Theoretically Based Optimal LES

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Introduction to Turbulence Simulations

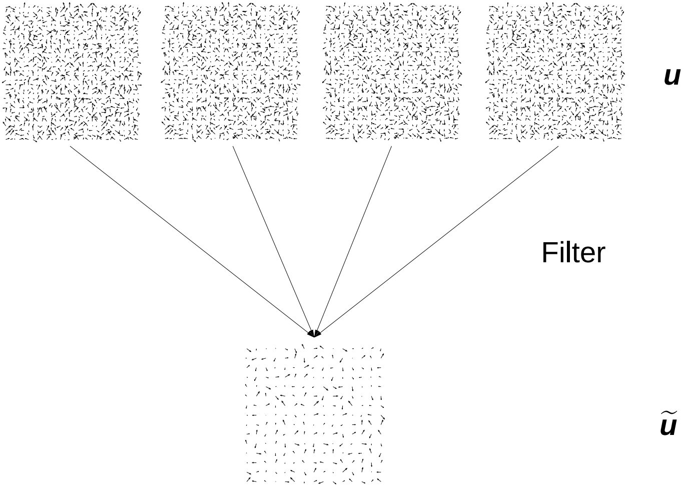
- Direct Numerical Simulation (DNS)
  - Simulate all scales of the flow.
  - Too expensive.
    - Cost scales with Re^3.
    - Complex geometries and/or high Reynolds number flows are impractical.
- Reynolds-Averaged Navier-Stokes (RANS)
  - Simulate a *mean* flow.
  - Models too much (effect of all fluctuating scales).
    - Models become flow dependent.
    - *Ad hoc* corrections must be used.

Large-Eddy Simulation

- Simulate the large scales, model the small scales.
  - Large scales dominate turbulence dynamics.
  - Small scales are important only in how they affect the large scales.
    - Small scales of turbulence are more universal $\Rightarrow$ Easier to model for a wide range of flows.
- Define scales through spatial filtering:

$$\widetilde{u}_i(\boldsymbol{x}) = \int g\left(\boldsymbol{x'}, \boldsymbol{x}\right) u_i\left(\boldsymbol{x'}\right) \mathrm{d}\boldsymbol{x'} \tag{1}$$

Stochastic Evolution of LES



Properties of the Ideal LES

- Defined by:

$$\frac{\mathrm{d}\boldsymbol{w}}{\mathrm{d}t} = \left\langle \widetilde{\frac{\mathrm{d}\boldsymbol{u}}{\mathrm{d}t}} \,\middle|\, \widetilde{\boldsymbol{u}} = \boldsymbol{w} \right\rangle \tag{2}$$

- Correct statistics and accurate short-time dynamics.
- Impossible to compute: Data requirement is excessive.

Formulating a Finite Volume Optimal Large Eddy Simulation

- Finite-volume filtered Navier-Stokes equation:

$$V^v \frac{\partial w_i^v}{\partial t} = -\underbrace{\int_s u_i u_j n_j^s \mathrm{d}\boldsymbol{x}}_{\mathcal{F}_i^s} - \underbrace{\int_s p n_i^s \mathrm{d}\boldsymbol{x}}_{P_i^s} + \underbrace{\frac{1}{\mathrm{Re}} \int_s \frac{\partial u_i}{\partial x_j} n_j^s \mathrm{d}\boldsymbol{x}}_{V_i^s}$$

u: unfiltered velocity $\qquad$ w: filtered velocity

- Finite volume averaging is the LES filter.
- Estimate convective fluxes through each volume face as linear and quadratic functions of resolved velocity w:

$$\mathcal{F}_i^s \approx \cancel{\mathcal{A}_i(s)} + \sum_{v_1} \mathcal{L}_{ij}(s, v_1) w_j^{v_1} + \sum_{v_1, v_2} \mathcal{Q}_{ijk}(s, v_1, v_2) w_j^{v_1} w_k^{v_2} \qquad (3)$$

- Approximation of *ideal* LES, given by conditional average (Pope 2000):
- Optimization: Minimize mean-square error $\left\langle (M - m)^2 \right\rangle$ with respect to dependencies.

Linear Stochastic Estimation

- The convective flux $\mathcal{F}_i^s$ is modeled using stochastic estimation.

The mean square error of our estimate is minimized when:

$$\left\langle \mathcal{F}_i^s \right\rangle = \mathcal{A}_i(s) + \cancel{\sum_{v_1} \mathcal{L}_{ij}(s, v_1) \left\langle \overline{u}_j^{v1} \right\rangle} + \sum_{v_1, v_1} \mathcal{Q}_{ijk}(s, v_1, v_2) \left\langle \overline{u}_j^{v1} \overline{u}_k^{v2} \right\rangle \quad (4)$$

$$\left\langle \mathcal{F}_i^s \overline{u}_l^{v3} \right\rangle = \cancel{\mathcal{A}_i(s) \left\langle \overline{u}_l^{v3} \right\rangle} + \sum_{v_1} \mathcal{L}_{ij}(s, v_1) \left\langle \overline{u}_j^{v1} \overline{u}_l^{v3} \right\rangle + \sum_{v_1, v_2} \mathcal{Q}_{ijk}(s, v_1, v_2) \left\langle \overline{u}_j^{v1} \overline{u}_k^{v2} \overline{u}_l^{v3} \right\rangle \quad (5)$$

$$\left\langle \mathcal{F}_i^s \overline{u}_l^{v3} \overline{u}_m^{v4} \right\rangle = \mathcal{A}_i(s) \left\langle \overline{u}_l^{v3} \overline{u}_m^{v4} \right\rangle + \sum_{v_1} \mathcal{L}_{ij}(s, v_1) \left\langle \overline{u}_j^{v1} \overline{u}_l^{v3} \overline{u}_m^{v4} \right\rangle + \sum_{v_1, v_2} \mathcal{Q}_{ijk}(s, v_1, v_2) \left\langle \overline{u}_j^{v1} \overline{u}_k^{v2} \overline{u}_l^{v3} \overline{u}_m^{v4} \right\rangle$$

Zero in isotropic turbulence, required correlations

- The velocity correlations are needed as input to solve the system of equations for the estimation coefficients (kernels) Q_{ijk}, and Lij.

Surface and Volume Integrals

$$\left\langle \mathcal{F}_i^{4s} \overline{u}_l^{v3\prime} \right\rangle = \frac{1}{v_3} \int_{v_3} \int_s \left\langle u_l'(\mathbf{x}^3) u_i'(\mathbf{x}) u_s'(\mathbf{x}) \right\rangle d\mathbf{x} \tag{6}$$

$$\left\langle \overline{u}_j^{v1\prime} \overline{u}_l^{v3\prime} \right\rangle = \frac{1}{v_3 v_1} \int_{v_3} \int_{v_1} \left\langle u_l'(\mathbf{x}^3) u_j'(\mathbf{x}^1) \right\rangle d\mathbf{x} \tag{7}$$

$$\left\langle \overline{u}_j^{v1\prime} \overline{u}_k^{v2\prime} \overline{u}_l^{v3\prime} \right\rangle = \frac{1}{v_3 v_1 v_2} \int_{v_3} \int_{v_1} \int_{v_2} \left\langle u_l'(\mathbf{x}^3) u_j'(\mathbf{x}^1) u_k'(\mathbf{x}^2) \right\rangle d\mathbf{x} = I \tag{8}$$

$$\left\langle \mathcal{F}_i^{4s} \overline{u}_l^{v3\prime} \overline{u}_m^{v4\prime} \right\rangle = \frac{1}{v_3 v_4} \int_{v_3} \int_{v_4} \int_s \left\langle u_l'(\mathbf{x}^3) u_m'(\mathbf{x}^4) u_i'(\mathbf{x}) u_s'(\mathbf{x}) \right\rangle d\mathbf{x} \tag{9}$$

$$\left\langle \overline{u}_j^{v1\prime} \overline{u}_k^{v2\prime} \overline{u}_l^{v3\prime} \overline{u}_m^{v4\prime} \right\rangle = \frac{1}{v_3 v_4 v_1 v_2} \int_{v_3} \int_{v_4} \int_{v_1} \int_{v_2} \left\langle u_l'(\mathbf{x}^3) u_m'(\mathbf{x}^4) u_j'(\mathbf{x}^1) u_k'(\mathbf{x}^2) \right\rangle d\mathbf{x} \tag{10}$$

(11)

- In the past, these inputs have been obtained from DNS fields, limiting the use of the optimal method.

Velocity correlations determined using Kolmogorov inertial range theory

- $\left\langle u_i(\boldsymbol{x}) u_j(\boldsymbol{x'}) \right\rangle$

$$= R_{ij}(\boldsymbol{r}) = \delta_{ij} u^2 + \frac{C_1}{6} \epsilon^{2/3} r^{-4/3} \left(r_i r_j - 4 r^2 \delta ij \right)$$

- $\left\langle u_i(\boldsymbol{x}) u_j(\boldsymbol{x}) u_k(\boldsymbol{x'}) \right\rangle$

$$= \frac{\epsilon}{15} \left(\delta_{ij} r_k - \frac{3}{2} \left(\delta_{ik} r_j + \delta_{jk} r_i \right) \right)$$

- $\left\langle u_i(\boldsymbol{x^1}) u_j(\boldsymbol{x^2}) u_k(\boldsymbol{x^3}) u_l(\boldsymbol{x^4}) \right\rangle$

$$= R_{ij}\left(\boldsymbol{r}^1\right) R_{kl}\left(\boldsymbol{r}^3 - \boldsymbol{r}^2\right) + R_{ik}\left(\boldsymbol{r}^2\right) R_{jl}\left(\boldsymbol{r}^3 - \boldsymbol{r}^1\right) + R_{il}\left(\boldsymbol{r}^3\right) R_{jk}\left(\boldsymbol{r}^2 - \boldsymbol{r}^1\right)$$

At this point, we only lack an expression for the three-point third-order correlation.

The three-point third-order correlation

- Kolmogorov inertial range theory is not sufficient to determine an expression for the three-point third-order correlation.
- Most general isotropic form satisfying all constraints (as in Proudman and Reed):

$$\mathbb{T}_{ijk}(\mathbf{r},\mathbf{s}) = \mathcal{P}^t_{im}\mathcal{P}^s_{jn}\mathcal{P}^r_{kp}[\delta_{np}\partial^s_m\psi(r,s,t) + \delta_{mp}\partial^r_n\psi(t,r,s) + \delta_{mn}\partial^s_p\psi(t,s,r)] \tag{12}$$

- Nevertheless, a model for $\mathbb{T}_{ijk}(\mathbf{r}^1,\mathbf{r}^2)$ that provides the final necessary input for OLES simulations was recently developed by H. Chang and R. D. Moser
[Phys. Fluids 19, 105111 (2007)]

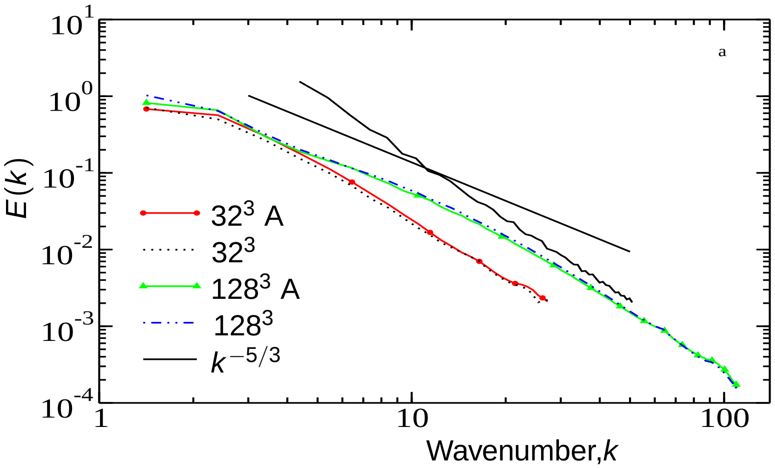
Asymptotics

- Three flow dependent parameters: C_1, ϵ and u^2.
  - C_1 is set to 2.0 (Kolmogorov's Constant)
- After nondimensionalization, kernels only depend on $\frac{\Delta\epsilon}{u^3} = \gamma$
  - Ratio between the filter scale to the largest turbulence scale.
- We are particularily interested in asymptotically small γ.
- The estimation kernels can be expanded as powers of $\gamma^{2/3}$,

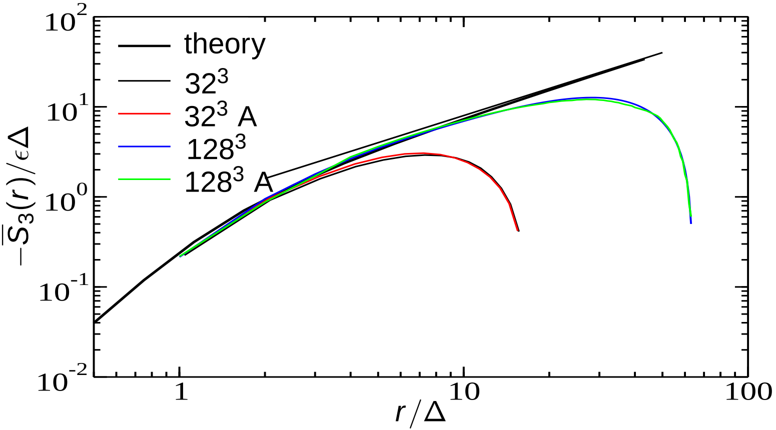
$$\tilde{\mathcal{L}} = \tilde{\mathcal{L}}^0 + \gamma^{2/3}\tilde{\mathcal{L}}^1 + \gamma^{4/3}\tilde{\mathcal{L}}^2 + \cdots \quad (13)$$

$$\tilde{\mathcal{Q}} = \tilde{\mathcal{Q}}^0 + \gamma^{2/3}\tilde{\mathcal{Q}}^1 + \gamma^{4/3}\tilde{\mathcal{Q}}^2 + \cdots \quad (14)$$

LES Results: 3-D Energy Spectra



LES Results: Third-order Structure Function

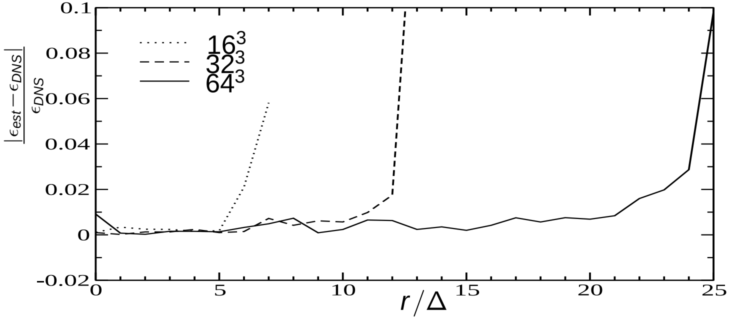


Shown is the $S_3 = -\frac{4}{5}\epsilon r$ line, as well as S_3 determined from I.

Dynamic Optimal LES: fluctuating ϵ and u^2

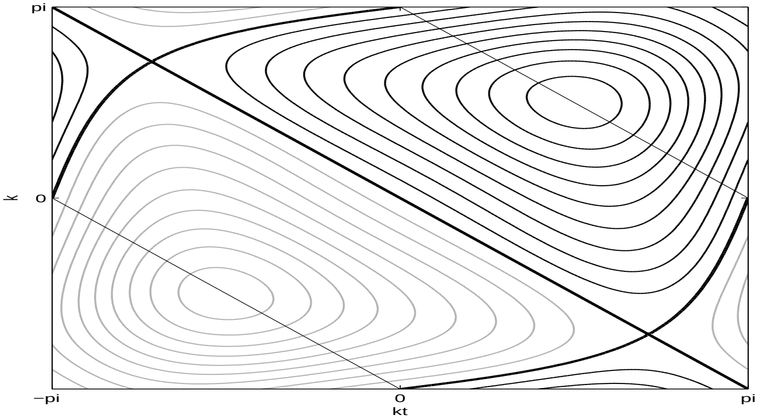
The longitudinal third-order structure function is used to estimate the dissipation:

$$\epsilon = \frac{\langle(\overline{u}'_1(v_1) - \overline{u}'_1(v_2))^3\rangle}{3\Delta(\tilde{I}_{111}(v_2,v_2,v_1) - \tilde{I}_{111}(v_2,v_1,v_1))} \tag{15}$$



Conclusions

- The multipoint velocity correlations needed as input for optimal FV-LES can be obtained from Kolmogorov, the quasi-normal approximation, and an expression for the three-point third-order correlation.
- Resulting LES simulations perform very well.
- Asymptotic and finite γ kernels yield consistent results.
  - only ϵ needs to be determined dynamically
  - There is a simple dynamic procedure for estimating ϵ
- These models are expected to be valid for high *Re* flows with isotropic small scales.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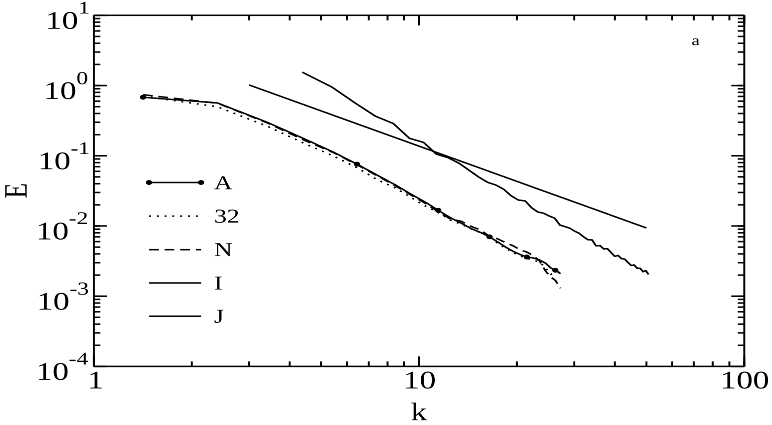

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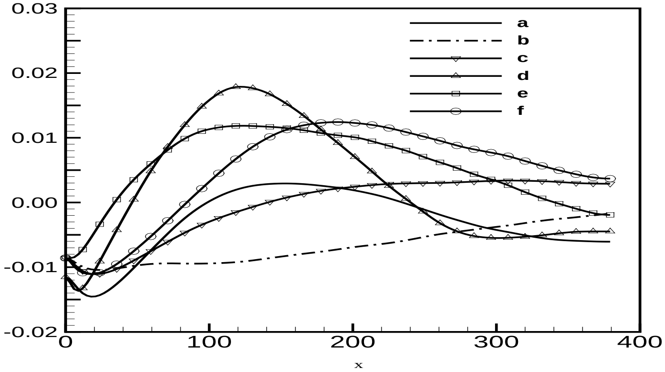
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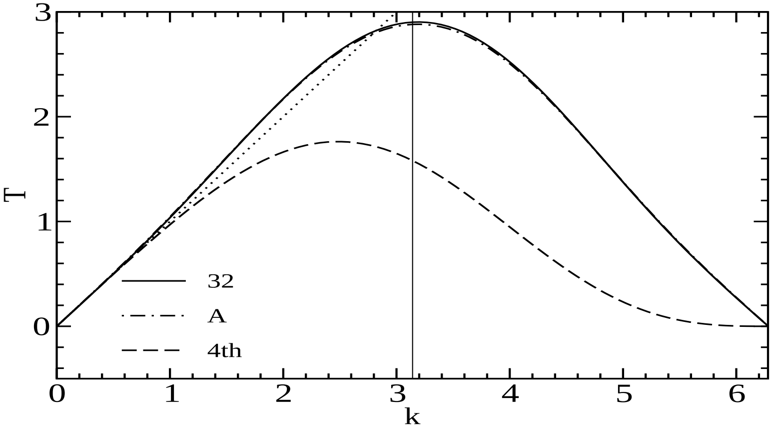
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