

Sub-Structure Modeling for Semi-Super-Parameterization

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Cloud Modeling Workshop



Sandia National Laboratories
Combustion Research Facility



Outline of presentation



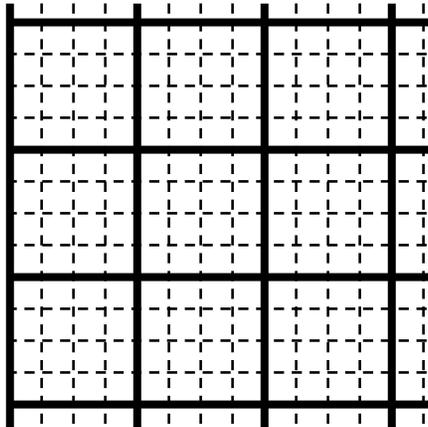
- **Introduction to semi-super-parameterization**
- **Sub-structure model**
 - Formulation
 - Illustrative applications
- **Features of semi-super-parameterization**



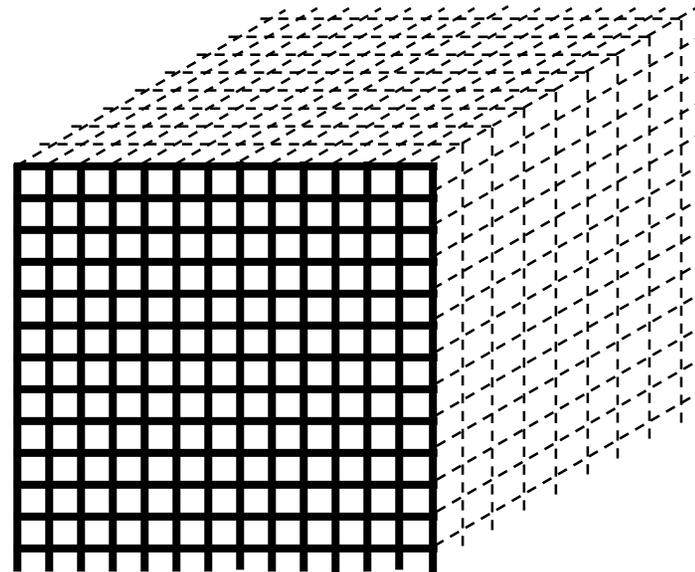
Super-parameterization combines two conventional CFD cost-reduction methods



Coarse graining:



Reduced dimensionality:



computational mesh



mesh needed to resolve all physics



Strategy: Use the mesh dimension best suited for each range of scales

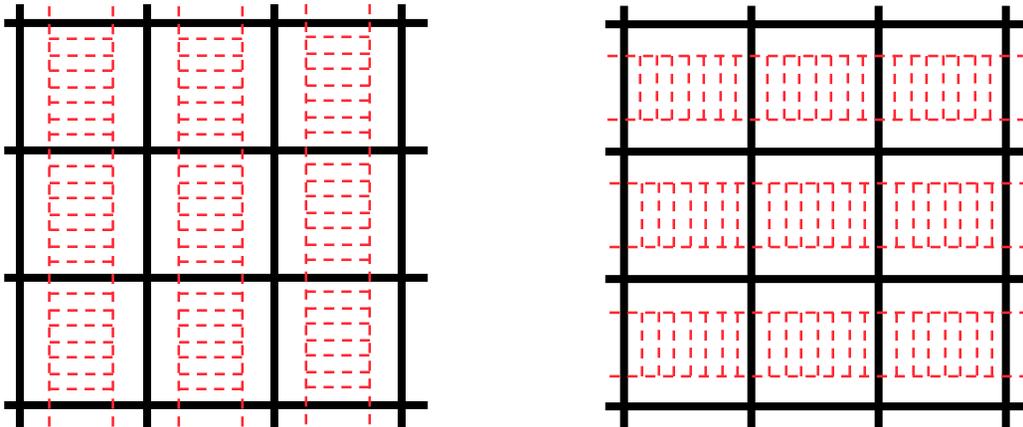


Large-scale advection is inherently 3D, but lower dimensionality can suffice at smaller scales, e.g.:

- 2D cloud-resolving model within a GCM: **super-parameterization**
- 1D model within a coarse-grained 3D simulation: **semi-super-parameterization**

Schematic of semi-super-parameterization:

1D substructure in each coordinate direction



Semi-super-parameterization is suitable for:

- Combustion
- Boundary layers
- Dry convection
- Cloud mixing/microphysics
- Stratocumulus?



Ideally, this can be implemented as autonomous flow advancement



Semi-super-parameterization concept:

- 1D resolution scale (small time step):
 - Substructures in each coordinate direction evolve independently
- 3D resolution scale (large time step):
 - Substructures in each direction interact by property fluxes
 - Substructures in the other directions determine those fluxes
 - This coupling communicates 3D effects to the 1D substructures

**The flow state is entirely represented within substructures;
spatial filtering of flow variables is done only for output**

**Current implementation: A related but distinct formulation
(Rod Schmidt's presentation)**

As in super-parameterization, there are many possible formulations



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Flow evolution within substructures is modeled using *One-Dimensional Turbulence* (ODT)



A one-dimensional model emulating 3D turbulence, including turbulence-microphysics interactions, has been developed and extensively demonstrated

- It combines two well-known 1D approaches:
 - *The 1D boundary-layer formulation* of the equations of motion, with ICs and BCs corresponding to various inhomogeneous flows: Captures the combined effects of advective and molecular transport
 - *Stochastic iterated maps*: capture the multiscale dynamics of the advection-dominated (inertial) subrange of homogeneous turbulence
- It incorporates widely used *mixing-length phenomenology*



Unlike other 1D (and 3D) approaches, ODT does not involve averaging



Exact equations of motion (Navier-Stokes equation, scalar transport equation):

$$\mathbf{u}_t + \mathbf{u} \cdot \nabla \mathbf{u} = \nu \nabla^2 \mathbf{u} - (1/\rho) \nabla p \quad \theta_t + \mathbf{u} \cdot \nabla \theta = \kappa \nabla^2 \theta$$

To obtain a turbulence model in 1D, apply the *boundary-layer approximation* and either

- replace ν and κ by ν_e and κ_e (conventional; represents advection by diffusion)
- or
- replace $\mathbf{u} \cdot \nabla$ by a different advection process (approach used here)

Simple example:

For constant-property time-developing flow, obtain the following **alternative modeling frameworks** for the *lateral (y) profile of streamwise velocity u*:

$$\begin{array}{lll} u_t = \nu_e(y,t) & \theta_t = \kappa_e(y,t) \theta & Pr_e \text{ (or } Sc_e) = \nu_e(y,t) / \kappa \\ u_t = \nu \frac{u_{yy}}{u} + \text{'advection'} & \theta_t = \kappa \frac{\theta_{yy}}{\theta} + \text{'advection'} & Pr \text{ (or } Sc) = \nu / \kappa \end{array}$$

neither framework is complete as written



ODT involves an explicit representation of turbulent eddies



On a 1D domain, molecular evolution based on a boundary layer formulation is supplemented by an ‘eddy process,’ e.g.,

$$u_t = \nu u_{yy} + \textit{eddies}$$

To specify the eddy process, need

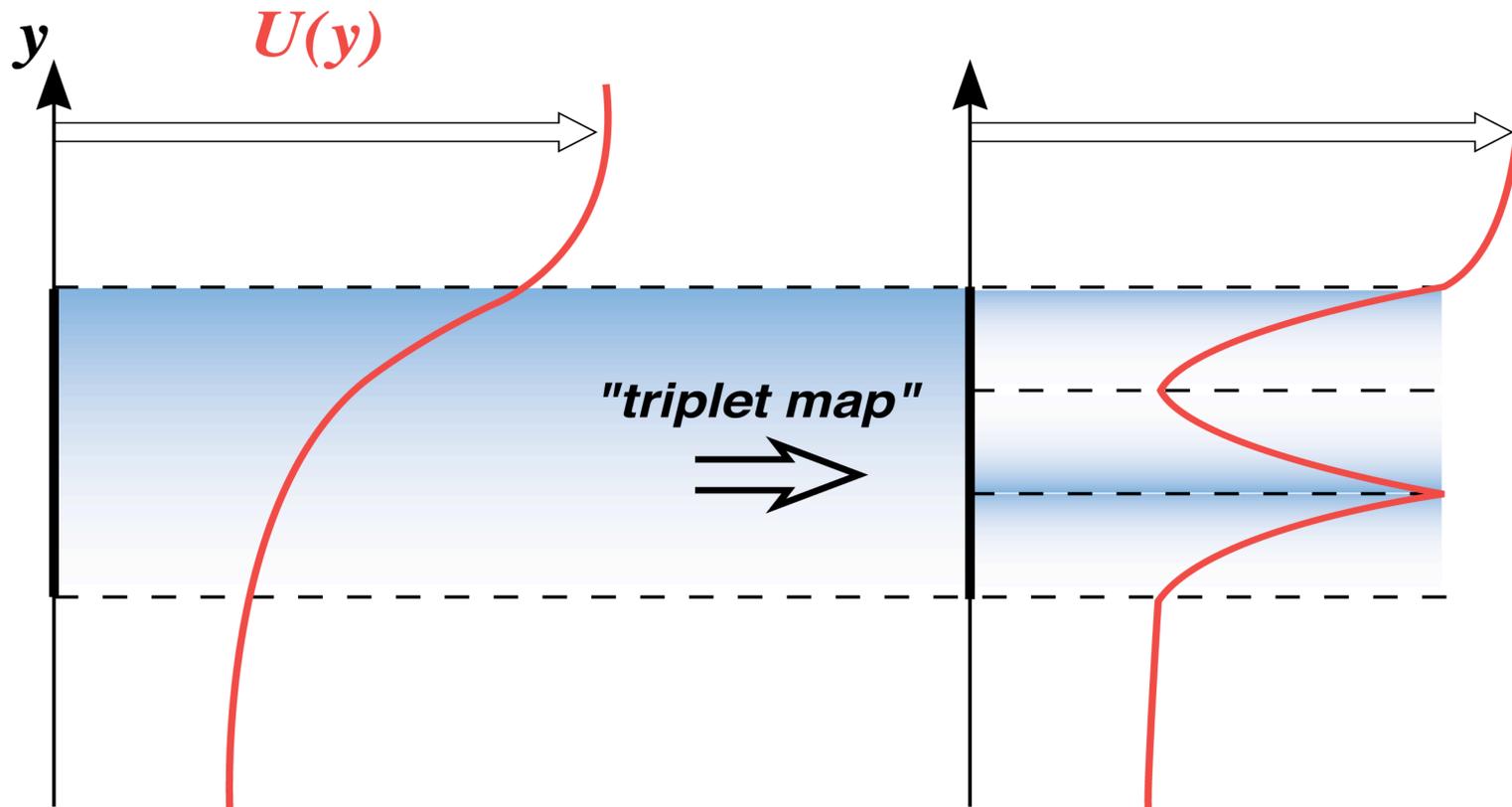
- Definition of an eddy (biography)
- Eddy selection procedure (demography)



The 1D turbulent 'eddy' amplifies shear; feedback induces an eddy cascade



- 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



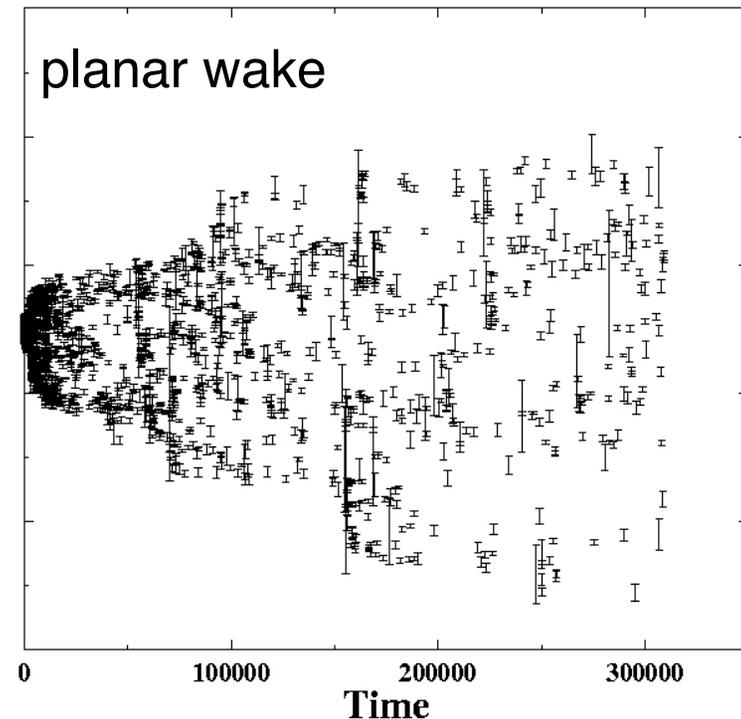
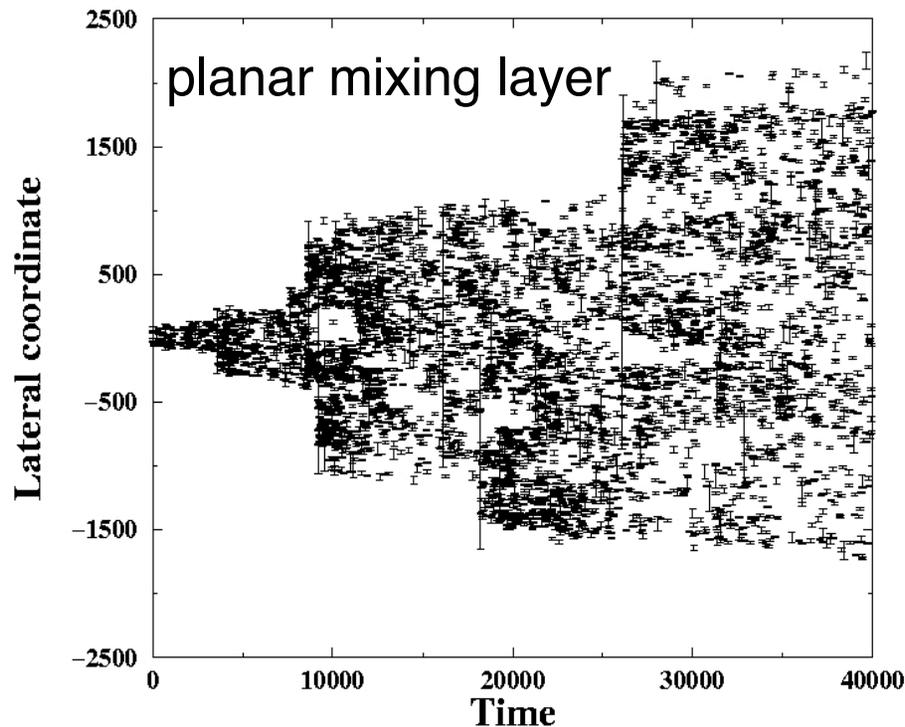
High shear at small scales drives small eddies, leading to an eddy cascade



ODT simulations provide detailed flow-specific representations of turbulence



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



These time-developing simulations are based on the evolution equation shown earlier, with flow-specific initial conditions (step-function and top-hat u profile, respectively), plus eddies



Eddy selection procedure



- Assign a time scale τ to each possible eddy, parameterized by eddy size and location within the computational domain
- The set of τ values defines an eddy rate distribution λ from which eddies are sampled

*The physics is in the determination of τ
(analogous to mixing-length theory)*



Determination of τ in ODT (schematic)



Principle: Enforce consistency of eddies and flow (velocity and density profiles)

Eddy: Eddy velocity $\sim l/\tau$ so eddy energy $\sim \rho l^3 / \tau^2$ (l = eddy size)

Flow: $P \equiv$ gravitational potential energy change caused by eddy

$K \equiv$ maximum kinetic energy extractable by adding *wavelets* to velocity components

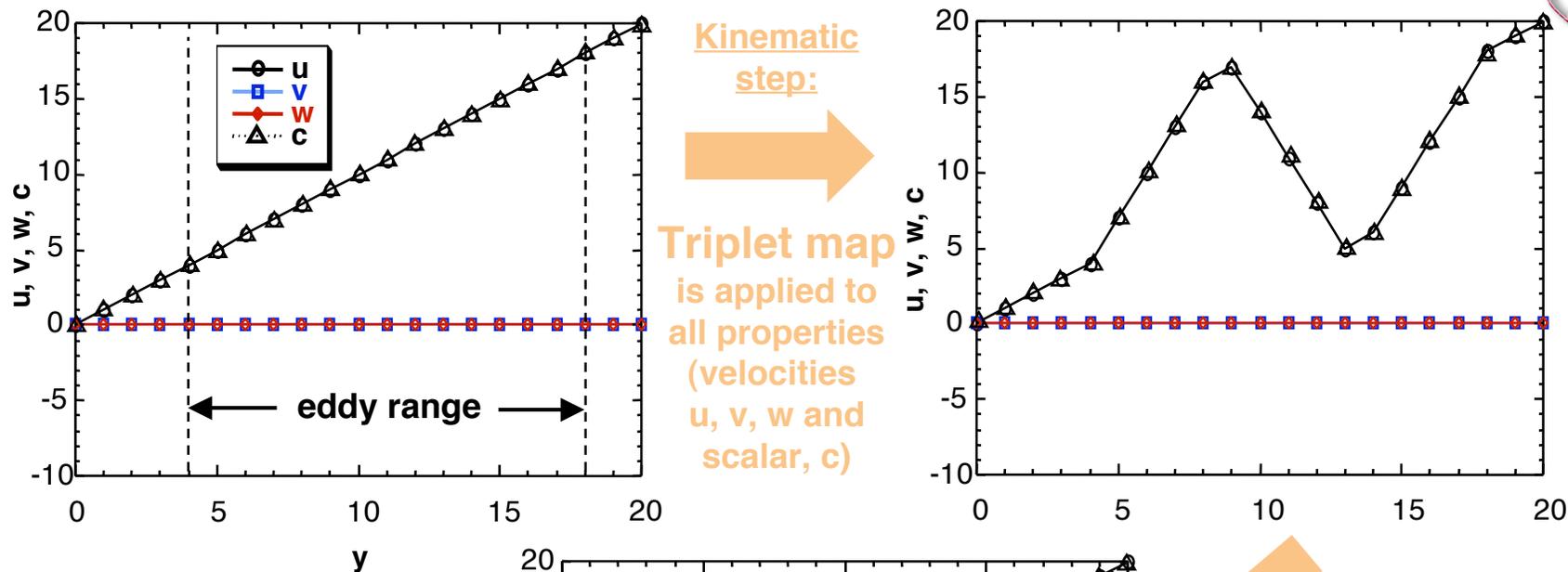
Relation determining τ :

$$\frac{\rho l^3}{\tau^2} = A \left(K - P - Z \frac{\mu^2}{\rho l} \right)$$

adjustable parameters viscous penalty (imposes a threshold Reynolds number)

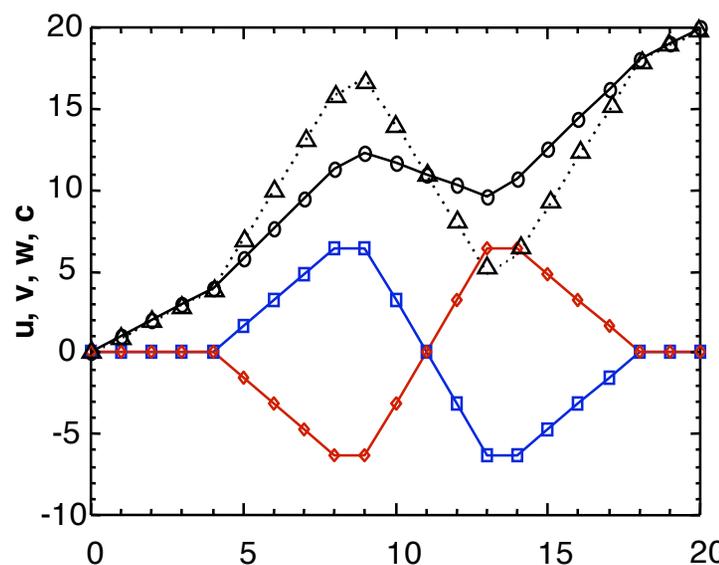


An eddy event consists of a triplet map followed by velocity profile changes



The dynamic step implements:

- Energy conversion (kinetic, potential, etc.)
- Pressure scrambling ('return to isotropy')



This approach is much like conventional mixing length theory



but

- The concept is applied to all l values, not to a single l value
- K and P are computed using the instantaneous state, not an average state
- Concurrent eddy and molecular processes are strongly coupled, thereby linking eddy dynamics to the flow configuration (ICs, BCs, body forces, fluid properties, etc.)



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One-Dimensional Turbulence (ODT) **captures fundamental turbulence properties**



Homogeneous turbulence:

- **Power spectra**
 - Inertial and dissipative subrange scalings (Kolmogorov)
 - Pr-dependent passive-scalar subrange scalings (Batchelor, etc.)
 - Buoyancy-driven scalar spectrum (Bolgiano-Obukhov)
- **Decay of grid turbulence**
- **Scalar mixing (variance decay, PDF evolution)**
- **Clustering of low-Stokes-number particles (or droplets)**

Inhomogeneous turbulence:

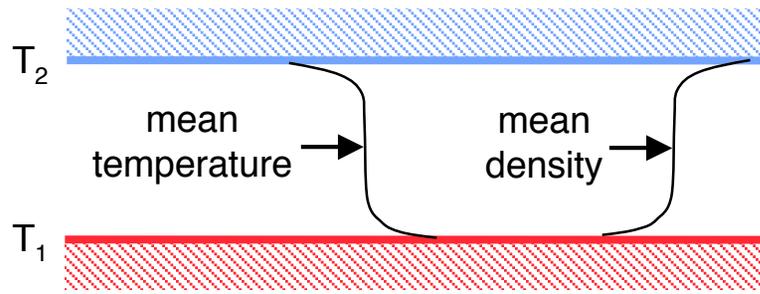
Representative examples are considered



Rayleigh-Benard convection is a simple flow configuration with complicated behaviors



Imposed temperature difference
 $T_1 > T_2$



Mean heat flux is independent of height, so mean temperature gradient is high where thermal diffusivity is low (near walls). Far from walls, eddy diffusivity dominates.

- **Parameters:**

- Ra: buoyant forcing scaled by viscous damping
- Pr: viscosity scaled by thermal diffusivity

- **Measured properties:**

- Nu: mean heat flux scaled by heat flux in motionless fluid
- Temperature and velocity fluctuations (variance, PDF)

- **Classical analysis (Priestley):**

- Near-wall flow unaffected by opposite wall
- Implication: $Nu \sim Ra^{1/3}$

- **Observation:** Scaling exponent depends on Ra and Pr



Nonclassical scaling implies wall interactions



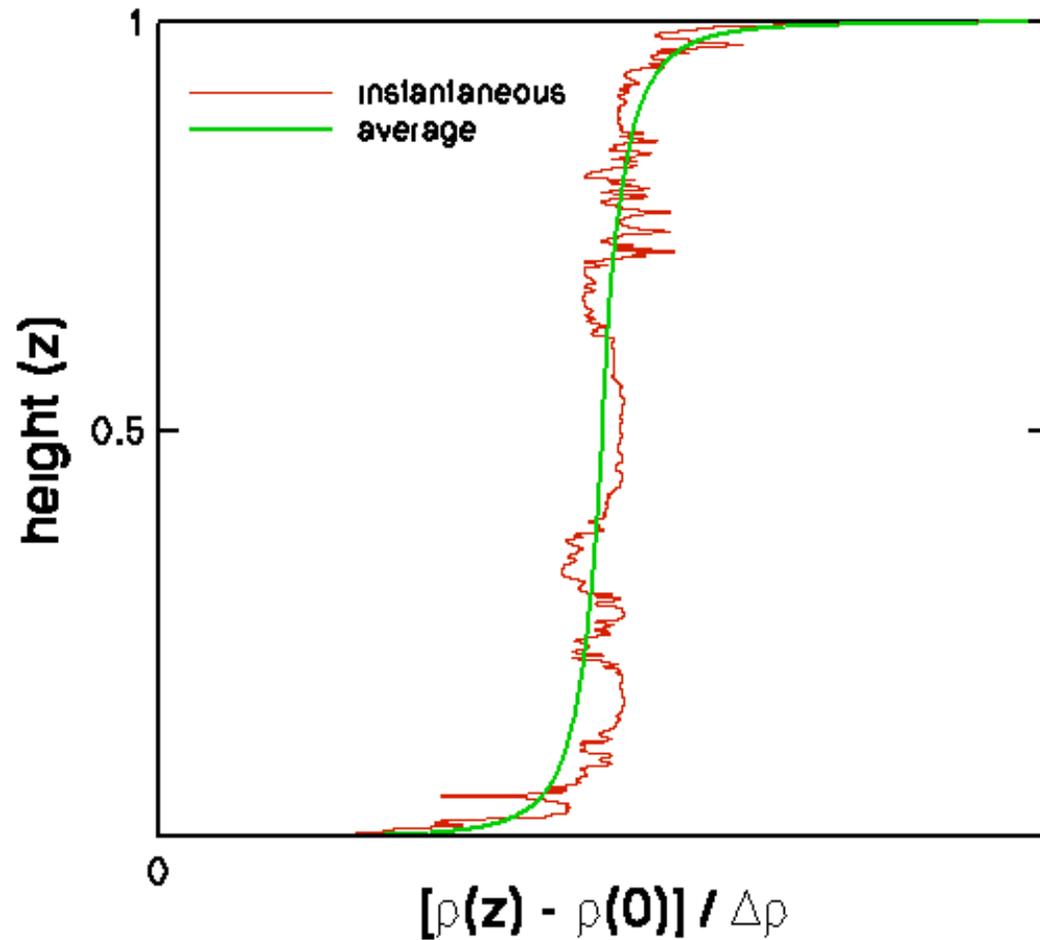
Two possible mechanisms:

- **Coupling via the mean density gradient in the central region**
- **Large scale motions**

**Large buoyant plumes
and large scale circulation
are seen in experiments**



Simulated Rayleigh-Benard density profile for $Ra = 1.4 \cdot 10^9$, $Pr = 0.7$



Other models need many parameters to fit $Nu(Ra,Pr)$ and say little about fluctuations

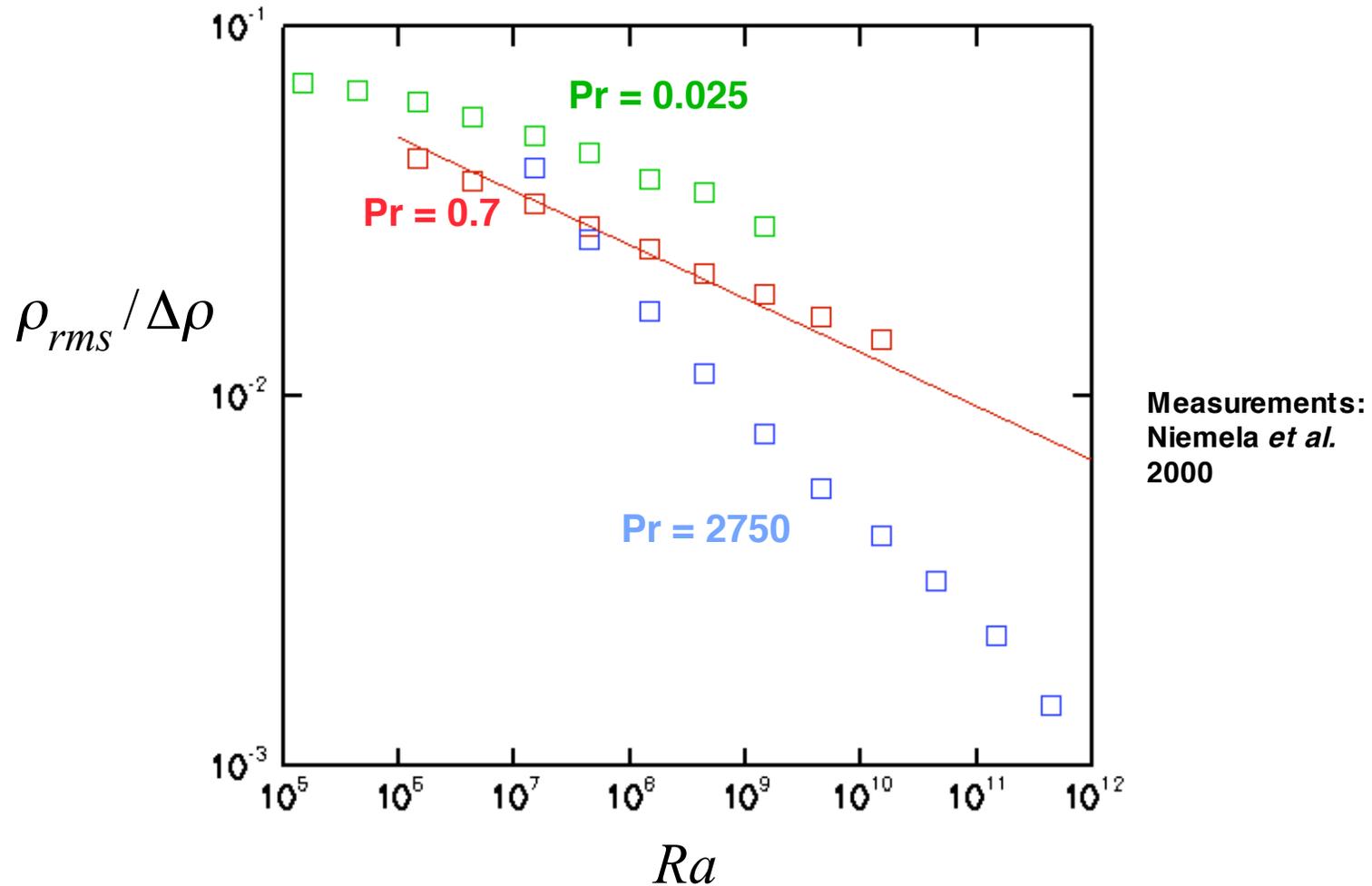


ODT application to Rayleigh-Benard convection:

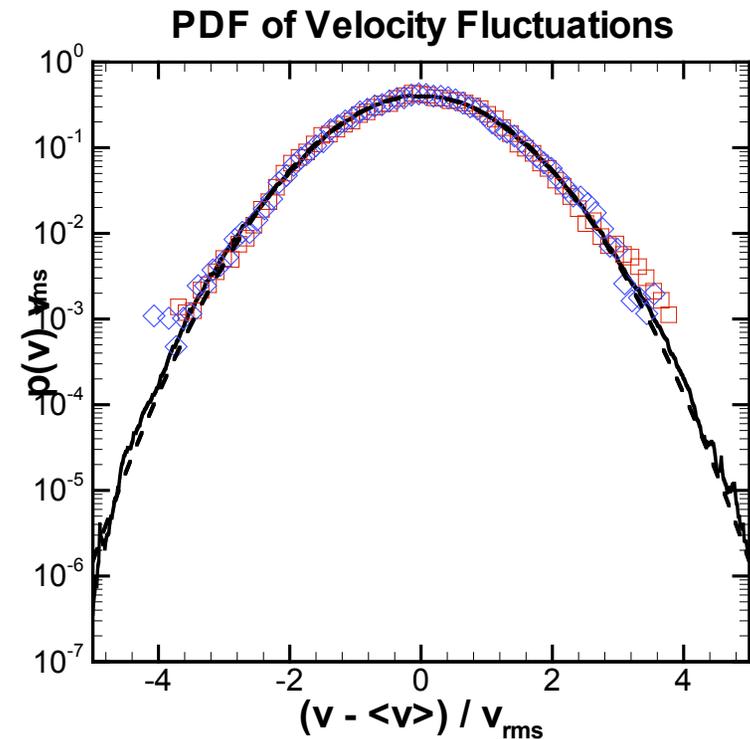
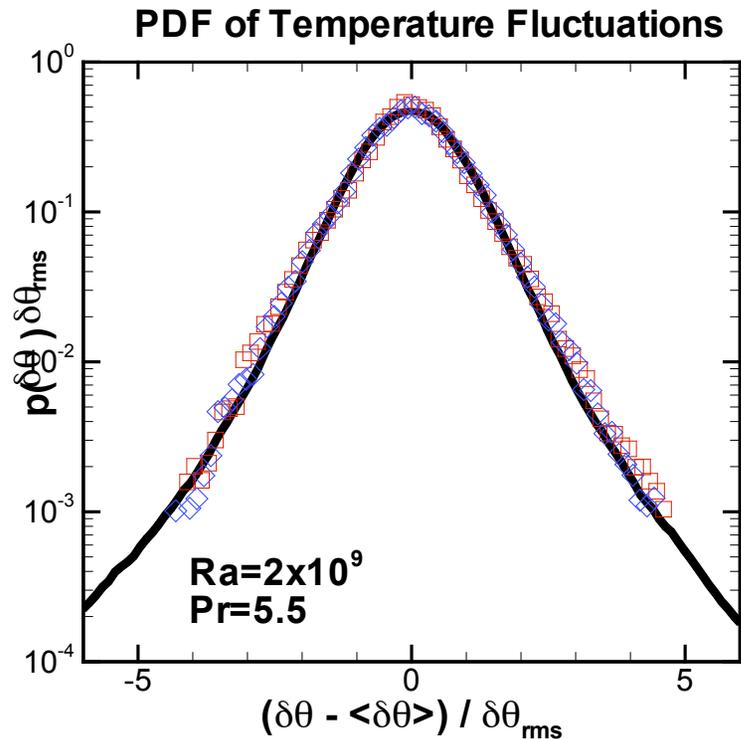
- **Adjust two parameters to fit $Nu(Ra,Pr)$**
- **Predict fluctuations**



Computed midplane density fluctuations match $Pr = 0.7$ data (curve) and predict Pr trend



and velocity PDFs match measurements



Measurements (Daya and Ecke 2002): □, cylindrical cell; ◇, rectangular cell

ODT: solid lines

Gaussian: dashed line



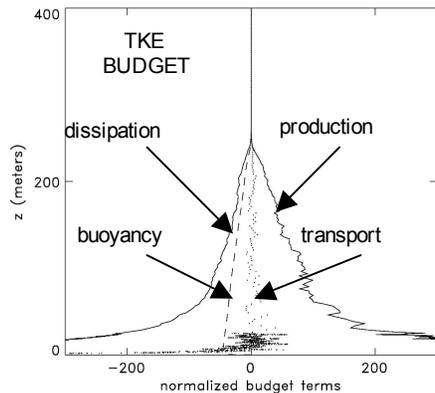
ODT is being used to study various environmental stratified-flow phenomena



- Penetrative convection
- Shear driven and convectively driven entrainment at stable density interfaces
- Stratified boundary layers
- Layering in stably stratified flow
- Mixing-induced buoyancy reversal
- Plume dispersal
- Mixing-controlled droplet growth in clouds
- Nuclear burning coupled to convection (supernovae)
- Multicomponent convection:
 - semiconvection (stars)
 - thermohaline staircase (oceans)

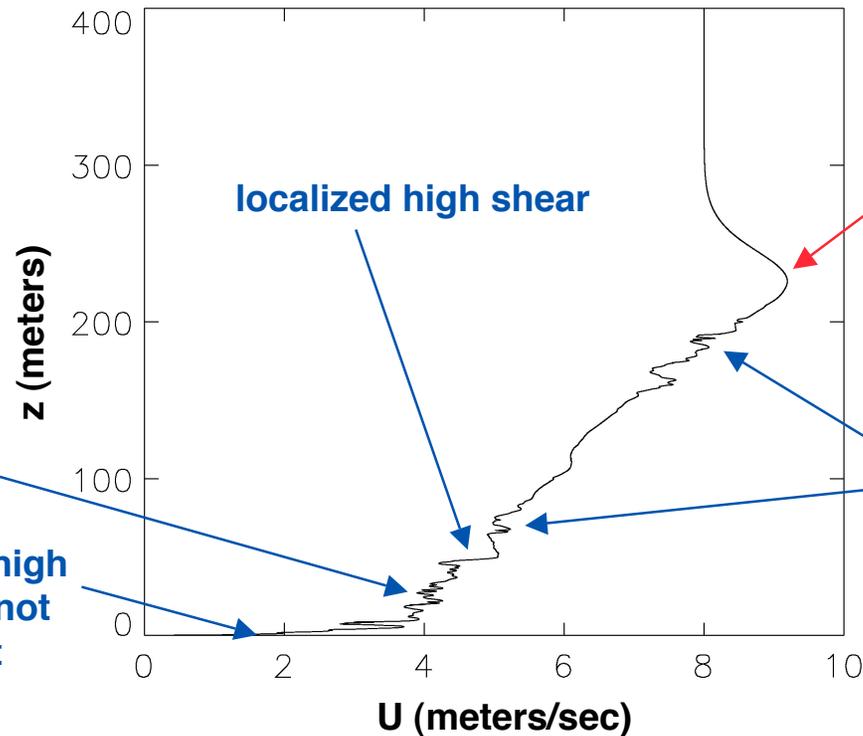


Eddy-viscosity closure within ODT enables atmospheric flow simulations



turbulence driven by near-surface shear

simulation resolves high near-surface shear not visible in the plot



low-level jet (resolved by coarse-grained simulations)

small turbulent patches

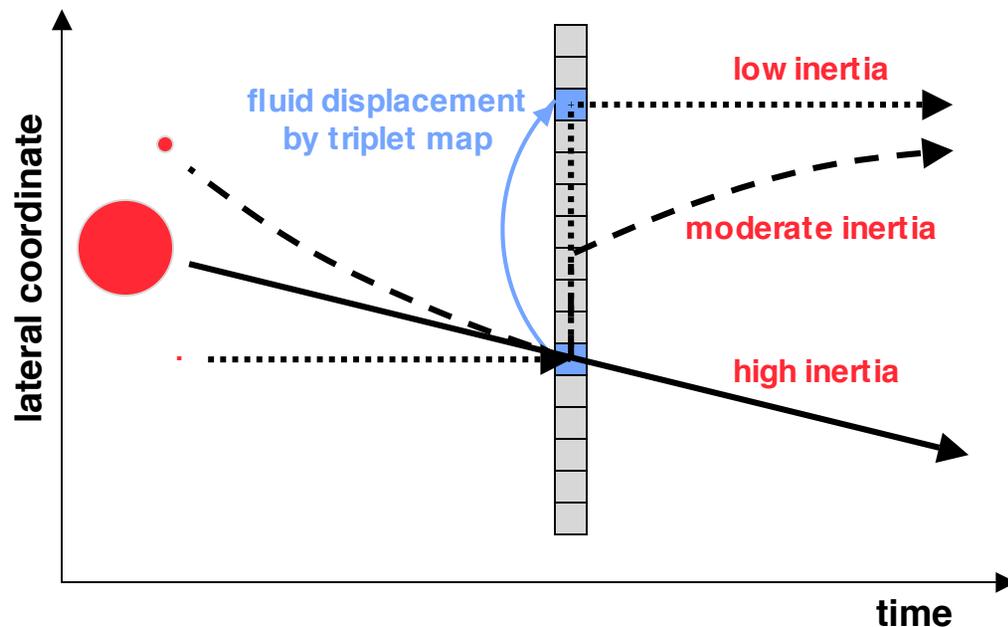
- An instantaneous vertical (z) profile of horizontal velocity (U) is shown
- Simulation corresponds to stably stratified conditions (surface cooling: GABLs inter-comparison case)
- 16000 computational cells, resolving 2.5 cm (roughness height)
- Approximately 100 eddy events / sec
- TKE budget resembles LES (Kosovic and Curry 2000, Cuxart *et al.* 2005)



A particle-eddy interaction couples entrained particles to fluid motion



- 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 τ



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

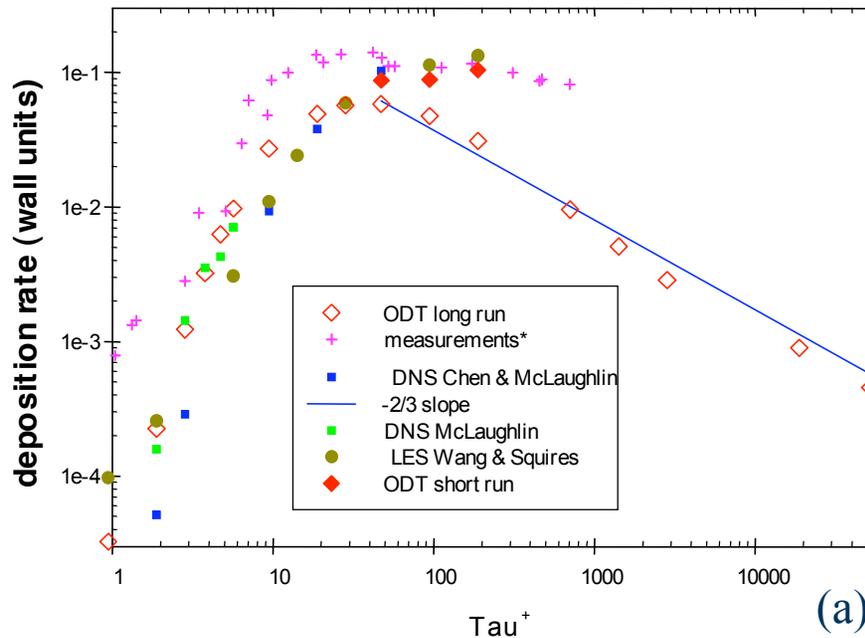


This approach provides a unified treatment of particle deposition regimes

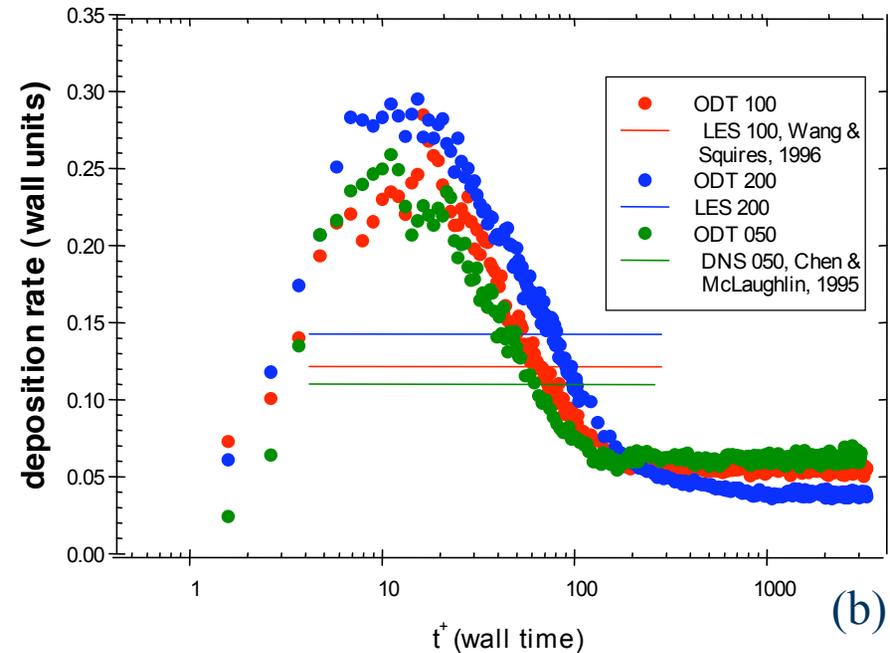


Wall deposition in turbulent channel flow (based on one-way coupling)

Dependence on Stokes number



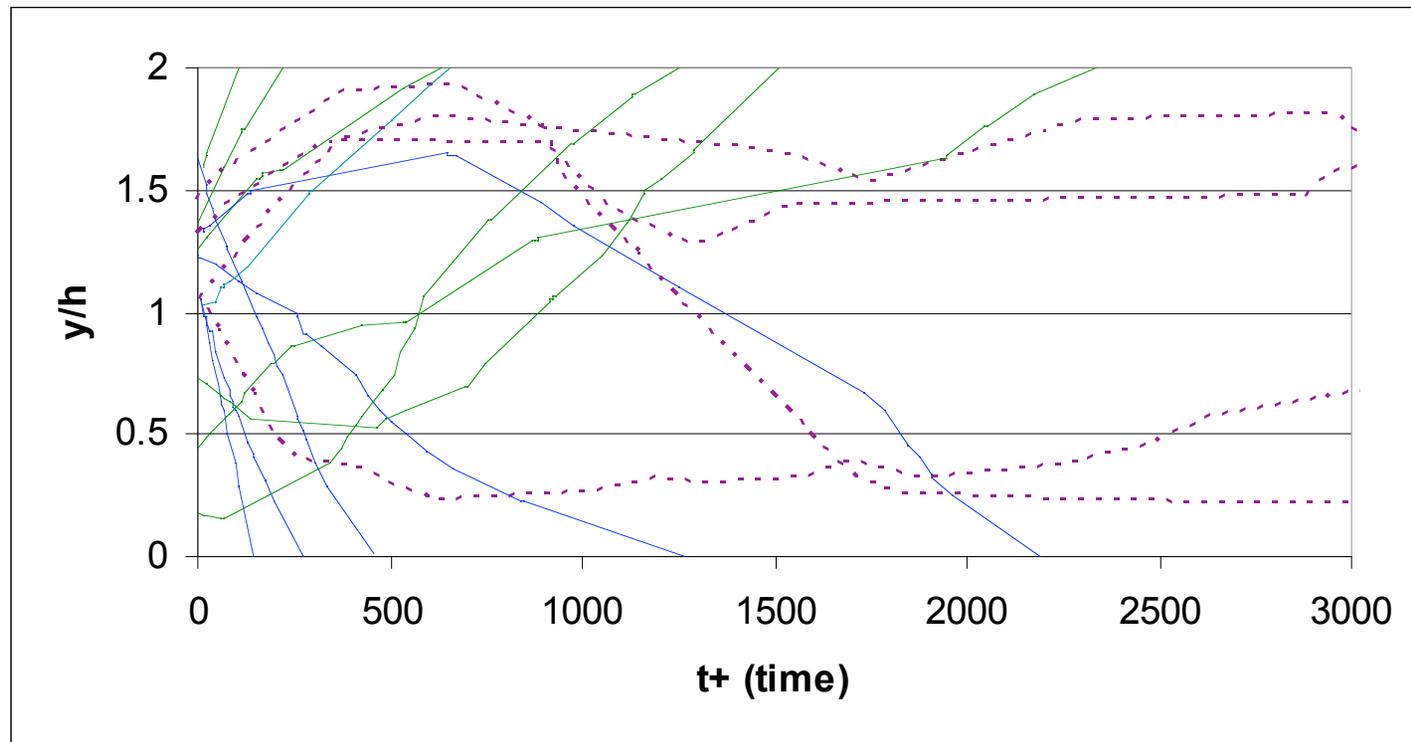
Time variation of deposition rate
(transient relaxation)



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



Representative particle trajectories



Disclaimer: DNS and LES results could be accurate long-time results; the true onset of the high-inertia asymptote might occur at larger Stokes number than predicted by ODT



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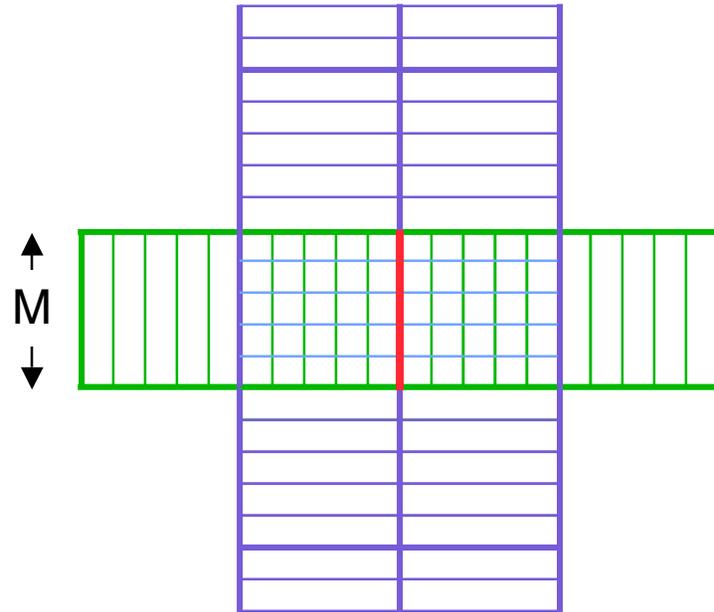
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Concept: 3D compressible turbulence simulation based on evolution on coupled ODT domains



- Along each domain:
 - 1D gas dynamics
 - ODT eddy events
- Lateral coupling of adjacent domains is based on fluxes in domains oriented in the direction of coupling
- This formulation:
 - Obeys applicable conservation laws
 - Reduces to DNS for flows resolved at scale M



ODT evolution on the *horizontal* domain determines fluxes that laterally couple the *vertical* domains across a *common face*

(Rod Schmidt will present an incompressible formulation)



With eddy-viscosity closure instead of ODT, this reduces to a conventional approach



- With eddy-viscosity subgrid-scale momentum closure instead of ODT, this becomes an alternating-direction advancement scheme for large-eddy simulation (LES) without 1D substructure
- Apart from the additional spatial and temporal resolution of micro-scale processes that ODT provides, **the roles of ODT and eddy viscosity with regard to impact on large-scale flow are analogous**



Conclusions



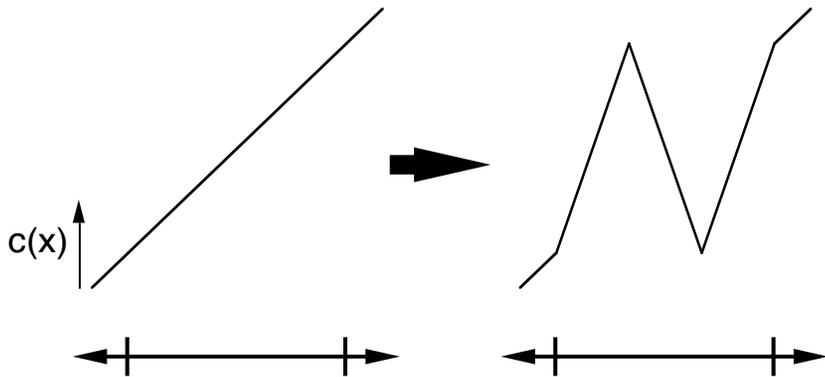
- **A new turbulent flow simulation approach, formulated in 1D but applicable in a 3D framework, provides a unified representation of processes at all scales**
- **This motivates the concept of semi-super-parameterization**
- **The performance of the 1D formulation indicates that the mixing-length concept, *applied locally* (in space and time), is a sound basis for modeling turbulence flow processes at all scales**



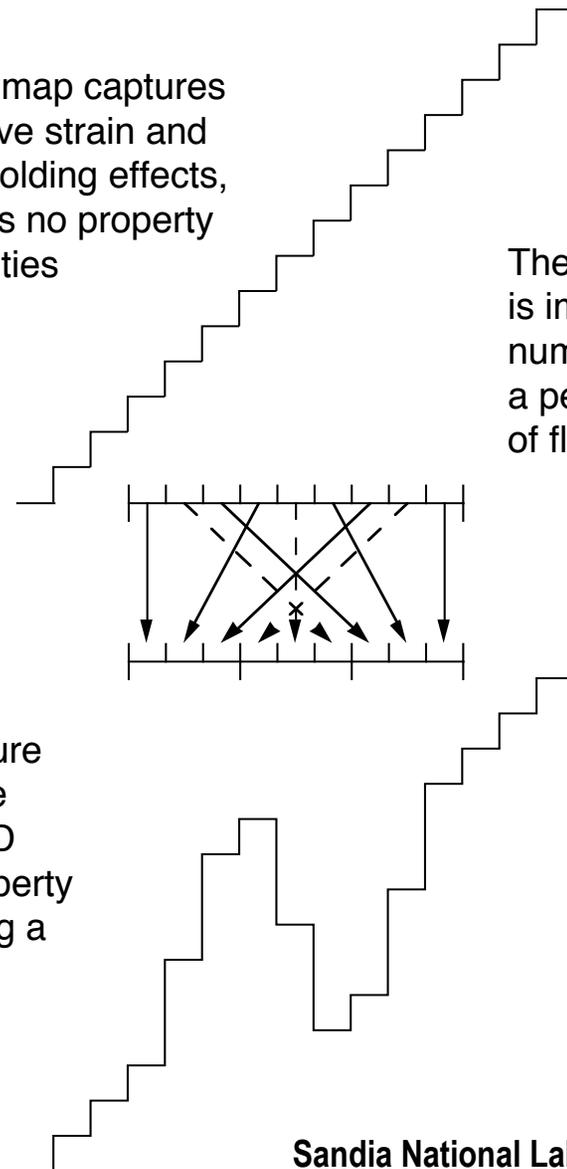
Backup slides follow



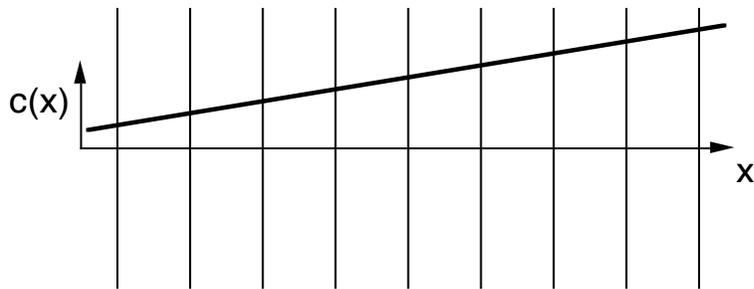
The *triplet map* is a 1D procedure that emulates 3D eddy kinematics



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



The triplet map is implemented numerically as a permutation of fluid cells



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

