Towards Large Eddy Simulation for Turbo-machinery Flows

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Presented at
International Conference on Flow Physics and Its Simulations
In Memory of Prof. Jaw-Yen Yang
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Outline

- Introduction to large eddy simulations (LES)
- Key pacing items enabling LES with high-order adaptive methods
  - High-order methods
  - High-order mesh generation
  - SGS models
- Sample demonstrations
- Conclusions
Introduction

Approaches to compute turbulent flows
- RANS: model all scales
- LES: resolve large scales while modeling small scales
- DNS: resolve all scales

What is LES
- Partition all scales into large scales and small sub-grid scales with a low pass filter with width $\Delta$
- Solve the filtered Navier-Stokes equations with a SGS closure model
- A compromise between RANS and DNS
RANS Inadequate for Many Applications
LES – the Challenges

- How to choose the filter width $\Delta$
- How to resolve the disparate length and time scales in the turbulent flow field
- How to handle complex geometries
- How to resolve very small turbulence scales in the boundary layer
- Discontinuity capturing
- Parallel performance on extreme scale computers
- Post-processing and visualization of large data sets
Key Pacing Items in LES

- High-order methods capable of handling unstructured meshes to deal with complex geometry
- High-order meshes resolving the geometry and viscous boundary layers
  - Coarse meshes (because internal degrees of freedom are added)
- Quality of SGS models
- Wall models to decrease the number of cells in the boundary layer
High order methods
High-Order CFD Methods Needed

- All of the challenges demand more accurate, efficient and scalable design tools in CFD
  - Better engine simulation tools
  - Better design tools for high-lift configurations

\[ \text{Error} \propto h^{p>2} \]
Popular High-Order Methods

- Compact difference method
- Optimized difference method
- ENO/WENO methods
- MUSCL, PPM and K-exact FV
- Residual distribution methods
- Discontinuous Galerkin (DG)
- Spectral volume (SV)/spectral difference (SD)
- Flux reconstruction/Correction procedure via reconstruction
- …

- Structured grid
- Unstructured grid
How to Achieve High-Order Accuracy

- Extend reconstruction stencil
  - Finite difference, compact
  - Finite volume, ENO/WENO, ...

- Add more internal degrees of freedom
  - Finite element/spectral element, discontinuous Galerkin
  - Spectral volume (SV)/spectral difference (SD), flux reconstruction (FR) or correction procedure via reconstruction (CPR), ...

- Hybrid approaches
  - PnPm, rDG, hybrid DG/FV, ...
Extending Stencil vs. More Internal DOFs

- Simple formulation and easy to understand for structured mesh
- Complicated boundary conditions: high-order one-sided difference on uniform grids may be unstable
- Not compact

- Boundary conditions trivial with uniform accuracy
- Non-uniform and unstructured grids
  - Reconstruction universal
- Scalable
  - Communication through immediate neighbor
Review of the Godunov FV Method

Consider

$$\frac{\partial u}{\partial t} + \frac{\partial f(u)}{\partial x} = 0$$

Integrate in $V_i$

$$\int_{V_i} \left( \frac{\partial u}{\partial t} + \frac{\partial f}{\partial x} \right) dx = \frac{\partial \bar{u}_i}{\partial t} \Delta x_i + \int_{i-1/2}^{i+1/2} \frac{\partial f}{\partial x} dx$$

$$= \frac{\partial \bar{u}_i}{\partial t} \Delta x_i + (f_{i+1/2} - f_{i-1/2}) = 0$$
FR/CPR

- Developed by Huynh in 2007 and extended to simplex by Wang & Gao in 2009, ...
- It is a differential formulation like “finite difference”

\[
\frac{\partial U_i(x)}{\partial t} + \frac{\partial F_i(x)}{\partial x} = 0, \quad U_i(x) \in P^k, \quad F_i(x) \in P^{k+1}
\]

- The DOFs are solutions at a set of “solution points”
CPR (cont.)

- Find a flux polynomial $F_i(x)$ one degree higher than the solution, which minimizes

$$\left\| \tilde{F}_i(x) - F_i(x) \right\|$$

- The use the following to update the DOFs

$$\frac{d u_{i,j}}{d t} + \frac{d F_i(x_{i,j})}{dx} = 0$$
CPR – DG

➢ If the following equations are satisfied

\[
\int_{V_i} \left[ \tilde{F}_i(x) - F_i(x) \right] dx = 0
\]

\[
\int_{V_i} \left[ \tilde{F}_i(x) - F_i(x) \right] x dx = 0
\]

➢ The scheme is DG!
High order mesh generation
The Need for Coarse, High-Order Meshes

- Internal degrees of freedom are added such that meshes with ~100,000 elements may be sufficient to achieve engineering accuracy.
- If boundaries are still represented by linear facets, large errors are generated.

![Diagram of projected to curved boundary](image)
Low versus High-Order Meshes: An Example in 2D

low-order

high-order
CAD Free, Low to High-Order Mesh Conversion

(released free of charge, just google meshCurve)
For high-order CFD simulations, we need to change this to this without smoothing away edges.
Main Features

- CGNS meshes: 3D, unstructured, multi-zone, multi-patch
- CAD-free operation
- Feature-curve preservation
- Easy-to-use, cross-platform graphical user interface
- Interactive 3D graphics
- Solid code base with minimal reliance on outside software libraries.
- Reasonably low memory footprint and fast operation on a desktop computer.
- Available for: Linux, MS Windows and Mac platforms
Demo Video
SGS Models with the Burgers’ Equation
Our Venture into LES

- Solve the filtered LES equations using
  - FR/CPR scheme
  - 3 stage SSP Runge-Kutta scheme for time marching

- Implemented 3 SGS models
  - Static Smagorinsky (SS) model
  - Dynamic Smagorinsky (DS) model
  - ILES (no model)

- Attempted several benchmark problems
  - Flow over a Cylinder (ILES)
  - Isotropic turbulence decay (SS, DS, ILES)
  - Channel flow (SS, DS, ILES)
LES Results – Isotropic Turbulence Decay

- DNS
- ILES
- Static
- Dynamic

Graphs showing decay of turbulence with time and wave number.
Why ILES Performs Better Consistently

- No good explanation!
- So we decided to evaluate SGS models using the 1D Burgers’ equation
  - High resolution DNS can be easily carried out
  - True stress can be computed based on DNS data
  - Both a priori and a posteriori studies can be performed
  - Yes, the physics of 1D Burger’s equation is vastly simpler than the Navier-Stokes equations, but if a SGS model has any chance for 3D Navier-Stokes equations, it must perform well for the 1D Burger’s equation
Filtered Burgers’ Equation

1D Burgers’ equation

\[
\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = \nu \frac{\partial^2 u}{\partial x^2}
\]

Filter the equation with a box filter

\[
\frac{\partial \bar{u}}{\partial t} + \bar{u} \frac{\partial \bar{u}}{\partial x} = \nu \frac{\partial^2 \bar{u}}{\partial x^2} - \frac{\partial \tau}{\partial x}.
\]

where

\[
\tau = \frac{1}{2} \bar{u} \bar{u} - \frac{1}{2} \bar{u} \bar{u}.
\]
SGS Models Evaluated

- Static Smagorinsky model (SS)
- Dynamic Smagorinsky model (DS)
- Scale similarity model (SSM)
- Mixed model (MM) of SSM and DS
- Linear unified RANS-LES model (LUM)
- ILES (no model)
Numerical Method and Problem Setup

Numerical method
- 3rd order FR/CPR scheme
- Viscous flux is discretized with BR2
- Explicit SSP 3 stage Runge-Kutta scheme

Problem setup
- Domain [-1, 1] with periodic boundary condition
- The initial solution contains 1,280 Fourier modes satisfying a prescribed energy spectrum with random phases
- The DNS needs 2,560 cells to resolve all the scales
- The filter width: $\Delta = 32 \Delta x_{DNS}$
- Various mesh resolutions for LES $\Delta x_{LES}/\Delta = 1, 1/2, 1/4, 1/8$
Initial Condition

\[ \frac{5}{3} \]
The DNS Results

Energy spectrum

Filtered DNS result used as “truth solution” for LES
Comparison of SGS Stresses (A Priori)

- True SGS stress
- SS
- DS
- SSM
- MM
- LUM

Graph showing SGS stress variations with X values from 0.1 to 0.3.
Lessons Learned about SGS Models

- In both a priori and a posteriori tests with the 1D Burgers’ equation
  - SGS stresses generated by static, dynamic Smagorisky and LUM models show no correlation with the true stress
  - SSM (and Mixed model) consistently produces stresses with the best correlation with the true stresses
- When the modeling error is dominant, SSM and MM perform the best. When the truncation error is dominant, no model shows any advantage. ILES is preferred
- For methods with dissipation, DO NOT use SGS models. For almost all LES simulations, truncation errors are dominant ($\Delta = h$), the best choice is ILES.
Example Applications
Parallel Efficiency: Strong Scalability Test

- Compare packing/unpacking vs direct data exchange
- P3 100 RK3 iterations on BlueWater; 125,000 Hex elements
- 3D inviscid vortex propagation: 72% at 8192 cores (15 elements/core)
- 3D viscous Couette Flow: 68% at 16384 cores (8 elements/core)
Periodic Hill

- Benchmark problem adopted by the international workshops for high-order CFD methods
- \( \text{Re} = 2,800 \) and \( 10,595 \)
- Accurate prediction of separation and reattachment points is a key challenge
- P3 FR/CPR+3\(^{rd}\) order SSP Runge-Kutta

16,384 P3 elements
Periodic Hill

Iso-surface of $Q$ colored by streamwise velocity at $Re_b=10595$ (hybrid)
Periodic Hill (Re = 2,900)

- Mean streamline

ILES

Hybrid
Periodic Hill (Re = 10,595)

- Mean streamline

ILES

Hybrid
Separation and Reattachment Points

![Graph showing separation and reattachment points with various lines representing different approaches such as ILES and HybridApproach, with x/h and Re_b axes.]
Velocity Profiles, $Re = 2,800$

$x/h = 2$

$x/h = 6$
Velocity Profiles, Re = 10,595

$x/h = 0.5$

$x/h = 6$
Uncooled VKI Vane Case - Benchmark

- Reynolds number: 584,000, Mach exit: 0.94
- No. of hexahedral elements: 511,744
- nDOFs/equ at p5 (6th order): 110.5M

Boundary conditions
- Inlet: fix total p and total T and flow angle
- Wall: no split and iso-thermal
- Exit: fix p
- Periodic on the rest

Some challenges
- There are supersonic regions and shock waves
- Heat transfer is difficult to predict
Simulation Process

- Start the simulation from \( p_0 \) (1\textsuperscript{st} order), and then restart at higher orders. This is much more robust than directly starting at high order.
- Monitor the Cl and Cd histories on the main blades to determine the start time for averaging.
- P-refinement studies used to assess the accuracy and mesh and order independence.
Q-Criterion and Computational Schlierens
Computational Schlierens

FDL3DI – sixth order compact scheme

FR/CPR - sixth order
Comparison of Heat Transfer
Summaries

- Outlined the challenges in LES
- Focused on several pacing items for LES
  - High order methods
  - High-order mesh generation
  - SGS models
- Presented several demonstration cases to show the capability
- Future work includes better wall models and efficient time integration schemes for extreme scale computers
Acknowledgements

- We are grateful to AFOSR, NASA, ARO and GE Global Research for supporting the present work.