Computational error-analysis for large-eddy simulation

Bernard J. Geurts

Multiscale Modeling and Simulation (Twente) Anisotropic Turbulence (Eindhoven)

Saarbrücken, June 23-24, 2008

Everyday flows: Wake-Vortex Hazard



Airport throughput limitations: separation up to 10 km



Flow over delta wing





Grid dependence



Reliability - Error-bounds - Computational costs?



Grid dependence



GTU/e

Reliability - Error-bounds - Computational costs?

Outline









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Filtering Navier-Stokes equations

$$\partial_j u_j = 0$$
 ; $\partial_t u_i + \partial_j (u_i u_j) + \partial_i p - \frac{1}{Re} \partial_{jj} u_i = 0$

Convolution-Filtering: filter-kernel G

$$\overline{u}_i = L(u_i) = \int G(x-\xi)u(\xi) d\xi$$
; $L(1) = 1$

Large-eddy equations:

$$\partial_{j}\overline{u}_{j} = 0$$

$$\partial_{t}\overline{u}_{i} + \partial_{j}(\overline{u}_{i}\overline{u}_{j}) + \partial_{i}\overline{p} - \frac{1}{Re}\partial_{jj}\overline{u}_{i} = -\partial_{j}(\overline{u_{i}u_{j}} - \overline{u_{i}}\overline{u}_{j})$$

Sub-filter stress tensor

$$\tau_{ij} = \overline{u_i u_j} - \overline{u}_i \overline{u}_j$$

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Shorthand notation:

$$NS(\mathbf{u}) = 0 \quad \Rightarrow \quad NS(\overline{\mathbf{u}}) = -\nabla \cdot \tau(\mathbf{u}, \overline{\mathbf{u}}) \iff -\nabla \cdot M(\overline{\mathbf{u}})$$

Basic LES formulation

Find
$$\mathbf{v}$$
: $NS(\mathbf{v}) = -\nabla \cdot M(\mathbf{v})$

After closure system of PDE's results:

- dynamic range restricted primarily to scales > Δ
- does solution v of closed system resemble u?

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 Goal in LES: determine the unique solution to system of PDE's that results after adopting explicit closure model



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Goal: approximate the unique solution to system of PDE's resulting after adopting explicit closure model

General (textbook) requirements:

- Filter separates scales $> \Delta$ from scales $< \Delta$
- Computational grid provides additional length-scale h
- Require Δ/h to be sufficiently large $(\Delta/h \to \infty)$
- Good numerics: $v(x, t : \Delta, h) \rightarrow v(x, t : \Delta, 0)$ rapidly

- computational costs $\sim N^4$: implies modest Δ/h
- potentially large role of numerical method in computational dynamics because of marginal resolution

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Consider central discretization:

$$\delta_{\mathbf{x}}(\mathbf{u})_{j} = \frac{1}{2h} \Big(u_{j+1} - u_{j-1} \Big)$$

$$= \frac{1}{2h} \int_{x_{j}-h}^{x_{j}+h} \partial_{\mathbf{x}} u(\xi) d\xi$$

$$= \frac{\partial}{\partial \mathbf{x}} \Big(\int_{x_{j}-h}^{x_{j}+h} \frac{u(\xi)}{2h} \Big)$$

$$= \partial_{\mathbf{x}} \Big(L_{2h}(u) \Big) = \partial_{\mathbf{x}}(\widehat{u})$$



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- Modified mean flux
- Computational Turbulent Stress Tensor

$$\xi = \overline{u^2} - \widehat{\overline{u}^2} = (\overline{u^2} - \overline{u}^2) + (\overline{u}^2 - \widehat{\overline{u}^2}) = \tau + \mathcal{H}(\overline{u}^2)$$

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Dynamic importance - subgrid resolution

Contributions associated with $u = e^{ikx}$:

$$au = A_{\tau}(k\Delta)e^{2\imath kx}$$
; $\mathcal{H}(\overline{u}^2) = A_{\mathcal{H}}(k\Delta, r)e^{2\imath kx}$



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3

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 $A_{\tau}\Delta$: solid $A_{\mathcal{H}}\Delta$ at r = 1 (- -) r = 2 (-.-) and r = 4 (o)

2nd order (thin) 4th order (thick)

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Strong effect r = 1 - 2; reduction as $r \ge 4$

LES treatment of convective term

Discretization and modeling introduce errors:

$$\partial_{j}(\overline{u_{i}u_{j}}) = \left[\delta_{j}(\overline{u}_{i}\overline{u}_{j}) + \mathcal{D}_{i}\right] + \partial_{j}\tau_{ij}$$

$$= \left[\delta_{j}(\overline{u}_{i}\overline{u}_{j}) + \mathcal{D}_{i}\right] + \left\{\partial_{j}m_{ij} + \mathcal{R}_{i}\right\}$$

$$= \delta_{j}(\overline{u}_{i}\overline{u}_{j}) + \delta_{j}m_{ij} + \left(\mathcal{D}_{i} + \mathcal{R}_{i} + \mathcal{D}_{i}^{(m)}\right)$$
wish:

Distinguish:

- \mathcal{D}_i : discretization error from using method δ_i
- $\mathcal{R}_i = \partial_i (\tau_{ij} m_{ij})$: total 'model-residue'
- $\mathcal{D}_{i}^{(m)}$: error when treating model m_{ij} , e.g., filtering
- **Q1:** Justified to ignore D_i ? Grid-(in)-dependent LES?
- Q2: Interacting errors? Error-decomposition? Dominance?
A priori test: snapshot turbulent mixing

Comparison discretization error and sub-filter flux



Sub-filter flux (solid): fixed grid, increasing Δ Discretization error: 2nd order (- -), 4th order (dotted) At r = 1 discretization dominant – relevance modeling? Bernard J. Geurts: Computational error-analysis for large-eddy simulation

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Total error decomposition

Total (ε_t)=Discretization (ε_d) + Modeling (ε_m)

Decomposition requires: DNS and LES at various $r = \Delta/h$

- Reference via (filtered) DNS data
- LES without discretization errors: fixed Δ , $r \rightarrow \infty$
- LES with both types of errors

Provides a posteriori decomposition:

$$\begin{split} \varepsilon_d(E) &= E_{\text{LES}}(\Delta, r) - E_{\text{LES}}(\Delta, \infty) \\ \varepsilon_m(E) &= E_{\text{LES}}(\Delta, \infty) - E_{\overline{\text{DNS}}}(\Delta, r) \\ \varepsilon_t(E) &= \varepsilon_d(E) + \varepsilon_m(E) = E_{\text{LES}}(\Delta, r) - E_{\overline{\text{DNS}}}(\Delta, r) \end{split}$$

Requires number of LES: various Δ , h, models, schemes ...



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- better model may result in worse predictions
- better numerics may result in worse predictions





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Observe:

- At marginal resolution the numerics strongly modifies the equations that should be solved
- Likewise, the introduction of a subgrid model modifies these equations

- Pragmatic guideline: minimal total error at given computational costs
- NOT: simply combine best numerics and best model

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Role of numerics in LES





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Experimental error-assessment

Pragmatic: minimal total error at given computational costs

Discuss:

- error-landscape/optimal refinement strategy
- optimality of MILES in DG-FEM



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Smagorinsky fluid

Homogeneous decaying turbulence at $Re_{\lambda} = 50, 100$



• Smagorinsky fluid — subgrid model:

$$m_{ij}^{\mathrm{S}} = -2(C_{\mathrm{S}}\overline{\Delta})^2|\overline{\mathrm{S}}|\overline{\mathrm{S}}_{ij} = -2\ell_{\mathrm{S}}^2|\overline{\mathrm{S}}|\overline{\mathrm{S}}_{ij}$$

introduces Smagorinsky-length ℓ_S

Accuracy measures

Monitor resolved kinetic energy

$$E = \frac{1}{|\Omega|} \int_{\Omega} \frac{1}{2} \overline{\mathbf{u}} \cdot \overline{\mathbf{u}} \, d\mathbf{x} = \frac{1}{2} \langle \overline{\mathbf{u}} \cdot \overline{\mathbf{u}} \rangle$$

Measure relative error: top-hat filter Δ , grid $h = \Delta/r$

$$\delta_{E}(\Delta, r) = \left\| \frac{E_{LES}(\Delta, r) - E_{\overline{DNS}}(\Delta, r)}{E_{\overline{DNS}}(\Delta, r)} \right\|$$

with error integrated over time

$$\|f\|^2 = \frac{1}{t_1 - t_0} \int_{t_0}^{t_1} f^2(t) dt$$

each simulation represented by single number

concise representation facilitates comparison

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Error-landscape: Definition

Framework for collecting error information:



Contours of δ_E — fingerprint of LES

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Total error-landscape



combination of central discretization and Smagorinsky
 optimum at C_S > 0: SGS modeling is viable here

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- optimum at $C_{\rm S} > 0$: SGS modeling is viable here



Error-landscape: optimal refinement



Optimal trajectory for $Re_{\lambda} = 50$ (a) and $Re_{\lambda} = 100$ (b)

- Under-resolution leads to strong error-increase
- Dynamic procedure over-estimates viscosity



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Near optimal parameter regions



(a) energy, (b) energy and enstrophy. In overlap both accurate.

- connected, overlapping region $N \ge 48$
- weighing of errors leads to 'multi-objective near optimum'



Observation:

- practical LES implies marginal resolution
- which implies large role of specific numerical discretization
- next to dynamics due to subgrid model
- and leads to strong interactions and complex error-accumulation

Proposal:

- obtain smoothing via appropriate numerical method alone
- accept that there is no grid-independent solution, other than DNS
- accept that predictions become discretization dependent



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DG-FEM of homogeneous turbulence

Discretization: Approximate Riemann solver

$$F = F_{central} + \gamma F_{dissipative}$$
; $HLLC - flux$



Three-dimensional accuracy charts

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LES with DG-FEM: dissipative numerics



Third order DG-FEM at $Re_{\lambda} = 100$

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Optimal refinement strategies: 2nd order



• left-to-right: $\gamma_c = 1$, $\gamma_c = 0.1$, $\gamma_c = 0.01$

- $C_{\rm S}^* = 0$ at $\gamma_c = 1$: MILES best option
- γ_c < 1 implies $C_{
 m S}^*$ \geq 0: MILES sub-optimal
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Optimal refinement strategies: 2nd order



• left-to-right: $\gamma_c = 1$, $\gamma_c = 0.1$, $\gamma_c = 0.01$

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Optimal refinement strategies: 3rd order



• left-to-right: $\gamma_c = 1$, $\gamma_c = 0.1$, $\gamma_c = 0.01$

• for all $\gamma_c \in [0, 1]$ find $C_S^* \ge 0$: MILES sub-optimal

• optimal C_S is less sensitive to γ_c value than 2nd order

GTU/e

Optimal refinement strategies: 3rd order



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Optimality of MILES ?



• (a): 2nd order ; (b): 3rd order

• $\gamma_c = 1.00$ (dot), $\gamma_c = 0.10$ (dash) and $\gamma_c = 0.01$ (–)

2nd: MILES-error larger than with explicit SGS model

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Outline



Role of numerics in LES







- error-decomposition: modeling, discretization effects
- LES-paradoxes and interacting errors: better models/numerics may not lead to better predictions
- error-landscape optimal refinement strategy
- MILES sub-optimal: examples in which explicit modeling more efficient/accurate
- Error-interaction and a priori error-bounds hard to include: direct minimization to account for modeling and numerics



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