Lecture 2

Turbulent Combustion Modeling
Linear Eddy Mixing Model for LES

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Regimes of Turbulent Combustion

- Perfect "mixing" requires a separate premixer
- All combustion devices incorporate mixing devices
  - Swirl is used to enhance mixing in most devices
- "Premixed" systems
  - Mixture entering the combustor is not perfectly mixed
  - Equivalence ratio variation: partially premixing
  - Lean mixture can occur *locally as well as globally*
- "Non-Premixed" liquid fueled systems
  - Mixing occurs after liquid vaporization
    - Many stages of mixedness
  - Spatial and temporal variation in mixing is very likely
- Can we develop a SINGLE formulation for ALL flows?

Strategy of Modeling

- Scale Separation implicit or explicit in ALL turbulent closure models (Peters, pg 4)
  - Scales of turbulence and combustion are separated in the inertial range
  - Mixing process in the inertial range independent of chemistry and simplify modeling considerable
  - Kolmogorov scaling laws are not modified by molecular mixing and heat release at the (even) smaller scales.
  - This seems reasonable is this true at very high Re?
- Without Scale Separation - any approach currently available?
  - Linear-Eddy Model in LES
- Why is that so important?
  - Simplified models can be "verified" (Peters, pg 6)

Classification of Turbulent Combustion Models in Terms of Chemistry and Mixing (Modified from Peters, pg 64)

	Premixed Combustion	Nonpremixed Combustion
Infinitely Fast Chemistry	Bray-Moss-Libby Coherent Flame	Conserved Scalar Equilibrium Model
Finite-rate w/o Molecular mixing	PDF Transport	PDF Transport
Finite-rate with filtered or modeled reaction rate	Flamelet Model G-equation, G-Z, ATF EBU, FSD, PaSR…	Flamelet Model Z, ATF, CMC, PaSr…
Finite-rate with Molecular mixing	Linear-Eddy Model	Linear-Eddy Model

LES Subgrid Combustion Modeling

$$\begin{cases} \partial_t(\bar{\rho}) + \nabla\cdot(\bar{\rho}\tilde{\mathbf{v}}) = 0 \\ \partial_t(\bar{\rho}\tilde{\mathbf{v}}) + \nabla\cdot(\bar{\rho}\tilde{\mathbf{v}}\otimes\tilde{\mathbf{v}}) = -\nabla\bar{p} + \nabla\cdot(2\mu\tilde{\mathbf{D}}_D - \mathbf{B}) + \bar{\rho}\tilde{\mathbf{f}} \\ \partial_t(\bar{\rho}\tilde{E}) + \nabla\cdot(\bar{\rho}\tilde{\mathbf{v}}\tilde{E}) = \nabla\cdot(-\bar{p}\tilde{\mathbf{v}} + \tilde{\mathbf{S}}\tilde{\mathbf{v}} + \bar{\mathbf{h}} - \mathbf{b}_E) + \bar{\rho}\tilde{\sigma} \\ \partial_t(\bar{\rho}\tilde{Y}_i) + \nabla\cdot(\bar{\rho}\tilde{\mathbf{v}}\tilde{Y}_i) = \nabla\cdot(D_i\nabla\tilde{Y}_i - \mathbf{b}_i) + \overline{M_i P_{ij}\dot{w}_j} \end{cases}$$

EVM, MM or ILES

Barlow thermal radiation model

How do we represent the filtered reaction rates?

Flamelet Model

Assume a thin flame

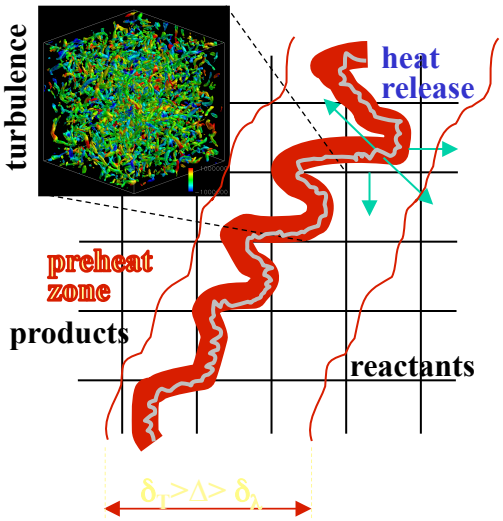
$\tilde{Y}_i = \hat{Y}_i(\tilde{c},\tilde{z})$

$D_t(\bar{\rho}\tilde{z}) = \nabla\cdot\mathbf{b}_z$

$D_t(\bar{\rho}\tilde{c}) = \nabla\cdot\mathbf{b}_c - \rho_u S_u \Xi\,|\nabla\tilde{\mathbf{c}}|$

Model Ξ and obtain S_u from a library $\hat{S}_u$

FW models of the form $\Xi = 1 + f(\mathrm{Re}, Da, Ka)$



Finite Rate Models

Assume that $\delta_T \geq \Delta$. Model $\overline{\dot{w}_j(Y)}$ using $\dot{w}_j(\tilde{Y})$ such that

$$\overline{\dot{w}_j(Y)} = \kappa()\dot{w}_j(\tilde{Y})$$

with κ estimated using different hypothesis'

- EDC, PaSR
- TFM
- T/P PDF

EVM: Eddy viscosity model, MM: Mixed Model, ILES: Implicit LES

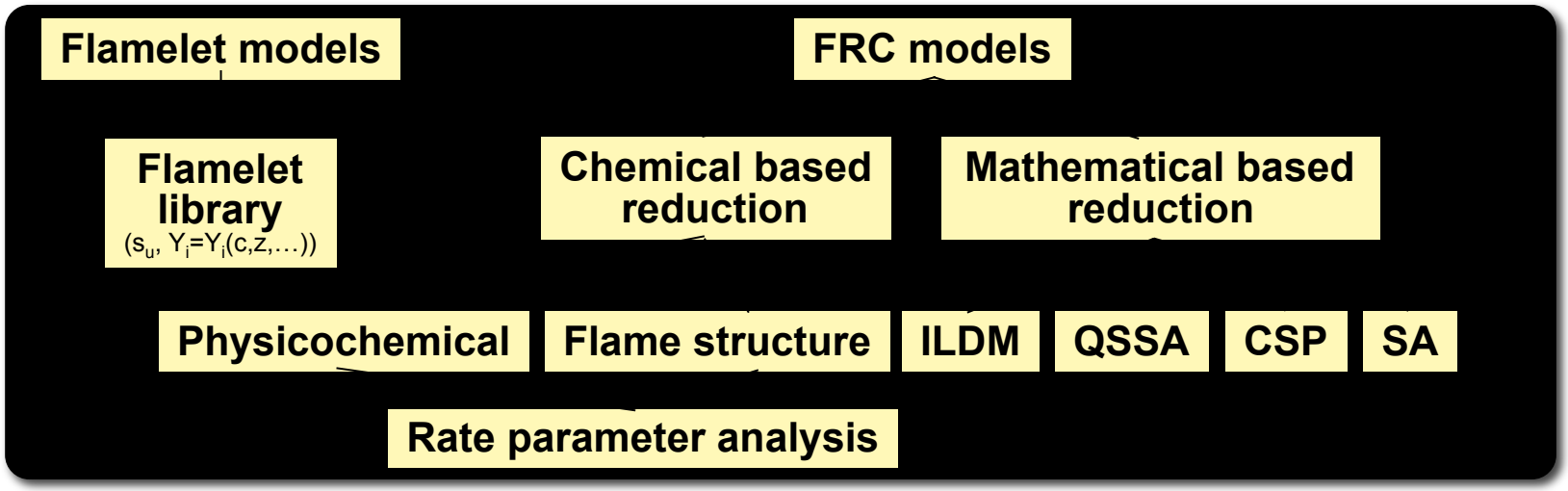
Reduced Chemical Kinetics

Detailed chemical kinetics too expensive to include in multi-dimensional unsteady CFD. Also produces too much information.

Two fundamental problems encountered in formulated reduced chemical kinetics multi-dimensional unsteady CFD:

- Formulation of reduced reaction mechanism (<15 species <20 reactions)
- Estimation of accurate rate parameters for the reduced mechanism

Different ways to address these coupled issues based on physical or mathematical considerations



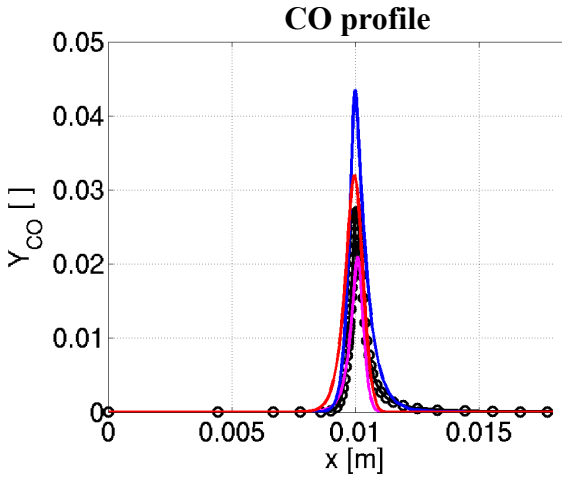
Reduced Chemical Kinetics cont'd

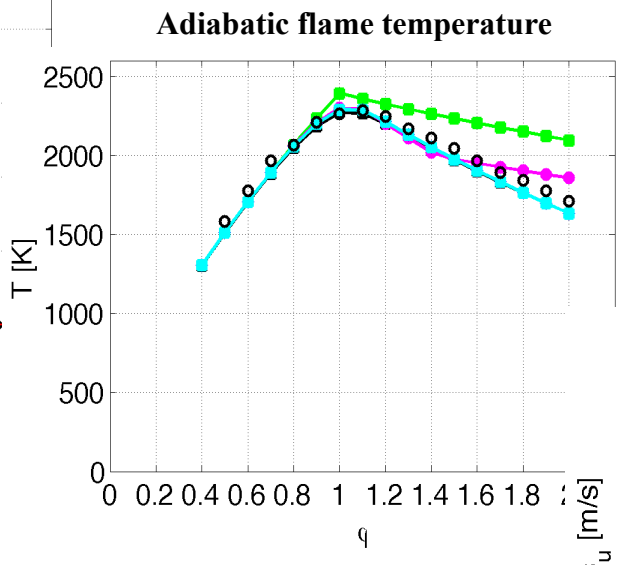
Overview of different approaches to reduce the chemical kinetics in CFD

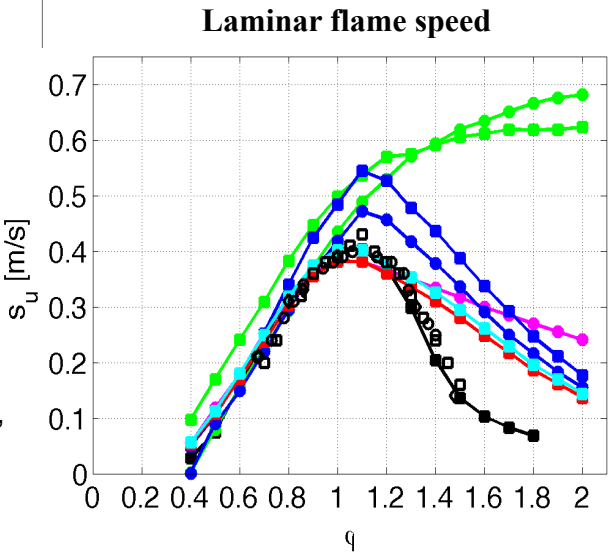
Method	Advantages	Disadvantages
Physicochemical and Flame structure	Intuitive, easy to apply and to implement accepted by nearly all CFD codes, efficient, includes a range of complexity.	Rate parameter estimations difficult, simple (1-step mechanisms) result in poor T predictions.
Intrinsic Low Dimensional Manifolds (ILDM)	Can be automated, CFD only requires the solution of 2 to 3 additional transport equations.	Requires massive amounts of data storage, generation of ILDM is a very slow process, difficult to get higher dimensionality.
Quasi Steady-State Assumptions (QSSA)	Matches detailed mechanisms well, good theoretical basis, can be automated.	Expensive, complicated to perform, non-standard implementation requiring sub-iterations to solve for steady-state species, rates not in Arrhenius form, requires advanced coding and numerics.
Sensitivity Analysis (SA)	No specialized implementation, can be quite accurate for conditions of interest.	Only valid close to conditions for which it was generated, typically 20 or more species required, expensive to generate.
Computational Singular Perturbation (CSP)	Number of steps in resulting mechanism can be specified, fairly accurate, can be used for all types of flames.	Non-standard implementation requiring sub-iterations to solve for steady-state species, rates not in Arrhenius form, requires advanced coding and numerics.
Laminar flamelet	Chemistry parameterized by c and/or z as well as $s_u=s_u(z, \ldots)$, computationally cheap, detailed chemistry can be included by means of a flamelet library.	Generation of laminar flamelet library, different models for premixed and diffusion flames, cannot deal with partially premixed flames, chemistry parameterized by s_u, lacks reaction-diffusion coupling effects.

LES Reduced Combustion Chemistry cont'd

Comparison of different detailed and reduced reaction mechanisms and experimental adiabatic temperature and flame speed data for C_3H_8-air combustion.







Legend: (–■–) A1, (–●–) A1M, (–●–) F2, (–■–) JL4, (–●–) JL4M, (–■–) KPY7, (–■–) KPY15, (–■–) C_3H_8 Williams *et al*, detailed reaction mechanism, (○) C_3H_8-air exp data Vagelopoulos *et al*., (□) C_3H_8-air exp data Boschaart & deGoey, (◇) C_3H_8-air exp data Marley & Roberts

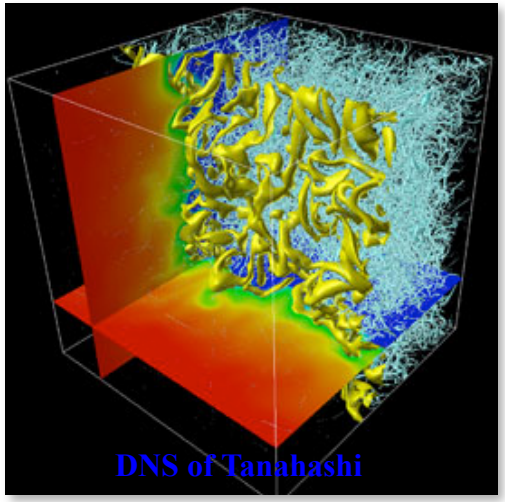
Fureby C. et al; 2012, Submitted to Comb. Inst.

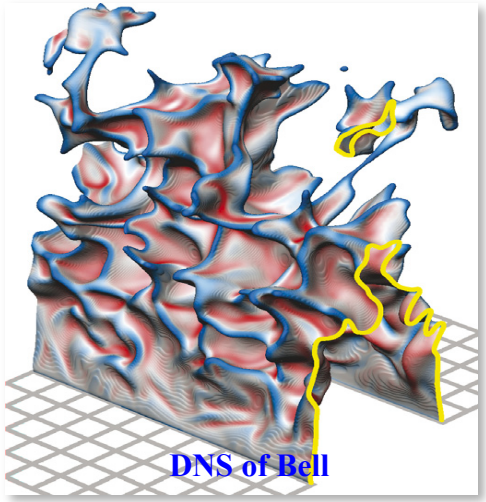
Turbulence Chemistry Interactions

Although most of the energy lies within the resolved scales all of the chemistry occurs on much smaller scales – mixing, chemical kinetics, exothermicity, volumetric expansion, …

Analysis of experiments (Batchelor & Townsend, Kuo & Corrsin, …) and DNS (Woodward *et al*, Tanahashi *et al*, Chen *et al*) suggests that:

- non-uniform spatial distribution of fine structures
- folded vortex sheets, ribbons and tubes
- exothermicity occurs in-between fine structures





Turbulence Chemistry Interactions cont'd

Given an arbitrary multi-step reaction of the form

$$\Sigma_{i=1}^{N}(P'_{ij}\Im_i)\Leftrightarrow\Sigma_{i=1}^{N}(P''_{ij}\Im_i),\ P_{ij}=P''_{ij}-P'_{ij}$$

we may examine the influence of the subgrid fluctuations by inserting $\rho=\bar{\rho}+\rho'$, $T=\tilde{T}+T''$ and $Y_i=Y_i+Y_i''$ into the rate expression to obtain

$$\overline{\dot{w}_i}=M_iP_{ij}\left[\overline{\Omega_f\tilde{\rho}^{m_f}\hat{A}_{f,j}T^{n_{f,j}}e^{-T_{a,f,j}/\tilde{T}}\Pi_{k=1}^{N}\tilde{Y}_k^{\hat{P}'_{kj}}-\Omega_b\bar{\rho}^{m_b}\hat{A}_{b,j}T^{n_{b,j}}e^{-T_{a,f,j}/\tilde{T}}\Pi_{k=1}^{N}\tilde{Y}_k^{\hat{P}''_{kj}}}\right]$$

$$\Omega_f=[1+\frac{m_f}{\bar{\rho}}\rho'+(\frac{m_f^2}{2\bar{\rho}^2}-\frac{m_f}{2\bar{\rho}^2})\rho'^2+\ldots]\Pi_{k=1}^{N}[1+\frac{\hat{P}'_{kj}}{\tilde{Y}_k}Y'_k+(\frac{\hat{P}'^2_{kj}}{2\tilde{Y}_k^2}-\frac{\hat{P}'_{kj}}{2\tilde{Y}_k^2})Y'^2_k+\ldots]\times$$

$$[1+\frac{T_a}{\tilde{T}^2}T'-(\frac{T_a}{T^3}-\frac{T_a^2}{2\tilde{T}^4})T'^2+\ldots]$$

$$\Omega_b=[1+\frac{m_b}{\bar{\rho}}\rho'+(\frac{m_b^2}{2\bar{\rho}^2}-\frac{m_b}{2\bar{\rho}^2})\rho'^2+\ldots]\Pi_{k=1}^{N}[1+\frac{\hat{P}''_{kj}}{\tilde{Y}_k}Y'_k+(\frac{\hat{P}''^2_{kj}}{2\tilde{Y}_k^2}-\frac{\hat{P}''_{kj}}{2\tilde{Y}_k^2})Y'^2_k+\ldots]\times$$

$$[1+\frac{T_a}{\tilde{T}^2}T'-(\frac{T_a}{T^3}-\frac{T_a^2}{2\tilde{T}^4})T'^2+\ldots]$$

where the Ω-terms represent the subgrid correlations to be modeled

- terms not necessarily convergent
- no closed expression
- large influence of the sgs T terms

Examples: Combustion Modeling Approaches

G-Eq. and/or Flamelet based LES

Flamelet model in which Z is solved for conventionally, whereas G is solved for by means of a level-set method. S_u is obtained through a library-look up and $\Xi = f(Re,Da,Ka)$

PaSR LES

Finite rate chemistry model in which κ is modeled as the ratio $\kappa=\tau_m/(\tau_c+\tau_m)$, in which τ_c and τ_m are estimated as $\tau_c=\delta_u/S_u$ and $\tau_c=\Delta/k^{1/2}$.

Thickened Flame Model LES

Thicken the flame by $F=\Delta/\delta_u$ and account for the subgrid flame wrinkling through Ξ=f(Re,Da,Ka)

$$\partial_t(\bar{\rho}\tilde{Y}_i) + \nabla\cdot(\bar{\rho}\tilde{\mathbf{v}}\tilde{Y}_i) = \nabla\cdot(EFD_i\nabla\tilde{Y}_i - \mathbf{b}_i) + M_i P_{ij} E\tilde{\dot{w}}_j / F$$

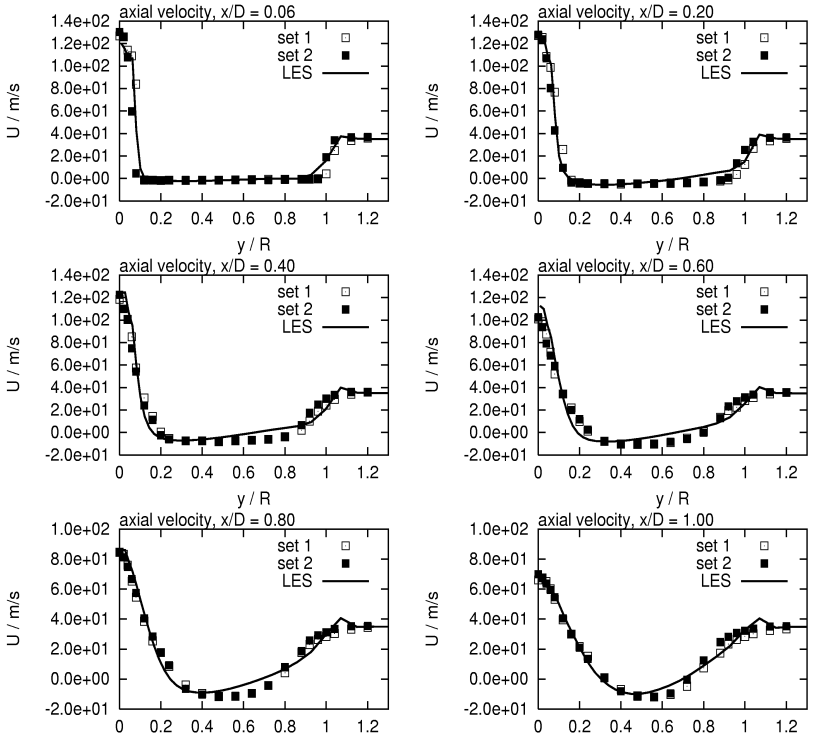
EDC LES

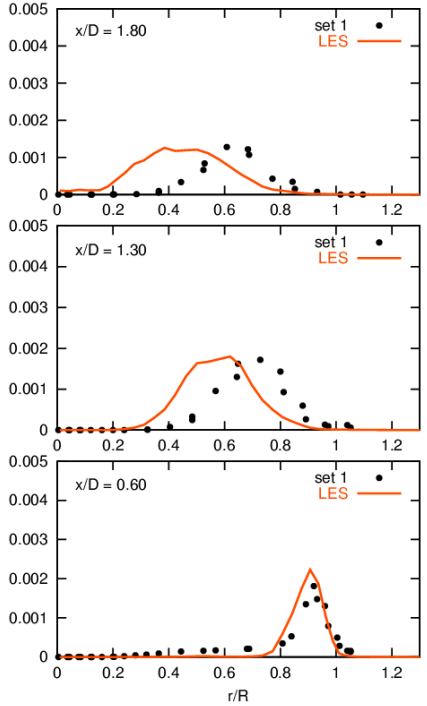
Multi-scale method in which subgrid balance equations are first solved for Y_i^* (flame region) and Y_i^0 (surrounding) from which

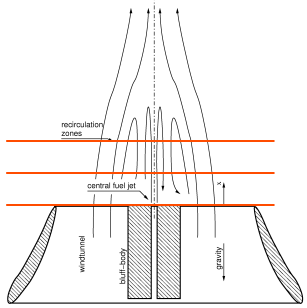
$$\overline{\dot{w}_i} = \gamma^* \dot{w}_i(\bar{\rho}, Y_i^*, T^*) + (1-\gamma^*)\dot{w}_i(\bar{\rho}, Y_i^0, T^0)$$

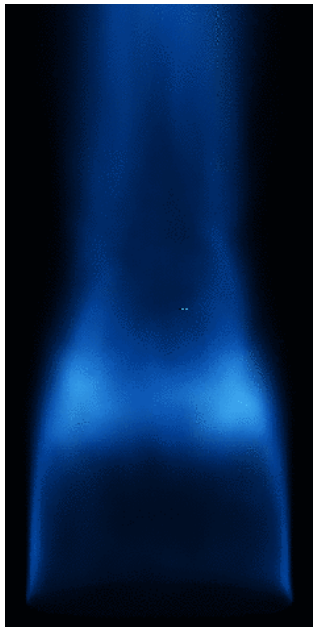
Steady LES-Flamelet-Model - Bluff-Body Flame

Velocity-profiles at axial positions









Kempf et. al. (2003, 2004)

(Exp. Masri et. al. (1998))

OH Profiles

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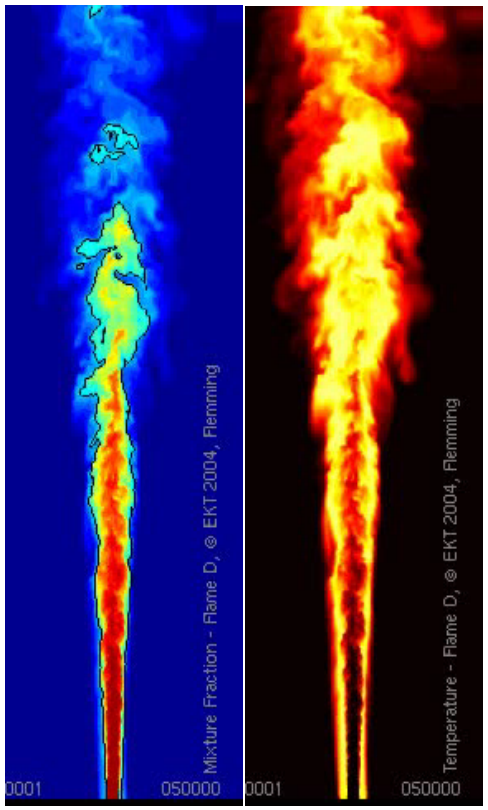
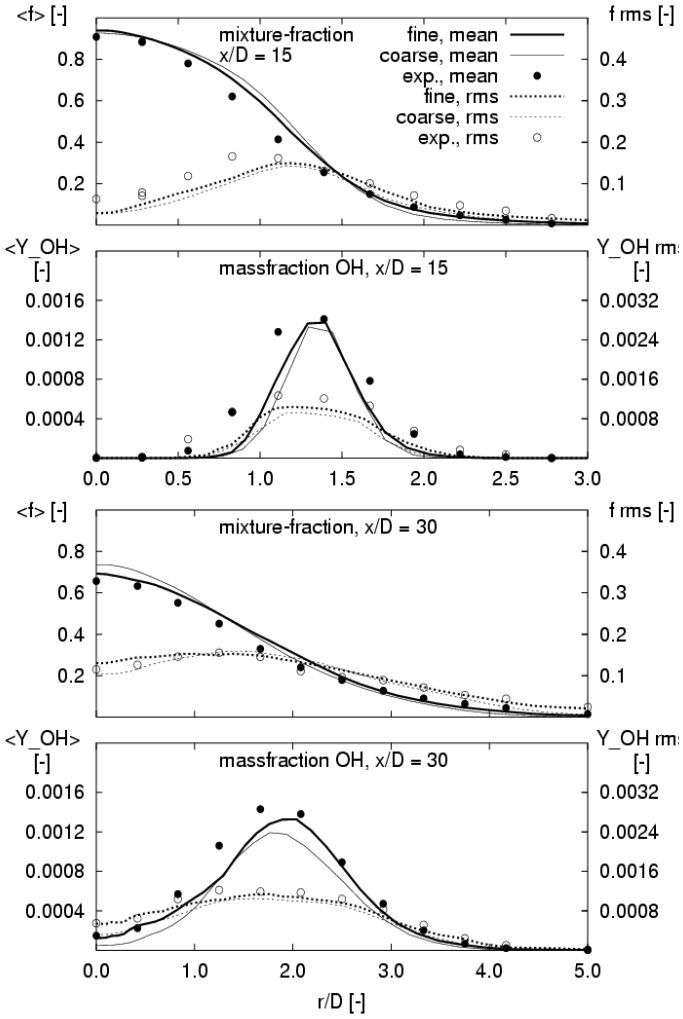
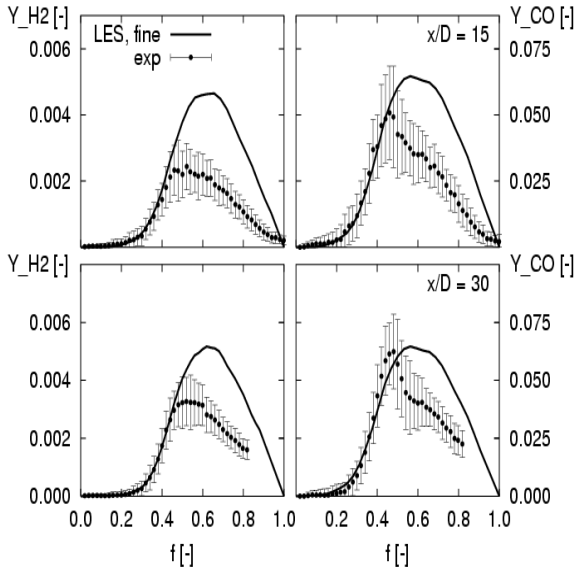
Courtesy: Janicka

Steady LES-Flamelet-Model D-Flame

Mixture fraction **T**







Kempf et. al. (2004)

(Exp. Barlow et. al. (1998))

Stable Species, T: OK

Minor Species: So-So

Extinction/Reignition: need more work!!

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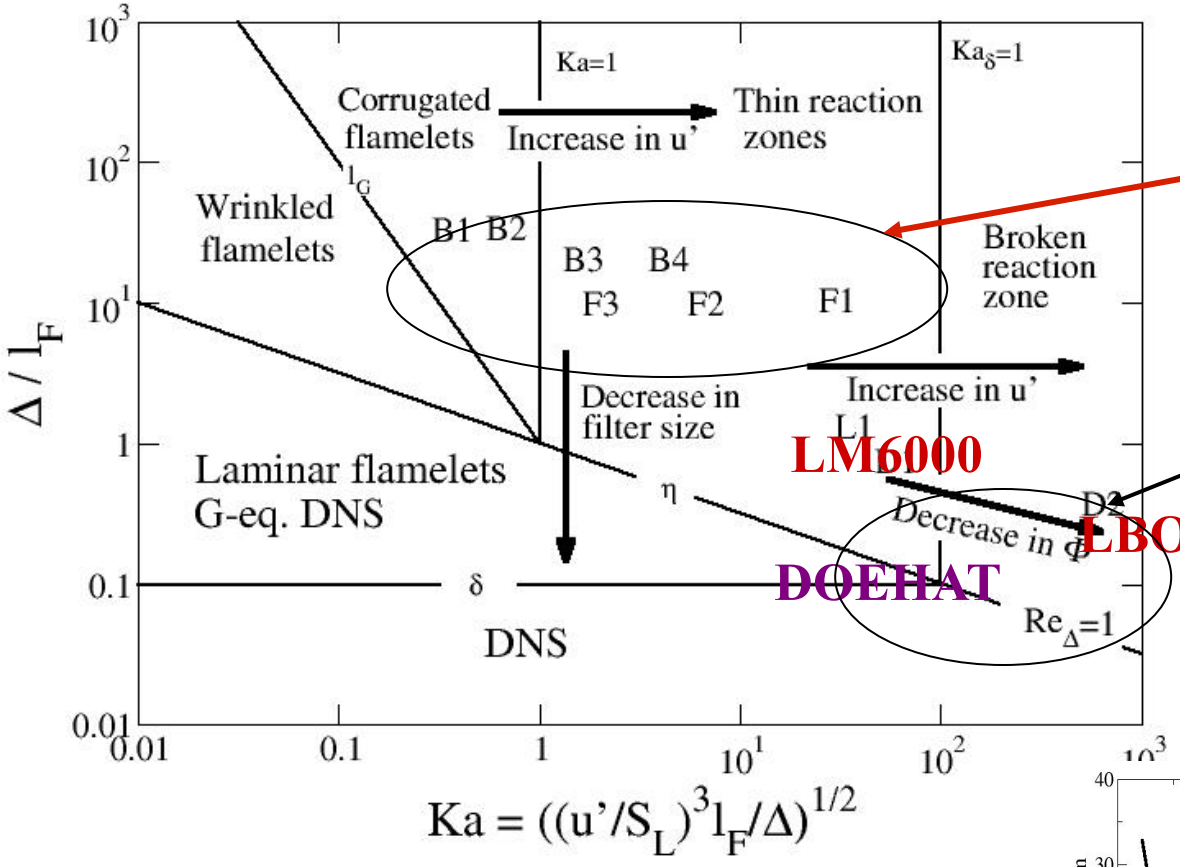
Courtesy: Janicka

Combustion Regimes (Pitsch, 2002)



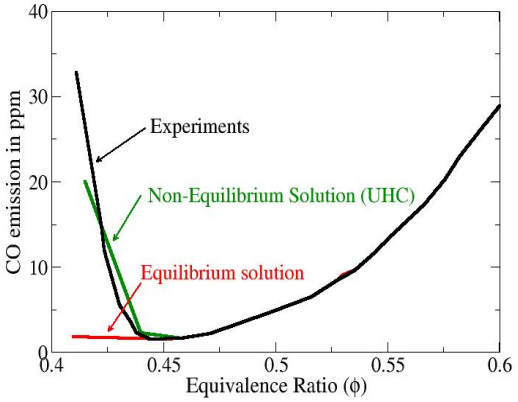
Laboratory Flame

Gas Turbine

LM6000

LBO

DOEHAT



- *TRZ-BRZ regimes relevance for lean systems*
- *LBO most likely to occur in Broken Reaction Zone Regime*
- *LES from Flamelet to TRZ to BRZ without model changes*

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Models for Premixed Combustion

- Subgrid BML-(Bray-Moss-Libby)-model
- Artificially thickened flame front model (Poinsot)
- Level set (G-equation: Kerstein, Williams, Peters, Pitsch)
  - Including partially premixed (G-Z) approach
- Linear-Eddy Mixing (LEM) Model (Kerstein)

Artificially Thickened Flames

- Thicken the flame to resolve it on the LES grid (Poinsot 2001, Colin et al., 2000), Vervisch et al. (1996)
- Species equations solved on the LES grid
  - Diffusion coefficient and reaction rate modified to achieve same flame speed and propagation
  - SGS wrinkling included using efficiency function
  - Easy to implement and efficient
  - Applied to complex combustors (shown later)
  - Reduced kinetics
  - Dynamically thickened flame for non-premixed flames

Processes in Turbulent Combustion

- Large-scale convection of scalars by coherent structures and mean flow controlled by geometry of the problem
  - Scalar interface is stretched/wrinkled but not molecularly mixed by these processes
- Small-scale processes
  - Turbulent mixing by smaller eddies (till Kolmogorov)
  - Molecular diffusion (including differential diffusion)
  - Reaction kinetics and heat release
- Small-to-large scale coupling
  - Volumetric expansion due to heat release
  - Modification of the velocity field by heat release
- *LEMLES resolves these processes independently and concurrently*

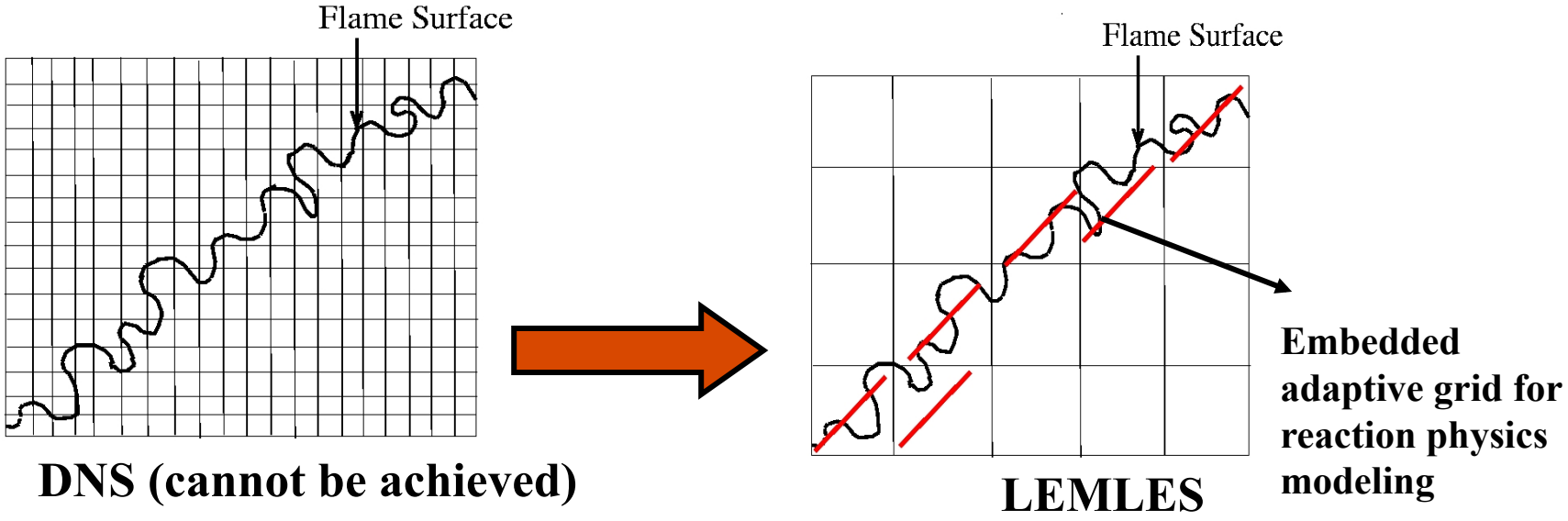
What is LEMLES?

- A multi-scale approach to solve the scalar conservation equations in any solver
  - Can be used in 2D or 3D
  - Can be used for RANS, URANS or LES
- It is a time-dependant method that employs a grid-within-grid strategy
  - Scalar field evolves at the small-scales where mixing, diffusion, kinetics and volumetric expansion all occur

Linear-Eddy Mixing (LEM) in LES

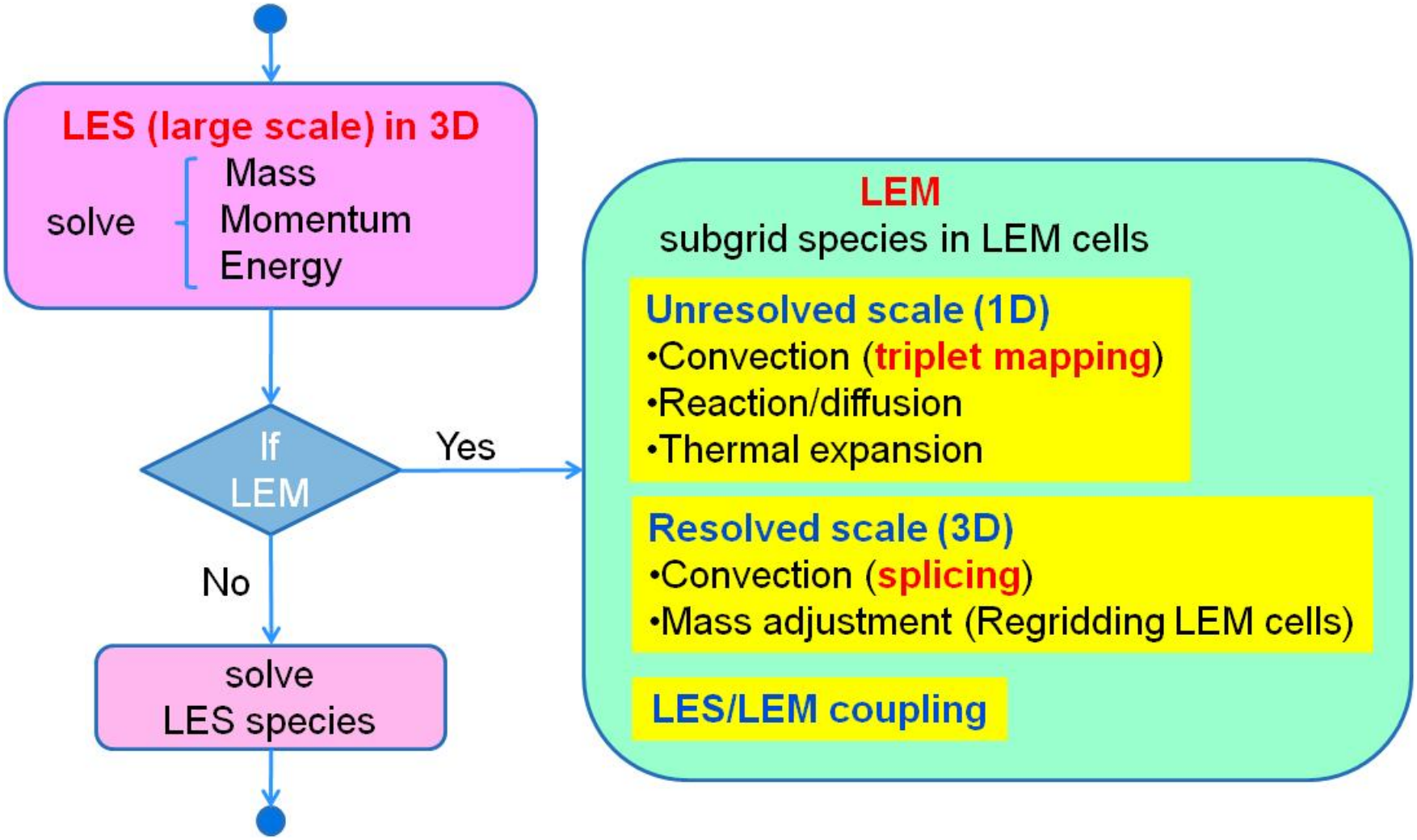
- LEM proposed by A. Kerstein (1989, 1990) is modified and used as a SGS reaction-diffusion "simulation" model
  - Model resides inside every LES cell
- Reaction kinetics closed exactly (as in FDF methods)
- Molecular diffusion is also closed
  - Ability to predict Schmidt number effects
- Parallel implementation is needed for efficiency
- Costly when compared to ATF, G-eqn or flamelet methods
  - Cost similar to FDF methods
- However, application to all types of combustion possible
  - No ad hoc parameters to adjust

Grid-Within-Grid Approach in LEMLES



- *Captures physics within complex geometries*
- *Grid resolution is reasonable compared to DNS*
- *Modeling approach has no "adjustable" parameters*
- *Single formulation validated for many real problems & systems*
  - *Premixed, Non-Premixed and Spray Flames*
  - *Gas Turbines, Afterburners, Rockets, Scramjets*
  - *Detonations, Explosions and Fires*

Linear Eddy Model in LES (LEMLES)



LEMLES Modules

- LES-to-LEM inputs
  - Grid resolution, Reynolds No., mass flux balance
- Internal LEM processes in each LES cell
  - Turbulent stirring, molecular diffusion and reactions
  - Volumetric expansion
  - Also Stand-Alone LEM (code provided)
- LEM transport across each LES cell
  - Scalar convection to maintain mass conservation
- LEM-to-LES coupling
  - Filtered scalar fields from each LES cell used in the energy conservation and equation of state

Subgrid LEM Processes

- Reaction-Diffusion processes
  - Similar to a stand-alone Chemkin but more general
- Subgrid turbulent stirring by eddies smaller than grid
  - Stochastic process using a mapping model
- Volumetric expansion of subgrid field due to heat release
- Computational issues for LEMLES for load balancing
  - Fixed LEM cells per LES volume
  - Re-gridding to maintain load balancing
  - Can be relaxed with some dynamic load balancing

Species Equation: Two Step Decomposition

- **Resolved Species Equation**

$$\frac{\partial(\rho Y_k)}{\partial t} + \underbrace{\frac{\partial(\rho u_i Y_k)}{\partial x_i}}_{\text{(Resolved + Unresolved) scale convection}} - \underbrace{\frac{\partial}{\partial x_i}\left(\rho D_k \frac{\partial Y_k}{\partial x_i}\right)}_{\text{Molecular diffusion}} = \underbrace{\dot{\omega}_k}_{\text{Chemical source term}} + \underbrace{\dot{S}_k}_{\text{Spray source term}}$$

- **Two scale procedure is used:** $u_i = \left(\tilde{u}_i + u'_{sgs}\right)_R + u'_{UR}$
  - **Unresolved Scale**

$$\frac{(\rho Y_k)^* - (\rho Y_k)^n}{\Delta t_{LES}} = \underbrace{-\frac{\partial\left(\rho^n u'_{iUR} Y_k^n\right)}{\partial x_i}}_{\text{Convection}} + \underbrace{\frac{\partial}{\partial x_i}\left(\rho^n D_k \frac{\partial Y_k^n}{\partial x_i}\right)}_{\text{Molecular diffusion}} + \underbrace{\dot{\omega}_k^n}_{\text{Chemical source}} + \underbrace{\dot{S}_k^n}_{\text{Spray source}}$$

  - **Resolved Scale**

$$\frac{(\rho Y_k)^{n+1} - (\rho Y_k)^*}{\Delta t_{LES}} = \underbrace{-\frac{\partial}{\partial x_i}\left[\rho^*\left(\tilde{u}_i^* + u'_{sgs}\right)_R Y_k^*\right]}_{\text{Convection}}$$

Energy Equation

- Resolved Energy Equation [Poinsot & Veynante, Pg. 20]

$$\rho C_p \frac{DT}{Dt} = \frac{DP}{Dt} + \frac{\partial}{\partial x_k}\left(\kappa \frac{\partial T}{\partial x_k}\right) - \left(\rho \sum_{k=1}^{N} C_{p,k} Y_k V_{k,i}\right)\frac{\partial T}{\partial x_i} + \tau_{ij}\frac{\partial u_i}{\partial x_j} + \omega_T^{'} + \dot{Q}_{spray}$$

- With low Mach No. approx and const pressure combustion [Poinsot & Veynante, Pg. 22]

$$\rho C_p \frac{\partial T}{\partial t} = \underbrace{-\rho C_p u_i \frac{\partial T}{\partial x_i}}_{\text{resolved + unresolved convection}} + \underbrace{\frac{\partial}{\partial x_k}\left(\kappa \frac{\partial T}{\partial x_k}\right)}_{\text{heat conduction}} - \underbrace{\left(\rho \sum_{k=1}^{N} C_{p,k} Y_k V_{k,i}\right)\frac{\partial T}{\partial x_i}}_{\text{diffusional enthalpy flux}} + \underbrace{\omega_T^{'}}_{\text{chem rxn}} + \underbrace{\dot{Q}_s}_{\text{spray source}}$$

Energy Equation: Two Step Decomposition

- **As before, a two-scale approach is used:**

$$u_i = \left(\tilde{u}_i + u'_{sgs}\right)_R + u'_{iUR}$$

  - **Small scale processes:**

$$\rho^n C_p \frac{T^* - T^n}{\Delta t} = -\rho^n u'^{n}_{i,UR} \frac{\partial T^n}{\partial x_k} + \frac{\partial}{\partial x_k}\left(\kappa \frac{\partial T^n}{\partial x_k}\right) - \left(\rho^n \sum_{k=1}^{N} C_{p,k}\left(Y_k^n V_{k,i}^n + V_{i,c}^n\right)\right)\frac{\partial T^n}{\partial x_i} + \omega'_T + \dot{Q}_s^n$$

  - **Large scale transport:**

$$V_{i,c}^n = \sum_{k=1}^{N} D_k \frac{W_k}{W} \frac{\partial X_k}{\partial x_i}$$

$$\rho C_p \frac{T^{n+1} - T^*}{\Delta t} = -\rho^* C_p \left(\tilde{u}_i^* + u'^{*}_{sgs}\right)_R \frac{\partial T^*}{\partial x_i}$$

LEM : Reaction Diffusion Equation

- 1-D domain resolve Kolmogorov scale

$$Y_k^* - Y_k^n = \frac{1}{\rho^n}\int_t^{t+\Delta t_{LES}} \left[\underbrace{F_{k\,stir}}_{\substack{\text{turbulent}\\ \text{convection}\\ \text{(stirring)}}} + \underbrace{\frac{\partial}{\partial s}\left(\rho^* D_k \frac{\partial Y_k^*}{\partial s}\right)}_{\substack{\text{molecular}\\ \text{diffusion}}} + \underbrace{\dot{\omega}_k^*}_{\substack{\text{chemical}\\ \text{reaction}}} + \underbrace{\dot{S}_k^*}_{\substack{\text{spray}\\ \text{source}}} \right] dt'$$

- Direction *S* is along the direction of the max. scalar gradient
- Time integ. (dt') corresponds to t_{stir}, t_{diff}, t_{chem}, respectively
  - Spray source is evaluated once at Δt_{LES} but can be called from within LEM solver to treat vaporization and spray mixing at the droplet timescales

LEM: Energy Equation

- 1-D domain: resolve Kolmogorov scale

$$T^* - T^n = \frac{1}{\rho^n C_p}\int_t^{t+\Delta t_{LES}} \left[\underbrace{F_{T\,stir}}_{\text{turbulent convection (stirring)}} + \kappa\frac{\partial T^n}{\partial s} - \underbrace{\frac{\partial T^n}{\partial s}\left(\rho^n \sum_{k=1}^{N} C_{p,k}(V_k^n Y_k^n + V_c^n)\right)}_{\text{molecular diffusion}} + \underbrace{\dot{\omega}_T^n}_{\text{chemical reaction}} + \underbrace{\dot{Q}^n}_{\text{spray source}} \right] dt'$$

Turbulent Transport

- Stochastic stirring
- Model (*Triplet Maps)*

Molecular Diffusion:

- Exact closure
- Mixture Averaged or
- Multi-Component

Reaction

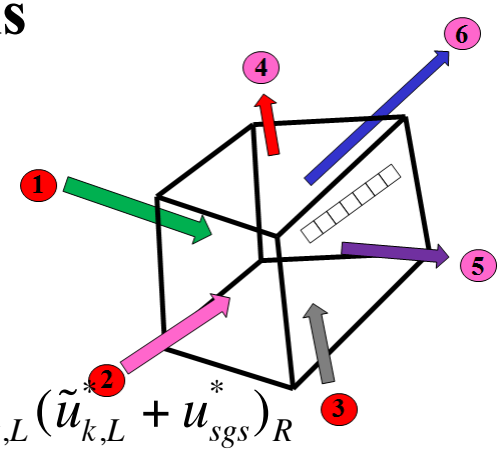
- Exact closure
- Direct integration
- ISAT
- ILDM
- ANN

LEM: Large Scale Transport

- **3D transport of scalar fields between LES cells**

$$Y_k: \quad \sum_{M=1}^{NLEM}\left(\rho_M^{n+1}Y_{k,M}^{n+1}-\rho_M^{*}Y_{k,M}^{*}\right)=\frac{\Delta t_{LES}}{\Delta V_{LEM}}\sum_{L=1}^{Nface}\overline{\rho}^{*}A_{k,L}(\tilde{u}_{k,L}^{*}+u_{sgs}^{*})_R$$

$$T: \quad \sum_{M=1}^{NLEM}\left(\rho_M^{n+1}C_{p,M}^{n+1}T_M^{n+1}-\rho_M^{*}C_{p,M}^{*}T_M^{*}\right)=\frac{\Delta t_{LES}}{\Delta V_{LEM}}\sum_{L=1}^{Nface}\overline{\rho}^{*}\overline{C}_{p,L}^{*}\tilde{T}_L^{*}A_{k,L}(\tilde{u}_{k,L}^{*}+u_{sgs}^{*})_R$$



- Implemented via a Lagrangian algorithm called splicing
- Resolved diffusion velocity is neglected in scalar convection
  - Cannot simulate Laminar flames using LEMLES
    - Note: Stand-alone LEM simulates Laminar flames
    - LEMLES valid and more accurate for high Re flows

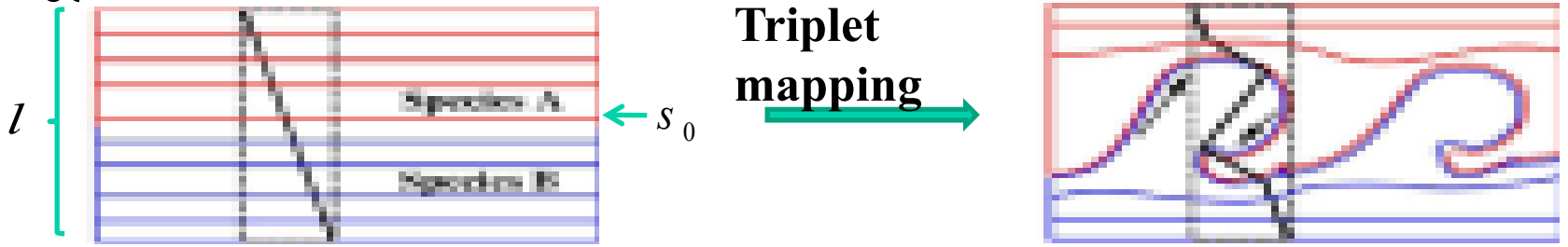
Small Scale Transport: Stirring

$$Y_k^* - Y_k^n = \frac{1}{\rho^n}\int_t^{t+\Delta t_{LES}} \left[\underbrace{F_{k\,stir}}_{\substack{\text{turbulent}\\ \text{convection}\\ \text{(stirring)}}} + \underbrace{\frac{\partial}{\partial s}\left(\rho^* D_k \frac{\partial Y_k^*}{\partial s}\right)}_{\substack{\text{molecular}\\ \text{diffusion}}} + \underbrace{\dot{\omega}_k^*}_{\substack{\text{chemical}\\ \text{reaction}}} + \underbrace{\dot{S}_k^*}_{\substack{\text{spray}\\ \text{source}}} \right] dt'$$

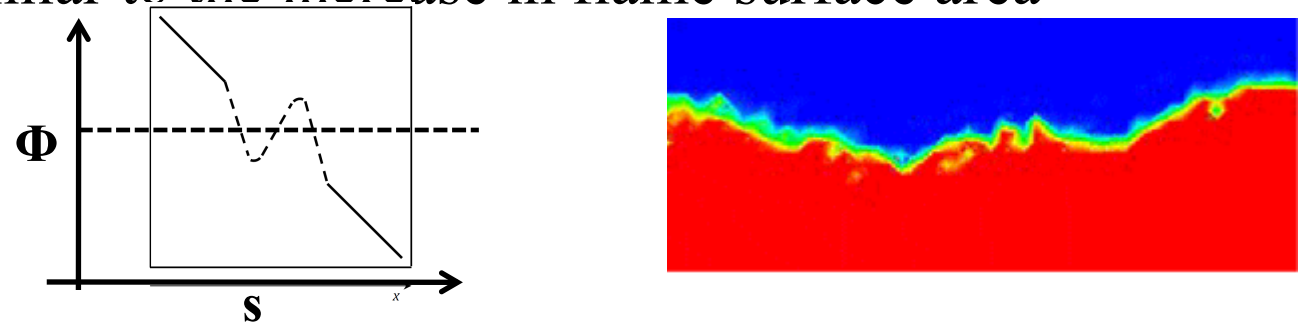
- Stirring is a
  - subgrid advection *model* for scalars via subgrid eddies
- Stirring is required because …
  - LES does not model down to dissipation scales η
  - As, $\Delta > \eta$, ($Re_{sub} > 1$) subgrid scalar transport still exists
  - Provides the effect of eddy-flame interaction

Triplet Mapping (Kerstein, 1989)

- Increases scalar gradients akin to the compressive action of an eddy on the scalar field



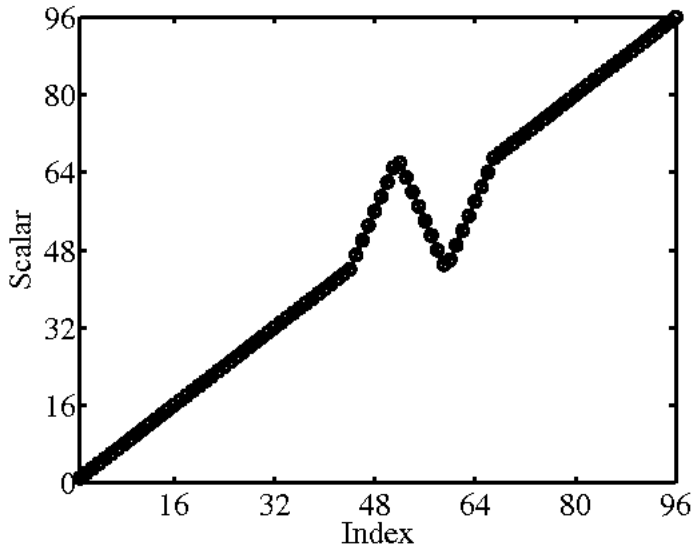
- Increases the number of crossings of a scalar value – this is similar to the increase in flame surface area



- The growth of flame surface area with the applied strain is captured quantitatively as in experimental observations

Triplet Mapping (Contd.)

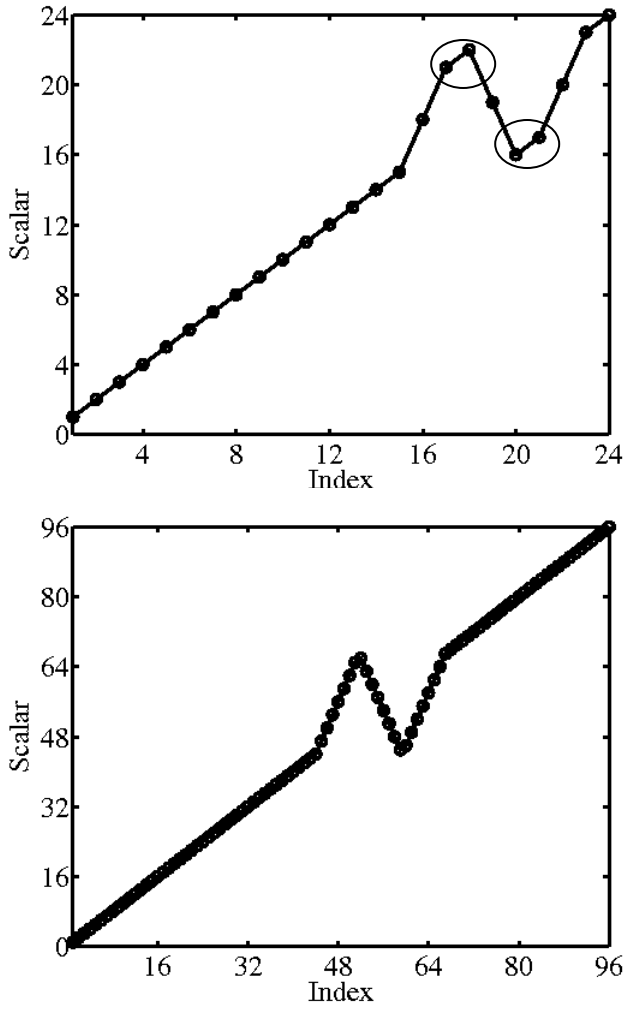
- Mapping procedure:
  - Three copies of stirred segment are made and the middle sub-segment is inverted
  - Triplet mapping offers the maximum compressive strain
  - Stirring by eddies $\{\eta < \ell \leq \Delta\}$ recovers turbulent diffusivity stochastically



$$D_T = \frac{2}{27}\lambda \int_{\eta}^{\bar{\Delta}} l^3 f(l) dl$$

Mapping Implementation

- **Scalar *re-arrangement***
  - Strictly not original Triplet mapping procedure
  - Conserves actual scalar values of the original field
    - No art. Diffusion via interp./averaging
  - Converges to a true triplet map for large LEM resolution



Mapping Implementation

- Eddy size, $\eta < \ell \leq L$, chosen from a PDF:

$$f(l) = \frac{5}{3}\frac{l^{-8/3}}{\eta^{-5/3} - L^{-5/3}} \qquad \eta = NL\,\mathrm{Re}^{-3/4}$$

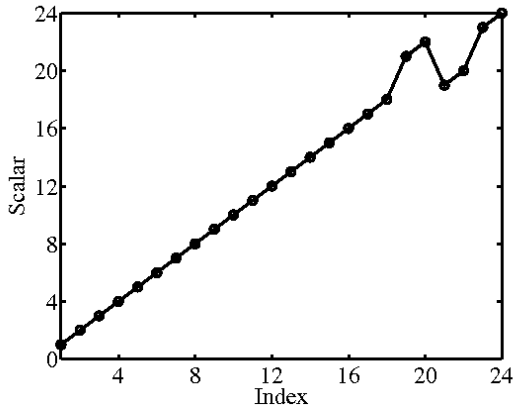
  - PDF obeys inertial range scaling laws for turbulent flows
  - Eddy subset depends on subgrid resolution ~ $O(N_{LEM}/3)$
- Eddy frequency is chosen from

$$\lambda = \frac{54}{5}\frac{\nu\,\mathrm{Re}\,C_\lambda}{L^3}\left(\frac{(L/\eta)^{5/3} - 1}{1 - (\eta/L)^{4/3}}\right)$$

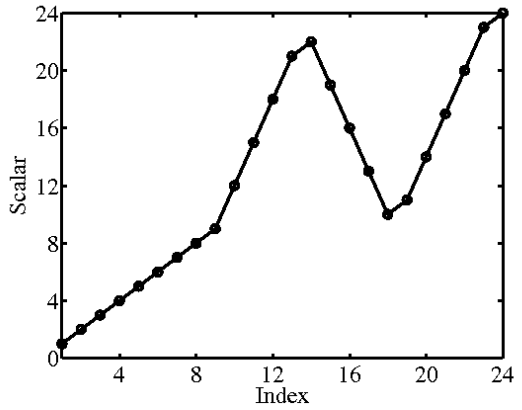
  - Time scale for stirring is $\Delta t_{stir} = 1/(\lambda L)$
- Eddy location is randomized within a subset of permissible locations such that the chosen eddy can be accommodated

Mapping Implementation

- Algorithmically, an eddy size must be of size 6 or more
  - Requires LEM grid-size, N_{LEM} a multiple of 3
- Physically eddy size must be above dissipation scales
  - $\Delta_{LEM} = \min(\eta, \eta_B)/6$ where is η_B the Batchelor scale, the dissipation scale for scalars, $\eta_B = \eta/Sc^{0.5}$
- Boundaries are not stirred
  - N_{LEM} must be greater than 9



Smallest computational eddy



A relatively larger eddy

Mapping Implementation

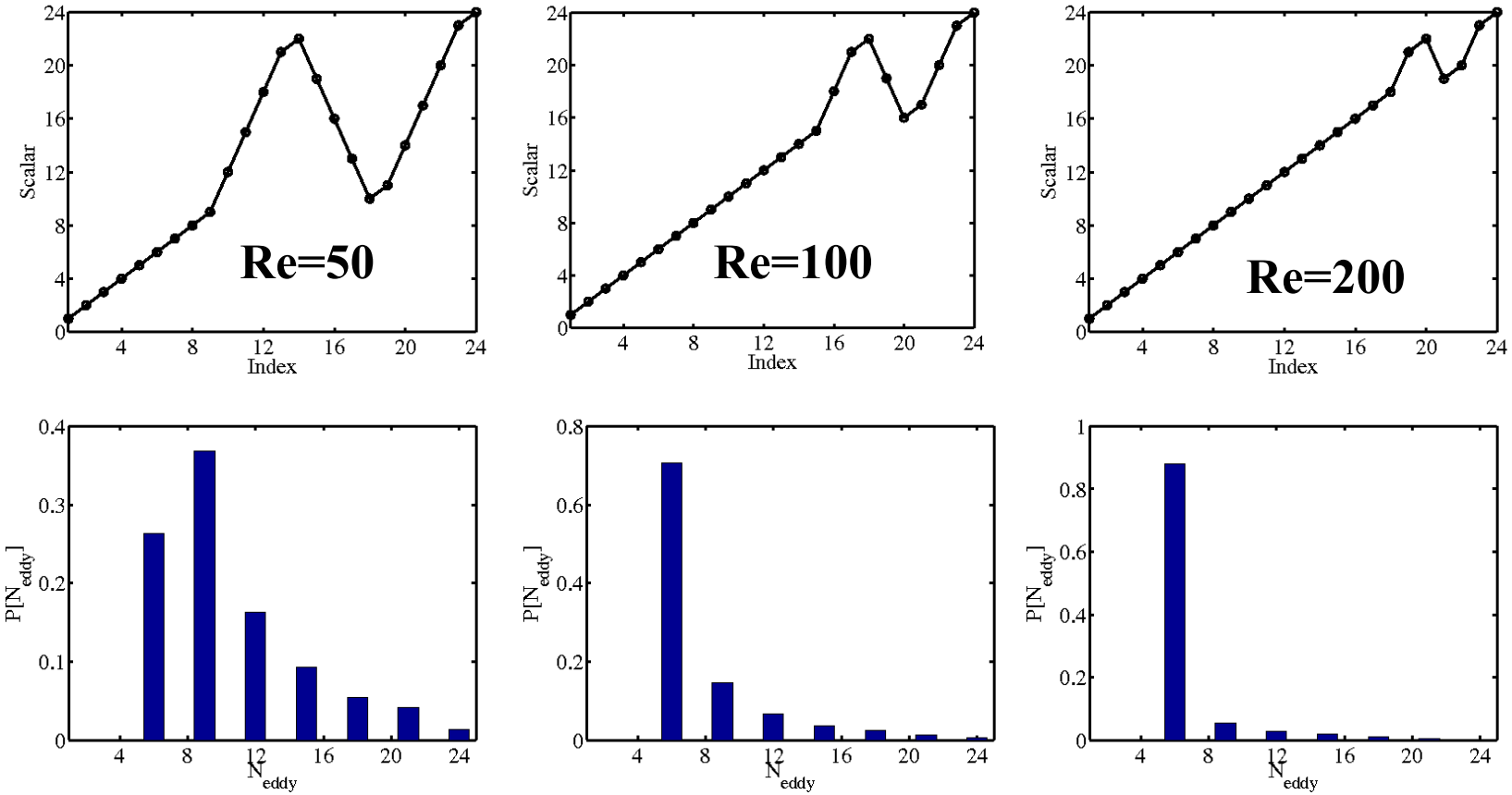
- Number of eddies in a resolution are finite
  - Smallest stirring eddy is of size 6
    - Size 6 eddies have triplet segments of length 2 (st. line)
    - Size 3 eddies have triplet segments that are points (zero-length segments), hence *do not perturb the profile!*
  - Boundaries cannot be stirred
  - Stirring eddy sizes are 6, 9, 12, 15 … N_{LEM}
  - For $N_{LEM} = 12$, eddy sizes are 6, 9, 12
- Physically, smaller the LEM grid-spacing..
  - Closer it is to dissipation scales
  - Smaller the number of stirring eddies

Triplet Mapping Code: Stirring.F

- Performs single stirring over of an unperturbed profile
- Specify in the code:
  - ISGS: LEM Resolution
  - RSCALE: LES grid size
  - RET: Subgrid Re
  - Initial profile in subroutine STIR
- Outputs:
  - stir.dat: prints the stirred field corresponding to the most probable eddy
  - prob.dat: PDF of eddies
- The next two plots were generated using this code

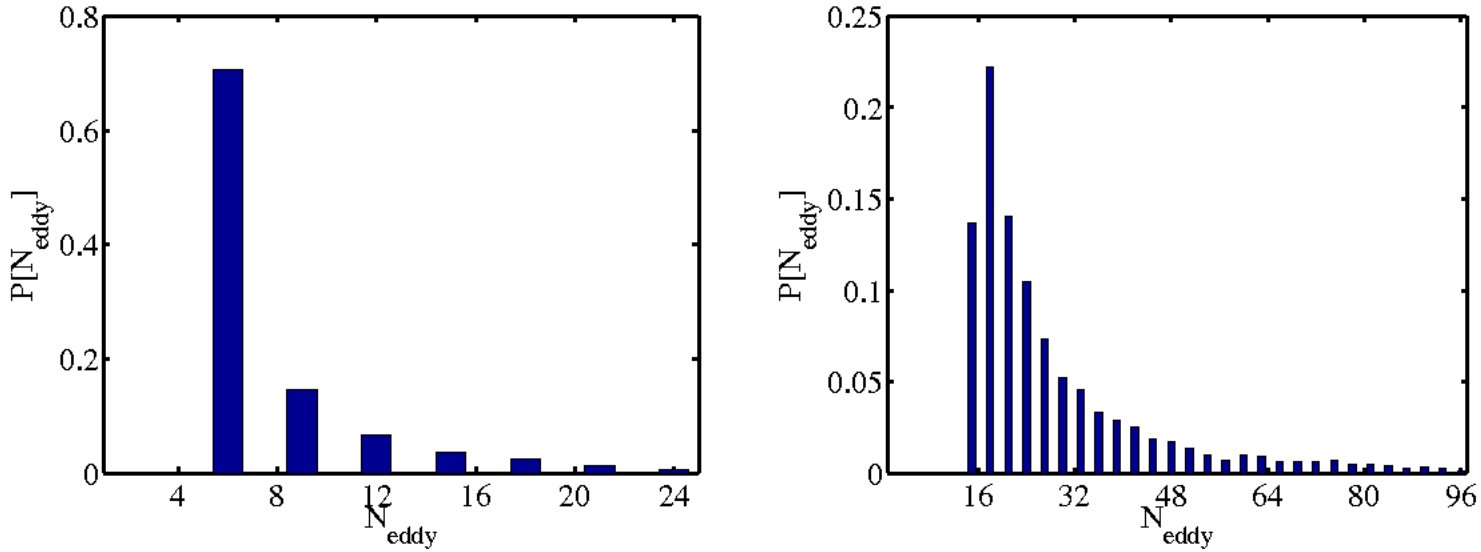
```
PROGRAM STIRRRR
IMPLICIT NONE
REAL (KIND=8) :: RSCALE,RET,DS,PROB(200),PMAX(1)
INTEGER :: ISGS,I,J,NITER,NEDDY
ISGS=24;RSCALE=0.2D-3;DS=RSCALE/DBLE(ISGS)
NITER=10000
PROB=0.D0
DO I=1,NITER
RET=20.D0
CALL STIR(RSCALE,RET,DS,ISGS,PROB,NEDDY)
PMAX=MAXLOC(PROB)*3
PRINT*,PMAX
IF(I.GT.NITER/2 .AND. PMAX(1)==NEDDY) THEN
OPEN(12,FILE='prob_020.dat',FORM='FORMATTED')
DO J=1,ISGS/3
WRITE(12,*),J,PROB(J)/DBLE(I)
ENDDO
CLOSE(12)
 STOP
ENDIF
ENDDO
STOP
END
```

Subgrid Re v/s Eddy Size



- Δ=0.2mm, N_{LEM}=24
- Most probable eddy is plotted on top followed by PDF of eddies based on size is plotted below

Effects of Subgrid Resolution



- Re_{sub}=100, N_{LEM}=24 Vs. N_{LEM}=96
- Most probable eddy=6(Δ/24) Vs. 18(Δ/96)
- A better representation of eddy cascade with better resolution

Stirring Frequency

- **Stirring frequency**

$$\lambda = \frac{54}{4}\frac{\nu \mathrm{Re}_\Delta}{C_\lambda \Delta^3}\frac{\left[\left(\Delta/\eta\right)^{5/3} - 1\right]}{1-\left(\eta/\Delta\right)^{4/3}}$$

$$T_{STIR} = 1/\lambda\Delta \qquad \eta = N_\eta \frac{\Delta}{\mathrm{Re}_\Delta^{3/4}}$$

Δ = local LES filter width (RSCALE)

η = Kolmogorov scale (ETA)

$\mathrm{Re}_\Delta = u'\Delta/\nu;\ u' = \sqrt{2k^{sgs}/3}$ (*REL*)

$C_\lambda = 0.067, N_\eta = 11$, constants (STSFAC,ETAFAC)

(fixed from scaling analysis)

```
REL=RET
ETA = RSCALE * (REL**(-R3D4))
IF (REL .NE. 1.0D0) THEN
   RLAM  = R54B5 * RNUS * REL * ((RSCALE / ETA)**R5D3
         - R1) / (R1 - (ETA / RSCALE)**R4D3) * RSCALE3
   TSTIR = STSCFAC / ( RLAM * RSCALE)
   ETA   = ETAFAC * ETA
   RESOL = ETA * RDXLEM

   TDELS  = TSTIR
   NTSMX  = INT(DTLES / TDELS) + 1
   TDELS  = DTLES / DBLE(NTSMX)

ELSE

   TSTIR  = 1.0D3
   TDELS  = TSTIR
   RESOL  = ETA * RDXLEM

ENDIF          !  ENDIF FOR REL = 1
```

Stirring Frequency (Contd.)

- Number of stirrings per iteration
  - $NTSMX=TSTIR/\Delta t_{LES}$
  - No stirring if $Re_{\Delta} \leq 1$

```
REL=RET
ETA = RSCALE * (REL**(-R3D4))
IF (REL .NE. 1.0D0) THEN
   RLAM  = R54B5 * RNUS * REL * ((RSCALE / ETA)**R5D3
        - R1) / (R1 - (ETA / RSCALE)**R4D3) * RSCALE3
   TSTIR = STSCFAC / ( RLAM * RSCALE)
   ETA   = ETAFAC * ETA
   RESOL = ETA * RDXLEM

   TDELS  = TSTIR
   NTSMX  = INT(DTLES / TDELS) + 1
   TDELS  = DTLES / DBLE(NTSMX)

ELSE

   TSTIR  = 1.0D3
   TDELS  = TSTIR
   RESOL  = ETA * RDXLEM

ENDIF         !  ENDIF FOR REL = 1
```

Triplet Mapping: Size Selection

- **RSCALE = Δ**
- **FAC1 = $\Delta^{-5/3}$**
- **FAC2 = $\eta^{-5/3}$**

$$f(l) = \frac{5}{3}\frac{l^{-8/3}}{\eta^{-5/3} - \Delta^{-5/3}}$$

$$CDF(l) = \int_{\eta}^{l} f(l)dl = \frac{l^{-5/3} - \eta^{-5/3}}{\Delta^{-5/3} - \eta^{-5/3}}$$

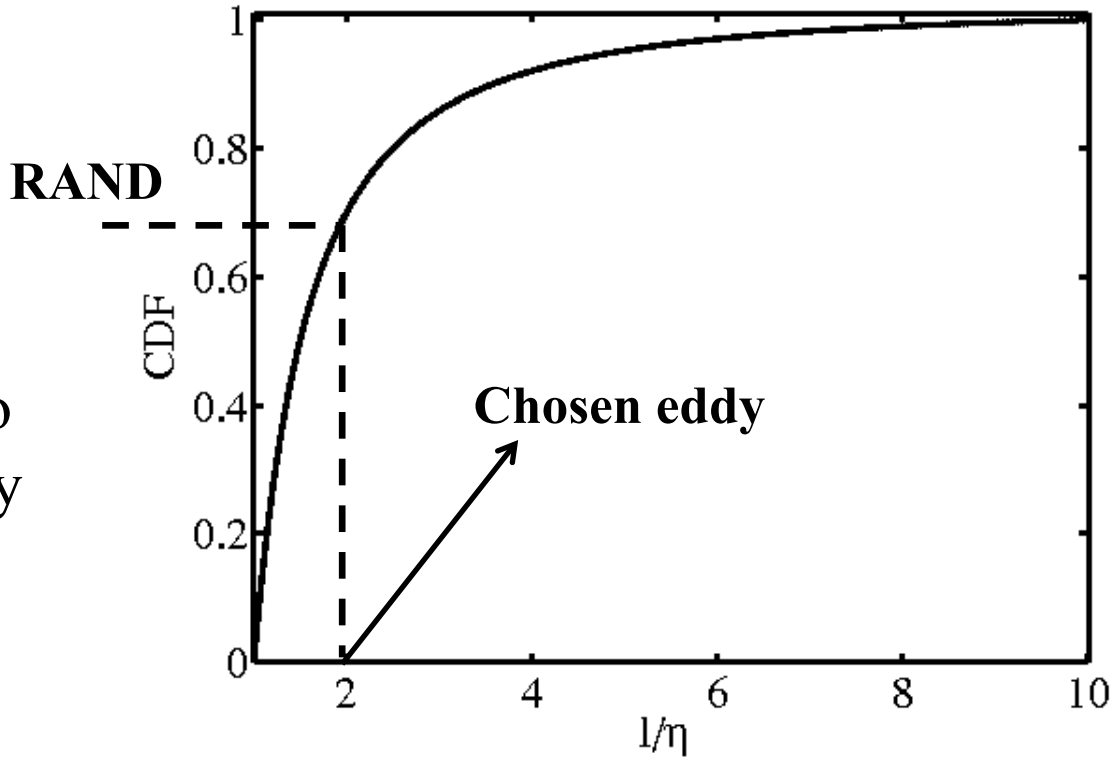
- **EVENT = ℓ, RAND = CDF(ℓ) =[0..1]**

$$l = [\eta^{-5/3} + RAND * (\Delta^{-5/3} - \eta^{-5/3})]^{-3/5}$$

```
FAC1  = RSCALE**(-R5D3)
FAC2  = ETA**(-R5D3)

CALL RANDOM_NUMBER(RAND)
EVENT = (RAND * (FAC1 - FAC2) + FAC2)**(-R3D5)

! We need EVENT to at least cover 6 LEM cells.
! So, multiply it by 6.1 to ensure later integer division
! still gives 6
IF(EVENT.LT.(6.1D0*DXLEM)) EVENT = 6.1D0*DXLEM

EDDY  = EVENT / RSCALE
EDDY  = EDDY * FSGS
! These two lines scale NEDDY to an integer multiple of 3
NEDDY = NINT(EDDY / 3.0D0 )
NEDDY = 3 * NEDDY
! This caps NEDDY to be no larger than ISGS
NEDDY = MIN(NEDDY, ISGS)
! This rounds NEDDY down to the nearest multiple of 3
NEDDY = NEDDY-MOD(NEDDY, 3)
```

Eddy Selection Algorithm

- RAND decides y-axis location on the CDF to determine stirring eddy



Triplet Mapping: Size Selection

- FSGS=NLEM
- EDDY = EVENT/DXLEM
  - Number of LEM Cells
- NEDDY= closest Integer to EDDY divisible by 3

```
FAC1  = RSCALE**(-R5D3)
FAC2  = ETA**(-R5D3)

CALL RANDOM_NUMBER(RAND)
EVENT = (RAND * (FAC1 - FAC2) + FAC2)**(-R3D5)

! We need EVENT to at least cover 6 LEM cells.
! So, multiply it by 6.1 to ensure later integer division
! still gives 6
IF(EVENT.LT.(6.1D0*DXLEM)) EVENT = 6.1D0*DXLEM

EDDY  = EVENT / RSCALE
EDDY  = EDDY * FSGS
! These two lines scale NEDDY to an integer multiple of 3
NEDDY = NINT(EDDY / 3.0D0 )
NEDDY = 3 * NEDDY
! This caps NEDDY to be no larger than ISGS
NEDDY = MIN(NEDDY, ISGS)
! This rounds NEDDY down to the nearest multiple of 3
NEDDY = NEDDY-MOD(NEDDY, 3)
```

Triplet Mapping: Size Selection

- Location of Eddy is randomized with the constraint that it fits in the LEM domain
- Size of Eddy = NEDDY
- LEM domain size = ISGS (NLEM)
- Randomization for start position over ISGS-NEDDY

```
C ------------------------------
C    FIND THE STIRRING LOCATION
C ------------------------------

CALL RANDOM_NUMBER(RAND)
LOC   = 1 + NINT(FLOAT(ISGS - NEDDY) * RAND)
! If NEDDY=ISGS, we need to at least start at 1
! hence the ISGS-NEDDY+1
LOC    = MIN(LOC, ISGS - NEDDY + 1)
```

Triplet Mapping: Rearrangement

- GDUM2 = Original Scalar Field
- GDUMM = Work Array
- NEDDY = Eddy Size
- LOC = Eddy location
- ISGS = LEM resolution, NLEM
- NSP3 = NSPECI+3 (Y_k, ρ, T, Vol)

$$\hat{Y}_k(s,t_0) = \begin{cases} Y_k(3s-2s_0,t_0) & s_0 \le s \le s_0 + l/3 \\ Y_k(-3s+4s_0+2l,t_0) & s_0 + l/3 \le s \le s_0 + 2l/3 \\ Y_k(3s-2s_0-2l,t_0) & s_0 + 2l/3 \le s \le s_0 + l \\ Y_k(s,t_0) & \text{otherwise} \end{cases}$$

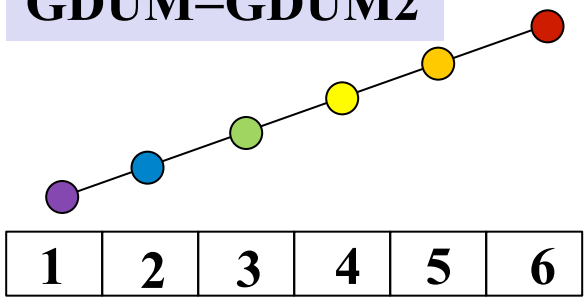
l : size of mapping event s_0 : location of mapping event

```
C ---------------------
C     TRIPLET MAPPING
C ---------------------
GDUMM(1:ISGS,1:NSP3) = GDUM2(1:ISGS,1:NSP3)
IL = NEDDY-1
! Define end points for each segment
IL1 = NEDDY/3
IL2 = 2*NEDDY/3

 DO IS = 1, IL1
GDUMM(IS+LOC-1,1:NSP3) = GDUM2(3*IS-3+LOC, 1:NSP3)
 END DO

 DO IS = IL1+1, IL2
    GDUMM(IS+LOC-1,1:NSP3) = GDUM2(-3*IS+3+2*IL+LOC,
         1:NSP3)
 END DO

 DO IS = IL2+1, NEDDY
    GDUMM(IS+LOC-1, 1:NSP3) = GDUM2(3*IS-3-2*IL+LOC,
         1:NSP3)
 END DO

 ! Loop unrolled to allow vectorization
 GDUM2(1:ISGS,1:NSP3) = GDUMM(1:ISGS,1:NSP3)
 GDUMM = 0.0D0
```

Triplet Mapping: Rearrangement

- ISGS = 6, Assume NEDDY = 6
  - In fact this is the only eddy for an LEM domain of size 6
- Set the bounds
  - IL = 5, IL1 = 2, IL2 = 4

GDUM=GDUM2

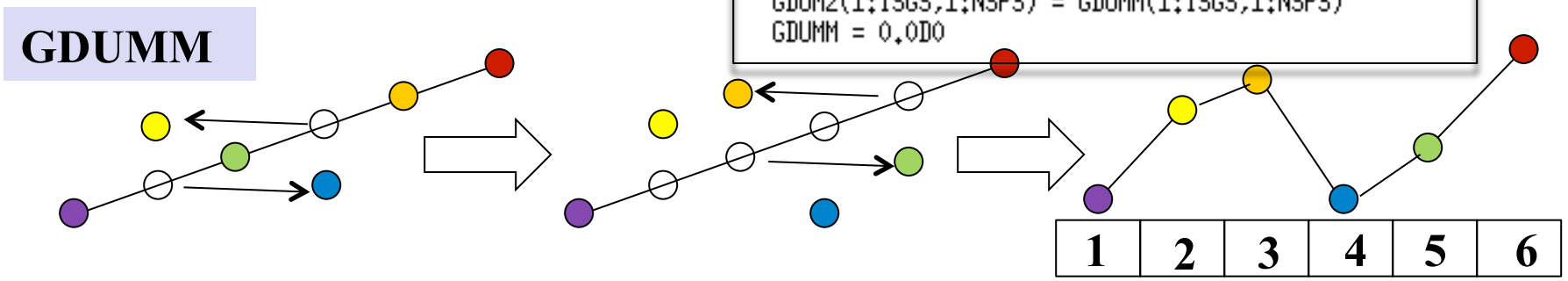



```
  GDUMM(1:ISGS,1:NSP3) = GDUM2(1:ISGS,1:NSP3)
  IL = NEDDY-1
  ! Define end points for each segment
  IL1 = NEDDY/3
  IL2 = 2*NEDDY/3

  DO IS = 1, IL1
GDUMM(IS+LOC-1,1:NSP3) = GDUM2(3*IS-3+LOC, 1:NSP3)
  END DO

  DO IS = IL1+1, IL2
     GDUMM(IS+LOC-1,1:NSP3) = GDUM2(-3*IS+3+2*IL+LOC,
          1:NSP3)
  END DO

  DO IS = IL2+1, NEDDY
     GDUMM(IS+LOC-1, 1:NSP3) = GDUM2(3*IS-3-2*IL+LOC,
          1:NSP3)
  END DO

  ! Loop unrolled to allow vectorization
  GDUM2(1:ISGS,1:NSP3) = GDUMM(1:ISGS,1:NSP3)
  GDUMM = 0.0D0
```

Triplet Mapping: Rearrangement

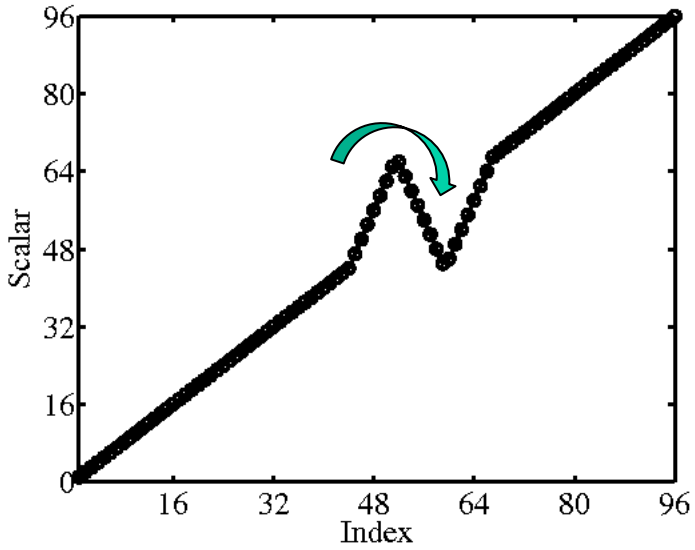
- LOC = 1
- @1 = @1, @2 = @4
- @3 = @5, @4 = @2
- @5 = @3, @6 = @6

```
  GDUMM(1:ISGS,1:NSP3) = GDUM2(1:ISGS,1:NSP3)

  IL = NEDDY-1
  ! Define end points for each segment
  IL1 = NEDDY/3
  IL2 = 2*NEDDY/3

  DO IS = 1, IL1
GDUMM(IS+LOC-1,1:NSP3) = GDUM2(3*IS-3+LOC, 1:NSP3)
  END DO

  DO IS = IL1+1, IL2
     GDUMM(IS+LOC-1,1:NSP3) = GDUM2(-3*IS+3+2*IL+LOC,
          1:NSP3)
  END DO

  DO IS = IL2+1, NEDDY
     GDUMM(IS+LOC-1, 1:NSP3) = GDUM2(3*IS-3-2*IL+LOC,
          1:NSP3)
  END DO

  ! Loop unrolled to allow vectorization
  GDUM2(1:ISGS,1:NSP3) = GDUMM(1:ISGS,1:NSP3)
  GDUMM = 0.0D0
```

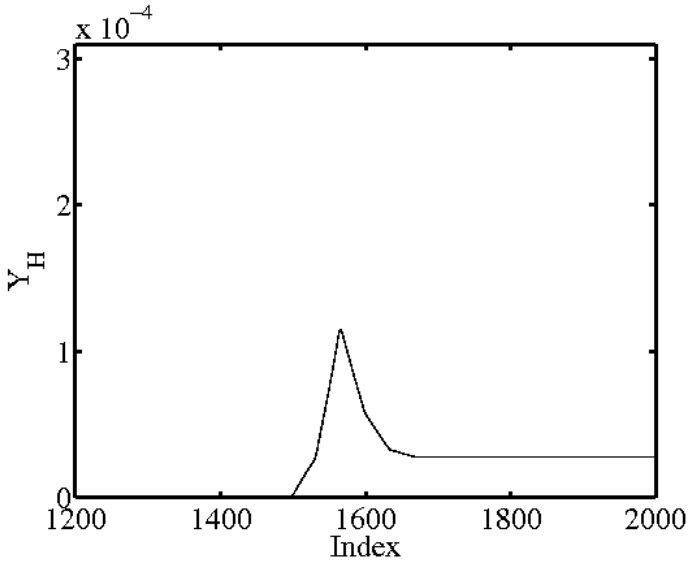


Triplet Mapping Example

- **Stirring in a freely propagating premixed flame**

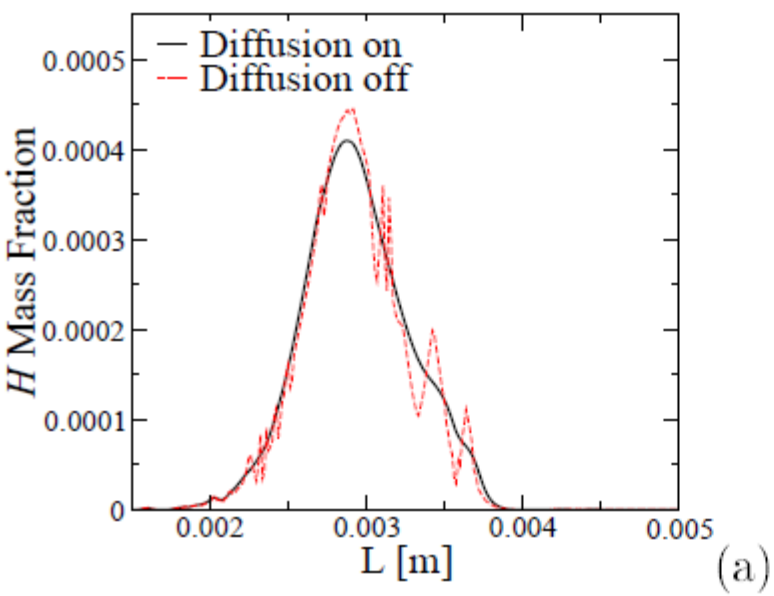


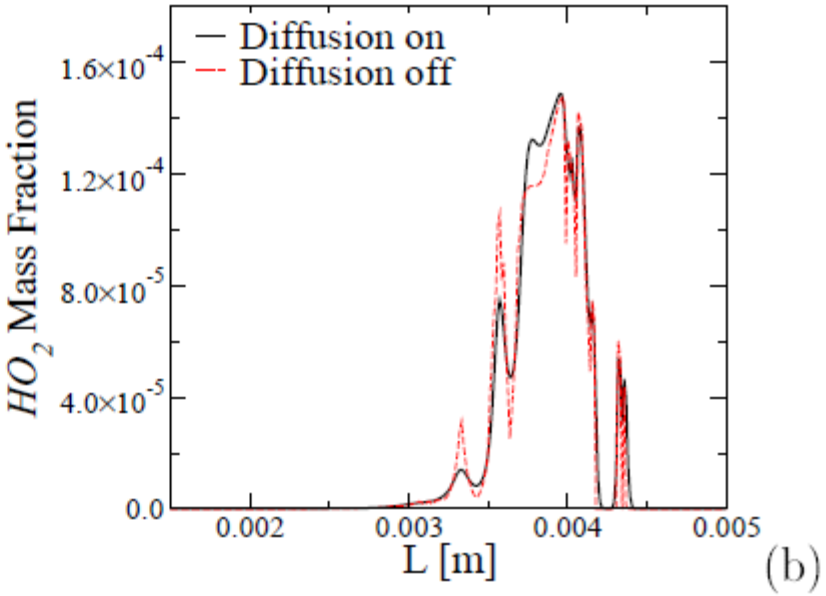
Schematic



Y_H in Freely propagating premixed turbulent CH_4/Air flame

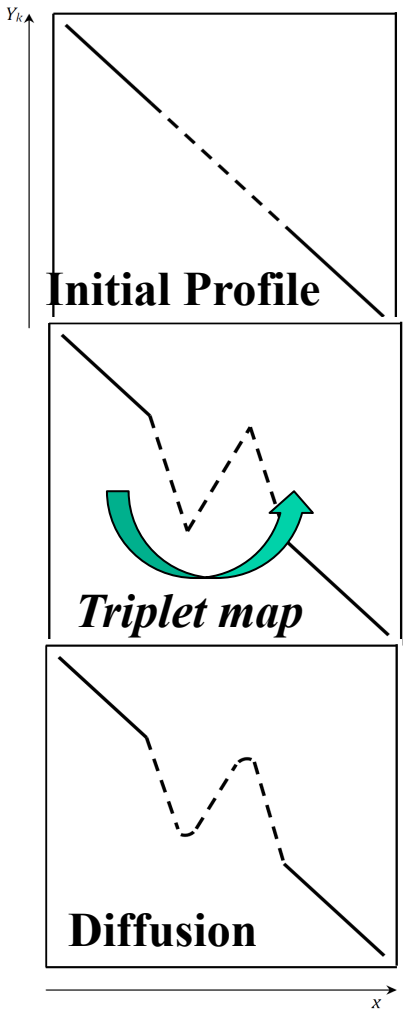
Comments (Contd.)

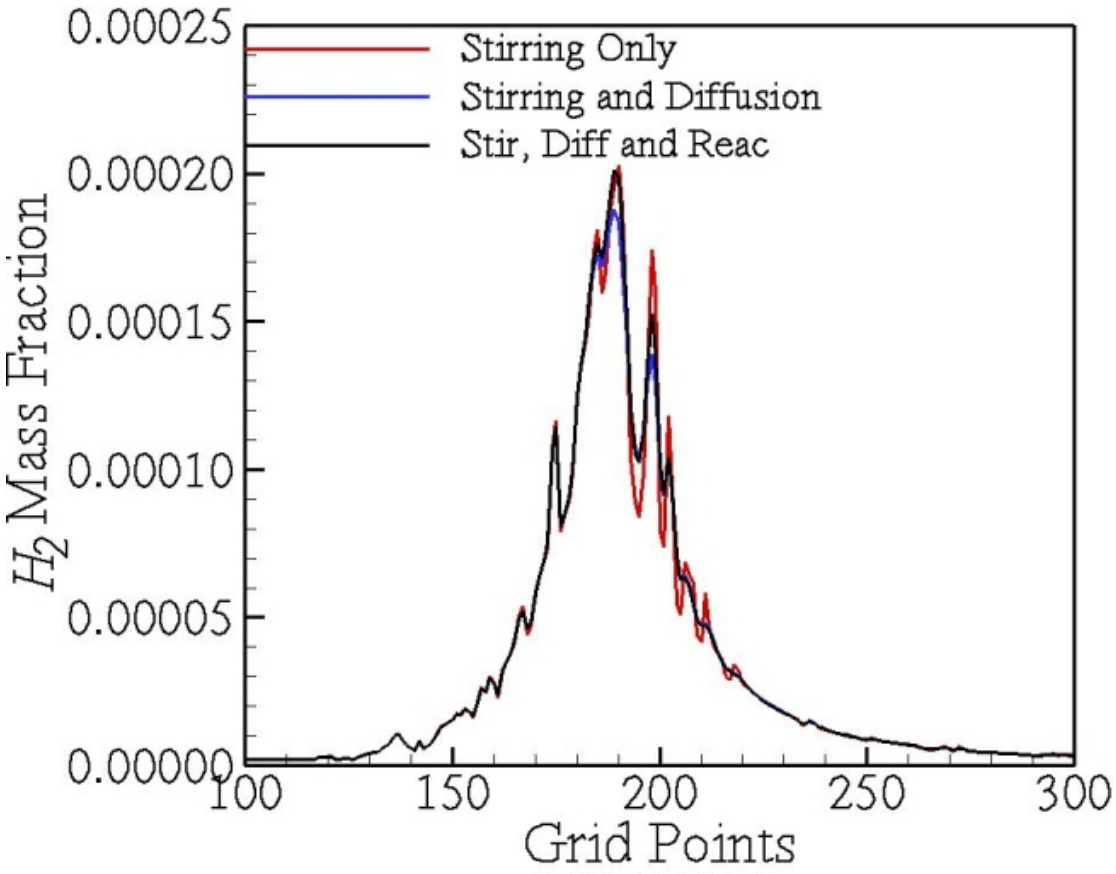




- Competition between stirring and diffusion
  - Highly diffusive H shows smoother profile Vs. HO_2

Interaction between Stirring, Diffusion and Reactions





Suresh Menon, Georgia Tech

Some Comments on Triplet Mapping

- Requires a uniform grid at this time
  - Resolution requirements stringent for thin flames
- Necessitates re-gridding of cells due to volumetric expansion or merger of cells from splicing
  - Leads to numerical diffusion of subgrid field
    - Higher resolution can reduce this numerical effect
- Local regridding and variable LEM resolution stirring being develop to address all these issues
- Instantaneous rearrangement of scalar field
  - In reality eddy acts over a finite turn-over time

Large Scale Transport: Splicing

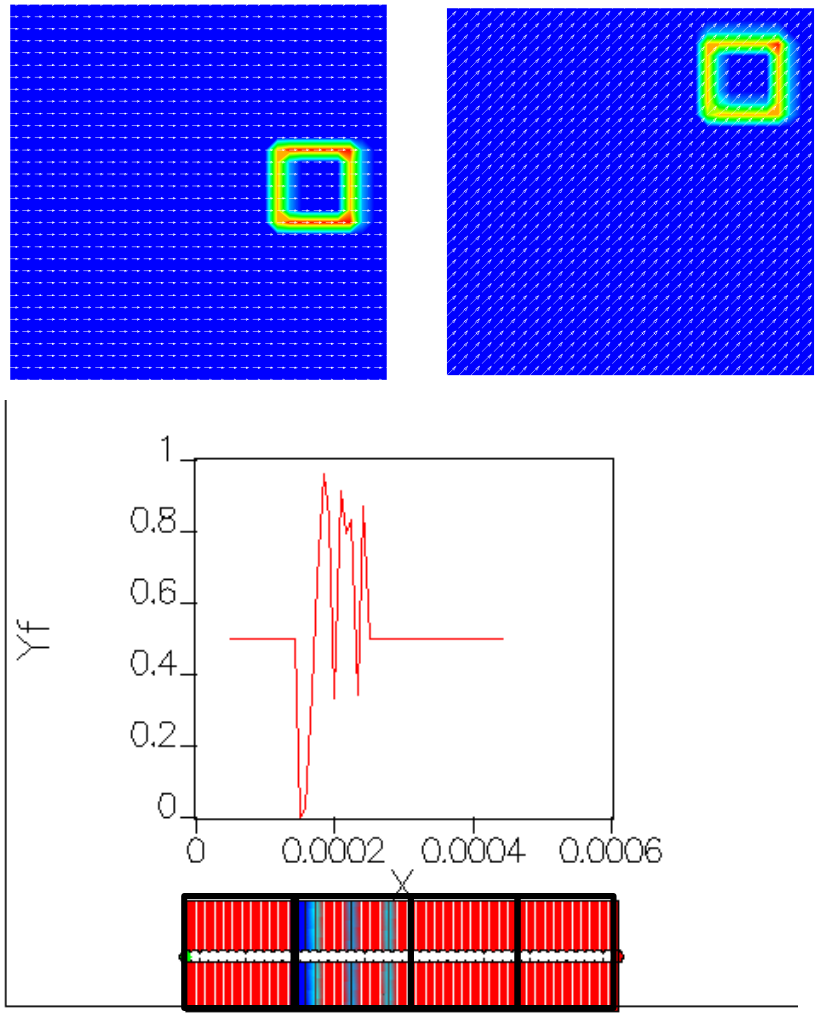
$$Y_k: \quad \sum_{M=1}^{NLEM}\left(\rho_M^{n+1}Y_{k,M}^{n+1} - \rho_M^{*}Y_{k,M}^{*}\right) = \frac{\Delta t_{LES}}{\Delta V_{LEM}} \sum_{L=1}^{Nface} \overline{\rho}^{*} A_{k,L}(\tilde{u}_{k,L}^{*} + u_{sgs}^{*})_R$$

$$T: \quad \sum_{M=1}^{NLEM}\left(\rho_M^{n+1}C_{p,M}^{n+1}T_M^{n+1} - \rho_M^{*}C_{p,M}^{*}T_M^{*}\right) = \frac{\Delta t_{LES}}{\Delta V_{LEM}} \sum_{L=1}^{Nface} \overline{\rho}^{*}\overline{C}_{p,L}^{*}\tilde{T}_L^{*} A_{k,L}(\tilde{u}_{k,L}^{*} + u_{sgs}^{*})_R$$

- Splicing facilitates large-scale 3D transport in LEMLES
  - Lagrangian convection of *scalar gradient* via LES fluxes
- Not integral part of LEM but facilitates LEMLES
- Scalars (Y, T, ρ, Vol) within LEM cell advected *en-masse*

Splicing Demonstration

- Splicing facilitates large-scale scalar transport
  - Convection of a Box
- Splicing maintains small-scale features during transport
  - 4 LES / 12 LEM cells
    - Rand number profile
    - Per. BC
    - Unif. flowfield
    - Stir/Diff/Rxn OFF!

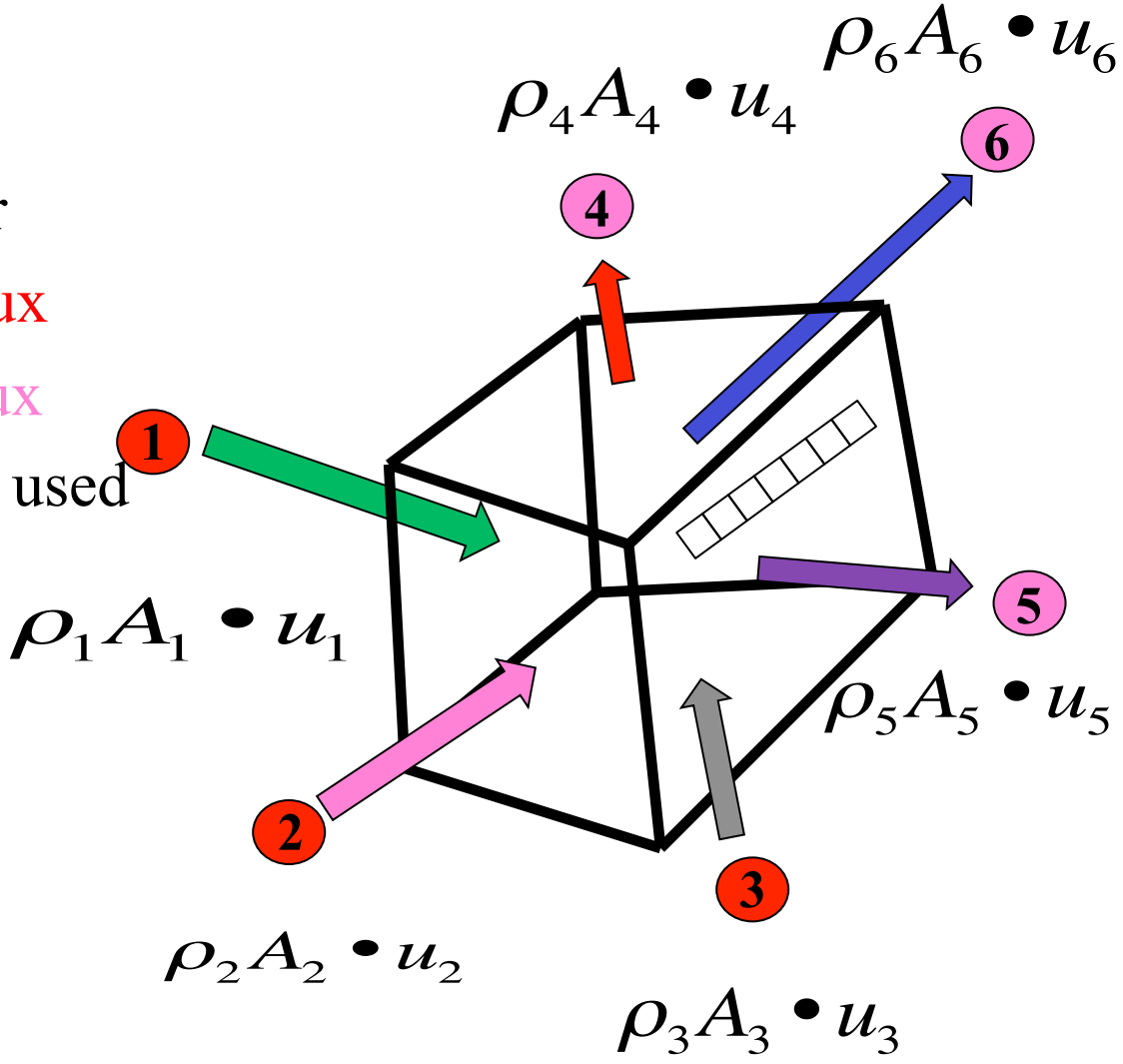


3D-Splicing Algorithm

- Step 1: Determine LES mass flux acting on each face
- Step 2: Rearrange Fluxes in order
  - Largest Influx first, Largest negative flux (outflux) last
- Step 3: Count x-ferable mass from abutting LES cells
  - Divide LEM cells to fractional values if required
- Step 4: Xfer mass from/to adjoining cells w.r.t. Flux order
  - Contiguous segments preserve scalar grad information
- Step 5: Interpolate the new subgrid field to a uniform grid
  - This is required due to triplet mapping

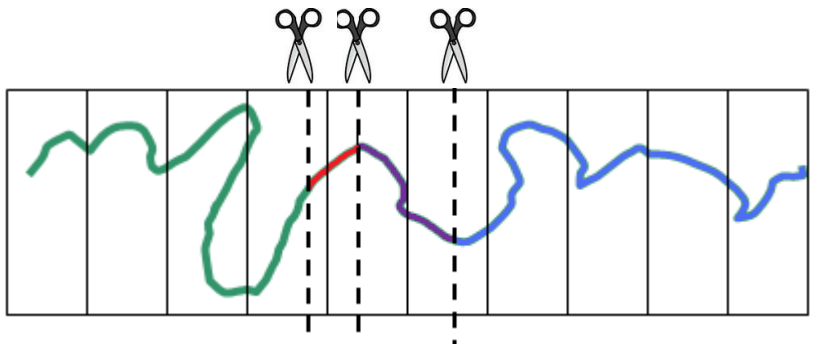
Splicing: Step 1 & 2

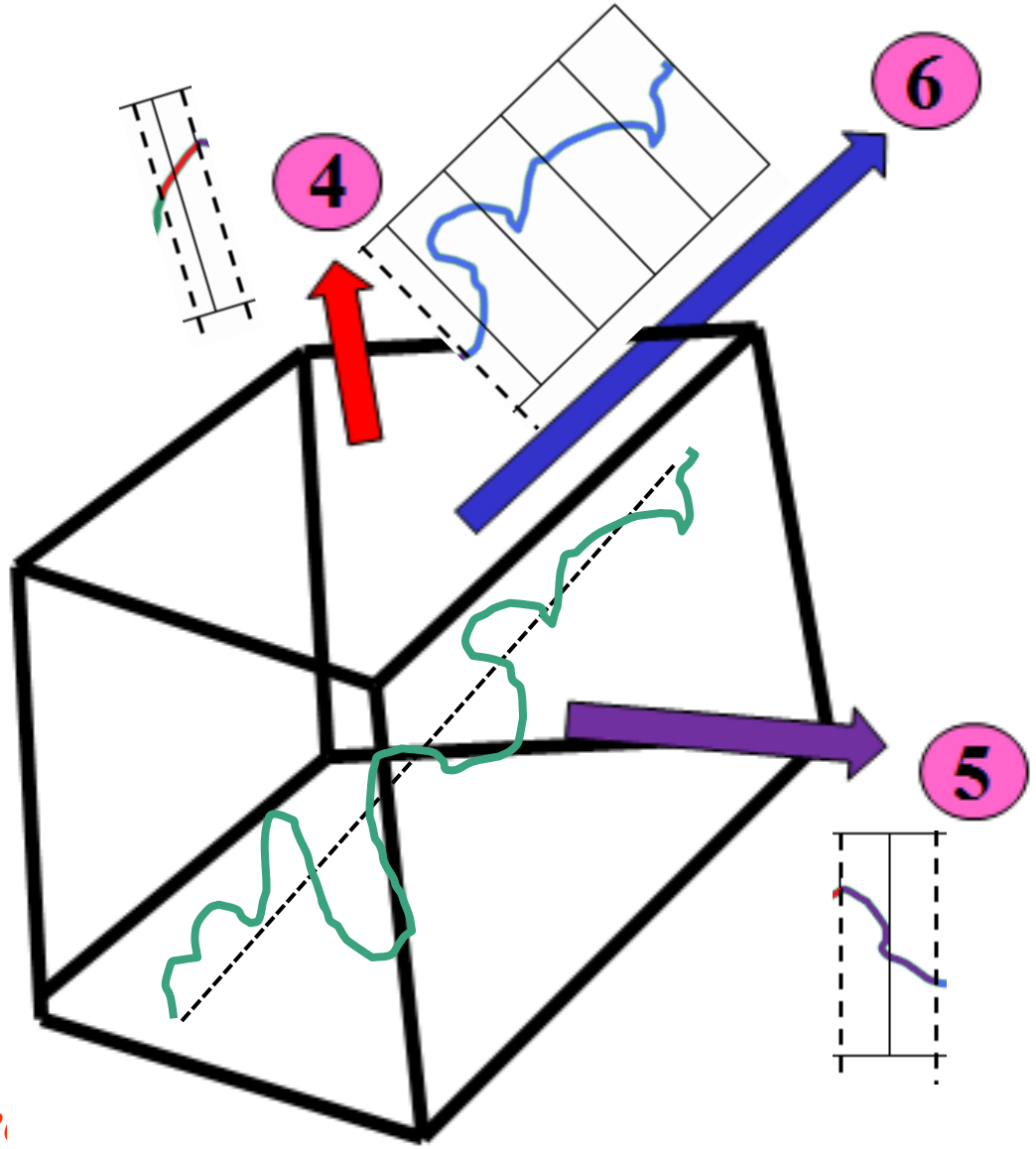
- Identify and arrange LES fluxes in decreasing order
- Red Circle : Incoming Flux
- Pink Circle: Outgoing Flux
- 2nd/4th order interpolation used to compute face fluxes



Step 3a: Outgoing Scalar Segments

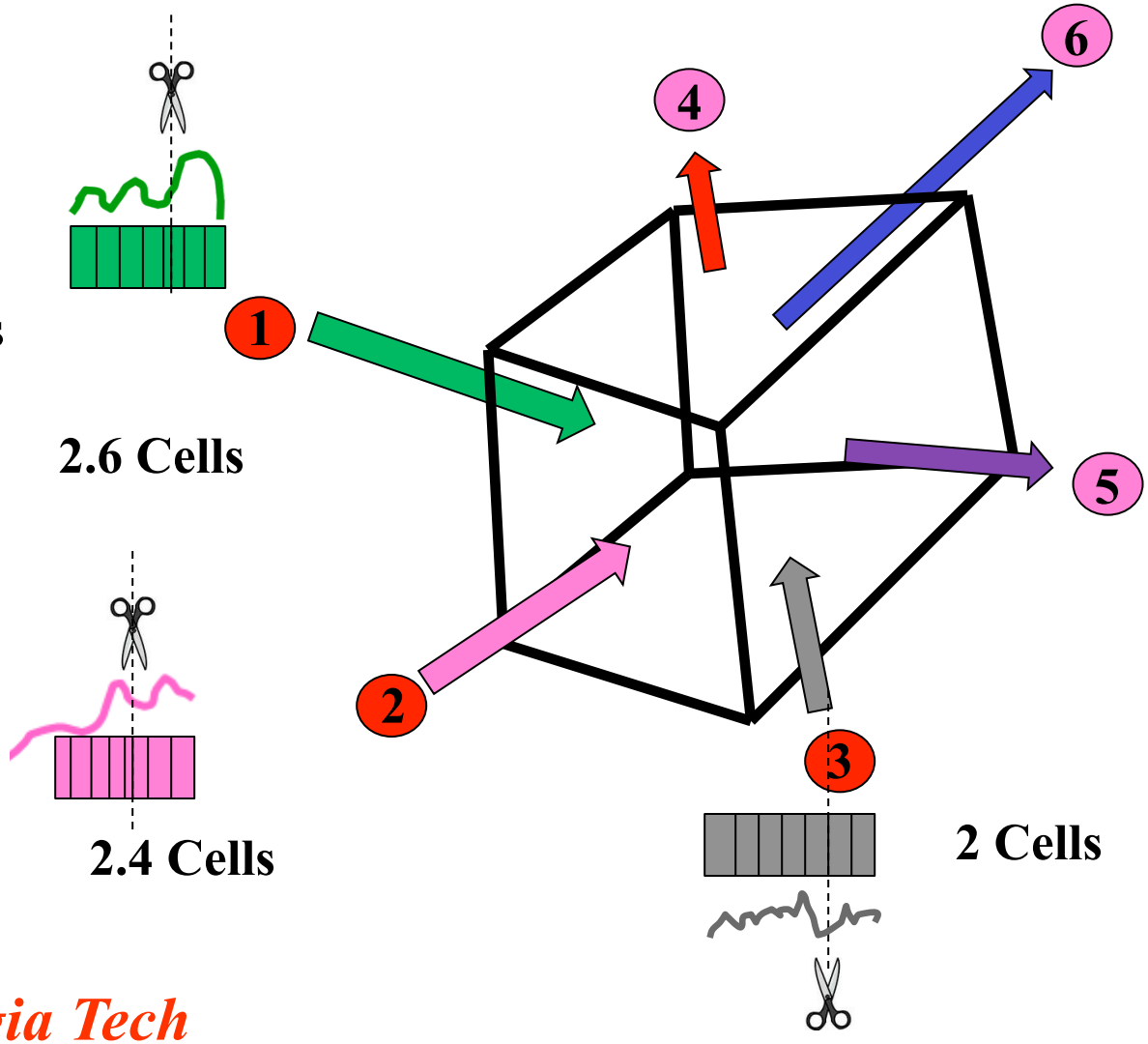
- Clip the scalar field inside the LES cell to match to neighbors' *mass flux*
- Start Clipping from the right end (outflux) sequentially
- Note that scalar gradients are preserved while clipping/ transport





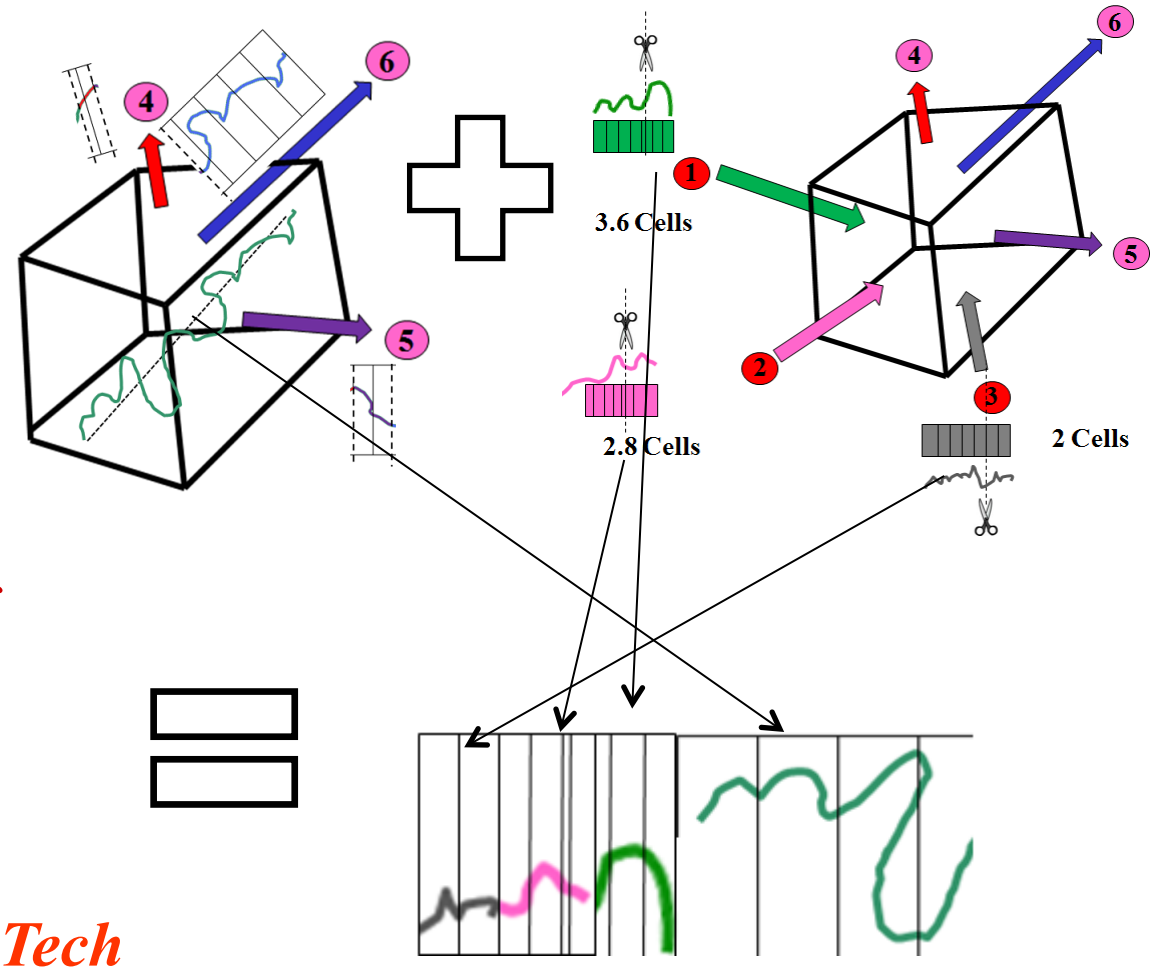
Step 3b: Incoming Scalar Segments

- Transferred mass may be fractional, so Scalar segments have to be "clipped"
- Note that the clipping is performed from the ends of Neighboring LEM fields,
  - First In - First Out Logic (FIFO)



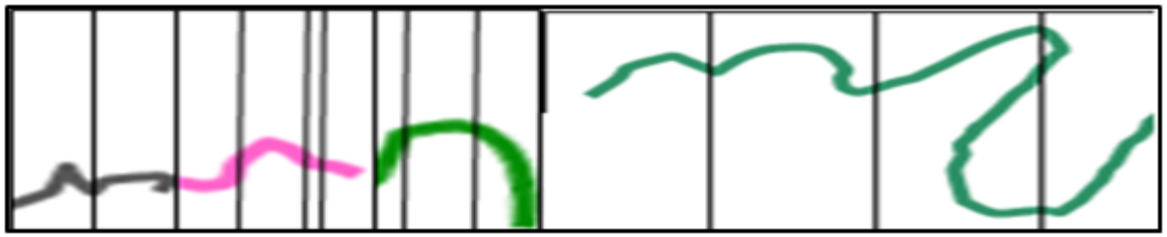
Step 4: Transfer mass (FIFO)

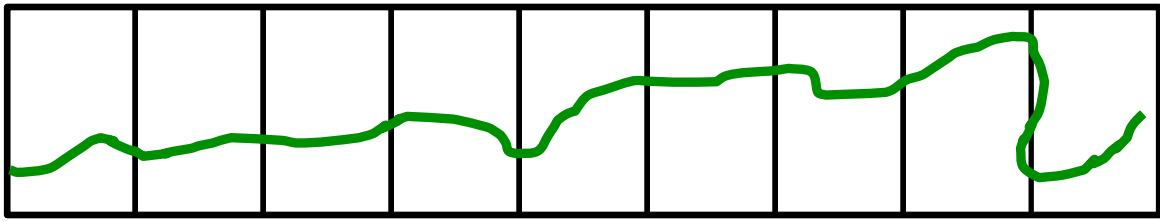
- Putting together the spliced masses based on FIFO logic
  - Outgoing masses moved out (not shown)
  - Remainder mass is shifted towards end
  - Incoming masses arranged in order of the magnitudes
- Non-uniform volumes!



Step 5: Re-gridding

- Performed to keep NLEM as constant and the volumes to be equal
  - NLEM=9 in this example
- Keep total volume constant in the new uniform grid
- Interpolate to get final scalar dist.





$$\sum_{i=1}^{NLEM^*} Vol_i = NLEM \times Vol$$

Splicing code : "splicing_demo.F"

- XLEN, YLEN, ZLEN [m]
- Dimensions: IMAX,JMAX,KMAX
  - Can simulate in 1D, 2D and 3D
- Time step: Convection time step
  - Should not violate mass conservation

$$\Delta t \oint_s \rho u ds \le \rho \forall$$

- ITER : Total number of iterations
- IFREQ : output file printing frequency

input.data

```
=====================================
XLEN  YLEN ZLEN
5.D-3  5.D-3   1.D-4
=====================================
IMAX JMAX KMAX
 51    51  2
=====================================
TIMESTEP, ITER IFREQ
1.D-5     200   10
=====================================
NSPECI
2
=====================================
U V W           THETA
8.D0 8.0D0 0.D0  60.D0
=====================================
# of SUBGRID CELLS
10
=====================================
INITIAL PROFILE: 2: 2D-BOX, 1: 2D-CIRCLE, 3: 1D-LINE
2
=====================================
INTEGER SPLICING
1
```

Splicing code : "splicing_demo.F"

- NSPECI: Number of species
  - 2 is sufficient for splicing demos
- U, V, W : Cartesian velocities
  - Choose values such that are consistent with TIMESTEP
- SUBGRID CELLS: LEM resolution
  - Since this is a convection demo, NLEM need not be a multiple of 3 (no triplet mapping) and only needs to be an integer greater than 1

input.data

```
========================================
XLEN  YLEN ZLEN
5.D-3  5.D-3   1.D-4
========================================
IMAX JMAX KMAX
 51    51  2
========================================
TIMESTEP, ITER IFREQ
1.D-5     200   10
========================================
NSPECI
2
========================================
U V W            THETA
8.D0 8.0D0 0.D0  60.D0
========================================
# of SUBGRID CELLS
10
========================================
INITIAL PROFILE: 2: 2D-BOX, 1: 2D-CIRCLE, 3: 1D-LINE
2
========================================
INTEGER SPLICING
1
```

Splicing code : "splicing_demo.F"

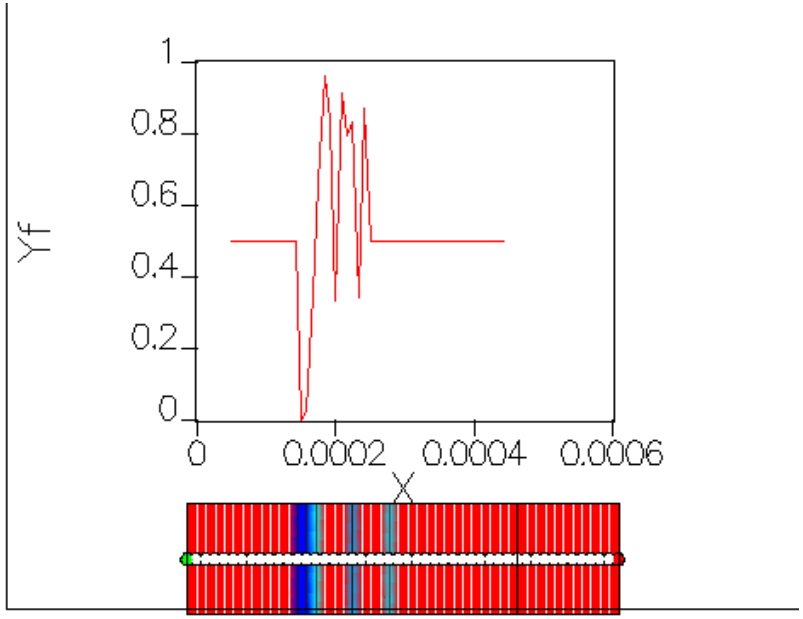
- **INITIAL PROFILE: Initial scalar distribution**
  - **1: BOX (2D), 2: Circle (2D), 3: random noise profile (1D)**
  - **User can define fields in Subroutine, USER_PROFILE() inside the code**
- **INTEGER SPLICING:**
  - **1: Perfect splicing (no regridding)**
  - **0: Realistic splicing (regridding and numerical diffusion)**

input.data

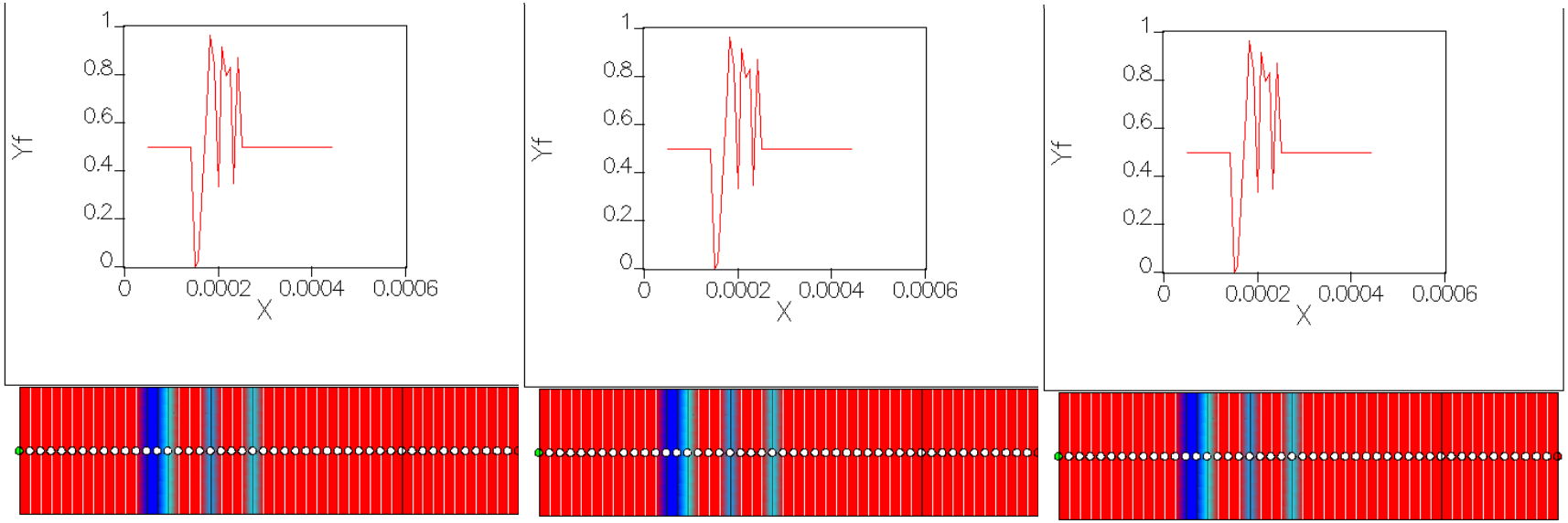
```
=====================================
XLEN  YLEN ZLEN
5.D-3  5.D-3   1.D-4
=====================================
IMAX JMAX KMAX
 51    51  2
=====================================
TIMESTEP, ITER IFREQ
1.D-5     200   10
=====================================
NSPECI
2
=====================================
U V W            THETA
8.D0 8.0D0 0.D0  60.D0
=====================================
# of SUBGRID CELLS
10
=====================================
INITIAL PROFILE: 2: 2D-BOX, 1: 2D-CIRCLE, 3: 1D-LINE
2
=====================================
INTEGER SPLICING
1
```

Perfect Splicing: 1D

- Re-gridding induces numerical diffusion due to interpolation
- In a perfect scenario, the fluxes on the LES volume would be perfectly matched with mass equivalent to integral number of LEM volumes
  - No splitting of LEM cell
  - No numerical diffusion



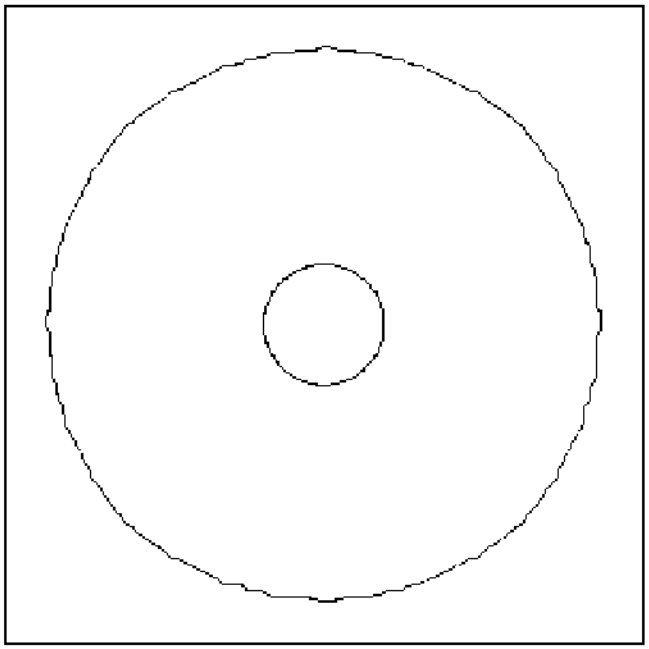
Errors Related to Splicing



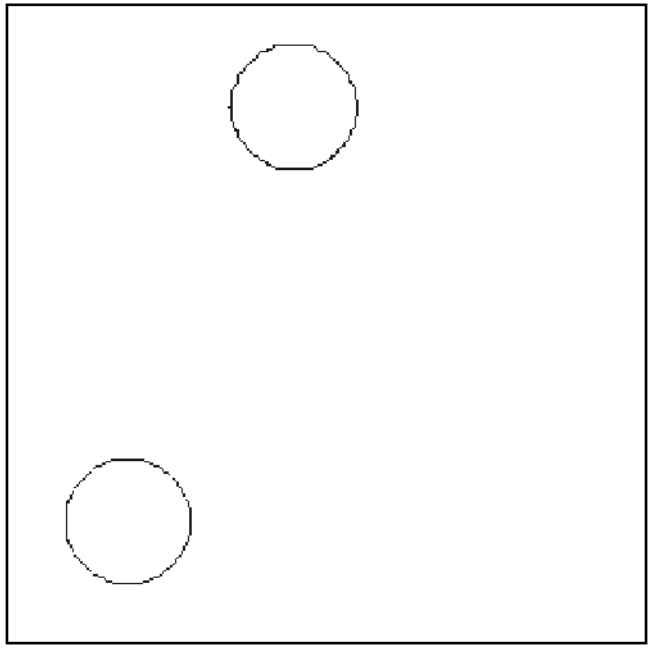
11.9 Spliced out **6.2 Spliced out** **0.1 Spliced out**

- Larger number of spliced cells reduces the error growth rate
- Larger number of spliced cells preserve scalar segments longer as they actually transport gradients as opposed to points related to fractional cell splicing
- Note: typical flame is quasi-stationary not propagating like this

Lagrangian Splicing Technique



Propagation of a Burning Front



Propagation of a Circular Front

LEM-LES Coupling

- **Filtered Species:**

$$\tilde{Y}_k = \left(\sum_{i=1}^{NLEM} \rho_i \right)^{-1} \sum_{i=1}^{NLEM} \rho_i Y_i^k \qquad \tilde{Q}_k = \overline{\rho} \tilde{Y}_k$$

  - Feeds back into the LES energy and EOS equations

- **Filtered Temperature:**

$$\tilde{T}_{LEM} = \left(\sum_{i=1}^{NLEM} \rho_i C_{p,i} \right)^{-1} \sum_{i=1}^{NLEM} \rho_i C_{p,i} T_i$$

  - Error in energy equation approximation

$$err(\tilde{T}_{LEM}) = (\tilde{T}_{LEM} - \tilde{T}) / \tilde{T}$$

Temperature Coupling

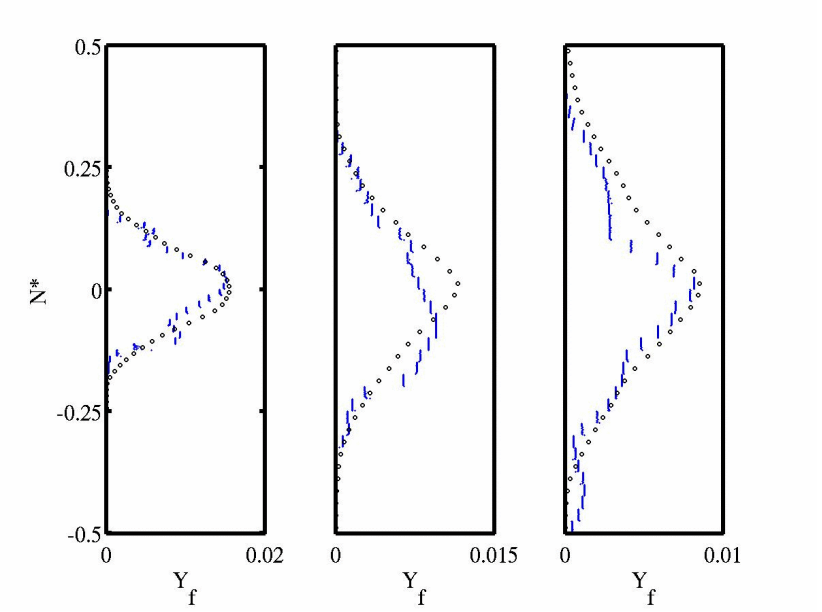
- Constrain LEM temperatures according to:

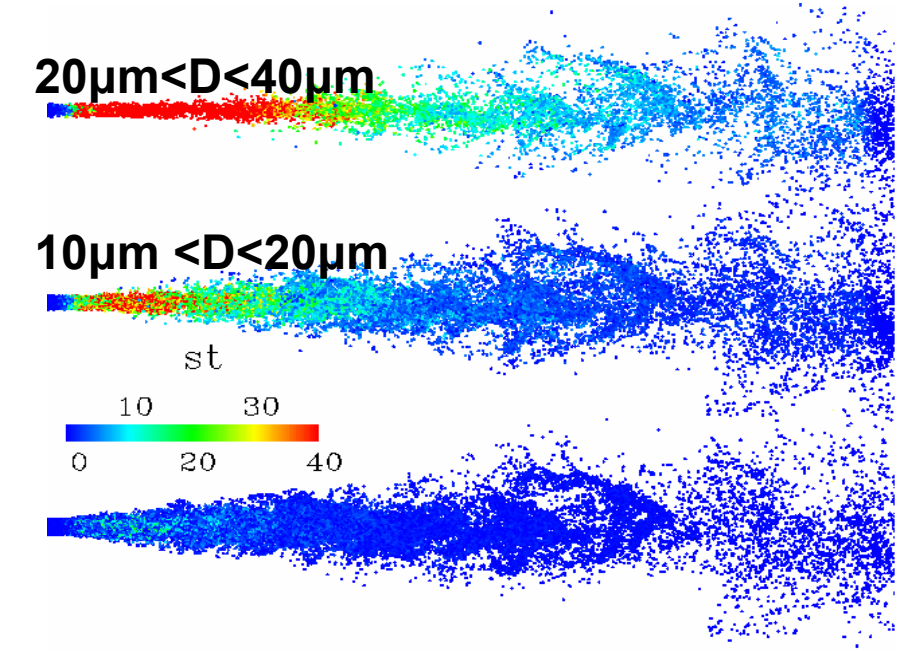
$$T_{i,rescaled} = T_i \times \tilde{T} / \left[\left(\sum_{i=1}^{NLEM} \rho_i C_{p,i} \right)^{-1} \sum_{i=1}^{NLEM} \rho_i C_{p,i} T_i \right]$$

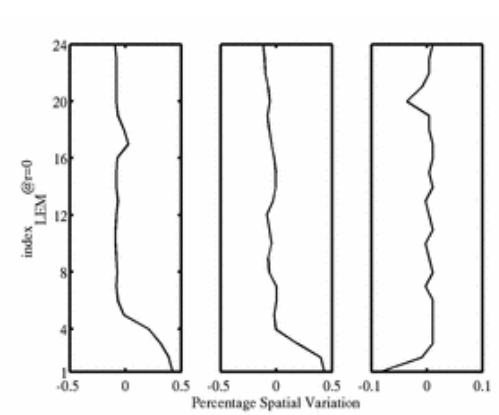
  - So that $\tilde{T}_{LEM,rescaled} = \tilde{T}$

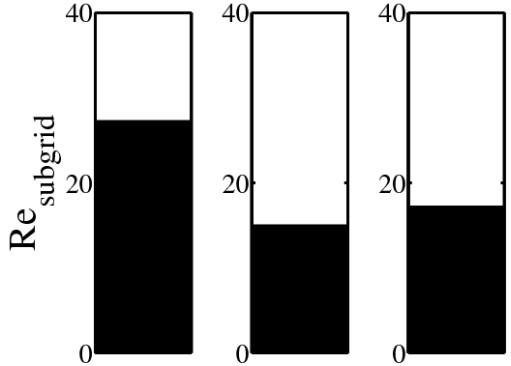
- Needs to be applied with care after making sure LES itself is predicting right temperatures (LES grid resolution)
- While forcing equality of LEM and LES filtered temperatures, the procedure can scale the internal temperature gradients

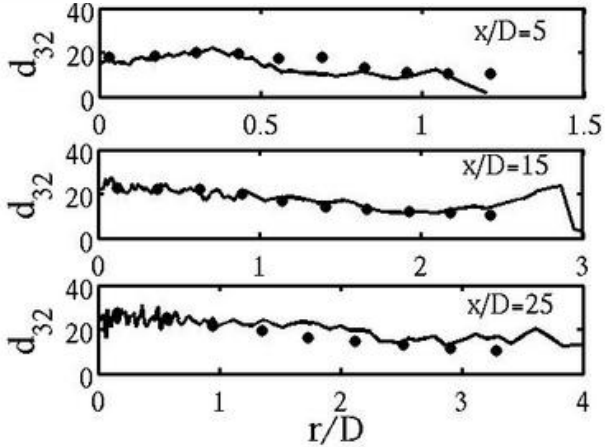
LEMLES of Vapor & Droplet Distribution*







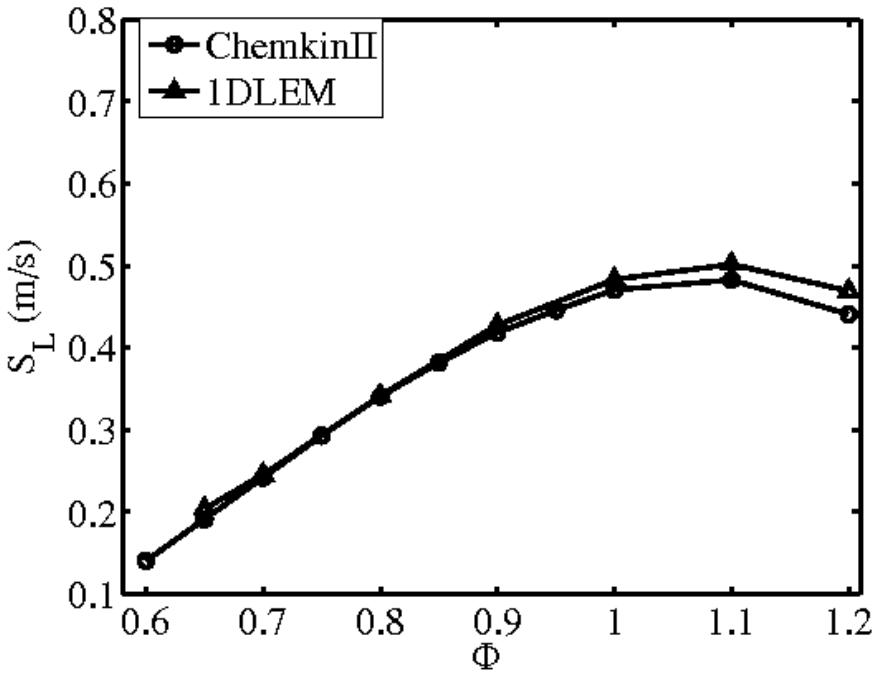




* Acetone spray Chen et al., 2006; Srinivasan et al. (DLES, 2010)

Laminar Flames using Standalone LEM

- Freely propagating premixed laminar CH4/Air flame
  - 4 step CH4/Air mechanism (Peters, 1991)
- S_L predictions compared with CHEMKIN and Peters' data
  - Stirring is disabled
  - 300K, 1 atm
  - Mix. ave. transport prop.
  - L=1cm, N_{LEM}=500



Standalone LEM

- **Timing Studies for a turbulent premixed flame for Re_t=42.5**

	Time/Step for Mech 1	Time/Step for Mech 2
Stirring Only	3.30×10^{-3}	1.20×10^{-3}
Diffusion Only (Le #)	2.24×10^{-2}	4.62×10^{-3}
Diffusion Only (M.A.)	3.60×10^{-2}	6.90×10^{-3}
Reaction Only	5.98×10^{-1}	9.80×10^{-3}

- Le# = Mixture averaged diffusivity with constant Lewis number
- M.A. = Mixture averaged diffusivity with multi-component mixture
- Mech 1 = 16 species, 12 steps; Mech 2: 5 species, 1 step
- Kinetics evaluation is the majority of the cost
- Nearly 96% cost is for kinetics for Mech 1
- Constant Le number approach is slightly faster

Standalone LEM: Timing Studies

For Re_t=42.5

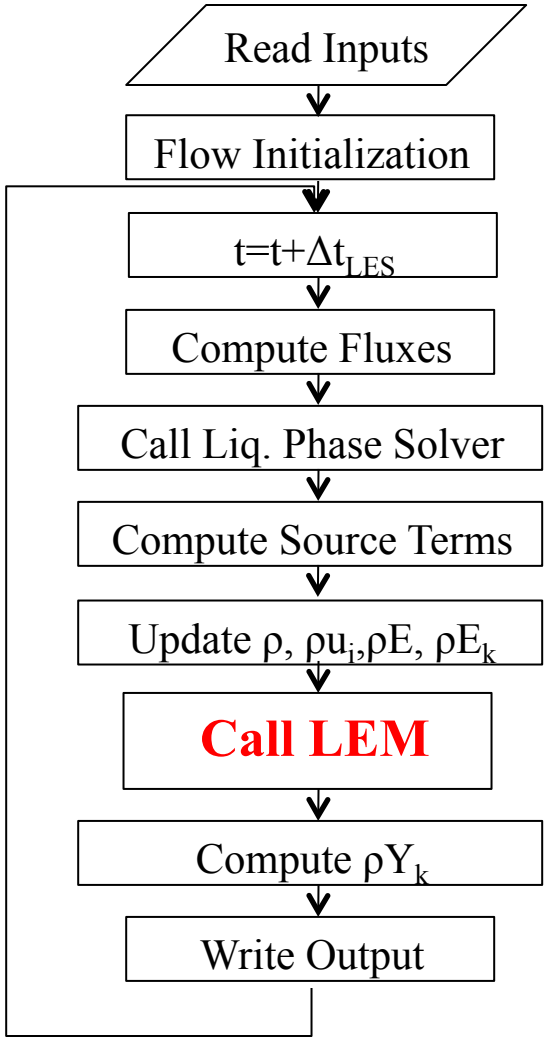
	Time/Step for Mech 1	Time/Step for Mech 2
Stirring Only	3.30×10^{-3}	1.20×10^{-3}
Diffusion Only (Le #)	2.24×10^{-2}	4.62×10^{-3}
Diffusion Only (M.A.)	3.60×10^{-2}	6.90×10^{-3}
Reaction Only	5.98×10^{-1}	9.80×10^{-3}

For Re_t= 175

	Time/Step for Mech 1	Time/Step for Mech 2
Stirring Only	9.80×10^{-3}	3.80×10^{-3}
Diffusion Only (Le #)	9.68×10^{-2}	1.99×10^{-2}
Diffusion Only (M.A.)	1.59×10^{-1}	2.94×10^{-2}
Reaction Only	1.88×10^{0}	2.83×10^{-2}

- As turbulent Reynolds number increases the number of grid points increases since is η decreasing
- Reaction rate calculations is even more time consuming
- LEM cost can decreased by faster kinetics evaluation – ISAT, ANN

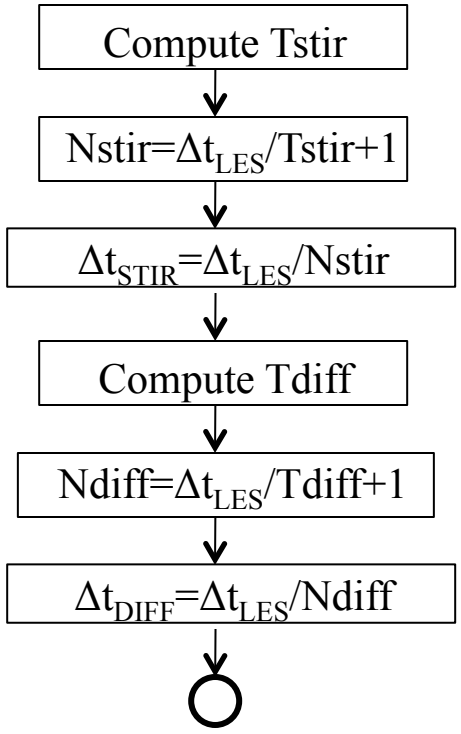
LEMLES Flowchart



- **Inputs: flow conditions, boundary conditions, thermal and transport property databases**
- **Explicit time-stepping**
- **Fluxes : viscous and inviscid components**
- **Liquid phase solver called as in LES**
- **No chemistry source terms, only those from liq. phase and ksgs (Prod and Diss)**
- **No update of species at this stage**
- **Call LEM solver (Energy and Species)**
- **Couple LEMLES via species and LES ρ**
- **Write output files for storage**
- **Repeat**

LEM Flowchart: Time Stepping

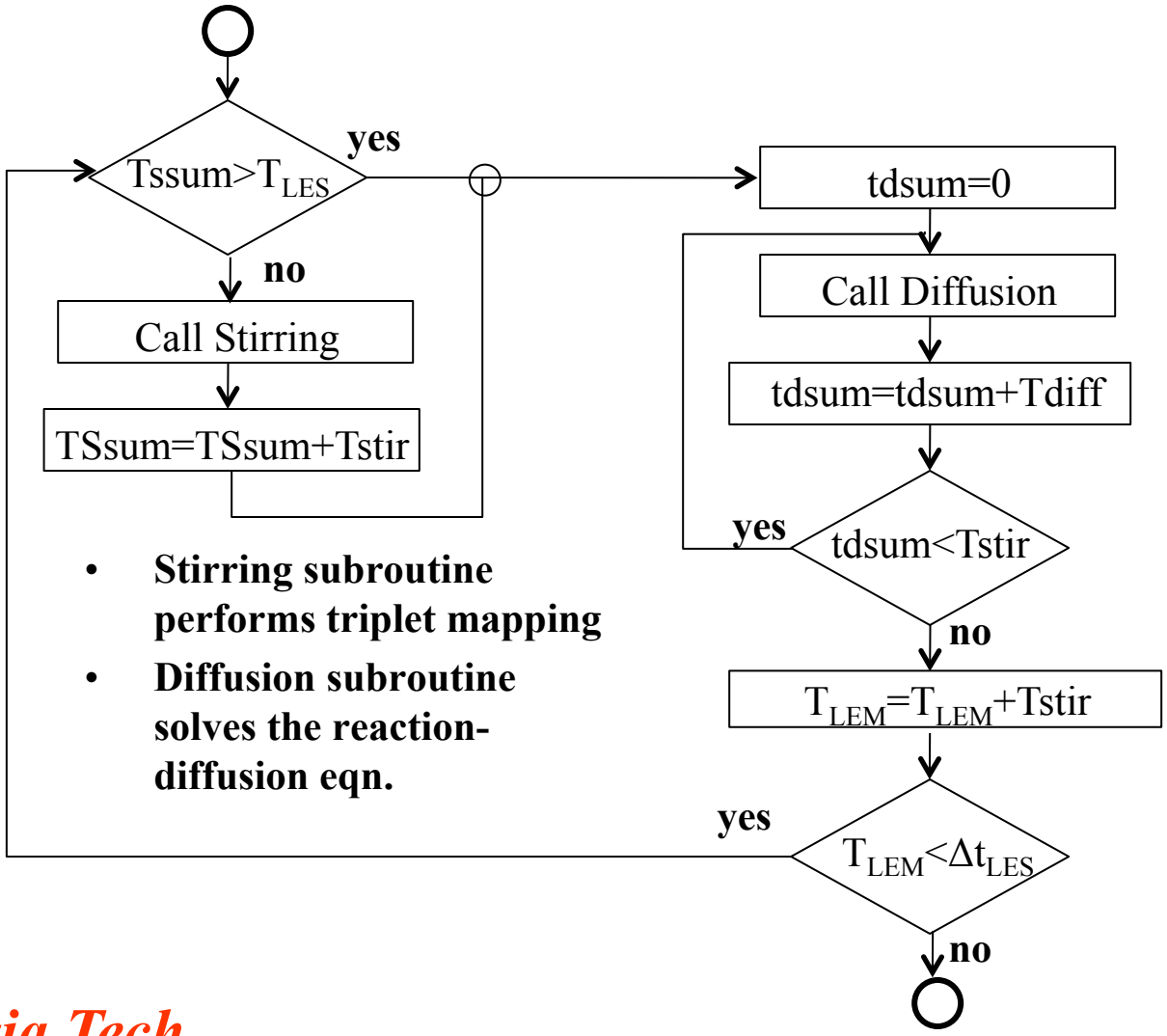
```
      RSCALE = EDDYSIZE
      RLAM = R54B5 * RNUS * REL * (1D0/RSCALE**3D0) *
     >       ((REL)**(5D0/4D0) - R1)/
     >       (R1 - (REL)**(-1D0))
      TSTIR = STSCFAC / ( RLAM * RSCALE)
      CALL RANDOM_NUMBER(RAND)
      RFAC = INT(10D0*RAND)
      IF (RFAC.EQ.0) RFAC = 1
      RAND = DBLE(RFAC/10D0)
      ETA  = ETA *ETAFAC
      SMAX   = INT(DELTA_T/TSTIR) + 1
      TNEXTS = DELTA_T/DBLE(SMAX)


      TDELG  = COOKG * DXLEM * DXLEM / DIFCOF
      SMAX   = INT(DELTA_T/TDELG) + 1
      TNEXTG = DELTA_T/DBLE(SMAX)
      TDELG  = TNEXTG
```



- **All processes in LEM resolved at their respective time scales**
- **DIFCOF = Max. Diff. coeff. in LEM domain**
- **COOKG=1/4**
- **Integer number of diffusion and stirring steps per LES time step**

LEM Flowchart: Time Stepping

```
LEMTIME = ODO
DO WHILE (LEMTIME.LT.DELTA_T)
  RET = ODO
IF (INIT.EQ.1) THEN

  IF (DELTA_T*JJ.GT.TSTR) THEN


    CALL STIR()

    TSTR = TSTR + TSTIR

  END IF

END IF

  DFT = ODO
  DO WHILE (DFT.LT.TNEXTS)
    CALL DIFFUSE(1)

    DFT = DFT + TNEXTG
  END DO
  LEMTIME = LEMTIME + TNEXTS
```



- **Stirring subroutine performs triplet mapping**
- **Diffusion subroutine solves the reaction-diffusion eqn.**

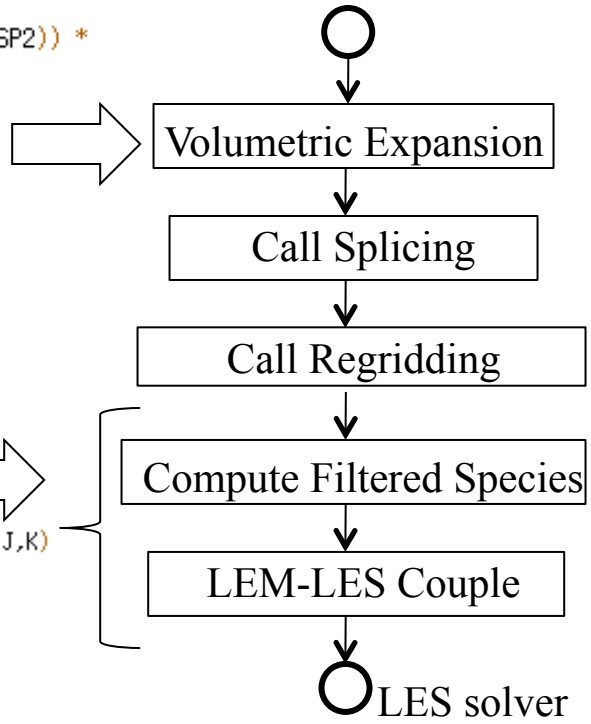
LEM Flowchart: Vol. Exp. and LEMLES

$$Vol^{n+1} = Vol^{n} \times \frac{\rho^{n}}{\rho^{n+1}}$$

```
DO IS = 1, ISGS
   GSGS(IS,NSP3,I,J,K) =
        (GSGS(IS,NSP2,I,J,K)/GDUMM(IS,NSP2)) *
         GSGS(IS,NSP3,I,J,K)
END DO
```

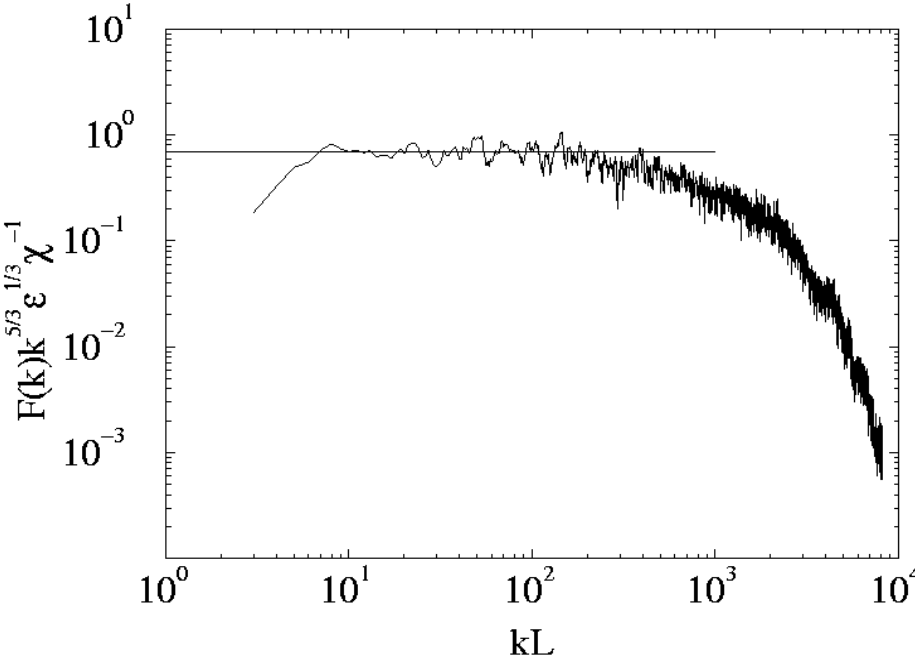
$$\overline{\rho}\widetilde{Y}_k = \overline{\rho}\frac{\sum_{i=1}^{ISGS}\rho_i Y_k}{\sum_{i=1}^{ISGS}\rho_i}$$

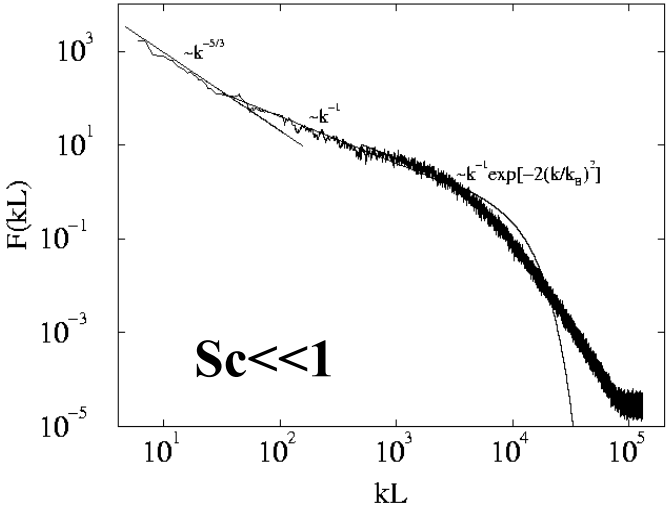
```
DO K = K1,K2
  DO J = J1,J2
    DO I = I1,I2
       SUMRO = RZERO
       DO IS = 1,ISGS
          SUMRO = SUMRO + GSGS(IS,NSP2,I,J,K)
       ENDDO
       DO NS = 1,NSPLEM
          SUMY = RZERO
          DO IS = 1,ISGS
             SUMY = SUMY+ GSGS(IS,NSP2,I,J,K)*GSGS(IS,NS,I,J,K)
          ENDDO
          CONC(I,J,K,NS)  = SUMY/SUMRO
          Q(I,J,K,INCHE+NS,M) = Q(I,J,K,1,M)*CONC(I,J,K,NS)
       ENDDO
    ENDDO
  ENDDO
ENDDO
```

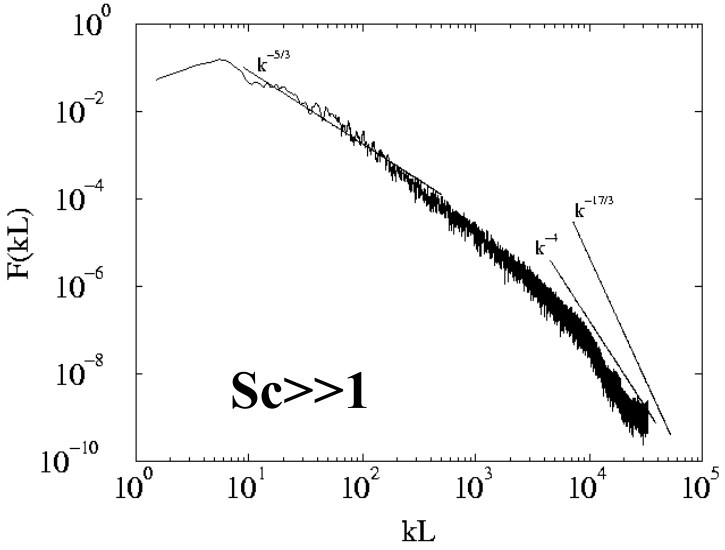


- **Splicing is not performed for the standalone LEM code**
- **ISGS=LEM resolution (N_{LEM})**
- **GSGS=subgrid species field, CONC=filtered species field (mass fraction)**
- **Index NS::1 to NSPECI=Species, NSP2=Subgrid Density, NSP3=Subgrid Volume**

Scalar Spectrum and Schmidt Number Effect







Prediction of χ(scalar dissipation) :

Mydlarski & Warhaft : $4.96s^{-1}$

LEM : $4.82s^{-1}$

Prediction of β (Obukhov - Corrsin constant) :

Sreenivasan (Phys. Fluids 1996, **8**) : 0.33-0.6

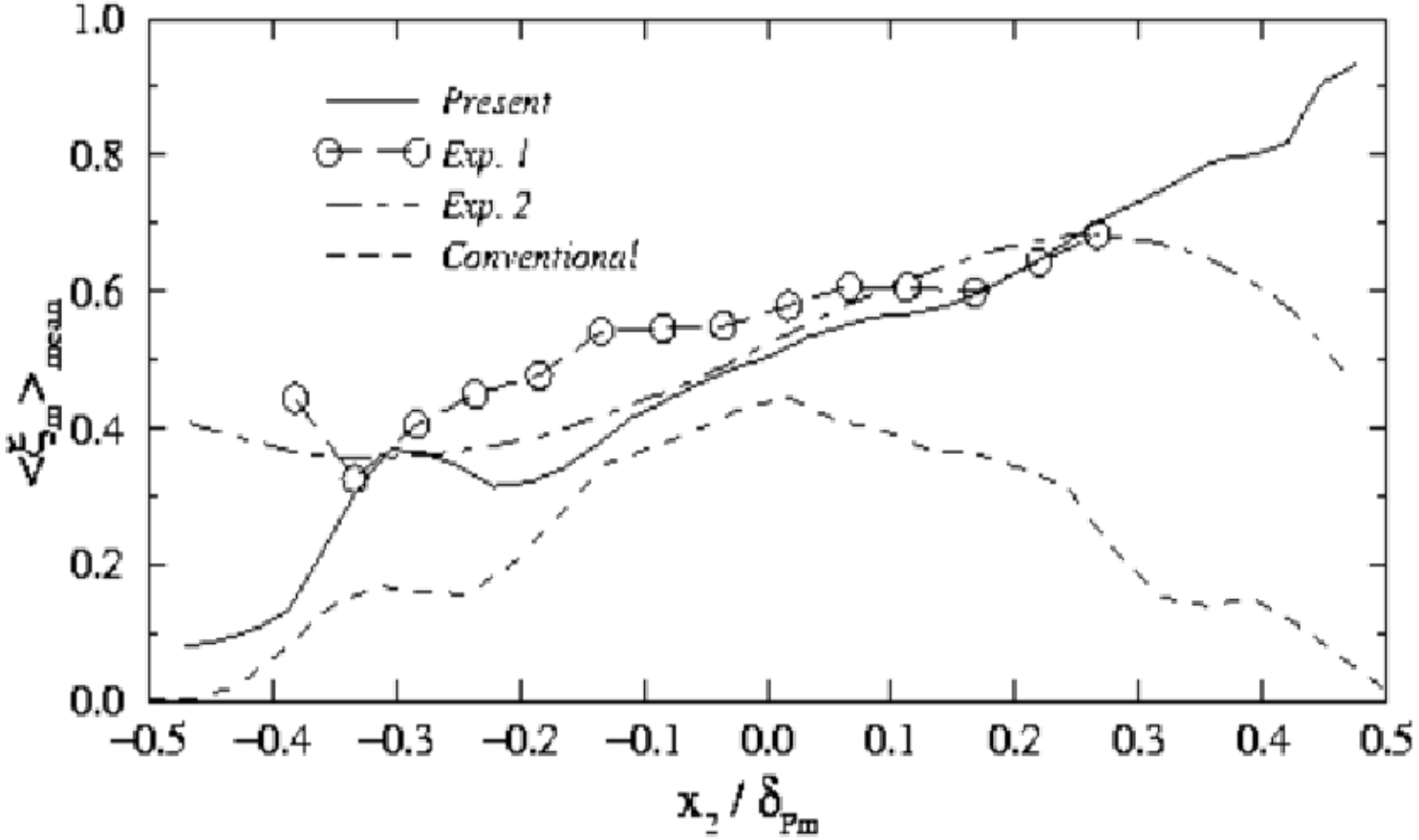
Mydlarski & Warhaft (JFM1998, vol.358): 0.45-0.5

LEM : 0.44

Suresh Menon, Georgia Tech

Phys. Fluid, Vol. 13, 2001

Mean Mixed Fluid Profile in Shear Layer (Menon and Calhoon, Symp. 96)



Flip Experiments: Filtered Product (Mungal and Dimotakis)

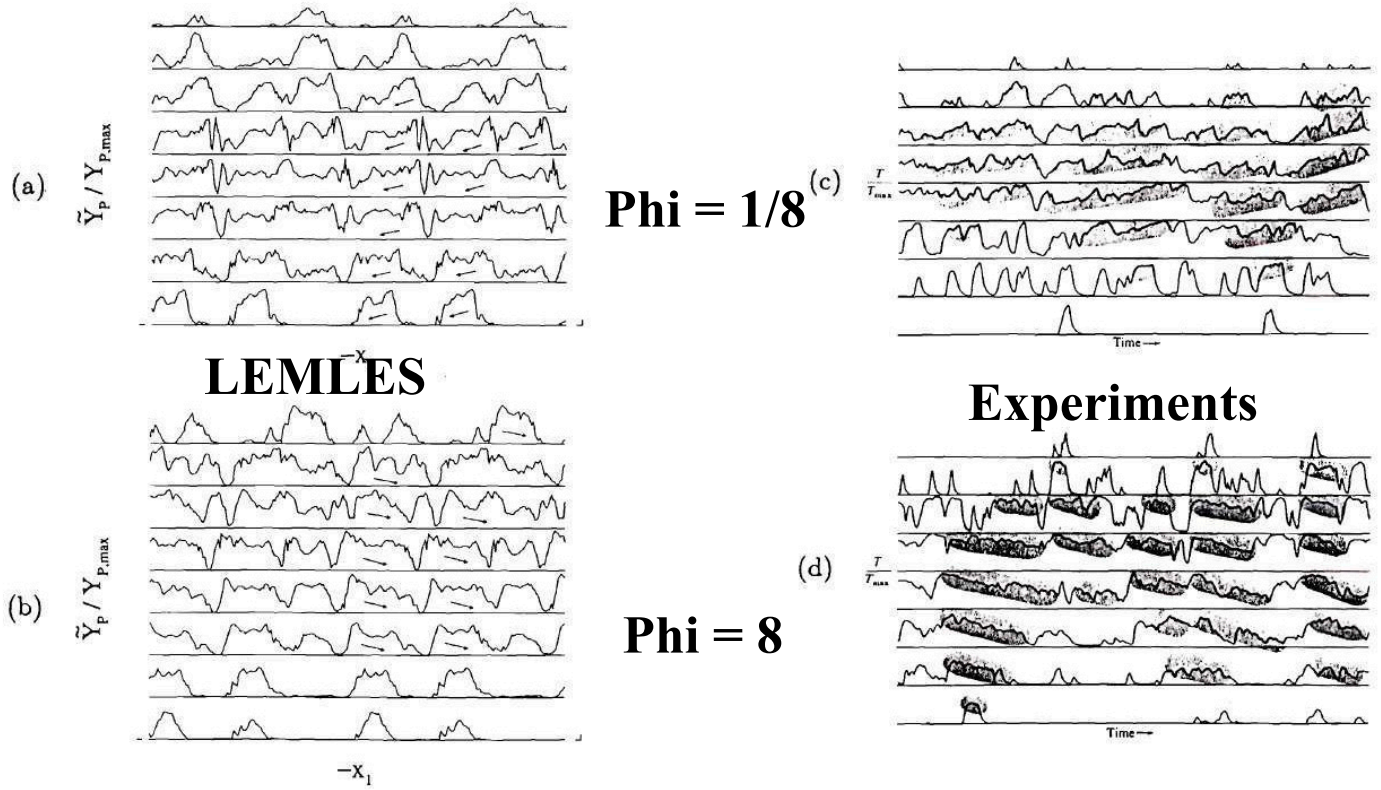
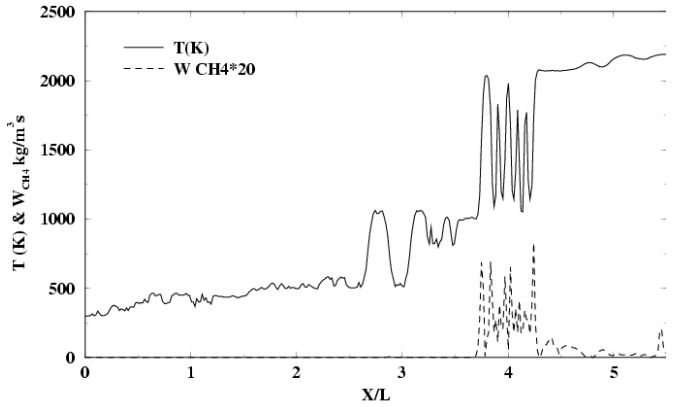
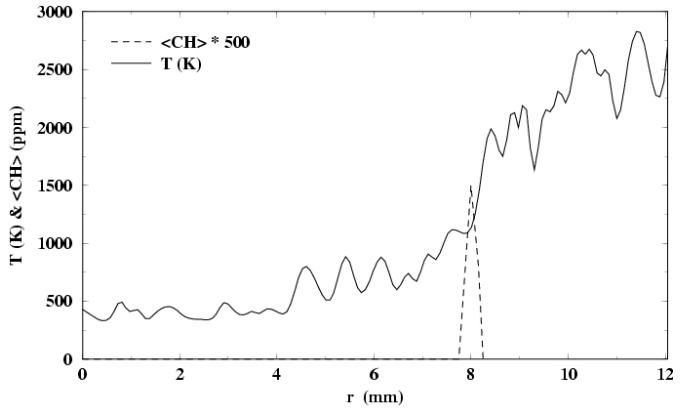


Figure 6.11. Trace plot of product in the layer. (a) and (b) are predicted filtered product for $\phi = 1/8$ and 8, respectively, measured at the same stations as in Figure 6.10. (c) and (d) are experimental temperature traces from Mungal and Dimotakis[169] (reproduced with permission) for $\phi = 1/8$ and 8, respectively, measured at $x_2/\delta_{Pm} = -.44, -.31, -.18, -.06, +.08, +.20, +.33$ and $+.46$.

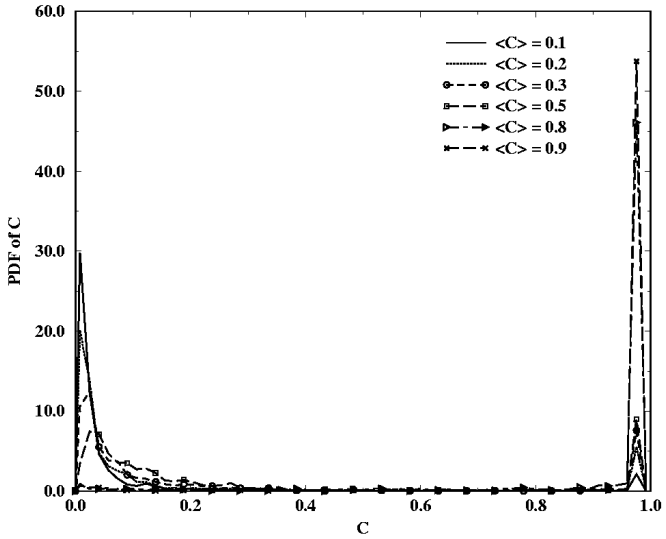
Prediction of Premixed Flames



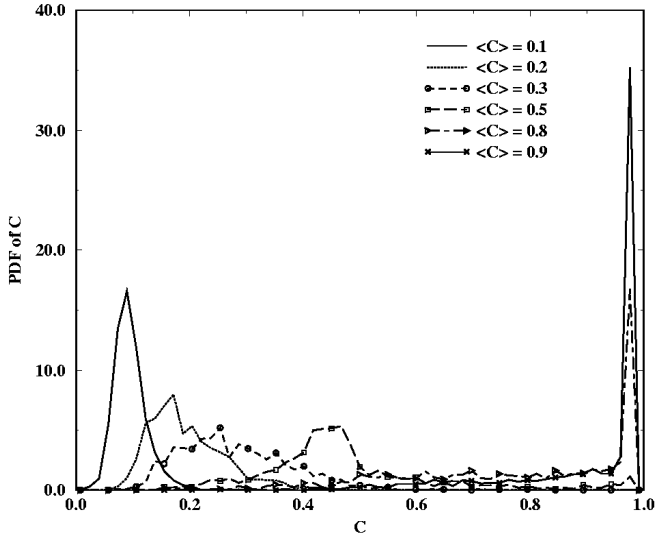
Flame F1 – Numerical



Flame F1 - Experimental



PDF of Flame B1 (Flamelet)



PDF of Flame F1 (TRZ)

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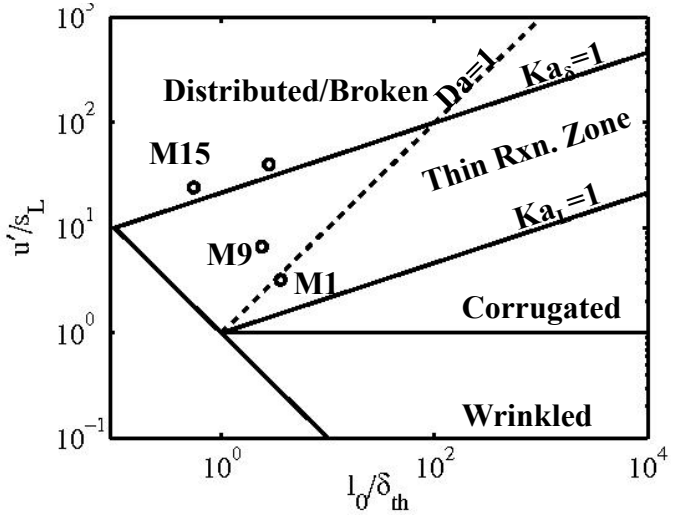
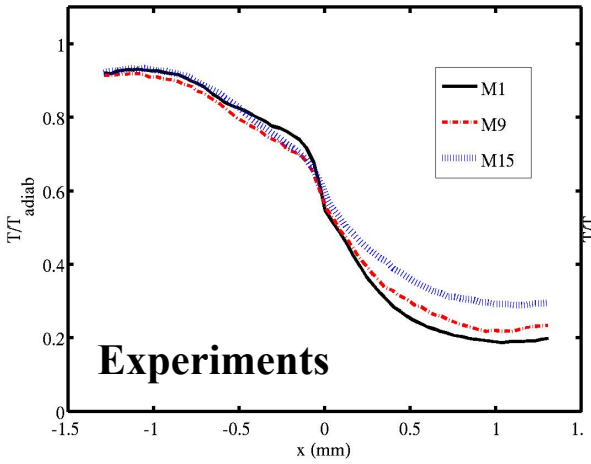
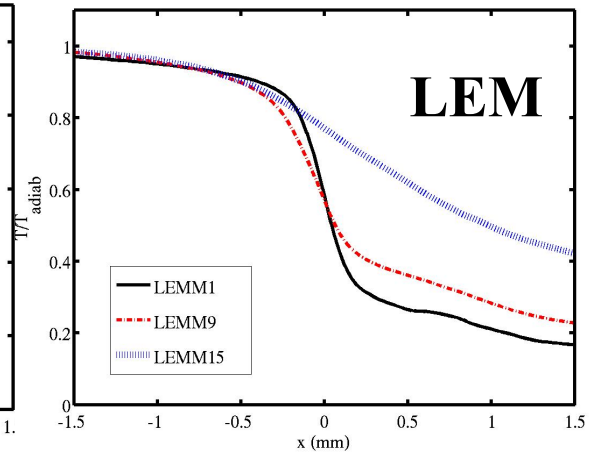
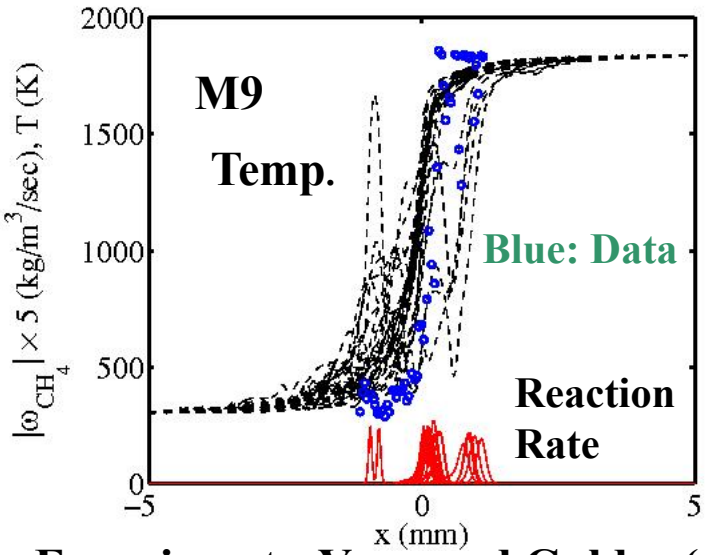
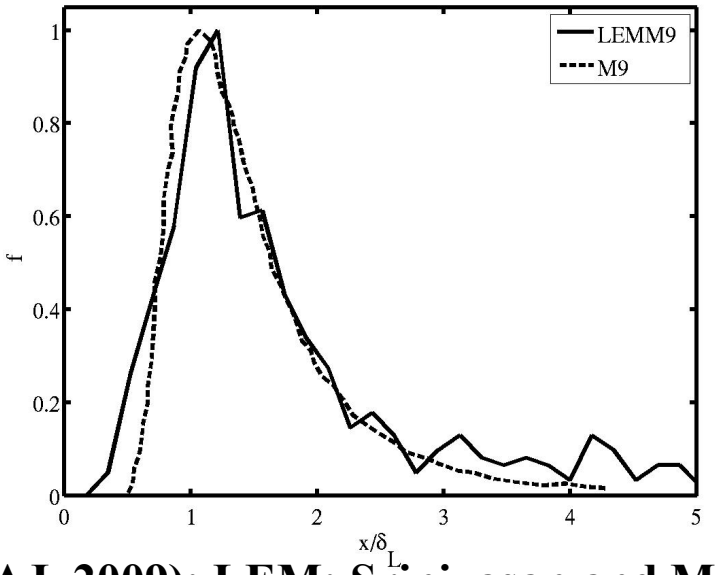
Predicting Flames in TRZ and BRZ Regimes







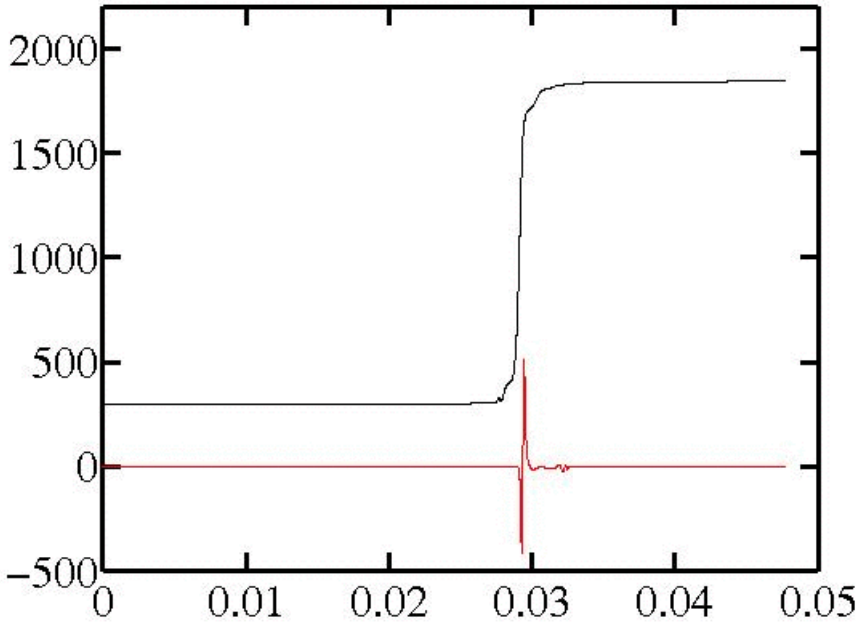


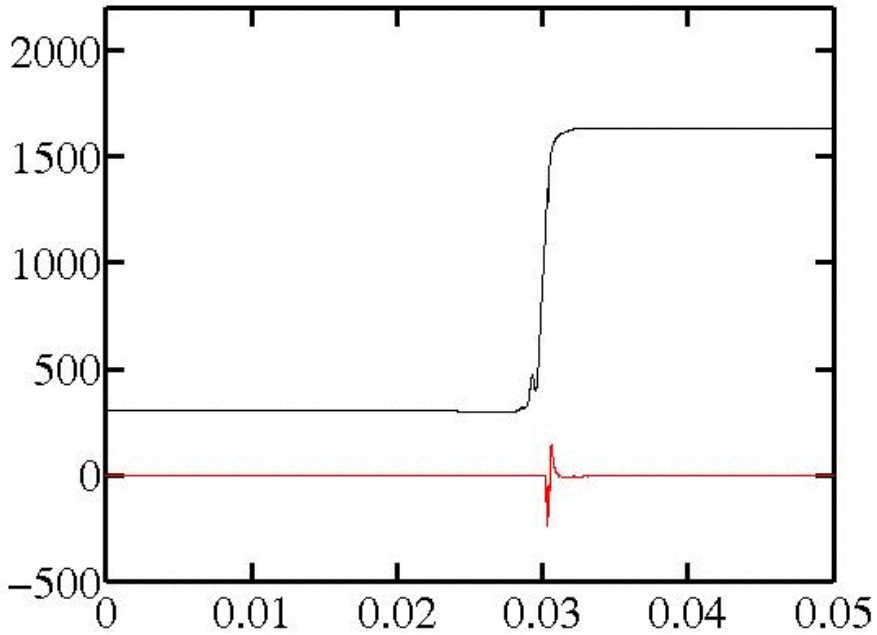


Histogram: Reaction Zone Thickness

Experiments, Yuen and Gulder (AIAAJ, 2009); LEM: Srinivasan and Menon, 2011

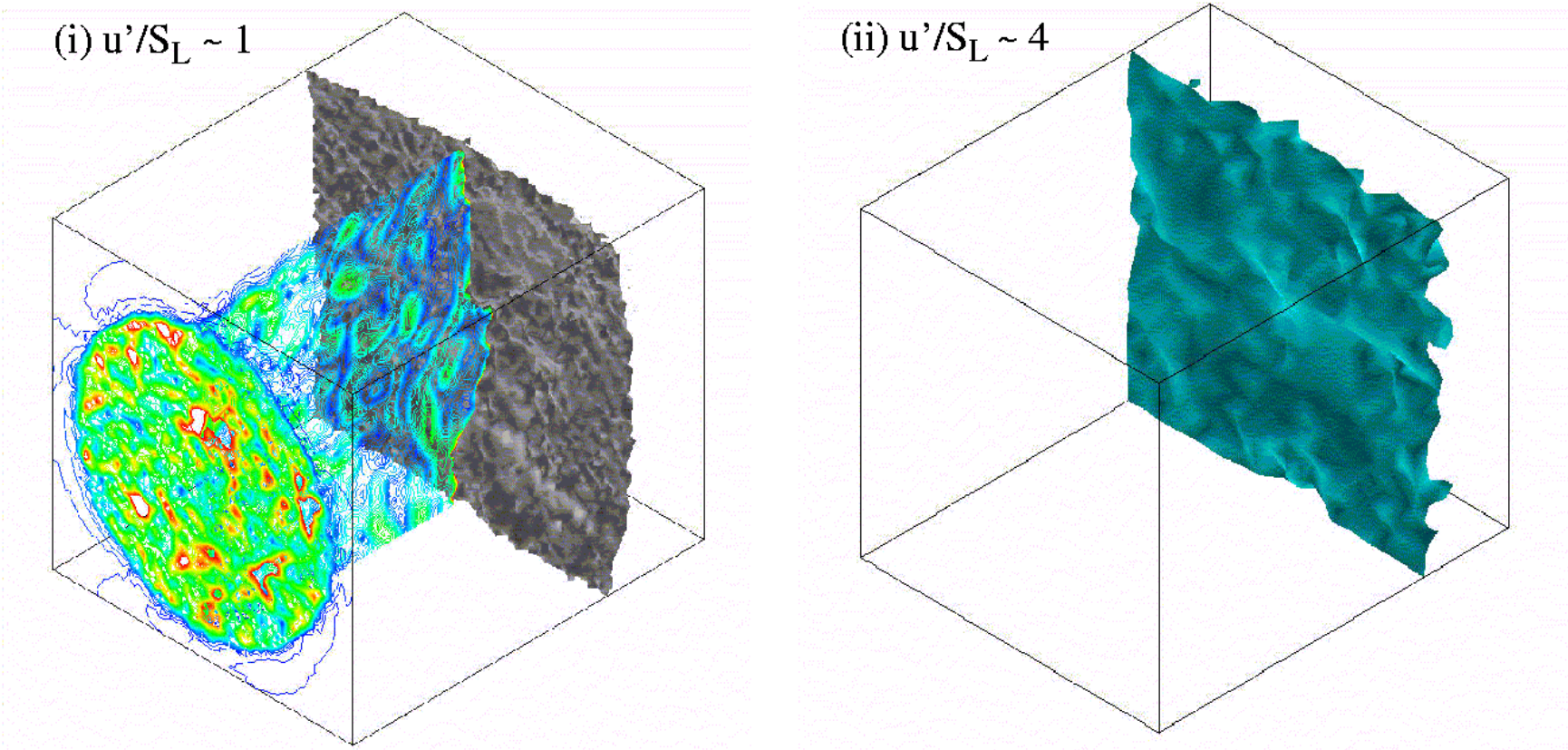
Flame Structure in LEM





M9 **M15**

Flame/flow structure

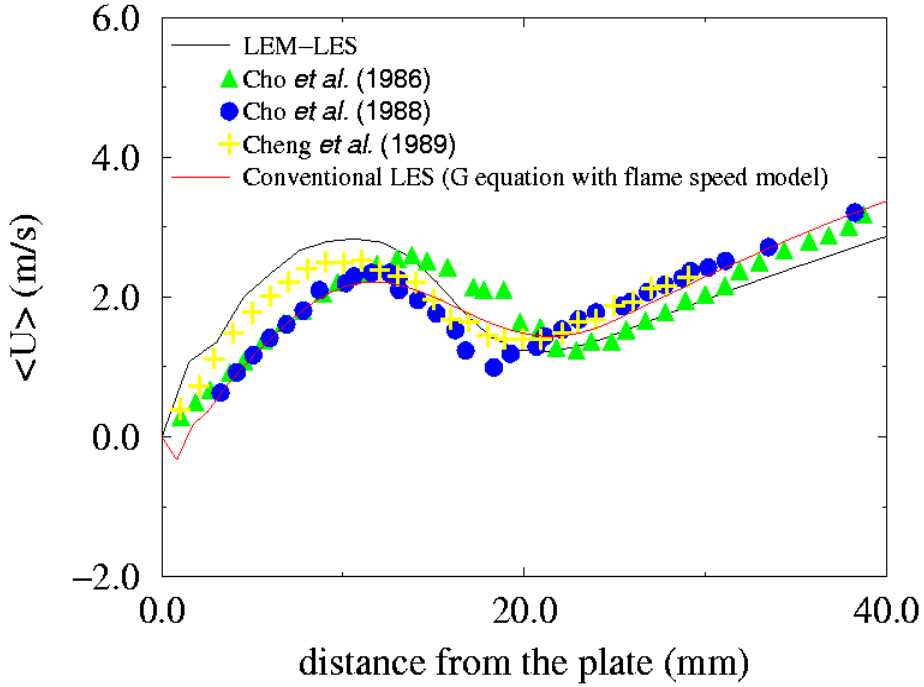


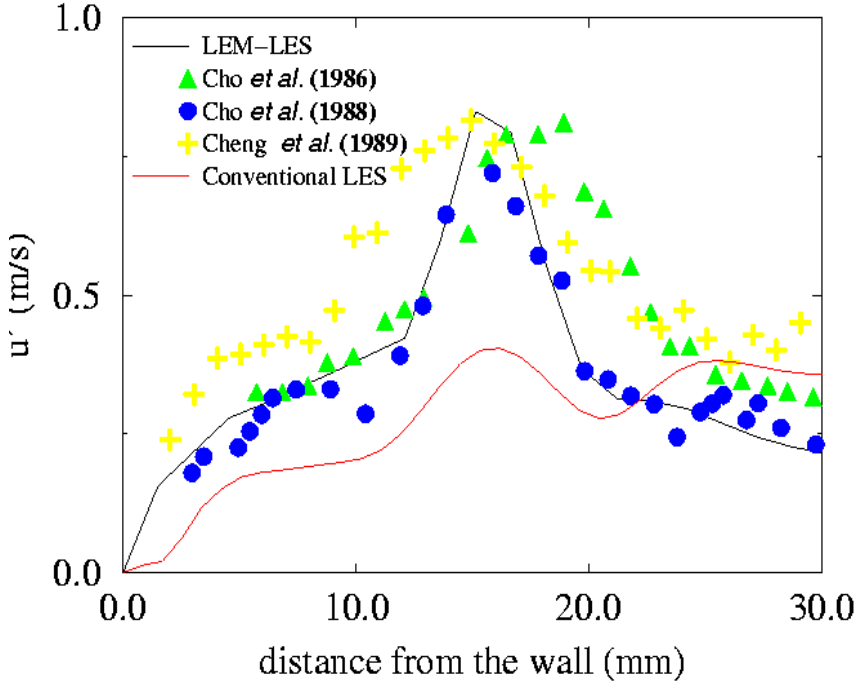
Shown in figure (i) are the vorticity contours on the inflow plane and one of the axial planes. Flame is visualized as an isosurface of the progress variable

LES resolution 67 x 59 x 59 for the region shown. LEM resolution : 100

Chakravarthy and Menon, CST (2002) FTC (2003)

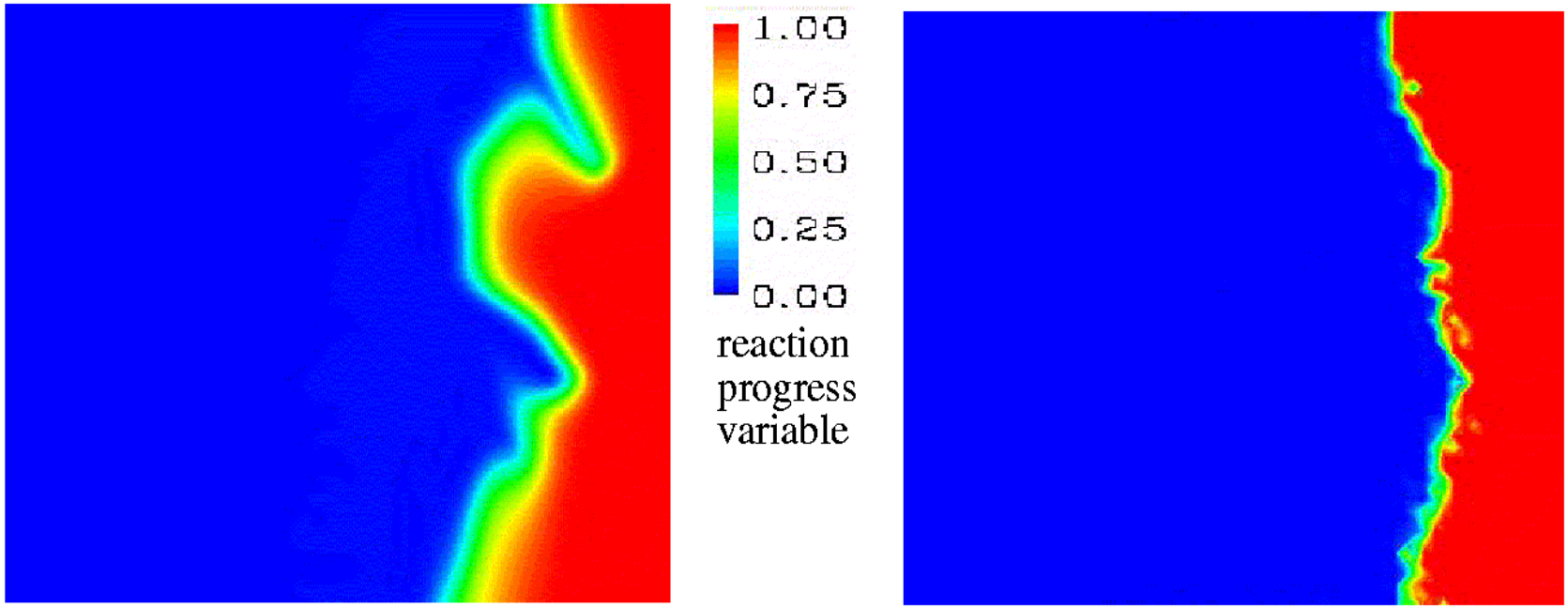
Effect of Flame Wrinkling on Mean and RMS





- Both GLEM-LES and LES-GEQN predict mean flow
- GLEM-LES show better agreement with RMS
- Flamelet regime flame structure captured in GLEM-LES

Resolution of the flame structure



Conventional (FD/FV) scheme using a flamespeed models

LEM-LES

* *Flame is captured over several LES cells in conventional approaches.*

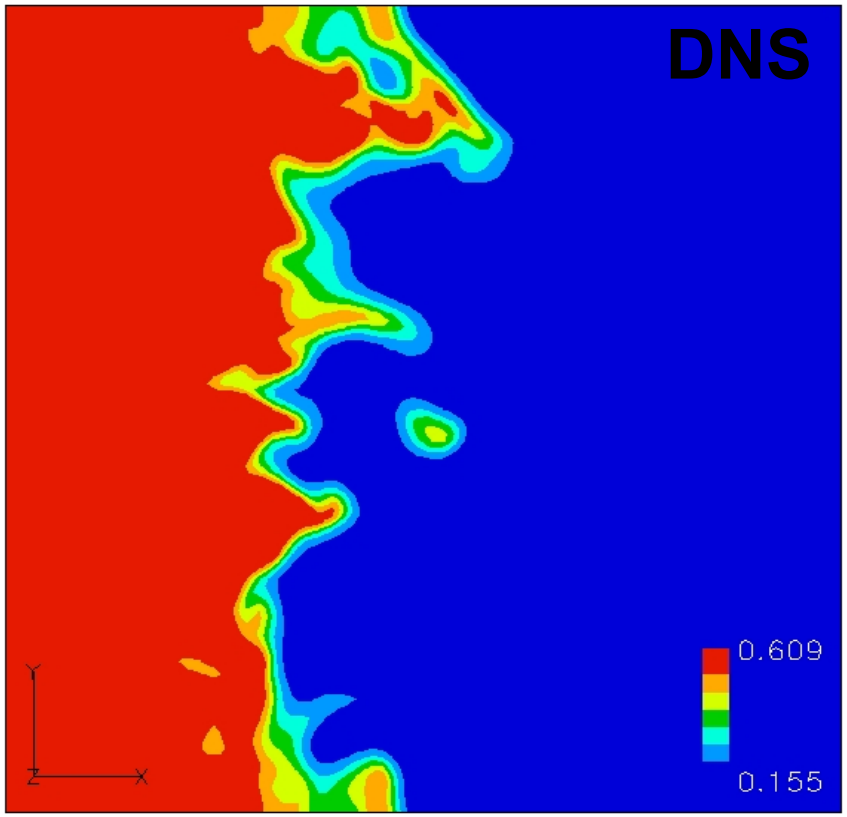
* Flow acceleration is gradual. Low velocity intermittency.

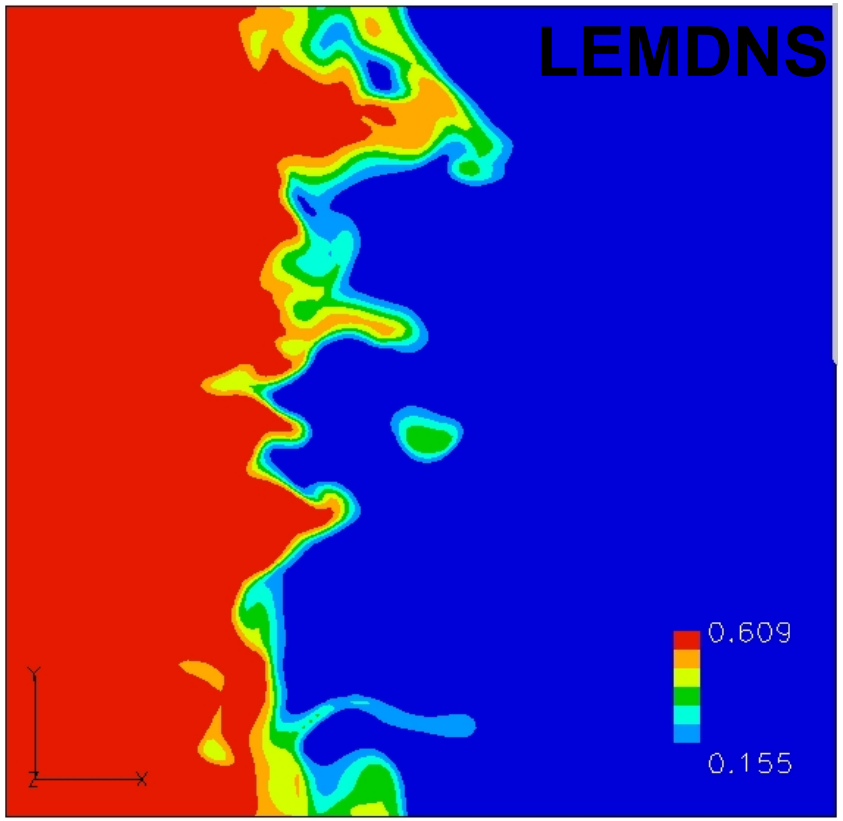
* *Flame is tracked as a thin front in LEM-LES*

* No fluid dynamic eddy can exist with the thickness of the flame.

* Flamelet type burning.

Contours of Density Stream-Wise (X)



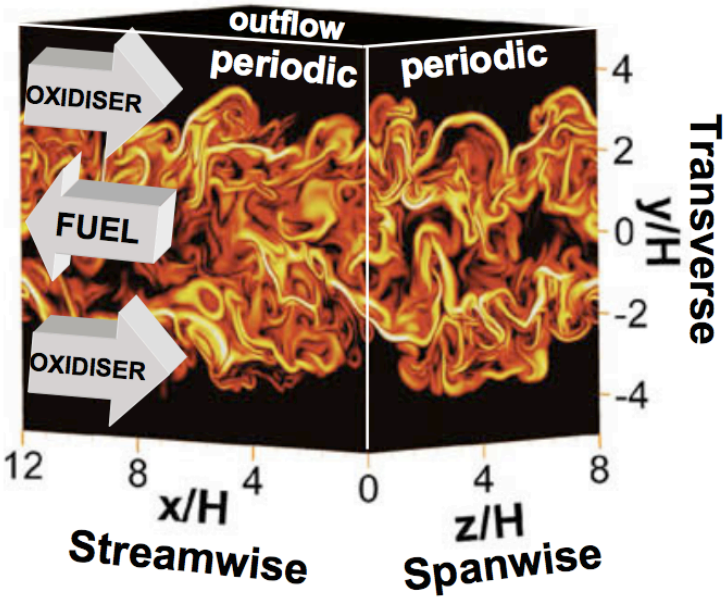


- DNS - Scalar field tracked with Eulerian formulation
- LEMDNS - Scalar field tracked with Lagrangian formulation

Sankaran and Menon, Symp 2004

Test Case

DNS of Extinction and Re-Ignition in a *CO/H*$_2$ Plane Jet Flame (Hawkes, E.R., et al., 2007 and 2009)



Re_{jet}=4478
Fuel: 50 % *CO*, 10 % H_2, 40 % N_2
350 M grid points, reduced kinetics with 11 species and 21 reactions

Case-M1: 96×112×64=700K grid points
Case-M2 192×224×128=5.5M grid points

	LEMLES	LANN-LEMLES	TANN-LES
Subgrid Turbulence	LDKM	LDKM	LDKM
Subgrid Combustion	LEM	LEM	TANN
Subgrid Chemistry	DI	LANN	—

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Turbulence-Chemistry Closure for Fast LES

- LEMLES is very accurate but is computational costly
- New approach to obtain filtered reactions rates using tabulated subgrid evolution of reactive scalars
- Include effect of turbulence on reaction-diffusion
- Off-line LEM simulations to generate the data base
  - Train ANN on the composition and turbulence
  - Employ TANN in the actual LES
- Look up based on *local composition, Re, time-step and scalar dissipation or gradient*
- Eliminate all stiffness of kinetics and LEM cost
- Cost is same as non-reacting scalar transport modeling

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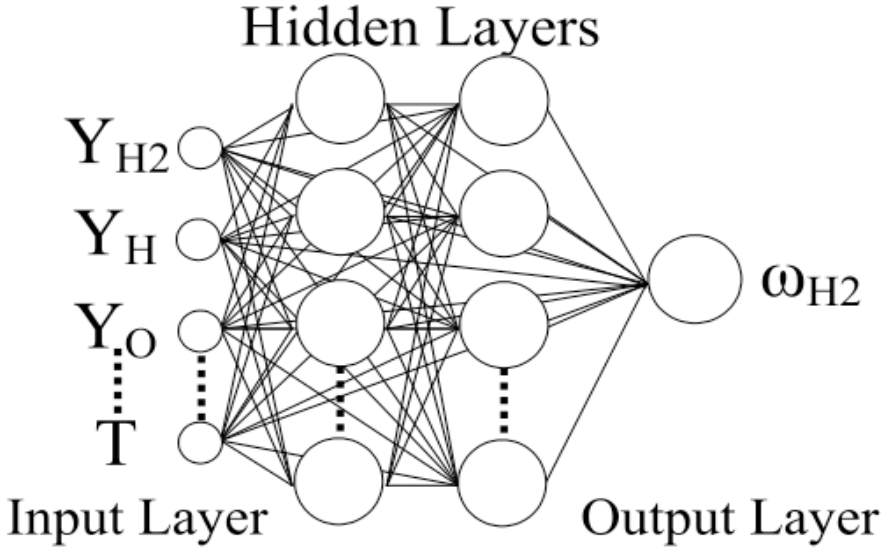
TANN for LES (or RANS)

- Optimal ANN strategy still under development
- All date used for training
- Training on composition and turbulent space not the actual geometry

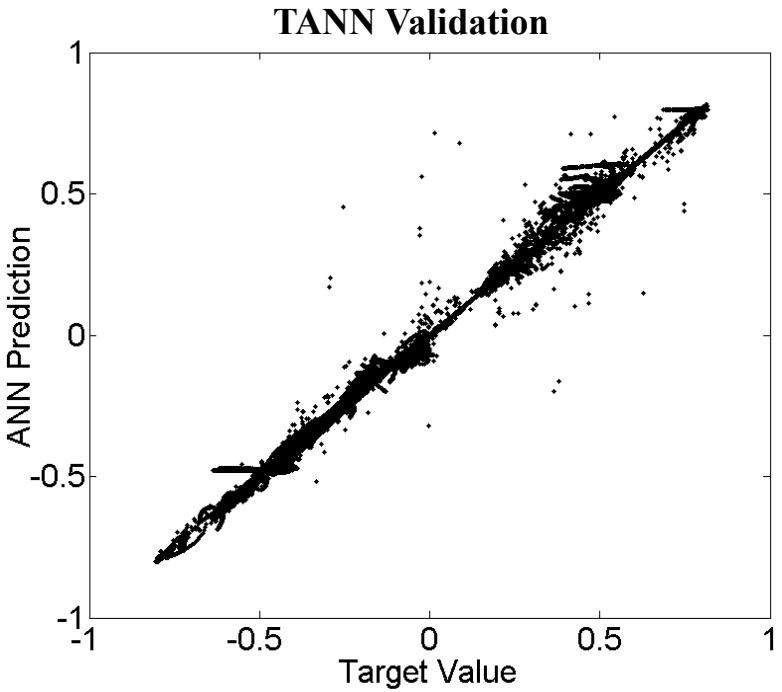


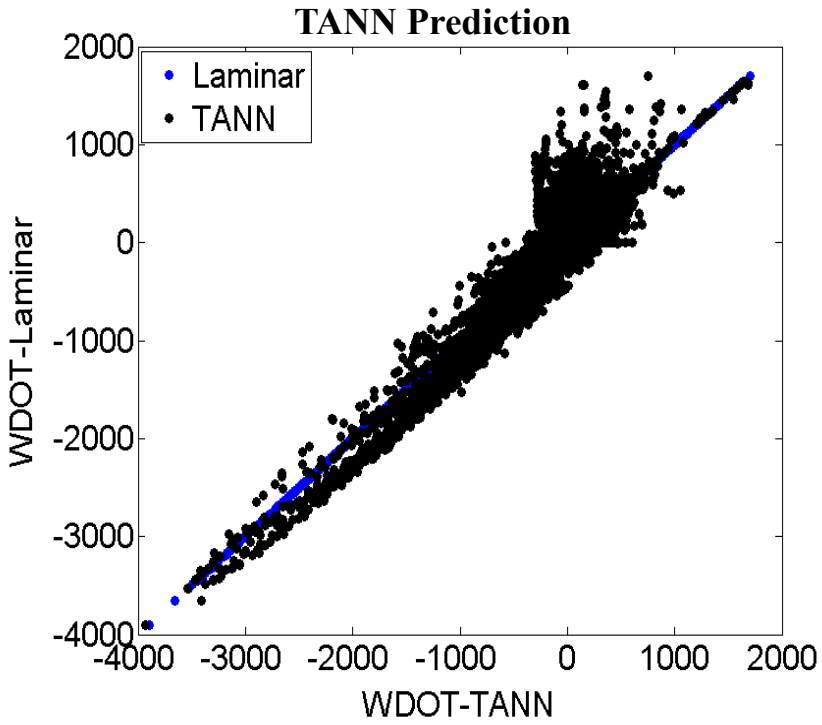
$$\frac{\partial \overline{\rho}\tilde{Y}_k}{\partial t} = \frac{\partial}{\partial x_j}\left(\overline{\rho}\tilde{Y}_k\tilde{u}_i - \overline{\rho}\tilde{Y}_k\tilde{V}_{i,k} + \phi_{i,k}^{sgs} + \theta_{i,k}^{sgs}\right) + \tilde{\omega}_k$$

$$\overline{\dot{\omega}}_k = TANN(\tilde{Y}_1, \tilde{Y}_2, ..., \tilde{Y}_{Ns}, \tilde{T}, \mathrm{Re}_\Delta, \partial\tilde{Y}_k/\partial x_i)$$

*** Sen and Menon (Symp. 32, 2009, Combustion and Flame 157, 2010a, 2010b)**

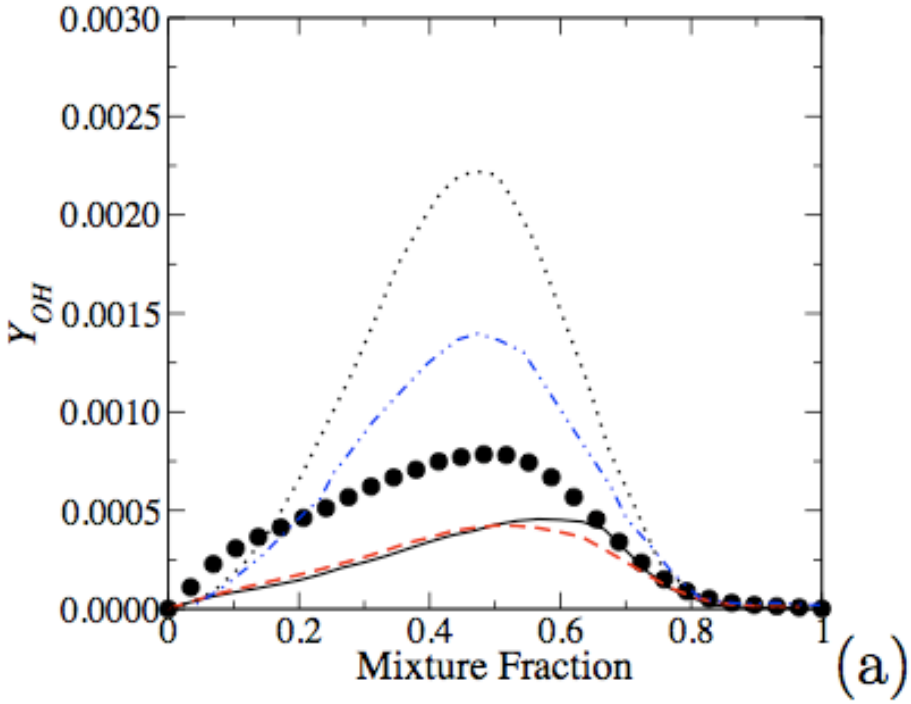
TANN Training and Validation



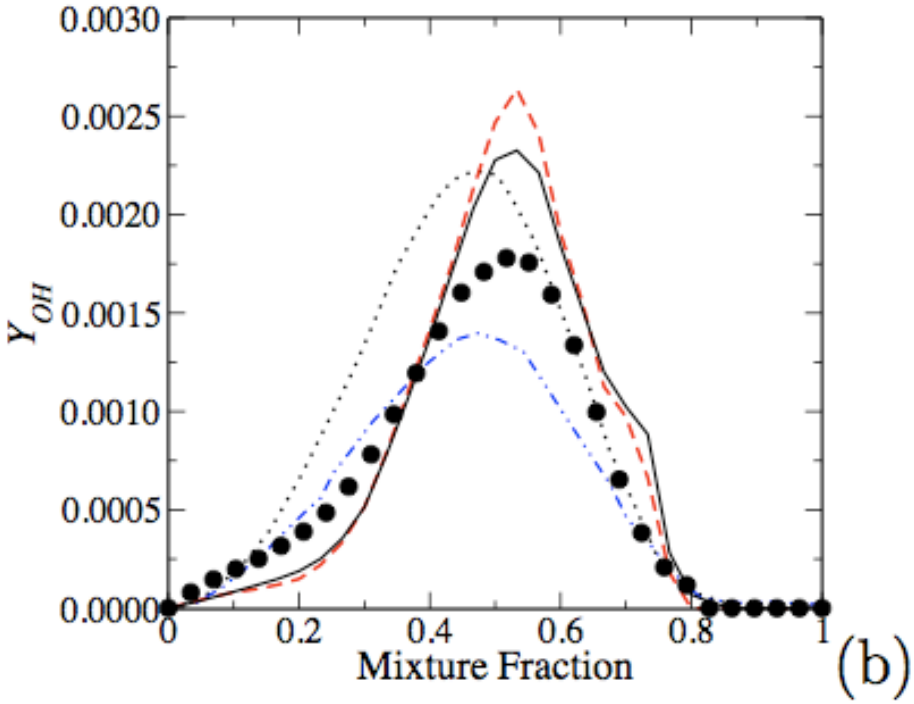


Same Composition but different Turbulent states

OH Statistics by LANN-LEMLES*



tj=20

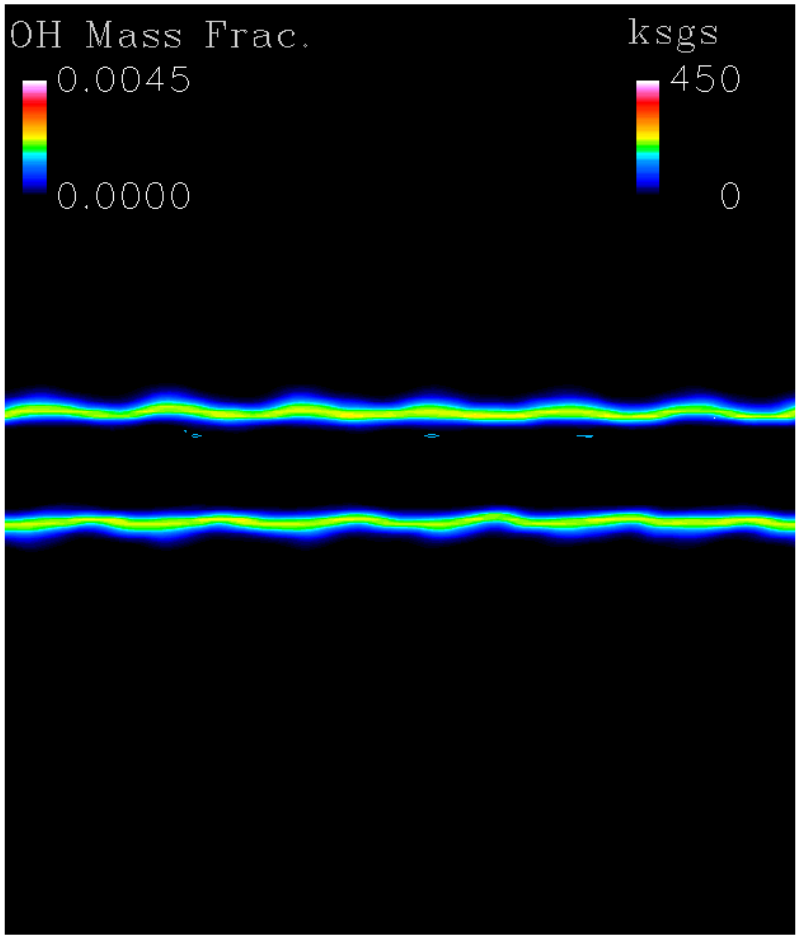


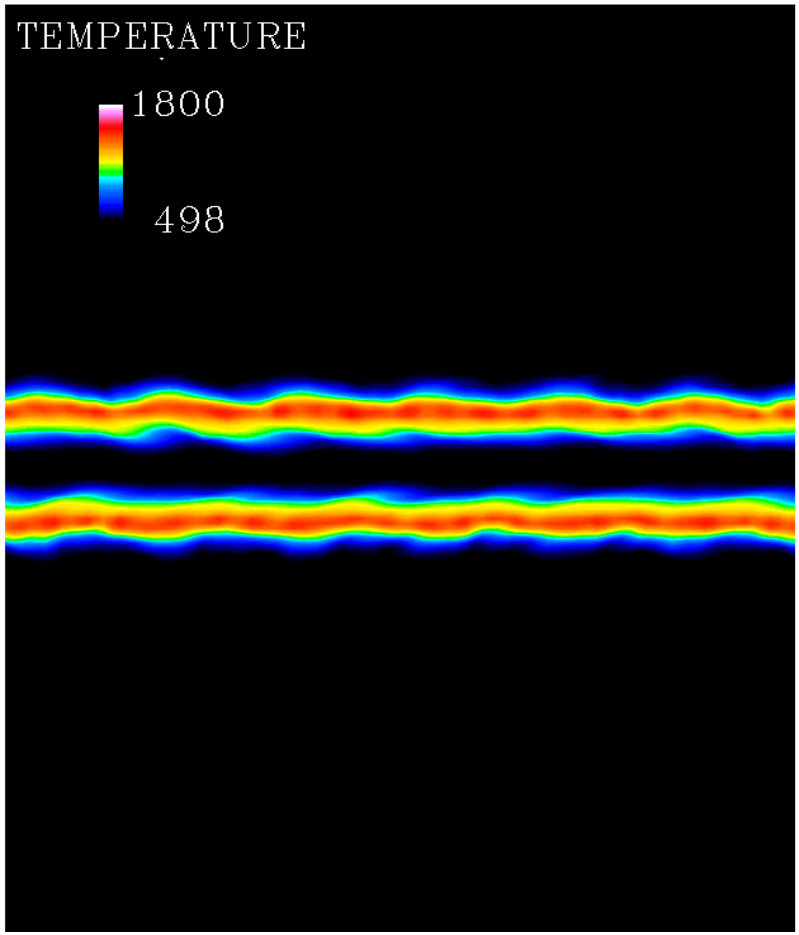
tj=40

- DNS data (•), Initial data (. . .), Laminar flamelet at extinction (- .. - ..), Case M-1 (- - -), Case M-2 (——)
- The LANN-LEMLES (Case M-1 and M-2) predict extinction and re-ignition with reasonable accuracy

*Sen, Hawkes and Menon, Comb. Flame, Vol. 157, 2010

OH Mass Fraction, K_{sgs} and Temperature LANN LES





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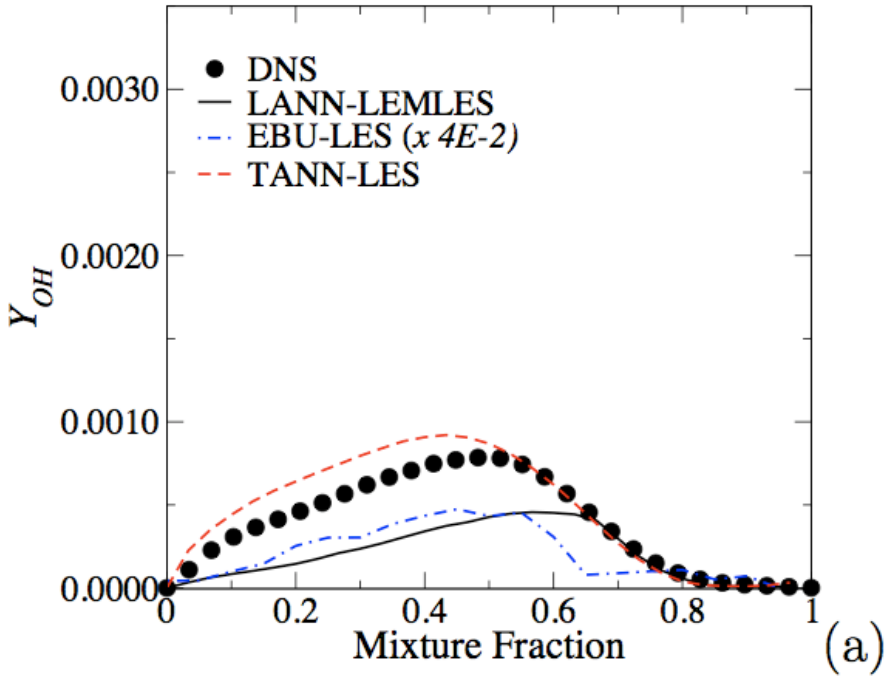
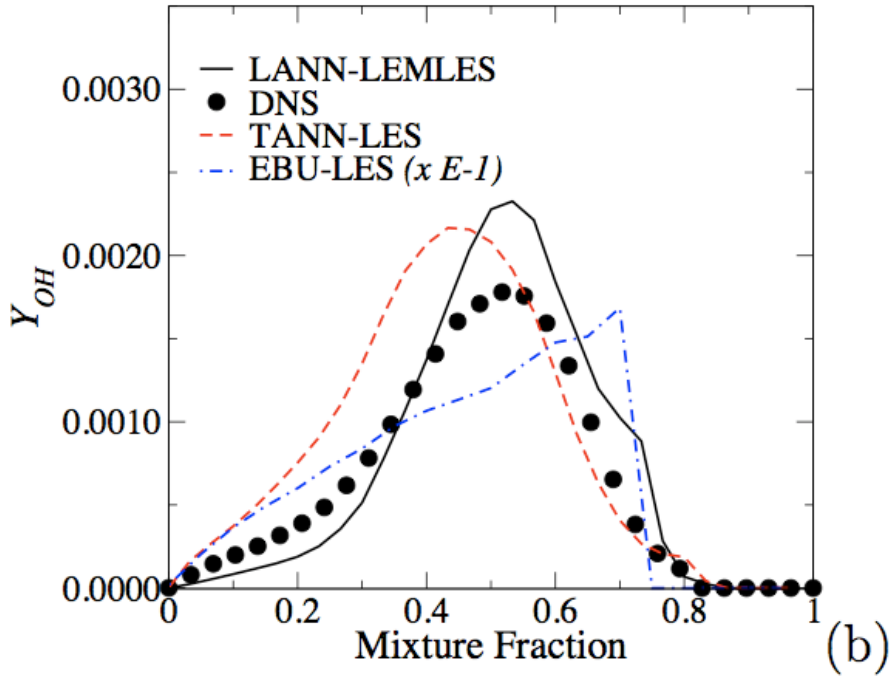
OH Statistics by TANN-LES



tj=20



tj=40

- At extinction TANN-LES seem better than LANN-LEMLES
  - may be due to the approach for scalar closure
- At re-ignition the peak is shifted by TANN-LES
- EBU: worst result with no extinction & re-ignition behavior

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Computational Time and Memory Savings

	Species Equation	Time/(step×cell)	Speed-Up
EBU-LES	LES level	0.36×10^{-2}	19.7
TANN-LES	LES level	0.39×10^{-2}	18.3
LANN-LEMLES	LEM level (12 cells/LES)	1.29×10^{-2}	5.5
DI-LEMLES	LEM level (12 cells/LES)	7.10×10^{-2}	1.0

- LANN table size: 2GB; Memory requirement in LES: 0.13 MB
- TANN table size: 380 MB; Memory requirement in LES: 0.14 MB
- TANN-LES cost is same as EBU-LES
- Speedup more significant for stiffer kinetics: 12-species, 16-species

	Species Equation	Time/(step×cell)	Speed-Up
TANN-LES	LES level	7.78×10^{-5}	134.9
LANN-LEMLES	LEM level (LES/12)	2.14×10^{-4}	49.2
DSTE-LEMLES	LEM level (LES/12)	8.79×10^{-3}	7.8
DI-LEMLES	LEM level (LES/12)	1.05×10^{-2}	1.0

The Baseline LES@GT Solver with LEMLES

- **Single comprehensive approach validated for**
  - **Non-premixed scalar mixing and combustion, and soot formation**
    - *JPP (1993), Comb. Symp. (1996, 2006), CST (1998), Phy. Fl (2001), Turbo Expo (2007), Comb. Flame (2008, 2010)*
  - **Premixed combustion: Flamelet, Thin-reaction and Broken-reaction zone regimes (DOE-HAT, LM6000, DLE), soot formation**
    - *CST (1999, 2000, 2001), Flow Turb. Comb (2001), J. Sup. Comp (2001), Comb. Symp. (2002, 2004), J. Turb. (2003), JPP (2005), Prog. CFD (2005), AIAA-06-0152, Comb. Symp, (2006, 2008), Comb. Flame (2007, 2008, 2010)*
  - **Spray Combustion (GE-TARS, DACRS, CFM56, NASA-LDI, JSF)**
    - *ASME-GT-225 (1998), ASME J (2003), Comb. Symp. (2002), J. Turb (2002), AIAA-04-3381, AIAAJ (2006), Comb. Symp. (2006), ASME (2006), CF (2008)*
  - **Supersonic Mixing/Combustion, Detonations, Plasma, Rockets**
    - *Comb. Symp. (2004), AIAA-03-7035, AIAA-04-3826, AIAA-04-4132, AIAA-05-3967, ICDERS (2005), AIAA-06-2891, AIAA-06-2894, AIAA (2007, 2008), Comp. & Fluids (2008*), Comb Symp. (2008), Phys. Plama (2008), AIAA (2011)*