Towards Discontinuous Galerkin Solution of the 3D RANS Equations

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Outline

1. Introduction
   - Motivation
   - Approach

2. The SA model

3. DG Discretization

4. Results
The Problem

- Engineers interested in solving the Navier Stokes equations for complex aerodynamic geometries
- Well-known that for most problems of interest, turbulence arises
  - Multiscale problem with lengths ranging from 70m (e.g. 747) to 0.1mm (smallest eddies)

Figure: Mach Number

Figure: Eddy Viscosity
Challenges of Turbulence

Kolmogorov Scales (1941)

- Kolmogorov describes the transfer of energy from large to small eddies (bulk-coherent region of turbulent motion)
  - At high $Re$, small scale eddies are statistically isotropic
  - Such small eddies (size $\eta$) are similar and governed by the energy dissipation $\epsilon = O(1)$ and the kinematic viscosity $\nu$

- Eddies have size $l$ and characteristic velocity $u_l$; largest eddies have $l_0 = L$, the flow length scale

- Dimensional analysis: $\epsilon = O(\frac{u_0^3}{l_0})$, $\eta = O((\frac{\nu^3}{\epsilon})^{1/4})$

- Length ratio: $\frac{l_0}{\eta} = O(Re^{3/4})$

- Time ratio: $\frac{l_0/u_0}{\tau} = O(Re^{1/2})$
Making Turbulence Manageable

A Multiscale Problem
- Aircraft (typical $Re > 10^7$) in 3D: more than $10^{15}$ elements to simulate all turbulent scales!
- Worse, more than $10^4$ time steps are required.

RANS
- Reformulate the problem by time-averaging and solving for the mean flow: Reynolds-Averaged Navier Stokes (RANS) Equations
- Make modeling assumptions about the remaining turbulent components to simplify the governing equations

We want to investigate...
- Whether a higher-order DG implementation of the RANS-SA equations is an efficient and accurate way of obtaining engineering accuracy on aerodynamic problems
Current State of the Art

AIAA Drag Prediction Workshop III

- Cases designed to exemplify common industry CFD usage patterns (e.g. turbulent flow: $Re$ around $5 \times 10^6$)
- Wing/Body/Nacelle geometries with as many as 25 million nodes
- Goal: Assess the current state-of-the-art CFD capabilities

Sample DPWIII surface mesh
Flow solution
Mavriplis studied drag convergence on two different initial meshes.

1 count ($= 0.0001C_D \approx 4$ counts) loss of 4-8 passengers on a 747-800.

- Meshes highly refined; typical industry meshes of $N = 1$ to 4 million elements.
- Observed large differences even after several refinements.
- Solutions are highly grid dependent; large numbers of refinements may not be sufficient for consistent results.
Approach

DPW: Same code can give inconsistent results, indicating that current best practices are insufficient.

DG for RANS

- We aim to provide an automated, accurate, and robust CFD-framework for solving the RANS equations
  - Higher-order solutions with the DG method
  - Output-based mesh adaptation via the adjoint problem
  - Direct interface to CAD models
- Believe the above will be effective in approaching the issues raised by the DPWs
- Solution of the RANS equations brings up many challenges:
  - Very stiff source terms
  - Non-canonical source terms not seen in standard problems, e.g. convection-reaction-diffusion
  - Lack of solution regularity due to turbulence model
Past Work: DG Discretizations of the RANS Equations

- Few publications to date on this subject (even for 2D)
- Nguyen et al (2007): SA model, artificial viscosity to regularize eddy viscosity
- Landmann (2007): several models, hard-limiting to improve robustness
- Oliver (2008): SA model, unsteady adaptation and dual-consistent source
- Oliver (2009): SA model, convergence-rate issues caused by model irregularity
Advantages of Higher-Order

Figure: Grid convergence study on a flat plate in 2D

Observed $O(h^p)$ drag convergence rate

Nguyen et al (2007)
- Experimentally observed that increasing $p$ results in less error than decreasing $h$, maintaining equal numbers of unknowns
- The higher $p$ case also required significantly less CPU time
Convergence Rate Issues Caused by Irregularity

NACA 0012 at: \( M_\infty = 0.25, \ Re_c = 1 \times 10^7, \ \alpha = 0^\circ \).

Figure: Drag error vs \( h \) for \( p = 1 \) (\( \square \)), \( p = 2 \) (\( \circ \)), \( p = 3 \) (\( \ast \)), \( p = 4 \) (\( \triangle \)), and \( p = 5 \) (\( \times \)). Error measured against \( p = 5 \) solution on the finest mesh.

Oliver (2009)

- Superconvergence achieved for \( p = 1 \) and \( p = 2 \) but not for higher \( p \).
  - Suboptimal rates due to a non-smooth solution and insufficient mesh resolution at the BL edge.
Convergence Rate Issues Caused by Irregularity

NACA 0012 at: \( M_\infty = 0.25, \) \( Re_c = 1 \times 10^7, \) \( \alpha = 0^\circ \).

Figure: Drag error vs \( NDOF \); shows several \( p \)-orders for different meshes. Error measured against \( p = 5 \) solution on the finest mesh.

Oliver (2009)

- \( p \)-refinement shows that exponential convergence: the rate stagnates
- Despite stagnation, higher \( p \) solutions sometimes reach lower error with fewer DOFs. \( (NDOF = O(1/h^2)) \)
Spalart Allmaras One-Variable Turbulence Model

**SA Overview**
- One-equation model for $\tilde{\nu}$, providing closure for eddy viscosity
- Popular in the aerospace community, especially for external flows

**Issues**
- Requires distance to the nearest solid wall.
- Potentially unstable when $\tilde{\nu} < 0$.
- Numerical difficulties from very stiff, nonlinear source terms
- $\tilde{\nu}$ varies rapidly near the BL edge (discontinuous first derivative in the 0 viscosity limit).
  - Needs additional mesh resolution at the BL edge as a result.

Using a modified SA model to mitigate issues when $\tilde{\nu} < 0$
Popular Choices

- Solve for distance exactly using a modified level-set equation over the entire flow-field.
- **Intelligent-search for the distance at points of interest.**

Approach

- Use kd-tree filled with surface quadrature points to perform a nearest-neighbor search from quadrature points in the flow field.
  - Assumes wall-curvature is small relative to quad-point spacing.
- Result initializes a Newton search to minimize wall-distance based on a polynomial representation of the geometry.
kd-Trees

kd-trees are essentially **k-dimensional** binary trees.
- Each node represents a k-dimensional point in space.
- Non-leaves also host splitting hyperplanes; points on the left/right become left/right children.

**Expected asymptotic performance:**
- $O(\log(N))$ to find a nearest-neighbor in a tree of $N$ points.
- $O(N)$ storage and $O(N \log(N))$ construction time.
For some triangulation ($T_h$) of the domain ($\Omega$), apply a polynomial basis ($V^p$) locally over each element to the governing equations in weak form.

$$
\sum_{\kappa \in T_h} \int_{\kappa} v_h^T \frac{\partial u_h}{\partial t} + R_{h,\text{Inv}}(u_h, v_h) + R_{h,\text{Vis}}(u_h, v_h) + R_{h,\text{Src}}(u_h, v_h) = 0
$$

where test functions $v_h$ and solution $u_h$ are represented in the discrete basis $V_h^p$ and $R_{h,\cdot}$ are the discrete residuals.

- $R_{h,\text{Inv}}$: evaluated using Roe’s method
- $R_{h,\text{Vis}}$: evaluated using the 2nd method of Bassi and Rebay (BR2)
- $R_{h,\text{Src}}$: optionally handled in a dual consistent manner (i.e. NOT as simple as $\int_{\kappa} v_h^T S(u, \nabla u)$)
Steady problem: $\mathbf{R}(\mathbf{U}) = 0$, where $\mathbf{R}$ is the discrete residual vector.

But $\mathbf{R}$ is nonlinear, so we solve a pseudo-time-dependent problem to slowly march to the steady-state solution:

$$M \frac{d\mathbf{U}}{dt} + \mathbf{R}(\mathbf{U}) = 0$$

where $M$ is the mass matrix.

Use Backward-Euler:

$$\frac{1}{\Delta t} M \left( \mathbf{U}^{m+1} - \mathbf{U}^m \right) + \mathbf{R}(\mathbf{U}^{m+1}) = 0$$

Each step requires the solution of a nonlinear problem; instead, only take 1 newton-step (i.e. linearize):

$$\mathbf{U}^{m+1} = \mathbf{U}^m - \left( \frac{1}{\Delta t} M + \frac{\partial \mathbf{R}}{\partial \mathbf{U}} \right)^{-1} \mathbf{R}(\mathbf{U}^m)$$

Use ILU-preconditioned GMRES to solve the linear system.
Preliminary Results

Extruded Flat Plate Test Case

- \( M_\infty = 0.25, \ Re_C = 1 \times 10^6, \ \alpha = 0^\circ \)
- 2D, 234 element triangular mesh extruded to 3D
  - Created 3 layers of tetrahedrons with total depth 1

### Table: Drag on a flat plate in 2D and 3D

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<thead>
<tr>
<th></th>
<th>2D</th>
<th>3D</th>
</tr>
</thead>
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<td>( p_5 )</td>
<td>2.03642280345054E-03</td>
<td>N/A</td>
</tr>
</tbody>
</table>
Figure: Output taken at $x = 0.45$ (2D, 3D) and $z = 0.5$ (3D).
Flat Plate Skin Friction

Figure: Output taken at $z = 0.5$ in 3D.
Remaining Challenges

- **Strong/Stiff source terms**
  - May be wiping out the matrix diagonal of the linear system

- **Non-physical updates and overshoots in time**
  - Pseudo-time stepping often leads to non-physical intermediate states before reaching a steady solution
  - Overshoots can be large enough to trigger unwanted modes, leading to non-convergence
  - Artificial solution oscillation in time can also result

- **Lack of regularity at the edge of the BL**
  - Could lead to non-convergence on coarse meshes by causing solution oscillation
  - Reduces optimal solution/output convergence rate
**Overall Goals**
- Improve robustness of current implementation
- Solve problems on DPW grids

**Immediate Tasks at Hand**
- ProjectX 3D capability remains largely untested
  - Create and run a battery of test cases to study the performance and robustness of the 3D laminar code
  - Problems to range from extruded 2D to wing-body configurations
- Solver is currently problematically slow
  - Large problems may not be feasible from a time perspective
  - Code profiling to attempt to improve performance (e.g. better cache/memory efficiency)
Questions?
In the core region, spread is about 10 drag counts (1 count $\approx 0.024+0.001C_D$): seems good?

By the Breguet Range Equation, raising the drag of a 747-400 by 1 count $\approx$ loss of 4-8 passengers

Uncertainty of 10 counts is actually huge!
Advantages of Higher-Order

Back of the Envelope Argument

- If the error converges at $O(h^{p+1})$, the computation time is estimated: $\log T \approx d \left( -\frac{1}{p+1} \log E \right) - \log F + \text{const}$
  - $d$ is the dimension, $F$ is the computational rate
  - For small $E$, the time depends exponentially on $\frac{d}{p+1}$
  - Increasing $p$ can significantly lower $T$


- Experimentally compared FV, SUPG, and DG schemes of various orders on the Euler and Navier-Stokes Equations
- Concluded that higher-order schemes are exceptionally efficient in smooth flows
  - But solution discontinuities “cap” convergence rates
- Higher-order schemes generally require update-limiting due to stronger, non-physical overshoots in pseudo-time stepping
Lift and Drag

- 3D RANS using $k - \omega$ model
- DG method (higher order)
- Body of revolution based on NACA 0012
Why DG?

Discontinuous Galerkin Finite Elements: Advantages

- Easier development of higher order schemes for convection dominated flows using upwinding ideas from FD and FV
- Compact stencils at any $p$: block-structured Jacobian with only 1st-neighbor connectivity
- Well-suited to unstructured meshes, mesh adaptation ($h$ and $p$), and parallelization
- Natural, weak enforcement of boundary conditions
- No global continuity constraint means maximal flexibility
- Optimally $O(h^{p+1})$ solution error and $O(h^{2p})$ output error
Compressible Reynolds-Averaged Navier Stokes Equations

Time-average the NS Equations, solving for the mean-state:

\[
\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial}{\partial x_i} (\bar{\rho} \bar{u}_i) = 0
\]

\[
\frac{\partial}{\partial t} (\bar{\rho} \bar{u}_i) + \frac{\partial}{\partial x_j} (\bar{\rho} \bar{u}_j \bar{u}_i + \bar{p} \delta_{ij}) = \frac{\partial}{\partial x_j} \left[ 2 (\mu + \mu_t) \left( \bar{s}_{ji} - \frac{1}{3} \frac{\partial \bar{u}_k}{\partial x_k} \delta_{ij} \right) \right]
\]

\[
\frac{\partial}{\partial t} \left[ \bar{\rho} \left( \bar{e} + \frac{1}{2} \bar{u}_i \bar{u}_i \right) \right] + \frac{\partial}{\partial x_j} \left[ \bar{\rho} \bar{u}_j \left( \bar{h} + \frac{1}{2} \bar{u}_i \bar{u}_i \right) \right] = \frac{\partial}{\partial x_j} \left[ c_p \left( \frac{\mu}{Pr} + \frac{\mu_t}{Pr_t} \right) \frac{\partial \bar{T}}{\partial x_j} \right] + \frac{\partial}{\partial x_j} \left[ 2 \bar{u}_i (\mu + \mu_t) \left( \bar{s}_{ij} - \frac{1}{3} \frac{\partial \bar{u}_k}{\partial x_k} \delta_{ij} \right) \right]
\]

where (\bar{\cdot}) and (\tilde{\cdot}) denote the Reynolds and Favre averages

- Neglect: turbulent kinetic energy, molecular diffusion, turbulent transport
- Require closure models for the Reynolds stress (Boussinesq Approximation) and eddy viscosity (\mu_t). . .
Derivation of the RANS Equations I

The (compressible) Navier Stokes (NS) equations are:

\[
\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i} (\rho u_i) = 0
\]

\[
\frac{\partial}{\partial t} (\rho u_i) + \frac{\partial}{\partial x_j} (\rho u_j u_i + p \delta_{ij}) = \frac{\partial \tau_{ij}}{\partial x_j}
\]

\[
\frac{\partial}{\partial t} \left( \rho (e + \frac{1}{2} u_i u_i) \right) + \frac{\partial}{\partial x_j} \left( \rho u_j (h + \frac{1}{2} u_i u_i) \right) = \frac{\partial}{\partial x_j} (u_i \tau_{ij}) - \frac{\partial q_j}{\partial x_j}
\]

where \( e \) is the specific internal energy, \( h \) is the specific enthalpy, \( \tau_{ij} \) is the (deviatoric) viscous stress tensor, and \( q_i \) is the heat flux vector.

Recall that \( \tau_{ij} = 2 \mu \left( s_{ij} - \frac{1}{3} \frac{\partial u_k}{\partial x_k} \delta_{ij} \right) \) where \( s_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \) is the strain rate tensor using Stokes’ Hypothesis. We also assume Fourier’s Law, \( q_i = -\kappa \frac{\partial T}{\partial x_i} \). Finally, we assume the working fluid is a perfect gas.
The NS equations apply to laminar and turbulent flows. As we have seen, turbulent flow is too complex to solve fully. Instead, we will derive the Reynolds Averaged Navier Stokes (RANS) equations which govern the mean flow by averaging out or modeling turbulent fluctuations.

Toward this end, we need two notions of “average”. First, the time average of a quantity \( \nu \) is,

\[
\bar{\nu}(x) = \lim_{T \to \infty} \int_{t_0}^{t_0+T} \nu(x, t) \, dt
\]

Now we can decompose \( \nu \) into mean and fluctuating parts, \( \nu = \bar{\nu} + \nu' \). \( \bar{\nu} \) is constant and \( \nu' \) has mean 0. The averaging process is also a linear operation. Observe that \( \nu' \) need not be small.
For compressible flow, a density weighted average (Favre average) is also useful:

\[
\tilde{u}(x) = \frac{1}{\bar{\rho}} \lim_{T \to \infty} \int_{t_0}^{t_0+T} \rho(x, t)u(x, t)dt
\]

We break \( u \) as \( u = \tilde{u} + u'' \). The Favre average has the same properties as the time average; after all they are quite similar.

As an example, consider computing

\[
\bar{u} \frac{\partial u}{\partial x} = \lim_{T \to \infty} \frac{1}{T} \int_{t_0}^{t_0+T} (\tilde{u} + u') \left( \frac{\partial \tilde{u}}{\partial x} + \frac{\partial u'}{\partial x} \right) dt
\]

for an incompressible flow. Using \( \bar{f'}g = 0 \), this reduces to \( \tilde{u} \frac{\partial \tilde{u}}{\partial x} + u' \frac{\partial u'}{\partial x} \).

So \( u_i \frac{\partial u}{\partial x_i} = \tilde{u}_i \frac{\partial \tilde{u}}{\partial x_i} + u'_i \frac{\partial u'}{\partial x_i} \). The nonlinear terms are evaluated as

\[
\lim_{T \to \infty} \frac{1}{T} \int_{t_0}^{t_0+T} \frac{\partial u'_i u'}{\partial x_i} + u' \frac{\partial u'_i}{\partial x_i} dt.
\]

Using continuity, the second term drops out, so \( u'_i \frac{\partial u'}{\partial x_i} = \frac{\partial u'_i u'}{\partial x_i} \).
\[
\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial}{\partial x_j}(\bar{\rho} \tilde{u}_i) = 0
\]

\[
\frac{\partial}{\partial t}(\bar{\rho} \tilde{u}_i) + \frac{\partial}{\partial x_j}(\bar{\rho} \tilde{u}_j \tilde{u}_i + \bar{p} \delta_{ij}) = \frac{\partial}{\partial x_j}(\bar{\tau}_{ij} - \bar{\rho} u''_j u''_i)
\]

\[
\frac{\partial}{\partial t} \left( \bar{\rho}(\tilde{e} + \frac{1}{2} \tilde{u}_i \tilde{u}_i) + \frac{1}{2} \bar{\rho} u''_i u''_i \right) + \frac{\partial}{\partial x_j} \left( \bar{\rho} \tilde{u}_j (\tilde{h} + \frac{1}{2} \tilde{u}_i \tilde{u}_i) + \tilde{u}_j \frac{1}{2} \bar{\rho} u''_i u''_i \right)
\]

\[
= \frac{\partial}{\partial x_j} \left( -q_j - \rho u''_j h'' + \tau_{ji} u''_i - \rho u''_j \frac{1}{2} u''_i u''_i \right) + \frac{\partial}{\partial x_j} (\tilde{u}_i (\bar{\tau}_{ij} - \bar{\rho} u''_i u''_j))
\]

Notice that the terms with large overlines (e.g. \( \bar{\rho} u''_i u''_i \)) do not have equivalents in the NS equations. In particular, these terms arose when we attempted to average nonlinear terms of the NS equations.
Additionally, these quantities are not in terms of the mean flow variables, implying that while the number of equations stayed the same, we have added “five” new unknowns. (Really there are many more than 5, since some of the new unknowns are tensors.)

Until now we have made no approximations or assumptions. But in order to make the RANS equations solvable, we need closure relations for our five new terms: the Reynolds stress tensor, $\rho u''_j u''_i$; the turbulent heat flux, $\rho u''_j h''$; the turbulent specific kinetic energy, $\bar{\rho}k = \frac{1}{2}\rho u''_i u''_i$; the molecular diffusion, $\tau_{ji}u''_i$; and the turbulent transport, $\rho u''_j \frac{1}{2}u''_i u''_j$.

Assuming $k \ll \tilde{h}$ (reasonable for most aerodynamic problems), we can neglect the latter three terms.

Boussinesq Approximation:

$$-\rho u''_j u''_i = 2\mu_t \left( \tilde{s}_{ij} - \frac{1}{3} \frac{\partial \tilde{u}_k}{\partial x_k} \delta_{ij} \right) - \frac{2}{3} \bar{\rho}k\delta_{ij}$$
where $\mu_t$ is an artificial quantity called the eddy viscosity; it is an additional, apparent addition to viscosity arising from the action of turbulent eddies. Keeping with $k \ll \tilde{h}$, the second term is neglected. Note that we still need a closure relation for $\mu_t$; this will be provided by the Spalart-Allmaras turbulence model. Using the Reynolds Analogy, we find that the turbulent heat flux is,

$$\rho u''' h''' = -\frac{\mu_t C_p}{Pr_t} \frac{\partial T}{\partial x_j}$$

where $Pr_t = 0.9$ is the turbulent Prandtl number.
The RANS equations have the strong form:

\[
\frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot \mathbf{F}^{\text{inv}}(\mathbf{u}) - \nabla \cdot \mathbf{F}^{\text{vis}}(\mathbf{u}, \nabla \mathbf{u}) = S(\mathbf{u}, \nabla \mathbf{u})
\]

- \( \mathbf{F}^{\text{inv}} \) and \( \mathbf{F}^{\text{vis}} \) are the inviscid and viscous fluxes, respectively.
- The corresponding weak form is obtained through multiplication by test functions \( v \) and integration by parts:

\[
\int_{\Omega} v \frac{\partial \mathbf{u}}{\partial t} + \int_{\Omega} \nabla v \cdot \mathbf{F}(\mathbf{u}, \nabla \mathbf{u}) + \int_{\partial \Omega} v \mathbf{F}(\mathbf{u}, \nabla \mathbf{u}) \cdot \hat{n} = \int_{\Omega} v S(\mathbf{u}, \nabla \mathbf{u})
\]

- Need a triangulation \( T_h \) of a domain \( \Omega \); both may be curved.
- \( p \)-th order polynomial basis in the reference space:

\[
\mathcal{V}^p \equiv \{ v \in L^2(\Omega) \mid v \circ f_k \in P^p(\kappa_{\text{ref}}), \forall \kappa \in T_h \} \subset L^2(\Omega)
\]
Nearest-Neighbor with kd-Trees

Algorithm

Given a tree $T$ and a query-point $Q$...
Idea: Use binary structure to quickly find a good candidate and then double-check the result

- Start at the root of $T$, traverse to find where $Q$ would be inserted
- The leaf-region where $Q$ “fits” is the current best-estimate, $d$
- Unwind the recursion of the search until the root is reached
  - At each node $S$, check if the kd-region could contain a better candidate than the current best
  - i.e. if a hypersphere of radius $d$ at $Q$ intersects the splitting hyperplane of $S$
  - If so, start another recursive search down the other branch of $S$
Complexity and Improvements

### Time Complexity
- Assuming balance and $N >> 2^k$, nearest-neighbor queries take $O(\log(N))$ time
  - This is optimal
- Worst-case occurs when the $N$ points are arranged roughly in a circle, for searches near the center of that circle

### Heuristics
- Search a sequence of points $\{A, B, C, \ldots\}$ such that A is near B, B is near C, etc
- Manual stack-management to avoid recursion
- Pre-sort inputs to obtain a balanced kd-tree
- Use squared-distances to avoid computation of square roots
Baseline SA Model

\[ \mu_t = \rho \tilde{\nu} f_{v1}, \quad f_{v1} = \frac{\chi^3}{\chi^3 + c_{v1}^3}, \quad \chi = \frac{\tilde{\nu}}{\nu} \]

\[ \frac{\partial}{\partial t} (\rho \tilde{\nu}) + \frac{\partial}{\partial x_j} (\rho u_j \tilde{\nu}) = c_{b1} \tilde{S} \rho \tilde{\nu} \]

\[ + \frac{1}{\sigma} \left[ \frac{\partial}{\partial x_j} \left( (\mu + \rho \tilde{\nu}) \frac{\partial \tilde{\nu}}{\partial x_j} \right) + c_{b2} \rho \frac{\partial \tilde{\nu}}{\partial x_j} \frac{\partial \tilde{\nu}}{\partial x_j} \right] - c_{w1} f_w \frac{\rho \tilde{\nu}^2}{d^2} \]

where \( d \) is the wall-distance.

\[ \tilde{S} = |\nabla \times u| + \frac{\tilde{\nu} f_{v2}}{k^2 d^2}, \quad f_{v2} = 1 - \frac{\chi}{1 + \chi f_{v1}} \]

\[ f_w = g \left( \frac{1 + c_{w3}^6}{g^6 + c_{w3}^6} \right), \quad g = r + c_{w2} (r^6 - r), \quad r = \frac{\tilde{\nu}}{\tilde{S}k^2 d^2} \]

Boundary Conditions: \( \tilde{\nu}_{\text{inflow}}/\nu = 5.0 \) (Allmaras); \( \tilde{\nu}_{\text{wall}} = 0 \); convective outflow
SA Model: Term Descriptions I

- Transport term: \( \rho \frac{D\tilde{\nu}}{Dt} = \frac{\partial}{\partial t} (\rho \tilde{\nu}) + \frac{\partial}{\partial x_j} (\rho u_j \tilde{\nu}) \). Naturally chosen as the substantial derivative, this will be balanced by production, destruction, and diffusion terms.

- Production: \( c_{b1} \tilde{S} \rho \tilde{\nu} \). Models the notion that turbulence is primarily found in regions of vorticity (which in turn arises near solid walls). Primarily this term should be proportional to the deformation tensor \( \frac{\partial U_i}{\partial x_j} \). \( \tilde{\nu} \) can only be created by the presence of vorticity.

- Destruction: \( -c_{w1} f_w \rho \tilde{\nu}^2 / \tilde{d}^2 \). Viscous effects are strongest near solid walls. The destruction of Reynolds shear stress is mainly felt at a distance through the pressure term. The form of destruction comes through dimensional analysis. \( f_w \) is a correction function which is calibrated to improve behavior in the log layer and over flat plates.
Diffusion: \( \frac{1}{\sigma} [\nabla \cdot ((\mu + \rho \tilde{\nu}) \nabla \tilde{\nu})] + c_{b2} \rho (\nabla \tilde{\nu})^2 \]. Contains a “classical” diffusive term along with a non-standard one. \( \tilde{\nu}^{1+c_{b2}} \) is conserved, not \( \tilde{\nu} \). \( c_{b2} \) is chosen so the conservation holds and so that a turbulent front propagates into a non-turbulent region.

All terms were chosen by analyzing previous turbulence models and/or through an educated guess. The constants were then tuned to match experimental data over some representative cases.
### SA Model Modifications

#### Lack of Robustness
- Issues when $\tilde{\nu} < 0$; difficult to force this condition.
  - Limiting of $\tilde{\nu}$ is hard because one must respect conservation and all the higher order DOFs.
- Our modifications to the SA model do not prevent this; in fact it is still very likely on under-resolved meshes.

#### Modifications to mitigate $\tilde{\nu} < 0$ issues
- Soft-limited $\mu_t \geq 0$.
- Modified source so turbulent energy decreases if $\tilde{\nu} < 0$.
- Source production term is non-negative.
The exact solution to the SA equation is non-negative, which follows the intuition that $\mu_t \geq 0$. Unfortunately the discretized equation is not guaranteed to preserve this property. In fact $\tilde{\nu}$ is likely to be negative near the BL edge where mesh resolution is typically lacking. The SA model may react unstably to $\tilde{\nu} < 0$; it can cause convergence issues. Allmaras has since suggested modifications to improve this problem. Note that the following changes at least preserve first derivative continuity, which is necessary to use Newton’s method for the nonlinear problem.

First, we can easily prevent $\mu_t < 0$ even if $\tilde{\nu} < 0$:

$$
\mu_t = \begin{cases} 
\rho \tilde{\nu} f_{v1} & \tilde{\nu} > 0 \\
0 & \tilde{\nu} \leq 0 
\end{cases}
$$
Modifications to the SA Model II

To motivate further changes, we will examine the energy of the SA working variable: $e_{\tilde{\nu}} = \frac{1}{2} \tilde{\nu}^2$. Multiplying the SA equation by $\tilde{\nu}$:

$$\frac{\partial}{\partial t} (\rho e_{\tilde{\nu}}) + \frac{\partial}{\partial x_j} (\rho u_j e_{\tilde{\nu}}) = \frac{1}{\sigma} \left[ \frac{\partial}{\partial x_j} (\eta \frac{\partial e_{\tilde{\nu}}}{\partial x_j}) + (c_{b2} \rho \tilde{\nu} - \eta) \frac{\partial \tilde{\nu}}{\partial x_j} \frac{\partial \tilde{\nu}}{\partial x_j} \right] + \tilde{\nu} (P - D)$$

where $\eta = \mu + \rho \tilde{\nu}$, $P = c_{b1} \tilde{S} \rho \tilde{\nu}$ and $D = c_{w1} f_w \rho \frac{\tilde{\nu}^2}{d^2}$. When $\tilde{\nu} < 0$ the RHS of the energy equation should be dissipative, causing $e_{\tilde{\nu}}$ to decrease in time. Let $\Omega_t^-$ denote the region where $\tilde{\nu} < 0$ and $E_{\tilde{\nu}}^{-}(t) = \int_{\Omega_t^-} \rho e_{\tilde{\nu}}(\mathbf{x}, t) d\mathbf{x}$ be the total energy in that region. Using Reynolds Transport,

$$\frac{dE_{\tilde{\nu}}^-}{dt} = \int_{\Omega_t^-} \frac{\partial}{\partial t} (\rho e_{\tilde{\nu}}) d\mathbf{x} + \int_{\partial \Omega_t^-} \rho e_{\tilde{\nu}} \tilde{\nu} \cdot \hat{n} ds$$
If $\partial \Omega_t^-$ is strictly in the interior and $\tilde{\nu}$ is continuous, then $\tilde{\nu} \Big|_{\partial \Omega_t^-} = 0$.

Substituting the energy equation into $\frac{dE_{\tilde{\nu}}^-}{dt}$ and applying the divergence theorem,

$$
\frac{dE_{\tilde{\nu}}^-}{dt} = \int_{\Omega_t^-} \left[ \frac{(c_{b2} \rho \tilde{\nu} - \eta)}{\sigma} \frac{\partial \tilde{\nu}}{\partial x_j} \frac{\partial \tilde{\nu}}{\partial x_j} + \tilde{\nu}(P - D) \right] dx
$$

We need the RHS of the above to be always negative, which corresponds to requiring:

$$(c_{b2} \rho \tilde{\nu} - \eta) < 0$$

$$\tilde{\nu}(P - D) < 0$$
Modifications to the SA Model IV

To accomplish this, it is necessary to modify the definitions of the diffusion coefficient $\eta$, the production $P$, and the destruction $D$ from the original SA paper. Summarizing,

$$\eta = \begin{cases} 
\mu(1 + \chi) & \chi \geq 0 \\
\mu(1 + \chi + \chi^2) & \chi < 0 
\end{cases}$$

$$P = \begin{cases} 
c_{b1}\tilde{S}\rho\tilde{\nu} & \chi \geq 0 \\
c_{b1}\tilde{S}\rho\tilde{\nu}g_n & \chi < 0 
\end{cases}$$

where $g_n = 1 - \frac{1000\chi^2}{1 + \chi^2}$.

$$D = \begin{cases} 
c_{w1}f_w\frac{\rho\tilde{\nu}^2}{d^2} & \chi \geq 0 \\
-c_{w1}\frac{\rho\tilde{\nu}^2}{d^2} & \chi < 0 
\end{cases}$$
Tests indicate that the modifications make $\tilde{\nu}$ less negative but do not guarantee $\tilde{\nu} > 0$. Additionally the changes do not significantly affect the final answer from a RANS-SA simulation.
SA Source Discretization

Standard Weighting

The direct approach: multiply by the test function and integrate.

\[ R_{h,S,DinC} (w_h, v_h) = - \sum_{\kappa \in T_h} \int_{\kappa} v_h^T S (w_h, \nabla w_h) \]

Unfortunately, this results in a \textbf{dual inconsistent} discretization.

Modified Standard Weighting

\[ R_{h,S,DC} (w_h, v_h) = - \sum_{\kappa \in T_h} \int_{\kappa} v_h^T S (w_h, \nabla w_h) + \int_{\Gamma_i} [w_h]^T \cdot \{ \vec{\beta} (w_h, \nabla w_h, v_h) \} + \int_{\partial \Omega} (u^b - w_h^+) \vec{\beta}_b (w_h, \nabla w_h, v_h) \cdot \vec{n} \]

This is \textbf{dual consistent} for the right choice of “dual” fluxes, \( \vec{\beta} \).
The Adjoint Problem

The adjoint (dual) solution is analogous to a Green’s Function relating the source of a PDE (e.g. truncation error) to an output, $J$, computed from the solution of the PDE.

Primal and Dual Problems

- **Discrete Primal**: find $u_h \in V_h^p$ satisfying $R_h(u_h, v_h) = 0$, $\forall v_h \in V_h^p$ where $R_h$ is the discrete primal residual.
  - Based on discretizing the continuous PDE $R(u, v) = 0$

- **Discrete Dual**: find $\psi_h \in V_h^p$ satisfying $R_h'(v_h, \psi_h) = J_h'(v_h)$, $\forall v_h \in V_h^p$ where $R_h'$ and $J_h'$ denote derivatives taken wrt components of $u_h$, evaluated at $u_h$
  - Notice that the arguments to $R_h$ are transposed.
  - The discrete dual can also be reached by discretizing the continuous dual problem: find $\psi \in V$ such that $R'(v, \psi) = J'(v)$, $\forall v \in V$.

When are $R_h'$ and the discretization of $R'$ the same?
Dual Consistency: Why do we care?

Dual Consistency

- Loosely, a discretization \((R_h, J_h)\) is **dual consistent** if the exact primal and dual solutions \((u, \psi \in V)\) satisfy the discrete dual problem:

  \[ R'_h(v, \psi) = J'_h(v), \forall v \in \{V + V^p_h} \]

- Not all primal discretizations lead to dual consistent adjoint discretizations!

Advantages of Dual Consistent (DC) Discretizations

- Dual inconsistency leads to suboptimal primal convergence, \((O(h^p) \text{ instead of } O(h^{p+1}))\) and output error \((O(h^p) < O(h^{2p}))\)

- Adjoint problems important in optimal control, design optimisation, etc.

- Many adjoint-based adaptation techniques will fail if the primal discretization is dual inconsistent.
Dual Consistency: Scalar Model Problem

\[-((1 + u)u_x)_x - \frac{1}{2}u_xu_x = g \quad \text{for} \quad x \in (0, 1)\]

\[u(0) = u(1) = 0\]

Optimal output error convergence rates for \textbf{dual consistent (left)} and \textbf{dual inconsistent (right)} discretizations for \(J(u) = \frac{1}{2} \int_0^1 (2 \sin(\pi x) - u)^2\).

Notice the difference between the convergence rates with a DC discretization and the standard weighting.
RAE 2822 at: $M_\infty = 0.6$, $Re_c = 6.3 \times 10^6$, $\alpha = 2.57^\circ$, using the dual consistent discretization.

Figure: Drag error vs $h$ for $p = 1$ (□), $p = 2$ (○), $p = 3$ (∗), $p = 4$ (△), and $p = 5$ (×).

Comments

- Error measured against $p = 5$ solution on the finest mesh.
- Optimal rate achieved for $p = 1$ and $p = 2$ but not for higher $p$.
- $p = 5$ obtains between $O(h^3)$ and $O(h^4)$ due to a non-smooth solution and suboptimal mesh resolution at the BL edge.
Started With...

- 2D RANS-SA capability with dual consistent source terms

In the last year...

- KD-Tree based distance function for 2D
- Cut-cell mesh capability for 2D problems
- Analysis indicating that non-physical solution overshoots can cause non-convergence
- Artificial viscosity to improve BL-edge resolution
- Extension of RANS-SA code for 3D problems with accompanying unit tests
- Assorted robustness improvements and bug fixes
Development Process II

Green = me; Blue = group; Black = others.

Current and Ongoing Work

- Improvements to the nonlinear solver (e.g. linesearch, limiting)
- DGLS stabilization for the SA model equation
- Source operator splitting to prevent ill-conditioning (which cause large updates)
- Improving the robustness of the 3D RANS capability
Dual Consistency: Linear Case I

Primal Problem: compute $J(u)$ for $u \in V$ s.t. $a(u, v) = \ell(v)$, $\forall v \in V$

Dual Problem: find $\psi \in V$ s.t. $a(v, \psi) = J(v)$, $\forall v \in V$

The discrete primal is obtained by finding $u_h \in V_h$ s.t.
\[ a(u_h, v_h) = \ell(v_h), \forall v \in V \text{ where } V_h \subset V \text{ is finite dimensional.} \]

Similarly the discrete dual: find $\psi_h \in V_h$ s.t.
\[ a(v_h, \psi_h) = J(v_h), \forall v \in V_h. \]
This can be obtained 2 ways: 1) discretize the (continuous) dual problem; 2) transpose the discrete primal; if they are the same then $a(u, v)$ is said to be dual consistent.

\[ |J(u) - J(u_h)| = |J(u - u_h)| \text{ (by linearity)} = |a(u - u_h, \psi)| \]
\[ \text{(definition of dual)} = |a(u - u_h, \psi - \psi_h)| \text{ (Galerkin Orthogonality on the primal)} \leq \beta \|u - u_h\|_V \|\psi - \psi_h\|_V. \]
If the discretization obtains $\|u - u_h\|_\mathcal{V} \leq O(h^s)$ and $\|\psi - \psi_h\|_\mathcal{V} \leq O(h^t)$, then the output error $|J(u) - J(u_h)| \leq O(h^{s+t})$. For many common problems, $h = s = p$, where $p$ is the order of the polynomial basis.
Roe’s Flux I

For a problem \( u_t + F(u)_x = 0 \), Roe’s approximate numerical flux is:

\[
F^n_{i+1/2} = \frac{1}{2} \left( F(u^n_i) + F(u^n_{i+1}) \right) - \frac{1}{2} \left| \frac{\partial F}{\partial u} \right|_{i'} (u^n_{i+1} - u^n_i)
\]

The evaluation at state \( i' \) involves Roe-averaging. This takes the form:

\[
\rho_{i'} = \sqrt{\rho_i \rho_{i+1}} \quad \text{and} \quad u_{i'} = \frac{\sqrt{\rho_i u_i + \rho_{i+1} u_{i+1}}}{\sqrt{\rho_i} + \sqrt{\rho_{i+1}}}
\]

Roe’s method solves a certain linear Riemann Problem exactly at cell interfaces. This problem has the form \( u_t + A u_x = 0 \), where \( A \) is only a function of \( u_L \) and \( u_R \). It satisfies the conditions: 1) \( F(u_R) - F(u_L) = A(u_R - u_L) \); 2) \( A \) has real eigenvalues and a complete set of eigenvectors; and 3) \( A \to \frac{\partial F}{\partial u} \bigg|_u \) as \( u_L, u_r \to u \).

These conditions ensure exactness for a single shock or expansion wave, consistency with the original equations, and solvability of the
linear Riemann problem.

We are also using Harten’s entropy correction, which fixes the Roe Flux near points where the velocity is near sonic. Here, expansions can go sonic, which is nonphysical. In fact Roe reduces to a central discretization and entropy-violation solutions may arise. Harten’s fix involves replacing near-0 eigenvalues.