On LES Modelling and Numerical Errors

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joint work with Ioan Teleaga

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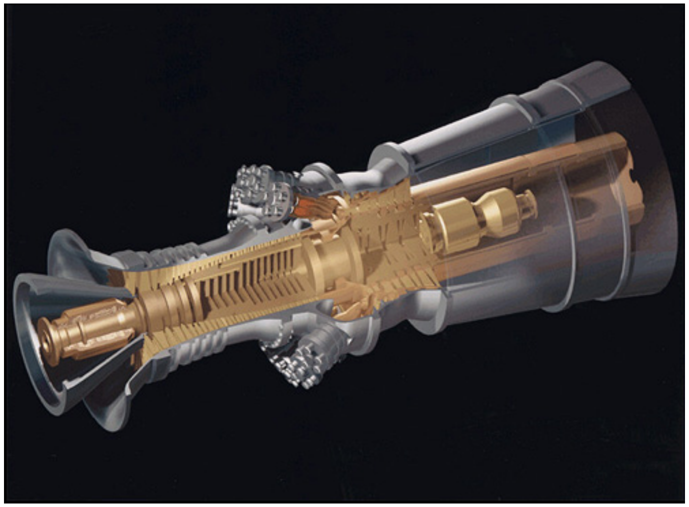
SFB568
Instationary Simulation of Gas Turbines



Introduction

- LES: Modelling and Discretization
- Errors in LES
- Dual Weighted Residual Method
- Computable Errors
- Illustrative Computational Result
- Current and Future Work

Model Equations

Incompressible Navier-Stokes equations for viscous flows on computational domain $[0,T] \times \Omega$, $\Omega \in \mathbb{R}^3$

$$\begin{aligned}
\partial_t \boldsymbol{u} + (\boldsymbol{u} \cdot \nabla)\boldsymbol{u} + \nabla p - \nabla \cdot (2\nu\, \boldsymbol{S}(\boldsymbol{u})) &= \boldsymbol{f}, \\
\nabla \cdot \boldsymbol{u} &= 0, \\
\boldsymbol{u} &= \boldsymbol{u}_b(t, \boldsymbol{x}), \quad \text{b.c.} \\
\boldsymbol{u}(0, \boldsymbol{x}) &= \boldsymbol{u}_0(\boldsymbol{x}), \quad \text{i.c.} \\
\int_\Omega p \, d\boldsymbol{x} &= 0
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with stress tensor $\boldsymbol{S} = (\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^T)/2$ and viscosity ν.

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Use explicit LES:

spatial filter, turbulence model, discretization method

LES: Step I

Apply spatial filter operator with width Δ to obtain space-averaged incompressible Navier-Stokes equations

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\partial_t \overline{\boldsymbol{u}} + (\overline{\boldsymbol{u}} \cdot \nabla)\overline{\boldsymbol{u}} + \nabla \overline{p} - \nabla \cdot (2\nu S(\overline{\boldsymbol{u}})) &= \overline{\boldsymbol{f}} - \nabla \cdot \tau(\boldsymbol{u}), \\
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Goal of LES: Compute only large flow structures accurately.

LES: Step II

Subgrid-scale models (sgs): $\tau_{mod}(\overline{\boldsymbol{u}}) \approx \tau(u) = \overline{\boldsymbol{u}\,\boldsymbol{u}^T} - \overline{\boldsymbol{u}}\,\overline{\boldsymbol{u}}^T$

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Here:

- Smagorinsky model

$$\tau_S(\overline{\boldsymbol{u}}) = -(c_s\,\Delta)^2\,\left(S(\overline{\boldsymbol{u}}) : S(\overline{\boldsymbol{u}})\right)^{1/2}\,S(\overline{\boldsymbol{u}}),\; c_s \in [0.01, 0.1]$$

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- Liu-Meneveau-Katz scale similarity model

$$\tau_{LMK}(\overline{\boldsymbol{u}}) = \left(\overline{\boldsymbol{u}}\,\overline{\boldsymbol{u}}^T\right)^{\Delta'} - (\overline{\boldsymbol{u}})^{\Delta'}(\overline{\boldsymbol{u}}^T)^{\Delta'},\; \Delta' > \Delta$$

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One-step s-stage integration methods and finite elements

Let $0 \leq t_0 < t_1 < \cdots < t_N = T$ be the chosen partition of $[0, T]$.

Construct continuous solutions (polynomials of order p)

$$\begin{aligned} \overline{\boldsymbol{u}}^h(t) &= \Pi_p(t; \overline{\boldsymbol{u}}^h_n, \overline{\boldsymbol{U}}^h_{n1}, \ldots, \overline{\boldsymbol{U}}^h_{ns}), \quad t \in [t_n, t_{n+1}] \\ \overline{p}^h(t) &= \Pi_p(t; \overline{p}^h_n, \overline{P}^h_{n1}, \ldots, \overline{P}^h_{ns}), \quad t \in [t_n, t_{n+1}] \end{aligned}$$

where $\overline{\boldsymbol{u}}^h_n, \overline{p}^h_n$ and $\overline{\boldsymbol{U}}^h_{ni}, \overline{P}^h_{ni}, i = 1, \ldots, s$, are FE-approximations at $t = t_n$ and at intermediate points, resp.

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Need for a posteriori quality assessment of LES!

Errors in LES II

Studies on error behaviour (selection)

- Ghosal (1996), Vreman et al. (1996)
- Geurts & Fröhlich (2002)
  computable subgrid activity
- Chow & Moin (2003)
- Meyers et al. (2003-2007)
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- Hoffmann & Johnson (2003-2007)
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How can we distinguish between modelling and discretization errors?

Dual Weighted Residual Method I

Goal: quantify the contributions of the subgrid-scale model and the numerical method to a user specified quantity of interest

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Linearize M in the neighbourhood of $\overline{\boldsymbol{u}}^h$

$$M(\overline{\boldsymbol{u}}) - M(\overline{\boldsymbol{u}}^h) = \overline{M}[\overline{\boldsymbol{u}}^h](\overline{\boldsymbol{u}} - \overline{\boldsymbol{u}}^h) + \text{H.O.T.}$$

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Set $\boldsymbol{e} = \overline{\boldsymbol{u}} - \overline{\boldsymbol{u}}^h$ and consider

$$\overline{M}[\overline{\boldsymbol{u}}^h](\boldsymbol{e}) = \int_0^T \int_\Omega \boldsymbol{e} \cdot \zeta[\overline{\boldsymbol{u}}^h]\, dx\, dt$$

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Examples: turbulent kinetic energy (lift, drag are also possible)

Dual Weighted Residual Method II

Exemplified: Smagorinsky model is used.

$$\nu_t(\overline{\boldsymbol{u}}^h) = -(c_s\,\Delta)^2 \left(S(\overline{\boldsymbol{u}}^h) : S(\overline{\boldsymbol{u}}^h)\right)^{1/2}$$

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$$\nu_t(\overline{\boldsymbol{u}}^h) = -(c_s\,\Delta)^2\left(S(\overline{\boldsymbol{u}}^h) : S(\overline{\boldsymbol{u}}^h)\right)^{1/2}$$

Define (linear) dual system with (ϕ, θ)

$$\begin{aligned}
-\partial_t\boldsymbol{\varphi} - (\overline{\boldsymbol{u}}\cdot\nabla)\boldsymbol{\varphi} + (\nabla\overline{\boldsymbol{u}}^h)^T\boldsymbol{\varphi} + \nabla\theta & \\
-\nabla\cdot\left((2\nu + \nu_t(\overline{\boldsymbol{u}}^h))S(\boldsymbol{\varphi})\right) - \nabla\cdot T^h[\overline{\boldsymbol{u}}^h](\boldsymbol{\varphi}) &= \zeta[\overline{\boldsymbol{u}}^h] \\
\nabla\cdot\boldsymbol{\varphi} &= 0 \\
\boldsymbol{\varphi} &= 0 \qquad \text{b.c.} \\
\boldsymbol{\varphi}(T,\boldsymbol{x}) &= 0 \qquad \text{i.c.}
\end{aligned}$$

where $T^h[\overline{\boldsymbol{u}}^h](\boldsymbol{\varphi}) = (c_s\,\Delta)^2\,||S(\overline{\boldsymbol{u}}^h)||_F^{-1}(S(\overline{\boldsymbol{u}}^h) : S(\boldsymbol{\varphi}))S(\overline{\boldsymbol{u}}^h)$.

Dual Weighted Residual Method III

Theorem [Error representation formula] Let $\overline{\boldsymbol{u}}^h$ be the numerical solution and ζ a given operator. Then

$$\overline{M}(\boldsymbol{e}) = \int_0^T \int_\Omega \boldsymbol{e} \cdot \zeta dx\, dt = e_M + e_N + O\left(\boldsymbol{e}^2\right)$$

Dual Weighted Residual Method III

Theorem [Error representation formula] Let $\overline{\boldsymbol{u}}^h$ be the numerical solution and ζ a given operator. Then

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with e_M and e_N are given by

$$\begin{aligned} e_M &= \int_0^T \int_\Omega \left(\nabla \cdot \tau_S(\overline{\boldsymbol{u}}^h) - \nabla \cdot \tau(\boldsymbol{u})\right) \cdot \varphi \, dx\, dt \\ e_N &= \int_0^T \int_\Omega \left(R(\overline{\boldsymbol{u}}^h) \cdot \varphi + (\nabla \cdot \overline{\boldsymbol{u}}^h)\, \theta\right) dx\, dt \end{aligned}$$

where $R(\overline{\boldsymbol{u}}^h)$ is the residual of the space-averaged momentum equation with Smagorinsky subgrid-scale model.

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Dual Weighted Residual Method IV

Computable Errors

- STEP 1a: Solve space-averaged NS-equations with τ_S.
- STEP 1b: Store continuous solutions $\overline{\boldsymbol{u}}^h(t)$ and $\overline{p}^h(t)$.

Dual Weighted Residual Method IV

Computable Errors

- STEP 1a: Solve space-averaged NS-equations with τ_S.
- STEP 1b: Store continuous solutions $\overline{\boldsymbol{u}}^h(t)$ and $\overline{p}^h(t)$.
- STEP 2a: Solve dual NS-equations backwards in time.
- STEP 2b: Compute approximations

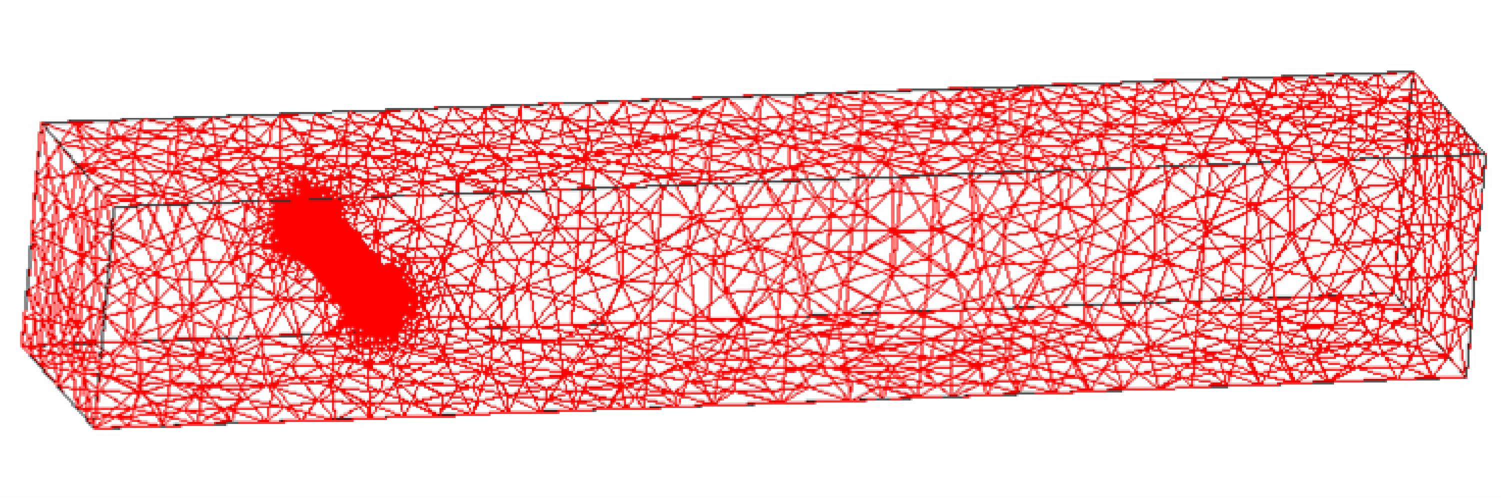
$$
\begin{aligned}
e_M^h &= \int_0^T \int_\Omega \big(\nabla \cdot \tau_S(\overline{\boldsymbol{u}}^h) - \nabla \cdot \tau_{DS}(\overline{\boldsymbol{u}}^h)\big) \cdot \varphi^h \, dx \, dt \\
e_N^h &= \int_0^T \int_\Omega \big(R(\overline{\boldsymbol{u}}^h) \cdot \varphi^h + (\nabla \cdot \overline{\boldsymbol{u}}^h)\, \theta^h\big) \, dx \, dt
\end{aligned}
$$

Example: Flow Around A Cylinder at $Re = 100$

Quantity of interest: time-integrated drag coefficient

$$M(\overline{\boldsymbol{u}}, \overline{p}) = \int_0^T \int_{Cyl} \boldsymbol{n} \cdot (\overline{p} I \; - 2\nu \boldsymbol{S}(\overline{\boldsymbol{u}})) \cdot \boldsymbol{a} \, dx \, dt$$

where $\boldsymbol{a}$ points in the direction of motion.



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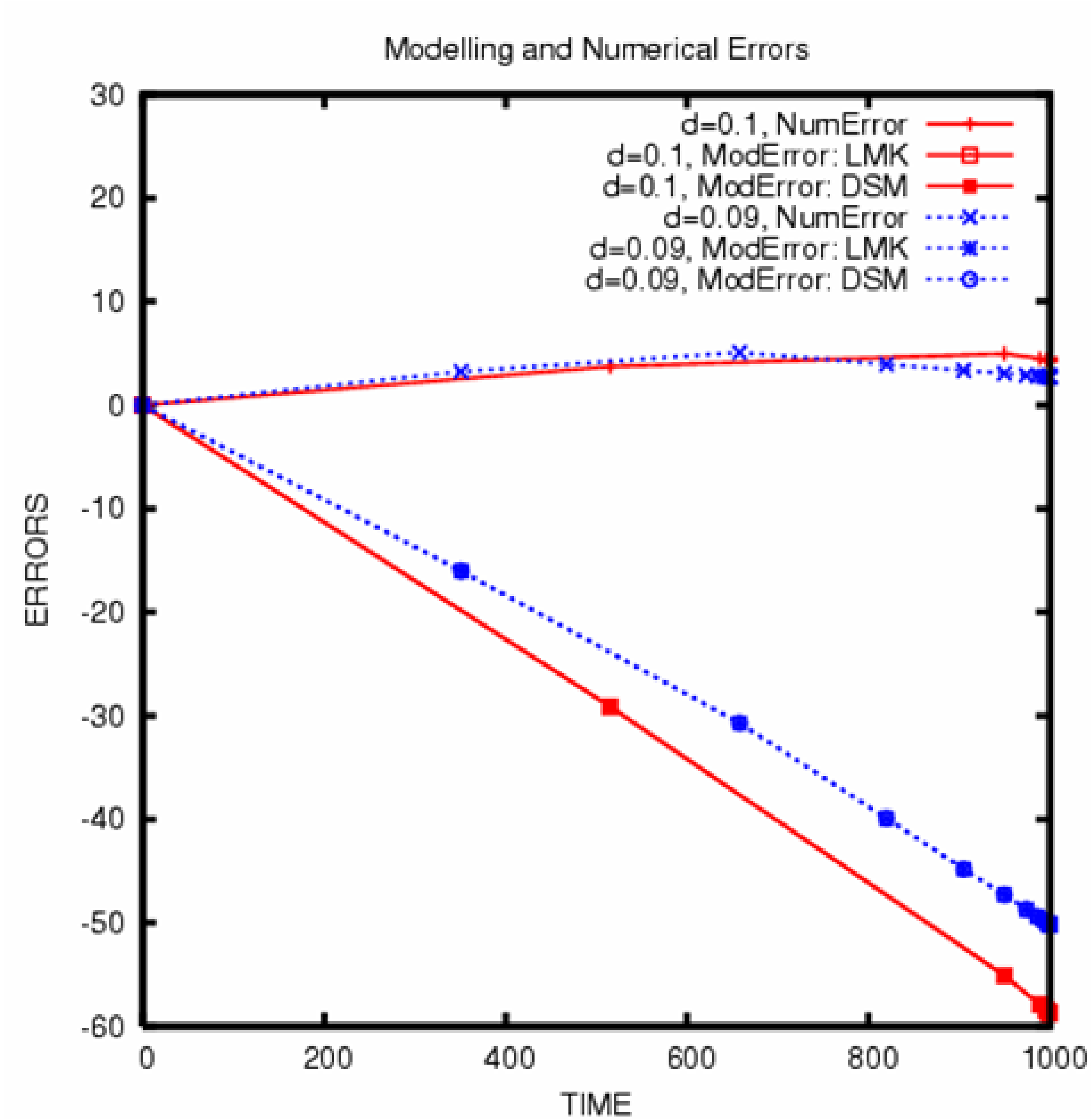

Current and Future Work

- Consider more complex turbulent flows.
- Study various quantities of interest.
- Use local error estimators to improve subgrid-scale model and numerical discretization where necessary (SPP1276 Metstroem)
- Balance errors by local adaptation.
- Develop reduced-order models, e.g., by using POD.
- Introduce framework to rigorously assess LES errors.