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Turbulence Simulation in One Spatial Dimension Using Map-Based Advection

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Exa Corporation

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Outline of presentation

- Map-based advection
- Introduction to One Dimensional Turbulence (ODT)
- Model and algorithm extensions
- Spontaneous layer formation in buoyant stratified flow
- Subgrid implementation (‘superparameterization’)
- Conclusions

The conventional representation of turbulent advection as enhanced diffusion omits important physics

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

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

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

- **average and replace ν and κ by ν_e and κ_e (usual: represents advection by diffusion)**

or

- **replace $u \cdot \nabla$ by a different advection process (approach used here: no averaging)**

Simple example:

For time-developing unforced flow, obtain the following alternative modeling frameworks for the lateral (y) profile of streamwise velocity u and a passive scalar θ:

$u_t = \nu_e(y,t)\, u_{yy}$ $\qquad$ $\theta_t = \kappa_e(y,t)\, \theta_{yy}$ $\qquad$ Pr_e (or Sc_e) $= \nu_e(y,t) / \kappa_e(y,t)$

$u_t = \nu u_{yy}$ + ‘advection’ $\qquad$ $\theta_t = \kappa \theta_{yy}$ + ‘advection’ $\qquad$ Pr (or Sc) $= \nu / \kappa$

neither framework is complete as written

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Basic properties of advection should be preserved

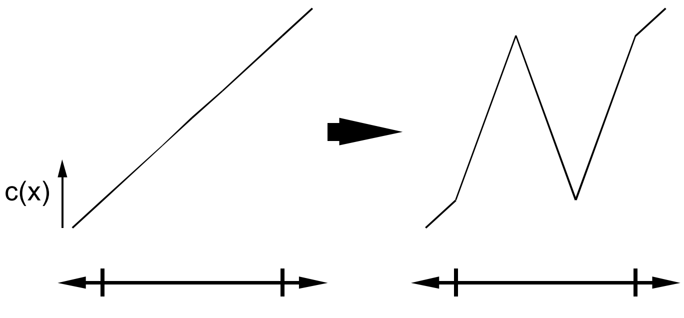
Advection

- moves fluid parcels without intermixing their contents
- conserves energy, momentum, mass, species, etc.
- changes the separation of neighboring parcels gradually

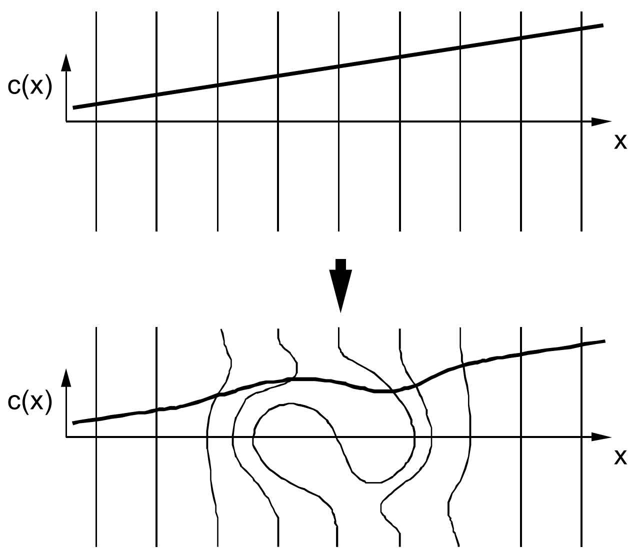
Key to a 1D advection model:

For many purposes, it is not essential to change the absolute fluid location gradually

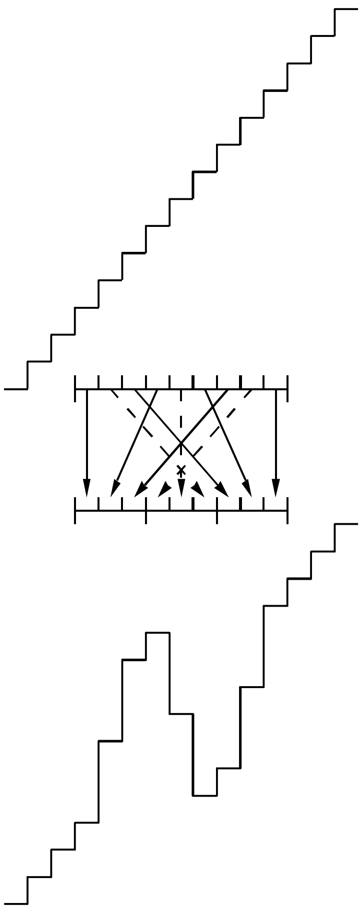
Advection is modeled as a sequence of *triplet maps*, which preserve desired advection properties



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



This procedure emulates 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)

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

- Linear-Eddy Model (LEM): Map occurrences and properties (size, location) are sampled from fixed distributions
  - Parameters determining these assignments based on the turbulent flow state at each location must be provided as input
  - LEM evolves scalar profiles but not velocity, hence is a turbulent mixing model, not a turbulence model

- One-Dimensional Turbulence (ODT): Eddy sampling is based on the flow state evolved by the model
  - After parameter adjustment, ODT predicts turbulence evolution
  - The required 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:

$u_t = \nu u_{yy}$ + 'eddies' — ODT only

$\theta_t = \kappa \theta_{yy}$ + 'eddies' — LEM or ODT

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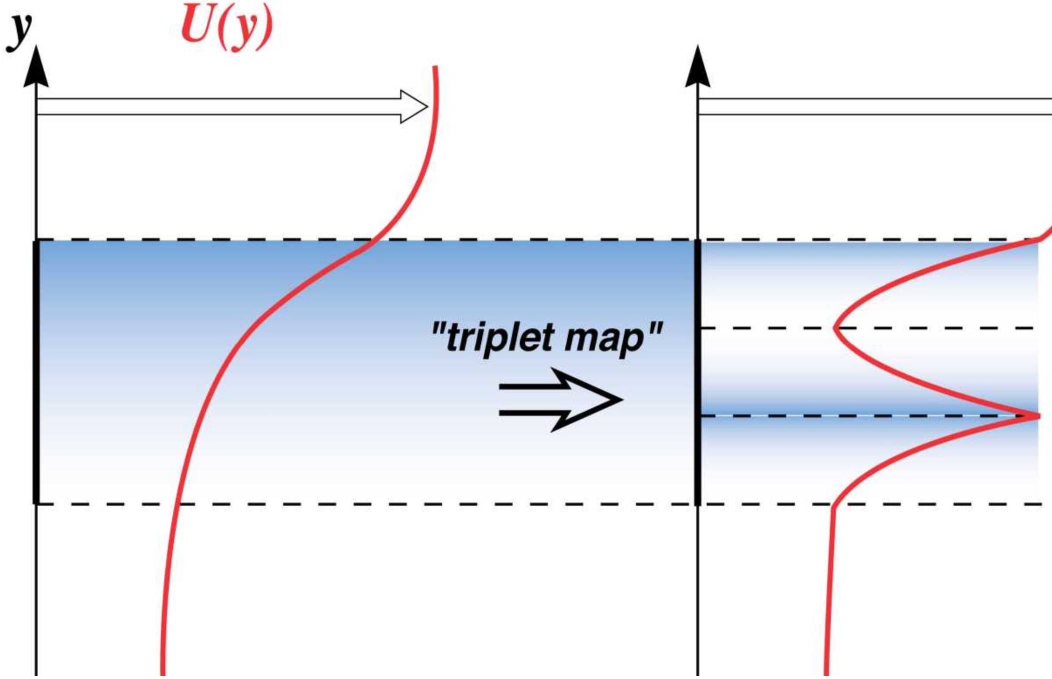
In ODT, the triplet map amplifies shear, inducing an *eddy cascade* (feedback mechanism)

- **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

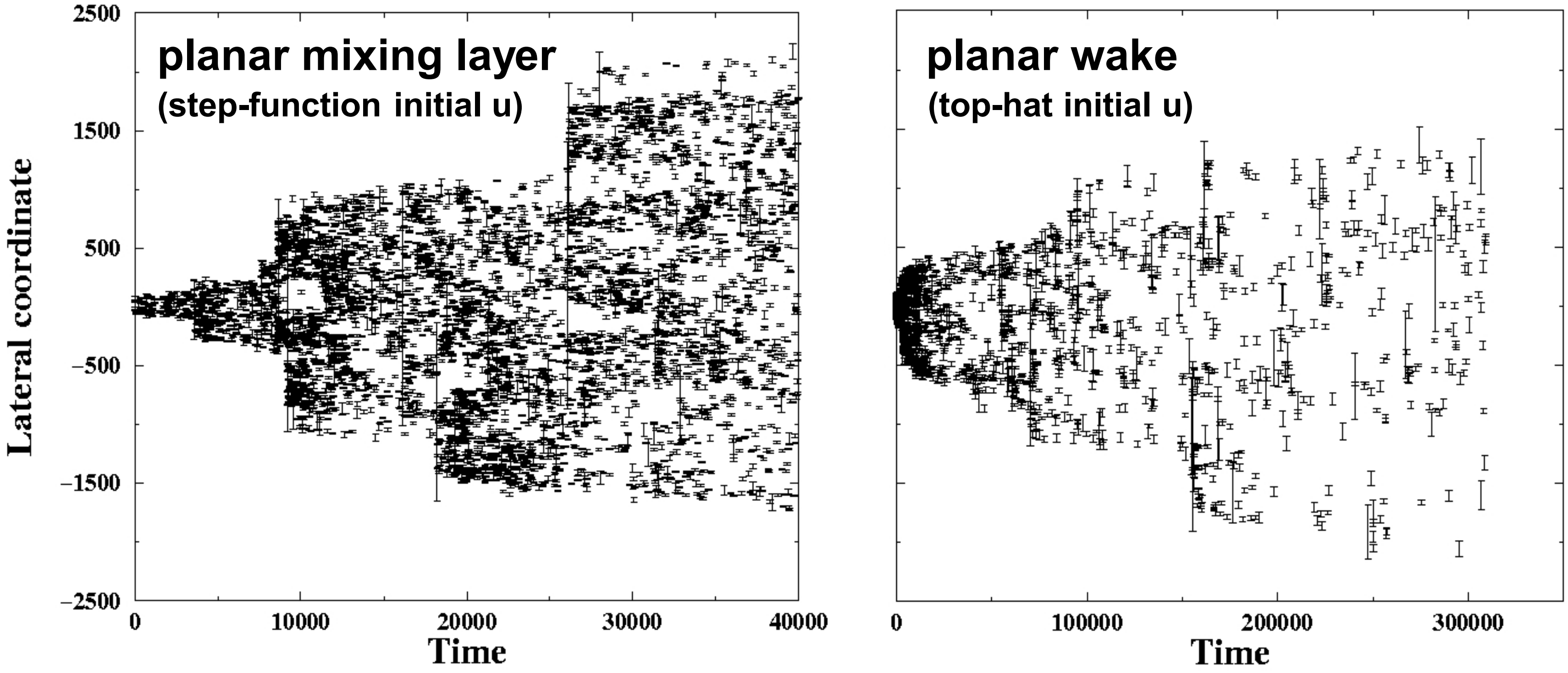
- Each possible eddy, defined by eddy spatial location and size (S), is assigned a time scale τ based on the local flow state
- A simple choice: $\tau \sim S / |U_+ - U_-|$ where +,– denote eddy endpoints
- The set of τ values determines an eddy rate distribution from which eddies are sampled
- Unlike 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), τ can be based on an energy balance

- **Energy balance (schematic): S E = C (K – P – Z V)**
  - **S is the eddy size**
  - **E = ρ (S/τ)^2 is the eddy kinetic-energy density**
  - **K is the ‘available’ kinetic energy of velocity profiles within the eddy**
  - **P is the gravitational potential energy change caused by the eddy**
  - **V is a ‘viscous penalty’ (imposes a threshold eddy Reynolds number)**
  - **C and Z are free parameters**
- **This relation determines the eddy time scale τ**
- **Within the size-S region, the velocity profile(s) are adjusted (wavelet method) so that total (kinetic + potential + …) energy is conserved**
- **This framework accommodates various energy couplings, e.g., pressure scrambling, compressibility effects, surface tension**

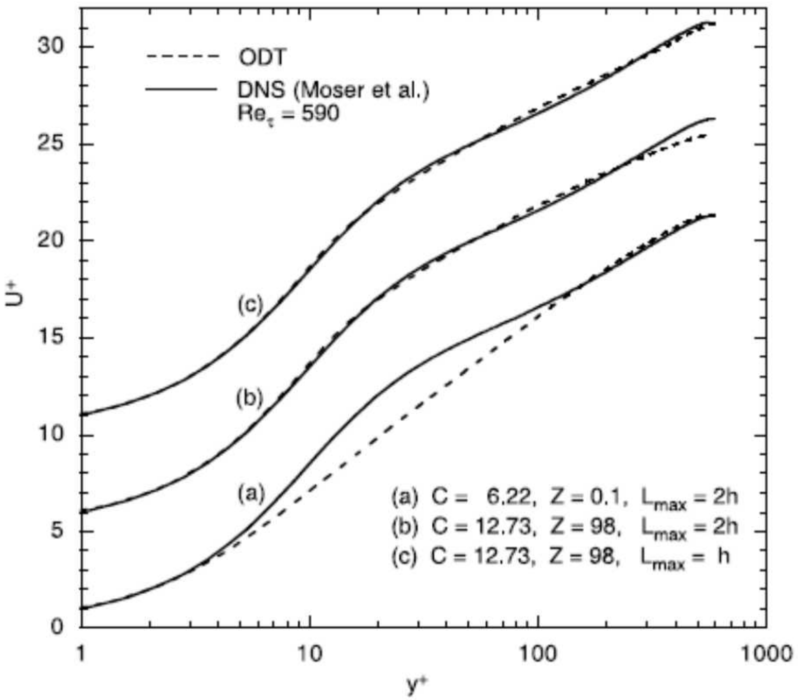
ODT simulations provide detailed flow-specific representations of turbulence

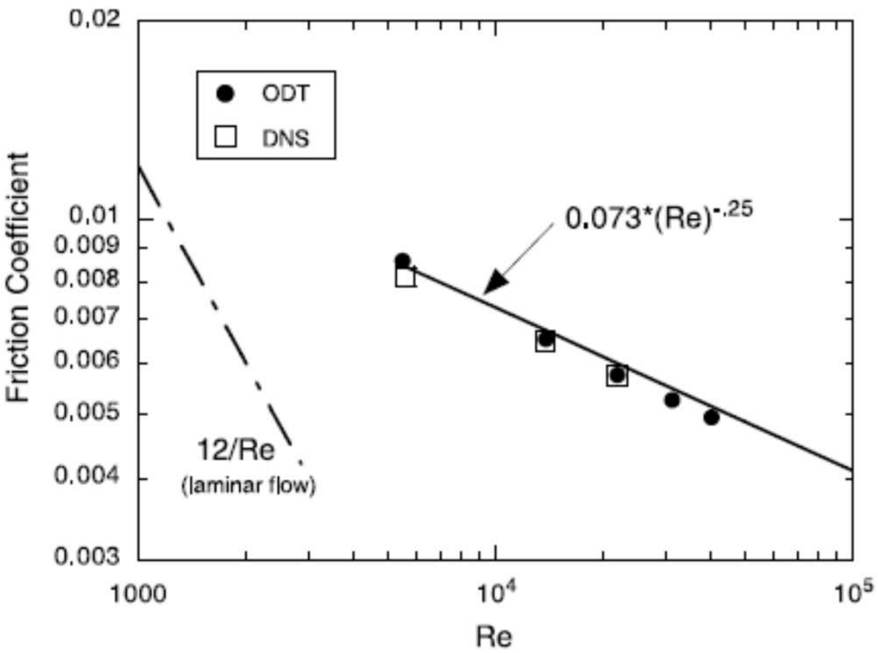
These simulations are based on time advancement of $u_t = \nu u_{yy}$ with flow-specific initial u profiles (see below), plus eddies



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

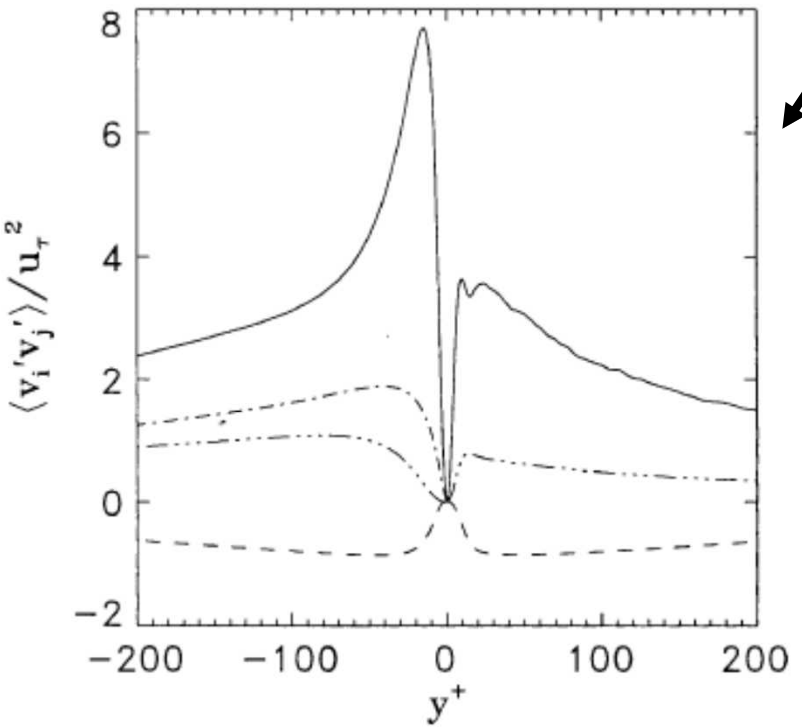
Channel flow: mean properties





Channel flow: fluctuation statistics

Fig. 5. Lateral profiles of Reynolds stress components in channel flow, scaled by u_τ^2: (—) $\langle v_1'^2 \rangle$; (–····–) $\langle v_2'^2 \rangle$; (–··–) $\langle v_3'^2 \rangle$; (–––) $\langle v_1' v_2' \rangle$. (The ODT $\langle v_3'^2 \rangle$ profile is identical to the ODT $\langle v_2'^2 \rangle$ profile.) ODT and DNS [33] results are plotted right and left of centerline, respectively.



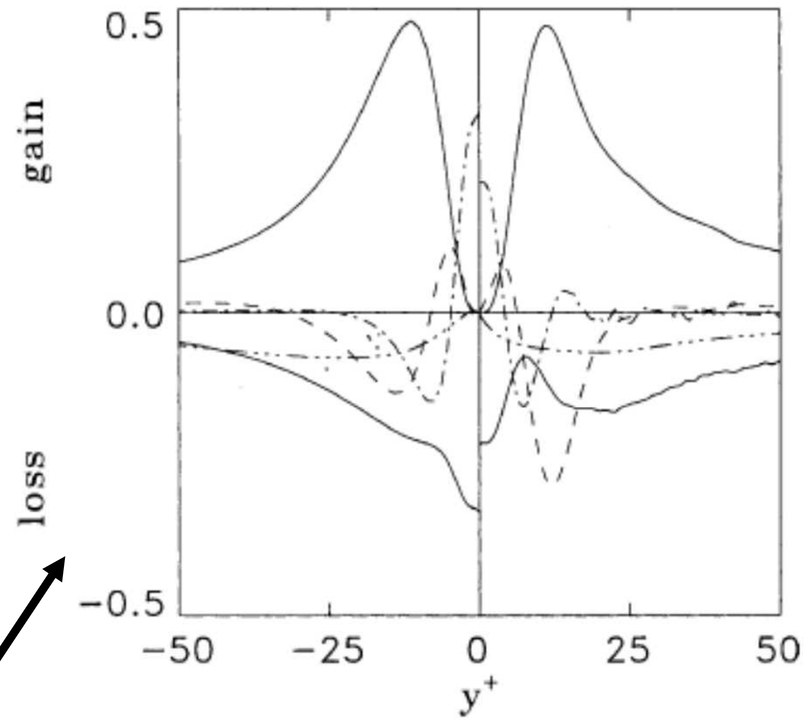


Fig. 6. Budget of $\langle v_1'^2 \rangle$ in channel flow, in wall coordinates: (—) production (upper), dissipation (lower); (–––) advective transport; (–··–) viscous transport; (–····–) scrambling. ODT and DNS [33] results are plotted right and left of centerline, respectively.

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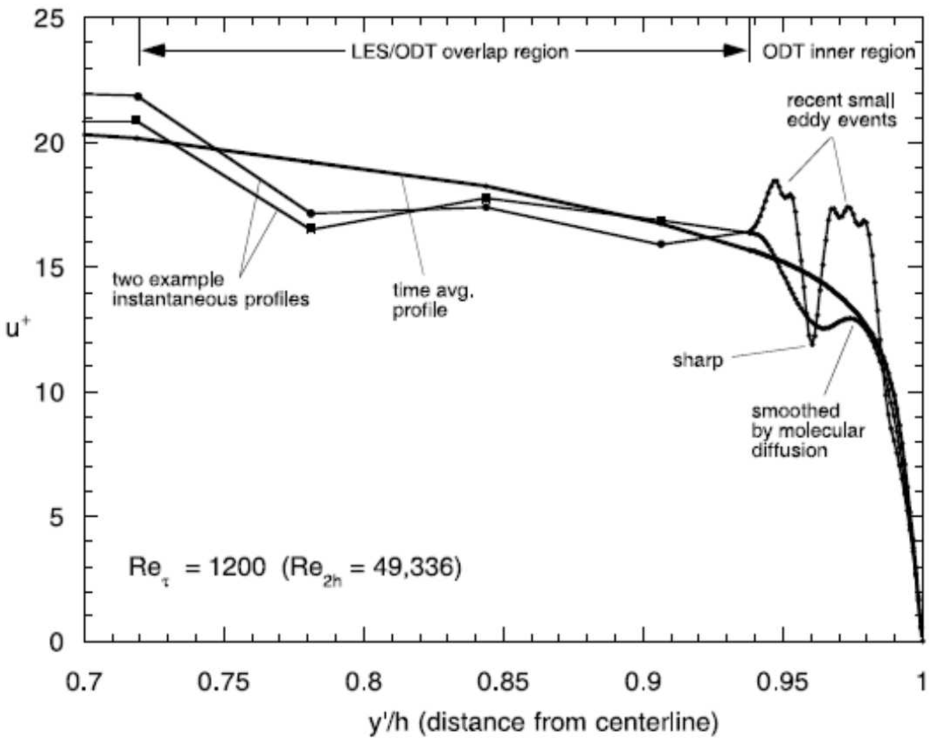
Use of ODT as an LES near-wall closure improves channel-flow fluctuation statistics

Fig. 15. Root-mean-square velocity fluctuation profiles normalized by the friction velocity for $Re_\tau = 590$ and computed from LES/ODT (open symbols), ODT stand-alone (filled symbols), and DNS [33] (solid and dashed lines).



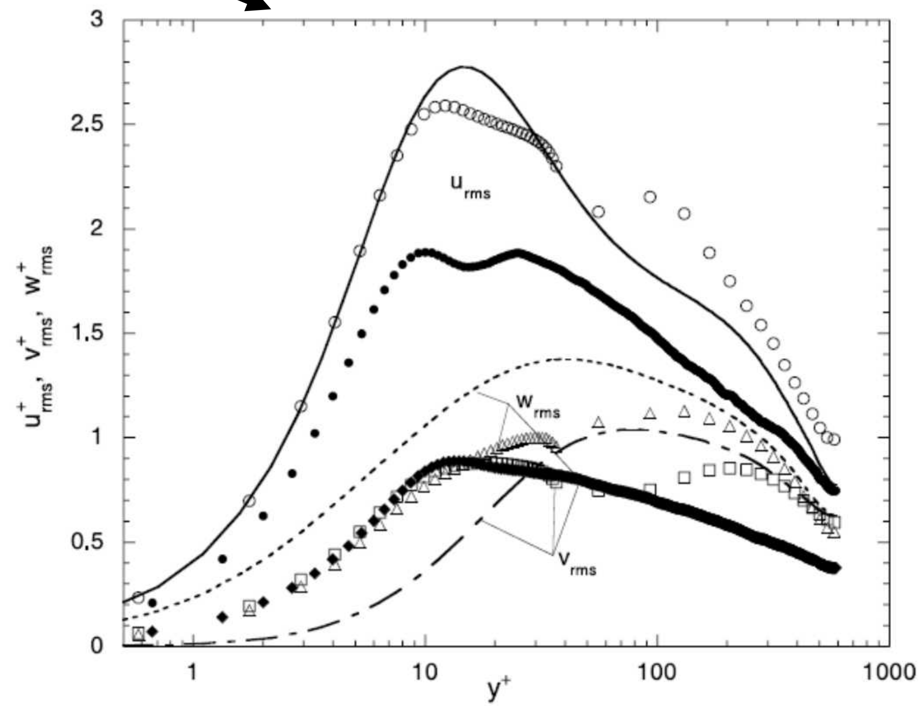
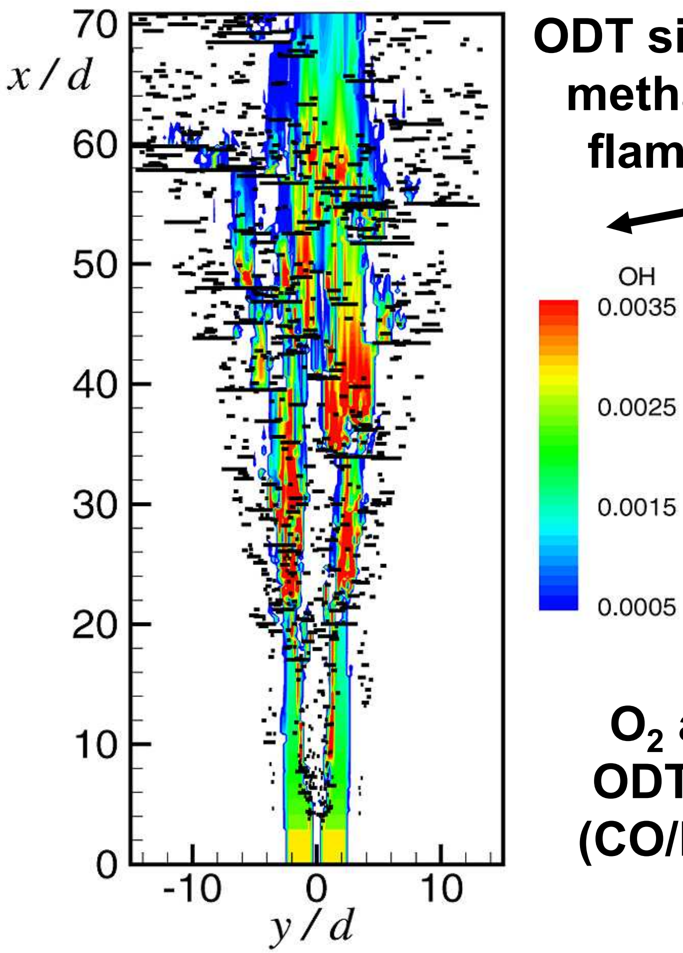


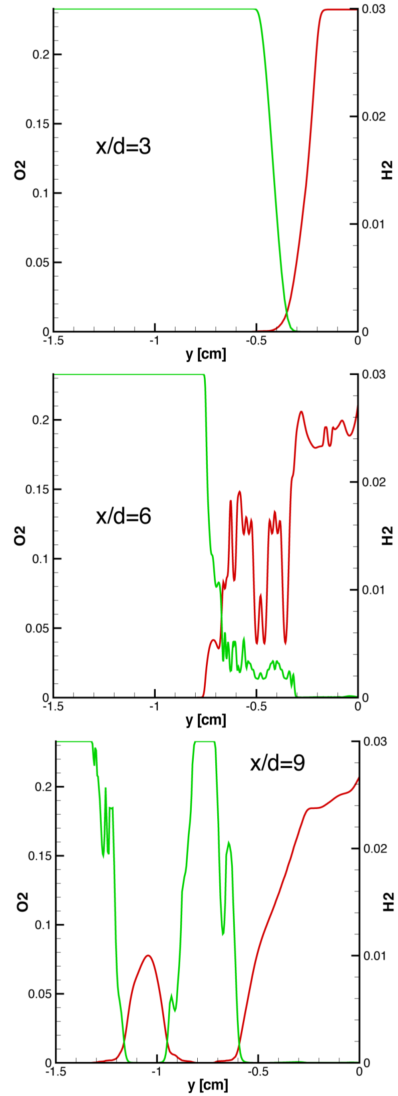
Fig. 12. Near-wall mean and sample instantaneous velocity profiles.

LEM and ODT resolve advective-diffusive-reactive couplings and hence all flame regimes

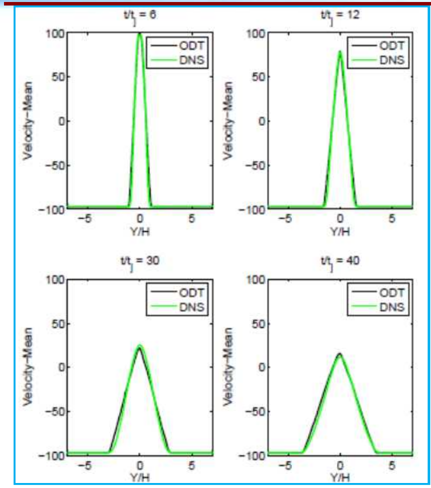


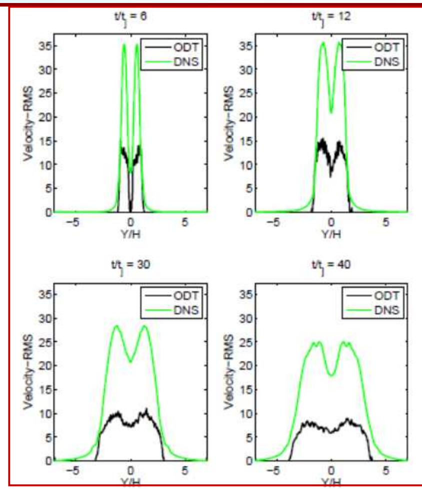
ODT simulation of a piloted methane-air jet diffusion flame (Sandia flame D)

O_2 and H_2 profiles from an ODT simulation of a syngas ($CO/H_2/N_2$) jet diffusion flame



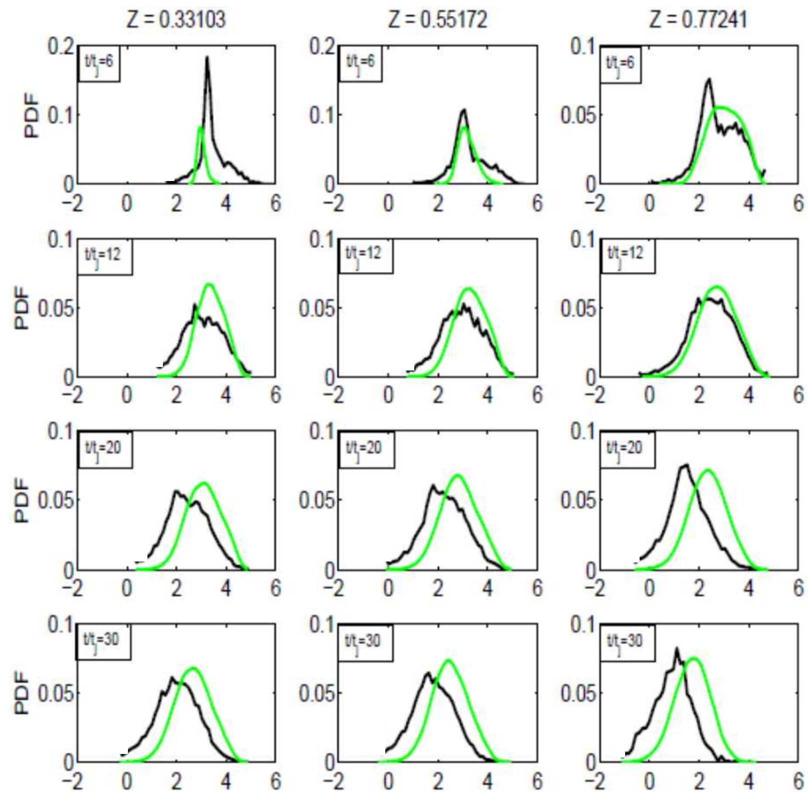
ODT (Punati et al.) captures extinction-reignition in DNS (Chen and Hawkes) of a planar temporal jet syngas flame

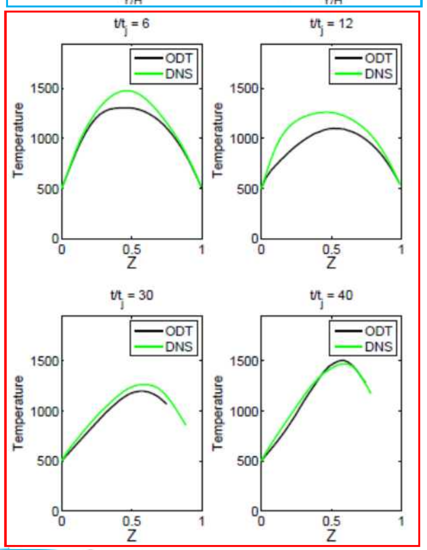


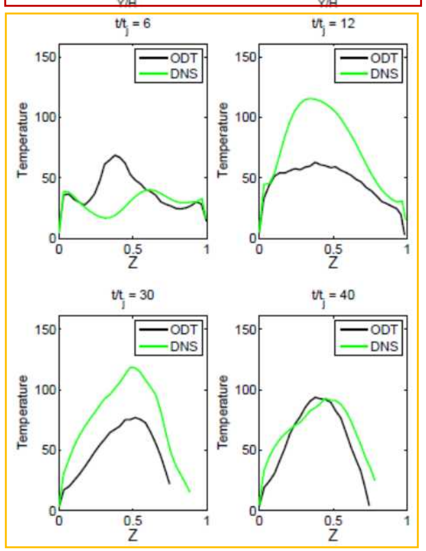


Lateral profiles of mean and rms streamwise velocity

PDF of $\log_{10}$(scalar dissipation) conditioned on mixture fraction







Temperature mean and rms conditioned on mixture fraction

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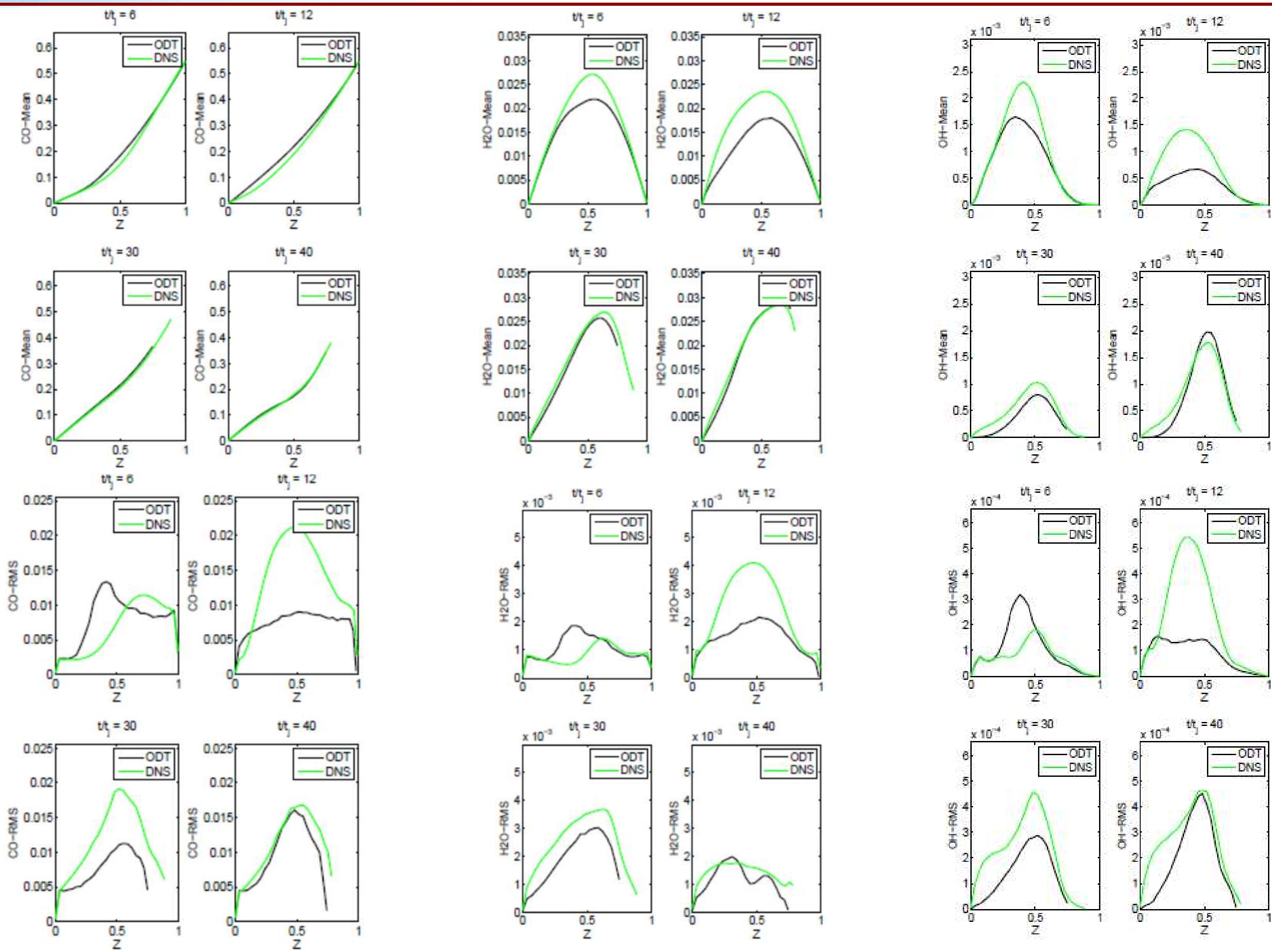
ODT has useful chemical predictive capability

Conditional mean

Conditional RMS



CO

H_2O

OH

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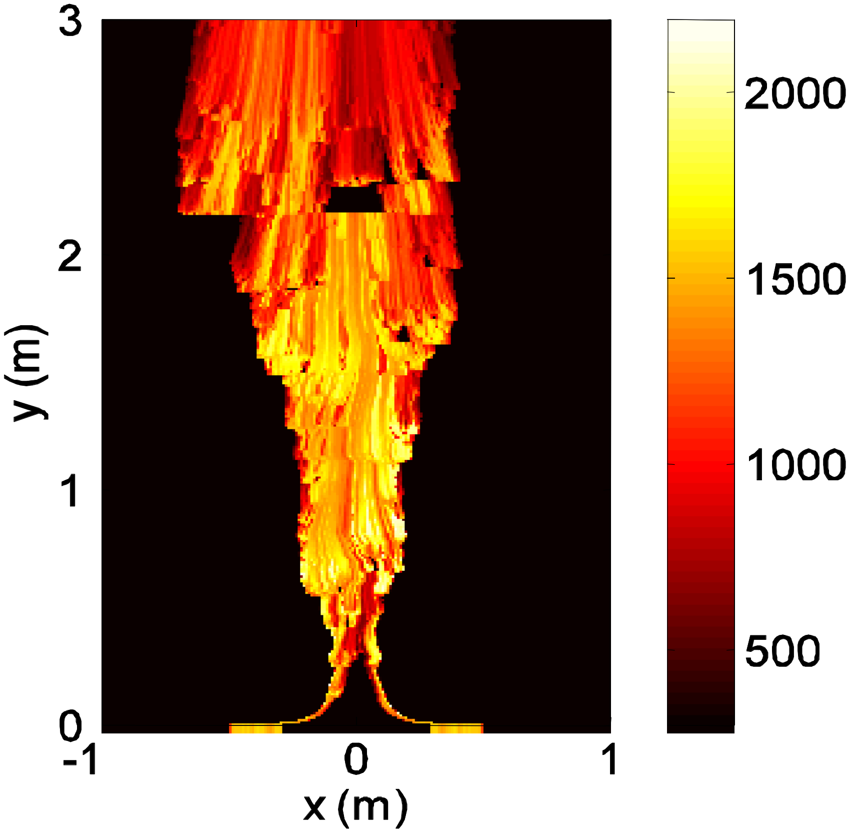
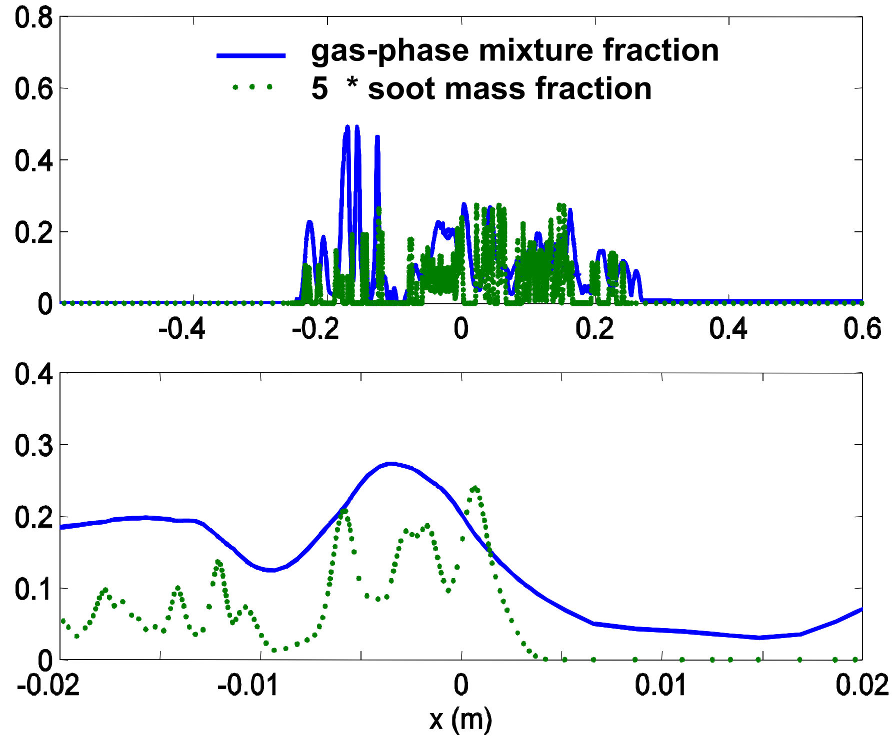
Adaptive-mesh ODT implementation has many benefits

- Full (Lagrangian) adaptivity is feasible in 1D (no mesh entanglement)
- Development of a c++ adaptive-mesh ODT code with full chemical-kinetic capability is ongoing (with D. Lignell, BYU)
- The adaptive mesh facilitates
  - **spatial advancement**
  - **cylindrical geometry**
  - **pseudo-compressible gas dynamics**
  - **domain coupling in 3D formulations**

The first adaptive-mesh ODT code was used to simulate an ethylene-air sooting plume

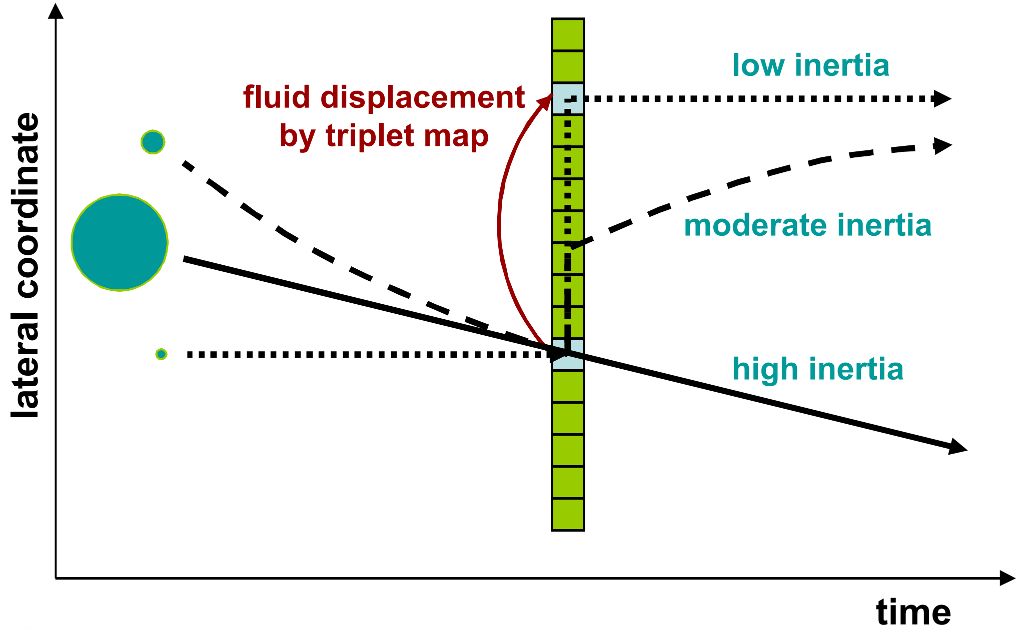




The adaptive mesh efficiently resolves small features – the new code allows different meshes for different properties, e.g., high-Sc scalars, enabling a big time-step increase

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

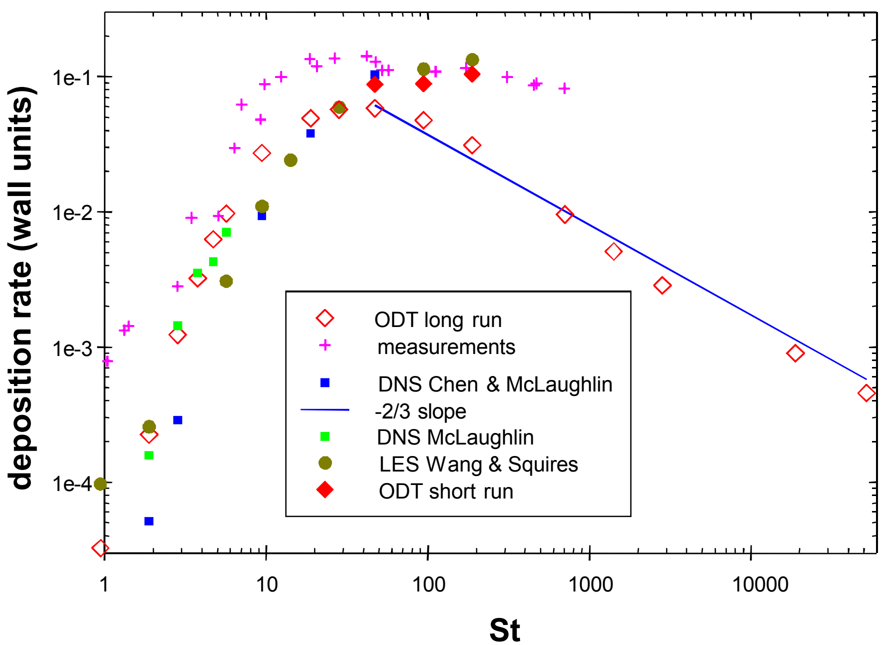


- **Eddy-time integration determines a trajectory 'jump condition' representing the eddy-induced trajectory change, adjusted so future motion is not double-counted**
- **Ballistic motion remains linear**
- **Zero-inertia (no-slip) particles follow the fluid**
- **Particle-fluid relative motion is realistic,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

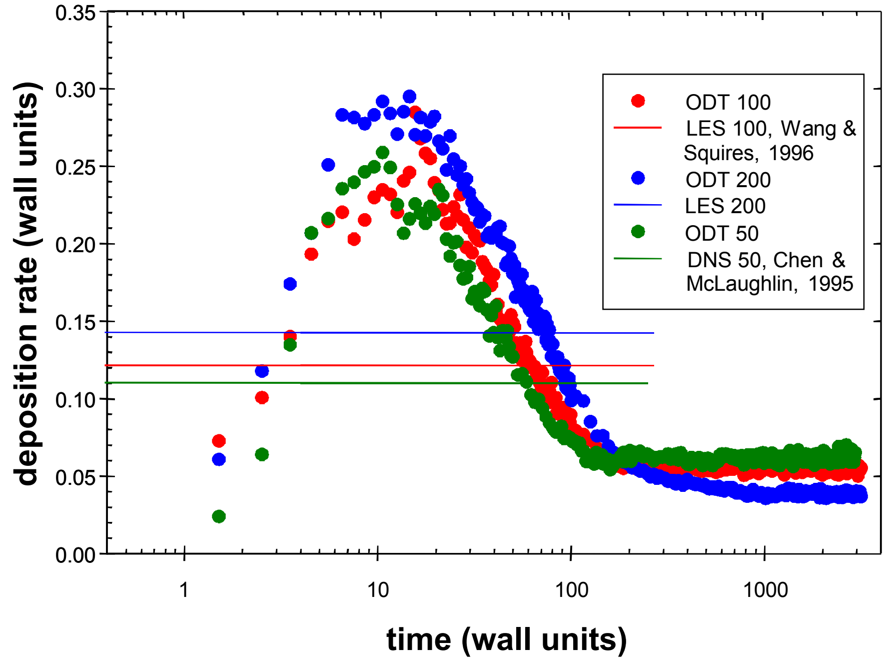
Measured and 3D-simulated wall deposition is reproduced, and a new regime is found

Wall deposition in turbulent channel flow

Dependence on Stokes number

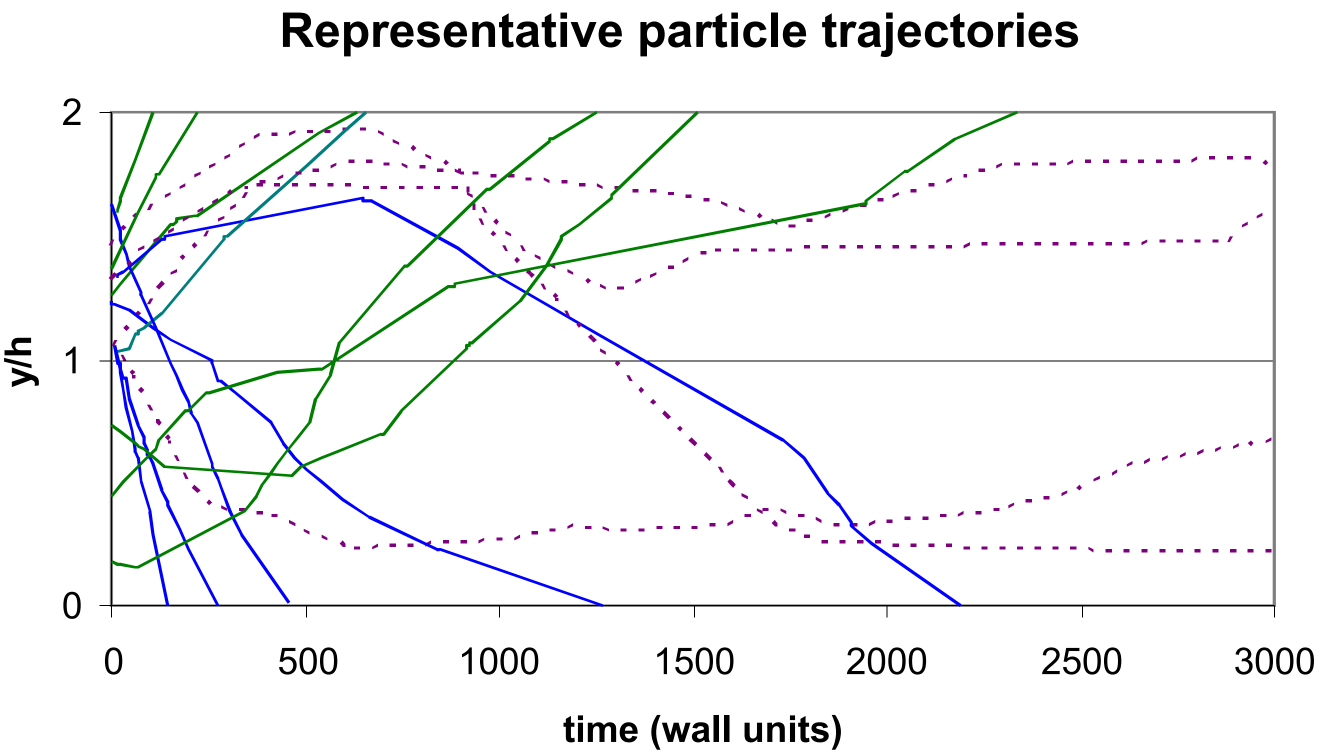


Time variation of deposition rate (transient relaxation)



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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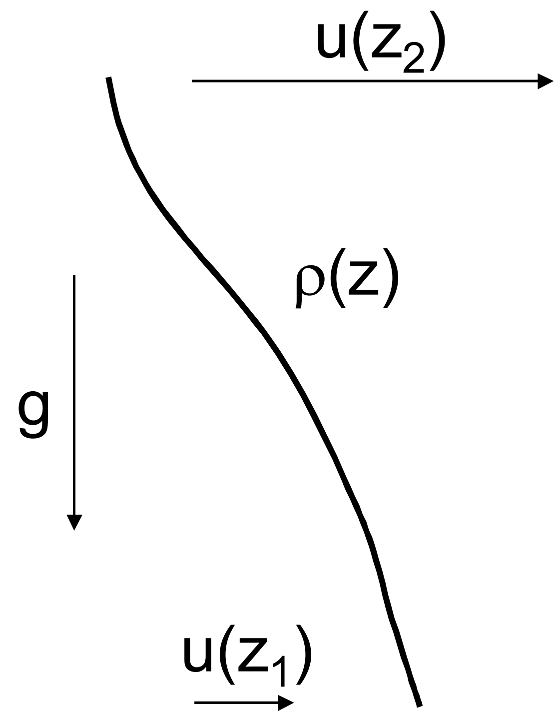
In a gravitationally stable fluid, apply enough shear to generate turbulence – what happens?



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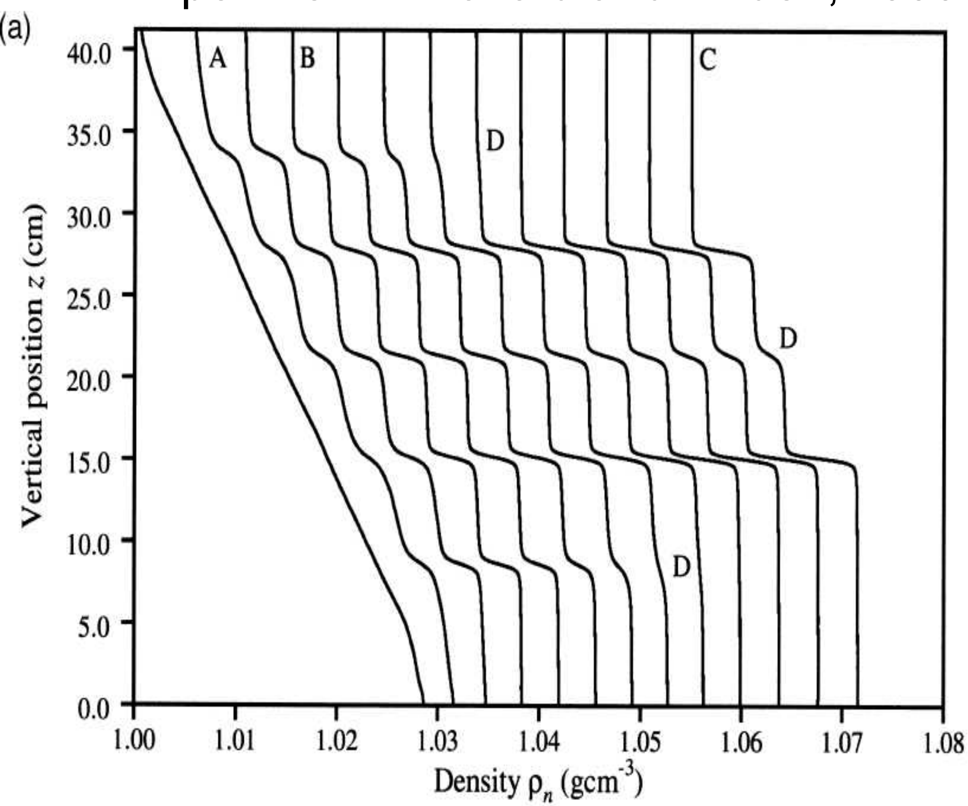
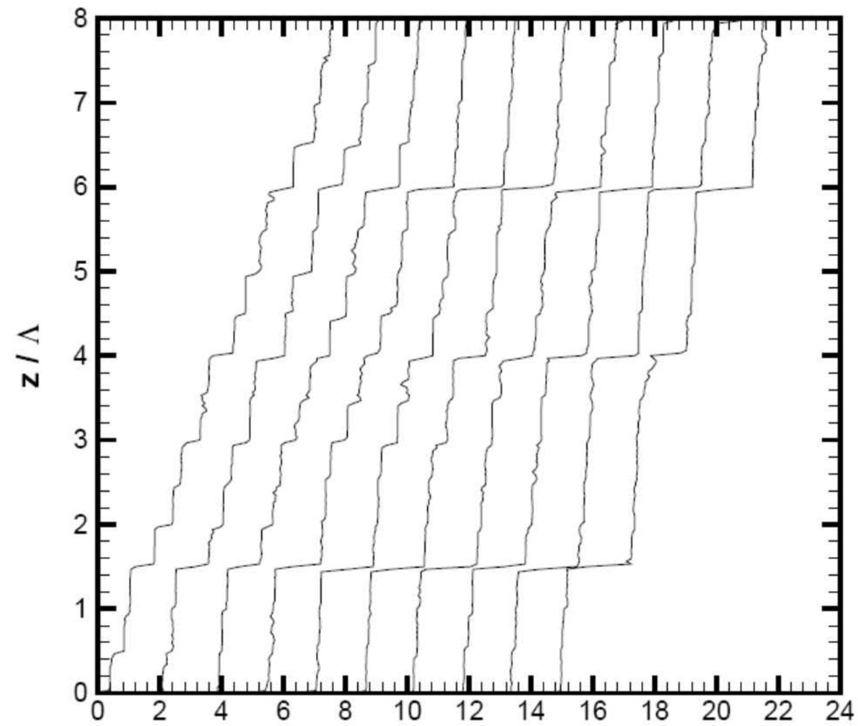
Layers form spontaneously!

Experiment: Holford and Linden, 1999



ODT: Wunsch and Kerstein, 2001



ODT parameter studies over a wider Pr range than is experimentally accessible led to new understanding and better collapse of data

A slow-diffusing stable species can cause layering of a convection process: *double-diffusive instability*

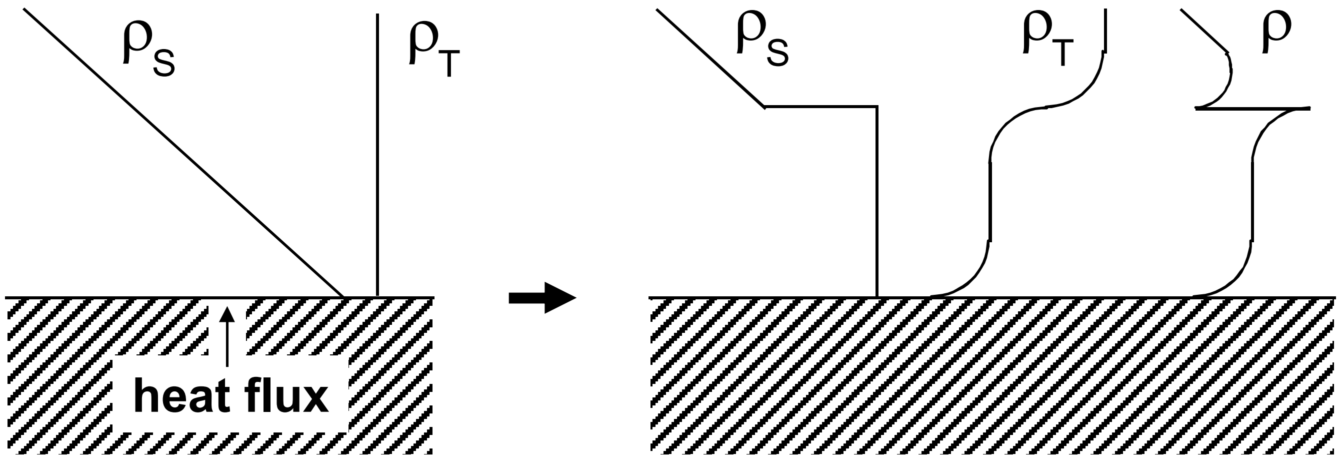
ρ_T **is the density variation due to temperature variation**

ρ_S **is the density variation due to salinity variation**

<u>Initial</u> <u>state</u>: constant temperature, salinity decreases with increasing height (stable, no motion)

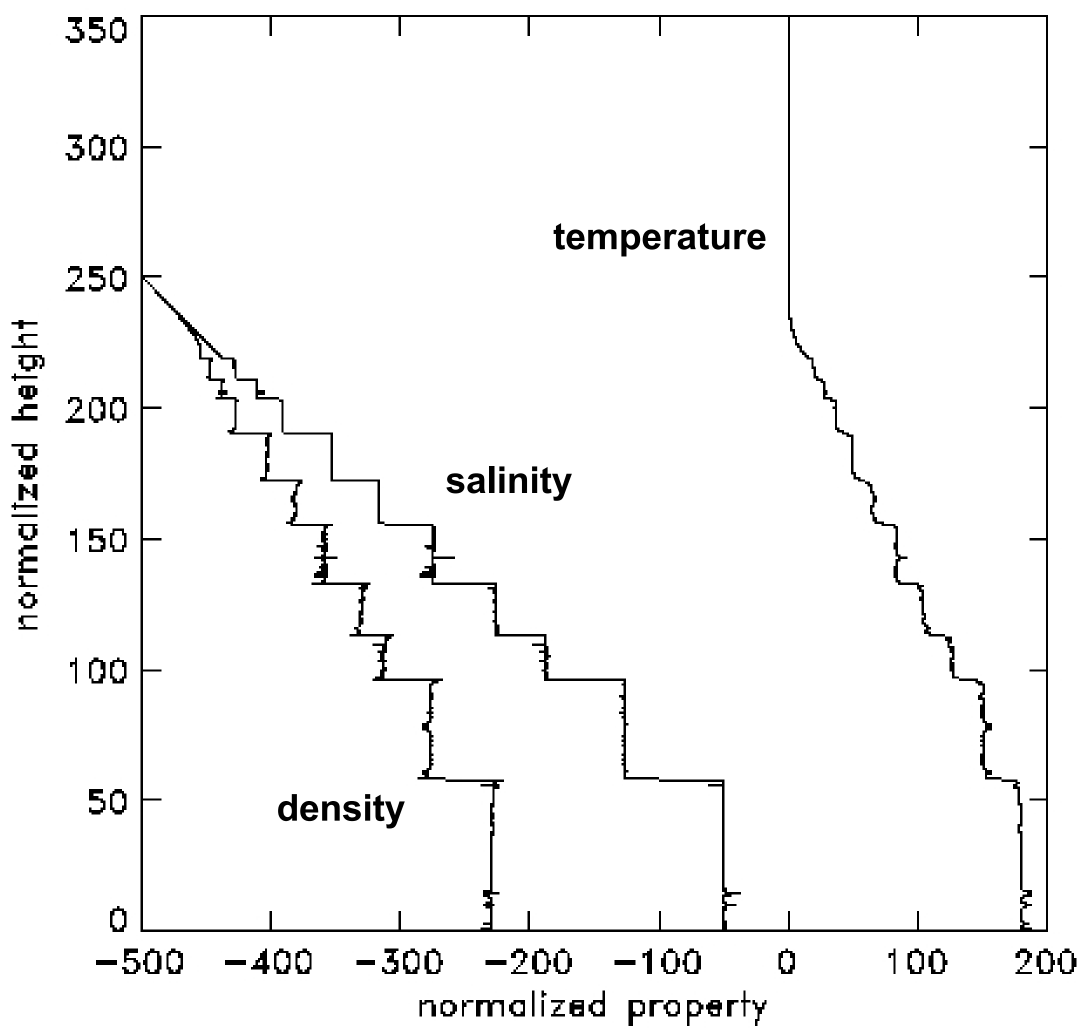
<u>Forcing</u>: heat from below causes gravitational instability leading to turbulent mixing

<u>Role</u> <u>of</u> <u>molecular</u> <u>transport</u>: salt diffusivity is negligible, so stable jump forms, but heat diffuses across, initiating a new turbulent layer above the jump

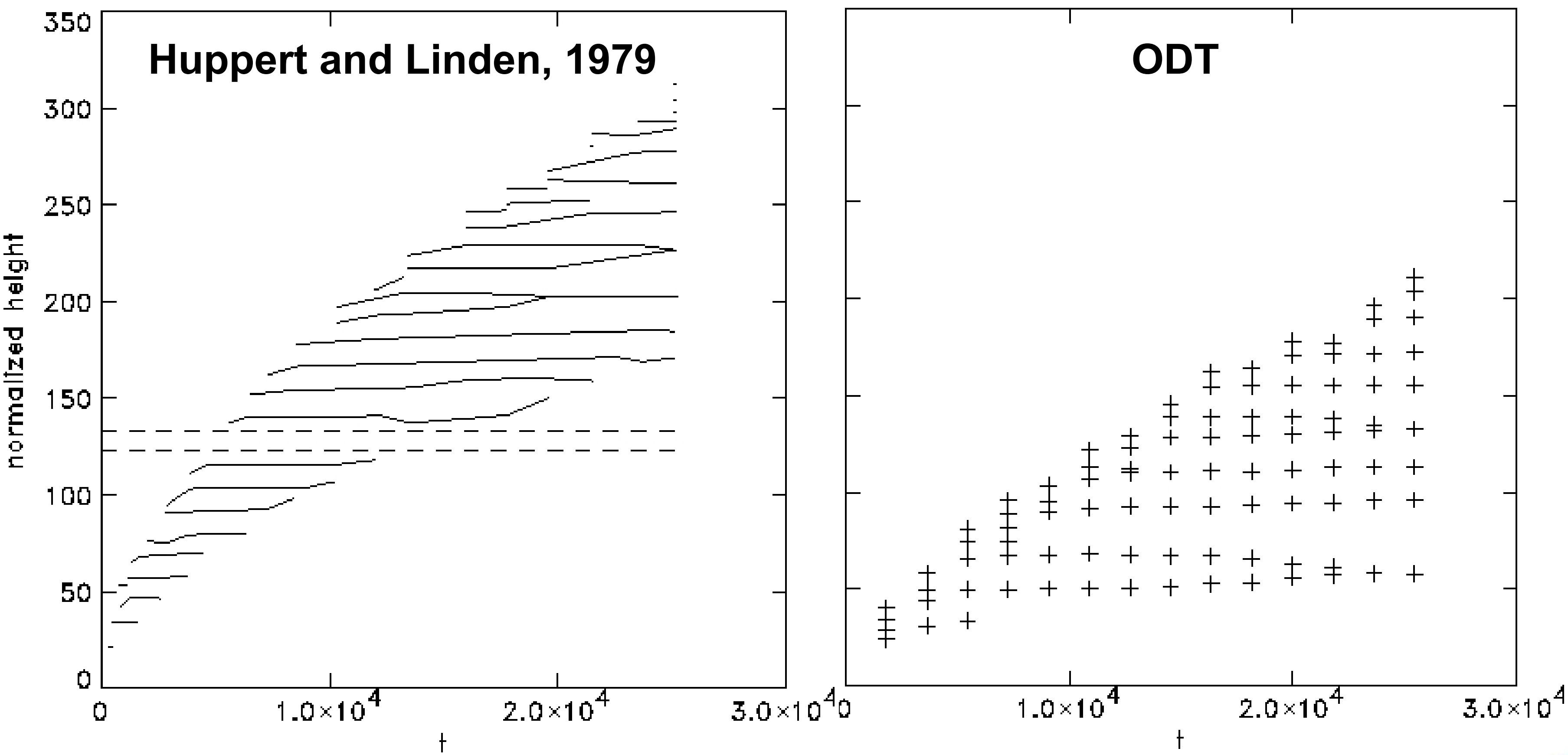


thermohaline staircase

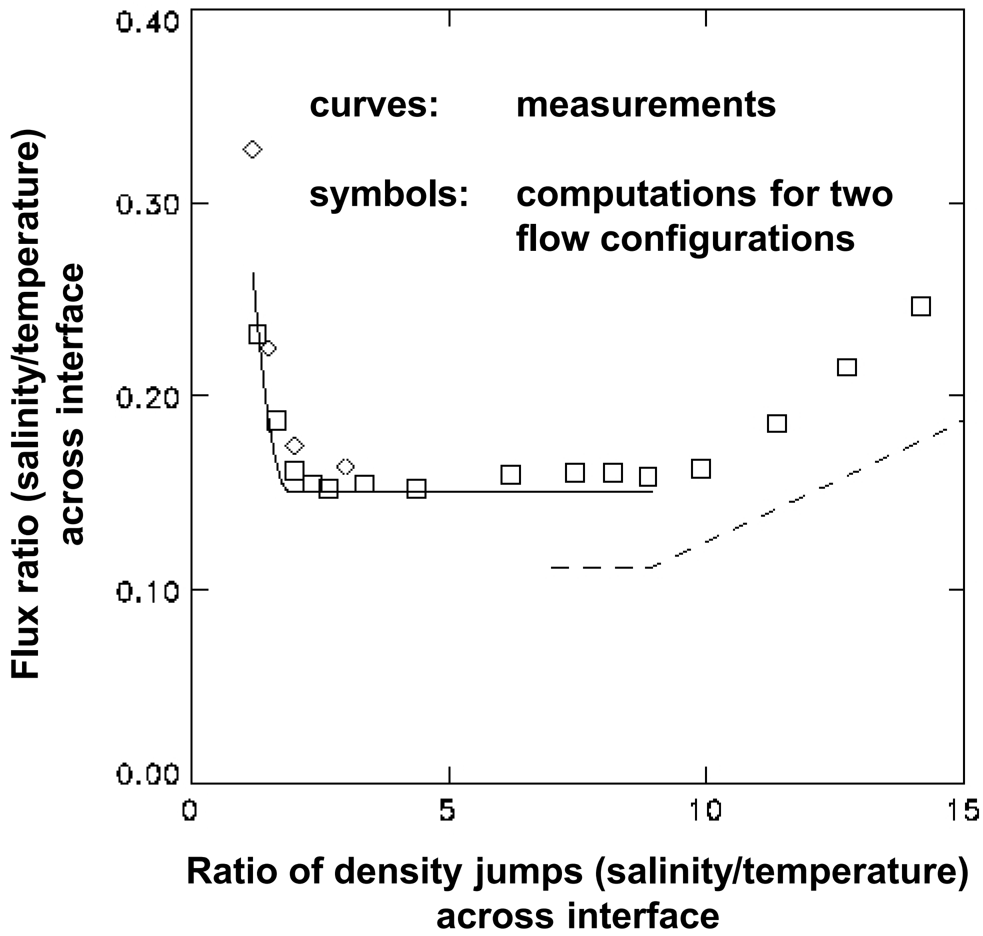
ODT captures the wide range of dynamically relevant time and length scales



An ODT formulation requiring no parameter adjustment is compared to measurements



ODT captures the observed regimes of diffusive interface structure



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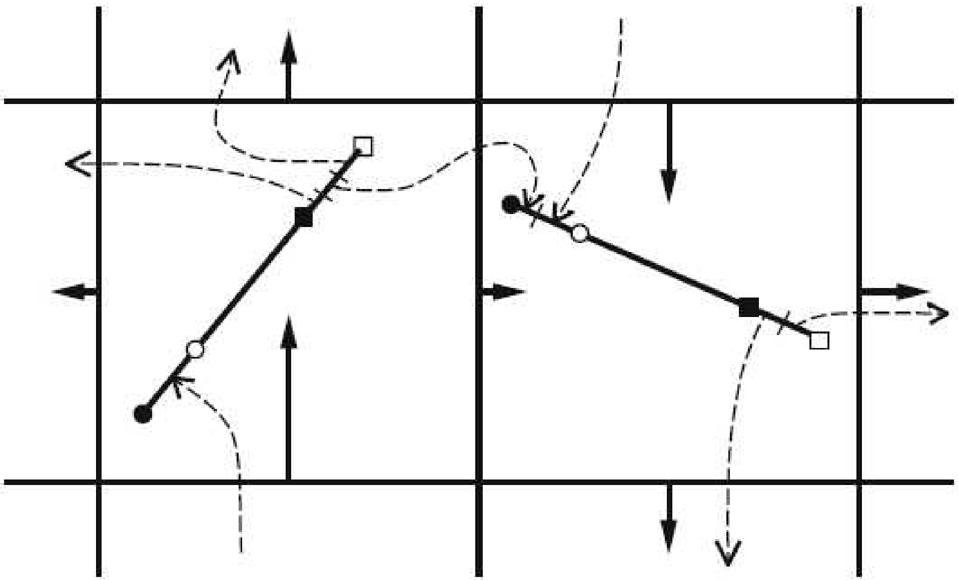
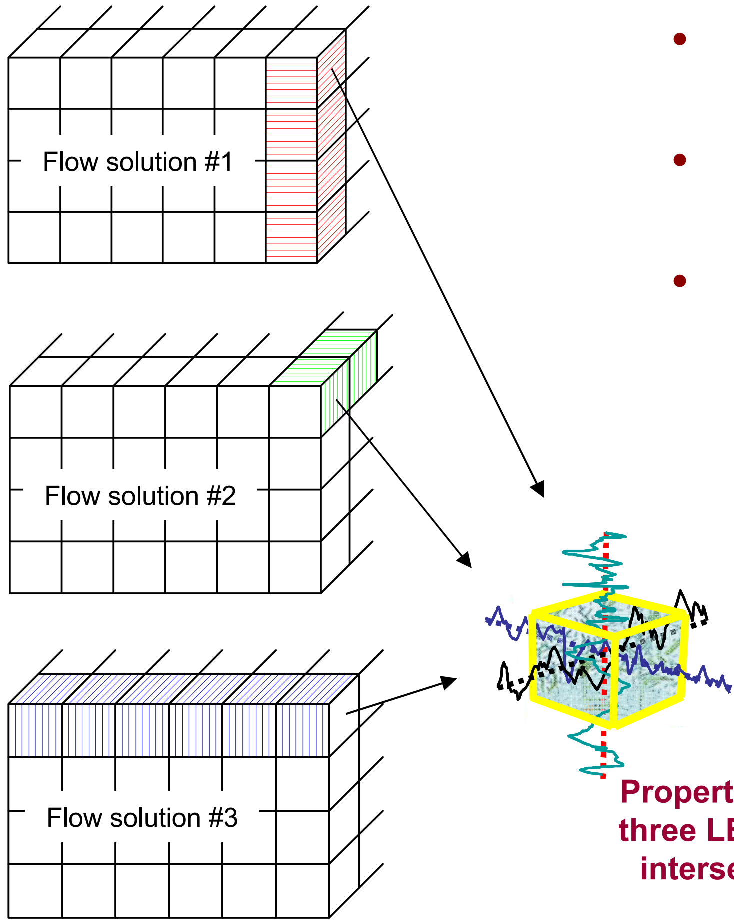
Suresh Menon implemented a ‘splicing’ method to couple LEM domains for LES mixing-reaction closure

- 1D domains are Lagrangian objects within control volumes (CVs) in one coordinate direction
- Each domain has an input end and an output end
- Mass transfer (splicing) between them is governed by CV face fluxes from a coarse-grained 3D flow solver



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

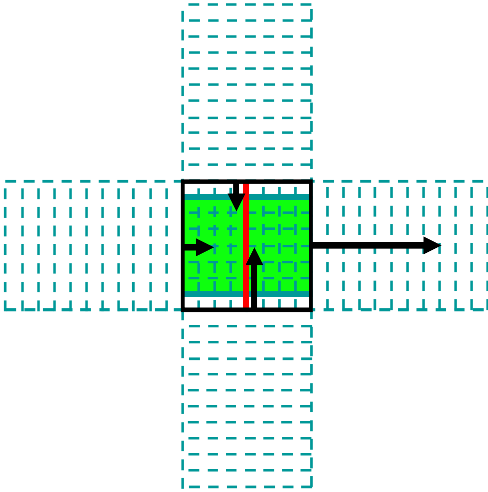


Property profiles on the three LEM domains that intersect a RANS CV

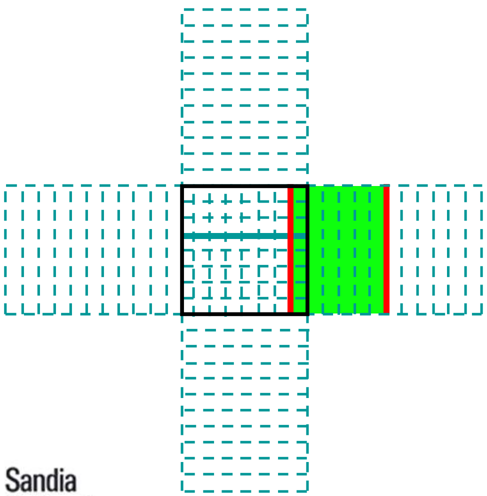
- Each LEM domain spatially refines RANS control volumes (CVs) in one coordinate direction
- Each CV is thus contained within three orthogonal LEM domains, each within a different flow solution
- Time-advancement cycle:
  - **Advancement on individual LEM domains**
    - **1D representation of small-scale 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>**

This approach can likewise be used for LES mixing-reaction closure

A 2D constant-density 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 chemically dissimilar fluids into contact
- Remedy: Use coarse CVs to minimize the artifact

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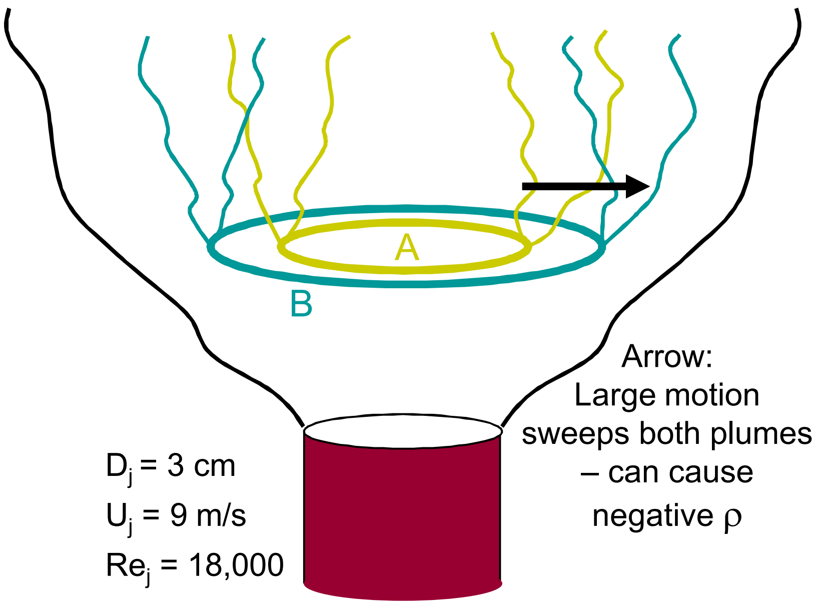
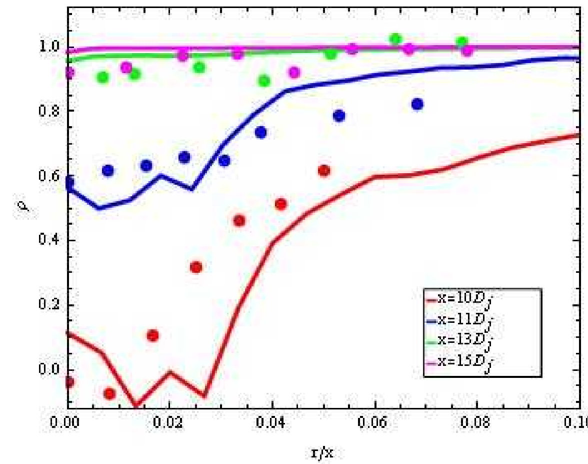
Using measured properties (surrogate RANS), LEM3D captures the mixing of scalars released within a jet

- 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

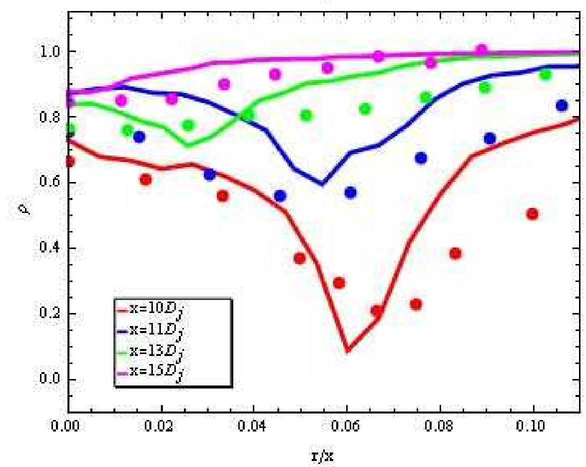


Radial profiles of ρ
(measurements: •, model: —)

Ring diameters



10 and 15 mm



35 and 40 mm

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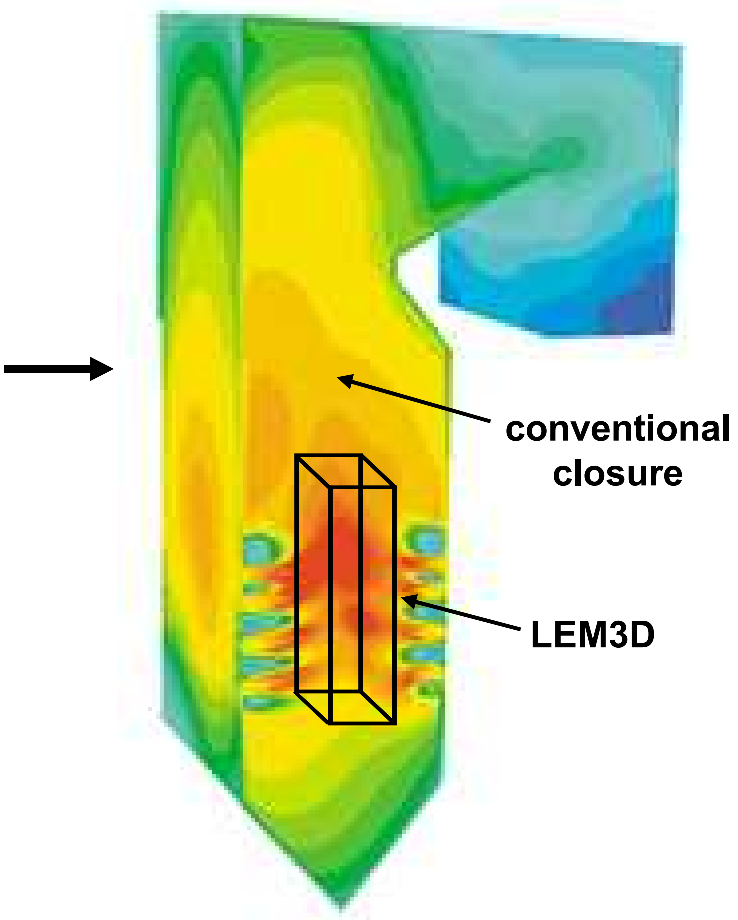
LEM3D is being generalized for combustion applications

- A variable-density formulation is under development (with 2-way RANS-LEM3D coupling); collaboration with SINTEF
- Chemical kinetics will be incorporated
- LEM3D sub-regions will be imbedded in flow simulations to resolve mixing locally
- Will couple LEM3D to an ODT-based 3D simulation (explained next)



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
    - **pulverized coal burners (by capturing recirculation)**
    - **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

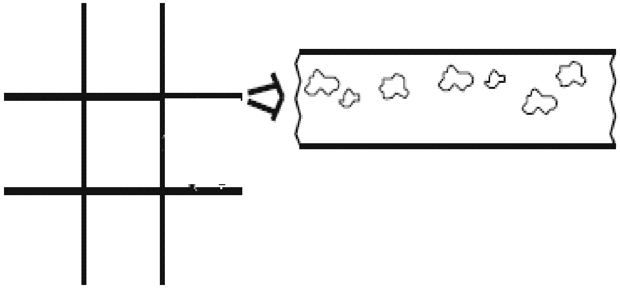
- Incompressible:
  - Continuity enforced using coarse-grained (CV scale) 3D pressure projection
  - ODT-resolved flow field is modified accordingly, a downscale coupling
- Pseudo-compressible:
  - Enables domain coupling with no coarse-graining or downscale coupling
  - Hence termed 'Autonomous Microscale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

Subgrid LEM inspired 'superparameterization' (SP) closure of atmospheric flow simulations

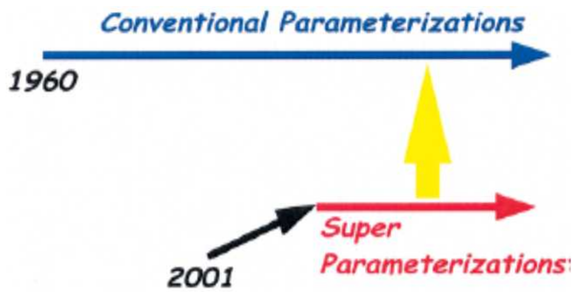
- Small scales resolved in 2D (vs. 1D in LEM and ODT)
- Deemed necessary despite high cost (NSF S&T Center)
- Cross-fertilization is ongoing, e.g., SP is adopting AME concepts

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

- Map-based advection
- Introduction to One Dimensional Turbulence (ODT)
- Model and algorithm extensions
- Spontaneous layer formation in buoyant stratified flow
- Subgrid implementation (‘superparameterization’)
- Conclusions

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 turbulent combustion and other turbulence-microphysics couplings

- Its uses include
  - Fundamental studies
  - Input to other modeling approaches
  - Engineering (e.g., design concept screening)
  - Building block for 3D simulation

- Downloadable code and documentation at http://groups.google.com/group/odt-research