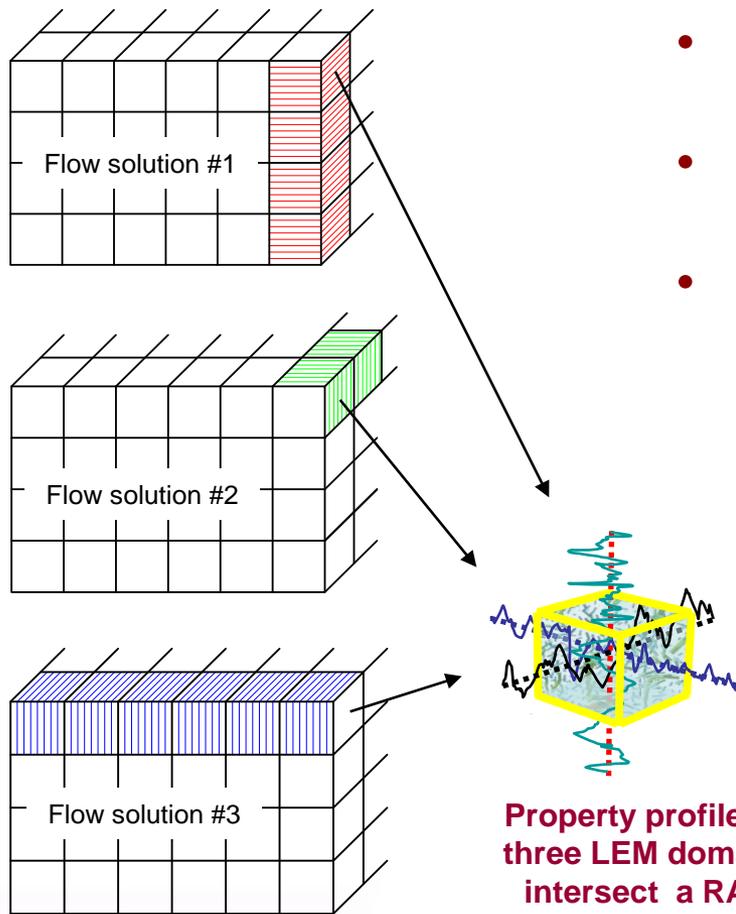
[turbulent diffusivity]/[kinematic viscosity]

ODT is uniquely applicable over wide ranges of Sc and Re values, allowing validation at high Sc and moderate Re (liquid-phase laboratory experiments) and subsequent application at $Sc \approx 1$ and high Re (atmospheric flow)

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

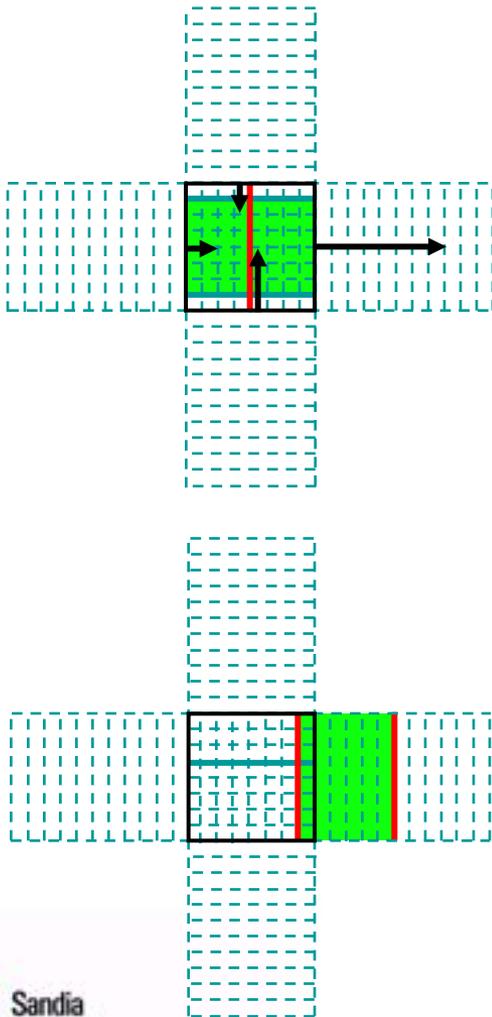


Property profiles on the three LEM domains that intersect a RANS CV

- 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 RANS eddy diffusivities to determine local eddy frequencies
 - Cell transfers (conservative mapping) couple domains
 - 3D representation of large-scale motions
 - Transfers implement displacements prescribed by RANS mean velocities

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

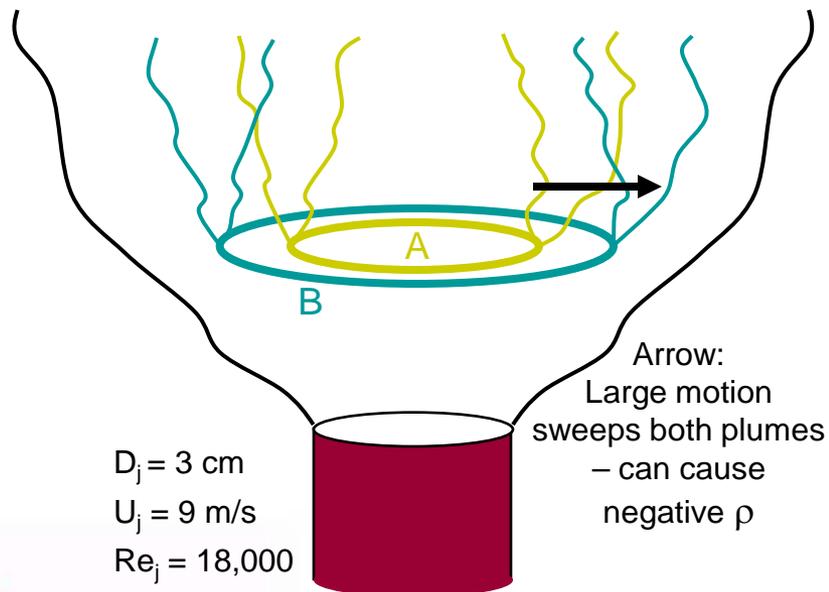
A 2D example illustrates the domain-coupling procedure



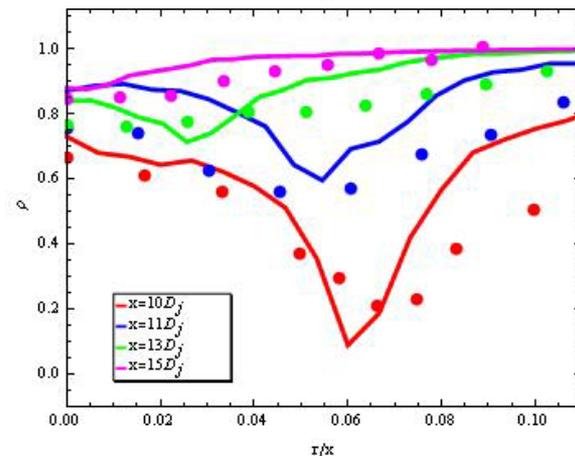
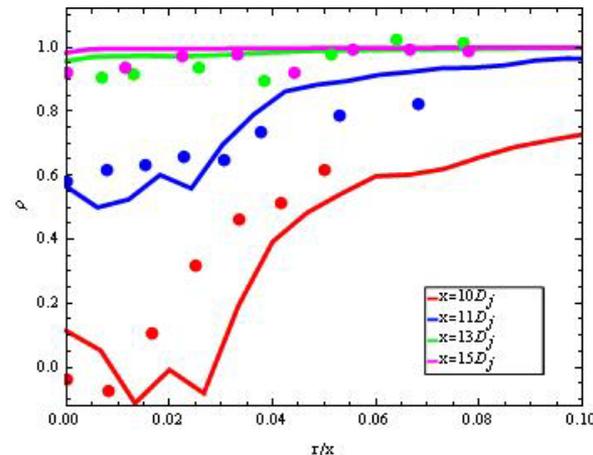
- Arrows are RANS CV face-normal displacements (velocities \times time step)
 - In this example, there is net vertical inflow and net horizontal outflow through CV faces (box)
 - Horizontal LEM domain: cut at **red** line and displace uniformly on either side, leaving a gap
 - Vertical LEM domain: remove **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: —)



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
- Implementation strategy:
 - Can use coarser 3D mesh than LES due to standalone ODT capabilities
 - Incorporates large scale 3D effects to improve ODT representation of
 - **stably stratified turbulence (by capturing internal waves)**
 - **Rayleigh convection (by capturing ‘wind of turbulence’)**
 - **etc. (greatly expands the range of possible applications)**

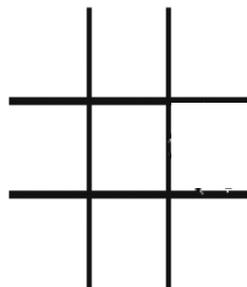
Treatment of 3D pressure-velocity coupling distinguishes two ODT3D formulations

- Incompressible formulation (used to date):
 - Continuity enforced using coarse-grained (CV scale) 3D pressure projection
 - ODT-resolved flow field is modified accordingly, a downscale coupling
- Pseudo-compressible formulation (under development):
 - Enables domain coupling with no coarse-graining or downscale coupling
 - Hence termed 'Autonomous Microscale Evolution' (AME)

ODT3D resembles superparameterization (SP) closure of atmospheric flow simulations

- SP: small scales resolved in 2D (vs. 1D in LEM and ODT)
- As with ODT3D, there are several SP implementation strategies

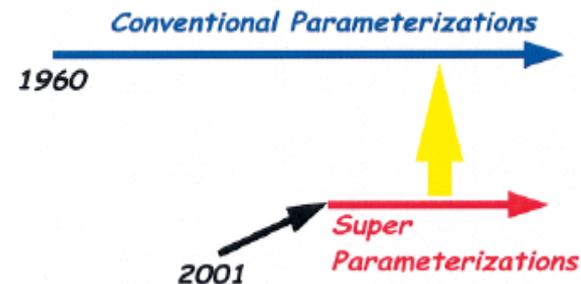
top view of a lattice-work of coupled vertical planar domains



side view of one domain (2D cloud simulation)



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



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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 Scott Wunsch
- 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 a cost-effective strategy for simulation of turbulence-microphysics couplings in diverse geophysical flows
- Its uses include
 - Fundamental studies
 - Input to other modeling approaches
 - Building block for 3D simulation