Small-scale turbulence; theory, phenomenology and applications

Physical models for small-scale structures

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Philip Saffman, Tom Lundgren, Paul O’Gorman
Overview

• Motivation; what can we predict (postdict?)

• Structure-based models of turbulent small scales

• Hills spherical vortex
  – *Longitudinal velocity structure functions*

• Generalized 2-Co-ordinate 3comPonent models (2C-3P)
  – *Burgers vortex tube/sheet*
  – *Stretched spiral vortex (Lundgren)*

• Stretched spiral vortex model of turbulent small scales
  – *Velocity (energy) spectrum*
  – *Scalar (variance) spectrum*
  – *Velocity-gradient/vorticity statistics (1-point)*
  – *Longitudinal velocity structure functions (2-point)*
Modeling Turbulence small scales

Turbulence forming and decaying downstream of a grid placed normal to the stream. Corke & Nagib.
Modeling Turbulence small scales

Laser induced fluorescence showing mixing in a turbulent jet.
Dimotakis, Lye & Papantoniou (1981)
Modeling Turbulence small scales

Mixing region in Richtmyer-Meshkov instability
Modeling Turbulence small scales

Spectral slope vs $Re_\lambda$. ● - grid turbulence, (Warhaft, 2000).
 ■ - Shear turbulence, (Sreenivasan, 1996).
Modeling Turbulence small scales

How does one build ``useful’’ analytical models of turbulence small scales?

• Construct general analytical solution of initial-value problem for 3D Navier Stokes equations
  – Hard (no one has yet done this)!
  – May not be very useful for turbulence prediction; one would still need to perform relevant statistics (e.g. Burgers equation)

• Strong phenomenology. E.G. model turbulence small scales by fractals, fractal systems
  – No connection with NS dynamics
  – Different model for each application
  – SGS models for LES (Meneveau, Burton & Dahm)?

• Structure-based physical models (weak phenomenology)
  – May be tractable but is there sufficient physics?
  – Are assumed structures observed?
  – Still need to do statistics
Structure-based models of turbulence fine scales

• Vortex blobs: Hill’s spherical vortex; Synge & Lin (1943), Aivazis, 1997

• 2-Co-ordinate, 3-comPonent (2C-3P) model
  – Burgers vortex; Burgers (1948), Townsend (1951, Chen, Kambe (1990s)

• One-point structure tensors; Reynolds and Kassinos (1995)

• Rapid distortion theory; Leonard (2000)
Hills Spherical Vortex; Singe & Lin (1943)

- Model turbulence by ensemble of translating Hills spherical vortices
- Main idea:
  - Fix two points in space separated by distance $r$
  - Calculate contribution to longitudinal, latitudinal structure functions contributed by HSV of given size, position, and orientation
- Perform statistics over size, position, orientation with assumed distributions
- Vortices do not interact with each other! Local dynamics.

FIG. 1. Case 1: When the vortex diameter is less than the distance between points $\lambda_0$ and $\lambda_e$, the volume can be partitioned into three distinct regions depending on the relative position of the vortex and the two points.

FIG. 3. The toroidal coordinate system. Each point in space is specified by $r = |\mathbf{r}|$, $\zeta = \theta$, and the polar angle $\phi$. 
Hills Spherical Vortex; Aivazis (PF, 1997)

- **Distributions:**
  - *Uniform in space, orientation (isotropy)*
  - *Lognormal in size (radii) (Kolmororov, Yaglom)*
  - *Turbulence of vortex blobs. Does not model breakdown process*

- **One-parameter model**

\[
\zeta(u, \sigma) = \begin{cases} 
  \left( \frac{2\pi}{\sigma u} \right)^{1/2} \exp \left[ - \frac{1}{2} \left( \frac{\log(u)}{\sigma} \right)^2 \right] & (a > 0) \\
  0 & (a \leq 0), 
\end{cases}
\]

\[u = a/a_0, \quad a_0 \text{ is a length scale}
\]

\[\sigma \text{ is a dimensionless variance}\]
Higher-order velocity structure functions

FIG. 9. Fourth order normalized longitudinal velocity structure function vs normalized separation, Eq. (5.36). Experiment, Tabeling et al. (Ref. 17).

FIG. 10. Fourth order normalized transverse velocity structure function vs normalized separation, Eq. (5.37).

FIG. 11. Fourth order mixed structure function vs normalized separation.

FIG. 12. Sixth order longitudinal velocity structure function. Experiment, Tabeling et al. (Ref. 17).
Evidence for existence of tube-like structures

- Ashurst et al (1987)
- Horiuti DNS data; scale 4
Evidence for existence of tube-like structures

Horiuti DNS data; scale 4 (detail)

Horiuti DNS data; scale 5 (detail)
Evidence for existence of spiral structures

Vortices/particle paths in turbulence. DNS, $R_\lambda = 60$ (Flohr 2002)

Generalized 2C-3P models

- Colinear vortex embedded in time varying linear velocity field (outer flow)
- Velocity field produced by vortex "cylindrical": 2-co-ordinate, 3 component
Generalized 2C-3P models

- Columnar vortex embedded in time varying linear velocity field (outer flow)
- velocity field produced by vortex `cylindrical': 2-Co-ordinate, 3 component (2C-3P)

\[
\tilde{q}_i = \tilde{A}_{ij}(t)x_j = \tilde{S}_{ij}(t)x_j + \tilde{Q}_{ij}(t)x_j
\]

\[
\tilde{\zeta}_i(r,t) = \tilde{\xi}_i - 2\Omega_i + \omega_i,
\]

\[
v_i(r,t) = \tilde{A}_{ij}r_j - \varepsilon_{ijk}\Omega_j r_k + u_i
\]

\[
\frac{\partial}{\partial t} (v_i + \varepsilon_{ijk}\Omega_j r_k) + v_j \frac{\partial v_i}{\partial r_j} + 2\varepsilon_{ijk}\Omega_j v_k = \frac{\partial P^*}{\partial r_i} + \nu \nabla^2 r_i v_i
\]

\[
\frac{\partial}{\partial t} (\tilde{\zeta}_i + 2\tilde{\Omega}_i) + v_j \frac{\partial \tilde{\zeta}_i}{\partial r_j} = (\tilde{\zeta}_j + 2\tilde{\Omega}_j) \frac{\partial v_i}{\partial r_j} + \nu \nabla^2 r_i \tilde{\zeta}_i
\]
Generalized 2C-3P models

\[ \Psi = \Psi(r_1, r_2, t), \]
\[ u_i = u_i(r_1, r_2, t), \]
\[ \omega_i = \omega_i(r_1, r_2, t), \]

(Definition of 2C-3P)

\[ u_i = \varepsilon_{ijk} \frac{\partial \Psi_k}{\partial r_j}, \quad \frac{\partial \Psi_i}{\partial r_i} = 0, \quad \omega_i = -\nabla_r^2 \Psi_i \]

(Vector potential)

\[ \Omega_1 = -\tilde{A}_{23} \]
\[ \Omega_2 = \tilde{A}_{13} \]
\[ \Omega_3 = -\tilde{A}_{12} \]

(Evolution of vortex axes)
Generalized 2C-3P models

- **Axial vorticity equation (plus 2 other vorticity equations):**

\[
\frac{\partial \omega_3}{\partial t} + \left( \tilde{S}_{11} r_1 + \frac{\partial \Psi_3}{\partial r_2} \right) \frac{\partial \omega_3}{\partial r_1} + \left( 2\tilde{S}_{12} r_1 + \tilde{S}_{22} r_2 - \frac{\partial \Psi_3}{\partial r_1} \right) \frac{\partial \omega_3}{\partial r_2} = 2 \tilde{S}_{13} \omega_1 + 2 \tilde{S}_{23} \omega_2 + \tilde{S}_{33} \omega_3 + \nu \nabla_{r_i}^2 \omega_3
\]

\[
\omega_3 = \omega_3(r_1, r_2, t) + \tilde{\xi}_i(t)
\]

- **Many special cases possible:** *e.g.*

\[
\omega_1 = \omega_2 = 0 \text{ at } t = 0, \quad \tilde{\xi}_i = 0
\]

\[
\frac{\partial \omega_3}{\partial t} + \left( \tilde{S}_{11} r_1 + \frac{\partial \Psi_3}{\partial r_2} \right) \frac{\partial \omega_3}{\partial r_1} + \left( 2\tilde{S}_{12} r_1 + \tilde{S}_{22} r_2 - \frac{\partial \Psi_3}{\partial r_1} \right) \frac{\partial \omega_3}{\partial r_2} = \tilde{S}_{33} \omega_3 + \nu \nabla_{r_i}^2 \omega_3
\]

- **Describes Burgers vortex sheet and tube. Stretched-spiral vortex**
Stretched-Vortex Models of Turbulent Fine Scales

- Townsend (1951), Lundgren (1982), Pullin & Saffman (1993), Pullin & Lundgren (2001)

- Turbulence consists of an ensemble of stretched "vortex tubes" (cylindrical 2C-3P) structures

- Vortex tube axis direction random on unit sphere (isotropy)

- Mutual vortex-vortex interaction not modeled

- At each time t, each tube is a different point in its unsteady evolution

- Turbulence statistics:
  - \( <\text{volume integral}> = <\text{time integral}> \) over lifetime of tube (ergodic hypothesis)
  - Average over all vortex axis orientation

- Class of tractable models
Burgers vortex tube (Burgers, 1948)

- Steady axisymmetric solution of axial vorticity equation

\[ \omega_0(r) = \frac{a\Gamma_0}{4\pi \nu} \exp\left( -\frac{r^2a}{4\nu} \right) \]

- Energy (velocity) spectrum for turbulence modeled by an ensemble of Burgers vortices (Townsend, 1951)

\[ \frac{E}{(\epsilon \nu^5)^{1/4}} = \frac{2C}{k\eta} \exp\left( -2Ck^2\eta^2 \right) \]

- No cascade dynamics or inertial range
Spiral-vortex models (2C-3P)

- Several Generic Spiral types

Pearson-Abernathy/Moore spiral

Lundgren spiral

“Mixed” spiral
Stretched-spiral Vortex (Lundgren, 1982)

- Asymptotic solution of Navier-Stokes equations

\[ \tilde{\omega}_3(r, \theta, t) = e^{at} \sum_{n} f_n(r) e^{in[\theta - \Omega(r) t] - \nu n^2 \Lambda(r)^2 t^3/3} \]

- Velocity (energy) spectrum \( E(k) \sim k^{-5/3} \)
Stretched-spiral vortex; velocity (energy) spectral dynamics

- Time-evolving spectrum
- Early time: $k^{\alpha(-2)}$ (sheet-like)
- Late time: $k^{\alpha(-1)}$ (tube like)
- $k^\alpha(-5/3)$ is time average

- time increasing, top-> bottom, left-> right
- Sheet-> tube transition
- Cascade is extraction of energy from outer linear flow
Phenomenology of scalar spectra

- **Obukhov-Corrsin spectrum**
  \[ E_c(k) \sim \epsilon_c \epsilon^{-1/3} k^{-5/3}, \quad L^{-1} \ll k \ll \left( \frac{\nu^3}{\epsilon} \right)^{-1/4} \]

- **Batchelor spectrum**
  \[ E_c(k) \sim \epsilon_c \nu^{1/2} \epsilon^{-1/2} k^{-1}, \quad \left( \frac{\nu^3}{\epsilon} \right)^{-1/4} \ll k \ll \left( \frac{D^2 \nu}{\epsilon} \right)^{-1/4} \]

- **Range of scales**
  \[ \frac{L}{\left( \frac{D^2 \nu}{\epsilon} \right)^{1/4}} \sim Re^{3/4} Sc^{1/2}, \quad Sc = \frac{\nu}{D} \quad (\text{Schmidt number}) \]
Scalar transport equation

- Scalar convected and diffused within stretched vortex

- Solve axial vorticity equation and passive scalar convection/diffusion equation inside stretched vortex

Axial vorticity

\[
\frac{\partial \tilde{\omega}_3}{\partial t} + \frac{1}{\rho} \left( \frac{\partial \tilde{\psi}_3}{\partial \theta} \frac{\partial \tilde{\omega}_3}{\partial \rho} - \frac{\partial \tilde{\psi}_3}{\partial \rho} \frac{\partial \tilde{\omega}_3}{\partial \theta} \right) = \nu \nabla^2_2 \tilde{\omega}_3, \quad \nabla^2_2 \tilde{\psi}_3 = -\tilde{\omega}_3
\]

Passive scalar

\[
\frac{\partial c}{\partial t} + \frac{1}{\rho} \left( \frac{\partial \tilde{\psi}_3}{\partial \theta} \frac{\partial c}{\partial \rho} - \frac{\partial \tilde{\psi}_3}{\partial \rho} \frac{\partial c}{\partial \theta} \right) = D \nabla^2_2 c
\]
Solution of Transport Equation

- $\tilde{\omega}_3$, $\tilde{\psi}_3$ obtained from solution of axial vorticity equation. E.G. diffusing line vortex, Burgers vortex, stretched-spiral vortex

- Two-time analysis

  Fast time variable $\Omega \tau$,
  Slow time variables $T_\nu = (\nu \Lambda^2)^{1/3} \tau$
  $T_D = (D \Lambda^2)^{1/3} \tau$, $\Lambda = \frac{d\Omega}{d\rho}$

- Seek solution of form

$$\tilde{\psi}_3 = \tilde{\psi}^{(0)}(\rho, T_\nu) + \tau^{-2} \sum_{-\infty, n \neq 0} \tilde{\psi}_n^{(2)}(\rho, T_\nu) \exp(i \nu (\theta - \Omega \tau)) + ..$$

$$c = \sum_{-\infty}^{\infty} \left( \phi_n^{(0)}(\rho, T_\nu, T_D) + \tau^{-1} c_n^{(1)}(\rho, T_\nu, T_D) + .. \right) \exp(i \nu (\theta - \Omega \tau))$$
“Wrapping” of a linear scalar field by a diffusing line vortex.

\[ a = 0 \text{ (no axial stretching). } \Gamma_0/(2\pi \nu) = 1000. \]
Scalar variance spectrum

\[ E_c(k) = E_c^{(0)}(k) + E_c^{(1)}(k) \]

- \( E_c^{(0)}(k) \) component
  \[ E_c^{(0)}(k) = \frac{2}{3} a^{-1} \epsilon_c^{(0)} k^{-1} \exp \left( -\frac{2 D k^2}{3 a} \right) \]

- \( a = \frac{1}{\sqrt{15}} \left( \frac{\epsilon}{\nu} \right)^{1/2} \rightarrow A = 2\sqrt{15}/3, \quad \eta_b = \left( \frac{D^2 \nu}{\epsilon} \right)^{1/4} \)

  \[ E_c^{(0)}(k) = A \nu^{1/2} \epsilon^{-1/2} \epsilon_c^{(0)} k^{-1} \exp \left( -A k^2 \eta_b^2 \right) \]

- \( E_c^{(1)}(k) \) component
  \[ E_c^{(1)}(k) = C_1(k) k^{-5/3} \exp \left( -\frac{D k^2}{3 a} \right) \]
Scalar Variance Spectrum

- Initial structure

\[ \omega_3(r, \theta, 0) = 2 f_0 g(r) \sin(2\theta), \quad c(r, \theta, 0) = 2 c_0 g(r) \cos \theta \]

- \( E_c = E_c^{(0)} + E_c^{(1)} \), strain: \( a = \left( \frac{\epsilon}{15 \nu} \right)^{1/2} \)

\[ E_c^{(0)} = 2.58 \epsilon_c \nu^{1/2} \epsilon^{-1/2} k^{-1} \exp(-2.58 S_c^{-1} (k \eta)^2) \]

\[ E_c^{(1)} = \frac{4.71}{(\Gamma/\nu)^{1/3}} \epsilon_c \epsilon^{-1/3} k^{-5/3} \exp(-2.58 (2 + S_c^{-1}) (k \eta)^2) \]
Scalar Variance Spectrum

3-D Scalar spectrum. $Sc = 7$. $Sc = 700$. $\frac{c}{\nu} = 10^3$

1-D Scalar spectrum. $Sc = 7$. $Sc = 700$. $\frac{c}{\nu} = 10^3$

Symbols, Data, Gibson & Schwarz (1963)
Modeling Turbulence small scales

Spectral slope vs $Re_\lambda$. ● - grid turbulence, (Warhaft, 2000).
■ - Shear turbulence, (Sreenivasan, 1996).
Velocity-Scalar co-spectrum

- Velocity field $u(x, t)$, scalar field $c(x, t)$

- Velocity-scalar cross-spectrum $C_{uc}(k)$ measures velocity-scalar correlations

- Important for small-scale turbulent transport of scalars, SGS scalar-flux models

- Homogeneous turbulence in presence of mean scalar gradient

- $C_{uc}(k) \sim k^{-7/3}$, Lumley (1967)
Velocity-Scalar co-spectrum
(P. O’Gorman)

## Spectral Exponents

<table>
<thead>
<tr>
<th>Quantity</th>
<th>SSV</th>
<th>“Classical”</th>
</tr>
</thead>
<tbody>
<tr>
<td>velocity</td>
<td>$-5/3$</td>
<td>$-5/3$</td>
</tr>
<tr>
<td>pressure</td>
<td>$-7/3$</td>
<td>$-7/3$</td>
</tr>
<tr>
<td>scalar</td>
<td>$-1$</td>
<td>$-1$</td>
</tr>
<tr>
<td>scalar</td>
<td>$-5/3$</td>
<td>$-5/3$</td>
</tr>
<tr>
<td>scalar-velocity</td>
<td>$-5/3, -7/3$</td>
<td>$-7/3$</td>
</tr>
<tr>
<td>(vorticity)$^2$</td>
<td>$0$</td>
<td>?</td>
</tr>
</tbody>
</table>

Spectral exponents postdicted by stretched-spiral vortex
Velocity-gradient and vorticity statistics

- **Fix point and direction in space** (relative to lab axes)
- **Assume isotropy**
- **Calculate longitudinal velocity gradient** at point within vortex structure in terms of local principal rates of strain
- **Average over Euler angles** (vortex axis) and vortex cross-section in space, from known internal vortex structure (SSV)

\[
\left\langle \left( \frac{\partial u}{\partial x} \right)^n \right\rangle = \frac{1}{4\pi} \int_0^{2\pi} \int_0^\pi (e_1 \sin^2 \phi \cos^2 \chi \\
+ e_2 \sin^2 \phi \sin^2 \chi + e_3 \cos^2 \phi)^n \times \sin \phi \, d\phi \, d\chi,
\]

\[
\left\langle \frac{\partial u}{\partial x} \right\rangle = 0,
\]

\[
\left\langle \left( \frac{\partial u}{\partial x} \right)^2 \right\rangle = \frac{2(e_1^2 + e_2^2 + e_3^2)}{15},
\]

\[
\left\langle \left( \frac{\partial u}{\partial x} \right)^3 \right\rangle = \frac{8(e_1 e_2 e_3)}{35},
\]

\[
\left\langle \left( \frac{\partial u}{\partial x} \right)^4 \right\rangle = \frac{8(e_1^4 + e_2^4 + e_3^4)}{105},
\]

- **Result; moments of velocity gradient and vorticity pdfs** as functions of order \(2^p, p \geq 2\), and Taylor Re

\[
F_{2p} = \hat{F}_{2p} R_\lambda^{p/2 - 3/4}, \quad S_{2p+1} = - \hat{S}_{2p+1} R_\lambda^{p/2 - 3/4}
\]

\[
G_{2p} = \hat{G}_{2p} R_\lambda^{p/2 - 3/4}
\]
FIG. 4. Flatness factor $F_4$ vs $R_\lambda$. 
---: $\phi = 0.35$; 
-----: $\phi = 0.475$; 
- - - : $\phi = 0.7$. Symbols are a compilation of experimental data, Van Atta and Antonia\textsuperscript{19} (reproduced with permission).
Longitudinal velocity structure functions

- Longitudinal velocity structure function of order $m$
  
  \[ B_m(r) = (u'_p - u_p)^m \]

- 2C-3P models; 5-dimensional integral as a function of separation $r$

- Monte-Carlo numerical integration

- Results for stretched-spiral vortex (PF, 1996)

- Agreement with experiment poor for large $m$

FIG. 4. Longitudinal velocity structure functions $(u'_p - u_p)^m/(\nu)^{3/4}$ for the stretched-spiral vortex versus $r/\eta$. Monte Carlo, $R_\lambda=500$. — $m=2$, --- $m=4$. ⋯ $m=6$, --- $m=8$: Symbols—experiment, Tabeling (Ref. 11), $R_\lambda=507$. Circles $m=2$, crosses $m=4$, up-triangles $m=6$, down-triangles $m=8$. 
Structure-based models of turbulence small scales

- Velocity/vorticity field based on assumed vortex structure; HSV, Burgers vortex, SSV
  - Requires solutions (approximate?) to Euler/NS
  - Complex integrations for statistics

- Stretched-spiral vortex (Lundgren, 1982)
  - Unifies Kolmogorov, Obukov-Corrsin/Batchelor, Lumley spectra
  - Good results for velocity-gradient/vorticity statistics (1-point)
  - Firm experimental/DNS evidence; open question?

- Problems:
  - Poor results for higher-order velocity structure functions (2-point)
  - Contains internal parameters (e.g. circulation etc.) not easily related to outer flow variables

- Basis for subgrid-scale modeling?
Small-scale turbulence; theory, phenomenology and applications

Stretched vortices as basis for SGS modeling

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Cargèse, August 13-26, 2007

Ashish Misra, Tobias Voelkl
Overview

• Motivation; why LES?

• Expectations of LES. Some present models.

• Stretched-vortex sub-grid scale model
  – Structure-based SGS model (2C-3P)
  – SGS stresses
  – SGS vortex orientations

• Example Applications
  – Decaying incompressible turbulence
  – Channel flow at moderate Re_\tau

• Subgrid-flux model for passive scalar
  – Overholt-Pope test
Why LES?

### Table 2.
Characteristics of some representative channel-flow simulations.

<table>
<thead>
<tr>
<th>$Re_\tau$</th>
<th>$L_x/\delta$</th>
<th>$L_z/\delta$</th>
<th>Points</th>
<th>Year</th>
</tr>
</thead>
<tbody>
<tr>
<td>590</td>
<td>6</td>
<td>3</td>
<td>40 M</td>
<td>1997  [12]</td>
</tr>
<tr>
<td>550</td>
<td>25</td>
<td>12</td>
<td>600 M</td>
<td>2001  [13]</td>
</tr>
<tr>
<td>950</td>
<td>25</td>
<td>9</td>
<td>4 G</td>
<td>2003  [14]</td>
</tr>
<tr>
<td>1900</td>
<td>3</td>
<td>1.5</td>
<td>450 M</td>
<td>2003  [14]</td>
</tr>
<tr>
<td>10000</td>
<td>12</td>
<td>6</td>
<td>900 T</td>
<td>2015?</td>
</tr>
</tbody>
</table>

- Jimenez (JOT, 2003)
Large-Eddy Simulation

physical space: fine-scale fluctuations not resolved, their influence is modeled.

spectral space: resolved range, $k < k_c$ (cutoff wavenumber $k_c$), subgrid range $k > k_c$.  
LES and SGS modeling

- LES equations

\[
\frac{\partial \tilde{U}_i}{\partial t} + \frac{\partial}{\partial x_j} (\tilde{U}_i \tilde{U}_j) = -\frac{\partial \tilde{P}}{\partial x_i} - \frac{\partial T_{ij}}{\partial x_j} + \nu \frac{\partial^2 \tilde{U}_i}{\partial x_j \partial x_j} + F_i
\]

Large-eddy simulation (LES) makes modeling assumptions;

- \( T_{ij} = \tilde{U}_i \tilde{U}_j - \tilde{\tilde{U}}_i \tilde{\tilde{U}}_j \); Subgrid stresses are replaced by some model \( T_{ij} \); subgrid stress (SGS) model:

\[
T_{ij} = T_{ij}[\tilde{U}_j, \partial \tilde{U}_i / \partial x_j, ...]
\]

- \( \tilde{U}_j \rightarrow \hat{U}_j \); Filtered field \( \tilde{U}_j \) is modeled by a computed under-resolved field \( \hat{U}_j \).
What can (should) we expect from LES?

- Robustness for different flows at large Re
- One-point statistics (velocity, density, concentration)
- Two-point statistics across full wavenumber range?
- Predictive for turbulent mixing
- Estimates for full turbulent fields
  - *Not just the ‘filtered’ part*
  - *Multiscale LES*
- Knowledge of Reynolds number; what is it?
- Fast convergence to DNS
  - *In some cases DNS is not available*
  - *DNS not possible for compressible turbulence containing strong shocks*
• Smagorinsky
• Dynamic Smagorinsky (CTR, Germano)
• Eddy-viscosity structure function (Lesieur)
• Scale-similarity (Bardina)
• MILES (Boris, Grinstein))
• Approximate deconvolution model (Leonard, Adams)
• Optimal LES (Adrian, Moser)
• Stretched-vortex subgrid model
Explicit SGS model; stretched-vortex model

512^3 DNS (scale 4)

• Small scales of turbulence Intense vorticity in form of “worms”
  Ashurst, Jimenez et al (1993)

• Can this be used as a basis of a structure-based sub-grid scale model?
Explicit SGS model; stretched-vortex model

- Structure-based approach
- Subgrid motion represented by nearly axisymmetric vortex tube within each cell
- Local solution of NS equations for stretched spiral vortex
  - Lundgren (1982), Pullin & Lundgren (2001)
- Subgrid transport:

\[
\tau_{ij} = \bar{\rho} \tilde{K}(\delta_{ij} - e_i^u e_j^u)
\]

\[
q_i^T = -\frac{\bar{\rho} \Delta_c}{2} \tilde{K}^{1/2}(\delta_{ij} - e_i^u e_j^u) \frac{\partial (\tilde{e}_p \tilde{T})}{\partial x_j}
\]

\[
q_i^\psi = -\frac{\bar{\rho} \Delta_c}{2} \tilde{K}^{1/2}(\delta_{ij} - e_i^u e_j^u) \frac{\partial \tilde{\psi}}{\partial x_j}
\]

\[
\tilde{K} = \int_{k_c}^{\infty} E(k) dk, \quad k_c = \pi / \Delta_c
\]
Model parameters

- Subgrid energy spectrum (Lundgren, 1982)

\[
E(k) = K_0 \varepsilon^{2/3} k^{-5/3} \exp \left[ -2k^2 \nu / (3|\tilde{a}|) \right]
\]

\[
\tilde{a} = \tilde{S}_{ij} e_i e_j, \quad \tilde{S}_{ij} = \frac{1}{2} \left( \frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right)
\]

- Parameters obtained from resolved-scale velocity structure-functions

\[
K_0 \varepsilon^{2/3} = \frac{\overline{F}_2(\Delta)}{\Delta^{2/3} A}, \quad A = 4 \int_0^{\pi} s^{-5/3} (1 - s^{-1} \sin \theta) ds \approx 1.90695
\]

\[
\overline{F}_2(\Delta) = \frac{1}{6} \sum_{j=1}^{3} \left( \delta \tilde{u}_1^2 + \delta \tilde{u}_2^2 + \delta \tilde{u}_3^2 + \delta \tilde{u}_1^2 + \delta \tilde{u}_2^2 + \delta \tilde{u}_3^2 \right)_j,
\]

- Subgrid vortex orientation, \( \mathbf{e} \)
  - \( \lambda \) : fraction aligned with principal extensional eigenvector of resolved rate-of-strain tensor (corresponding eigenvalue, \( \lambda_3 \))
  - \( (1- \lambda) \) : fraction aligned with resolved vorticity vector, \( \mathbf{\omega} \) (Misra & Pullin 1997)

\[
\lambda = \frac{\lambda_3}{\lambda_3 + \|\mathbf{\omega}\|}
\]
Decay of homogeneous turbulence

- 32^3 LES of decaying turbulence; $R_\lambda = 70$ (PF, 1997)
- Data; Comte-Bellot & Corssin (1971)

Resolved-scale energy
Subgrid-scale-scale energy
Decay of homogeneous turbulence

- $32^3$ LES of decaying turbulence; $R_\lambda = 70$ (PF, 1997)
- Data; Comte-Bellot & Corssin (1971)

Velocity (energy) spectrum
LES of turbulent channel flow

Domain size: $2.5\pi\delta \times \pi\delta \times 2\delta$, effective resolution: $48 \times 64 \times 65$. 
LES of turbulent channel flow

\[ Re_\tau = 180, \quad \omega_z = 15u_\tau/h \text{ (purple)} \]
\[ \text{and} \quad \omega_z = -15u_\tau/h \text{ (yellow)} \]
Rotating channel flow

Resolution: $48 \times 64 \times 43$ (DNS: $128 \times 128 \times 128$)

$Ro_T = 1.56$, $\omega_z = \pm 15u_T/h$

$Ro_T = 7.625$, $\omega_z = \pm 15u_T/h$
Filtered equation for a passive scalar $\phi$ is

$$\frac{\partial \tilde{\phi}}{\partial t} + \frac{\partial}{\partial x_j} \left( \tilde{\phi} \tilde{U}_j \right) = - \frac{\partial g_j}{\partial x_j} + D \frac{\partial^2 \tilde{\phi}}{\partial x_j \partial x_j}$$

$$g_j = \phi \tilde{U}_j - \tilde{\phi} \tilde{U}_j$$

$g_j$ is the subgrid flux of $\phi$ by the turbulent velocity field.

We model $g_j$ by the winding of $\tilde{\phi}$ field by an axisymmetric model subgrid vortex.
SGS model for subgrid flux of a passive scalar

- Subgrid velocity field. Scalar convection equation

\[ u_\theta = r \Omega(r), \quad u_r = u_{x_3} = 0, \quad \frac{\partial \phi}{\partial t} + \Omega(r) \frac{\partial \phi}{\partial \theta} = 0 \]

\[ \phi(r, \theta, t) = r \cos[\theta - \Omega t] \left( \frac{\partial \tilde{\phi}}{\partial x_1} \right) + r \sin[\theta - \Omega t] \left( \frac{\partial \tilde{\phi}}{\partial x_2} \right) + \text{background} \]
SGS model for subgrid flux of a passive scalar

- Average over cylinder, \( R_1 = \Delta \), stirring time \( T \) and pdf of \( \Gamma \)

\[
g'_1 + i g'_2 = \frac{1}{\pi R_1^2 T} \int_{-\infty}^{\infty} \int_{0}^{2\pi} \int_{0}^{R_1} \int_{0}^{T} \phi(r, \theta, t) i u_\theta e^{i \theta} p(\Gamma) \, d\theta \, r \, dr \, dt \, d\Gamma
\]

- In laboratory co-ordinates

\[
g_j = -\frac{1}{2} KT \left( \delta_{jp} - e^v_j e^v_p \right) \frac{\partial \tilde{\phi}}{\partial x_p}, \quad K = \frac{1}{R_1^2} \int_{0}^{R_1} r^3 \Omega^2(r) \, dr
\]

- Assume \( T = \gamma \Delta x / K^{1/2} \). Argument based on scalar, velocity structure functions then gives

\[
\gamma = \frac{2}{\pi \beta} \left( \frac{2}{3K_0} \right)^{1/2}, \quad K_0 = 1.67, \quad \beta = 0.67 \rightarrow \gamma = 0.74
\]
SGS model for subgrid flux of a passive scalar

- Scalar flux subgrid model - tensor diffusivity

\[ g_i = -\frac{\gamma \pi}{2 k_c} K^{\frac{1}{2}} (\delta_{ip} - e_i^v e_p^v) \frac{\partial \phi}{\partial x_p} \]

SGS \[ T_{ij} = K (\delta_{ij} - e_i^v e_j^v) \]

- Model parameter \( \gamma = 1 \) (present demonstration)

- Model appropriate for \( Sc = \nu/D = O(1) \)

- Model suggests scalar gradient is orthogonal to small scale vorticity (Ruetsch & Ferziger, DNS, 1997).
Passive scalar with imposed mean scalar gradient in forced homogeneous turbulence

- Forced turbulence in $(2\pi)^3$ box $(32^3)$. $\tilde{\phi} = \alpha_1 x_1 + \phi$

$$\frac{1}{2} \frac{\partial}{\partial t} \langle \tilde{\phi}^2 \rangle + \alpha_1 \langle \tilde{\phi} \tilde{U}_1 \rangle = \left\langle g_i \frac{\partial \tilde{\phi}}{\partial x_i} \right\rangle - D \left\langle \left( \frac{\partial \tilde{\phi}}{\partial x_i} \right)^2 \right\rangle$$

- $\alpha_1$ is preserved by the evolution

- Statistical steady state for $\langle \tilde{\phi}^2 \rangle$

- DNS, $R_\lambda = 27 - 180$ [Overholt and Pope, Phys Fluids, 1996]
Passive scalar with imposed mean scalar gradient in forced homogeneous turbulence

Scalar variance $\langle \phi^2 \rangle / (\alpha_1 L_s)^2$ versus $t$. $Sc = 0.7$

$L_c = w^3 / \varepsilon$, $T_L = L/u' \approx 2.2$

Scalar variance, $32^3$ LES compared to DNS - Overholt & Pope (1996), $32^3 - 256^3$. $Sc = 0.7$. 
Stretched-vortices for SGS modeling

- Structure-based sub-grid-scale model for LES
- Uses stretched-spiral vortex as subgrid vorticity element
- 2-point SGS statistics known (spectrum, structure function)
- Uses second order velocity structure functions to dynamically determine model parameters
- Need model for SGS vortex orientations
- Good performance for standard LES tests; decaying turbulence and channel flow at moderate Reynolds number
- Problems:
  - Each new/different SGS physics problem requires new analysis
  - Contains internal parameters (e.g. circulation etc.) not easily related to outer flow variables. Not needed for simple SGS momentum/scalar flux modeling but may be important for more complex SGS physics.
- Promise; may admit SGS extension of some turbulence statistics, i.e. multi-scale modeling.
Small-scale turbulence; theory, phenomenology and applications

Large-eddy simulation with stretched-vortex SGS model

D.I. Pullin
Graduate Aeronautical Laboratories
California Institute of Technology

Cargèse, August 13-26, 2007

Carlos Pantano, David Hill, Ralf Deiterding, Daniel Chung
Ravi samtaney, Branko Kosovic
Overview

• LES of compressible, shock-driven turbulence
  – Extension of SGS model to compressible flow
  – Issues of numerical methodology
  – Adaptive Mesh Refinement (AMR)

• LES of Richtmyer-Meshkov instability with re-shock
  – Growth of mixing layer thickness
  – Resolved-scale turbulence statistics
  – Multi-scale modeling; subgrid extension of turbulence statistics
  – Effect of magnetic field
  – Cylindrical RM instability

• Near-wall SGS modeling
  – No large eddies near the wall
  – Local inner scaling and near-wall modeling
  – Virtual-wall model
  – LES of channel flow at large Re_\tau
• SGS models need extension to deal with compressible flow

• Standard LES methodology not well suited to LES of shock-driven turbulence
  – Numerical methods for shock-capturing and LES `orthogonal'.
    • LES with explicit SGS model requires dissipation-free numerical scheme
    • Shock-capturing numerical schemes are essentially SGS models for shocks; they are generally extremely numerically dissipative even away from shocks.

• Owing to its largely hyperbolic character, gas-dynamic turbulence can benefit greatly from Adaptive-Mesh-Refinement (AMR) technology
SAMR and AMROC (R. Deiterding)

- Structured Adaptive Mesh Refinement (SAMR)
- Adaptive Mesh Refinement Object Oriented C++ (AMROC)
- Berger & Colella's algorithm for conservation laws of the form:
  \[ \frac{\partial q}{\partial t} + \frac{\partial}{\partial x_k} f^k(q) = 0, \]
- Hierarchical data structure contains the solution vector and fluxes
- On each patch, a standard Cartesian fluid solver is applied to march the solution (e.g. WENO/TCD)
- Boundary conditions and synchronization between patches is accomplished by filling ghost cells with interpolated data.
  - ghost cell interpolation is an approximation for non-linear systems of equations

Figure 1. AMR hierarchy.
LES of compressible turbulence. LES and strong shocks (D. Hill).
Hybrid WENO-TCDS algorithm:

- Numerical methods for shock-capturing and LES `orthogonal’.
- Our solution: hybrid technique: blending Weighted Essentially Non-Oscillatory (WENO) scheme with Tuned Centered-Difference (TCD) stencil.
- WENO in regions of very-large density ratio (Shocks)
  - But WENO is not suitable for LES in smooth regions away from shocks.
  - Upwinding strategy is too dissipative
- TCD stencil in smooth regions away from shocks
  - Low numerical dissipation (centered method)
  - optimized for minimum resolved-scale discretization error in LES (Ghosal, 1996)
  - 5- or 7-point stencil trades off formal order of accuracy for small dispersion errors
- Target WENO stencil = TCD stencil
- In practice, target TCD stencil not always achieved; switch is used based on acceptable WENO smoothness measure
- Hybrid method designed for LES in presence of strong shocks
Test I: decay of compressible homogeneous turbulence

- $256^3$ DNS of compressible decaying turbulence. Fully resolved (R. Samtaney)
- 10-th order compact Pade scheme
- $R_{\lambda} \sim 70$, $M_t = 0.49$ (shocklets in turbulence)

[Images of Density slices and Vorticity slices]
Test 1; decay of compressible homogeneous turbulence

Density slices. Shocklets (weak shocks) evident
DNS and LES of decaying compressible turbulence; decay of TKE

- $M_t = 0.488$, $R_{\lambda} = 70$.
- Black; $256^3$ DNS (10-th order Pade)
- Other; $32^3$ LES
- Stretched-vortex SGS model

![Graphs showing resolved KE over time](image)

- **DNS**
- **Weno - LES**

**5-pt Stencils.**

- Ghosal-Optimal (2nd order)
- Standard (4th order)

**WENO scheme**

**Hybrid WENO-TCD scheme**
Test II: Riemann 1D Wave Exact solution of 1D Euler

Hybrid WENO-TCD scheme
Richtmyer-Meshkov (R-M) Instability

\[
\frac{\partial \omega}{\partial t} + u \cdot \nabla \omega = \omega \cdot \nabla u - \omega \nabla \cdot u + \frac{1}{\rho^2} \nabla(p) \times \nabla(p)
\]

Incident shock
Interface
Self-stretching and dilatation
Barotropic vorticity Generation
Advection
Shock reflects off end
Misalignment of contact and shock
Richtmyer-Meshkov (R-M) Instability

- Astrophysics: A role in the description of the explosion of supernovae (Smarr 1981, Arnett 1989.)
  - *Supernova 1987A* R. McCray (JILA)  *Images from HST*

- A role in Inertial confinement fusion design (Lund 1997)
  - *Laser pulse drives pressure waves*
- National lab applications
- Canonical example of shock-turbulence interaction
Flow Description

Shock tube, flow conditions (Vetter & Sturtevant 1995) and 1-D wave diagram

Table 1: The test conditions and growth rates of the interface thickness from Vetter & Sturtevant (1995).
Computational runs: unigrid

- Unigrid simulations
- QSC supercomputer (Los Alamos)

<table>
<thead>
<tr>
<th></th>
<th>II$^b$</th>
<th>VI$^b$</th>
<th>VI$^e$</th>
<th>VII$^b$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Incident Mach number</td>
<td>1.24</td>
<td>1.50</td>
<td>1.50</td>
<td>1.98</td>
</tr>
<tr>
<td>Computational grid</td>
<td>616x128$^2$</td>
<td>388x128$^2$</td>
<td>776x256$^2$</td>
<td>327x128$^2$</td>
</tr>
<tr>
<td>Computational resolution:$\Delta x$ (cm)</td>
<td>0.21</td>
<td>0.21</td>
<td>0.105</td>
<td>0.21</td>
</tr>
<tr>
<td>Simulation time (ms)</td>
<td>16.62</td>
<td>6.35</td>
<td>12.0</td>
<td>2.57</td>
</tr>
<tr>
<td>CPU hours</td>
<td>3,982</td>
<td>972</td>
<td>38,400</td>
<td>544</td>
</tr>
</tbody>
</table>

Table 1: The computational cost in CPU hours for each of the runs. Simulation $VI^e$ is a higher resolution version of $VI^b$ computed to about twice the experimental time.
LES of planar Richtmyer-Meshkov instability

- Vetter & Sturtevant (1995) RMI with reshock off end wall
- Air/SF$_6$, Mach=1.5
- 3 levels of refinement
Growth of turbulent mixing zone

T = 0. ms
T = 3.6 ms
T = 10.0 ms
Growth of turbulent mixing zone

\[ \langle f(x, t) \rangle = \frac{1}{A} \int \int f(x, y, z, t) dydz \]
\[ \delta_{MZ}(t) = 4 \int_{\text{tube}} (1 - \langle \psi \rangle) \langle \psi \rangle dx \]

y-z plane-averaged mixing-layer width compared with Vetter & Sturtevant (1995)

Case VI\textsuperscript{b} (Mach 1.24)

Case VII\textsuperscript{b} (Mach 1.98)

Case Vle; 776x256x256
Kinetic energy in mixing layer
Turbulence statistics

\[
\langle \tilde{K}_{res} \rangle = \frac{1}{2} \left( \frac{\langle \rho \tilde{u}_k \tilde{u}_k \rangle}{\langle \rho \rangle} - \frac{\langle \rho \tilde{u}_k \rangle \langle \rho \tilde{u}_k \rangle}{\langle \rho \rangle^2} \right), \quad \langle \tilde{K}_{sgs} \rangle = \frac{\langle \tau_{kk} \rangle}{2\langle \rho \rangle} \\
\langle \epsilon_{res} \rangle = \frac{\langle \sigma_{ij}' \tilde{S}_{ij}' \rangle}{\langle \rho \rangle}, \quad \langle \epsilon_{sgs} \rangle = -\frac{\langle \tau_{ij}' \tilde{S}_{ij}' \rangle}{\langle \rho \rangle} \\
K = \langle \tilde{K}_{res} \rangle + \langle \tilde{K}_{sgs} \rangle, \quad u' = \sqrt{\frac{2K}{3}}, \quad M_t = \frac{u'}{\langle c \rangle} \\
Re_T = \frac{u' \ell}{\langle \nu \rangle}, \quad \ell = \frac{u'^3}{\epsilon} \\
\eta = \left( \frac{<\nu^3>}{<\epsilon_{res} > + <\epsilon_{sgs} >} \right)^{1/4}
\]
y-z plane-averaged quantities after reshock (10 ms)

- Turbulent (rms) Mach number and sound speed
- Density variance
- Density and gamma
- Decay of Reynolds number
y-z plane-averaged quantities after reshock

Resolved and subgrid scale TKE
\[ t = 10\text{ms (after reshock)} \]

Resolved and subgrid scale dissipation
\[ t = 10\text{ms (after reshock)} \]

Solid; resolved. Dashed; subgrid
Resolved-scale radial spectra in y-z plane

Radial spectrum of x-velocity, center of mixing layer

Radial spectrum of density (solid) and mixture fraction, center of mixing layer
Subgrid continuation

- Stretched-spiral vortex SGS model used for subgrid continuation
  - Contains description of local anisotropy
  - Computation of local and plane-averaged Kolmorogov scale $\eta$
  - Parameters computed from LES (structure functions)

\[
E(k) = C_0 \epsilon^{2/3} k^{-5/3} \exp[-2k^2 \nu / (3|\bar{u}|)]
\]

\[
\tilde{a} = \tilde{S}_{ij} e_i^v e_j^v, \quad \tilde{S}_{ij} = \frac{1}{2} \left( \frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right)
\]

\[
E_{qq}^{2D}(k_r, \alpha_0) = \frac{2k_r}{\pi} \int_{k_r}^{[k_r/\cos \alpha_o]} \frac{E(\kappa)}{\left(\kappa^2 - k_r^2\right)^{1/2}\left(\kappa^2 - \kappa^2 \cos^2 \alpha_o\right)^{1/2}} \, d\kappa.
\]

\[
E_{33}^{2D}(k_r, \alpha_0) = \frac{2k_r}{\pi} \int_{k_r}^{[k_r/\cos \alpha_o]} \frac{(k_r^2 - \kappa^2 \cos^2 \alpha_o)^{1/2} E(\kappa)}{\kappa^2 (\kappa^2 - k_r^2)^{1/2}} \, d\kappa.
\]
Subgrid continuation of radial velocity spectra

• Radial (in k-space) velocity spectrum on center plane of mixing layer
  – Resolved-scale spectrum (solid)
  – Subgrid continuation (dashed)
  – Parameters computed from LES (structure functions)

• Subgrid velocity spectrum in dissipation range
  – Log-linear scale
  – Note exponential roll-off
Subgrid continuation of radial velocity spectra. Anisotropy of in-plane and normal velocity spectra

- Radial spectrum of $u$ (top) and $u+w$ (below)
  - Resolved-scale spectrum (solid)
  - Subgrid continuation (dashed)

- Measure of anisotropy for radial velocity spectra
  - Resolved-scale spectrum (solid)
  - Subgrid continuation (dashed)
Subgrid continuation of scalar spectrum in y-z plane

Scalar spectrum for stretched-spiral vortex

Pullin & Lundgren (2000)

\[ E_{\psi}(k) = K_{\psi} \left( k^{-5/3} \exp\left(-\frac{(4\nu + 2D)k^2}{3\bar{a}}\right) + \frac{8}{5\pi} \left( \frac{2\Gamma}{\bar{a}} \right)^{1/3} k^{-1} \exp\left(-\frac{2Dk^2}{3\bar{a}}\right) \right) \]

\[ \tilde{F}_{2}^{\psi}(\Delta) = 4K_{\psi} \Delta^{2/3} \int_{0}^{\pi} s^{-5/3} + \frac{8}{5\pi} \left( \frac{2\Gamma}{\bar{a}\Delta^2} \right)^{1/3} s^{-1} \left( 1 - \frac{\sin s}{s} \right) ds \]

Resolved-scale and continued scalar spectrum in center y-z plane, \( t = 10\,\text{ms} \). Left to right, \( Sc = 1, 1000, 1000,000 \)
Favre P.D.F. $P(\psi)$ of mixture fraction (resolved scales)
P.D.F. of mixture fraction with subgrid correction

\[
\tilde{P}_{sgs}(\psi, \tilde{\psi}, \sigma_\psi^2; x, t) = \tilde{P}_{sgs}(\psi|\tilde{\psi}, \sigma_\psi^2)\tilde{P}_{sgs}(\tilde{\psi}, \sigma_\psi^2; x, t)
\]

\[
\tilde{P}_{sgs}(\psi; x, t) = \int \int \tilde{P}_{sgs}(\psi|\tilde{\psi}, \sigma_\psi^2)\tilde{P}_{sgs}(\tilde{\psi}, \sigma_\psi^2; x, t)\, d\tilde{\psi}d\sigma_\psi^2
\]

\[
\tilde{P}(\psi; x, t) \approx \frac{\langle \tilde{p}\tilde{P}_{sgs}(\psi; x, t) \rangle}{\langle \tilde{p}(x, t) \rangle}
\]

\[
\tilde{P}_{sgs}(\psi; x, t) = \frac{\Gamma(a + b)}{\Gamma(a)\Gamma(b)}\psi^{a-1}(1 - \psi)^{b-1}
\]

\[
a = \psi(1 - \psi)\sigma_\psi^{-2} - 1, \quad b = a(\psi^{-1} - 1)
\]

P.D.F. of mixture fraction in center y-z plane, t = 10ms. Resolved-scale and Sc = 1, 1000,000
Suppression of RM instability by Magnetic Field
(V. Wheatley, R. Samtaney)

- Suppression due to change in shock refraction process at interface when $B \neq 0$ (Wheatley, Pullin & Samtaney, JFM 2004)
- Linear initial-value problem for impulsive acceleration of interface in presence of magnetic field solved exactly

Vorticity (top) and $\rho$ (bottom) at $t = 1.8$, $B = 0$, interface unstable

Vorticity (top) and $\rho$ (bottom) at $t = 1.8$, $B \neq 0$, instability suppressed
Analysis: Solution Features

Solution consists of:

• Inner region of rotational flow
• 2 small amplitude Alfvén shocks that carry circulation
• 2 outer irrotational regions

Notes:

• $w^*(0, t)$ is interfacial growth rate
• this decays to zero as Alfvén shocks propagate away
Cylindrical RMI: Flow Description

Flow conditions and 1-D wave diagram \((r,t)\)
Cylindrical RMI; $M_0=1.3$, 90 degree wedge (M. Lombardini)

- WENO-TCD with LES (SV model)
- Adaptive Mesh Refinement (AMROC)
  Ghost Fluid Method (inner and outer cylindrical boundaries)
- Initial conditions:
  - $M_0 = 1.3$ or 2.0 or 3.0
  - Air/SF$_6$ (Atwood number = 2/3)
  - “egg-carton” + smaller symmetry breaking perturbation with random phase
  - Chisnell’s converging flow behind the shock wave
- Resolution:
  - Base grid 83 x 83 x 51
  - 2 additional levels of refinement
  - Equivalent refined resolution 332 x 332 x 204
Growth of turbulent mixing zone ($M_0=2.0$)

- $t = 0. \text{ ms}$: Initial condition
- $t = 1.45 \text{ ms}$: After first shock interaction
- $t = 5.13 \text{ ms}$: After first reschock
Turbulent channel flow

\[-\delta \frac{\partial p}{\partial x_1} = \nu \left( \frac{\partial u_1}{\partial x_3} \right)_{\text{wall}} \equiv u_\tau^2, \quad \text{Re}_\tau = u_\tau \delta / \nu\]
A physical-space version of the stretched-vortex subgrid-stress model for large-eddy simulation

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FIG. 8. Model “dissipation” ratio $\varepsilon_{\text{sgs}}/(\bar{\varepsilon}_{\text{elc}} + \varepsilon_{\text{sgs}})$, - - - - $Re_{\tau} = 1017$; - - - - $Re_{\tau} = 590$. $Re_{\tau} = 180$. 
No large eddies near wall

Ten questions concerning the large-eddy simulation of turbulent flows

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A second example is high Reynolds number near-wall flows, the simplest specific case being the turbulent boundary layer on a smooth wall. The wall shear stress—all-important in aerodynamic applications—arises from momentum transfer from the outer flow through the boundary layer to the wall. In the viscous near-wall region, the momentum transfer is effected by the near-wall structures, the length scale of which scales with the tiny viscous length scale. As Bradshaw has succinctly put it: in the viscous near-wall region there are no large eddies. But, as has been appreciated at least since Chapman [15], the near-wall motions cannot be resolved in high-Reynolds number LES, but must instead be modelled (to avoid impracticable computational requirements that increase as a power of Reynolds number, as in DNS).
Near-wall filtering

Streamwise and spanwise Gaussian filter

$$\tilde{Q}(x_1, x_2, x_3, t) \equiv \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} Q(x'_1, x'_2, x_3, t) G_1(x_1, x'_1; \Delta_1) G_2(x_2, x'_2; \Delta_2) \, dx'_1 \, dx'_2$$

$$\Delta_1, \Delta_2 \gg \nu/u_\tau$$

Wall-normal top-hat filter

$$\langle Q \rangle(x_1, x_2, t) \equiv \frac{1}{h} \int_{0}^{h} \tilde{Q}(x_1, x_2, x'_3, t) \, dx'_3$$

$$\nu/u_\tau = \delta/Re_\tau \ll h \ll \delta$$

$$\delta = 1900\nu/u_\tau$$

$$\Delta_2 = 3000\nu/u_\tau$$

$$\Delta_1 = 6000\nu/u_\tau$$

http://torroja.dmt.upm.es/ftp/channels/
Local inner scaling

Filtered streamwise momentum equation

$$\frac{\partial \langle u_1 \rangle}{\partial t} = \left( -\frac{1}{h} u_3 u_1 - \frac{\partial \tilde{p}}{\partial x_1} + \frac{\nu}{h} \left[ \frac{\partial \tilde{u}_1}{\partial x_3} - u'_0 \right] \right)_{x_3=h}$$

$$u'_0 (x_1, x_2, t) \equiv \left( \frac{\partial \tilde{u}_1}{\partial x_3} \right)_{x_3=0} = \frac{\tilde{u}_r^2 (x_1, x_2, t)}{\nu}$$

Law of the wall in a local sense

$$\tilde{u}_1^+ = F \left( x_3^+ \right) \iff \frac{\tilde{u}_1 (x_1, x_2, x_3, t)}{(\nu u'_0)^{1/2}} = F \left( \frac{x_3}{(\nu / u'_0)^{1/2}} \right)$$

$$\frac{\partial \langle u_1 \rangle}{\partial t} = \frac{\langle \tilde{u}_1 \rangle}{2 u'_0} \frac{\partial u'_0}{\partial t}$$

Local shear stress equation

$$\frac{\partial u'_0}{\partial t} = \frac{2 u'_0}{\langle u_1 \rangle_{x_3=h}} \left( -\frac{1}{h} u_3 u_1 - \frac{\partial \tilde{p}}{\partial x_1} + \frac{\nu}{h} \left[ \frac{\partial \tilde{u}_1}{\partial x_3} - u'_0 \right] \right)_{x_3=h}$$
Fluctuating virtual-wall BC

\[ \tilde{u}_1^+ (x_1, x_2, h_0, t) = F(h_0^+) = h_0^+, \quad h_0^+ \leq 10 \]
Extended stretched-vortex SGS model

LES decomposition

\[ u_i (x, t) = \widetilde{U}_i (x, t) + U_i (x, t) \]

Dynamic alignment of subgrid vortices

\[ \frac{\partial e_i^v}{\partial t} = e_j^v \frac{\partial \widetilde{U}_i}{\partial x_j} - e_i^v e_k^v e_j^v \frac{\partial \widetilde{U}_k}{\partial x_j} \]

Additional stresses from subgrid stretched-vortex wrapping axial velocity.


\[ T_{1j} = \widetilde{U}_i \widetilde{U}_j + \widetilde{U}_i \widetilde{U}_j + \widetilde{U}_i \widetilde{U}_j \]

\[ = K (\delta_{ij} - e_i^v e_j^v) - \gamma \frac{1}{2} \Delta c K^{1/2} \left( e_j^v e_k^v \frac{\partial \widetilde{U}_k}{\partial x_l} (\delta_{li} - e_i^v e_j^v) + e_i^v e_k^v \frac{\partial \widetilde{U}_k}{\partial x_l} (\delta_{lj} - e_l^v e_j^v) \right) \]

\[ (e_1^v, e_2^v, e_3^v) = (1, 0, 0) \Rightarrow T_{13} = -\gamma \frac{1}{2} \Delta c K^{1/2} \frac{\partial \widetilde{U}_1}{\partial x_3} \]
1) Time march local shear stress equation.

\[
\frac{\partial u_0'}{\partial t} = \frac{2 u_0'}{(u_1)_{x_3=h}} \left( -\frac{1}{h} \bar{u}_3 \bar{u}_1 - \frac{\partial \bar{p}}{\partial x_1} + \frac{\nu}{h} \left[ \frac{\partial \bar{u}_1}{\partial x_3} - u_0' \right] \right)_{x_3=h}
\]

2) Obtain fluctuating slip BC from shear stress.

\[
\bar{u}_1^+ (x_1, x_2, h_0, t) = F (h_0^+) = h_0^+, \quad h_0^+ \leq 10
\]

3) Time march filtered N-S with extended SGS model.

\[
T_{ij} = \bar{U}_i \bar{U}_j + \bar{U}_i \bar{U}_j + \bar{U}_i \bar{U}_j
\]

\[
= K (\delta_{ij} - e_i^v e_j^v) - \gamma \frac{1}{2} \Delta_c K^{1/2} \left( e_j^v e_k^v \frac{\partial \bar{U}_k}{\partial x_l} (\delta_{lj} - e_l^v e_j^v) + e_i^v e_k^v \frac{\partial \bar{U}_k}{\partial x_l} (\delta_{lj} - e_l^v e_j^v) \right)
\]

4) Time march dynamic subgrid vortex alignment model.

\[
\frac{\partial e_i^v}{\partial t} = e_j^v \frac{\partial \bar{U}_i}{\partial x_j} - e_i^v e_k^v e_j^v \frac{\partial \bar{U}_k}{\partial x_j}
\]
Results ($Re_{\tau} = 600$ to $60k$)

<table>
<thead>
<tr>
<th>$Re_{\tau} = u_{\tau}\delta/\nu$</th>
<th>$Re = u_{CL}\delta/\nu$</th>
<th>log($z^+$/0.41 + 5.2)</th>
<th>$N_1 \times N_2 \times N_3$</th>
<th>$L_1 \times L_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>5.9 $\times$ 10^{2}</td>
<td>1.2 $\times$ 10^{4}</td>
<td>1 - $z/\delta$</td>
<td>DNS (Moser et al. 1999)</td>
<td>384 $\times$ 384 $\times$ 257</td>
</tr>
<tr>
<td>2.0 $\times$ 10^{3}</td>
<td>4.9 $\times$ 10^{4}</td>
<td>DNS (Hoyas &amp; Jiménez 2006)</td>
<td>6144 $\times$ 4608 $\times$ 633</td>
<td></td>
</tr>
<tr>
<td>5.9 $\times$ 10^{2}</td>
<td>1.2 $\times$ 10^{4}</td>
<td>LES</td>
<td>32 $\times$ 32 $\times$ 32</td>
<td>8$\pi\delta \times 3\pi\delta$</td>
</tr>
<tr>
<td>2.0 $\times$ 10^{3}</td>
<td>4.9 $\times$ 10^{4}</td>
<td>LES</td>
<td>64 $\times$ 64 $\times$ 64</td>
<td>8$\pi\delta \times 3\pi\delta$</td>
</tr>
<tr>
<td>6.0 $\times$ 10^{3}</td>
<td>1.6 $\times$ 10^{5}</td>
<td>LES</td>
<td>64 $\times$ 64 $\times$ 64</td>
<td>8$\pi\delta \times 3\pi\delta$</td>
</tr>
<tr>
<td>2.0 $\times$ 10^{4}</td>
<td>5.9 $\times$ 10^{5}</td>
<td>LES</td>
<td>64 $\times$ 64 $\times$ 64</td>
<td>8$\pi\delta \times 3\pi\delta$</td>
</tr>
<tr>
<td>6.0 $\times$ 10^{4}</td>
<td>1.9 $\times$ 10^{6}</td>
<td>LES</td>
<td>64 $\times$ 64 $\times$ 64</td>
<td>8$\pi\delta \times 3\pi\delta$</td>
</tr>
</tbody>
</table>
Reynolds stresses

\[ \text{Re}_\tau = 2.0 \times 10^3 \]
Future work

- Higher Reynolds number.
- Dynamic gamma from structure function matching.
- Application to flow over airfoil.
- Two-vortex SGS model to improve Reynolds stresses.
- Plug for related presentation:
LES of turbulent channel flow; virtual wall model

- LES of turbulent channel flow
- Turbulent flow between two parallel plates driven by pressure gradient
  - Flow contains many features of complex wall-bounded flows
  - Viscous sublayer, stream-wise vortices, log layer
- Stringent test of SGS/LES model for wall-bounded turbulence
- SGS model must accurately model turbulent transport processes
- Near-wall LES; frontier problem in present research
- Special "virtual-wall" near-wall SGS model
- Allow LES of wall bounded flows at large $Re_{\tau} = 20,000$; $Re_U = 650,000$
- Comparison with DNS;
- $Re_{\tau} = 590$ (Moser et al, 1999)
- $Re_{\tau} = 2000$ (Hoyas et al, 2006)
Summary

• LES methodology
  – Two-component Favre-filtered Navier-Stokes equations
  – Stretched-vortex subgrid-scale (SGS) model; structure based

• Computational method: hybrid WENO-TCD
  – Shock capturing low numerical dissipation
  – Verification
    • Decaying compressible turbulence
    • Riemann 1D wave (Exact Euler)

• Large-eddy simulation of Richtmyer-Meshkov instability with reshock
  – RM instability in plane channel with end wall; Air-SF6
  – Modeled on experiments of Vetter & Sturtevant (1995)

• Traditional Statistics
  – Mixing-layer growth
  – Turbulence statistics, velocity, density & scalar spectra

• “Multi-scale modeling”
  – Subgrid continuation statistics; spectra and anisotropy
  – Scalar p.d.f.s, including subgrid contribution
  – Effect of Schmidt number

• Adaptive Mesh Refinement (AMROC)
  – Berger & Colella’s algorithm for conservation laws
  – Hierarchical data structure
  – WENO-TCD and stretched-vortex SGS model implemented
Conclusions

• Large-eddy simulation of plane Richtmyer-Meshkov instability with reshock
  – Hybrid WENO-TCD scheme with SV SGS model
  – Air-SF6; modeled on experiments of Vetter & Sturtevant (1995)
• Growth of mixing-layer width
  – Initial linear growth of interface following first shock impact
  – Period of nonlinear bubble/spike growth
  – Reshock produces rapid transition to turbulent mixing layer
  – Strong mixing layer growth
  – Enhanced by interaction with reflected expansion
  – Eventual saturation of growth
• Traditional Statistics
  – Mixing-layer growth
  – turbulence statistics, velocity, density & scalar spectra
• “Multi-scale modeling”
  – SV SGS model provides basis for subgrid continuation statistics; spectra and anisotropy
  – Scalar p.d.f.s, including subgrid contribution
  – log-dependence of scalar p.d.f. on Schmidt number
Reynolds number and integral length

Decay on Reynolds number

Decay of integral length
Scalar spectrum from stretched-spiral vortex

Schematic showing winding of scalar field by ‘subgrid vortex’. Contours of passive scalar.

1-D scalar spectrum for homogeneous turbulence, Pullin & Lundgren (2001)

_____ Sc = 7, ------ Sc = 700. Symbols, Data

(Gibson & Schwarz 1963)
Numerical algorithm (D. Hill, C. Pantano)

- **WENO-TCD hybrid method** (Hill & Pullin, JCP, 2004)
  - Tuned-Centered Difference (TCD); away from shocks exploit smoothness of flow
  - Order of accuracy traded for minimization of one-step truncation error in LES equations (Ghosal, 1995)
  - 5-point stencil -> 2-nd order accuracy
  - At shocks (only) revert to full WENO
  - Optimal WENO stencil matched to TCD stencil

- **Flux-based finite difference**
  - Naturally integrated in AMROC
  - Conservative, skew-symmetric

- **Skew-symmetric**
  - Energy conserving
  - Satisfies summation-by-parts

- **Tested in 1D, 2D, 3D**
  - Decaying compressible turbulence

- **No explicit filtering**

![Riemann 1D Wave](image)

Exact solution of 1D Euler

![Graph](image)
Idea: Improve $K(k)$ for center-difference

- Finite-difference operator

$$D f(x) = \frac{1}{\Delta x} \sum_{j=-3}^{j=3} d_j [f(x + j \Delta x) - f(x - j \Delta x)]$$

$$d_1 = \frac{2}{3}, \quad d_2 = -\frac{1}{12}, \quad d_3 = 0, \quad \rightarrow 5 - pt, \ 4^{th} \ order$$

$$d_1 = \frac{3}{4}, \quad d_2 = -\frac{1}{10}, \quad d_3 = -1/2, \quad \rightarrow 7 - pt, \ 6^{th} \ order$$

- Tuned 5-point with parameter $\alpha$

$$d_1 = \frac{1}{2} - 2\alpha, \quad d_2 = \alpha, \quad d_3 = 0, \quad \rightarrow 5 - pt, \ 2^{nd} \ order$$

- Tuned 7-point with parameter $\alpha$

$$d_1 = \frac{2}{3} + \alpha, \quad d_2 = -\frac{1}{12} - 4\alpha, \quad d_3 = \alpha, \quad \rightarrow 7 - pt, \ 4^{th} \ order$$
Performance for LES of decaying turbulence

DNS and LES of Decaying compressible turbulence, \( M_t = 0.488, R_{\lambda} = 70 \).

Decay of total TKE. Black; \( 256^3 \) DNS (10-th order Pade)
Numerical algorithm (D. Hill, C. Pantano)

- **WENO-TCD hybrid method** (Hill & Pullin, JCP, 2004)
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- No explicit filtering
Conservation and time adaptation

- Hanging nodes exist because cells at different levels are logically conforming.

- A special correction, fixup, must be applied to satisfy global conservation.

- Fluxes at coarse cells next to fine cells are replaced by the sum of those fluxes at the fine cells.
  \[
  \delta F_{i-\frac{1}{2},j}^{1,l+1} := \delta F_{i-\frac{1}{2},j}^{1,l+1} + \frac{1}{r_{l+1}} \sum_{m=0}^{r_{l+1}-1} F_{v+\frac{1}{2},w+m}^{1,l+1}(t + \kappa \Delta t_{l+1})
  \]

- This correction impacts the spatial as well as temporal integration scheme.
  \[
  Q_{i,j}^{n+1} := Q_{i,j}^{n+1} + \frac{\Delta t_l}{\Delta x_{1,t}} \delta F_{i-\frac{1}{2},j}^{1,l+1}
  \]

- Ghost cell values of fine patches are obtained by linear time interpolation from the coarse patch solution.
LES in the absence of strong shocks and density contacts

- The nonlinear term $\frac{\partial}{\partial x_i}(\rho u_i u_j)$ is responsible primarily for the energy cascade.
- The most successful Eulerian methods are global:
  - Spectral
  - High-Order Pade
- Good response across all (spectral) or most (Pade) of the resolved scales, i.e. modified wavenumber:
  $$F(\partial / \partial x) = ik \quad F(D_x) = i\tilde{K}(k)$$
- Limitations of spectral methods:
  - *global nature results in (fatal?) ringing at discontinuities like shocks and contacts*
  - *Limited to simple geometries*
Conservation and time adaptation

- Hanging nodes exist because cells at different levels are logically conforming.
- A special correction, fixup, must be applied to satisfy global conservation.
- Fluxes at coarse cells next to fine cells are replaced by the sum of those fluxes at the fine cells:
  \[ \delta F_{j+1}^{i,j+1} = \delta F_{j-\frac{1}{2},j}^{i,j+1} + \frac{1}{t+1} \sum_{m=0}^{r_{j+1}-1} F_{j+\frac{1}{2},j+1}^{i,j+1}(t + \Delta t_{j+1}) \]
- This correction impacts the spatial as well as temporal integration scheme:
  \[ Q_{i,j}^{n+1} = Q_{i,j}^{n+1} + \frac{\Delta t_i}{\Delta x_{1,i}} \delta F_{i,j}^{n+1} \]
- Ghost cell values of fine patches are obtained by linear time interpolation from the coarse patch solution.
Idea: Improve $K(k)$ for center-difference

- Finite-difference operator

$$D f(x) = \frac{1}{\Delta x} \sum_{j=-3}^{j=3} d_j [f(x + j \Delta x) - f(x - j \Delta x)]$$

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$$d_1 = \frac{3}{4}, \quad d_2 = -\frac{1}{10}, \quad d_3 = -1/2, \quad \rightarrow 7\text{-pt, } 6^{th}\text{ order}$$

- Tuned 5-point with parameter $\alpha$

$$d_1 = \frac{1}{2} - 2\alpha, \quad d_2 = \alpha, \quad d_3 = 0, \quad \rightarrow 5\text{-pt, } 2^{nd}\text{ order}$$

- Tuned 7-point with parameter $\alpha$

$$d_1 = \frac{2}{3} + \alpha, \quad d_2 = -\frac{1}{12} - 4\alpha, \quad d_3 = \alpha, \quad \rightarrow 7\text{-pt, } 4^{th}\text{ order}$$
Tuned Center-Difference Stencil (TCD)

- Error in resolved-scale energy spectrum produced by one step of Navier-Stokes equations using given discretization; Ghosal (1996)
- Assume –
  - Von-Karman energy spectrum
  - Joint normal velocity pdf

- \( E^{(FD)}(\kappa, \tilde{\kappa}(\kappa, \alpha)) \) is spectrum of truncation error for numerical method with modified wavenumber behavior \( \tilde{\kappa}(\kappa, \alpha) \)

- Define total discretization error:

\[
E_G(\alpha) = \int_0^{\Delta x} E^{(FD)}(\kappa, \tilde{\kappa}(\kappa, \alpha)) d\kappa
\]
Optimized 5-point TCD stencil (second order)

Truncation error

Modified wavenumber of minimal error stencil
Shock capturing solvers; WENO

- True shocks have a thickness on the mean free path order
- The shocks are not resolved: Euler equations are solved in conservative form
- Euler solver shocks are ‘captured’, i.e. smeared across a few cells – first-order accurate at shocks

\[
\frac{dq}{dt} + \frac{\partial F(q)}{\partial x} + \frac{\partial G(q)}{\partial y} + \frac{\partial H(q)}{\partial z} = 0
\]

\[
q = (\rho, \rho u, \rho v, \rho w, E)^T
\]

\[
F(q) = \begin{pmatrix}
\rho u \\
\rho u^2 + P \\
\rho uv \\
\rho uw \\
\rho u(E + P)
\end{pmatrix}
\]

Weighted Essentially Non-Oscillatory (WENO) method (Osher)
Hybrid WENO-TCDS algorithm: LES and strong shocks (D. Hill)

- Hybrid technique: blending Weighted Essentially Non-Oscillatory (WENO) scheme with Tuned Centered-Difference (TCD) stencil.
- WENO in regions of very-large density ratio (Shocks)
  - But WENO is not suitable for LES in smooth regions away from shocks.
  - Upwinding strategy is too dissipative
- TCD stencil in smooth regions away from shocks
  - Low numerical dissipation (centered method)
  - optimized for minimum resolved-scale discretization error in LES (Ghosal, 1996)
  - 5- or 7-point stencil trades off formal order of accuracy for small dispersion errors
- Target WENO stencil = TCD stencil
- In practice, target TCD stencil not always achieved; switch is used based on acceptable WENO smoothness measure
- Hybrid method designed for LES in presence of strong shocks
Cylindrical RM instability with AMROC (R.Deiterding)

- AMROC – Adaptive Mesh Refinement engine
- Exploratory 2D Richtmyer-Meshkov instability with reshock in wedge geometry
- Passage of the shock results in vorticity deposition by means of baroclinic generation
- Canonical model of phase 2 experiments
- Incident shock modeled by Chisnell (1998) approximation to Guderley solution for similarity shock
- Euler simulation
- Initial density interface; sinusoidal perturbation corresponding to n = 24 on circle
Reacting Hydrogen Jet flame (C. Pantano)

- Planar hydrogen jet flame of Rehm & Clemens (1999), Mach=0.28
- 5 $10^6$ grid cells and 4 levels of refinement
- 128 processors at LLNL ALC, 50,000 cpu/hours
- Cantera chemistry solver by D. Goodwin for flamelet model