A New Approach to LES Modeling

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Optimal LES: Trading in the Navier-Stokes Equations for Custom Designed Discrete LES
Large Eddy Simulation

- Simulate only the largest scales of High-Reynolds number turbulence
  - Models of small scales required
- Numerous models developed recently
  - E.g. scale similarity, dynamic, structure function, stretched vortex, deconvolution
- Difficulties remain
  - Wall-bounded turbulence
  - Impact of numerical discretization
- LES is for making predictions!
  - Predict (some) statistical properties of turbulence
  - Predict large-scale dynamics of turbulence
Optimal LES Development Map

- Dynamic Treatment of Correlations
- Theoretical Correlation Models
- Optimal LES Formulation
- DNS Correlation Data
- Practical Optimal LES Models
- Finite Volume Optimal LES
- Validation + Testing
- DNS + Experiment Validation Data
- Critical Formulation Checks
- Optimal LES Design Approach

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Filtering and LES

- Filters precisely define the large scales to be simulated
  - Not absolutely necessary, but useful
  - Provides a framework in which to develop models

- Two flavors of filtering and LES
  - Continuously filtered LES
  - Discretely filtered LES
Many filters are invertible or nearly so (e.g. Gaussian)

A hypothetical exercise: suppose filter can be inverted
- Determine evolution by defiltering and advancing N-S
- Best “model” would be a DNS $\Rightarrow$ DNS resolution
- Coarse resolution determines accuracy limits
- Best models must depend explicitly on discretization
Discrete LES

Examples: Fourier cut-off, sampled top-hat (finite volume), MILES

Filter is not invertible & stochastic modeling tools are applicable
  • Many turbulent fields map to same filtered state
  • Evolution of filtered state considered stochastic

This is the formulation used here

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Stochastic Evolution of LES

\[ u \]

Filter

\[ \tilde{u} \]
Stochastic Evolution of LES
Stochastic Evolution of LES

Mapping from filtered field to filtered evolution?

replacements

\( \frac{du}{dt} \)
Best deterministic LES evolution: Average of filtered evolutions of fields mapping to the current LES state

\[ \frac{dw}{dt} = \left\langle \frac{d\tilde{u}}{dt} \right\rangle \tilde{u} = w \]

- Equivalently average of model terms: \( m = \langle M | \tilde{u} = w \rangle \)
- Two Theorems:
  1) 1-time statistics of \( w \) and \( \tilde{u} \) match (Pope 2000, Langford & Moser 1999)
  2) Mean-square difference between \( \frac{dw}{dt} \) and \( \frac{d\tilde{u}}{dt} \) minimized but finite.
**Optimal LES**

- Statistical data requirements for Ideal LES are outrageous
  - # of conditions = # DOF in LES

- Stochastic estimation as an approximation to conditional average
  - Pick functional form of $m(w)$
  - Minimize mean-square error of approximation to conditional average
  - Results in model formulation first proposed by Adrian (1979, 1990)
Optimal LES
An example

- Estimate conditional average $m \approx \langle M | \tilde{u} = w \rangle$

- Suppose $m(w) = A + Bw + Cw^2 + Dw^3$, then

$$
\langle (M - m(\tilde{u}))E_j \rangle = 0 \quad \Rightarrow \quad \langle ME_j \rangle = \langle m(\tilde{u})E_j \rangle
$$

where $E = (1, \tilde{u}, \tilde{u}^2, \tilde{u}^3)$ is the event vector

- Equations solved for coefficients $A$, $B$, $C$ and $D \Rightarrow$ Optimal model

- Must know $\langle ME_j \rangle$ and $\langle E_i E_j \rangle$
  - Try using DNS correlation data
  - Then get correlations from theory

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Ideal vs. Optimal LES

For a given turbulent flow and filter, Ideal LES is uniquely defined but unknown.

In contrast, several choices must be made to define Optimal LES:

- Selection of modeled term $M$
  
  E.g. $\frac{d\tilde{u}}{dt}$, $\tau_{ij}$ or $\partial_j \tau_{ij}$
  
  Matters because error minimized is different

- Selection of model dependencies
  
  E.g. spatial locality, nonlinearity
  
  Matters because changes space in which minimum error is sought
Developing Optimal LES Models

- Modeler needs to design the Optimal model
  - Guidance provided by $\langle ME_j \rangle = \langle mE_j \rangle$
  - Arrange so $\langle ME_j \rangle$ includes terms of dynamical interest
    Model reproduces them \textit{a priori}
    Example: Terms in 2-point correlation or Reynolds stress equation

- Statistical information required as input
  - For quadratic estimates need correlations:
    $\langle u_i(x)u_j(x') \rangle$ $\langle u_i(x)u_j(x')u_k(x') \rangle$ $\langle u_i(x)u_j(x')u_k(x'')u_l(x'') \rangle$
    with separations of order the non-locality of the model

- Use DNS correlations for testing,

- Theoretically determined correlations later.
Optimal LES Development Map

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Tests of Optimal LES with DNS Statistical Data

- Evaluate modeling approach without other uncertainties
- Principles of Optimal model design
- Test Cases:
  - Forced isotropic turbulence ($Re_\lambda = 164$)
    Fourier cutoff filter
  - Turbulent flow in a plane channel ($Re_\tau = 590$)
    Spectral representation/filter
    Severely filtered ($\Delta x^+ = 116$, $\Delta z^+ = 58$)
  - Forced isotropic turbulence
    Finite volume filter

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Optimal LES of Forced Isotropic turbulence

Energy spectrum, $E(k)$

$\log_{10}$ replacement

$Wavenumber, k$

$E^{(16)}$, $Q^{(16)}$

DNS

Smagorinsky $Cs = 0.228$

Smagorinsky $Cs = 0.819$

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Optimal LES of Turbulent Channel at $Re_\tau = 590$
Constructing Good Optimal Models

- Optimal model was formulated to reproduce the $y$–transport term in the Reynolds stress equation ($\partial_y u_k \tau_{ij}$).

- Simpler optimal model that doesn’t reproduce transport yields:

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Responsibilities of an LES Model

- An LES model must represent several effects of the subgrid turbulence
  - Dissipation of energy (and $R_{ij}$) - standard requirement
  - Subgrid contribution to mean equation (unresolved Reynolds stress).
  - Subgrid contribution to $R_{ij}$ transport
  - Subgrid contribution to pressure redistribution of $R_{ij}$

- Optimal LES provides a mechanism to construct models that do this
  - Select $M$ and $E_j$, so that $\langle ME_j \rangle$ includes terms in $R_{ij}$ equation
Optimal LES Development Map

- Dynamic treatment of correlations
- Theoretical correlation models
- Optimal LES formulation
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Finite Volume Optimal LES

- Like standard finite volume schemes, except:
  - Cell size not small compared to turbulence scales
  - Standard reconstruction techniques to determine finite volume fluxes are not applicable
    True solution is not smooth on scale of the grid volume.

- Fluxes must be modeled.
  - Use Optimal model of the fluxes.
  - Estimate consistent with turbulence statistics, not numerical convergence.

- Need FV formulation for complex geometries

- Similar approach for Finite Difference and Finite Element discretizations
Performance of FV LES, $Re_\lambda = 164$

$32^3$ Isotropic LES

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Optimal LES Development Map

DYNAMIC TREATMENT OF CORRELATIONS

THEORETICAL CORRELATION MODELS

OPTIMAL LES FORMULATION

DNS CORRELATION DATA

FINITE VOLUME OPTIMAL LES

DNS + EXPERIMENT VALIDATION DATA

VALIDATION + TESTING

OPTIMAL LES DESIGN APPROACH

CRITICAL FORMULATION CHECKS

PRACTICAL OPTIMAL LES MODELS

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Making Optimal LES Useful

- Simulations shown so far relied on DNS statistical data
  - Allowed properties and accuracy of OLES models to be explored
  - Allowed formulation details to be determined
  - Has not produced useful models
    Need to do a DNS first

- Statistical input is needed
  - Rely as much as possible on theory
High Reynolds Number Optimal FV LES

- Estimation equations are of the form:

\[
M'_{ij} = \sum_{\alpha} L_{ijk}^{\alpha} w_k^{\alpha} + \sum_{\alpha, \beta} Q_{ijkl}^{\alpha\beta} (w_k^{\alpha} w_l^{\beta})'
\]

\[
\langle w_m^{\gamma} M'_{ij} \rangle = \sum_{\alpha} L_{ijk}^{\alpha} \langle w_k^{\alpha} w_m^{\gamma} \rangle + \sum_{\alpha, \beta} Q_{ijkl}^{\alpha\beta} \langle (w_k^{\alpha} w_l^{\beta})' w_m^{\gamma} \rangle
\]

\[
\langle (w_m^{\gamma} w_n^{\delta})' M'_{ij} \rangle = \sum_{\alpha} L_{ijk}^{\alpha} \langle w_k^{\alpha} (w_m^{\gamma} w_n^{\delta})' \rangle + \sum_{\alpha, \beta} Q_{ijkl}^{\alpha\beta} \langle (w_k^{\alpha} w_l^{\beta})' (w_m^{\gamma} w_n^{\delta})' \rangle
\]

- **Green** terms are correlations of LES variables
  - Can compute from LES “on the fly” (dynamically)

- **Red** terms require modeling input

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Modeling the Red Terms

- The red correlations are surface/volume integrals of:

\[
\langle u_i(x)u_j(x)u_m(x') \rangle \quad \langle u_i(x)u_j(x)u_m(x')u_n(x'') \rangle
\]

- Assume \( Re \to \infty \), separations in inertial range \( (r = x - x') \)

- Small-scale isotropy, Kolmogorov \( \frac{2}{3} \) and \( \frac{4}{5} \) laws, Quasi-normal approximation

\[
\begin{align*}
\langle u_i(x)u_j(x') \rangle &= u^2 \delta_{ij} + \frac{C_1}{6} \epsilon^{2/3} r^{-4/3} (r_i r_j - 4r^2 \delta_{ij}) \\
\langle u_i(x)u_j(x)u_m(x') \rangle &= \frac{\epsilon}{15} (\delta_{ij} r_m - \frac{3}{2} (\delta_{jm} r_i + \delta_{im} r_j)) \\
\langle u_i(x)u_j(x)u_m(x')u_n(x'') \rangle &= \langle u_i(x)u_j(x) \rangle \langle u_k(x')u_l(x'') \rangle \\
&\quad + \langle u_i(x)u_k(x') \rangle \langle u_j(x)u_l(x'') \rangle \\
&\quad + \langle u_i(x)u_l(x'') \rangle \langle u_k(x')u_l(x) \rangle
\end{align*}
\]
Theoretical Optimal LES

- Forced Isotropic Turbulence
  - DNS at $Re_\lambda = 164$
  - LES at $Re_\lambda = \infty$

PSfrag replacements

- filtered DNS, $Re_\lambda = 164$
- DNS-based optimal LES, $Re_\lambda = 164$
- Theoretical optimal LES, $Re_\lambda = \infty$
- theoretical optimal LES, $Re_\lambda = 164$

$k$

$E(k)$
High ($\infty$) $Re$ Wall-Bounded Turbulence

- Assumptions of isotropy and inertial range not valid near wall
- Green terms can still be determined dynamically
- Need red correlations:
- A variety of modeling tools are being evaluated:
  - Log-layer similarity (Oberlack)
  - Anisotropy expansion & scaling (Procaccia)
  - Constraints from N-S equations
  - Quasi-Normal approximation
Test of Quasi-Normal Approximation
Channel Flow at $Re_\tau = 590$

- Normalized error, $\phi_{11,11}(r) = \frac{Q_{11,11}(r) - Q_{NA}}{L(r)}$ where

$$L(r) = \langle Q_{pq,rs}(r) Q_{pq,rs}(r) \rangle^{1/2}$$
Similarity Scaling of Expansion Coefficients
in Channel at $Re_\tau = 940$, Expansion of Procaccia

1 = 0 m = 0 q = 1

\[ \log_{10}(r/y) \]

1 = 2 m = 0 q = 4

\[ \log_{10}(r/y) \]

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Conclusions

- Discrete LES formulations are useful, avoid problems with discretization

- Optimal LES is a rational basis for discrete LES modeling
  - Yields remarkably good LES
  - But needs extensive statistical data as input

- For $Re \to \infty$, correlations available theoretically (away from walls)
  - Kolmogorov theory, Quasi-normal approximation, small-scale isotropy & a dynamic procedure.

- Near walls, need more information

- Also need models for subgrid contribution to statistical quantities of interest (e.g. turbulent energy).