CFD for Combustion Modeling

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DAY 2

Day 2, Lecture 1: Suresh Menon, Georgia Tech

Day 2: Summary of Presentations

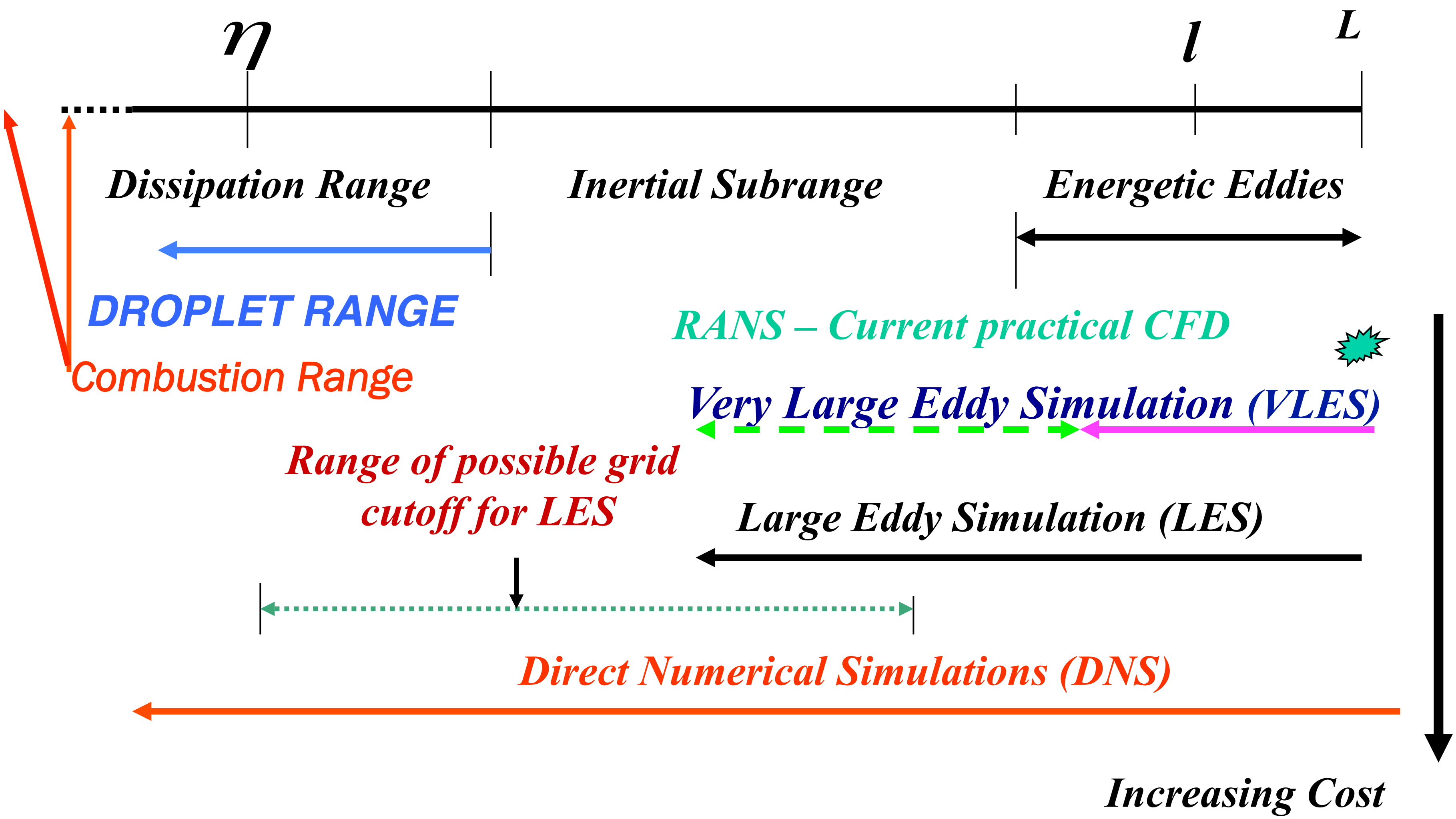
- Introduction, Review of Length/Time Scales
- Filtering and Closure Issues
- Closures for Momentum and Energy Transport
- RANS/URANS Closures for Turbulent Combustion
- LES Closures for Turbulent Combustion
- Special Topics: Applications*
  - Gas Turbines both premixed and liquid fueled
  - Bluff Bodies
  - Ramjets/Scramjets/Rockets

* *Some results provided by: Poinsot, Janicka, Fureby, Flohr, Oefelein, Hasse*

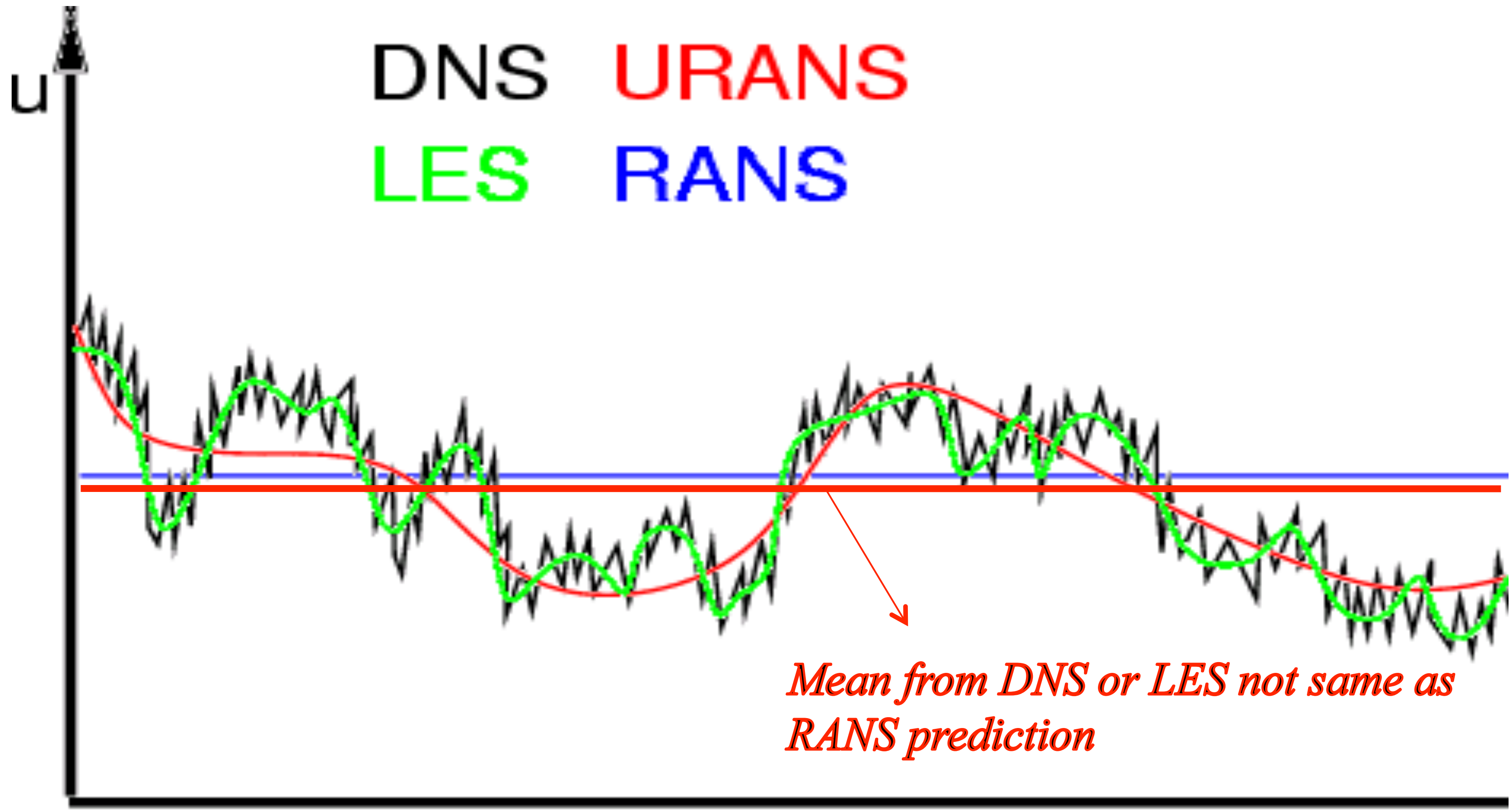
Some Goals for these Lectures

- Identify practical needs for combustion devices
- Identify where CFD can contribute (if at all!)
- Identify the critical issues that have to be considered
  - time and length scales, modeling approach
- Identify approaches (RANS, URANS, LES), their use and predictive capability to specific test cases
- Define numerical and algorithmic issues
  - Grid generation, boundary conditions
  - Accuracy, physics and cost
- Backup slides provided for additional information
  - Additional slides provided for completeness

Modeling of Turbulent Reacting Flows



Turbulent Signal and Modeling Strategy



Turbulence Modeling Approaches

- Direct numerical simulation (DNS)
  - Transient, 3-D, resolve all fluctuations, no modeling
- Moment formulation (RANS/URANS-Models)
  - Mean, variances, co-variance predicted
  - Model the complete spectrum
- Large-Eddy-Simulation (LES or VLES)
  - Transient, 3-D, resolve large-scales, model 'unresolved' scale effect on the 'resolved' scale
  - Only 'energy-containing' scales resolved in VLES
  - Energy-containing and inertial scales resolved in LES
- Hybrid Schemes: Detached Eddy Simulation, RANS-LES

New Combustion System Challenges

- Efficient performance at *idle (lean)* and full-power
  - Low emission – CO, NO, UHC, Soot, "Noise"
  - Stable combustion (i.e., without instability/dynamics)
  - "Fuel-Flexible" robust designs without instability
- Very high pressure (> 40 atm) "compact" combustors
  - High T, Sub-Trans-Super-critical combustion
- Some Designs Challenges
  - Lean blow out (LBO)
  - Ignition, Extinction/Re-ignition
  - Combustion instability, flame extinction
  - Engine un-start (e.g., dual-mode scramjets)

Combustion Modeling Relevance

- All easy solutions have been reached in practice!!
- New designs will operate at the "edge" of combustion limits
- Problems (e.g. LBO) avoided at present "by not going there"
- Future designs will "go there" and operate at the "edge"
- Testing and measurements in actual rigs at high pressure economically prohibitive and technically very challenging
- Need to put modeling and simulations into the design cycle
  - reduce cost, get better insight into "new" physics
  - Reliable predictions but how quickly?
  - Even if done quickly can it be analyzed in time?

Some Practical Systems of Interest

- Gas Turbine Engines: Premixed and Spray systems
- Internal Combustion Engines: Spray systems
- Micro-combustors: Premixed and Spray systems
- SCRAMJETS: Gaseous (H2) and Liquid (HC) systems
- Liquid-Fueled Rocket Motors: LOX-GH2, LOX-LCH4
- Solid-Fueled Rocket Motors: Solid phase combustion
- Fires: Non-premixed multi-phase systems
- Pulse Detonation Engines
- *Are these diverse systems all that different?*

Some Practical Realities

- Nearly all operational systems have complex geometries
- Nearly all systems involve very high Re No flows
  - Resolution of near walls (?) and shear layers
  - Highly 3D swirling flow
- All real systems: finite-rate kinetics and heat release
  - Resolution of molecular and turbulent mixing scales
  - Resolution of finite-rate kinetics effects locally
  - Modeling of finite-rate kinetics locally
- All systems involve some time-dependent interactions
  - Excursions about the "mean" is critical

What is the underlying Theme?

FUEL-AIR MIXING Is the KEY

It is an Unsteady Process

It occurs over a range of time & length scales

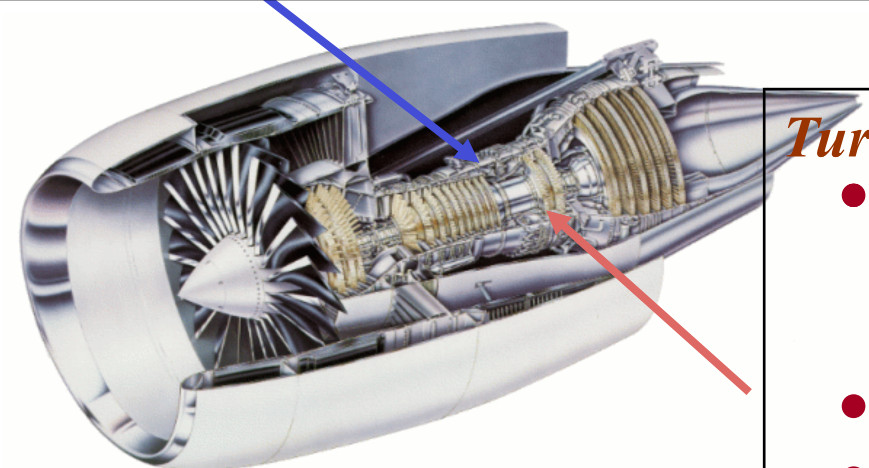
Mixing by Turbulent Eddies

Mixing by Molecular Diffusion

Fuel-Air Mixing

Fuel-air mixing

- **Varies with power, pressure, equivalence ratio, etc.**
- **Use mixing "control" to:**
  - ***Reduce size***
  - ***Improve off-design performance – high altitude relight***
  - ***Improve stability - lean blowout***



Turbine inlet temperature profile

- ***Mix exhaust gases, remove hot/ cold spots => longer turbine lifetime***
- ***Film cooling optimization***
- ***Minimize cooling air needs***

Reality of Fuel-Air Mixing

- Perfect "mixing" requires a separate premixer
- All combustion devices incorporate mixing devices
  - Swirl is used to enhance mixing in most devices
- "Premixed" systems
  - Mixture need <u>not</u> be perfectly mixed
  - Equivalence ratio variation: partially premixing
  - Very lean mixture can occur *locally in lean systems*
- "Non-Premixed" liquid fueled systems
  - Mixing occurs after liquid vaporization
  - Spatial and temporal variation in mixing
  - premixed to non-premixed state of combustion
    - Partial premixed combustion

CFD for Design

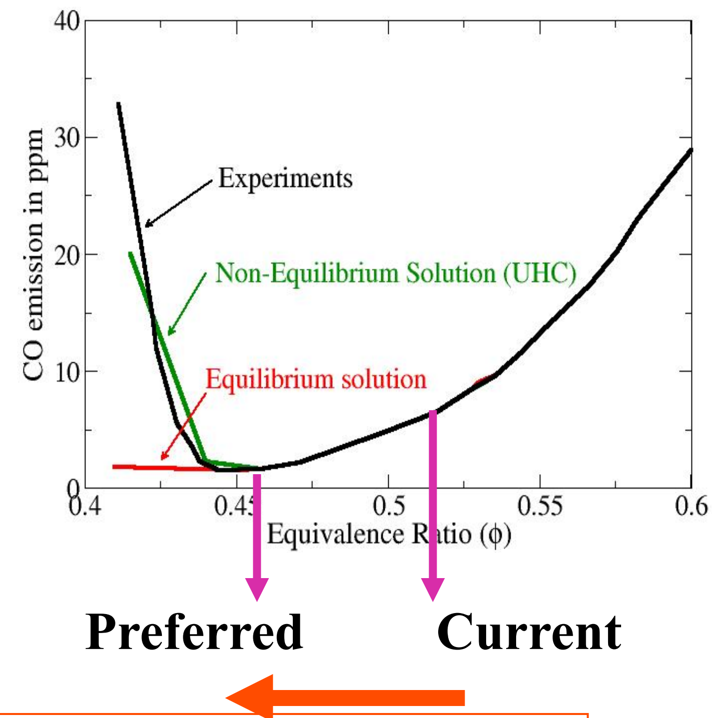
- Need to carry out many parametric studies
  - Complex geometry and conditions to be modeled
  - qualitative agreement & trends of primary concern
    - quick turn-around of results: 1-2 days per run
- Modeling based on RANS and/or empirical models
  - time-averaged results
  - inaccuracy in prediction of dynamical properties
- Past focus has been on averaged properties
  - mean temperature, pattern factor, heat flux, etc.
- New focus is likely to be on emission, LBO, instability
  - Unsteady effects

CFD for Design

- RANS still the cornerstone of research studies
  – Typically employ commercial codes
  – Steady state solutions
  – higher resolution (e.g., 4-20 million grid points)
  – more advanced models (e.g., flamelet, PDF)
  – Turnaround on parallel systems – 2-3 weeks
- *MANY new designs employ unsteady processes to enhance and/or control mixing*
  – URANS or LES option is needed
  – Closure and applicability of models need to be re-assessed based of simulation goal

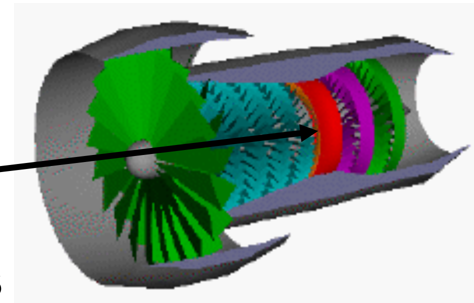
Challenge for Power Generation Gas Turbine Engines

- Lean-Prevaporized-Premixed system
  - Low CO and NO emission
  - Avoid Lean Blowout (LBO)
- Combustion signature near LBO
  - Rapid increase in CO/UHC as equivalence ratio decreases
  - Rapid increase in pressure oscillation (in some combustors)
- Challenges for CFD
  - Predict emission over a range of equivalence ratio and fuel types
  - Predict sensitivity to LBO
  - Predict sensitivity to onset of combustion instability



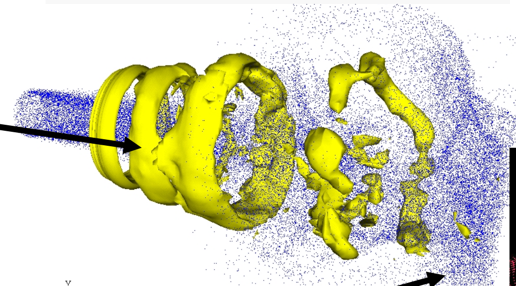
Enormous reduction in emission and increase in Profits besides being Environmentally green!

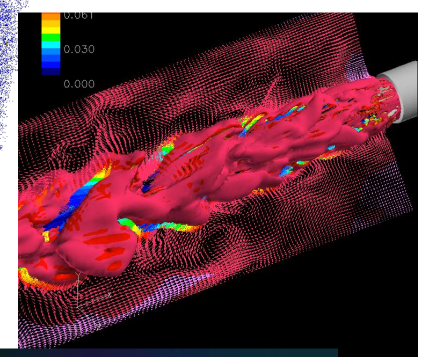
The Computational Spatial-Scale Dilemma!!

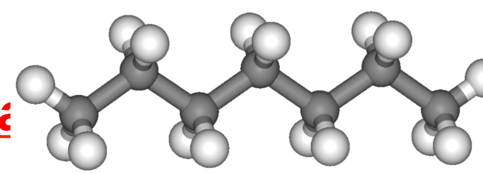


CFM56-5B

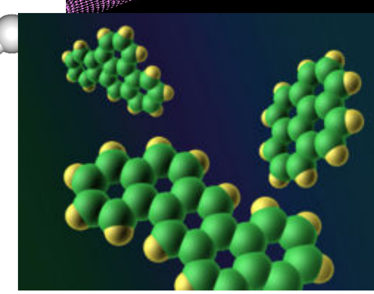
- Scale of the combustor
  - *10-100 cm*
- Large "eddies" in real combustors
  - *1-10 cm*
- Small-scale mixing occurs at
  - *0.1-10 mm*
- Droplets with distinct "identity"
  - *1-100 microns*
- Molecular/chemical processes
  - *0.1 – 1 nm*
- *<u>O(8) dynamic range of scales tha</u>* *<u>must be resolved accurately</u>*







Heptane

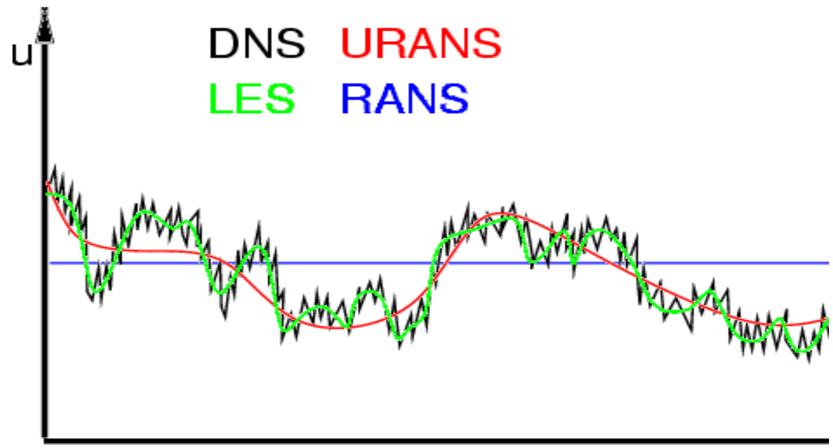


PAHs (soot precursor)

Other Length/Time Scales

- Fluid Dynamics in shear layers
  - Vortex Shedding: f H/U = 0.017; 0.001 – 0.0001 sec
  - Jet Preferred Mode: f D/U = 0.1-1.0; 0.01-0.001 sec
- Acoustic time scales
  - 0.01-0.001 sec (100-1000 Hz in longitudinal modes)
  - 1-10 KHz in azimuthal modes
- Flame Scales (Flamelet–Thin-reaction-Broken Zones)
  - Flame response time scale: 0.01 – 0.001 sec
- Acoustics and Flames can interact without turbulence
  - Acoustically forced laminar flame
- Acoustics & Vortices can interact without flame
  - Acoustically forced turbulent jets

Resolution Requirements and Implications



Some Requirements for Realistic (?) Problems

Human Vision Simulation	**100**	**Teraflops**
Aerodynamic (URANS) Analysis	**1**	**Petaflop**
Laser Optics	**10**	**Petaflops**
Molecular Biology Dynamics	**20**	**Petaflops**
Aerodynamic (URANS) Design	**1**	**Exaflop**
Computational Cosmology	**10**	**Exaflops**
Turbulence in Physics	**100**	**Exaflops**
Computational Chemistry	**1**	**Zettaflop**
Turbulent Combustion		**???**

1+ Petaflop Hardware 2010

Real Simulation codes achieve only 3-15% of peak of OEM systems

Source: Business Week, NASA, Energy Dept, NSF: May 2004

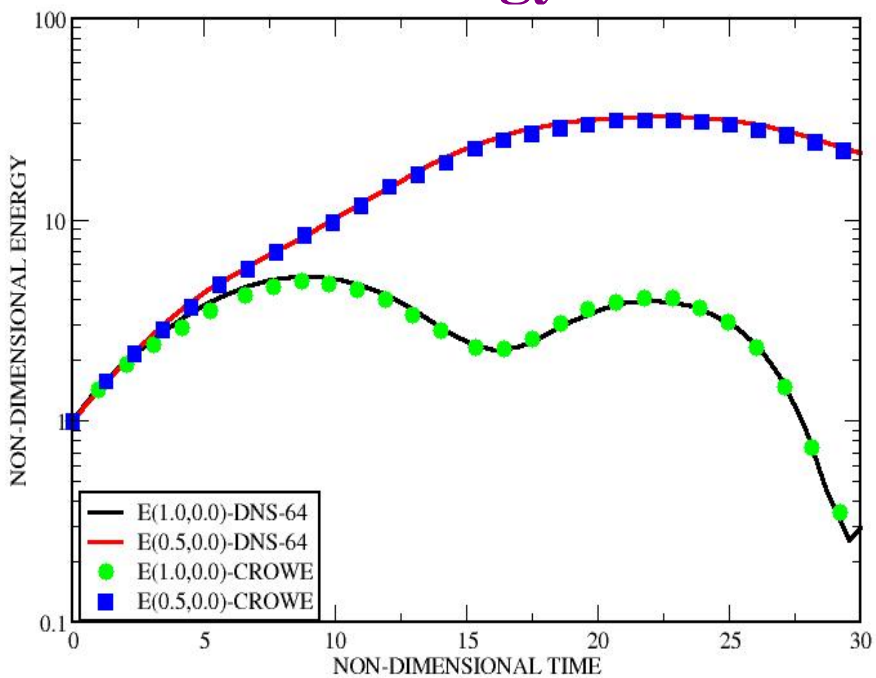
Some Key Issues to Consider

- Numerical Algorithm
  - Compressible or low-Mach number ?
  - Numerical accuracy O(2-4) or higher?
  - Numerical dissipation – understand and quantify
  - Unstructured or Structured Grid ?
  - Grid resolution and quality
- Simulation Algorithm
  - Closure for momentum and energy transport
  - Closure for scalar transport and kinetics
  - Boundary conditions!!
- Parallel Efficiency, Scale-up

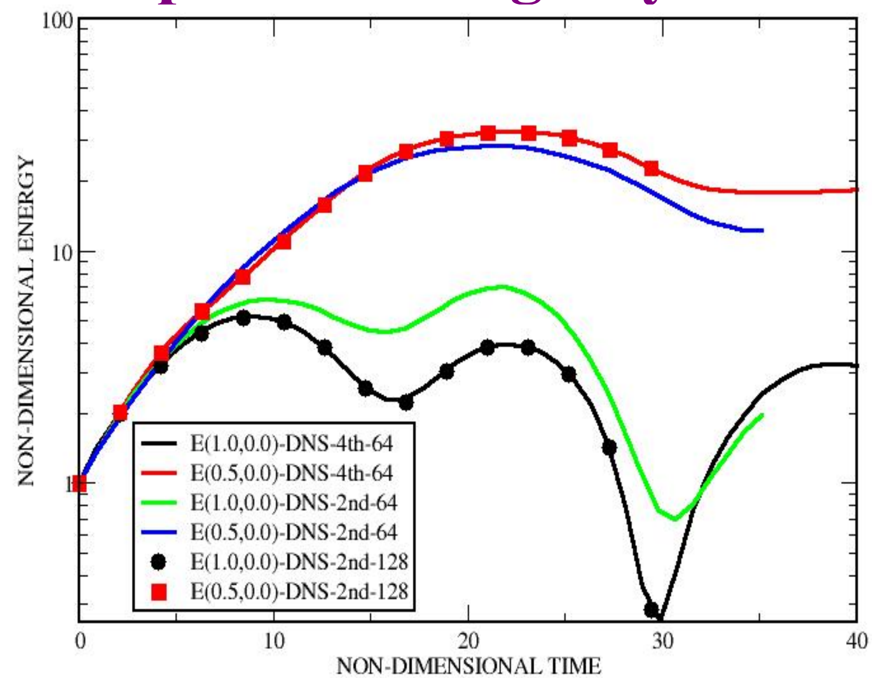
Comments on these Lectures

- Simulations by only few researchers are highlighted
  - There are many others not included
- Simulations at Georgia Tech are highlighted more
  - Due to past experience and availability of data
- Other results highlight key issues when carrying out CFD of turbulent combustion
- Many slides are included for completeness only and may not be fully covered
- Wherever possible past "experience" of researchers will be indicated during the presentations
  - The "art" of CFD is important to appreciate

Example of Grid and Numerical Accuracy
Modal Energy Growth in Temporal Mixing Layer



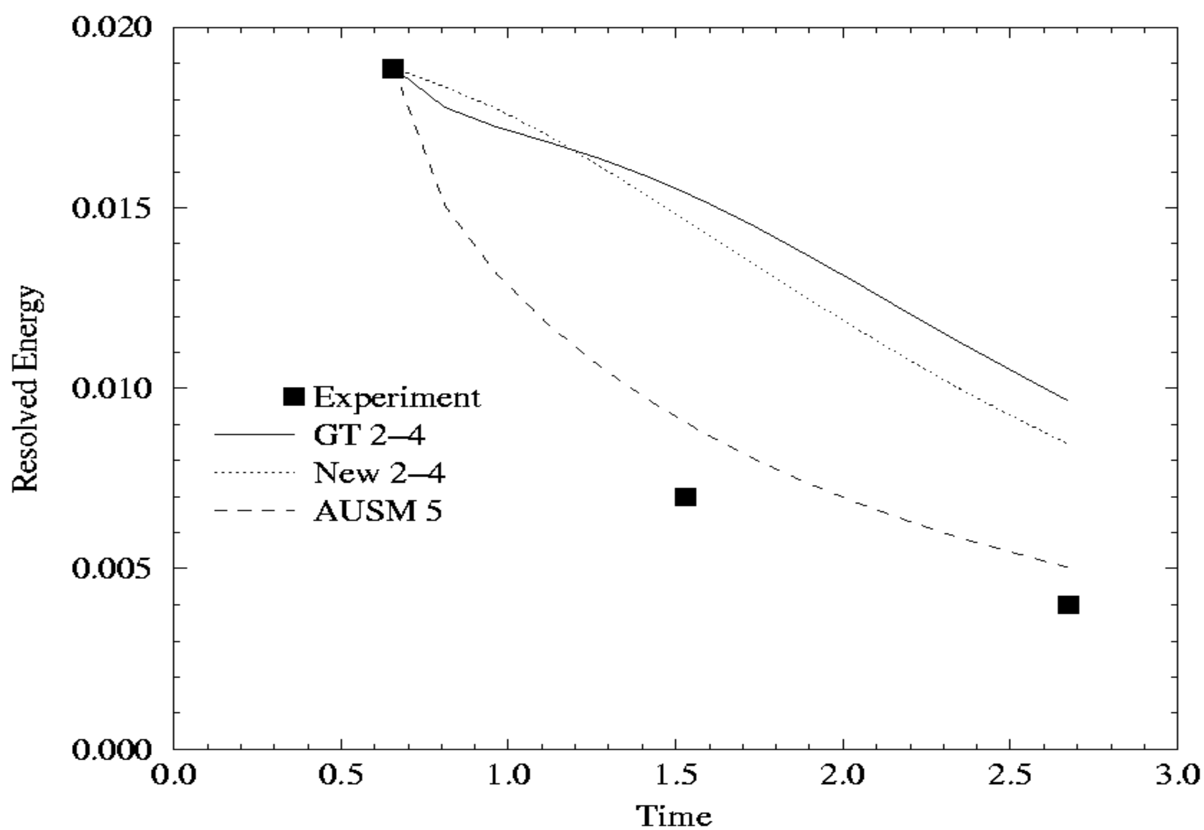
O(4) FV-DNS comparison with Spectral DNS using same 643 grid resolution**



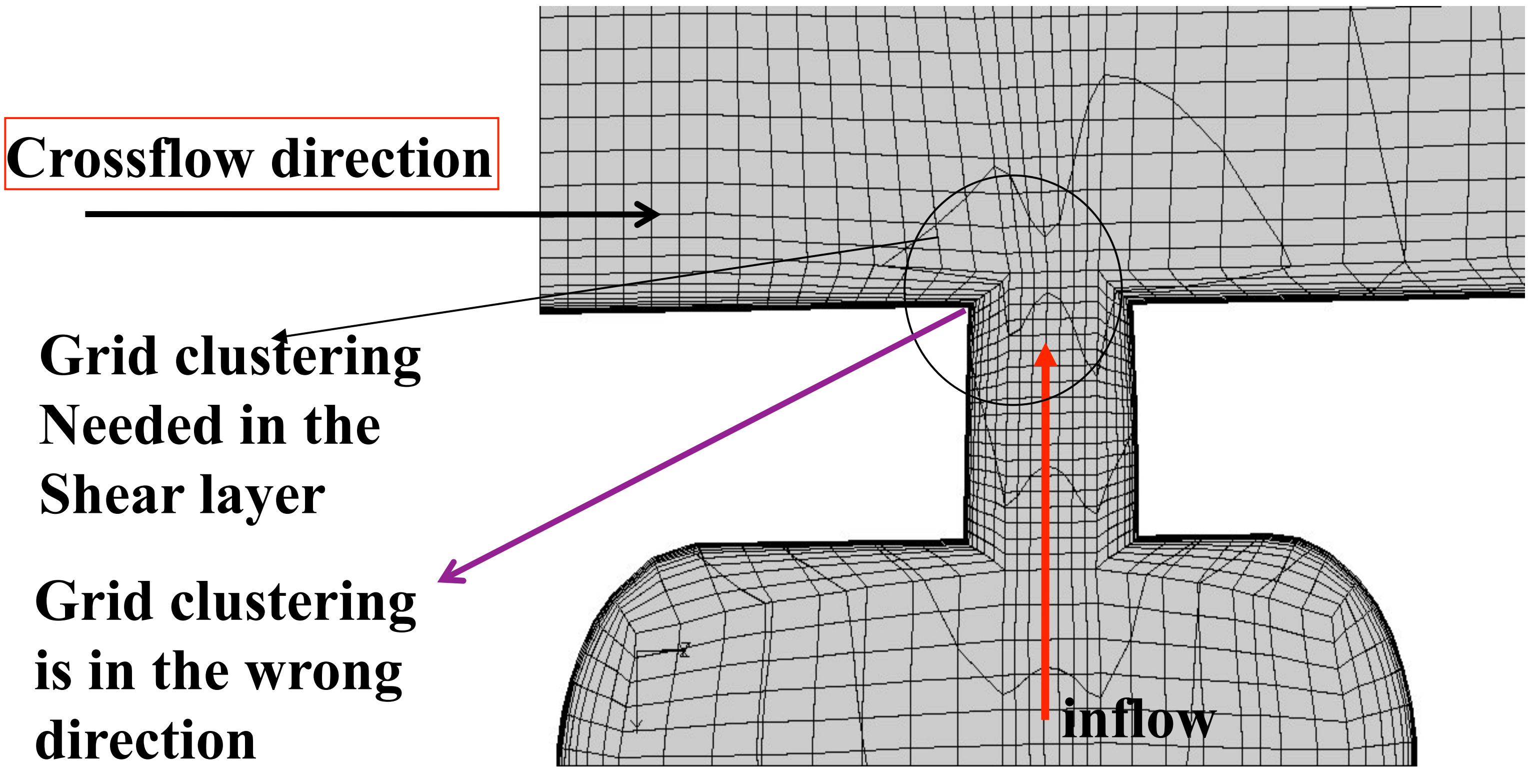
Comparison of numerical scheme's accuracy for 643 and 128**3 grid**

Impact of Numerical Dissipation in the LES Solver

Isotropic Turbulence Decay without SGS model

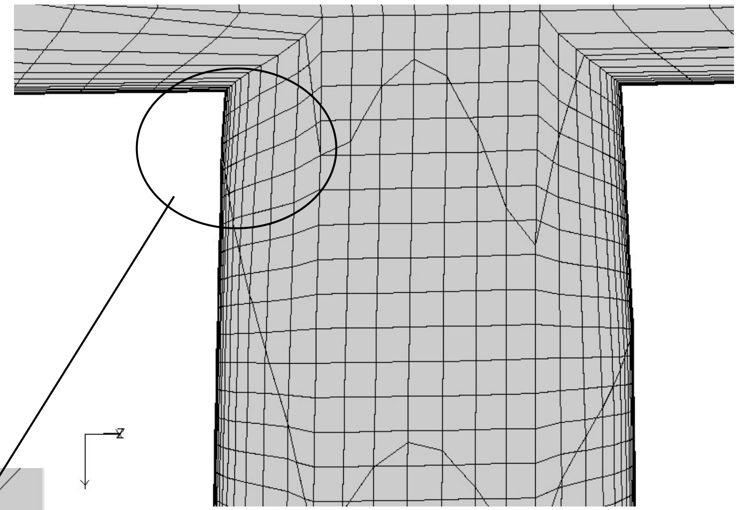


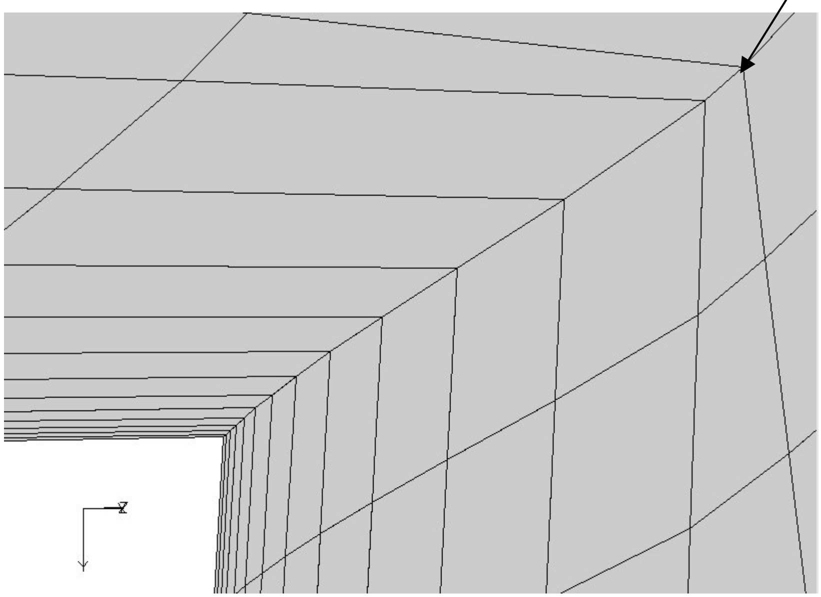
Grid Generation using Commercial Software

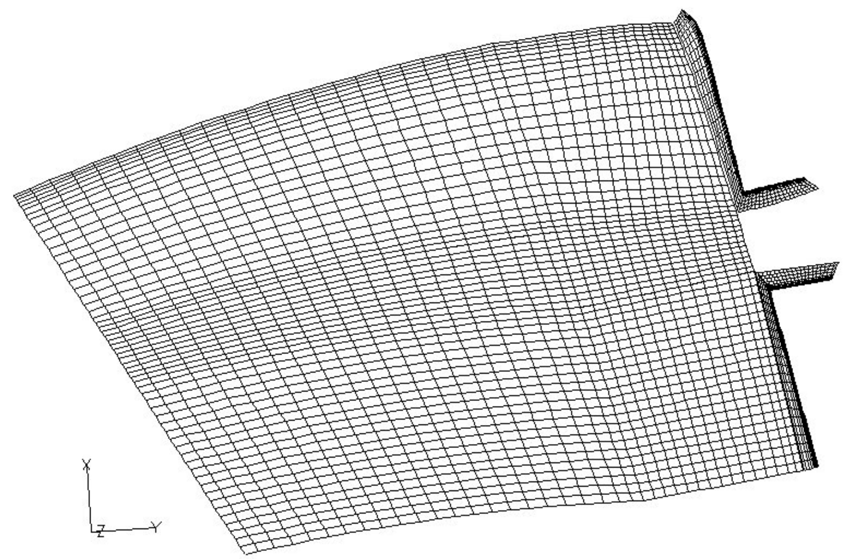


- **Multi-block unstructured Cartesian grids are needed to satisfy both wall and shear layer resolution requirements**
- **Unstructured solvers can address this but have their own issues**

Clustering at walls – too high aspect
Ratio and clustered in region where
There is no real flow







Physics versus Numerics

- Need to distinguish between numerical accuracy and physics (model) accuracy, if possible
- Numerical scheme and accuracy may be limited by availability and the complexity of the problem
  - Grid resolution for LES needs to be 2-3 order of magnitude coarser than an equivalent DNS
  - Grid resolution for many RANS (and/or URANS) have been similar to LES grid resolution (Why?)
- However, physics in the model can be improved (?)
  - Simple models will require very fine grids
  - Higher order models may need only "coarser" grid
  - Potential area for further advancements

Numerical Issues

- Accuracy of the Spatial Scheme
  - O(2) or higher is the question !! (O(4) is optimal?)
    - Accuracy at lower resolution with high order scheme
  - Complex geometry may restrict to O(2) but need to ensure space and time accuracy
  - Scheme's dissipation must be well understood
- Accuracy of the Algorithm
  - More physics in the model versus cost
- Scheme and algorithm can have different errors
  - Difficult to quantify in real systems
- Validate same scheme & algorithm in canonical flows

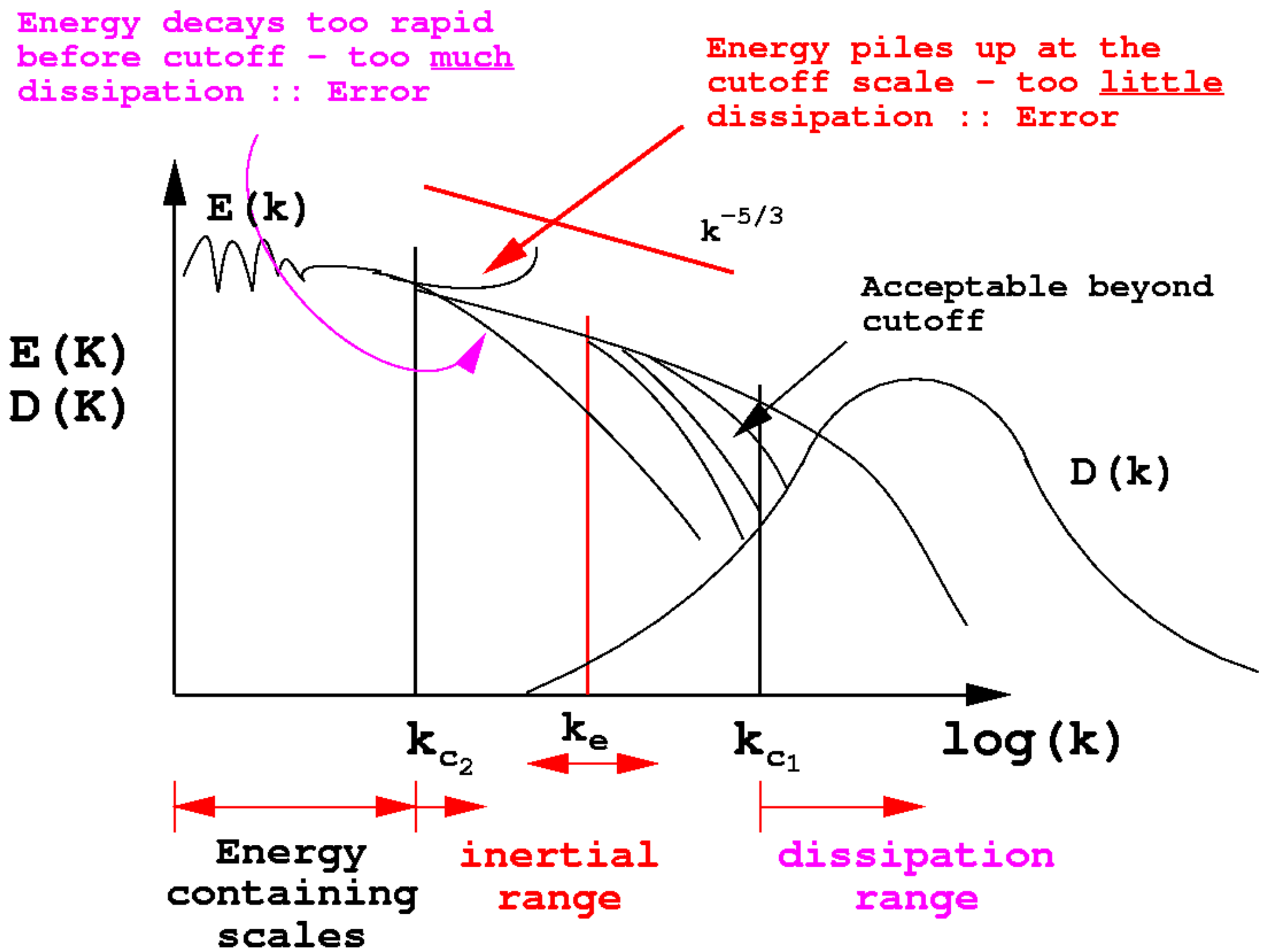
Numerical Issues

- Structured or unstructured scheme ?
- Grid quality is very important for structured solvers
  - Stretching should be < 3-5% in high shear regions
  - Grid generated to resolve complex geometries sometime do not capture turbulent physics
  - Orthogonality of the grid preferred
- Explicit dissipation should be avoided if possible
  - its behavior in canonical flows should be known
- Boundary conditions must be carefully implemented
  - Accuracy should be same as scheme
  - Inflow-outflow is very important
- Parallel implementation is very important

LES of Turbulent Flows: Current Trends

- Solve the "filtered" Navier-Stokes Equations
- Model unresolved terms in terms of resolved variables
  - similar to RANS closure approach
- Simple "eddy viscosity" type subgrid models very popular
  - requires a length and a velocity scale
- Grid scale is the length scale
- Two approaches to determine the velocity scale
  - resolved strain-rate and grid scale (Smagorinsky)
  - subgrid kinetic energy (Schumann)

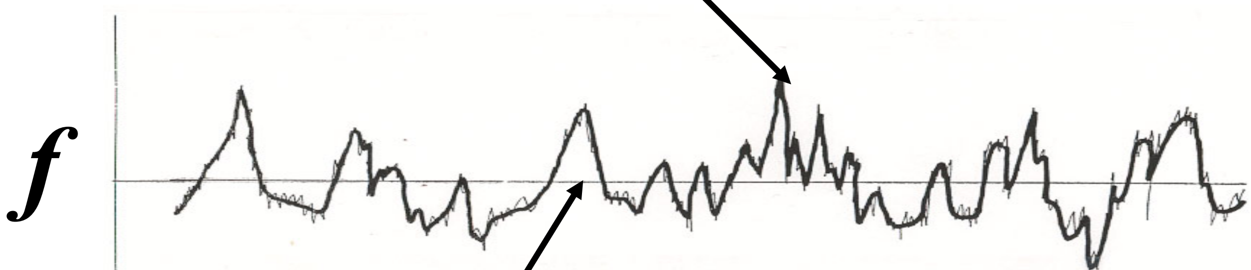
Impact of Filtering on the Turbulent Spectrum



Filtering in LES: Separate the Scales

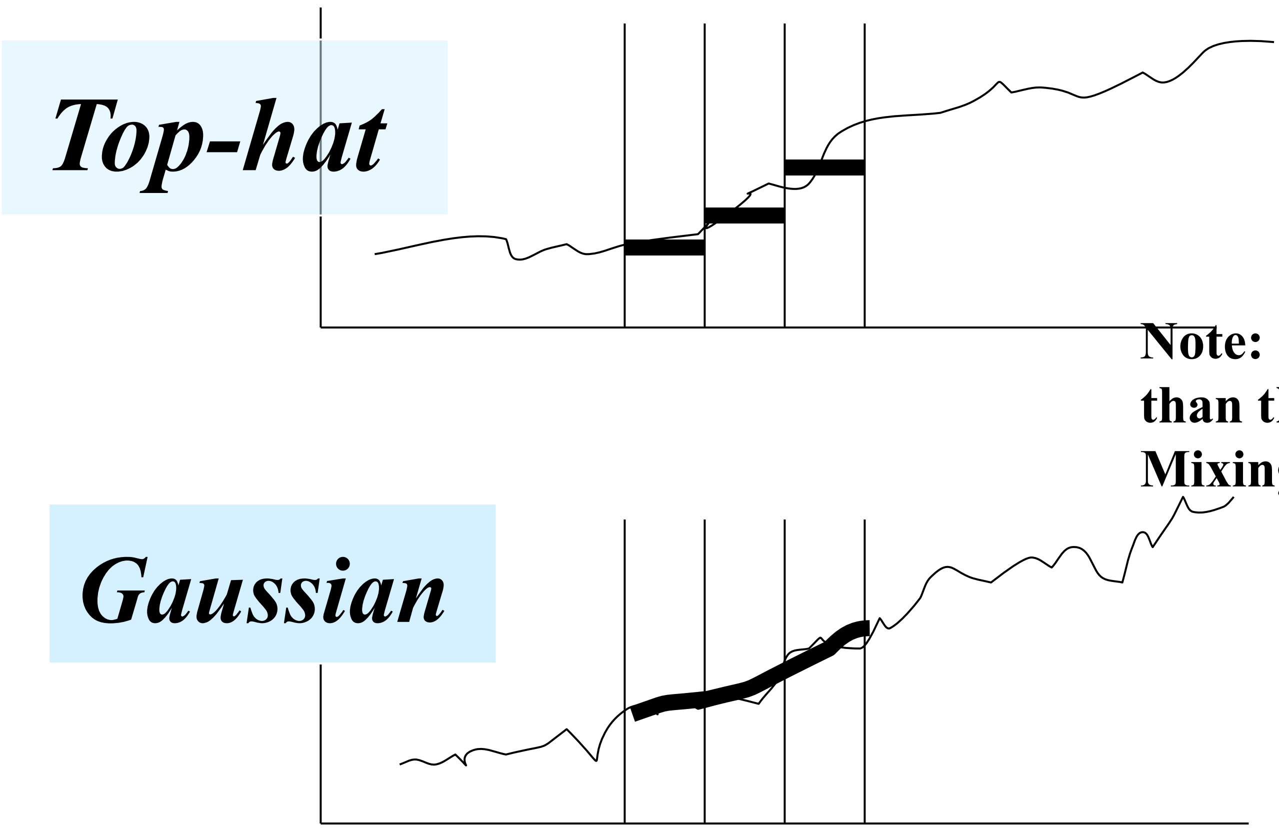
- **Define a filter** $\tilde{f}(x,t) \equiv \int f(x',t)G(x,x')dx'$

$$f''(x,t) = f(x,t) - \tilde{f}(x,t)$$



$$f(x,t) \Rightarrow \bar{f}(x) + f'(x,t)$$

Examples of filter functions



Note: filter width is larger than the scales of scalar Mixing and combustion

LES Filtering

*** Spatially low-pass filtering (e.g. top-hat filter)**

$$\overline{\varphi}(\underline{x},t) = \iiint_V F(\underline{x}-\underline{s})\varphi(\underline{s},t)\,d\underline{s} \longrightarrow \varphi = \overline{\varphi} + \varphi'$$

- ***LES filtering is not the same as RANS filtering***
  - ***impacts accuracy depending on the scheme***

$$\frac{\partial\overline{\varphi}}{\partial x_i} \neq \overline{\frac{\partial\varphi}{\partial x_i}} \quad \textbf{or} \quad \overline{\varphi'} \neq 0$$

Favre filtering (density weighted)

$$\tilde{\varphi} = \overline{\rho\varphi} / \overline{\varphi} \qquad \varphi = \tilde{\varphi} + \varphi''$$

Low-Mach Number or Compressible Formulation ?

- Low Mach Number approximation
  - Eliminate acoustic waves (can be added separately)
  - Evolution at convective time (>> acoustic time)
    - May not be feasible if chemical time is very small
  - Density not a function of pressure (acoustic)
    - However density changes due to heat release
    - Large change in time-step can create acoustic wave
      - Implicit or explicit filtering to eliminate these waves
    - Pressure solver convergence issues
  - Most laboratory flames and combustors away from unstable limit can be simulated using this approach
  - Most commercial solvers are low-M methods

Low-Mach Number or Compressible Formulation ?

- **Compressible formulation**
  - Acoustic field included naturally
    - Fully coupled acoustic-vortex-entropy interactions
  - Thermo-acoustic instability captured naturally
    - Combustion instability, LBO
  - Necessary for supersonic flows
  - Applicable in low-M flow but can be expensive
    - Need to use pre-conditioner, dual-time stepping
  - One formulation for all Mach regime possible
  - Inflow-outflow needs careful treatment to deal with waves entering and leaving the domain
  - Easy to parallelize and scale-up

Low Mach Number Equation

Low Mach number assumption :

$$p = p_0(t) + \gamma M^2 p_1(\vec{x},t) + O\left(M^3\right)$$

Conservation of Mass

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} = 0$$

Conservation of Momentum

$$\left(\frac{\partial \rho u_j}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_i}\right) = -\frac{\partial p_1}{\partial x_j} + \frac{\partial}{\partial x_i}\left(\mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3}\frac{\partial u_k}{\partial x_k}\delta_{ij}\right)\right)$$

Conservation of Species

$$\left(\frac{\partial \rho Y_k}{\partial t} + \frac{\partial \rho u_i Y_k}{\partial x_i}\right) = -\sum_{k=1}^{N} \rho Y_k V_{k,i} + \dot{\varpi}_k \qquad k = 1,\ldots,N$$

Conservation of Energy

$$\left(\frac{\partial \rho c_p T}{\partial t} + \frac{\partial \rho c_p u_i T}{\partial x_i}\right) = \frac{\partial}{\partial x_i}\left(\lambda \frac{\partial T}{\partial x_i}\right) + \sum_{k=1}^{N} h_0^k \dot{\varpi}_k - \frac{\partial \rho T}{\partial x_j}\sum_{k=1}^{N} c_{p,k} Y_k V_{k,i} + \frac{dp_0}{dt}$$

Ideal gas law

$$p_0 = \rho R T$$

Thermodynamic Pressure in Zero-M Limit

- Non-dimensional form of EOS: $p_0 = \rho_0 T_0$
- Global thermodynamic pressure $p_0(t)$ only due to compressibility and heat transfer from the boundaries

$$\frac{dp_0}{dt} = -\lambda p_0 \nabla.\vec{u} + \frac{\gamma}{\Pr \mathrm{Re}} \nabla.(\lambda \nabla T)$$

- Generalization of the divergence-free condition of incompressible flow for heat release
- The kinematic or dynamic pressure p_1 appears in the momentum equation
- LES form quite similar to compressible equations
- Density (Favre) weighted filtering used for all Mach flow

Other Requirements to Consider

- Gallilean invariance of the LES equations (Speziale, 85)
  - Modeled equation must satisfy this property
- Realizability of the modeled subgrid stresses (Schumann, 77; Vreman, 94)
  - Certain properties must be satisfied locally and in time
- Commutativity errors
  - Filtering and gradient operators do not commute when the grid is stretched
- Truncation and/or roundoff errors
  - Depends on the scheme

Compressible LES Equations

- **Favre Filtered equations (Equations look same as RANS BUT…)**
  - **Conservation of mass**

$$\frac{\partial \overline{\rho}}{\partial t} + \frac{\partial \overline{\rho}\widetilde{u}_i}{\partial x_i} = 0$$

  - **Conservation of momentum**

$$\frac{\partial \overline{\rho}\widetilde{u}_i}{\partial t} + \frac{\partial}{\partial x_j}\left[\overline{\rho}\widetilde{u}_i\widetilde{u}_j + \overline{P}\delta_{ij} + \tau_{ij}^{sgs} - \overline{\tau_{ij}}\right] = 0$$

  - **Conservation of energy**

$$\frac{\partial \overline{\rho}\widetilde{E}}{\partial t} + \frac{\partial}{\partial x_j}\left[\overline{\rho}\widetilde{u}_j\widetilde{E} + \widetilde{u}_j\overline{P} + \overline{q_j} - \widetilde{u}_i\overline{\tau_{ji}} + H_j^{sgs} + \sigma_j^{sgs}\right] = 0$$

  - **Conservation of Species**

$$\frac{\partial \overline{\rho}\widetilde{Y}_k}{\partial t} + \frac{\partial}{\partial x_i}\left[\overline{\rho}\left(\widetilde{Y}_k\widetilde{u}_i + \widetilde{Y_k V_{i,k}}\right) + Y_{i,k}^{sgs} + \theta_{i,k}^{sgs}\right] = \overline{\dot{\omega}_k}$$

LES Governing Equations

- The filtered quantities are now *averaged* over a cell volume, and are in the resolved scales
- The subgrid scale (SGS) terms represent the unresolved properties in the resolved scales – require closure

Reynolds Stress	$\tau_{ij}^{sgs} = \overline{\rho}\left(\widetilde{u_i u_j} - \widetilde{u}_i \widetilde{u}_j\right)$
Enthalpy Flux	$H_i^{sgs} = \overline{\rho}\left(\widetilde{E u_i} - \widetilde{E}\widetilde{u}_i\right) + \left(\overline{p u_i} - \overline{p}\widetilde{u}_i\right)$
Viscous Work	$\sigma_i^{sgs} = \widetilde{u_j \tau_{ij}} - \widetilde{u}_j \overline{\tau}_{ij}.$
Convective-Species Flux	$Y_{i,k}^{sgs} = \bar{\rho}[\widetilde{u_i Y_k} - \tilde{u}_i \tilde{Y}_k]$
Heat Flux	$q_{i,k}^{sgs} = [\overline{h_k D_k \partial Y_k / \partial x_i} - \tilde{h}_k \tilde{D}_k \partial \tilde{Y}_k / \partial x_i]$
Species-Diffusive Flux	$\theta_{i,k}^{sgs} = \bar{\rho}[\widetilde{V_{i,k} Y_k} - \widetilde{V}_{i,k} \widetilde{Y}_k]$

Eddy viscosity models for LES

- SGS Stress: $$\tau_{ij}^{sgs} = -2\overline{\rho}\nu_t(\widetilde{S_{ij}} - \tfrac{1}{3}\widetilde{S_{kk}}) + \tfrac{1}{3}\tau_{kk}\delta_{ij}$$
- Characteristic length provided by the local grid spacing Δ
- Smagorinsky algebraic model for the subgrid stress

$$\nu_t = C\Delta^2|\widetilde{S}| \qquad |\widetilde{S}| = \sqrt{2S_{ij}S_{ij}}$$

- One-equation model for subgrid kinetic energy (Schumann)

$$\nu_t = C_\nu\sqrt{k^{sgs}}\,\overline{\Delta}$$

$$\frac{\partial\overline{\rho}k^{sgs}}{\partial t} + \frac{\partial}{\partial x_i}\left(\overline{\rho}\tilde{u}_i k^{sgs}\right) = P^{sgs} - \epsilon^{sgs} + \frac{\partial}{\partial x_i}\left(\overline{\rho}\frac{\nu_t}{Pr_t}\frac{\partial k^{sgs}}{\partial x_i}\right)$$

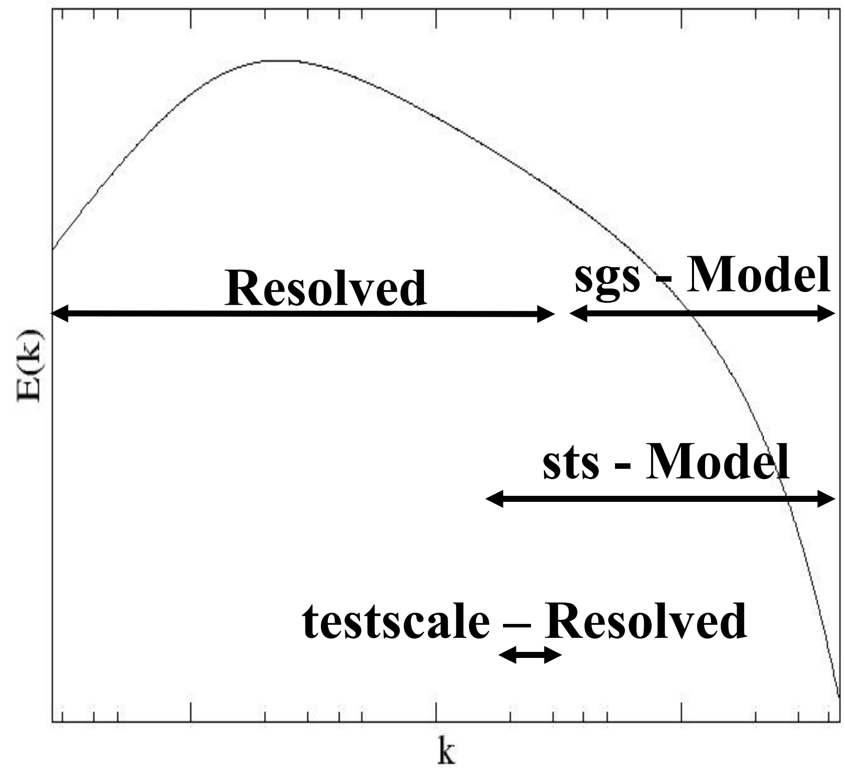
Dynamic Germano's Model

- The subgrid stress requires modeling (here for incompressible flows – density is dropped):

- Applying an *explicit* filter at a test scale (greater than the subgrid scale) to the velocity field, the *sub testscale* (sts) stress is:

$$\widehat{\tau_{ij}^{sgs}} = \underbrace{\left(\widehat{\widetilde{u_i u_j}} - \widehat{\tilde{u}_i}\widehat{\tilde{u}_j}\right)}_{\tau_{ij}^{sts}} - \underbrace{\left(\widehat{\tilde{u}_i \tilde{u}_j} - \widehat{\tilde{u}_i}\widehat{\tilde{u}_j}\right)}_{\mathcal{L}_{ij}}$$

- The model used for the subgrid stress should be applicable to the sub-testscale stress!



Dynamic Smagorinsky Model

- Assuming the model coefficient is constant over the width of the explicit filter (Germano *et al,* PoF 1991):

$$C = \frac{\langle (L_{ij} - \frac{1}{3} L_{kk}\delta_{ij}) M_{ij} \rangle_h}{\langle M_{ij} M_{ij} \rangle_h} \qquad L_{ij} = (\widehat{\bar{\rho}\tilde{u}_i\tilde{u}_j}) - \frac{1}{\widehat{\bar{\rho}}}\widehat{\bar{\rho}\tilde{u}_i}\widehat{\bar{\rho}\tilde{u}_j}$$

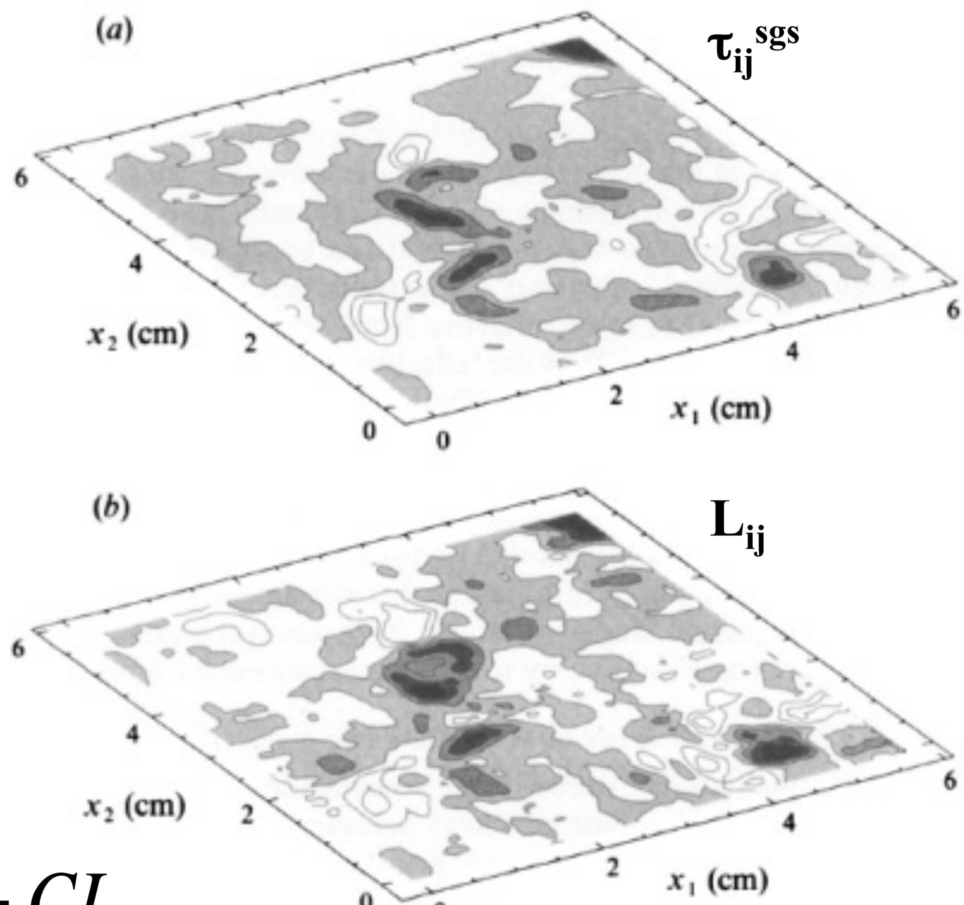
$$M_{ij} = 2\Delta^2 \widehat{\overbrace{(\bar{\rho}|\tilde{S}|(\tilde{S}_{ij} - \frac{1}{3}\tilde{S}_{kk}\delta_{ij}))}} - 2\widehat{\Delta}^2 \widehat{\bar{\rho}}|\widehat{\tilde{S}}|(\widehat{\tilde{S}}_{ij} - \frac{1}{3}\widehat{\tilde{S}}_{kk}\delta_{ij})$$

- Ill-posed subject to numerical instability
- Various solutions devised: averaging, Lagrangian, etc.
- Otherwise very efficient and no ad hoc model adjustments

Sagaut: LES for Incompressible Flows

Localized Dynamic Kinetic Energy Model – LDKM (Kim and Menon, 1995, 1999)

- The ill-posed nature of the Germano's dynamic formulation comes from the difference between filtered subgrid and subtestscale stresses
- Liu *et al* (JFM, 1994) found experimentally in high Re jet flows, $\mathcal{L}_{ij}$ and τ_{ij}^{sgs} are similar and proposed a model
- Model was not dissipative enough: $\tau_{ij}^{sgs} = CL_{ij}$



From Liu *et al* (JFM, 1994)

LDKM Approach

- Scale similarity is extended to test filter level and a model is assumed for

$$\tau_{ij}^{test} = C_l L_{ij}$$

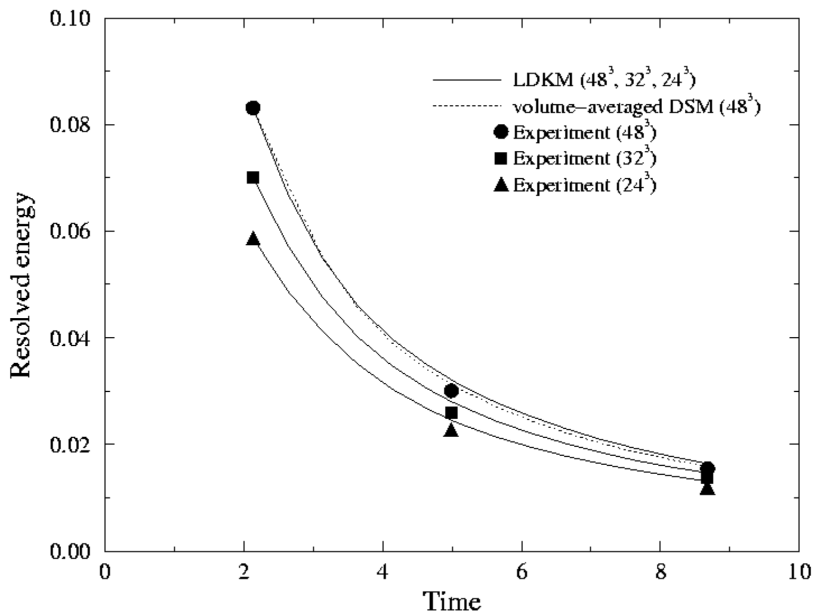
- Does not employ Germano's identity

$$\mathcal{L}_{ij} = -2C_\nu \sqrt{k^{test}}\widehat{\bar{\rho}}\widehat{\Delta}\left(\frac{\widehat{\bar{\rho}\widetilde{S}_{ij}}}{\widehat{\bar{\rho}}} - \frac{1}{3}\frac{\widehat{\bar{\rho}\widetilde{S}_{kk}}}{\widehat{\bar{\rho}}}\delta_{ij}\right) + \frac{1}{3}\mathcal{L}_{kk}\delta ij$$

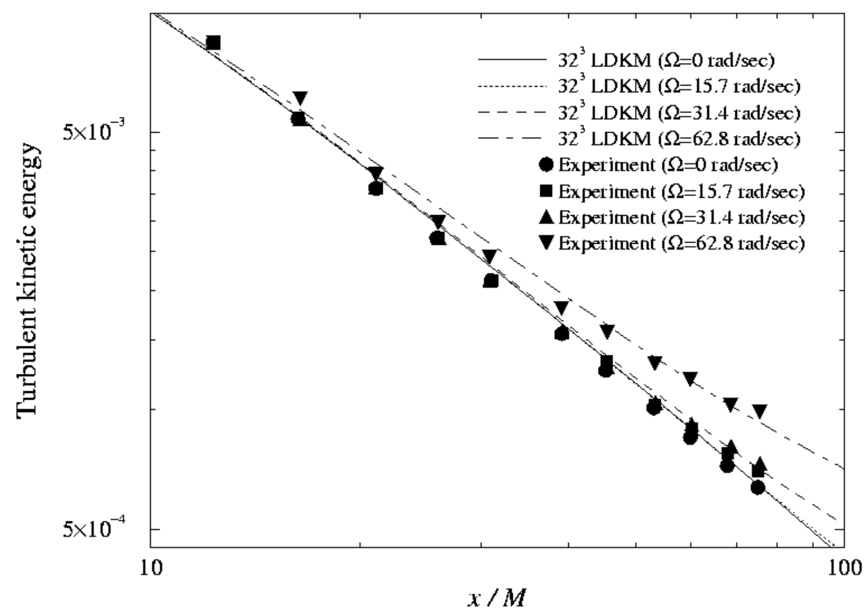
$$C_\nu = -\frac{\mathcal{M}_{ij}\mathcal{L}'_{ij}}{2\mathcal{M}_{ij}\mathcal{M}_{ij}} \qquad \mathcal{M}_{ij} = \sqrt{k^{test}}\widehat{\Delta}\left(\widehat{\bar{\rho}\widetilde{S}_{ij}} - \frac{1}{3}\widehat{\bar{\rho}\widetilde{S}_{kk}\delta_{ij}}\right) \qquad \mathcal{L}'_{ij} = \mathcal{L}_{ij} - \frac{1}{3}\mathcal{L}_{kk}\delta_{ij}$$

- Denominator is well defined at the test filter level and non-zero
- Approach is stable and robust without averaging in complex flows
- can be used for any model, including Smagorinsky's model
- Model is available in commercial codes (e.g. FLUENT)

Localized Dynamic Kinetic Energy Model Predictions



Decaying Isotropic Turbulence



Rotating Isotropic Turbulence

DSM and LDKM captures real turbulence at high Re accurately even when a very coarse grid is employed. LDKM also capture the effect of rotation (i.e., the backscatter increase with rotation) accurately (Kim and Menon, 99).

Alternate Models for LES

- Other models:
  - Spectral cut-off models
  - Approximate de-convolution models
  - Structure function models
  - Scale similarity models
  - Second order algebraic models
  - Reynolds stress transport models
- Finally, some models are combinations of previous models to combine the strengths of each
  - Mixed Model combines Smagorinsky (good levels of dissipation) and Similarity models (good physical representation of the stresses principal direction)

Book: Sagaut: LES for Incompressible Flow

Practical Constraints (Numerical)

- Even on parallel clusters simulations need to be completed in a reasonable time frame
  - 1-2 weeks?
- Very few people have access to 1000+ processors with high-speed dedicated switches
  - 300+ processors may be more realistic
- Grid resolution of 10^7 points may be reasonable but 10^8 points is beyond current access for majority
- With finite-rate kinetics even 10^7 points may be questionable (unless kinetics cost is eliminated)
- Can we get accurate predictions using 10^6+ points?

Boundary Conditions

- Wall: Slip/No-Slip, isothermal/adiabatic
- Inflow-Outflow critical for compressible flow
  - Finite computational region
  - Incorrect BCs will cause wave reflection
  - 1D Euler equation (Thompson 1987)
  - Navier-Stokes (Poinsot & Lele 1992, Baum et at. 94)
  - Characteristic waves @ inflow/outflow
  - Full viscous equations solved at inflow/outflow
- BCs needed for arbitrary directions
- Modifications needed for acoustic modeling
  - Non-reflecting
  - Absorbing

Boundary conditions for compressible Navier-Stokes equations

- Boundary conditions (velocity, pressure) with acoustic wave motion (impedance, incoming/outgoing)
  - Accurate control of wave reflections without any addition of numerical dissipation
  - Avoiding non physical coupling between inlet and outlet due to propagation of numerical waves (Wiggles …)
- Most methods are based on characteristic analysis of the Euler equations or Navier-Stokes equations (Engquist & Majda,1979, Thomson,1990, Poinsot & Lele,1992)

Navier Stokes Characteristic Boundary Conditions (NSCBC)

- Navier Stokes apply everywhere including boundaries
- Correction of the solution on the boundaries:
  - On each boundary, *incoming waves must be specified*
    - must be modified using the *physical boundary conditions* (Velocity, pressure, mass flow rate …)
  - *Outgoing waves* are prescribed from the *computed flow*
    - Do not need any corrections
- Characteristic analysis of the Navier Stokes
  - Inlet/outlet are perpendicular to the x_1 (flow) direction
  - Acoustic waves are propagating in the x_1 direction
  - Incoming/outgoing waves are in the derivatives normal to the x_1 boundary.

Identification of the Acoustic terms in the Navier-Stokes equations

$$\frac{\partial \rho}{\partial t} + d_1 + \frac{\partial \rho u_2}{\partial x_2} + \frac{\partial \rho u_3}{\partial x_3} = 0$$

$$\frac{\partial \rho E}{\partial t} + \frac{1}{2}\left(\sum_{k=1}^{3} u_k^2\right) d_1 + \frac{d_2}{\gamma - 1} + \rho u_1 d_3 + \rho u_2 d_4 + \rho u_3 d_5$$

$$+ \frac{\partial}{\partial x_2}\left[u_2\left(\rho e_s + p\right)\right] + \frac{\partial}{\partial x_3}\left[u_3\left(\rho e_s + p\right)\right] = \frac{\partial}{\partial x_i}\left(\lambda \frac{\partial T}{\partial x_i}\right) + \frac{\partial u_i \tau_{ij}}{\partial x_i} + \dot{\varpi}_T$$

$$\frac{\partial \rho u_1}{\partial t} + u_1 d_1 + \rho d_3 + \frac{\partial \rho u_2 u_1}{\partial x_2} + \frac{\partial \rho u_3 u_1}{\partial x_3} = \frac{\partial \tau_{1j}}{\partial x_j}$$

$$\frac{\partial \rho u_2}{\partial t} + u_2 d_1 + \rho d_4 \frac{\partial \rho u_2}{\partial t} + u_2 d_1 + \rho d_4 + \frac{\partial \rho u_2 u_2}{\partial x_2} + \frac{\partial \rho u_3 u_2}{\partial x_3} + \frac{\partial p}{\partial x_2} = \frac{\partial \tau_{2j}}{\partial x_j}$$

$$\frac{\partial \rho u_3}{\partial t} + u_3 d_1 + \rho d_5 + \frac{\partial \rho u_2 u_3}{\partial x_2} + \frac{\partial \rho u_3 u_3}{\partial x_3} + \frac{\partial p}{\partial x_3} = \frac{\partial \tau_{3j}}{\partial x_j}$$

$$\frac{\partial \rho Y_k}{\partial t} + Y_k d_1 + \rho d_{5+k} + \frac{\partial \rho u_2 Y_k}{\partial x_2} + \frac{\partial \rho u_3 Y_k}{\partial x_3} = \frac{\partial M_{kj}}{\partial x_j} - \dot{\varpi}_k$$

$$d = \begin{pmatrix} d_1 \\ d_2 \\ d_3 \\ d_4 \\ d_5 \\ d_{5+k} \end{pmatrix} == \begin{pmatrix} \dfrac{\partial \rho u_1}{\partial x_1} \\ \rho c^2 \dfrac{\partial u_1}{\partial x_1} + u_1 \dfrac{\partial p}{\partial x_1} \\ u_1 \dfrac{\partial u_1}{\partial x_1} + \dfrac{1}{\rho} u_1 \dfrac{\partial p}{\partial x_1} \\ u_1 \dfrac{\partial u_2}{\partial x_1} \\ u_1 \dfrac{\partial u_3}{\partial x_1} \\ u_1 \dfrac{\partial Y_k}{\partial x_1} \end{pmatrix}$$

Amplitude of the characteristic waves

- The d_i terms contain both incoming and outgoing information
- Characteristic analysis of the 1D Euler equations link d_i with the amplitude of the characteristic waves L_i

$$d = \begin{pmatrix} d_1 \\ d_2 \\ d_3 \\ d_4 \\ d_5 \\ d_{5+k} \end{pmatrix} = \begin{pmatrix} \frac{1}{c^2}\left[L_2 + \frac{1}{2}(L_5 + L_1)\right] \\ \frac{1}{2}(L_5 + L_1) \\ \frac{1}{2\rho c}(L_5 - L_1) \\ L_3 \\ L_4 \\ L_{5+k} \end{pmatrix}$$

$$L_1 = \lambda_1\left(\frac{\partial p}{\partial x_1} - \rho c\frac{\partial u_1}{\partial x_1}\right) \qquad L_5 = \lambda_5\left(\frac{\partial p}{\partial x_1} + \rho c\frac{\partial u_1}{\partial x_1}\right)$$

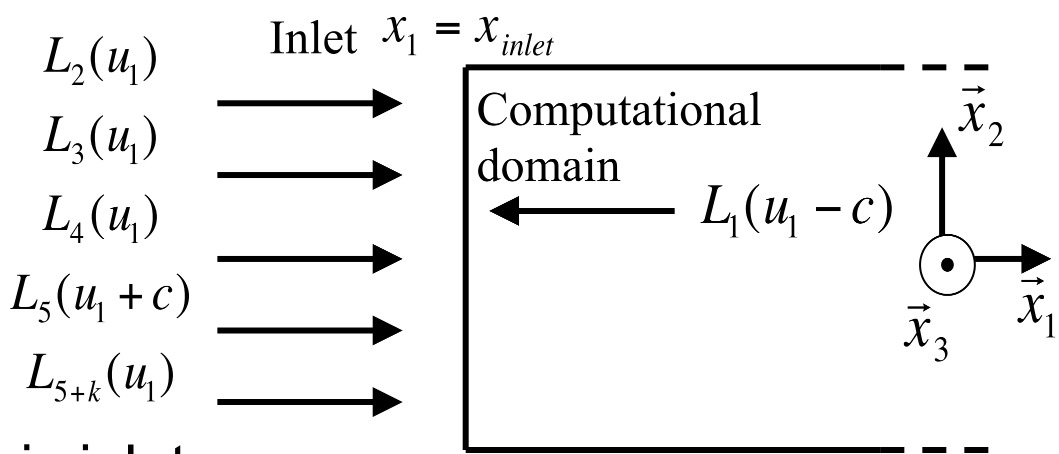
$$L_2 = \lambda_2\left(c^2\frac{\partial \rho}{\partial x_1} - \frac{\partial p}{\partial x_1}\right) \qquad L_{5+k} = \lambda_5\frac{\partial Y_k}{\partial x_1} \quad \text{for } k = 1,N$$

$$L_3 = \lambda_3\frac{\partial u_2}{\partial x_1} \quad \text{and} \quad \mathrm{L}_4 = \lambda_4\frac{\partial u_4}{\partial x_1}$$

- Each wave is associated with a characteristic velocity:

$$\lambda_1 = u_1 - c \qquad \lambda_2 = \lambda_3 = \lambda_4 = \lambda_{5+k} = u_1 \qquad \lambda_5 = u_1 + c$$

Incoming and outgoing waves



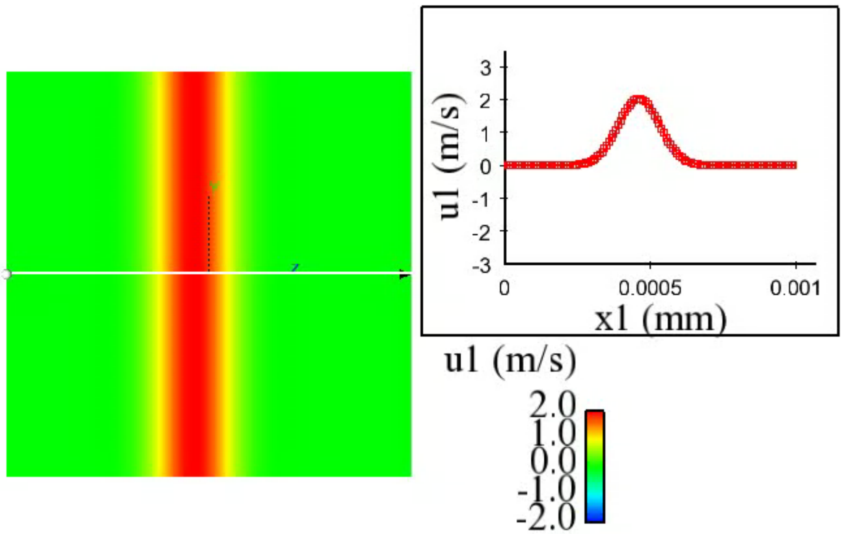
- For a subsonic inlet:
  - 4 incoming waves (L_2, L_3, L_4, L_5) and 1 outgoing wave (L_1)
  - A model must be applied to compute the incoming characteristic waves using the physical boundary values (Velocity, pressure …)
  - LODI hypothesis (Poinsot & Lele1992): The waves L_i are computed assuming flow is Locally One Dimensional and Inviscid
- Supersonic flow: all incoming or all outgoing waves
  - All properties can be prescribed
  - Note: Supersonic boundary layer has a subsonic portion!

Reflecting or Non-Reflecting Inflow/Outflow

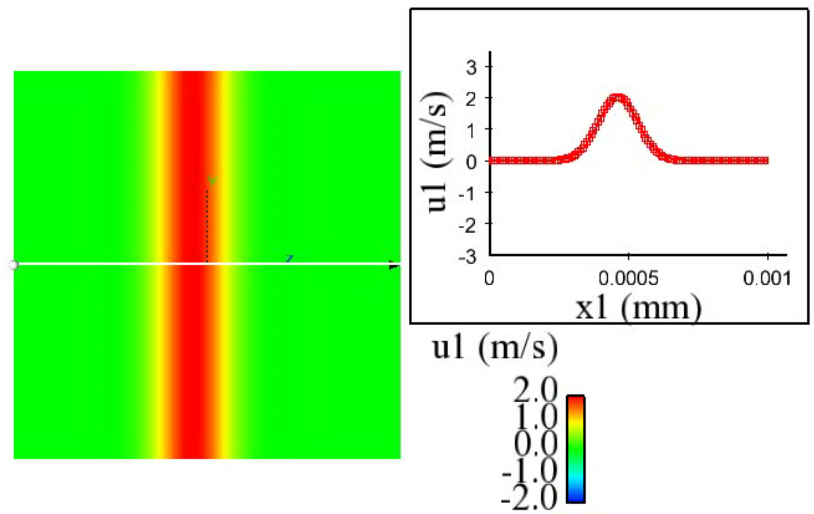
- Use LODI system to impose fixed in/outflow conditions
- Reflecting Conditions:
  - Acoustic waves reflect from computational boundaries
    - Can be weak or strong reflection
- Non-Reflecting Conditions
  - Acoustic waves leave domain without reflection
    - Match impedance at the boundary (can be tricky!)
- Sponge Outflow Conditions
  - Damp all pertubations as the outflow is reached
    - Requires an increased domain size
- Advantages and disadvantages of all approaches

Comparison of reflecting and non reflecting boundary conditions

- Interaction between a characteristic inlet and an outgoing acoustic wave



Non-reflecting inflow

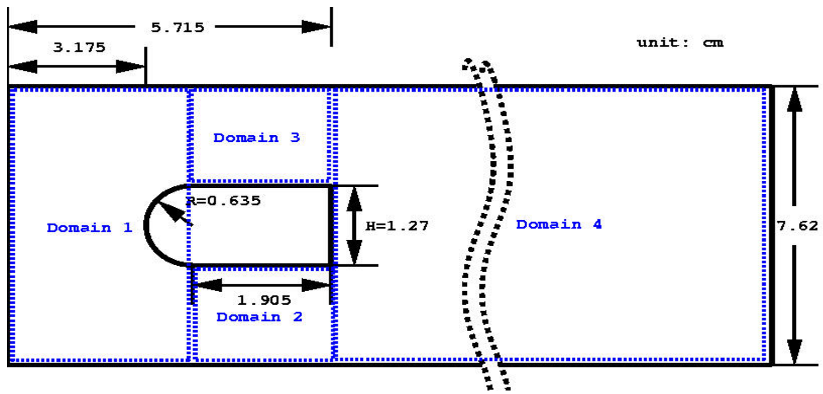


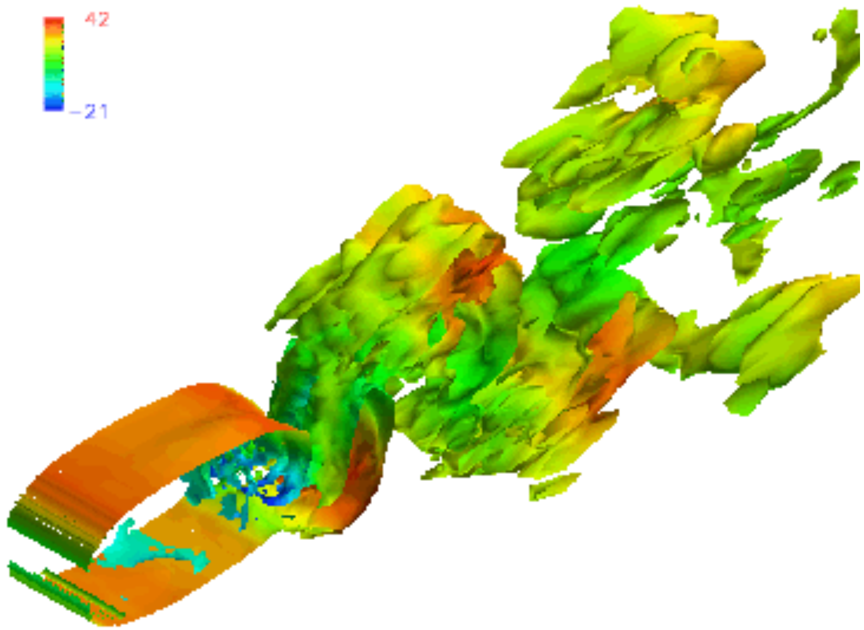
Reflecting inflow

Limitations and Extensions of LODI formulation

- If the boundary is not aligned with a Cartesian direction
  - Generalized coordinate system: one direction is normal to the boundary (Moureau et al. 2005)
- The LODI formulation assumes that the transverse effect are negligible (1D assumption):
  - Transverse terms included (Yoo et al., 2005, 2007)
- 3D NSCBC for edge/corners (Lodato, 2008)
- Cross-term viscous terms are also included
- Extension for reacting flows also developed and employed
  - Baum et al.

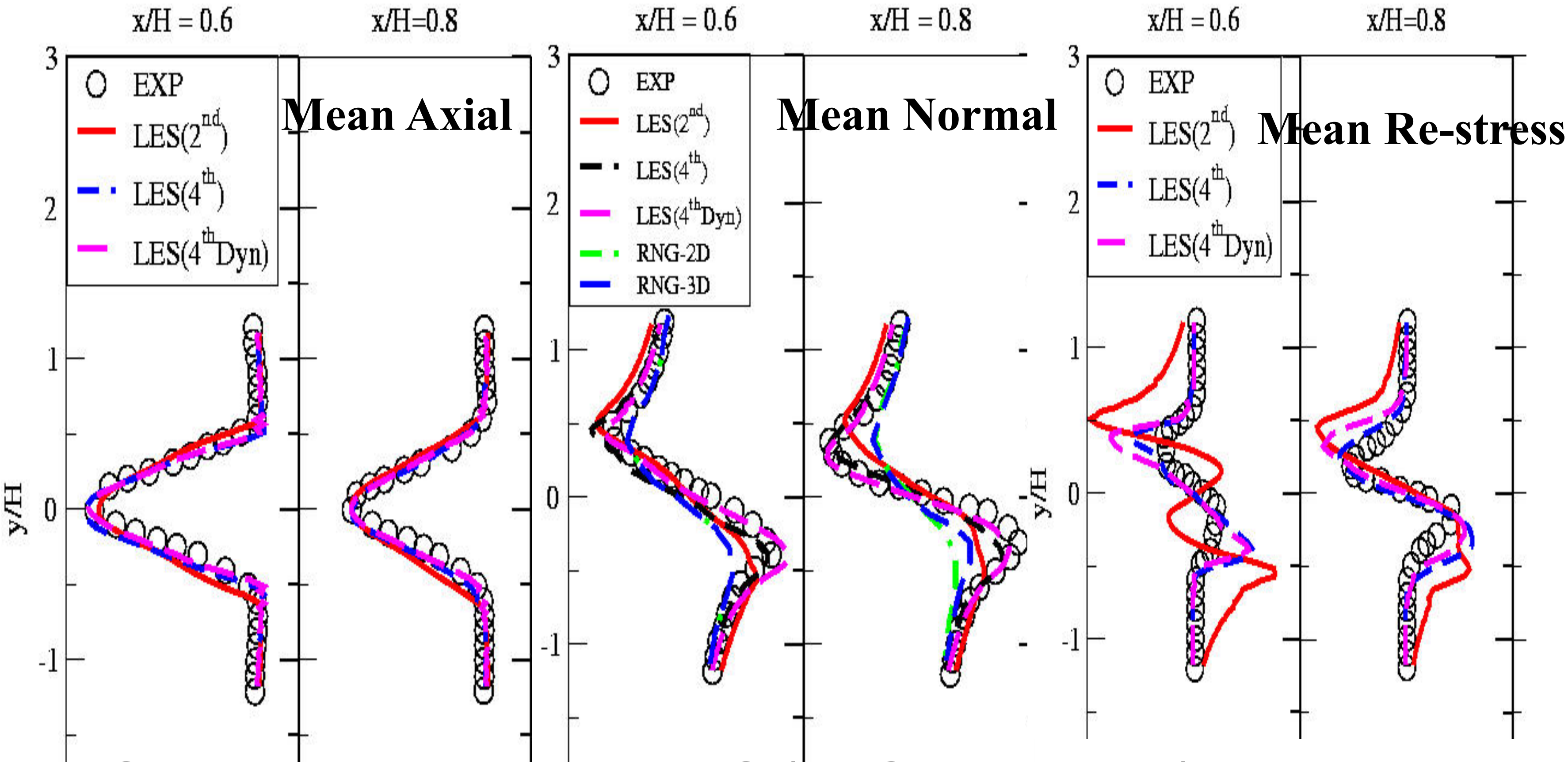
Comparison of RANS/LES of Flow past a Bluff Body





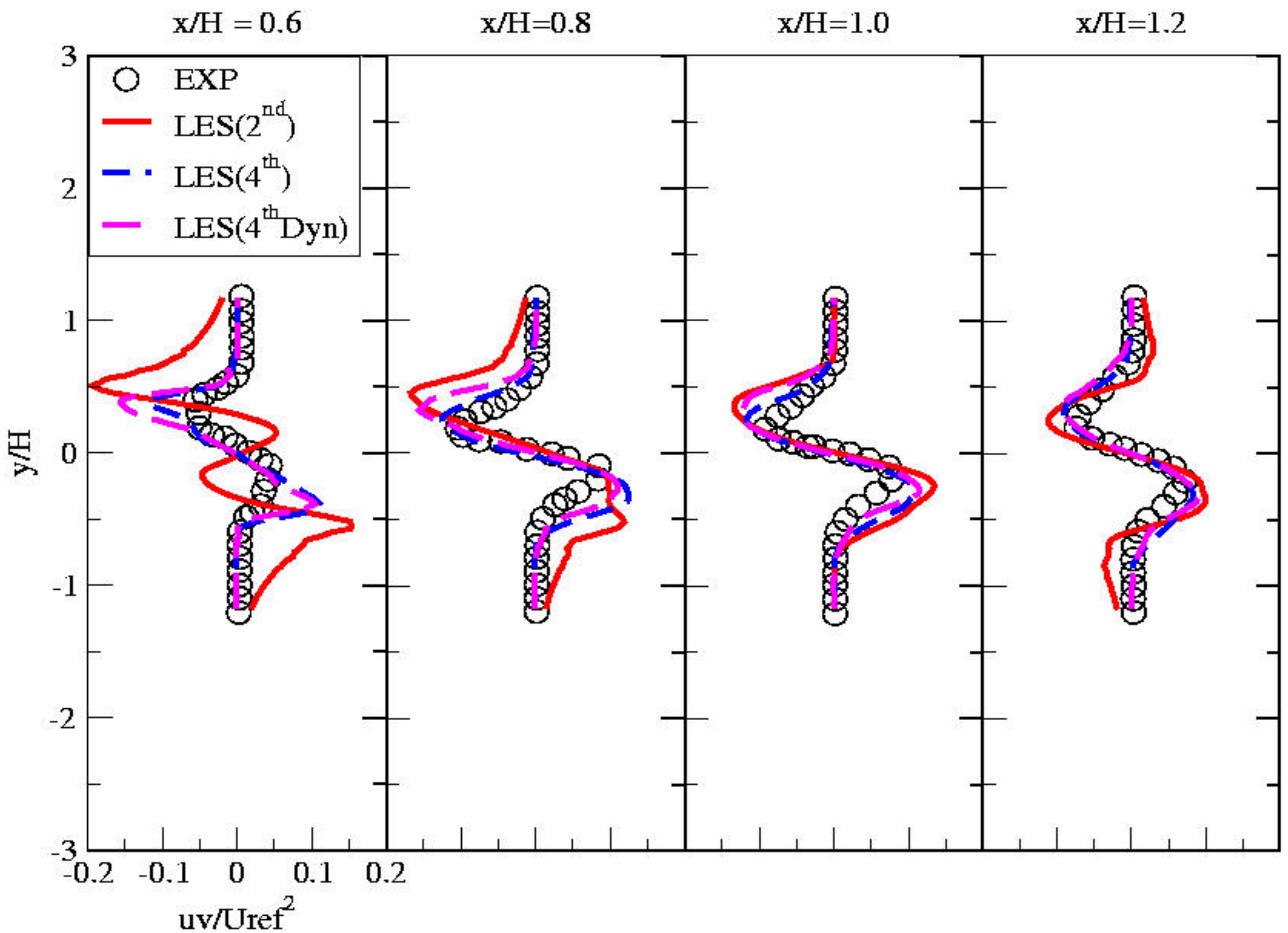
- Non-reacting flow
- LES using “coarse” grid: ~ 750,000 cells
    - O(2-4) accuracy in application of BCs
    - LDKM dynamic closure
- RANS: Commercial code with standard 2-equation closure

Velocity Profiles in the Wake of the Bluff Body



- LES more accurate than RANS (RNG k-e closure)
- O(4) more accurate than O(2) for a given resolution
- Dynamic O(4) LES somewhat more accurate

Turbulent Stress (uv) Profiles



Codes Used for Results Discussed

- Most of the studies reported here employ in-house codes at various research labs
- Some studies employ commercial codes as well
  - FLUENT, OpenFOAM, CFX, STARCD etc.
- Important to become aware of code's strengths and limitations before attempting realistic problems
  - Sometimes a simple test case with well defined boundary conditions can be used to verify the accuracy and reliability of the solver
- Verification and Validation strategy
- Uncertainty Quantification

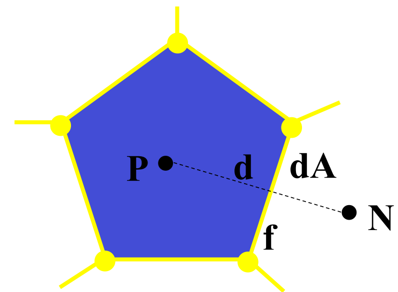
Some Definitions of Codes

- OpenFOAM
  - Christer Fureby, FOA
- LESLIE3D
  - Suresh Menon, Georgia Tech
- AVBP
  - Thierry Poinsot, IMF Toulouse, CNRS, France
- FLUENT
  - Peter Flohr, Alstom
- SNL-LES
  - Joe Oefelein, Sandia National Laboratory
- CFX
  - Christian Hasse, BMW

LES Code: Fureby (FOA)

Unstructured Finite Volume (FV) discretization

Reynolds transport theorem



$$\bar{\mathbf{u}} = [\bar{\rho},\ \bar{\rho}\tilde{Y}_i,\ \bar{\rho}\tilde{\mathbf{v}},\ \bar{\rho}\tilde{E}]^T$$

$$\partial_t(\bar{\mathbf{u}}_P) + \tfrac{1}{\delta V_P}\sum_f \left[\mathbf{F}_f^C(\bar{\mathbf{u}}) - \mathbf{F}_f^D(\bar{\mathbf{u}}) + \mathbf{F}_f^B(\mathbf{u},\bar{\mathbf{u}})\right] = s_P(\mathbf{u},\bar{\mathbf{u}})$$

$$\bar{\mathbf{u}} = [\bar{\rho},\ \bar{\rho}\tilde{Y}_i,\ \bar{\rho}\tilde{\mathbf{v}},\ \bar{\rho}\tilde{E}]^T$$

$$\partial_t(\bar{\mathbf{u}}_P) + \tfrac{1}{\delta V_P}\sum_f \left[\mathbf{F}_f^C(\bar{\mathbf{u}}) - \mathbf{F}_f^D(\bar{\mathbf{u}}) + \mathbf{F}_f^B(\mathbf{u},\bar{\mathbf{u}})\right] = -(\nabla p)_P + s_P(\mathbf{u},\bar{\mathbf{u}})$$

Semi-Implicit Algorithm: Linear/cubic reconstruction of convective fluxes

Central difference approximations of inner derivatives in other fluxes

Crank Nicholson time integration, Co≈0.5

Fully Explicit algorithm

Monotone (van-Leer/FCT) reconstruction of convective fluxes

Central difference approx. for inner derivatives other fluxes

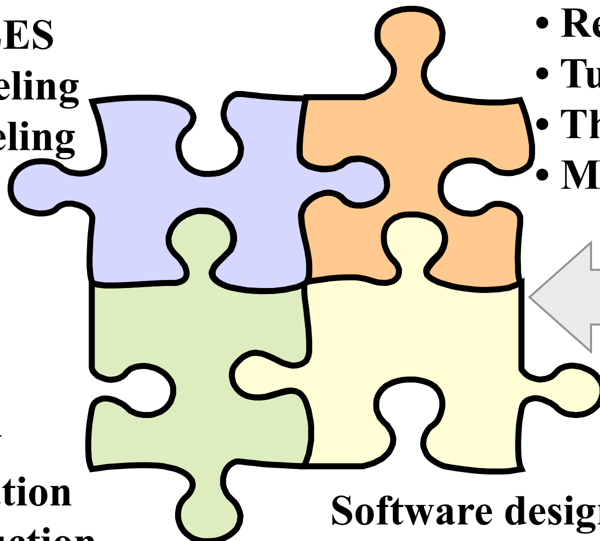
Modified Equations Analysis (MEA)

Drikakis D., Fureby C., Grinstein F.F. & Liefendahl M.; 2007, "ILES with Limiting Algorithms", In Implicit Large Eddy Simulation: Computing Turbulent Fluid Dynamics, Eds. Grinstein F.F., Margolin L. & Rider B., Cambridge University Press, p 94.

LES Code (Fureby) Architecture

Turbulence
- LES or ILES
- Wall modeling
- SGS modeling

Complex Chemistry
- Reduced reaction mech.
- Turbulence/chemistry interactions
- Thermal radiation
- Multi-phase effects

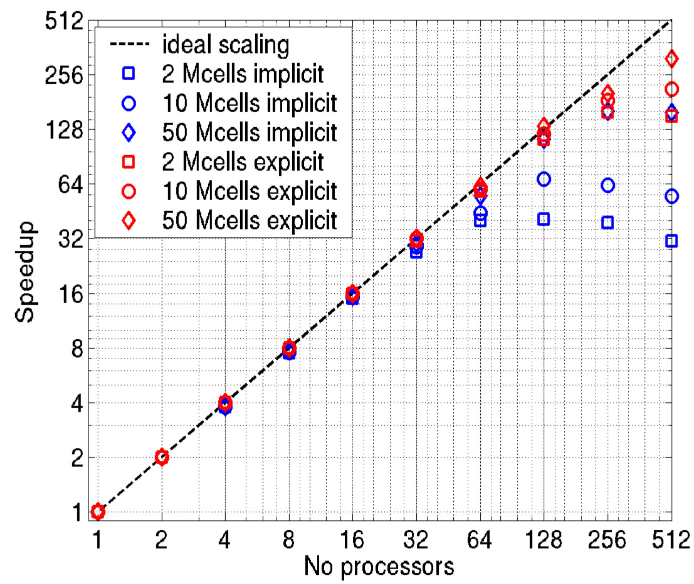


Additional Physics
- Acoustics
- FSI

Visualization

Numerics
- Geometry
- Discretization
- Reconstruction
- Solvers
- AMR

Software design
- Platforms
- Parallelization
- Comunication

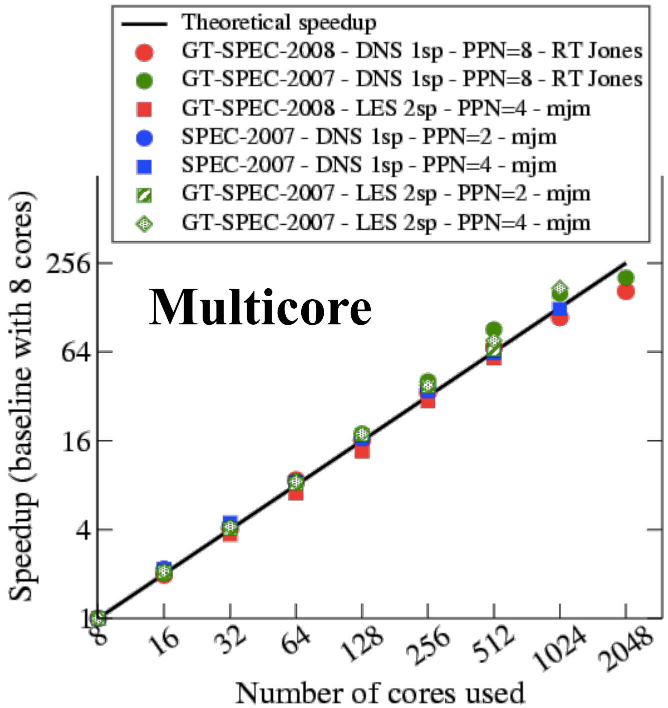


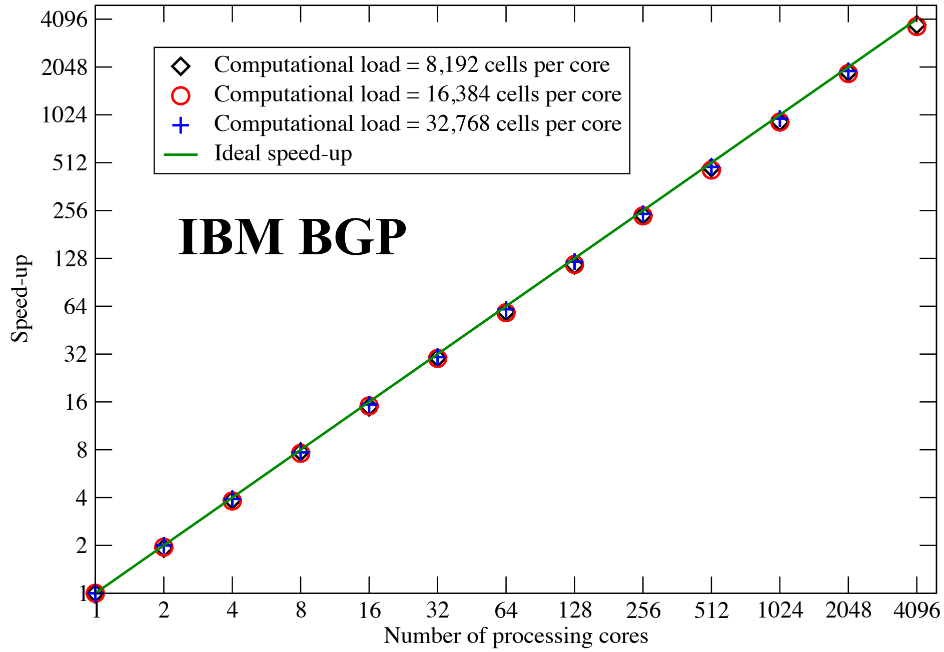
Software
Use OpenFoam C++ library
running on large linux systems
MPI + gigabit ethernet / infiniband

LES Code (LESLIE3D) – Georgia Tech

- Fully compressible finite-volume solver, O(2-4) in space, O(2) in time, explicit time integration
- Eulerian gas -Lagrangian particle (liquid and/or solid) solver with full coupling
- Capability to do real gas, dense sprays, breakup
- Multi-block, structured grid
- Hybrid solvers that combines shock capturing (MUSCL + HLL) with O(4) central scheme
  - Shock capturing used only for discontinuities
- No explicit artificial dissipation
- Dynamic subgrid closures, subgrid mixing models
  - G-eqn, ATF, Flamelet, LEM, EBU/EDC

Scalability of LESLIE3D





- 107.leslie is a SPEC 2007 MPI Benchmark for ALL OEMs
- Achieve 1+ TFLOP on our dual-core cluster (>15% peak!)
- Multi-core with GPU optimization underway

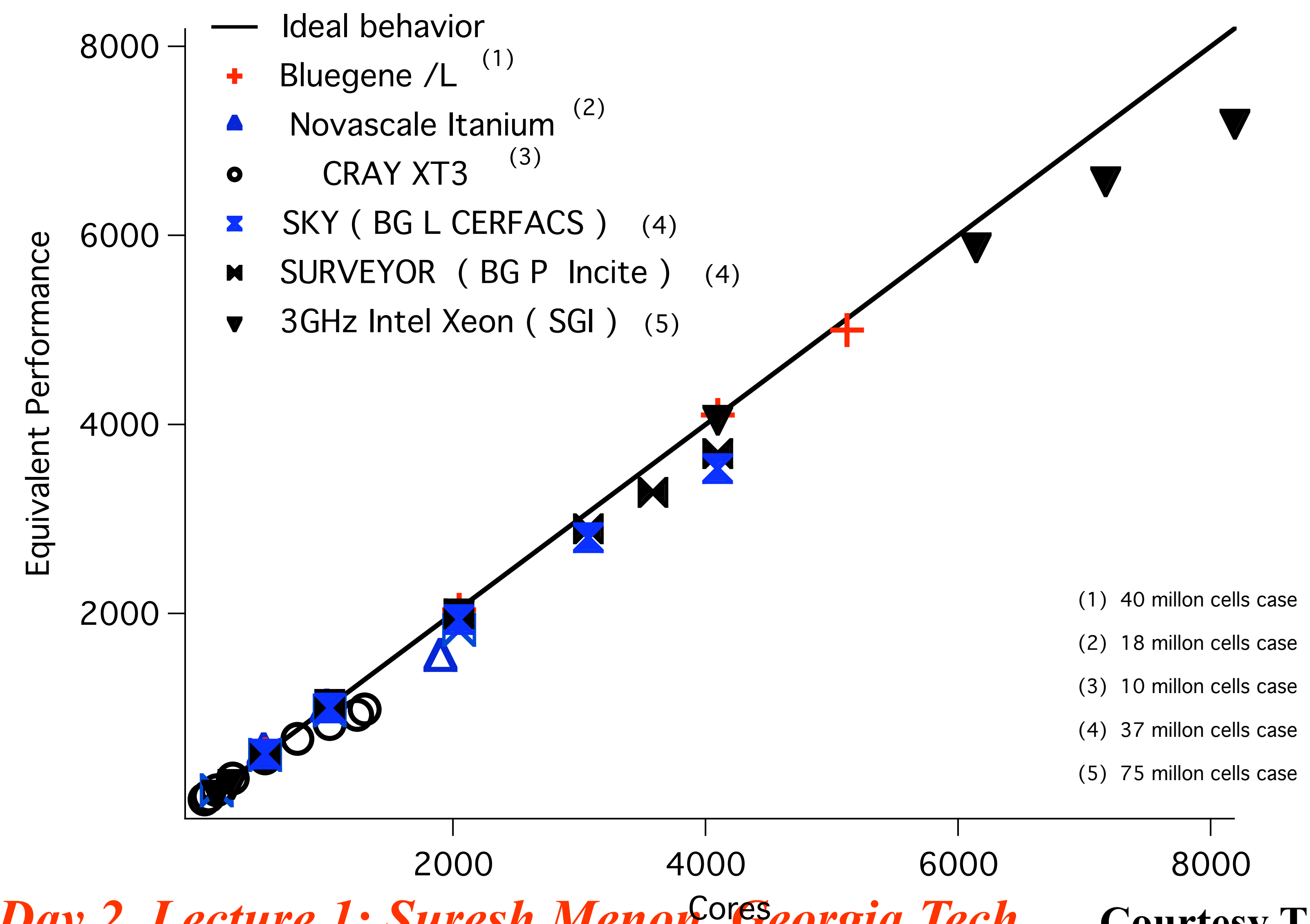
LES Code AVBP – Poinsot et al.

- 3D turbulent compressible reactive Navier-Stokes solver [2]
- Unstructured explicit parallel solver
- WALE model for sub-grid scale viscosity [3]
- Euler-Euler monodisperse formulation for two-phase flow [6]
- Single and multi-step kinetics [4]
- Dynamic Flame Thickening TFLES [5]
  - Applicable to premixed and non-premixed combustion

[2] V. Moureau *et al.*, High-order methods for DNS and LES of compressible multi-component reacting flows on fixed and moving grids, J. Comp. Phys., 2005
[3] F. Nicoud, F. Ducros, Subgrid-scale stress modelling based on the square of the velocity gradient, Flow Turb. and Combustion, 1999
[4] S. Li *et al.*, Chemistry of JP-10 ignition, AIAA Journal, 2001
[5] O. Colin, F. Ducros, D. Veynante, T. Poinsot, A thickened flame model for large eddy simulations of turbulent premixed combustion, Phys. Fluids, 2000
[6] Boileau M., Pascaud S., Riber E., Cuenot B., Gicquel L., Poinsot T. and Cazalens M. Investigation of two-fluid methods for Large Eddy Simulation of spray combustion in Gas Turbines. Flow, Turbulence and Combustion, 80(3):291-321, (2008).

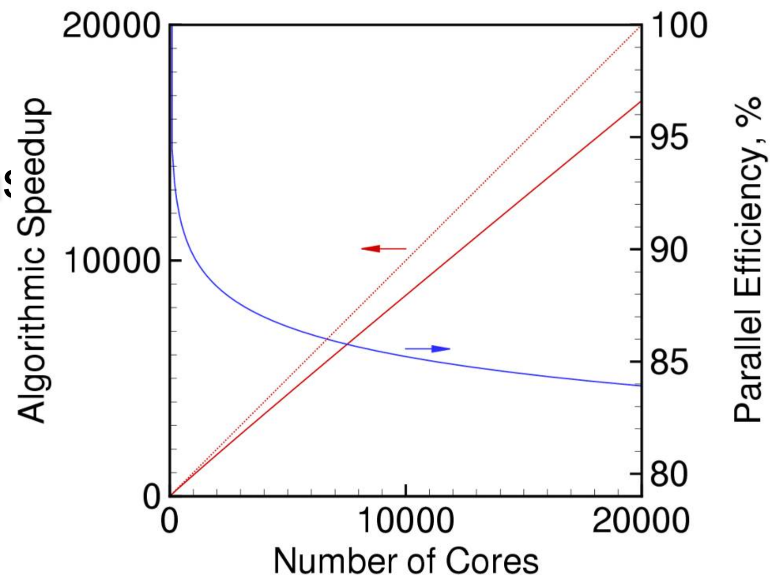
 Courtesy T. Poinsot

Speed up of AVBP (CNRS, CERFAC):



Courtesy T. Poinsot

LES code – Oefelein, SNL



- Theoretical framework
  - Compressible conservation equations
  - Real-fluid equation(s) of state
  - Multiphase flow, spray
  - Dynamic SGS modeling
- Numerical framework
  - Dual-time stepping integration
  - Staggered finite-volume differencing (non-dissipative, conservative)
  - Generalized body-fitted coordinates (adaptive or moving mesh via ALE)
  - Generalized multi-block connectivity (complex geometry)
  - Massively-parallel (MPI)

J. C. Oefelein (2006). Large eddy simulation of turbulent combustion processes in propulsion and power systems. *Progress in Aerospace Sciences*, 42: 2-37.