Adaptive Meshing, Adaptive Physics, Advanced Numerics for Reacting-LES Computations

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Reacting-LES

**Unstructured Mesh**
- Rarely automated
- Very inefficient
- Usually limited to 2nd order
- Difficult to adapt
- Good at capturing geom
- Very good for boundary layers

**Cartesian Mesh**
- Automatic generation
- Highly efficient
- High-order accuracy
  - Usually 5th or 7th order
- Amenable to adaption
- Poor geometry defn
- Poor for boundary layer
Dual-Mesh Paradigm

Combine unstructured near-body with Cartesian off-body

Use domain connectivity to exchange data between two mesh systems
Goals

Develop dual-mesh algorithms for reacting-LES

1. Extend existing automated strand-Cartesian gridding techniques for internal flows
2. Develop off-body Cartesian adaptive meshing strategies for turbulent reacting flows
3. Devise adaptive physics approach for combustion
4. Employ optimal numerics for reacting-LES

Project is part of the AFOSR/Test and Evaluation Portfolio
- Dr. Michael Kendra as Program Officer
- Dr Terrance Dubreus - AEDC - as tech transition advisor
Strand Grids and Internal Flows

Strand Grids
Automated volume grid
High-order accuracy
Enhanced scalability

Protypical Internal Geometries

(a) Nozzle.
(b) Curved Duct.
(c) Bluff Body.
(d) Internal-External Flow.
(e) Internal-External Flow with Forebody.
(f) Annulus.
(g) Co-axial Injector.
(h) Regenerative Cooling.
Adaptive Meshing

Adaptive Algorithms

- Current methods
  - New grid level based on vorticity detection
  - Refinement terminated based on Richardson extrapolation

Reacting-LES

- Is vorticity sufficient?
- Use other detection & termination methods?
- Heat release, temperature gradients, etc.
Adaptive Physics

- **Combustion calculations are extremely expensive**
  - Detailed combustion kinetics
    - Large number of species and reaction steps
  - Turbulent combustion closures
    - Linear Eddy Model involves sub-grid solutions

- **Silver Lining**
  - Detailed chemistry & closures needed only locally
  - Most of the flowfield has unburnt or burned propellants

- **Devise adaptive physics approach**
  - Apply detailed models only in local blocks
  - Block-based solver structure is ideally suited to adaptive physics implementation
Modular Physics

Different grid blocks can use different physics

Domain connectivity provides data transfer between blocks
Advanced Numerics

Challenges: Reacting LES

Premixed flame:

Algorithm comparisons:
- Identical SGS
- Differences in numerical schemes’ dissipation

MUSCL scheme
LESIE3D (Geol Tech)
Central scheme


Need to determine OPTIMAL discretization schemes for Reacting
The Role of Artificial Dissipation

Backward Euler (BDF-1)

21 points per wave
5 cycles

GOAL: Damp high frequency errors while preserving low wave content (i.e.: low-pass response)
Artificial Dissipation:

\[
\frac{\partial Q}{\partial t} + A \frac{\partial Q}{\partial x} = \sum_m (-1)^{m-1} (\Delta x)^{2m-1} \epsilon_{2m} \lambda_{u+c} \left| \frac{\partial^{2m} Q}{\partial x^{2m}} \right|
\]

\[\varepsilon_2 = 1/2; \quad \varepsilon_4 = 1/12; \quad \varepsilon_6 = 1/60\]

Higher order terms better preserve
Explicit Filter: Growth Factor

Shapiro Filter:

\[ Q_i = \left[ 1 - \left( -\frac{\Delta x^2}{4} \right)^m \frac{\partial^2 Q^*}{\partial x^2} \right] Q_i^* \]

Higher order terms better preserve low
$2^{nd}$ Order Padé Filter: Growth Factor

Long Filter: 

$$Q_i = \left[ 1 + \frac{(\Delta x)^2}{4} \frac{\partial^2}{\partial \chi^2} \right] Q_i^* \text{ with } \delta \in [0,1]$$

Low-pass response achieved with compact
Explicit Filtering as an Artificial Dissipation Scheme

\[
Q_{j}^{n+1} = \left[ 1 + \frac{1}{4} (\Delta x)^{2} \frac{\partial^{2}}{\partial x^{2}} \right] Q_{j}^{*}
\]

\[
= \left[ 1 + \frac{1}{4} (\Delta x)^{2} \frac{\partial^{2}}{\partial x^{2}} \right] \left[ Q_{j}^{n} - \Delta t (1 - \theta) \frac{\partial E^{n}}{\partial x} + \Delta t \theta \frac{\partial E^{*}}{\partial x} \right] \text{ with } \theta \in [0, 1]
\]

\[
\frac{Q_{j}^{n+1} - Q_{j}^{n}}{\Delta t} + (1 - \theta) \frac{\partial E^{n}}{\partial x} + (\theta) \frac{\partial E^{*}}{\partial x} = \frac{1}{4} (\Delta x)^{2} \frac{\partial^{2} Q^{n}}{\partial x^{2}} - (1 - \theta) \frac{1}{4} (\Delta x)^{2} \frac{\partial^{3} E^{n}}{\partial x^{3}} - (\theta) \frac{1}{4} (\Delta x)^{2} \frac{\partial^{3} E^{*}}{\partial x^{3}}
\]
Growth Factor: Effect of CFL

- Artificial dissipation adjusts for CFL

[Graph showing the effect of CFL on growth factor with curves for different CFL values (0.01, 0.1, 1) and order of filters (10th and 6th)]
Cumulative Effect of CFL

$\text{CFL}_{u+c} = 10^{-4}$ with 10,000 steps
Computational Test: Dissipation

$CFL_{u+c} = 1$ at Mach = 0.5 with 100 cycles
21 points per wave (PPW)

4th Order Artificial Dissipation

4th Order Padé Filter (Lele)

Padé filter preserves low wavenumber
Computational Test: Dispersion

\[ \text{CFL}_{u+c} = 1 \text{ at Mach } = 0.5 \text{ with 100 cycles} \]

21 points per wave (PPW)

**4th Order Padé Filter (Lele)**

<table>
<thead>
<tr>
<th>Phase Error:</th>
<th>21 PPW</th>
<th>5 PPW</th>
</tr>
</thead>
<tbody>
<tr>
<td>2nd order</td>
<td>2.36%</td>
<td>40.8%</td>
</tr>
<tr>
<td>4th order</td>
<td>0.82%</td>
<td>25.0%</td>
</tr>
<tr>
<td>4th order (*)</td>
<td>0.80%</td>
<td>15.4%</td>
</tr>
<tr>
<td>6th order</td>
<td>0.79%</td>
<td>19.4%</td>
</tr>
<tr>
<td>6th order (4th order AD)</td>
<td>0.79%</td>
<td>18.3%</td>
</tr>
<tr>
<td>8th order</td>
<td>0.79%</td>
<td>17.0%</td>
</tr>
</tbody>
</table>

* optimized 9pt stencil (Bogey & Bailly 2004)

**Phase error is substantial over long periods**

exact numerical: - 6th order
High-Order Time Schemes

Phase error for high-order spatial schemes without accounting for temporal discretization

Phase error for high-order temporal schemes
Summary

- **New LRIR project awarded in FY15**
  - Research in technologies for the next-gen CFD solver for reacting LES for rocket propulsion

- **Focus areas**
  - Dual mesh paradigm for internal flows
  - Cartesian adaptive meshing for reacting-LES
  - Adaptive physics for kinetics and turbulent combustion
  - Optimal numerics for minimal dissipation/discretization