

USM3D-ME Revised SA-neg Implementation and Assessment for Seventh Drag Prediction Workshop Solutions

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Simulations performed by an unstructured-grid, cell-centered, finite-volume, mixed-element flow solver USM3D-ME were presented at the Seventh Drag Prediction Workshop (DPW-7). Reynolds-averaged Navier-Stokes (RANS) solutions for the NASA high-speed common research model wing-body configuration were computed using a new implementation of the negative variant of the Spalart-Allmaras turbulence model (SA-neg) with hierarchical adaptive nonlinear iteration method (HANIM). This USM3D-ME enhancement improved efficiency and robustness of RANS solutions resulting in fast iterative convergence to machine zero residuals on mixed-element unstructured grids provided by the DPW-7 organizing committee. This paper presents theoretical foundations for the new implementation of the SA-neg model and analyzes USM3D-ME solutions for flow conditions corresponding to the required DPW-7 cases.

Nomenclature and abbreviations

b	=	face-based diffusion coefficient
C_D	=	total drag coefficient
$C_{D,v}$	=	viscous drag coefficient
C_L	=	lift coefficient
C_f	=	magnitude of vector of skin friction
$C_{f,x}$	=	x component of vector of skin friction
C_m	=	pitching moment coefficient
C_p	=	pressure coefficient
c	=	airfoil chord
d	=	distance to wall
h	=	characteristic mesh size
M	=	Mach number
N	=	total number of cells
Re	=	Reynolds number
$\mathbf{s}$	=	outward directed area vector
T	=	temperature
t	=	time
$\mathbf{u}$	=	flow velocity vector
u, v, w	=	Cartesian components of flow velocity vector
x, y, z	=	spatial coordinates

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α	=	angle of attack
κ	=	von Karman constant
η	=	normalized spanwise coordinate of wing
μ	=	dynamic laminar viscosity
μ_t	=	turbulent eddy viscosity
ν	=	kinematic laminar viscosity
$\tilde{\nu}$	=	working variable used in Spalart-Allmaras (SA) turbulence models
ρ	=	density
Ω	=	magnitude of vorticity
∇	=	formal vector of spatial derivatives
$\frac{D\tilde{\nu}}{Dt}$	=	material derivative of $\tilde{\nu}$
∂_t	=	partial time derivative
$\partial_x, \partial_y, \partial_z$	=	partial spatial derivatives

Subscripts

i, j	=	cell index
$face$	=	face-based quantity
ref	=	reference quantity

Abbreviations

AE	=	aeroelastic
AIAA	=	American Institute of Aeronautics and Astronautics
CFD	=	computational fluid dynamics
CFL	=	Courant, Friedrichs, Lewy
CRM	=	common research model
DPW	=	drag prediction workshop
FDS	=	flux difference splitting
FVS	=	flux vector splitting
GCR	=	generalized conjugate residual
G-S	=	Gauss, Seidel
HANIM	=	hierarchical adaptive nonlinear iteration method
HiQ	=	high dynamic pressure
HLLC	=	Harten, Lax, van Leer – Contact
HLLE	=	Harten, Lax, van Leer, Einfeldt
LaRC	=	Langley research center
LE	=	leading edge
LoQ	=	low dynamic pressure
ME	=	mixed elements
PDE	=	partial differential equation
RANS	=	Reynolds-averaged Navier Stokes
rms	=	root mean square
SA	=	Spalart, Allmaras
TetrUSS	=	tetrahedral unstructured software system
TMR	=	turbulence modeling resource
QCR	=	quadratic constitutive relation

I. Introduction

The American Institute of Aeronautics and Astronautics (AIAA) Computational Fluid Dynamics (CFD) Drag Prediction Workshop (DPW) series [1] is sponsored by the AIAA Applied Aerodynamics Technical Committee. Since 2001, seven workshops have been held [2-8]. The main focus of the DPW series is on establishing the confidence level in predicting aerodynamic forces and moments for industry-relevant cases. The predictions by various CFD solvers from multiple organizations have been submitted for cases defined by the DPW organizing committee and

subjected to rigorous statistical analysis. Most of the submitted solutions have been computed using Reynolds-averaged Navier Stokes (RANS) models. Over the time, the spread between solutions computed by different solvers reduced dramatically. For example, the spread in predicting total drag for a wing-body configuration at a fixed-lift condition reduced from 270 drag counts (DPW-1) to less than 10 drag counts (DPW-6).

The spread reduction was achieved through improved description of the geometry, availability of high quality experimental data, careful selection of grids used in grid-refinement studies, and verification of CFD solvers contributing solutions for workshop configurations. Since DPW-4, the NASA Common Research Model (CRM) [9], a wing-body configuration with and without tail and nacelle-pylons, has been used allowing better documentation of the geometry and collection of high-quality experimental data at multiple facilities. Ability to compute on grids with higher resolution, grid convergence studies, and detailed guidelines for generation of families of grids reduced grid dependence of the computed solutions. Reference solutions provided by the NASA Turbulence Modeling Resource (TMR) website [10] were extensively used for the verification of the implementations of specific turbulence models.

A potential reason for the remaining spread in aerodynamic predictions is insufficient iterative convergence. Due to complexity of grids, geometry, and turbulence models, iterative solutions rarely converge to machine zero residuals, and engineers usually apply best-practice guidelines to judge if a solution has sufficiently converged. Iterative solvers may truncate numerical solutions to satisfy various realizability constraints, which may lead to stall or divergence of discrete residuals. In particular, the working variable in the Spalart-Allmaras (SA) turbulence model [11] is often truncated to force positivity because the eddy viscosity of turbulent flows is defined only for positive values of the working variable. The negative variant of the SA model (SA-neg) introduced in Ref. [12] avoids truncation by allowing negative values of the working variable. The SA-neg formulation and advancements in nonlinear iteration methods have led to significant improvements in iterative convergence of RANS solvers. Positivity and boundness of the steady-state solution (working variable), rigorously proved for the SA-neg partial differential equation (PDE) in Ref. [12], ensure that the SA and SA-neg models have the same steady-state solutions. However, discrete implementations of the SA-neg model in many practical CFD codes violate conditions of this rigorous proof. Stalling or diverging iterative solutions are still common even with the SA-neg turbulence model. One of the contributions of this paper is an SA-neg finite-volume implementation methodology that satisfies conditions of the rigorous proof for positivity and boundness of discrete SA-neg solutions in the limit of zero residuals.

DPW-7 was conducted in June 2022 in conjunction with the 2022 AIAA AVIATION Forum. The main challenge of the workshop was to predict the effect of shock-induced separation on the lift and pitching-moment coefficients of the NASA CRM wing-body configuration with the increasing angles of attack at transonic conditions. Participants were required to submit solutions for at least three cases: a grid convergence study (Case 1), an angle-of-attack sweep at constant Reynolds number (Case 2), and a study of Reynolds number effects at constant lift (Case 3). Optional studies include solutions on adapted grids (Case 4), solutions with high-fidelity models (Case 5), and coupled aerostructural simulations (Case 6).

This paper presents RANS solutions computed by the NASA cell-centered, finite-volume, mixed-element, unstructured-grid, flow solver USM3D-ME. Solutions are computed with the SA-neg-QCR2000 turbulence model on a family of mixed-element grids provided by the DPW organizing committee for the three required cases. Grids are fixed but incorporate aeroelastic deformations corresponding to specific flow conditions. The USM3D-ME flow solver features a recently developed hierarchical adaptive nonlinear iteration method (HANIM) and a new discrete implementation of the SA-neg model. Machine-zero residual convergence has been achieved on all grids used in the study. The material in this paper is organized as follows. Salient features of USM3D-ME are described in Section II. Section III presents theoretical foundations and discusses the new implementation of the SA-neg turbulence model. Section IV describes the CRM model and the family of unstructured grids used in USM3D-ME computations. Sections V, VI, and VII assess USM3D-ME solutions for the three DPW-7 cases. The contributions of this paper are summarized in Section VIII.

II. USM3D-ME Flow Solver

The USM3D-ME [13-17] is a second-order accurate, finite-volume, cell-centered, mixed-element, unstructured-grid CFD solver that is developed at the NASA Langley Research Center (LaRC). The USM3D-ME is a successor to the USM3D solver of the NASA Tetrahedral Unstructured Software System (TetrUSS) [18] that was customized for tetrahedral grids and, for many years, served as a reliable computational aerodynamic analysis tool for U.S. government and industry [18-23]. In distinction from the legacy USM3D solver, the USM3D-ME solves CFD equations on unstructured grids that can include arbitrary combinations of tetrahedra, prisms, hexahedra, and pyramids. Extension to mixed-element grids improved the accuracy and robustness of numerical simulations by allowing flow-aligned anisotropic hexahedral or prismatic cells in boundary layers.

The discretization scheme of the USM3D-ME places independent flow variables used by the governing equations at the cell centers. A reconstruction process based on solution gradients computed within cells is used to obtain the second-order spatial discretization of inviscid fluxes. The cell gradients are computed by a Green-Gauss integration procedure using solution values interpolated to grid nodes. Inviscid fluxes are computed at cell faces using various upwind schemes, such as Roe’s Flux Difference Splitting (FDS) [24], van Leer’s Flux Vector Splitting (FVS) [25], Harten, Lax, van Leer, Einfeldt (HLLC) [26], or Harten, Lax, van Leer – Contact (HLLC) [27] schemes, among others. A library of cell-based and face-based gradient limiters including Barth-Jespersen, van Albada, and Venkatakrishnan is available in the flow solver. Several verified variants of the SA one-equation turbulence model have been implemented including a nonlinear model that uses a quadratic constitutive relation (QCR) [28]. The convective term of the SA turbulence model equation can be approximated with either second- or first-order accuracy. Face gradients needed for the diffusion fluxes of the meanflow and turbulence model equations are evaluated from Mitchell’s stencil [29, 30]. A face-area weighted average of face-based velocity gradients provides cell-based gradients for the SA source term.

Several important modifications to the discretization schemes were made to improve the USM3D-ME accuracy, efficiency, and robustness. The modifications include: (1) a fully-implicit formulation that is entirely based on cell-centered solutions; (2) a compact nodal-averaging scheme for efficient flow solver parallelization; (3) a more consistent Jacobian used by the USM3D-ME preconditioner; (4) an adaptive face-based catastrophic limiter for improved robustness; (5) improved turbulence models including a more robust version of the SA-neg model and the SA-QCR2000 model [31] to better capture the physics of the corner flows.

The baseline simple iterative solver of USM3D-ME is based on an approximate Jacobian, a point-implicit Gauss-Seidel (G-S) relaxation scheme, and a prescribed schedule for the pseudotime step that is controlled by a Courant-Friedrichs-Lewy (CFL) number. A new solution methodology, HANIM, has been implemented in the USM3D-ME [14-16]. HANIM is a strong nonlinear solver that is based on a hierarchy of modules including a preconditioner, a matrix-free linear solver, realizability check, and nonlinear control of solution update. HANIM enhances the baseline iterative solver with a mechanism for an automatic adaptation of the pseudotime step to increase convergence rates and overcome instabilities occurring in transient solutions. The HANIM preconditioner is similar to the baseline iterative solver. The matrix-free linear solver [32-35] uses Fréchet derivatives and a generalized conjugate residual (GCR) method [33] from the family of Krylov methods. HANIM prescribes the residual reduction targets for the preconditioner, the GCR solver, and nonlinear solution updates and specifies the maximum number of G-S iterations allowed in the preconditioner and the maximum number of search directions to be used in the GCR solver. The CFL number is increased if all the HANIM modules have reported success. If any of the modules fails, HANIM discards the correction and aggressively reduces the CFL number.

USM3D-ME has been parallelized for maximizing the CFD solution throughput. The parallelization is based on a message passing interface (MPI) paradigm [36]. The internal grid decomposition method follows the current state of the art [37]. Interpartition communication is performed judiciously and efficiently such that excellent strong scalability and weak scalability are achieved [17]. USM3D-ME solutions have been extensively verified and validated for many benchmark flows [17], and through participation in AIAA workshops and other community activities [41-43]. USM3D-ME provides reference solutions for several verification cases at the TMR website [10].

The following is a brief description of USM3D-ME discretization parameters that are used in computing all solutions in the paper.

- 1) The turbulence model is SA-neg-QCR2000.
- 2) The meanflow inviscid fluxes use Roe’s FDS and second-order reconstruction with no limiters.
- 3) The SA-model convection term is upwind and first order.
- 4) The cell gradients for meanflow inviscid terms are based on the Green–Gauss method with nodal solutions.
- 5) The face gradients for meanflow and SA model diffusion terms include Mitchell’s method.
- 6) The mean-flow diffusion terms are second order.
- 7) The SA-model diffusion term is second order.
- 8) The meanflow approximate-Jacobian inviscid terms use linearization of the first-order Roe’s FDS fluxes.
- 9) The approximate-Jacobian diffusion terms use thin-layer approximation.
- 10) The cell gradients for the SA-model source term are computed from area-weighted face gradients.
- 11) The initial conditions include freestream flow.
- 12) The Prandtl numbers for diffusion fluxes are 0.72 for meanflow and 0.90 for the SA model.

III. SA-neg Turbulence Model

This section discusses a rigorous proof of positivity and boundness of solutions of the SA-neg model equation. First, arguments suggested in Ref. [12] for positivity and boundness of steady-state SA-neg PDE solutions are described in

details. Then a new finite-volume discretization of the SA-neg model equation is presented. This discretization satisfies conditions for positivity and boundness of discrete solutions in the limit of zero residual.

A. Positivity and Boundness of SA-neg PDE Solution

The SA-neg model [10-12] PDE is the following. For the positive turbulence working variable, $\tilde{v} > 0$,

$$\frac{D\tilde{v}}{Dt} = c_{b1}(1 - f_{t2})\tilde{S}\tilde{v} - \left(c_{w1}f_w - \frac{c_{b1}}{\kappa^2}f_{t2}\right)\left(\frac{\tilde{v}}{d}\right)^2 + \frac{1}{\sigma}[\mathbf{\nabla} \cdot ((v + \tilde{v})\mathbf{\nabla}\tilde{v}) + c_{b2}(\mathbf{\nabla}\tilde{v} \cdot \mathbf{\nabla}\tilde{v})]. \quad (1)$$

For the negative working variable, $\tilde{v} \leq 0$,

$$\frac{D\tilde{v}}{Dt} = c_{b1}(1 - c_{t3})\Omega\tilde{v} + c_{w1}\left(\frac{\tilde{v}}{d}\right)^2 + \frac{1}{\sigma}[\mathbf{\nabla} \cdot ((v + \tilde{v}f_n)\mathbf{\nabla}\tilde{v}) + c_{b2}(\mathbf{\nabla}\tilde{v} \cdot \mathbf{\nabla}\tilde{v})]. \quad (2)$$

The boundary conditions are

$$\tilde{v}_{wall} = 0, \quad \tilde{v}_{farfield} = 3v_{ref}. \quad (3)$$

Here, d is the distance to the nearest wall, $\nu = \mu/\rho$ is the kinematic laminar viscosity, ν_{ref} is the freestream kinematic laminar viscosity, $\mathbf{\nabla} \equiv (\partial_x, \partial_y, \partial_z)$ denotes a formal vector of spatial derivatives, $\frac{D\tilde{v}}{Dt}$ denotes the material derivative that is defined as

$$\frac{D\tilde{v}}{Dt} \equiv \partial_t \tilde{v} + \mathbf{u} \cdot \mathbf{\nabla} \tilde{v}, \quad (4)$$

∂_t is the partial time derivative, and $\mathbf{u}$ is the flow velocity vector.

$$\tilde{S} = \Omega + \frac{\tilde{v}}{\kappa^2 d^2} f_{v2}, \quad (5)$$

where Ω is the magnitude of vorticity,

$$\Omega = \sqrt{(\partial_y w - \partial_z v)^2 + (\partial_z u - \partial_x w)^2 + (\partial_x v - \partial_y u)^2}, \quad (6)$$

$$f_n = \frac{c_{n1} + \chi^3}{c_{n1} - \chi^3}, \quad f_{v1} = \frac{\chi^3}{c_{v1}^3 + \chi^3}, \quad \chi = \frac{\tilde{v}}{\nu}, \quad f_{v2} = 1 - \frac{\chi}{1 + \chi f_{v1}}, \quad f_{t2} = c_{t3} \exp(-c_{t4} \chi^2), \quad (7)$$

$$f_w = g \left[\frac{1 + c_{w3}^6}{g^6 + c_{w3}^6} \right]^{\frac{1}{6}}, \quad g = r + c_{w2}(r^6 - r), \quad r = \min \left[\frac{\chi}{\kappa^2 d^2 \Omega / \nu + \chi f_{v2}}, 10 \right], \quad (8)$$

and the constants are

$$\kappa = 0.41, \quad \sigma = \frac{2}{3}, \quad c_{b1} = 0.1355, \quad c_{b2} = 0.622, \quad c_{w1} = \frac{c_{b1}}{\kappa} + \frac{1 + c_{b2}}{\sigma}, \quad c_{w2} = 0.3, \quad (9)$$

$$c_{w3} = 2, \quad c_{v1} = 7.1, \quad c_{t3} = 1.2, \quad c_{t4} = 0.5, \quad c_{n1} = 16.$$

The auxiliary functions $f_n, f_{v1}, f_{v2}, f_{t2}$, and f_w are chosen to ensure, besides properties motivated by physics, the mathematical properties of solution differentiability, boundness, and non-negativity. The turbulent eddy viscosity is computed as

$$\mu_t = \rho \tilde{v} f_{v1} \quad (10)$$

when $\tilde{v} \geq 0$ and set to zero when $\tilde{v} < 0$.

Non-negativity of the SA-neg PDE solution at steady state is rigorously proved by the arguments suggested in [12]. The solution non-negativity at steady state follows if the material derivative is strictly positive, $\frac{D\tilde{v}}{Dt} > 0$, at any local minimum of a transient solution where $\tilde{v} < 0$. Indeed, $\frac{D\tilde{v}}{Dt} = 0$ at a steady-state local extremum where $\mathbf{\nabla}\tilde{v} = 0$. If there is any local minimum of a transient solution with $\frac{D\tilde{v}}{Dt} > 0$ and $\tilde{v} < 0$, then this solution increases (becoming less negative) in time and is not at steady state.

Thus, to prove non-negativity of the steady-state solution, it is sufficient to show that the right side of Eq. (2) is positive at local minimum. The following terms are non-negative by construction:

$$c_{b1}(1 - c_{t3})\Omega\tilde{v} \geq 0, \quad c_{w1}\left(\frac{\tilde{v}}{d}\right)^2 \geq 0, \quad c_{b2}(\mathbf{\nabla}\tilde{v} \cdot \mathbf{\nabla}\tilde{v}) \geq 0. \quad (11)$$

The diffusion term $\nabla \cdot ((\nu + \tilde{\nu}f_n)\nabla \tilde{\nu})$ is a second-order differential operator. If the diffusion coefficient $(\nu + \tilde{\nu}f_n)$ is positive, then the operator is elliptic and evaluates to a positive number at any local minimum. In fact, the coefficient c_{n1} in Eq. (9) is chosen to ensure

$$\nu + \tilde{\nu}f_n > 0 \text{ for } \tilde{\nu} < 0. \quad (12)$$

An auxiliary function,

$$\tilde{\nu}f_n = g(\chi) = \nu\chi \frac{c_{n1} + \chi^3}{c_{n1} - \chi^3}, \quad (13)$$

is constructed to have a single extremum (minimum) in the semi-space $\chi \leq 0$. This minimum can be found as follows.

$$0 = \frac{dg}{d\chi} = \nu \frac{(c_{n1})^2 - (\chi^3)^2 + 6c_{n1}\chi^3}{(c_{n1} - \chi^3)^2}, \quad \chi^3 = c_{n1}(3 \pm \sqrt{10}). \quad (14)$$

Since we are interested in $\chi \leq 0$, we choose the root

$$\chi_{min} = (c_{n1}(3 - \sqrt{10}))^{\frac{1}{3}}. \quad (15)$$

The value of this minimum is

$$\min(\tilde{\nu}f_n) = g(\chi_{min}) = \nu (c_{n1}(3 - \sqrt{10}))^{\frac{1}{3}} \frac{1 + (3 - \sqrt{10})}{1 - (3 - \sqrt{10})}. \quad (16)$$

Condition in Eq. (12) is satisfied if $\min(\tilde{\nu}f_n) > -\nu$ or

$$(c_{n1}(3 - \sqrt{10}))^{\frac{1}{3}} \frac{1 + (3 - \sqrt{10})}{1 - (3 - \sqrt{10})} > -1. \quad (17)$$

From Eq. (17),

$$c_{n1} < -\frac{1}{(3 - \sqrt{10})} \left(\frac{(1 - (3 - \sqrt{10}))}{(1 + (3 - \sqrt{10}))} \right)^3 = 16.4577568967328. \quad (18)$$

The rounded down $c_{n1} = 16$ ensures that $\nu + \tilde{\nu}f_n > 0$. Thus, $\frac{D\tilde{\nu}}{Dt} > 0$ at any local minimum with $\tilde{\nu} < 0$, and the steady-state solution of the SA-neg PDE is non-negative.

Using similar arguments, one can show that the SA-neg PDE solution is bounded if the material derivative is negative at any local maximum with large enough positive value of $\tilde{\nu}$. At any local maximum, $\nabla \tilde{\nu} = 0$. The diffusion operator $\nabla \cdot ((\nu + \tilde{\nu})\nabla \tilde{\nu})$ is elliptic because $\nu + \tilde{\nu} > 0$ and thus $\nabla \cdot ((\nu + \tilde{\nu})\nabla \tilde{\nu}) < 0$ at any local maximum. The source term in Eq. (1) is the following.

$$\begin{aligned} c_{b1}(1 - f_{t2})\tilde{S}\tilde{\nu} - \left(c_{w1}f_w - \frac{c_{b1}}{\kappa^2}f_{t2}\right)\left(\frac{\tilde{\nu}}{d}\right)^2 &= c_{b1}(1 - f_{t2})\left(\Omega + \frac{\tilde{\nu}}{\kappa^2 d^2}f_{v2}\right)\tilde{\nu} - \left(c_{w1}f_w - \frac{c_{b1}}{\kappa^2}f_{t2}\right)\left(\frac{\tilde{\nu}}{d}\right)^2 \\ &= c_{b1}(1 - f_{t2})\Omega\tilde{\nu} + \frac{c_{b1}}{\kappa^2}(f_{v2} - f_{t2}f_{v2} + f_{t2})\left(\frac{\tilde{\nu}}{d}\right)^2 - c_{w1}f_w\left(\frac{\tilde{\nu}}{d}\right)^2. \end{aligned} \quad (19)$$

Functions f_{v2} and f_{t2} approach zero as $\tilde{\nu}$ increases toward infinity. Thus, for a large enough $\tilde{\nu}$, the source term is simplified to

$$\left[c_{b1}\Omega\tilde{\nu} - c_{w1}f_w\left(\frac{\tilde{\nu}}{d}\right)^2 \right]. \quad (20)$$

For a large enough $\tilde{\nu}$, $r = 10$, and $f_w \approx c_{w3} = 2$ (Eqs. (8) and (9)). Since vorticity magnitude, Ω , is finite, there is a large enough $\tilde{\nu} > 0$, such that

$$c_{b1}\Omega\tilde{\nu} - c_{w1}f_w\left(\frac{\tilde{\nu}}{d}\right)^2 < 0. \quad (21)$$

Thus, $\frac{D\tilde{\nu}}{Dt} < 0$ for a large enough local maximum value of $\tilde{\nu}$, which proves boundness of SA-neg solutions.

Remark: One exception to the proof logic is that a local solution extremum can be at the boundary. In this case, one cannot claim that $\nabla \tilde{\nu} = 0$ and $\frac{D\tilde{\nu}}{Dt} = 0$, and that, at least, boundness of the steady-state solution remains in question.

In practice, the steady-state solution can be bounded even if some extrema are at the boundary or one can use a special treatment of near-boundary solutions to ensure that no negative minimum or positive maximum occur at the boundary.

B. Positivity and Boundness of SA-neg Discrete Solution

Many finite-volume codes avoid implicit discretization of the $(\nabla \tilde{v} \cdot \nabla \tilde{v}) \equiv (\partial_x \tilde{v})^2 + (\partial_y \tilde{v})^2 + (\partial_z \tilde{v})^2$ term. Contributions from this term to the linearization matrix have an unpredictable and uncontrollable effect because of a relatively large neighbor-based stencil, lack of diagonal dominance, and variation of the sign of $\tilde{v}$ derivatives. These considerations are especially important for iterative methods that use simple point- and line-implicit iterations, which, in their core, invert the diagonal blocks. To have a fully implicit discretization and, at the same time, avoid the need to discretize the $(\nabla \tilde{v} \cdot \nabla \tilde{v})$ term, the following transformation is performed.

$$\nabla \tilde{v} \cdot \nabla \tilde{v} = \nabla \cdot (\tilde{v} \nabla \tilde{v}) - \tilde{v} (\nabla \cdot \nabla) \tilde{v}. \quad (22)$$

This transformation is exact for the differential operators. The first term, $\nabla \cdot (\tilde{v} \nabla \tilde{v})$, is a nonlinear diffusion operator that can be conservatively discretized by a finite-volume method; the second term, $\tilde{v} (\nabla \cdot \nabla) \tilde{v} = \tilde{v} (\partial_{xx} \tilde{v} + \partial_{yy} \tilde{v} + \partial_{zz} \tilde{v})$, is the Laplace operator multiplied by the local solution. The Laplace operator is a particular example of a linear diffusion operator that also can be conservatively discretized by a finite-volume method. The overall formulation is not conservative because the Laplacian is multiplied by the local solution.

The nonlinear diffusion term in Eq. (1) can be reformulated as

$$\nabla \cdot ((v + \tilde{v}) \nabla \tilde{v}) + c_{b2} (\nabla \tilde{v} \cdot \nabla \tilde{v}) = \nabla \cdot ((v + (1 + c_{b2}) \tilde{v}) \nabla \tilde{v}) - c_{b2} \tilde{v} (\nabla \cdot \nabla) \tilde{v} \quad (23)$$

and discretized using a finite-volume method. Let us consider a face of cell i . The contribution from the nonlinear diffusion flux defined at the face to the residual at cell i can be expressed as

$$b_i (\nabla \tilde{v} \cdot \mathbf{s})_{face}, \quad b_i = (v + (1 + c_{b2}) \tilde{v})_{face} - c_{b2} \tilde{v}_i. \quad (24)$$

Here, subscripts *face* indicate quantities evaluated at the face, $\tilde{v}_i$ is evaluated at the center of cell i , and $\mathbf{s}$ is the outward directed area vector.

To prove non-negativity of a steady-state discrete solution, the steady-state residual (the right side of discretized Eq. (2)) should be positive for any local minimum with $\tilde{v}_i < 0$. To prove boundness of a steady-state discrete solution, the steady-state residual (the right side of discretized Eq. (1)) should be negative for any local maximum with large enough solution $\tilde{v}_i > 0$. From Eqs. (11), (19), and (21), the source terms at local extrema have the correct sign. To ensure that residual contributions from the nonlinear diffusion flux (Eq. (24)) have the correct sign, the diffusion coefficient should be positive, $b_i > 0$. Indeed, $(\nabla \tilde{v} \cdot \mathbf{s})_{face} > 0$ for faces of the cell containing a local minimum and $(\nabla \tilde{v} \cdot \mathbf{s})_{face} < 0$ for faces of the cell containing a local maximum.

For some common finite-volume discretizations, requirements of positivity for the diffusion coefficient can be violated even if cell solutions are positive because solution at a face is reconstructed using gradients. For other common discretizations, e.g., cell-centered discretization of USM3D-ME, the solution at a face is averaged from solutions at two cells separated by this face, $\tilde{v}_{face} = \frac{\tilde{v}_i + \tilde{v}_j}{2}$. For such discretizations, the condition $b_i > 0$ is naturally satisfied if $\tilde{v}_i > 0$ and $\tilde{v}_j > 0$. In this specific case, the diffusion coefficient is simplified to

$$b_i = v_{face} + (1 + c_{b2}) \frac{\tilde{v}_i + \tilde{v}_j}{2} - c_{b2} \tilde{v}_i = v_{face} + (1 + c_{b2}) \frac{\tilde{v}_j}{2} + (1 - c_{b2}) \frac{\tilde{v}_i}{2}. \quad (25)$$

In case when cell solutions are allowed to be negative, one can extend the treatment developed in the SA-neg formulation to ensure positivity of b_i in the diffusion flux.

$$b_i = v_{face} + ((1 + c_{b2}) \tilde{v}_{face} - c_{b2} \tilde{v}_i) f_{n,i} = v_{face} (1 + \zeta_i f_{n,i}), \quad (26)$$

$$f_{n,i} = \begin{cases} \frac{c_{n1} + \zeta_i^3}{c_{n1} - \zeta_i^3}, & \text{if } \zeta_i < 0, \\ 1, & \text{if } \zeta_i \geq 0. \end{cases} \quad \zeta_i = \frac{1}{v_{face}} ((1 + c_{b2}) \tilde{v}_{face} - c_{b2} \tilde{v}_i), c_{n1} = 16. \quad (27)$$

The same analysis as in Eqs. (13)–(18) proves that $b_i > 0$. This formulation leads to the following modification of the nonlinear diffusion term in Eq. (2).

$$\nabla \cdot ((v + (1 + c_{b2}) \tilde{v} f_n) \nabla \tilde{v}) - c_{b2} \tilde{v} f_n \nabla \cdot \nabla \tilde{v} = \nabla \cdot ((v + \tilde{v} f_n) \nabla \tilde{v}) + c_{b2} (\nabla(\tilde{v} f_n) \cdot \nabla \tilde{v}). \quad (28)$$

The SA-neg equation for $\tilde{v} \leq 0$ becomes

$$\frac{D \tilde{v}}{Dt} = c_{b1} (1 - c_{t3}) \Omega \tilde{v} + c_{w1} \left(\frac{\tilde{v}}{d} \right)^2 + \frac{1}{\sigma} [\nabla \cdot ((v + \tilde{v} f_n) \nabla \tilde{v}) + c_{b2} (\nabla(\tilde{v} f_n) \cdot \nabla \tilde{v})]. \quad (29)$$

IV. Configuration and Grids

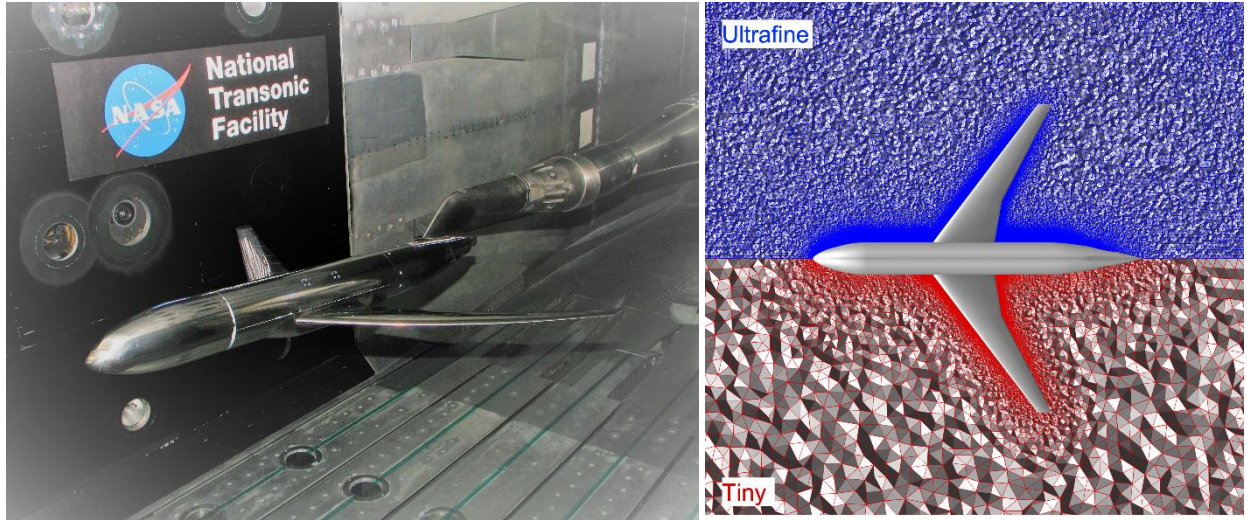
The CRM [9] used in the DPW-7 cases is a wing-body configuration representative of contemporary transonic transport aircraft. The reference characteristics of the full-scale configuration are shown in Table 1. USM3D-ME solutions have been computed on six unstructured mixed-element grids generated by Japan Aerospace Exploration Agency (JAXA). The grids incorporate aeroelastic deformations. Grid statistics are shown in Table 2. Figure 1a illustrates the CRM configuration in the NASA National Transonic Facility and Fig. 1b shows tiny and ultrafine grids from the JAXA family.

Table 1. Reference parameters of full-scale CRM configuration.

Aspect ratio	9.00 in
Model span	2313.50 in
Reference area	594,720.00 in ²
Reference length	275.80 in
x moment center	1325.89 in
y moment center	0.00 in
z moment center	177.96 in

Table 2. Statistics of unstructured grids generated by JAXA.

Grid level	Grid name	Tetrahedra (millions)	Prisms (millions)	Hexahedra (millions)	Pyramids (millions)	Total cells (millions)	Total nodes (millions)
L1	tiny	16.3	6.1	2.7	0.1	25.3	8.7
L2	coarse	47.9	18.8	9.1	0.3	76.1	26.9
L3	medium	100.0	41.7	21.8	0.5	164.1	60.2
L4	fine	173.4	78.8	42.2	0.8	295.2	111.8
L5	extrafine	265.9	142.7	66.5	1.3	476.4	184.1
L6	ultrafine	404.8	223.4	109.2	1.8	739.2	291.2



a) NASA Common Research Model (CRM) [Source: NASA]

b) Tiny and ultrafine JAXA grids

Fig. 1. CRM configuration and JAXA grids.

V. Case 1a: Grid Convergence

Solutions presented in this section are computed for the flow conditions corresponding to the freestream Mach number of $M = 0.85$, the Reynolds number of $Re = 20 \times 10^6$, and the reference temperature of $T = -250^\circ F$. The JAXA family grids have been generated for the Reynolds number of $Re = 30 \times 10^6$ and incorporate static aeroelastic (AE)

deformations corresponding to the angle of attack of $\alpha = 3^\circ$ and a low dynamic pressure (LoQ). This geometry, provided by the committee, was determined using optical techniques in a previous wind-tunnel test.

Simulations are performed for the specified lift coefficient $C_L = 0.58$. All simulations are initialized at the freestream conditions. Each individual iteration is conducted for a specific angle of attack. The angle of attack is periodically adjusted to match the prescribed lift coefficient after residuals have been reduced by 1.5 orders of magnitude. The lift-matching iterations converge well; the lift coefficient tolerance of ± 0.0001 specified by the DPW organizing committee is met on all grids. USM3D-ME reduces the combined root-mean-square (rms) norm of meanflow and turbulence-model residuals below 10^{-13} on all grids. The force and moment coefficients converge to six significant digits. Iterative convergence on medium and ultrafine grids is illustrated in Fig. 2. The logarithm of the rms norm of combined residuals and lift, drag, and pitching moment coefficients are shown versus HANIM iterations. Convergence of medium-grid residuals below 10^{-13} was achieved in about 3000 iterations and 9.7 hours of computing on 600 Ivy Bridge central processor unit (CPU) cores. This 10^{-13} level of residual convergence on the ultrafine grid required 7000 iterations and 20.2 hours of computing on 2500 Ivy Bridge CPU cores. Aerodynamic coefficients converged much earlier: all coefficients converged in fewer than 1500 and 2500 HANIM iterations on the medium and ultrafine grids, respectively. The operational CFL number was close to 300 and 400, respectively, on the medium and ultrafine grids.

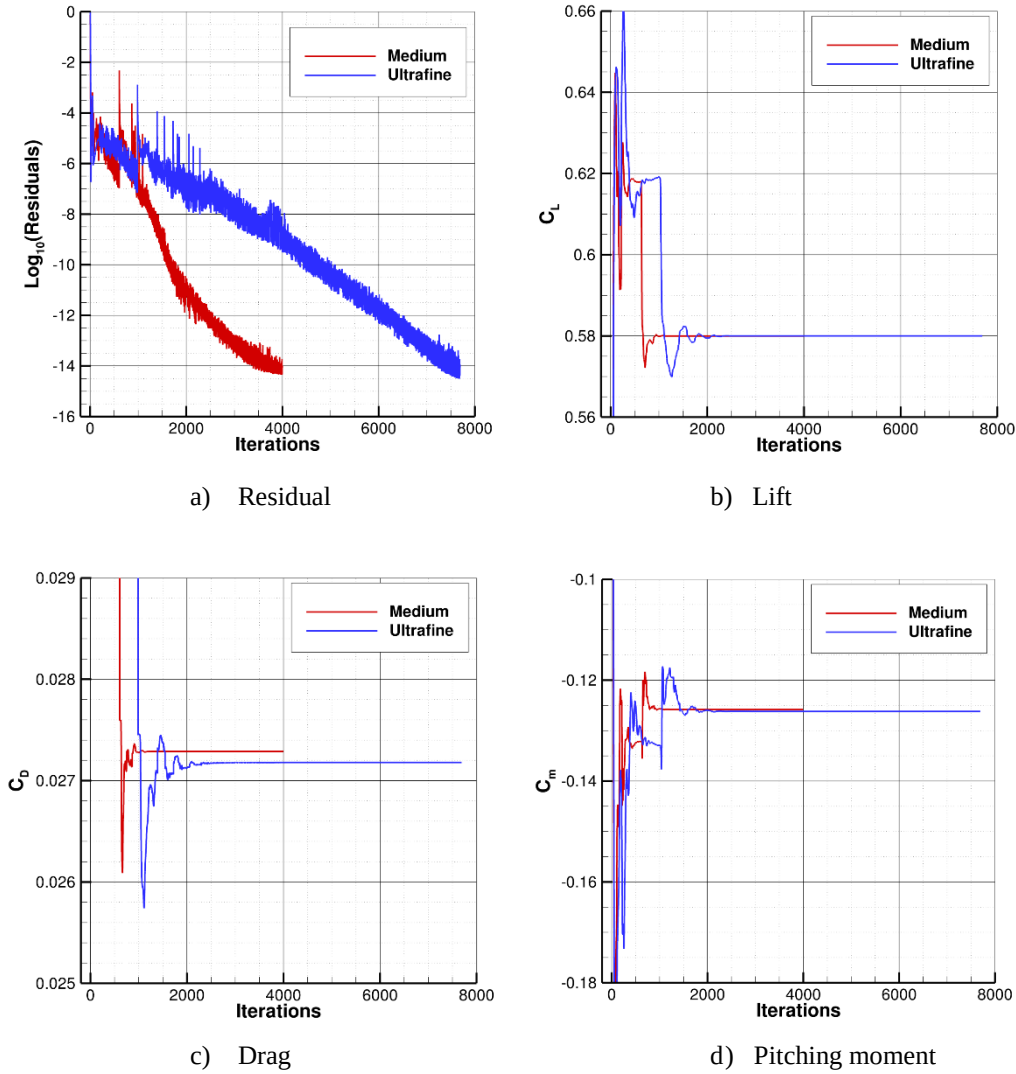


Fig. 2. Iterative convergence on medium and ultrafine grids.

Figure 3 shows grid convergence of total drag coefficient, viscous drag coefficient, pitching moment coefficient, and angle of attack versus the characteristic grid spacing that is computed as inverse of cubic root of the total number of cells (N). All quantities appear well converged in grid refinement: the variation of the total drag coefficients computed on the two finest grids is less than 0.14 counts or less than 0.05%, the corresponding pitching moment coefficients differ by less than 0.03%, and the corresponding angles of attack match up to five significant digits.

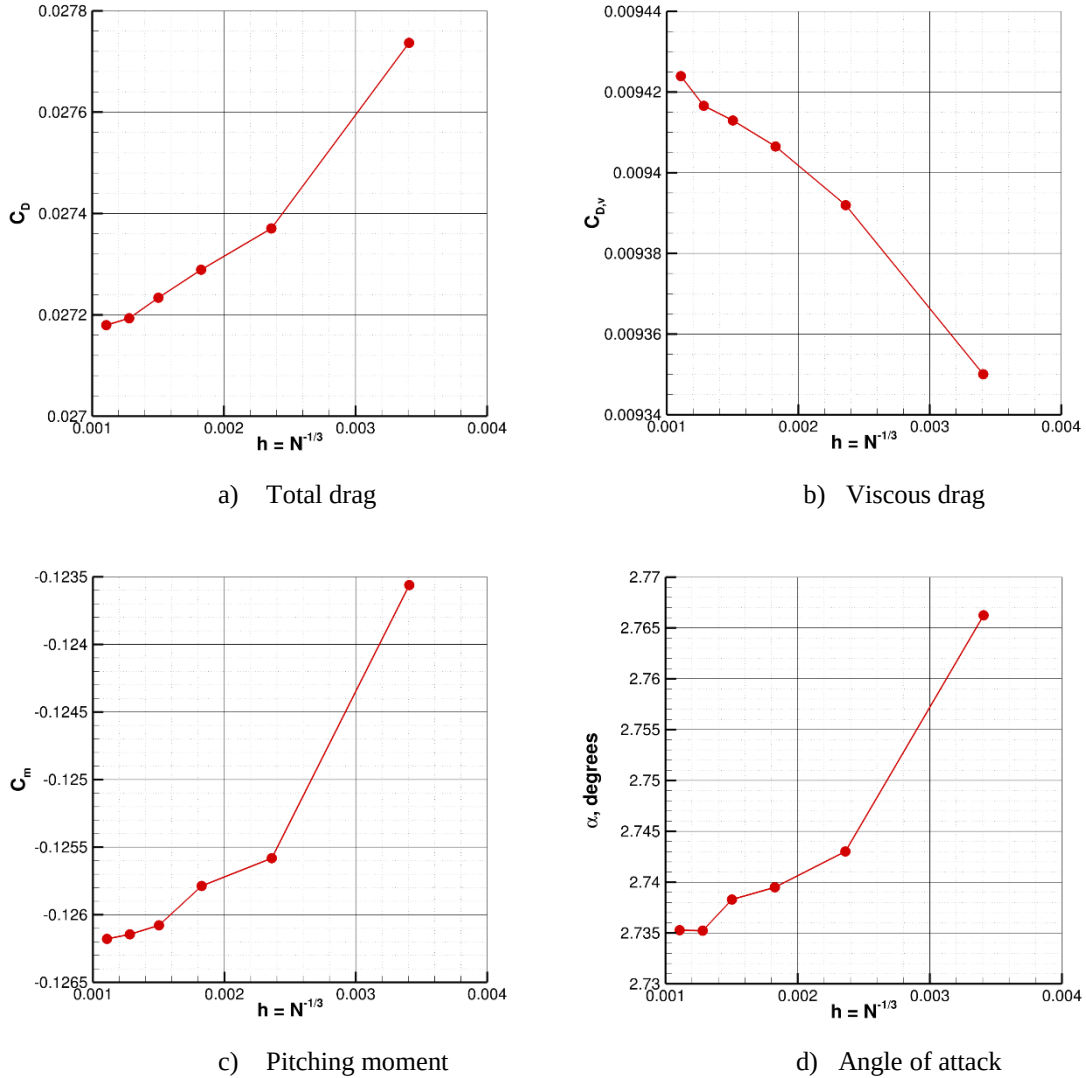


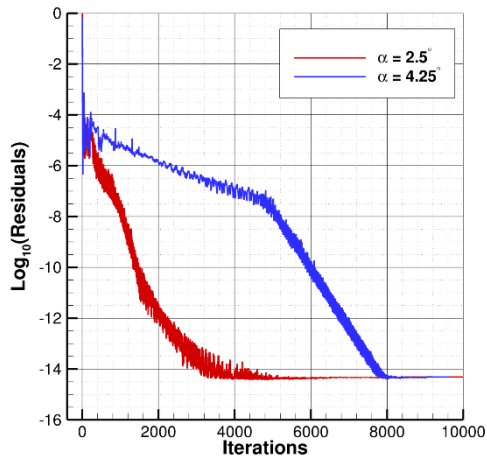
Fig. 3. Grid convergence of drag, pitching moment, and angle of attack at fixed lift, $C_L = 0.58$.

VI. Case 2a: Angle of Attack Sweep

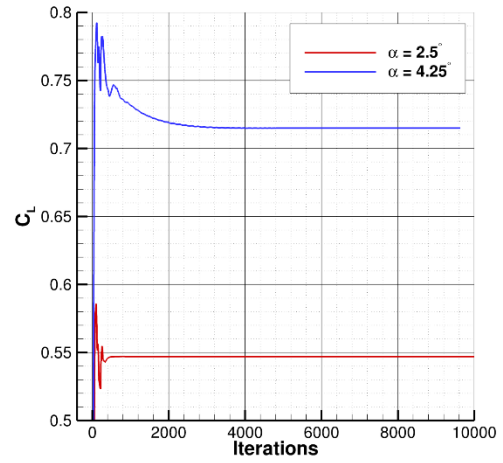
Solutions presented in this section are computed for the flow conditions corresponding to the freestream Mach number of $M = 0.85$, the Reynolds number of $Re = 20 \times 10^6$, and the reference temperature of $T = -250^\circ F$. Solutions are computed for eight angles of attack ranging from $\alpha = 2.5^\circ$ to $\alpha = 4.25^\circ$ with an increment of 0.25° . Additionally, a separate solution is computed for the $C_L = 0.50$ condition. USM3D-ME solutions are computed on medium grids generated for the Reynolds number of $Re = 30 \times 10^6$. The grids incorporate aeroelastic deformations corresponding to the LoQ AE CRM geometries and specific angles of attack. The grid for the fixed-lift solution incorporates the aeroelastic deformation that corresponds to the angle of attack of $\alpha = 2.5^\circ$. The size of a medium grid is representative of current industry practices.

All USM3D-ME solutions quickly converge the residuals to the levels below 10^{-13} . Figure 4 illustrates iterative convergence for two angles of attack, $\alpha = 2.5^\circ$ and $\alpha = 4.25^\circ$. The iterative convergence for the higher angles of

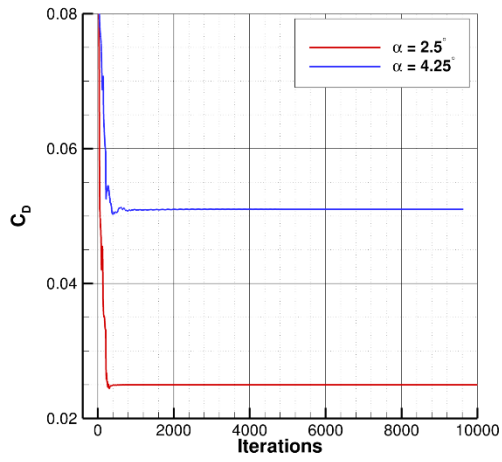
attack is somewhat slower than the convergence for the lower angles of attack. The convergence of pitching moment requires more iterations than the convergence of aerodynamic forces. Figure 5 shows the variations of the converged aerodynamic coefficients corresponding to different angles of attack. The lift and drag coefficients monotonically increase for higher angles of attack. The rate of increase is negative for lift and positive for drag. The pitch break occurs for a lift coefficient within the range $0.65 > C_L > 0.62$, an angle of attack within the range $3.25^\circ > \alpha > 3.00^\circ$, and a pitching moment coefficient $C_m \approx -0.133$. To illustrate flow separation induced by shock, the contours of skin-friction magnitude and streamlines are shown in Fig. 6 on the wing surface for three angles of attack. The flow is attached at $\alpha = 2.75^\circ$, a moderate separation zone is observed at the wing midspan at $\alpha = 3.00^\circ$, and a much more significant separation is seen at $\alpha = 3.25^\circ$. These observations are consistent with the pitch break in Fig. 5. Figures 7 and 8 show sectional variations of pressure and skin-friction coefficients. The organizing committee specified 16 wing sections to show variations of pressure and skin-friction coefficients for different angles of attack. The variations in Fig. 7 are shown for an inboard wing section 5 ($\eta = 0.2009$) that corresponds to the airfoil with the leading-edge coordinates $(x, y, z)_{LE,5} = (1076.873, 232.444, 177.509)$ and chord $c_5 = 400.743$. Figure 8 shows variations for a midspan wing section 10 ($\eta = 0.5024$) that corresponds to the airfoil with the leading edge coordinates $(x, y, z)_{LE,10} = (1342.440, 581.148, 188.658)$ and chord $c_{10} = 248.312$. For the inboard section, the shock is moving toward the trailing edge and getting stronger for higher angles of attack. The x -component of skin friction in this section remains strictly positive for all tested angles of attack indicating absence of reverse-flow conditions. The midspan section represents the region of the earliest flow separation. The strength of the shock increases for higher angles of attack, but the shock position varies nonmonotonically. The shock position closest to the trailing edge is observed for $\alpha = 3.00^\circ$; for higher angles of attack the shock moves toward the leading edge. For angles of attack $\alpha < 3.00^\circ$, the x -component of skin friction remains strictly positive. A small zone with negative x -component of skin friction appears near $(x - x_{LE,10})/c_{10} \approx 0.65$ for $\alpha = 3.00^\circ$. Reverse flow is an indication of a separation bubble. The reverse-flow zone is expanded upstream and downstream for higher angles of attack. At $\alpha = 4.25^\circ$, reverse flow covers almost half of the section near the trailing edge.



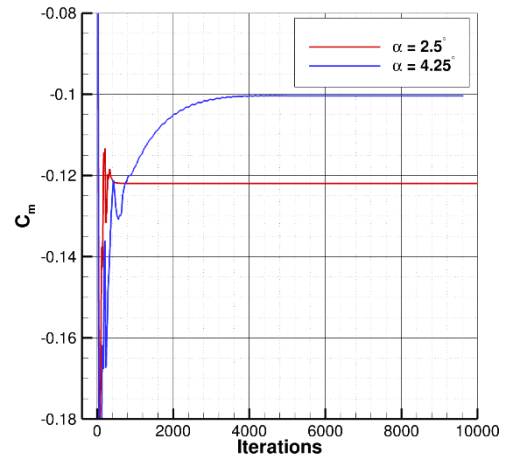
a) Residual



b) Lift

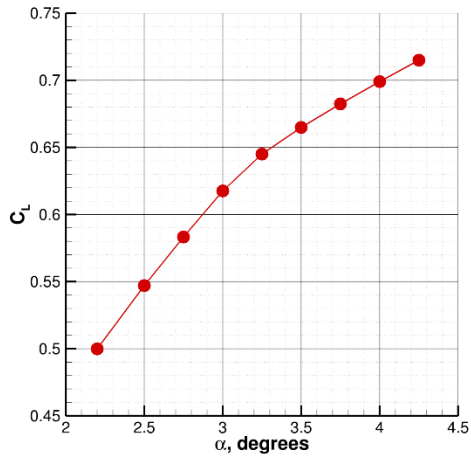


c) Drag

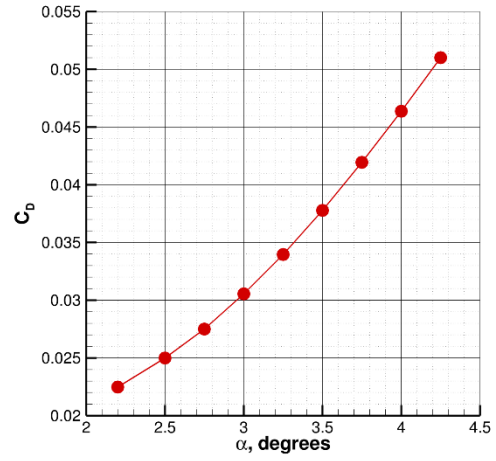


d) Pitching moment

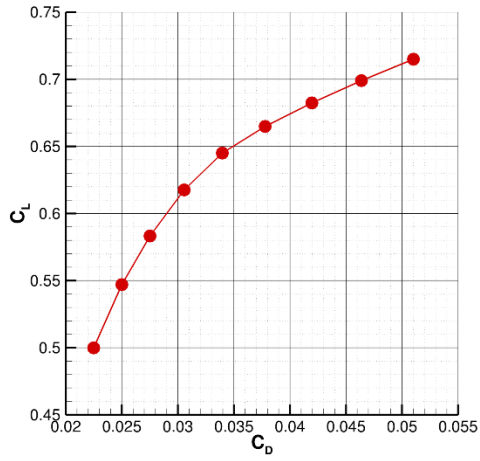
Fig. 4. Iterative convergence for two angles of attack.



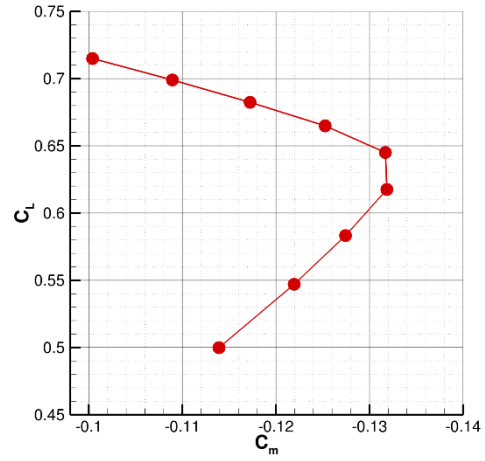
a) Lift versus angle of attack



b) Drag versus angle of attack



c) Lift versus drag



d) Lift versus pitching moment

Fig. 5. Variation of aerodynamic coefficients.

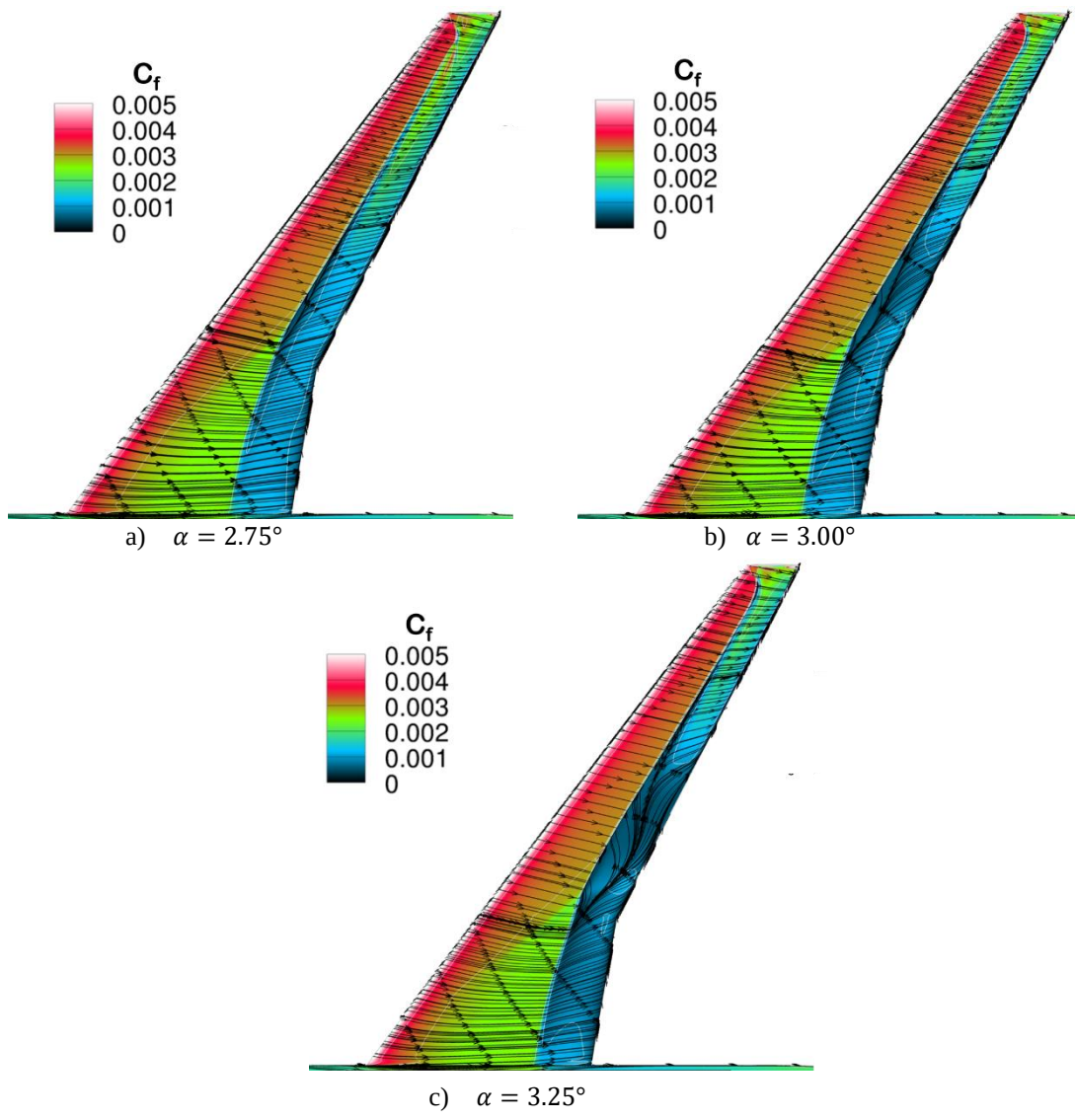
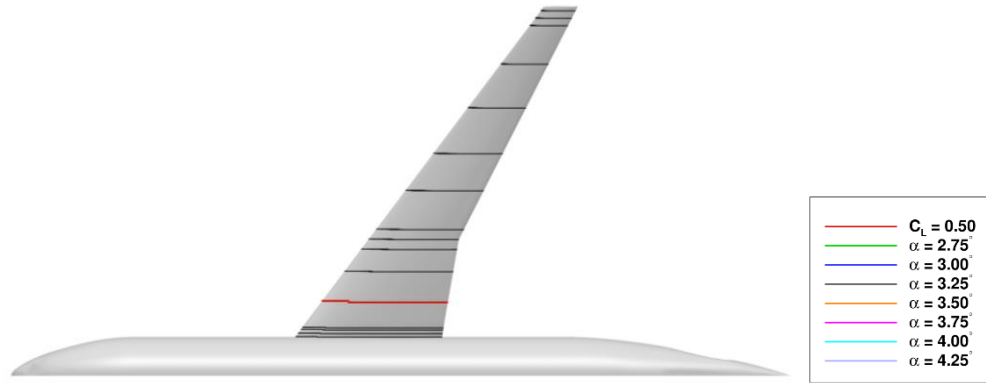
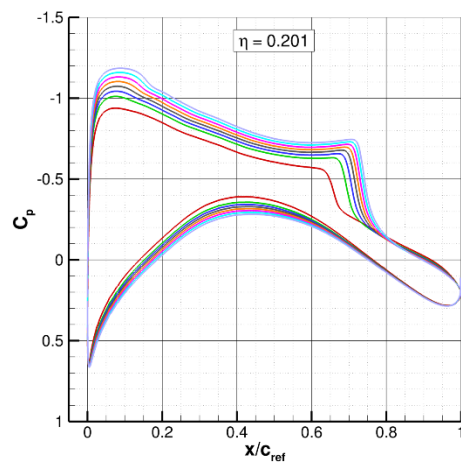


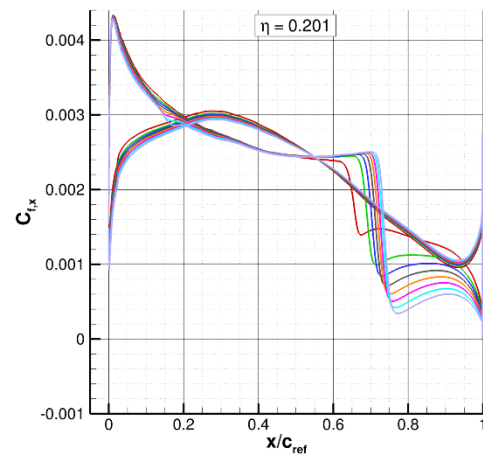
Fig. 6. Skin-friction contours and streamlines.



a) Location of wing section

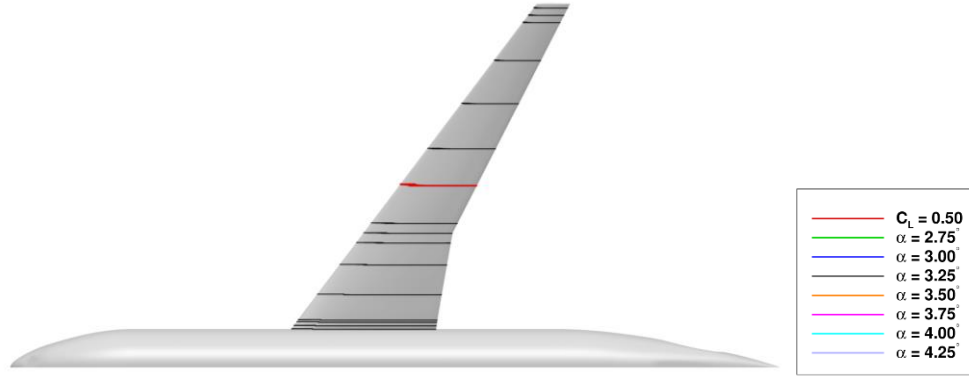


b) Pressure coefficient

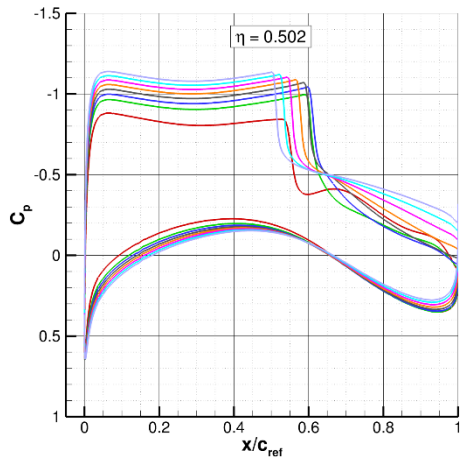


c) Skin-friction coefficient

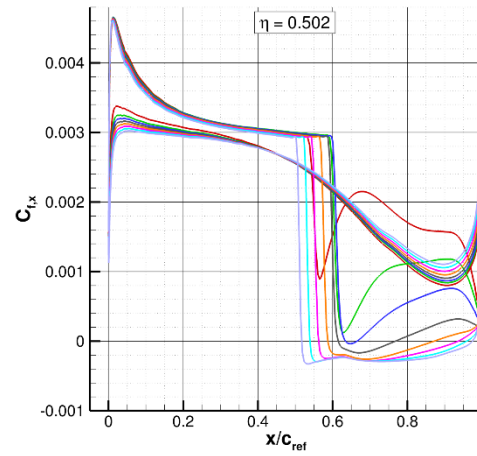
Fig. 7. Inboard wing section.



a) Location of wing section



b) Pressure coefficient



c) Skin-friction coefficient

Fig. 8. Midspan wing section.

VII. Case 3: Reynolds Number Effects

In this section, USM3D-ME solutions are computed for three Reynolds numbers. All solutions correspond to a Mach number of $M = 0.85$ and lift coefficient of $C_L = 0.5$. The first solution, defined by the authors to be simulated at Condition 1, is computed for Reynolds number of $Re = 5 \times 10^6$, reference temperature of $T = 100^\circ F$ on a medium grid that has been generated for $Re = 5 \times 10^6$ and incorporates aeroelastic deformations corresponding to $\alpha = 2.5^\circ$ angle of attack and the corresponding LoQ AE CRM loft. The second condition, Condition 2, was prescribed to capture the Reynolds number effect by specifying the same dynamic pressure as Condition 1 but with a Reynolds number of $Re = 20 \times 10^6$. Condition 3 was chosen to have the same Reynolds number but higher dynamic pressure (HiQ) relative to Condition 2. Given the same freestream Mach and Reynolds number, comparisons between Conditions 2 and 3 primarily capture the effect of different aeroelastic deformations. Condition 4 was chosen such that a representative flight Reynolds number, 30×10^6 , in this case, could be simulated. The appropriately deformed lofts, provided by the committee, were used to simulate each condition.

Figure 9 shows the effect of Reynolds number on angle of attack, drag, and pitching moment. As expected, a dramatic decrease in aerodynamic performance is observed at off-design conditions, such as a Reynolds number of 5 million. This is evidenced by a significant increase in drag and also increased angle of attack needed to achieve the target C_L . The effect of aeroelastic deformations can be seen through comparison of two solutions computed for the same flow conditions ($Re = 20 \times 10^6$) on medium grids that incorporate different aeroelastic deformations. The drag coefficients from these two solutions are similar, but there is a 15% difference between pitching moments. The pitching moment computed on the grid incorporating aeroelastic deformation corresponding to low dynamic pressure is higher by 0.016 than the coefficient computed on the grid incorporating the deformation corresponding to high

dynamic pressure. Figure 10 shows the pressure contours and streamlines on the wing surface for two different Reynolds numbers, $Re = 5 \times 10^6$ and $Re = 30 \times 10^6$. The pressure distributions look qualitatively similar. The flow corresponding to the lower Reynolds number exhibits some spanwise streamlines aligned with the y direction in the wing midspan, while streamlines of higher-Reynolds number flow are mainly aligned with the x direction.

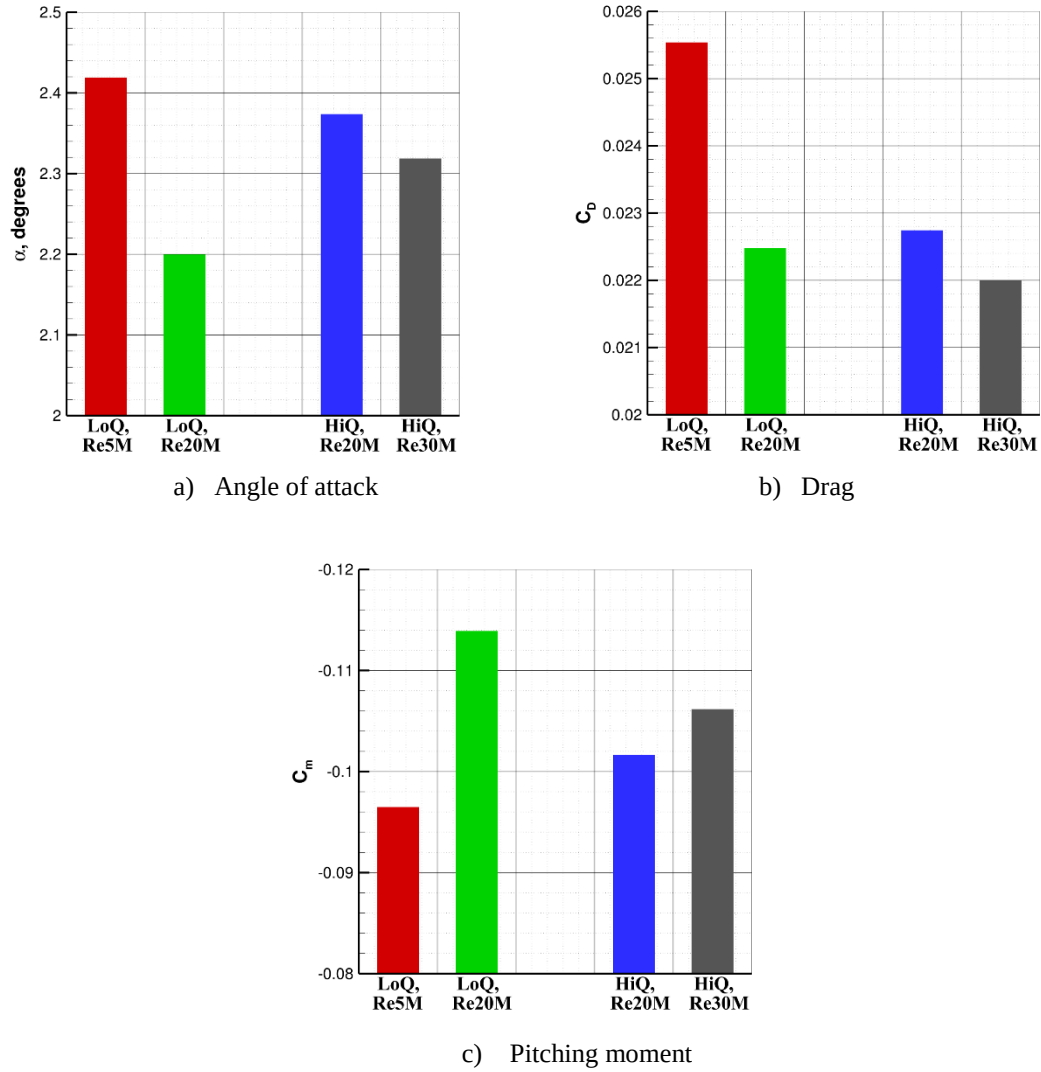


Fig. 9. Effect of Reynolds number.

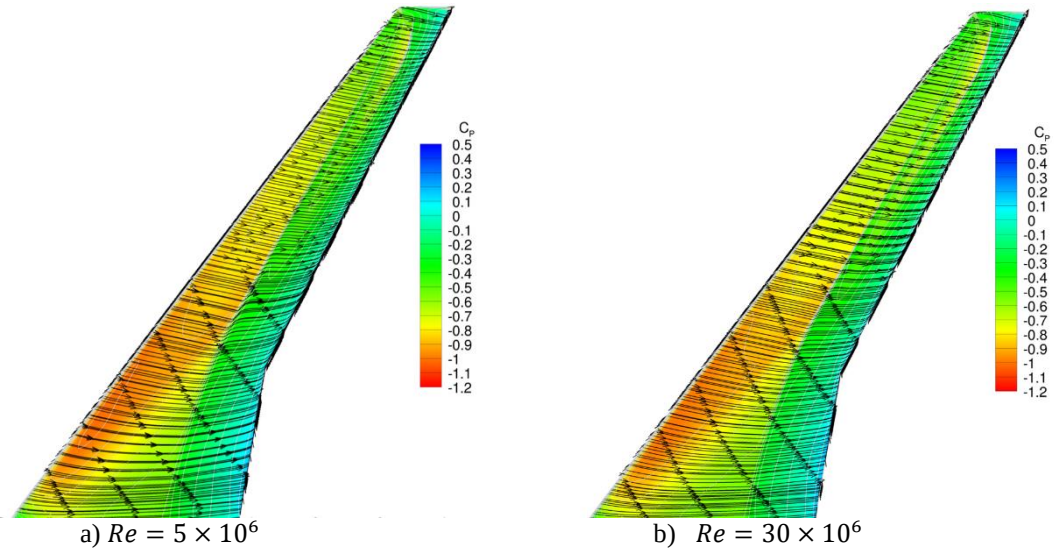


Fig. 10. Effect of Reynolds number on surface flow.

VIII. Summary

The seventh drag prediction workshop (DPW-7) was held in conjunction with the 2022 AIAA AVIATION Forum and focused on prediction of the drag and pitching moment for the NASA Common Research Model (CRM) wing-body configuration at transonic flight conditions representative of high-speed commercial transport aircraft. USM3D-ME, a cell-centered, finite-volume, mixed-element, unstructured-grid flow solver, developed and supported at NASA Langley research center, computed solutions for three required cases that include a grid convergence study at a fixed lift condition and the studies of the effects of variations in the angles of attack and Reynolds numbers. USM3D-ME solutions feature a new implementation of the negative variant of Spalart-Allmaras turbulence model (SA-neg) and a hierarchical adaptive nonlinear iteration method (HANIM) that improve efficiency and robustness of iterative solutions on unstructured grids. The paper presented theoretical foundations for the new implementation of SA-neg model.

For the DPW-7 cases, USM3D-ME solutions have been computed using the nonlinear SA-neg-QCR2000 model that is appropriate for wing-body configurations. Solutions have been computed on a family of unstructured mixed-element grids generated by JAXA. The grid size ranges from 25 million cells to almost 740 million cells. The grids incorporate aeroelastic deformations corresponding to particular flight conditions. USM3D-ME quickly converged the combined (meanflow and turbulence-model) residuals to the machine-zero levels (root-mean-square norm is less than 10^{-13}) on all grids, eliminating the error due to incomplete iterative convergence. The aerodynamic coefficients converged to six significant digits on each grid. Grid convergence studies demonstrated good convergence for the aerodynamic coefficients: drag and pitching moment converge monotonically and differ by less than 0.05% on the two finest grids.

The study of effects of angle-of-attack variation indicates onset of flow separation in the wing midspan at the angle of attack of $\alpha = 3.0^\circ$. The pitch break occurs for the pitching moment coefficient of $C_m \approx -0.133$ within lift coefficient range $0.65 > C_L > 0.62$ and angle of attack range $3.25^\circ > \alpha > 3.00^\circ$. The study of effects of Reynolds-number variation shows that drag increases for low Reynolds number in off-design conditions. Aeroelastic deformations for high-Reynolds flow have a small effect on drag, but a significant effect on pitching moment.

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