Building a Turbulent Combustion Numerical Simulation from the Bottom Up

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Outline of Presentation

- Why a bottom-up strategy?
- A small-scale formulation using map-based advection
- Economical simulation of small-scale *mixing,* illustrated by:
  - **Pipe mixing**
  - **Astrophysical flames**
  - **HCCI engine combustion**
- Coupling the mixing model to a large-scale-flow solver
  - **Formulation**
  - **Validation**
- Economical simulations of small-scale *flow*
- All-scale flow simulation using coupled small-scale-flow simulations
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- Summary

The prevailing turbulent combustion modeling paradigm faces challenges

- Stringent efficiency and environmental requirements drive increasing complexity of combustor design
- Combustor performance is increasingly sensitive to details of turbulence-chemistry interactions
- The current modeling paradigm is 3D coarse-grained simulation supplemented by combustion closures
- *Is this approach close to the point of diminishing returns?*

An alternative that uses ***map-based advection*** is described here:

- Captures details of flame structure and evolution in 1D
- Enables 1D 'flow simulation'
- Building block for 3D *'bottom-up' simulation strategy*

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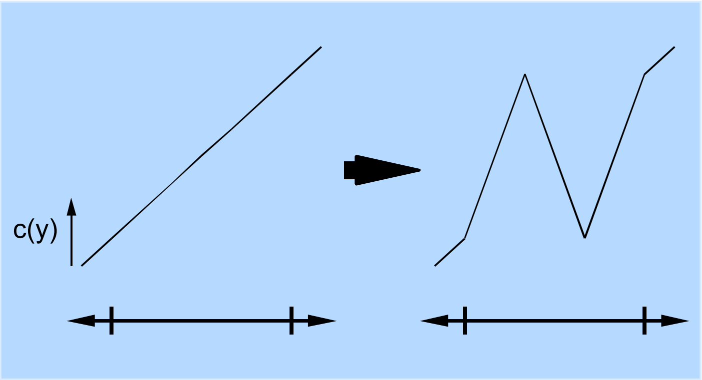
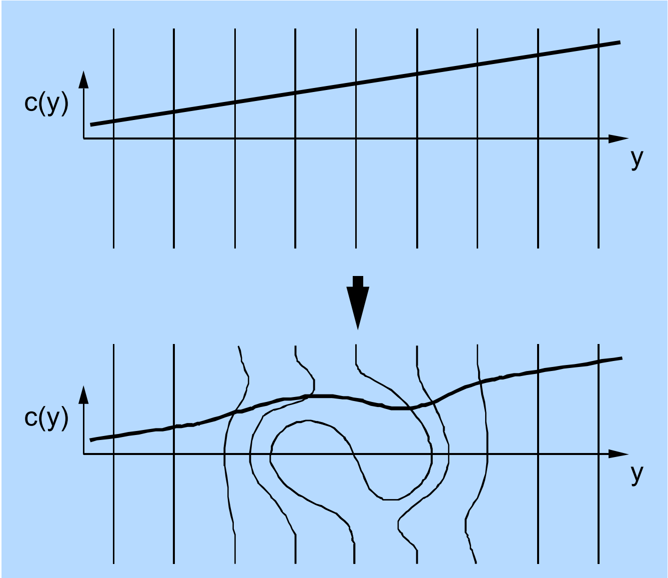
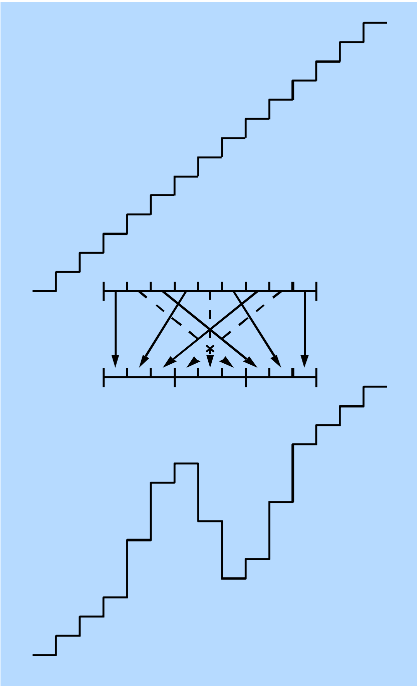
Advection is modeled as a sequence of *triplet maps*, which preserve desired advection properties



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



This procedure 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 (optimal in this respect)

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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:

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

scalar $\qquad$ **velocity component (ODT only)**

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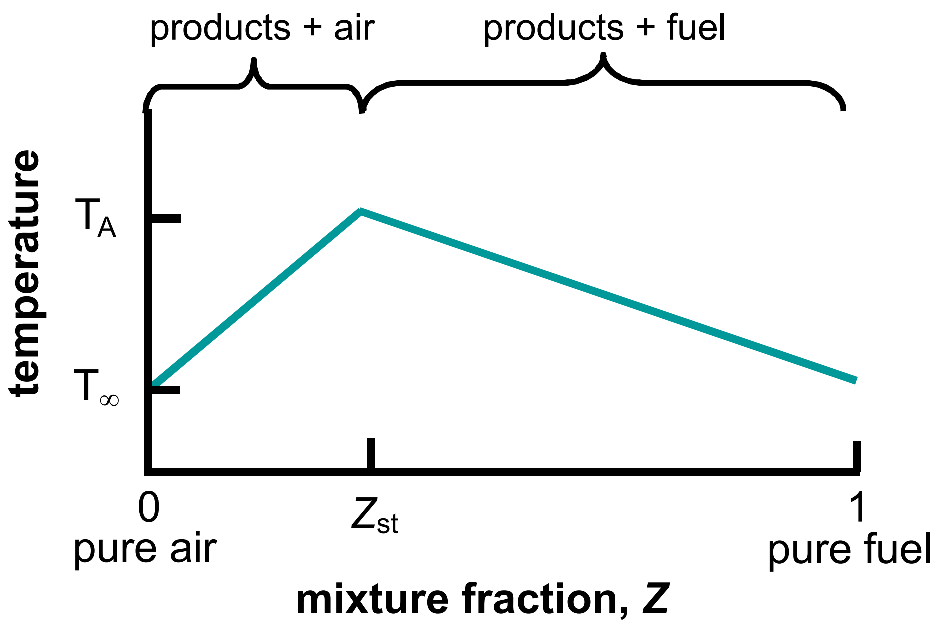
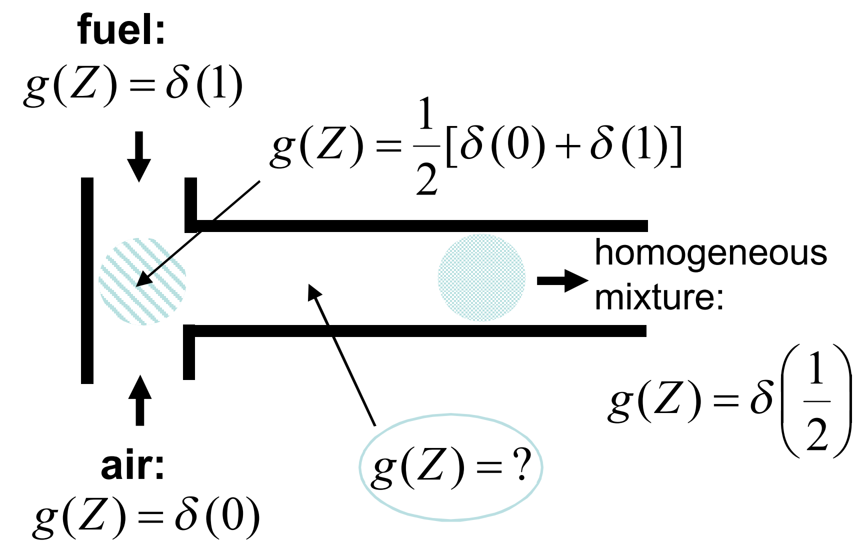
For two-stream (e.g. fuel-air) mixing, the mixture-fraction PDF is often sufficient

For fast chemistry (relative to mixing), the mixture fraction determines the (equilibrium) chemical state



The combustion problem is thus reduced (under certain approximations) to a passive mixing problem



Need to predict:

- Sequence of mixture-fraction PDF shapes $g(Z)$
- Rate of evolution through shape sequence

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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?

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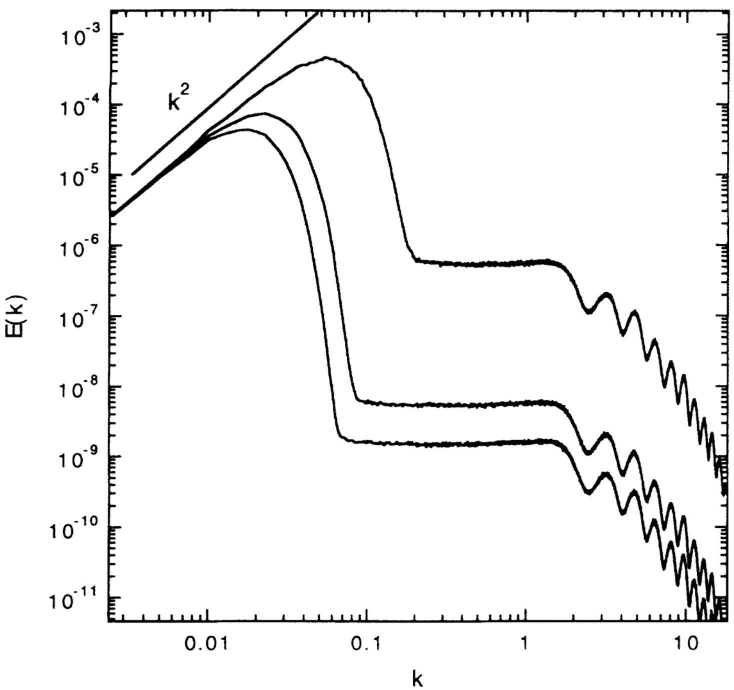
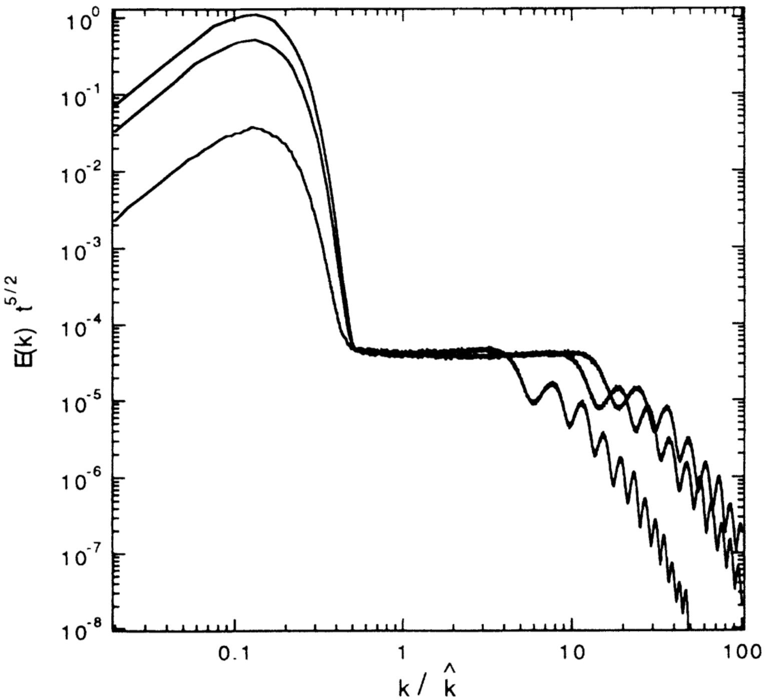
The result was surprising (amazing!) – then an explanation was found



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

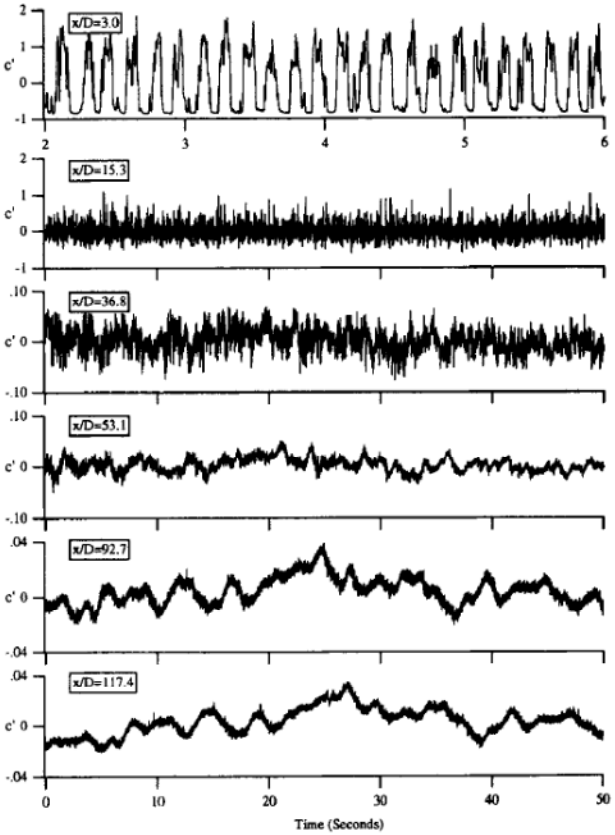
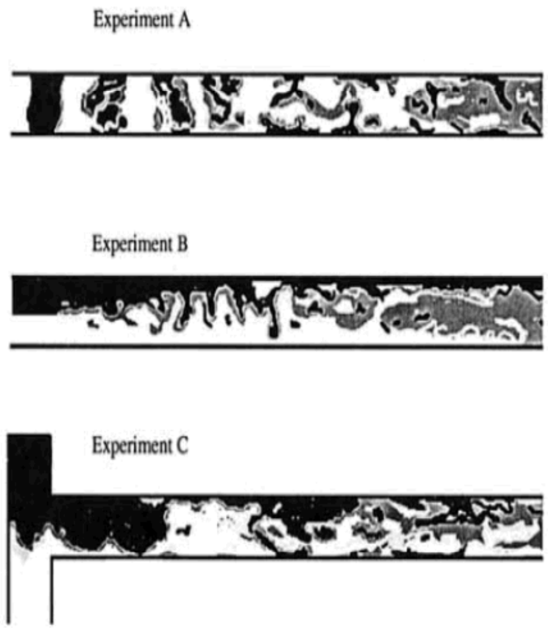


Figure 3. Time series of measured scalar field at the center of the pipe for experiment A.
A 4-s period is shown for $x/D = 3.0$ to show the idealized inlet condition achieved. At all other locations a 50-s time series is shown.



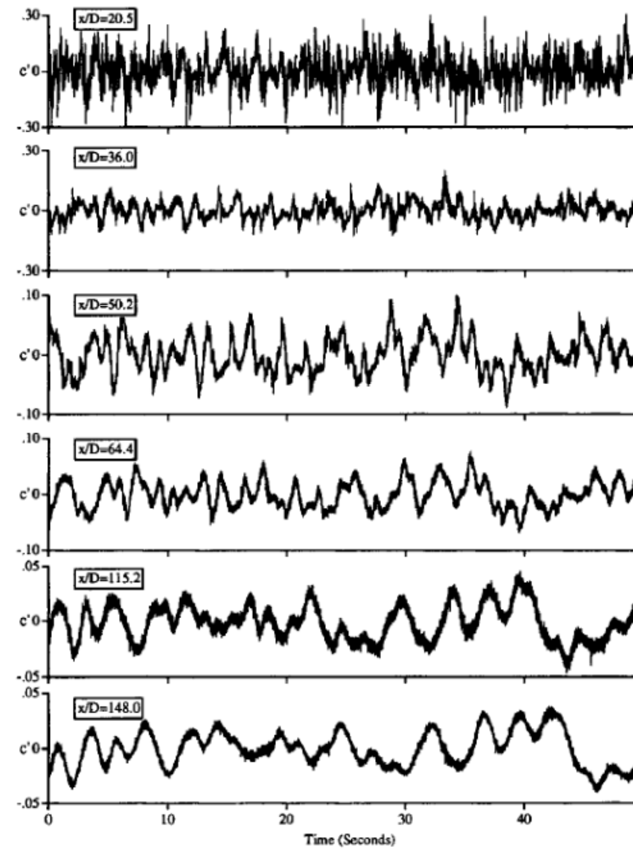


Figure 11. Time series of measured scalar field at the center of the pipe for experiment C.

Guilkey, McMurtry, and Klewicki, 1997

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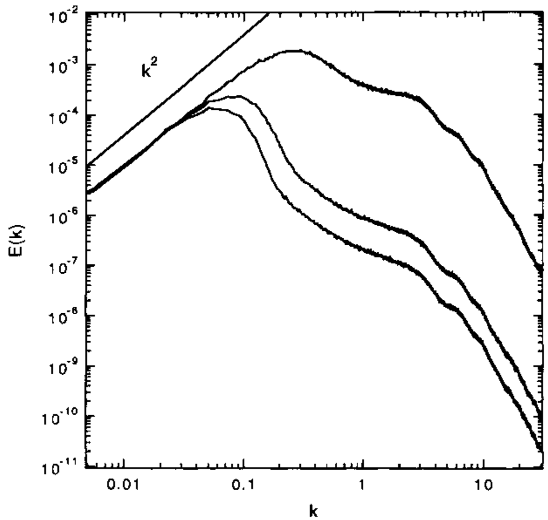
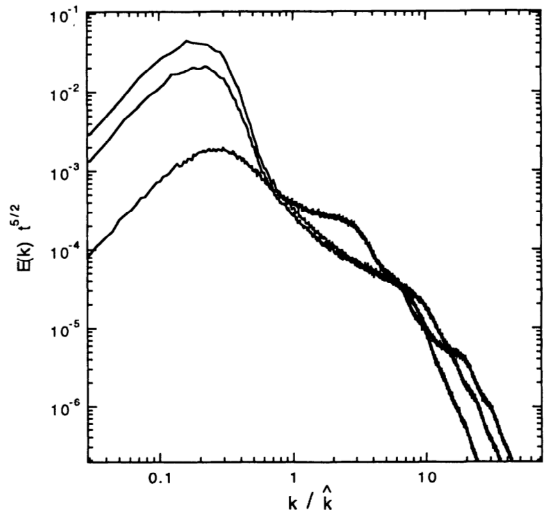
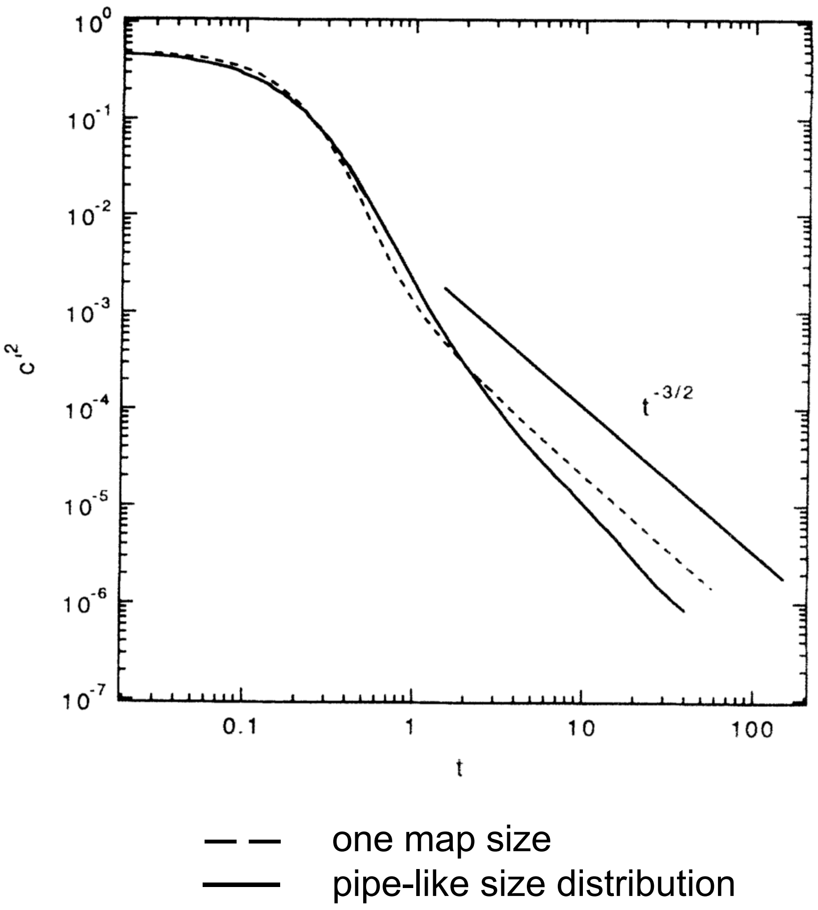
Simulations were performed for a 'pipe-like' map-size distribution





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



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Scalar power-spectrum measurements exhibit the predicted features

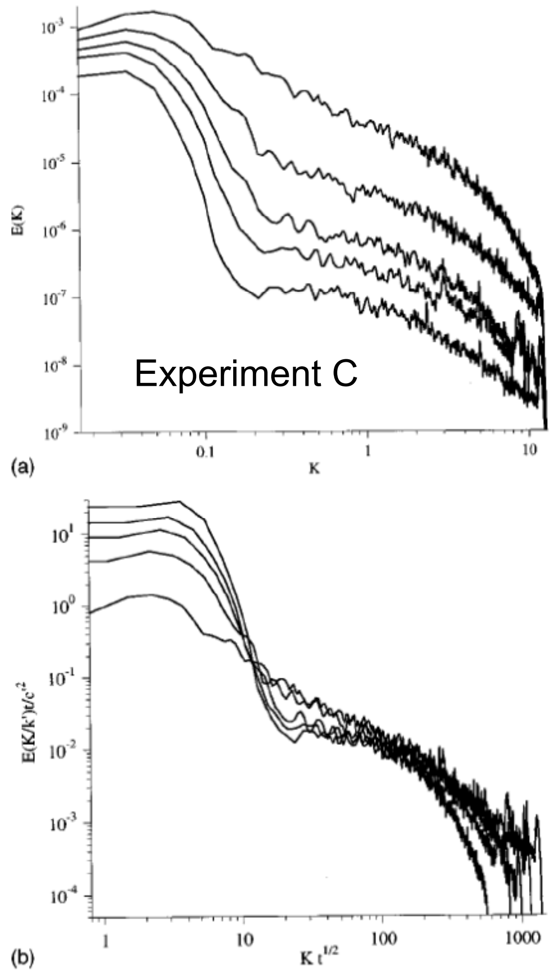

FIG. 5. (a) Power spectral densities of scalar fluctuations, experiment 2. Axial locations (from top to bottom) are $x/D = 20.5$, 36.0, 50.2, 64.4, and 90.3. (b) Spectra subject to ''equilibrium'' range scalings, indicating self-preserving behavior.

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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

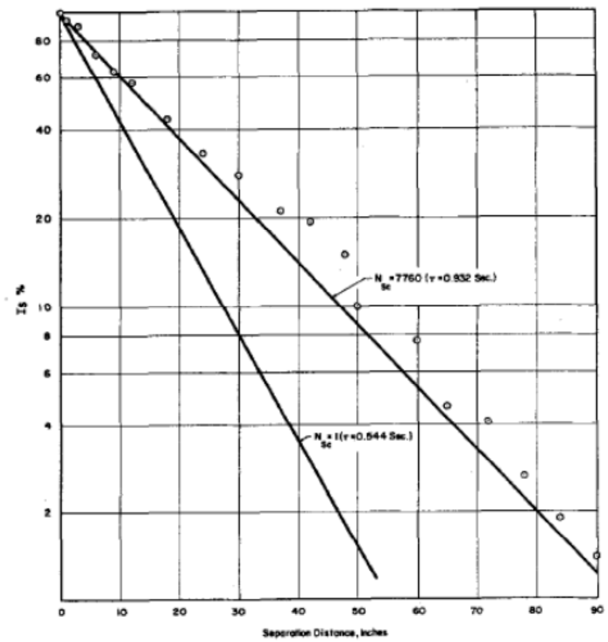
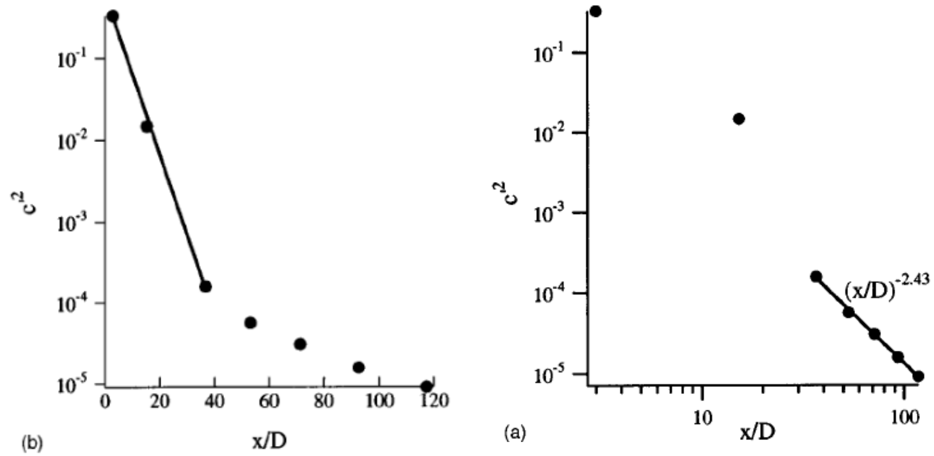
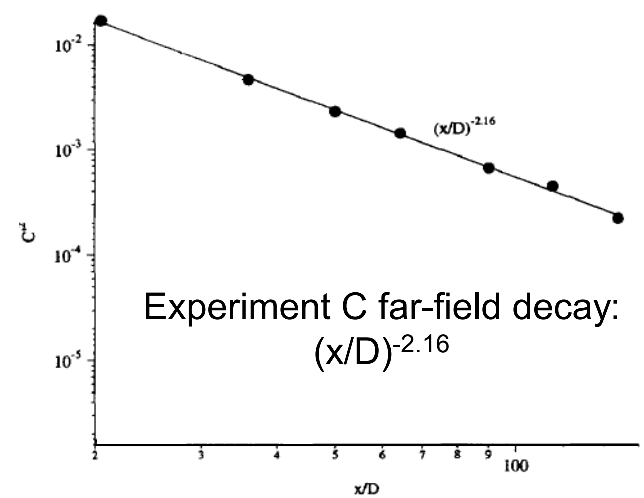


Fig. 1. Intensity of segregation.

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)

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Turbulent premixed flames extinguish when the eddy time scale falls below the chemical time scale

- So there's little empirical information about strongly turbulent premixed flames
- But nuclear flames in exploding supernovae are subject to very strong turbulence, and never extinguish
- ***How do these flames behave?***

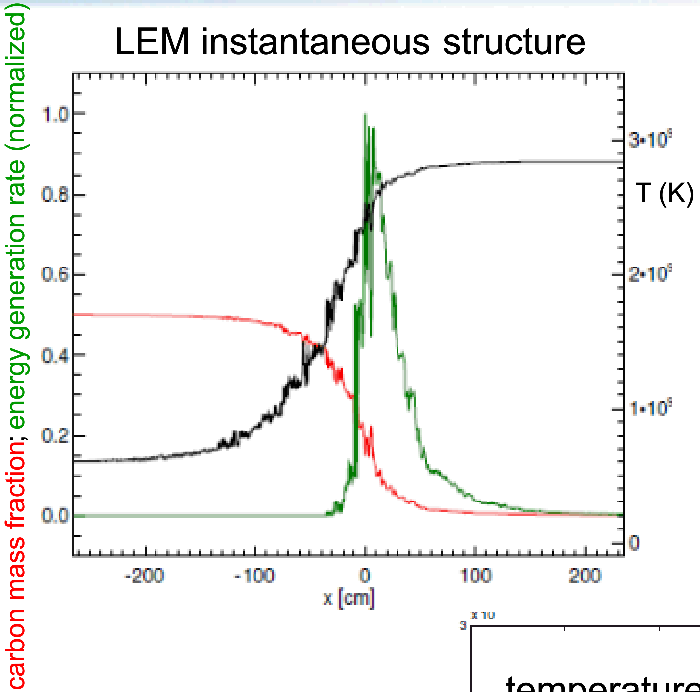
Linear-eddy model (LEM): distribution of eddy sizes, obeys inertial-range scalings

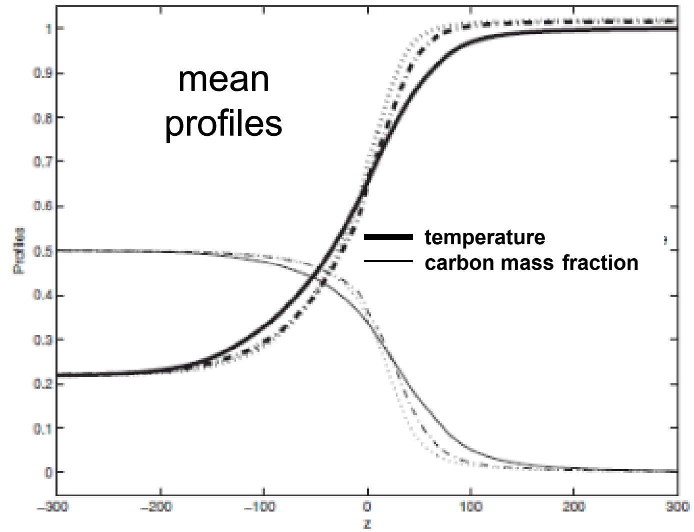
Evolve $\theta_t = \kappa \theta_{yy}$ + 'eddies' where

- The map distribution is spatially uniform (homogeneous turbulence)
- Map size ranges from smallest (η) to largest (L) turbulence scale
- In this range, the known (power-law) dependence of turbulent dispersion on the scale of motion determines the map size PDF
- Need an input value of the 'turbulent diffusivity' to set the overall map frequency

In the ‘well-stirred-reactor’ (WSR) limit, the flame is relatively featureless

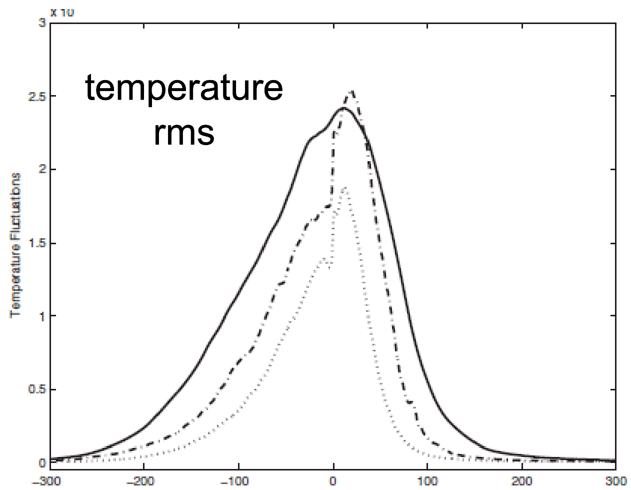
LEM instantaneous structure

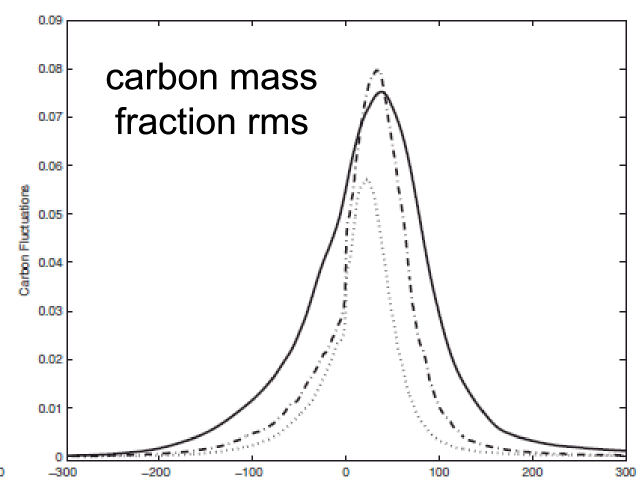




Two LEM parameters were tuned to fit DNS profiles and turbulent burning velocity (one-step kinetics)

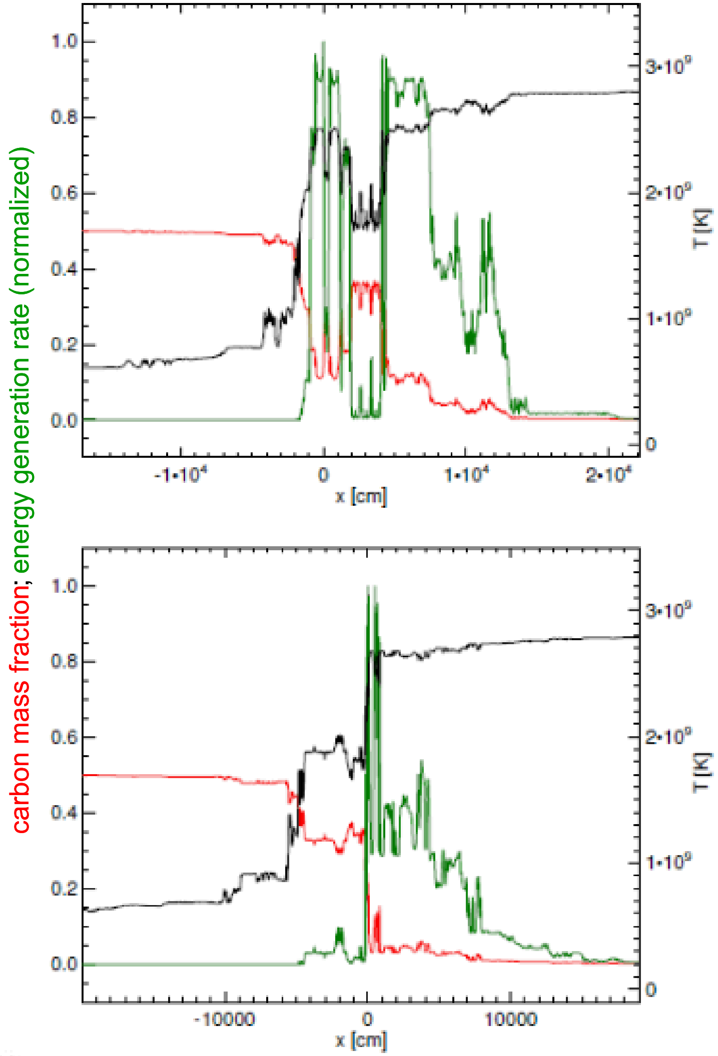
DNS (LBNL group)
LEM best fit
LEM excursion



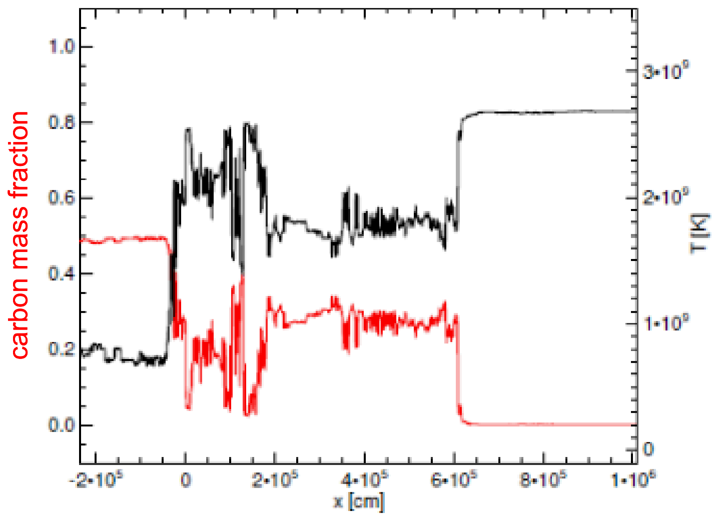


Woosley, Kerstein, Sankaran, Aspden, and Roepke (2009)

LEM, but not DNS, can reach the ‘stirred-flame regime’ between flamelet and WSR limits



Regions of relatively uniform mixing are seen



These cases used a multistep nuclear reaction mechanism

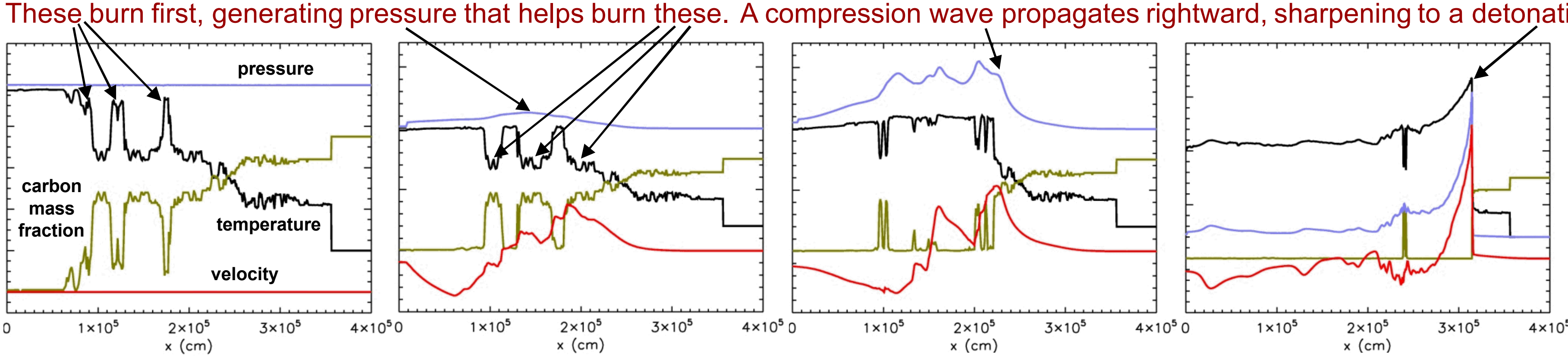
LEM flow states were used to initialize compressible hydro simulations that indicate a new DDT pathway

<u>Context</u>: New physics (e.g., dark energy) is implied if type 1A supernovae are 'standard candles' – but are they?

<u>Prior status</u>: Observations require a 'delayed' deflagration-to-detonation transition (DDT), but nuclear and fluid physics seemed to preclude this.

<u>New insight</u>: DDT in a supernova could result from the sequential interaction of several distinct mixture states, analogous to a pyrotechnic (igniter, primer, main charge), but in this case unconfined.

These burn first, generating pressure that helps burn these. A compression wave propagates rightward, sharpening to a detonation.



initial state

(vertical scale of each property is different on each plot)

Step-like property profiles are central to this picture – but are they real?

- Step-like structure is well known, e.g., as shown below.
- Proposed explanations invoke details of turbulence dynamics.
- Its occurrence in LEM implies a more general mathematical origin. <u>This will be investigated.</u>

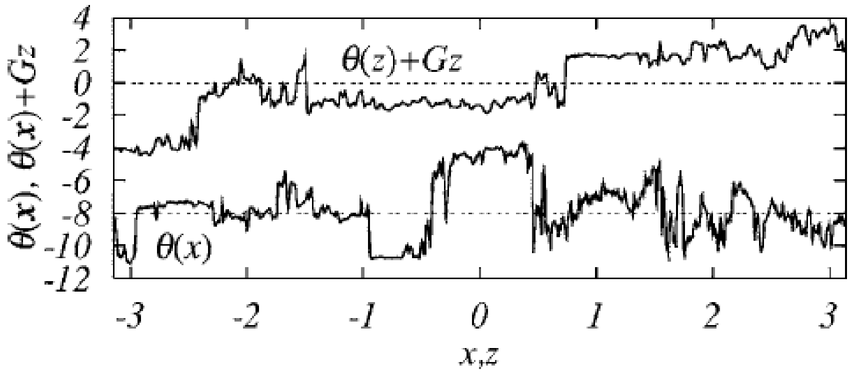


FIG. 4. One-dimensional profile of $\theta+Gz$ (upper) and θ (lower) along the directions of $e_{\parallel}$ and $e_{\perp}(=e_x)$ obtained from case G, respectively. The lower curve is shifted by −8 for clarity. Horizontal dot lines denote the zero levels.

DNS of passive scalar mixing:

Watanabe & Gotoh, 2006

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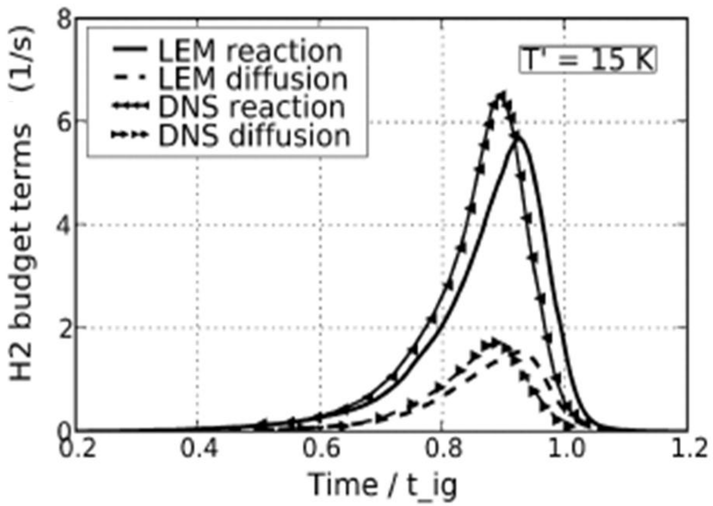
LEM is being used for both fundamental and applied HCCI combustion studies

Fundamental study: Comparison to 2D DNS by J. Chen et al.

(with M. Oevermann , TU Berlin, & H. Schmidt, TU Cottbus)



- Homogeneous charge compression ignition (HCCI) engine combustion relies on autoignition rather than flame propagation to burn the fuel
- DNS: Constant-volume H_2-air combustion with initial T fluctuations (rms: T′)
- Shown here: LEM captures the relative contributions of autoignition and flame propagation to H_2 consumption
- Will compare to planned 3D DNS with hydrocarbon fuel
- With LEM, can affordably explore sensitivity to details of the chemical mechanism

LEM HCCI application at GM

A General Motors team is using LEM to study mixing-chemistry (n-heptane, iso-octane) interactions under HCCI conditions and other HCCI performance issues.

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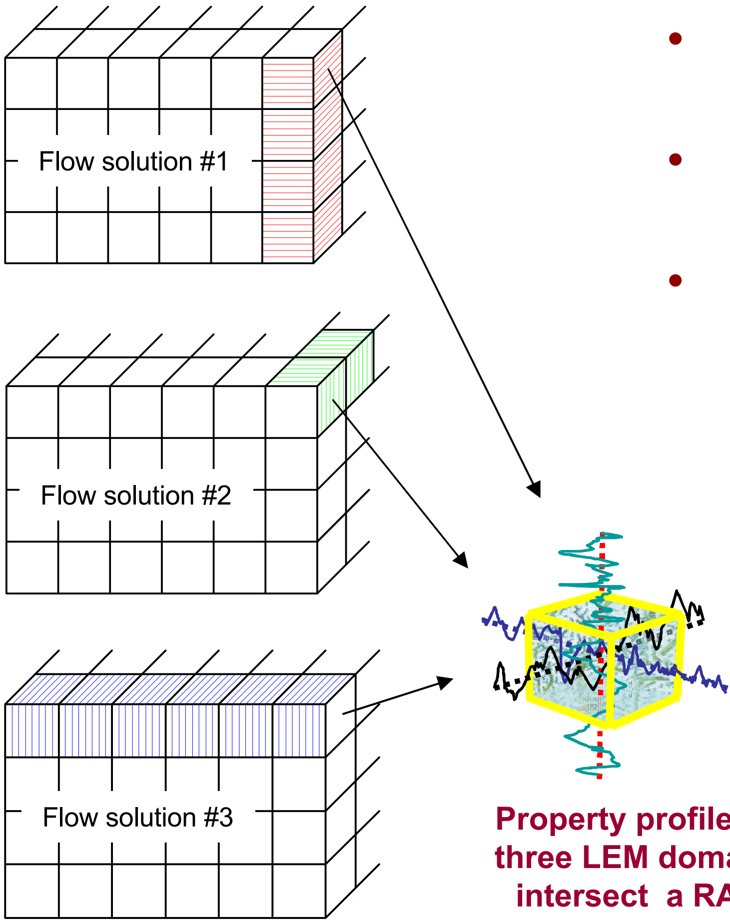
Time advancement of a 3D lattice-work of coupled LEM domains can be driven by RANS input: ‘LEM3D’

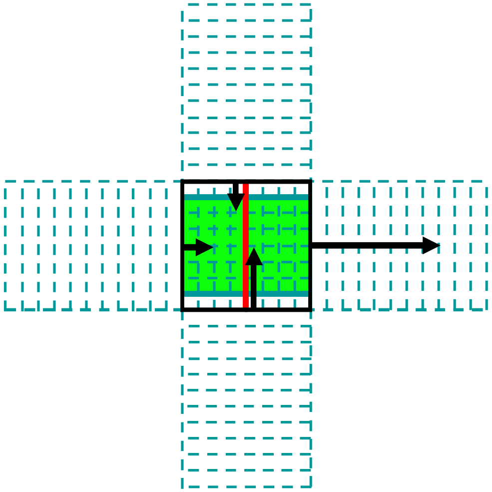


Property profiles on the three LEM domains that intersect a RANS CV

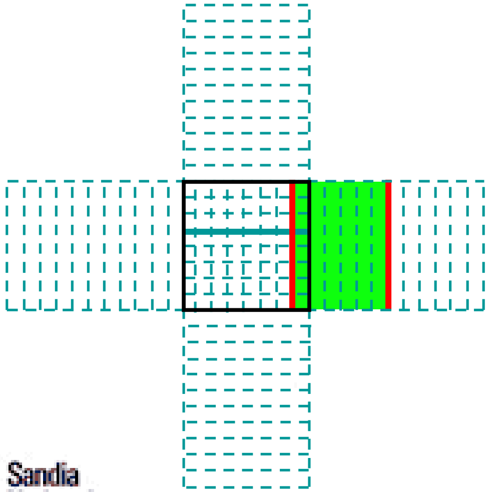
- Each LEM domain spatially refines RANS control volumes (CVs) in one coordinate direction
- Each CV is thus contained within three orthogonal LEM domains, each within a different flow solution
- Time-advancement cycle:
  - **Advancement on individual LEM domains**
    - **1D representation of small-scale 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 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, 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 chemically dissimilar fluids into contact
- Remedy: Use coarse CVs to minimize the artifact

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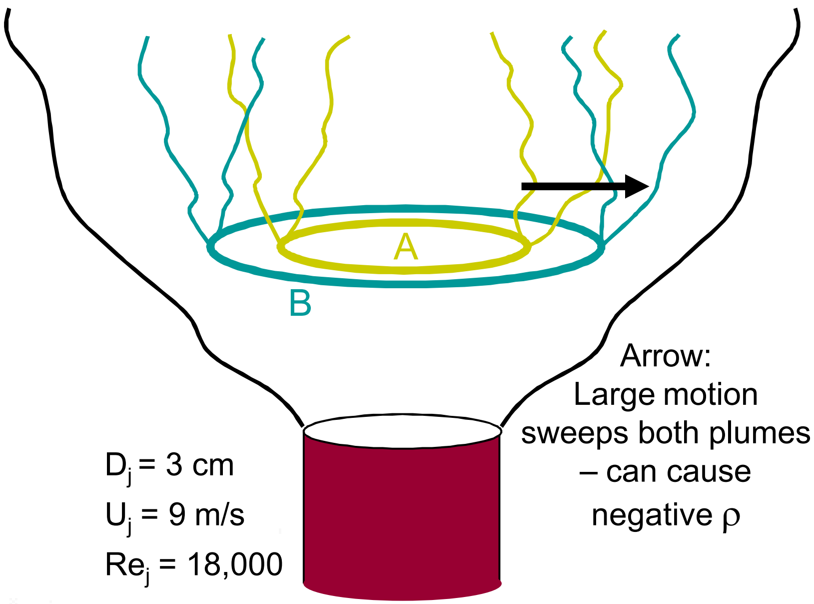
Using measured properties (surrogate RANS), LEM3D captures the mixing of scalars released within a jet

- 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



D_j = 3 cm

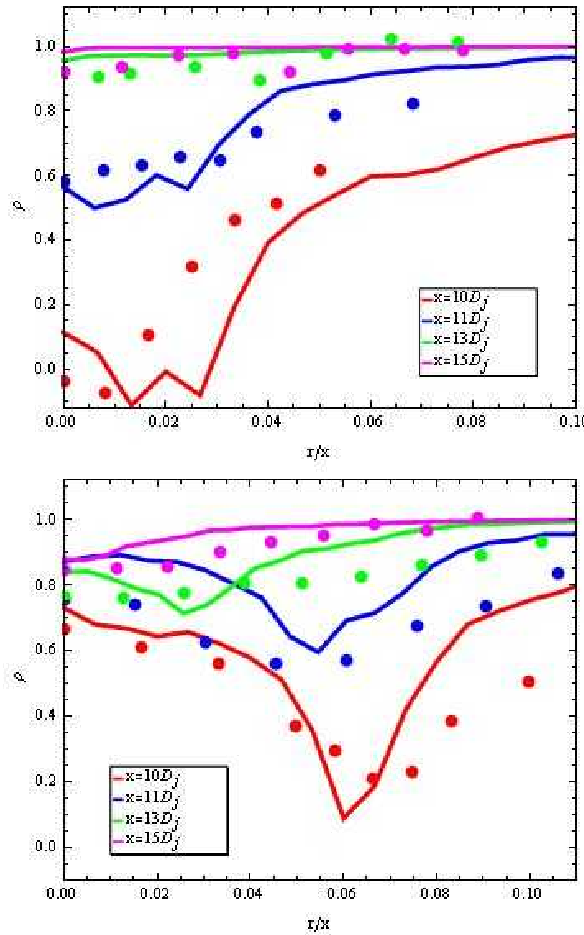
U_j = 9 m/s

Re_j = 18,000

Arrow:
Large motion sweeps both plumes – can cause negative ρ

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

Ring diameters



10 and 15 mm

35 and 40 mm

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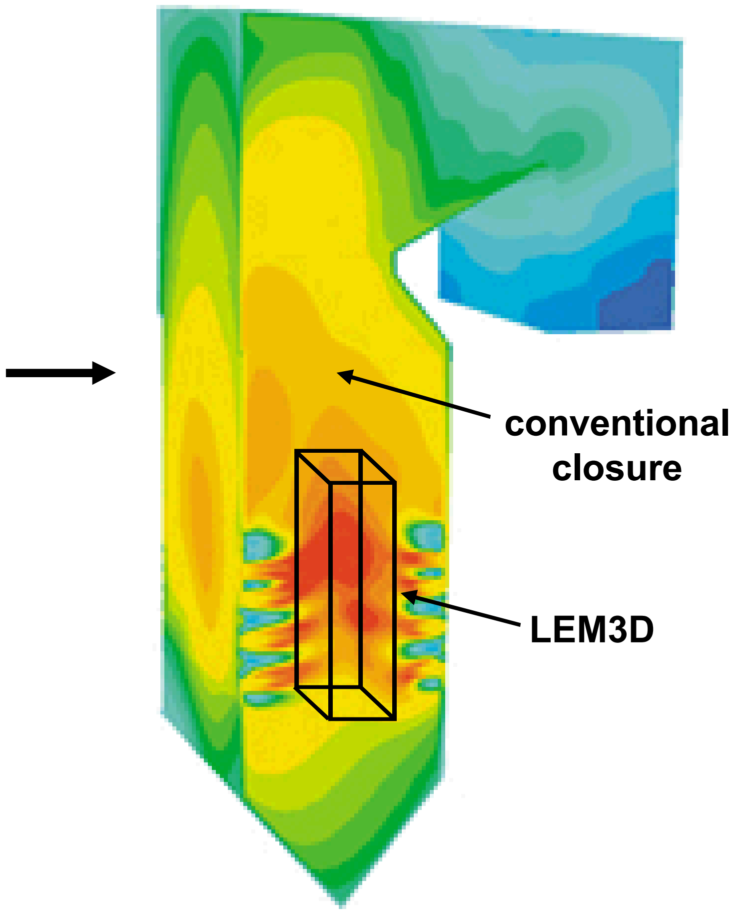
LEM3D is being configured for combustion applications

- A variable-density formulation is under development (with 2-way RANS-LEM3D coupling)
- Chemical kinetics is being incorporated
- LEM3D sub-regions will be imbedded in flow simulations to resolve mixing locally
- Will validate against a purpose-built confined-jet-mixing experiment (SINTEF)
- Will couple LEM3D to an ODT-based 3D simulation (explained next)
- This work is a collaboration with SINTEF (I. Gran, S. Sannan, T. Weydahl)



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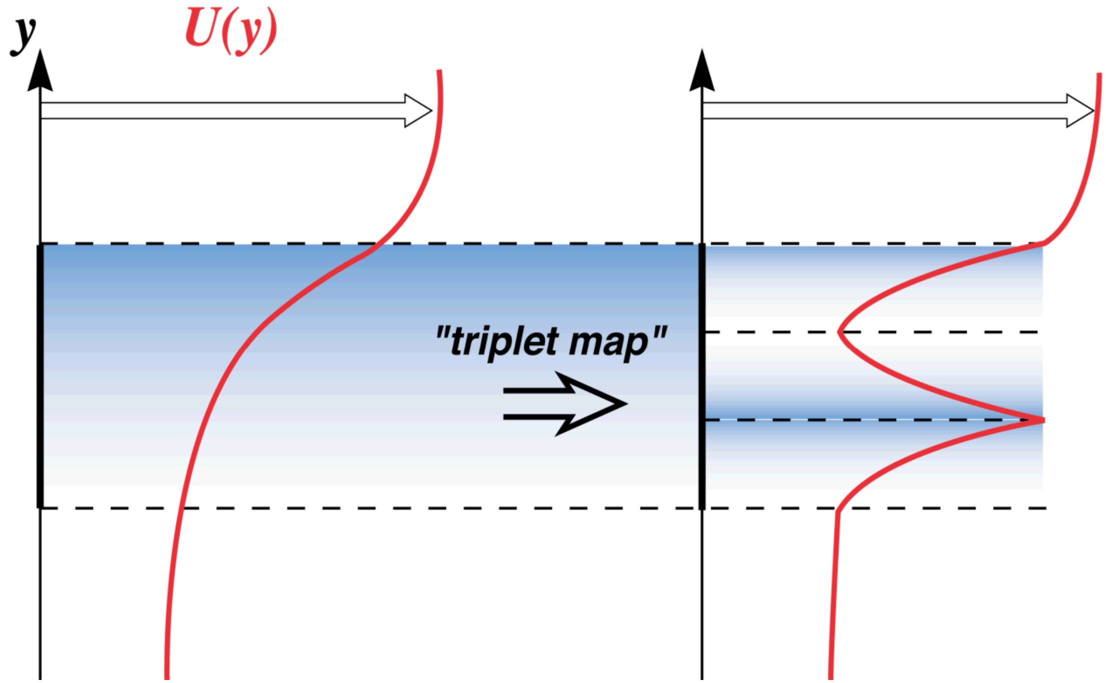
In ODT, the triplet map amplifies shear, inducing an *eddy cascade* (feedback mechanism)

- **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



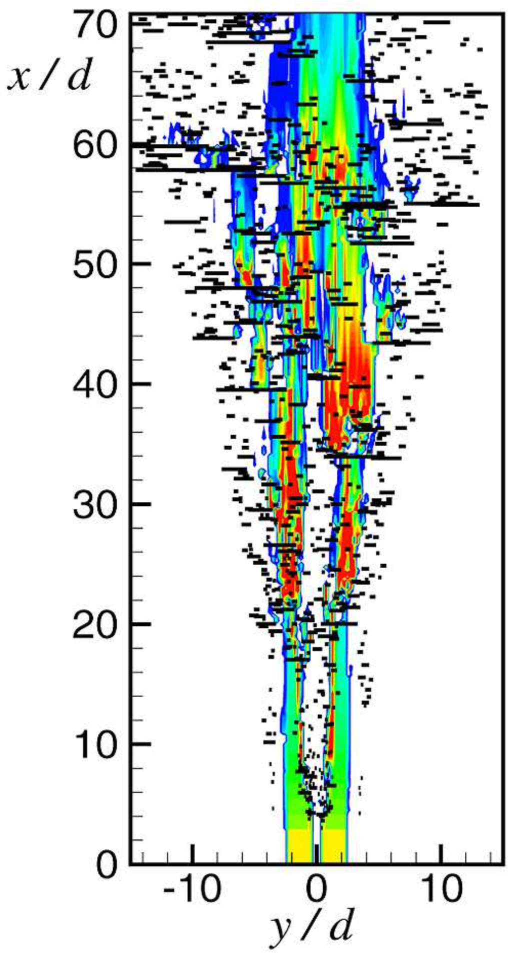
High shear at small scales drives small eddies, leading to an eddy cascade

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

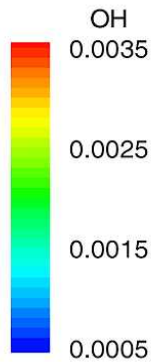
ODT eddy selection is based on the mixing-length concept, applied locally

- 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')

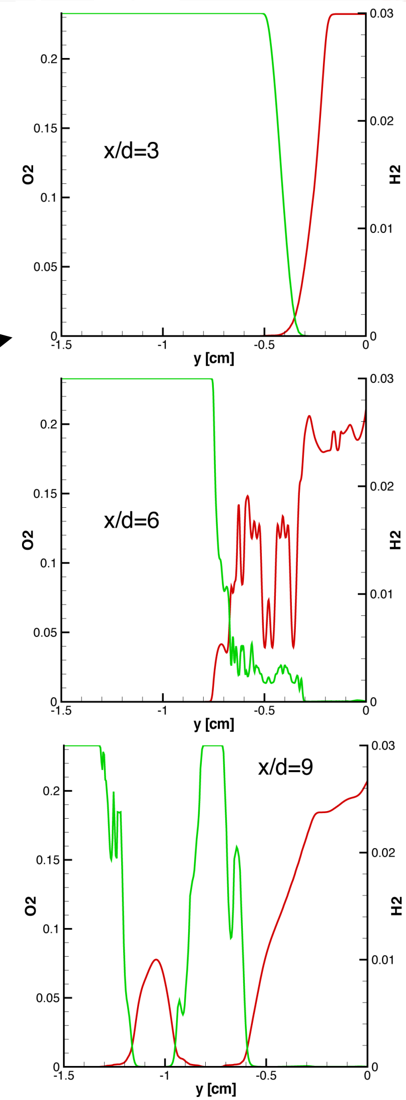
LEM and ODT resolve advective-diffusive-reactive couplings and hence are 'regime-independent'



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



Caveat:
Simulations are planar temporal, interpreted as cylindrical spatial advancement

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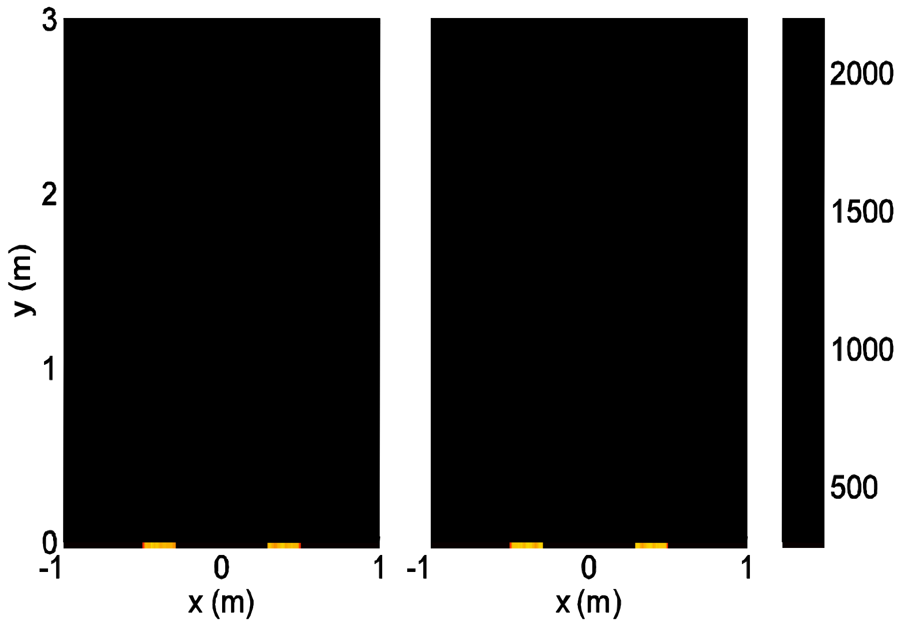
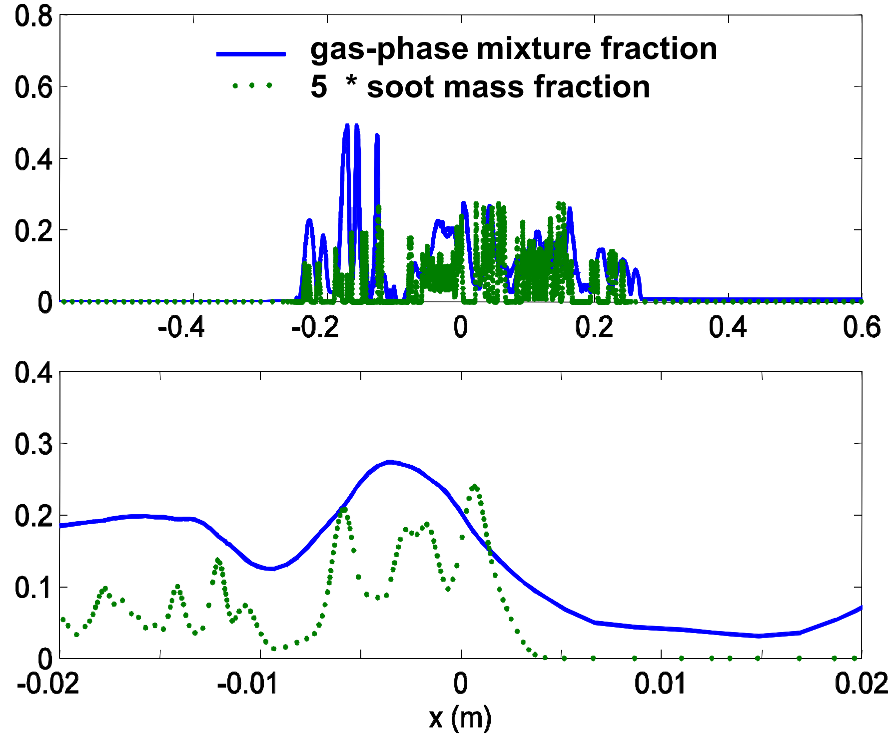
Spatially advancing ODT captures the structure of an ethylene-air sooting plume

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

- Why a bottom-up strategy?
- A small-scale formulation using map-based advection
- Economical simulation of small-scale *mixing,* illustrated by:
  - **Pipe mixing**
  - **Astrophysical flames**
  - **HCCI engine combustion**
- Coupling the mixing model to a large-scale-flow solver
  - **Formulation**
  - **Validation**
- Economical simulations of small-scale *flow*
- All-scale flow simulation using coupled small-scale-flow simulations
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- Summary

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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
- Status
  - Incompressible ODT3D has been implemented and validated (shown next)
  - A reformulation targeting combustion applications is underway

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ODT3D captures subtle 3D flow effects while fully resolving wall layers

Validation cases:

- Open channel (no-slip wall and free-slip surface): Captures free-surface upwelling/downwelling
- Square duct: Captures secondary recirculations (spontaneous symmetry breaking)
- Lid-driven cavity: Captures wall-layer distortions induced by the primary recirculation

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

- Map-based advection is an advantageous approach for cost-effective simulation of turbulent combustion and other turbulence-microphysics couplings

- Its current uses include
  - Fundamental studies yielding new insights
  - Engineering (e.g., design concept screening)
  - Building block for 3D simulation

- It enables a bottom-up strategy that offers opportunities for improving the capabilities of turbulent combustion simulations