Transport Equations: Mathematical and Discrete Issues

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Turbulence and Modeling

- For this subject, let me quote Heisenberg.
  - "*When I meet God, I am going to ask him two questions: Why relativity? And Why turbulence? I really believe he will have an answer for the first.*"
  - "*An expert is someone who knows the worst mistakes that can be made in his subject, and how to avoid them*"
- Caveat: I certainly do not consider myself an expert in either turbulence or the modeling of turbulence.
  - However, I have studied these subjects with experts. In addition, my graduate work and dissertation concerned turbulence.
  - My focus is on Mathematics and Numerical Analysis

Outline of Discussion

- Brief discussion of 3 hierarchel models
  - One-equation model
  - Two-equation model
  - Some issues in solving two-equation model
  - Full Reynolds stress model (RSM)
- Brief discussion of current solution algorithm
- Some numerical results
- Perspective on solving transport equations
  - Mathematical foundation and formulation
  - Strong solution algorithms
  - Stiffness issues
  - Positivity and realizability
  - Linear and nonlinear stability
  - Summary of some key solution algorithm properties

Compressible Reynolds-Averaged Navier-Stokes Equations

Integral form of the 3-D Reynolds-averaged Navier-Stokes equations

$$\iiint_{\mathcal{V}} \frac{\partial \mathbf{W}}{\partial t} d\mathcal{V} + \iint_{\mathcal{S}} \mathcal{F} \cdot \mathbf{n} d\mathcal{S} = 0,$$

where the solution vector

$$\mathbf{W} = [\rho \quad \rho u \quad \rho v \quad \rho w \quad \rho E]^T$$

and the flux density tensor $\mathcal{F} = \mathcal{F}_c + \mathcal{F}_v$, with

$$\mathcal{F}_c = [\rho q \quad \rho u q + p\mathbf{e}_x \quad \rho u q + p\mathbf{e}_y \quad \rho w q + p\mathbf{e}_z \quad \rho H q]^T$$

$$\mathcal{F}_v = -[0 \quad \overline{\tau} \cdot \mathbf{e_x} \quad \overline{\tau} \cdot \mathbf{e_y} \quad \overline{\tau} \cdot \mathbf{e_z} \quad \overline{\tau} \cdot \mathbf{q} + k\nabla T]^T$$

where $\mathbf{q} = u\mathbf{e}_x + v\mathbf{e}_y + w\mathbf{e}_z$, and $\overline{\tau}$ is the stress tensor.

One Equation Turbulence Model

- One-equation model of Spalart-Allmaras (La Recherche Aerospatiale 1 1994)

$$\frac{\partial \tilde{\nu}}{\partial t} + u_j \frac{\partial \tilde{\nu}}{\partial x_j} = C_{b1}(1 - f_{t2})\hat{S}\tilde{\nu} - \left[C_{w1} f_w - \frac{C_{b1}}{\kappa^2} f_{t2} \right] \left(\frac{\tilde{\nu}}{d} \right)^2 + \frac{1}{\sigma} \left[\frac{\partial}{\partial x_j} \left((\nu + \tilde{\nu}) \frac{\partial \tilde{\nu}}{\partial x_j} \right) + C_{b2} \frac{\partial \tilde{\nu}}{\partial x_j} \frac{\partial \tilde{\nu}}{\partial x_j} \right]$$

  where the eddy viscosity is determined from

$$\mu_t = \rho \tilde{\nu} f_{v1},$$

  and

$$f_{v1} = \frac{\chi^3}{x^3 + c_{v1}^3}, \quad \chi = \frac{\tilde{\nu}}{\nu}, \quad \nu = \frac{\mu}{\rho}, \quad \hat{S} = \Omega + \frac{\tilde{\nu}}{k^2 d^2} f_{v2}$$

- Implementation
  - Advection terms: First order, non-conservative discretization
  - Boundary Conditions: solid surfaces ($\tilde{\nu} = 0$); free stream ($\tilde{\nu} = 3\nu_\infty$)

Two Equation Turbulence Model

- A form of the two-equation k-ω model of Wilcox (Turbulence Modeling for CFD 2006) is given by

$$\frac{\partial k}{\partial t} + \tilde{u}_j \frac{\partial k}{\partial x_j} = \frac{1}{\bar{\rho}} \frac{\partial}{\partial x_j} \left[\left(\mu + \sigma^* \frac{\bar{\rho} k}{\omega} \right) \frac{\partial k}{\partial x_j} \right] + P_k - D_k$$

$$\frac{\partial \omega}{\partial t} + \tilde{u}_j \frac{\partial \omega}{\partial x_j} = \frac{1}{\bar{\rho}} \frac{\partial}{\partial x_j} \left[\left(\mu + \sigma \frac{\bar{\rho} k}{\omega} \right) \frac{\partial \omega}{\partial x_j} \right] + \frac{\sigma_d}{\omega} \frac{\partial k}{\partial x_j} \frac{\partial \omega}{\partial x_j} + P_\omega - D_\omega$$

where the production and destruction terms are given by

$$P_k = \frac{\mu_t}{\bar{\rho}} |\mathbf{\Omega}|^2, \quad P_\omega = \alpha \frac{\omega}{k} \frac{\mu_t}{\bar{\rho}} |\mathbf{\Omega}|^2, \quad D_k = \beta^* k \omega, \quad D_\omega = \beta \omega^2$$

- To reduce the magnitude of μ_t when the production of the turbulence energy exceeds the dissipation rate, a stress limiter is introduced:

$$\tilde{\omega} = \max \left\{ \omega, \quad C_{lim} \sqrt{\frac{2 \bar{\Omega}_{ij} \bar{\Omega}_{ij}}{\beta^*}} \right\}, \qquad C_{lim} = 0.95.$$

Two Equation Turbulence Model

- Solid wall boundary conditions (Menter [AIAA J. 1994]):

$$k = 0, \qquad \omega = \omega_w = \frac{60\mu_1}{\rho_1 \beta (d_1)^2}.$$

- Free-stream boundary conditions [NASA TM 1998-208444]:

$$k = k_\infty = 9 \times 10^{-9}\, u_\infty^2, \quad \omega = \omega_\infty = 1 \times 10^{-6} \left(\frac{u_\infty^2}{\nu_\infty} \right).$$

- The turbulent viscosity is computed by

$$\mu_t = \frac{\rho k}{\tilde{\omega}}$$

Issues in Solving Two-Equation Model

- Ensuring positivity of dependent variables of turbulence model equations
- Imbalance between production and destruction terms
  - Such an imbalance occurs in regions where ω becomes small
    - Allows disturbances in the strain rate
    - Results in large values of μ_t
    - Production term becomes very large when ω goes to zero and μ_t is finite
  - To prevent excessively large P_k term, we use the constraint suggested by Menter

$$\tilde{P}_k = \min(P_k, 20D_k)$$

Full Reynolds Stress Model (RSM)

- A form of the SSG/LRR full RSM [Eisfeld, 2004] is given by

$$\frac{\partial \bar{\rho}\hat{R}_{ij}}{\partial t} + \frac{\partial \bar{\rho}\hat{u}_k\hat{R}_{ij}}{\partial x_k} = \bar{\rho}P_{ij} + \bar{\rho}\Pi_{ij} - \bar{\rho}\varepsilon_{ij} + \bar{\rho}D_{ij} + \bar{\rho}M_{ij}$$

$$\frac{\partial \bar{\rho}\omega}{\partial t} + \frac{\partial \bar{\rho}\hat{u}_k\omega}{\partial x_k} = \frac{\alpha_\omega \omega}{\hat{k}}\frac{\bar{\rho}P_{kk}}{2} - \beta_\omega \bar{\rho}\omega^2 + \frac{\partial}{\partial x_k}\left[\left(\bar{\mu} + \sigma_\omega \frac{\bar{\rho}\hat{k}}{\omega}\right)\frac{\partial \omega}{\partial x_k}\right] + \sigma_d \frac{\bar{\rho}}{\omega}\max\left(\frac{\partial \hat{k}}{\partial x_j}\frac{\partial \omega}{\partial x_j}, 0\right)$$

  where the production term is given by

$$\bar{\rho}P_{ij} = -\bar{\rho}\hat{R}_{ik}\frac{\partial u_j}{\partial x_k} - \bar{\rho}\hat{R}_{jk}\frac{\partial u_i}{\partial x_k}$$

  and the dissipation is modeled with ($\varepsilon = C_\mu \hat{k}\omega$, $\hat{k} = \hat{R}_{ii}/2$)

$$\bar{\rho}\varepsilon_{ij} = \frac{2}{3}\bar{\rho}\varepsilon\delta_{ij}$$

Full Reynolds Stress Model (RSM)

- Note the following

$$\bar{\rho}\hat{R}_{ij} = -\tau_{ij} = \overline{\rho u_i'' u_j''}$$

- The diffusion term is modeled by

$$\bar{\rho}D_{ij} = \frac{\partial}{\partial x_k}\left[\left(\bar{\mu}\delta_{k\ell} + D\frac{\bar{\rho}\hat{R}_{k\ell}}{C_\mu \omega}\right)\frac{\partial \hat{R}_{ij}}{\partial x_\ell}\right]$$

- For details on modeling of the pressure-strain correlation ($\bar{\rho}\Pi_{i,j}$)
  - NASA Turbulence Modeling Resource (TMR)
  - Eisfeld [DLR, ISSN 1614-7790, 2004]

- Reynolds stresses are zero at solid wall boundary, and BC for ω is the same as for Wilcox 2006 model.

RK/Implicit Scheme

- Consider a multistage scheme (e.g, Runge-Kutta)

$$\mathbf{W}^{(0)} = \mathbf{W}^{n}$$
$$\mathbf{W}^{(q)} = \mathbf{W}^{(0)} - \alpha_q \, \mathcal{L} \, \mathbf{W}^{(q-1)}, \quad q = 1, ..., s$$
$$\mathbf{W}^{n+1} = \mathbf{W}^{(q)}$$

  $\mathcal{L}$ is the complete difference operator.

- Suppose we introduce an implicit preconditioner $\mathcal{P}^{-1}$ on stage q

$$\mathbf{W}^{(q)} = \mathbf{W}^{(0)} - \alpha_q \, \mathcal{P}_q^{-1} \, \mathcal{L} \, \mathbf{W}^{(q-1)}$$

  where

$$\mathcal{P}_q = \left(\frac{1}{CFL\,(\Delta t)}\right) I + \left(\frac{\partial \mathbf{R}}{\partial \mathbf{W}}\right)_q$$

- The resulting scheme $\in$ of the general class of implicit RK schemes
- Now, we have to determine the discrete implicit operator.

Inverse of Implicit Operator

- Consider the preconditioner

$$\mathcal{P}_q = \left(\frac{1}{CFL\,(\Delta t)}\right) I + \left(\frac{\partial \mathbf{R}}{\partial \mathbf{W}}\right)_q$$

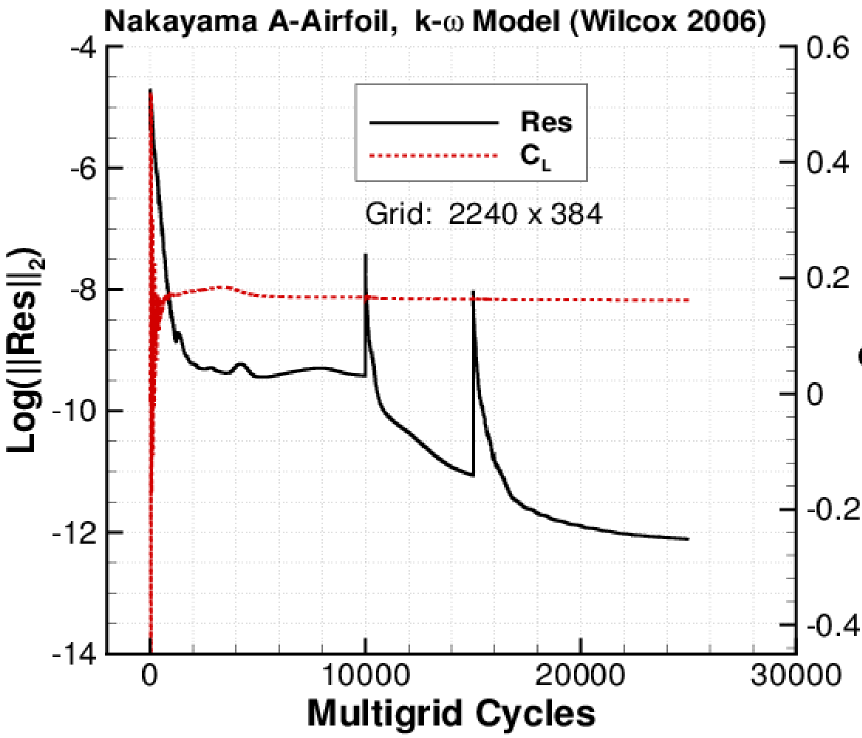
- The inverse of the preconditioner $\mathcal{P}_q$ is approximated.
- Stiff discrete equations are considered.
  - Point SGS and partial line SGS relaxation used to approx. $\mathcal{P}_q^{-1}$.
  - Sufficient approx. with 2 SGS sweeps for each relaxation type
  - CFL is between 10^3 and 10^6
- Implementation details of RK/Implicit scheme given in
  - Rossow [JCP 2007]
  - Swanson et al. [JCP 2007],
  - Swanson, Rossow [Comput. Fluids 2011]

Numerical Results

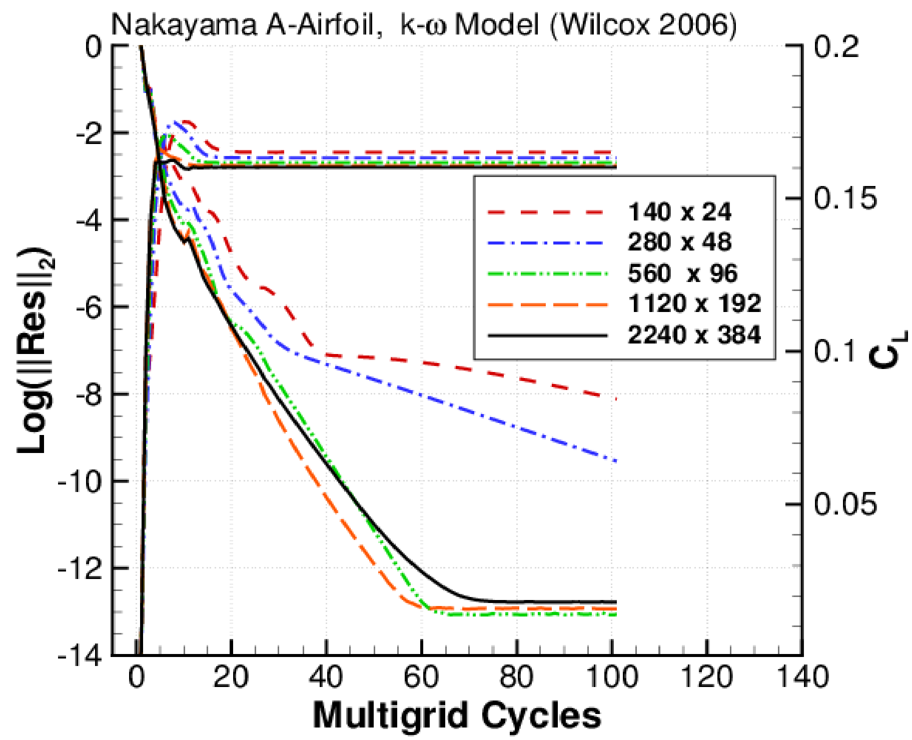
- Numerical solutions for airfoil flows
  - Nakayama A-Airfoil
  - RAE Airfoil
  - NACA 4412 Airfoil

Convergence Histories for Nakayama A-Airfoil

k-ω Model, $\alpha = 0^o$, $M = 0.088$, $Re = 1.2 \times 10^6$



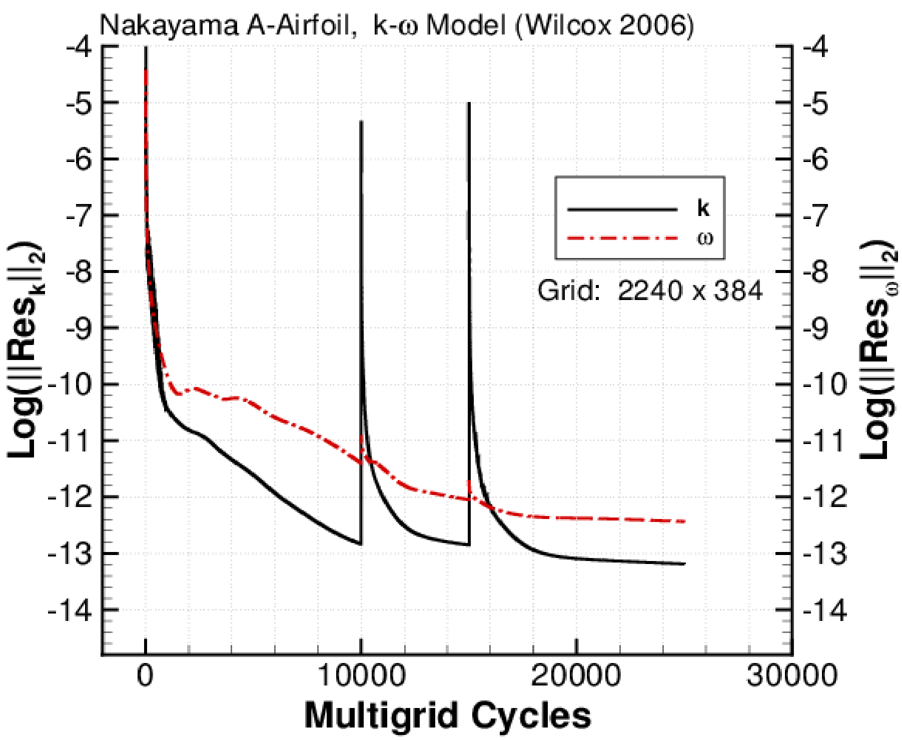
(a) Implicit AF Scheme



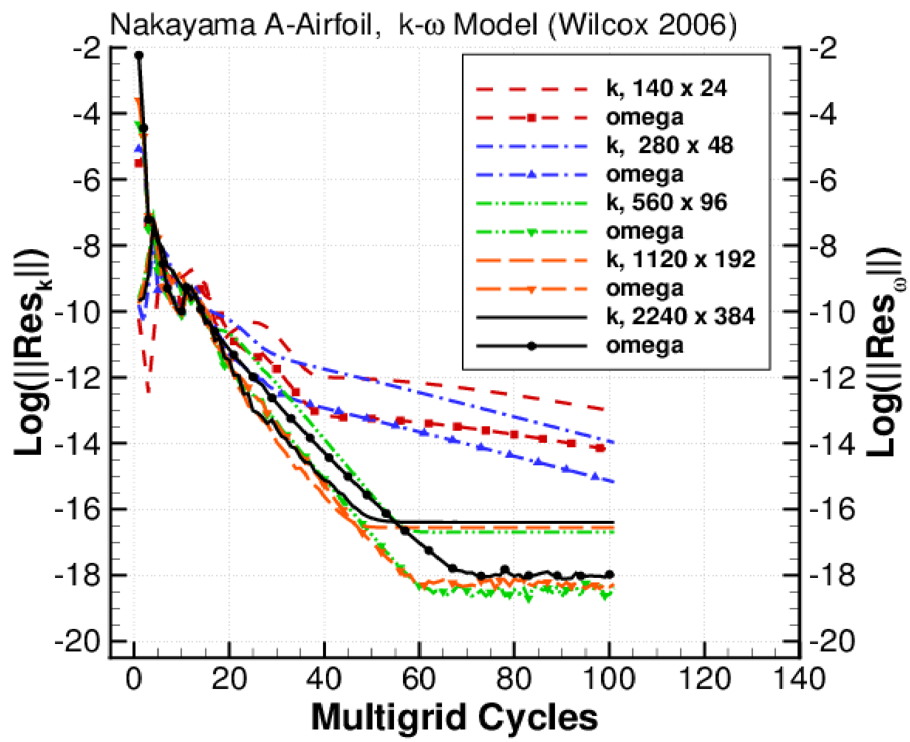
(b) RK/Implicit Scheme

Convergence Histories for Nakayama A-Airfoil

k-ω Model, $\alpha = 0^o$, $M = 0.088$, $Re = 1.2 \times 10^6$



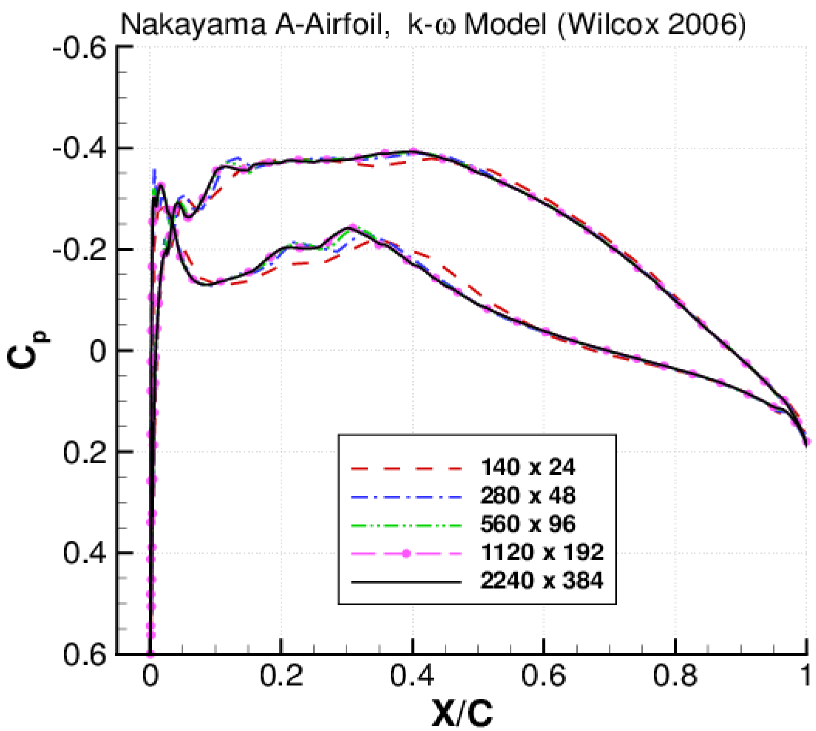
(a) Implicit AF Scheme

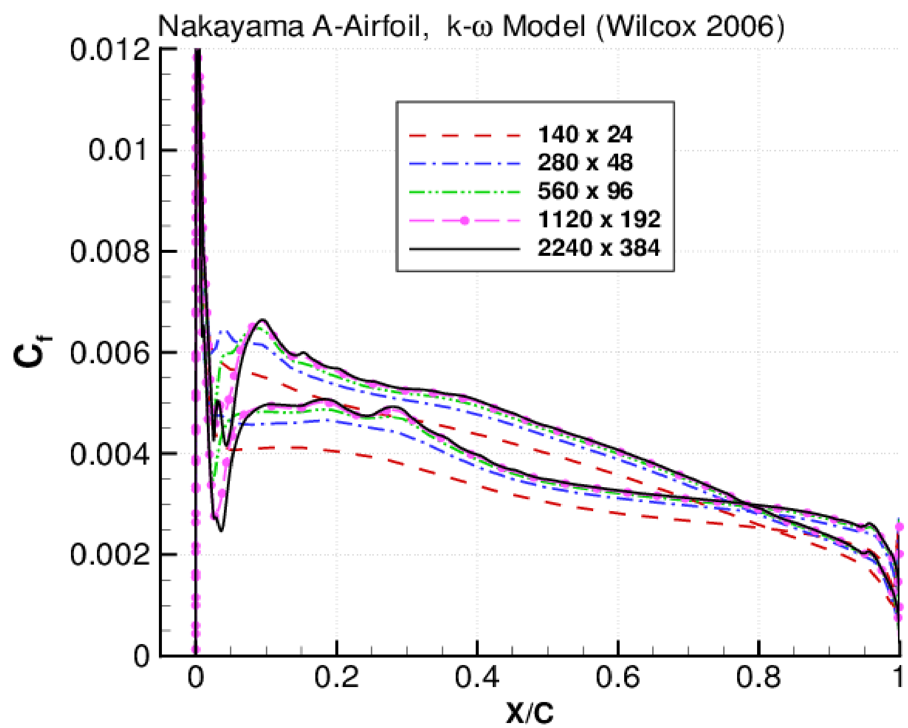


(b) RK/Implicit Scheme

Results for Nakayama A-Airfoil

k-ω Model, $\alpha = 0^o$, $M = 0.088$, $Re = 1.2 \times 10^6$

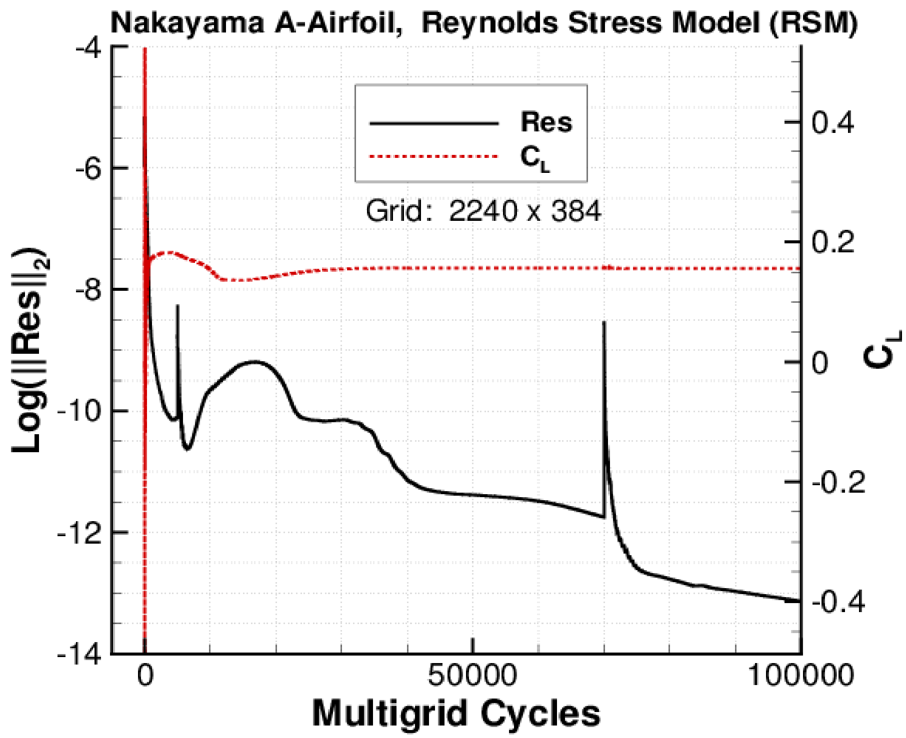


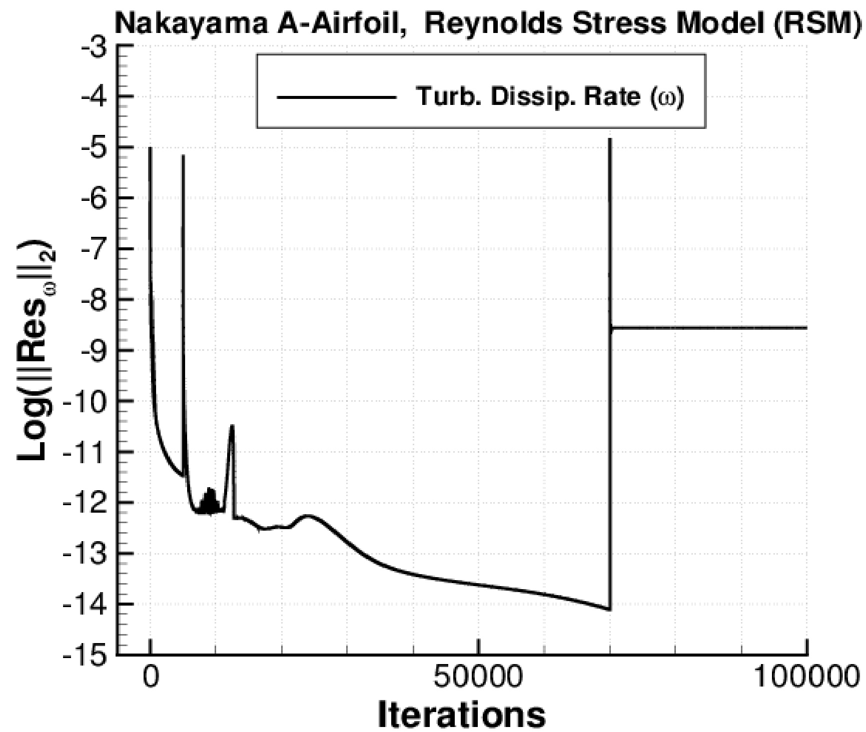


Surface Pressure and Skin-Friction Distributions (RK/Implicit Scheme)

Convergence Histories with RSM for Nakayama A-Airfoil

Reynolds Stress Model, $\alpha = 0^o$, $M = 0.088$, $Re = 1.2 \times 10^6$

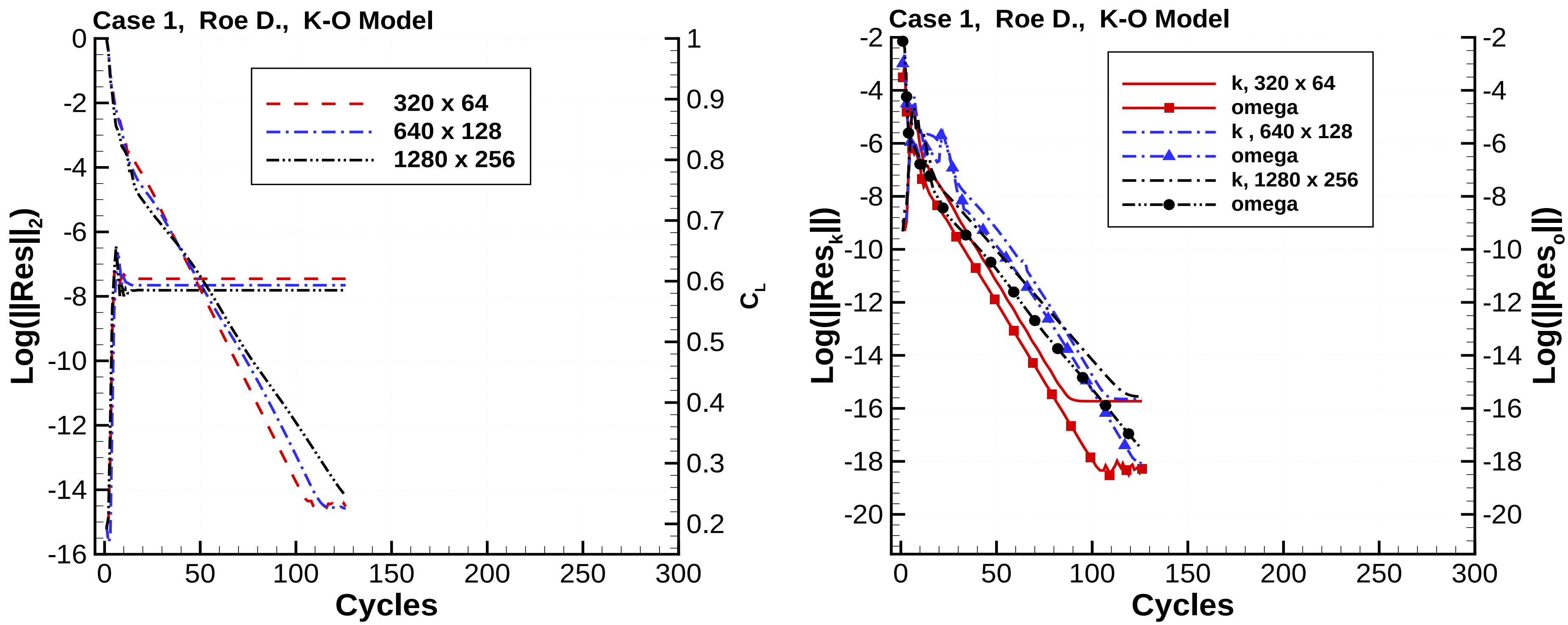




Computations with Implicit AF Scheme and Reynolds Stress Model

Convergence Histories for RAE 2822 Airfoil: Subsonic

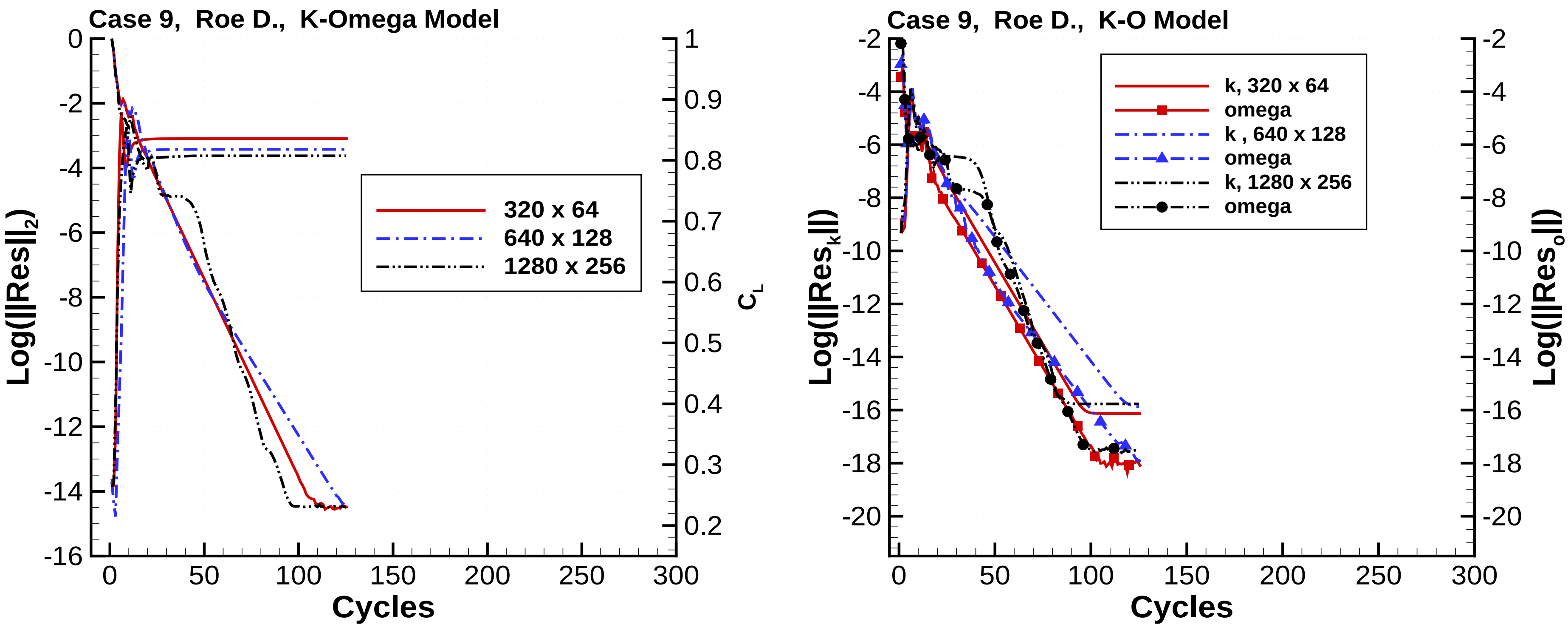
$$\alpha = 1.93^o,\ M = 0.676,\ Re = 5.7 \times 10^6$$



Case 1: RK/Implicit scheme, k-ω model

Convergence Histories for RAE 2822 Airfoil: Transonic

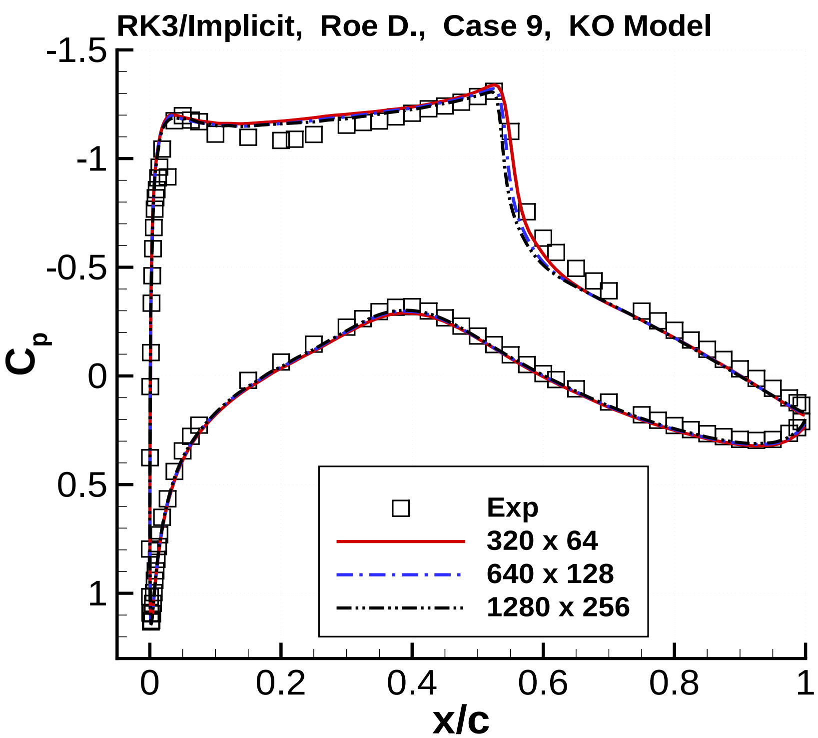
$$\alpha = 2.79^o,\ M = 0.730,\ Re = 6.5 \times 10^6$$

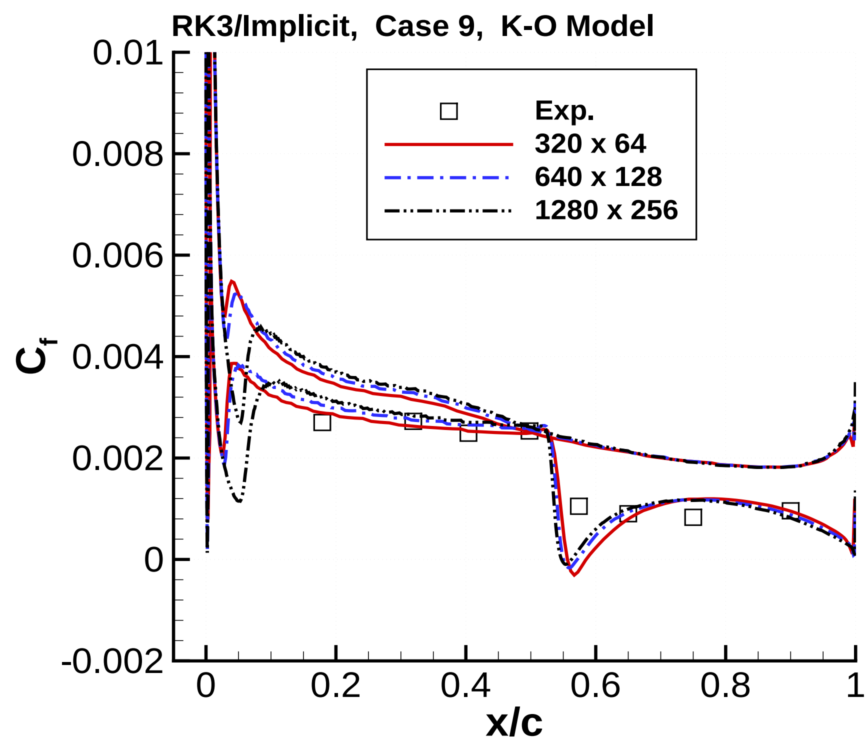


Case 9: RK/Implicit scheme, k-ω model

Results for RAE 2822 Airfoil: Transonic

$$\alpha = 2.79^o,\ M = 0.730,\ Re = 6.5 \times 10^6$$

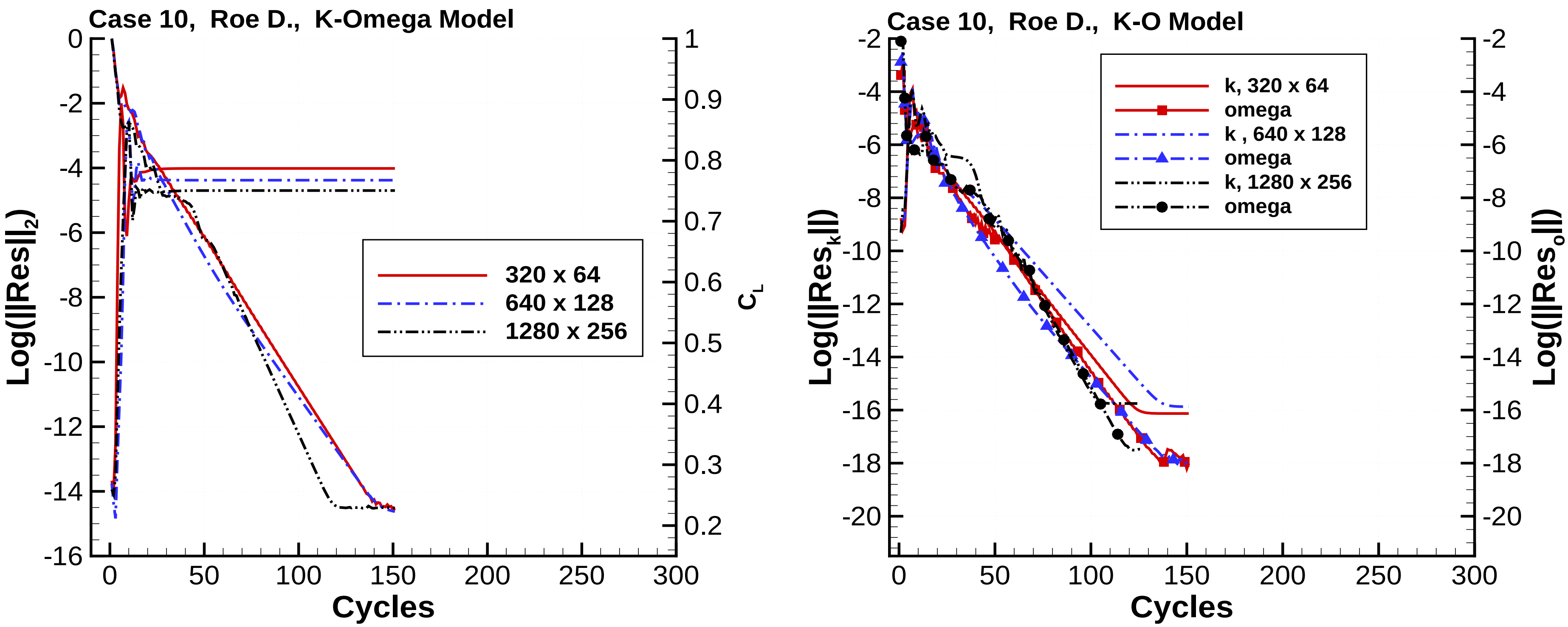




Computations with RK/Implicit Scheme and k-ω model

Convergence Histories for RAE 2822 Airfoil: Transonic

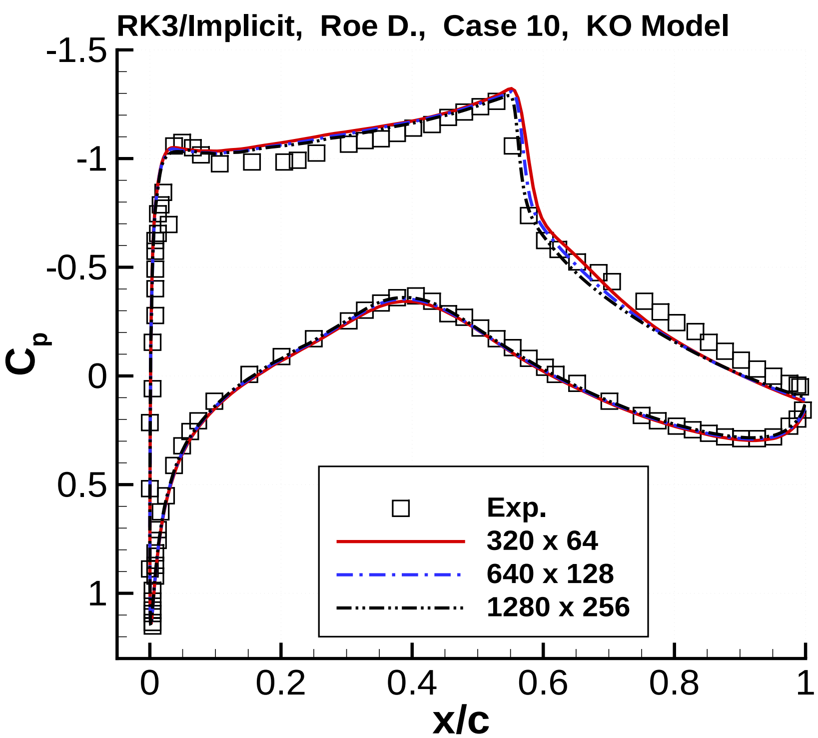
$$\alpha = 2.81^o,\ M = 0.750,\ Re = 6.2 \times 10^6$$

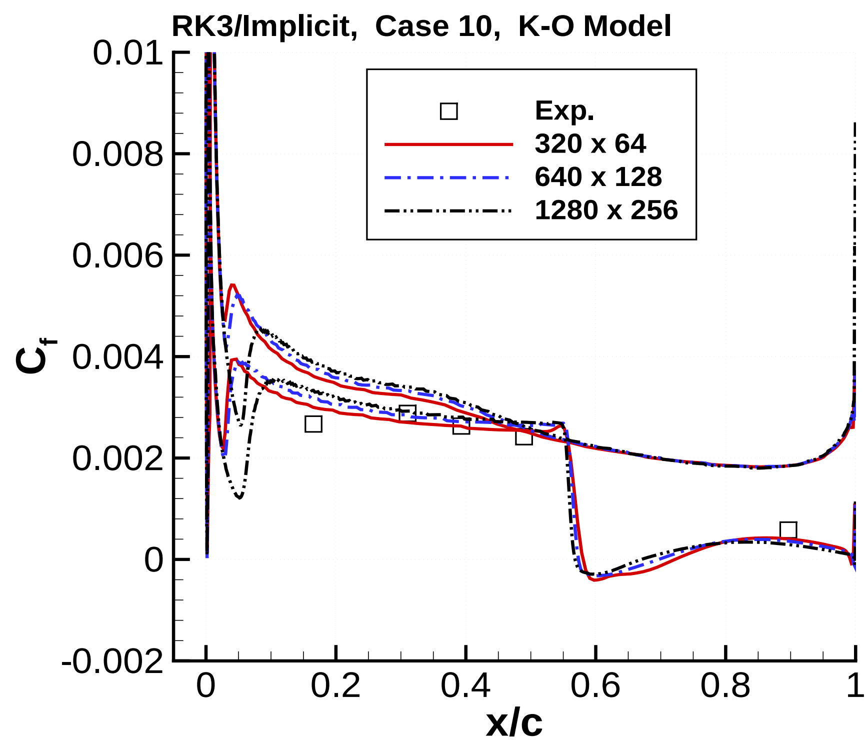


Case 10: RK/Implicit scheme, k-ω model

Results for RAE 2822 Airfoil: Transonic

$\alpha = 2.81^o,\ M = 0.750,\ Re = 6.2 \times 10^6$



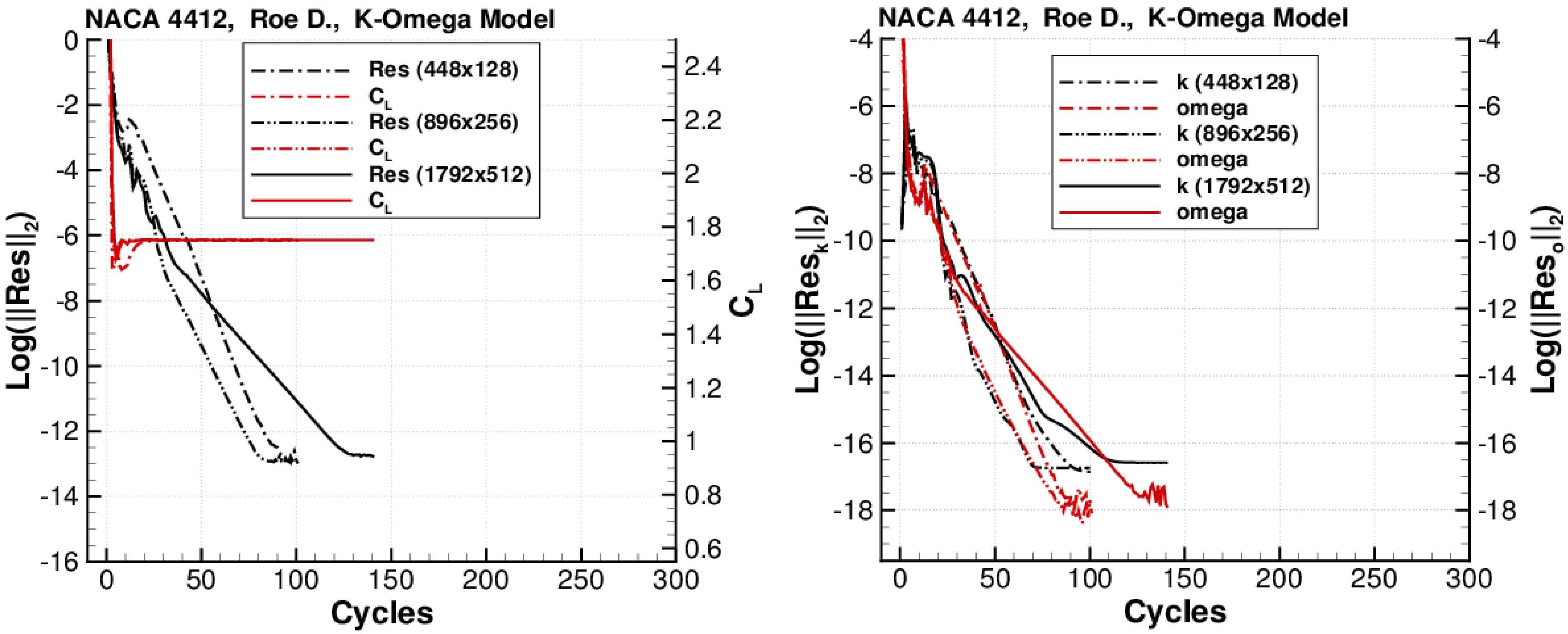


Computations with RK/Implicit Scheme and k-ω model

Convergence Histories for NACA 4412 Airfoil

High Angle of Attack (α)

$$\alpha = 13.87^o,\ M = 0.09,\ Re = 1.52 \times 10^6$$

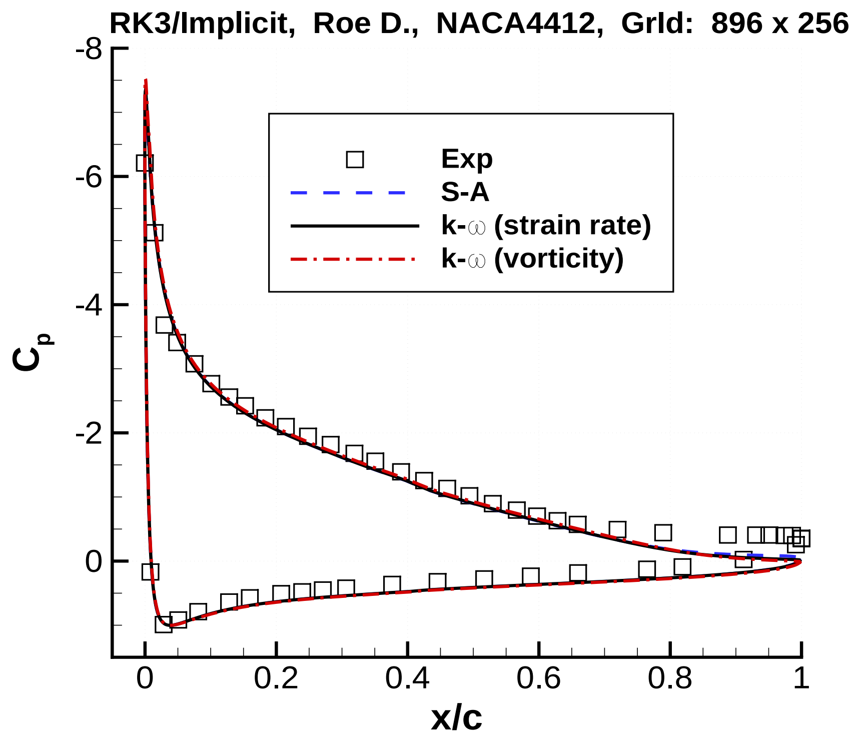


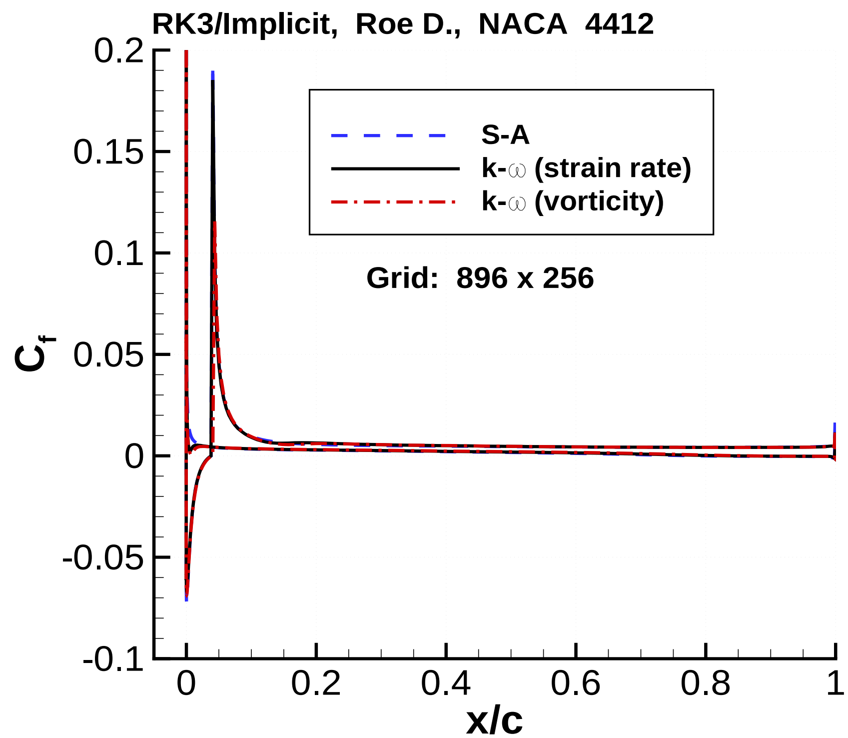
NACA 4412: RK/Implicit scheme, k-ω model

Results for NACA 4412 Airfoil

High Angle of Attack (α)

$$\alpha = 13.87^o,\ M = 0.09,\ Re = 1.52 \times 10^6$$





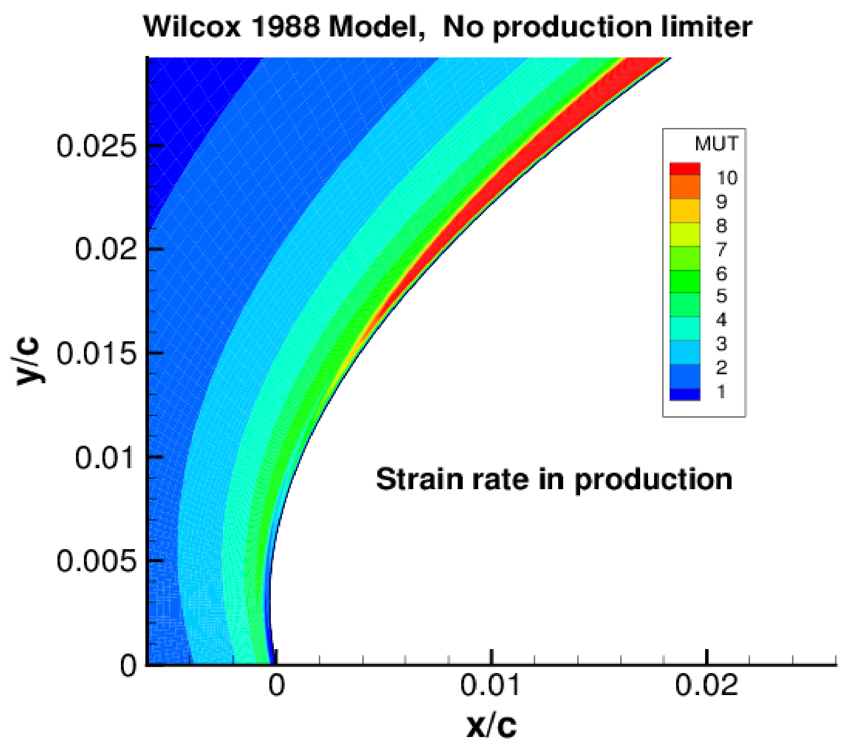
Computations with RK/Implicit Scheme and k-ω model

Turbulent Viscosity Contours

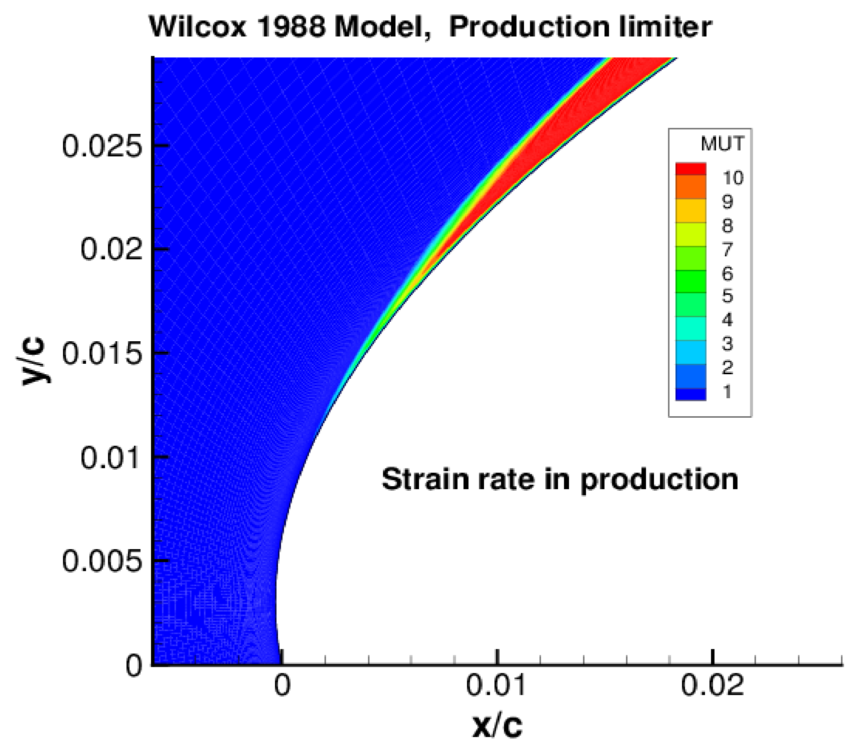
High Angle of Attack (α)

$\alpha = 13.87^o$, $M = 0.09$, $Re = 1.52 \times 10^6$

Upper LE Region, 1988 Wilcox Model



(a) No production limiter



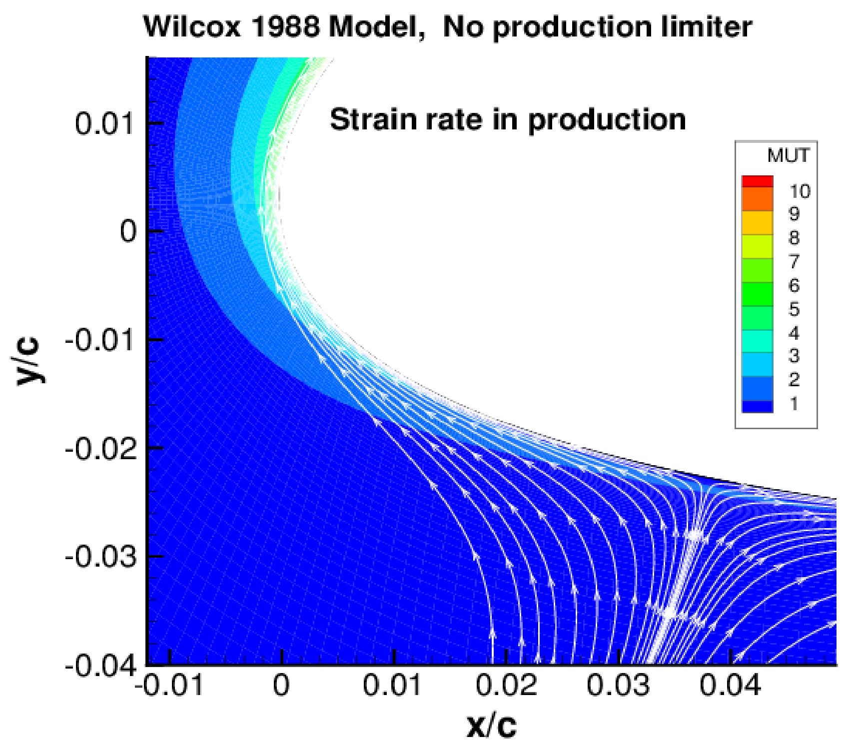
(b) Production limiter

Turbulent Viscosity Contours and Streamines

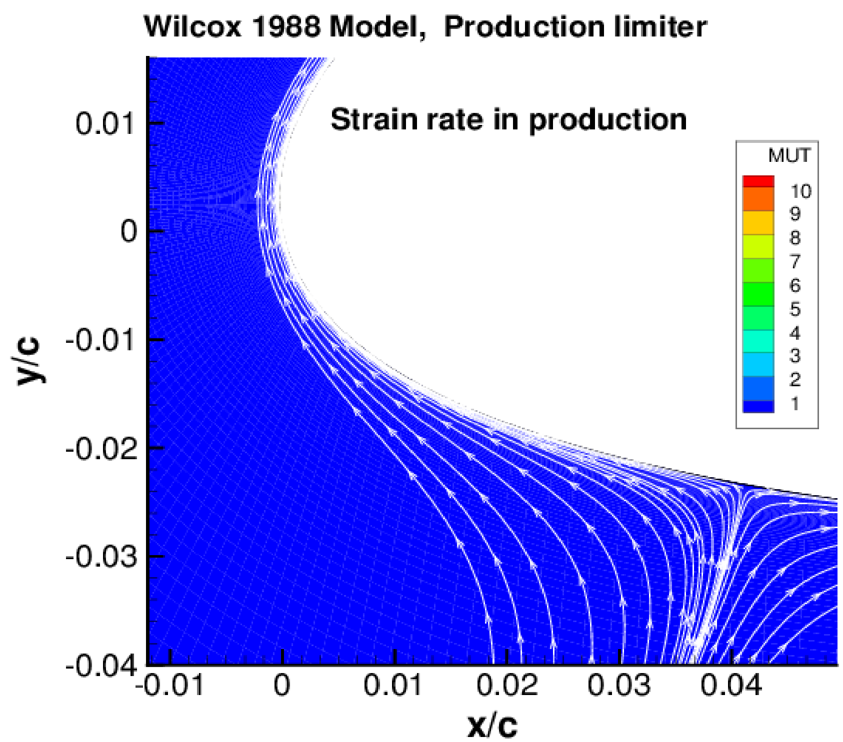
High Angle of Attack (α)

$\alpha = 13.87^o$, $M = 0.09$, $Re = 1.52 \times 10^6$

Lower LE Region, 1988 Wilcox Model



(a) No production limiter



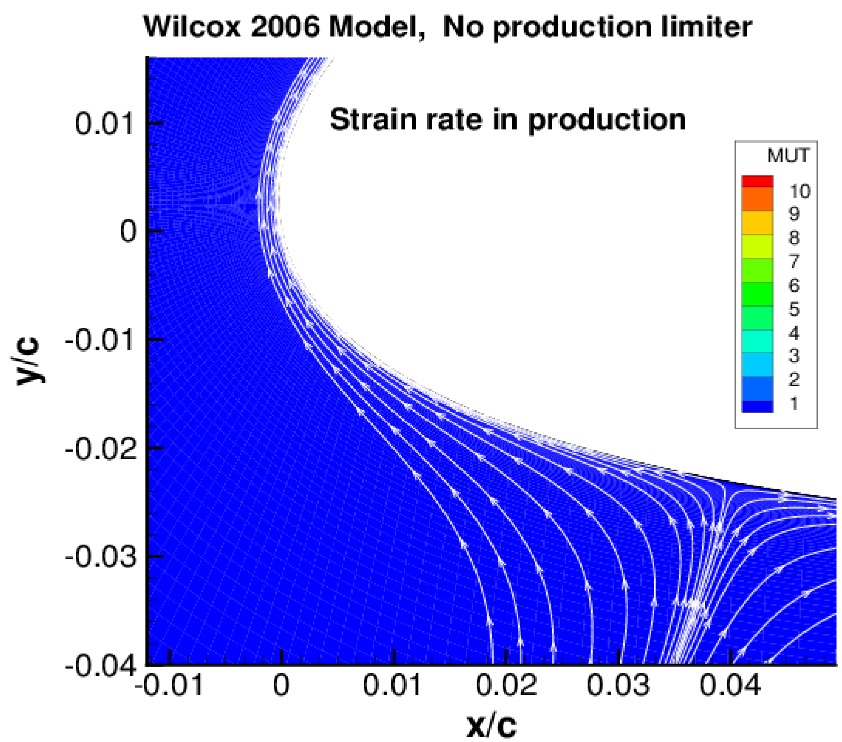
(b) Production limiter

Turbulent Viscosity Contours and Streamines

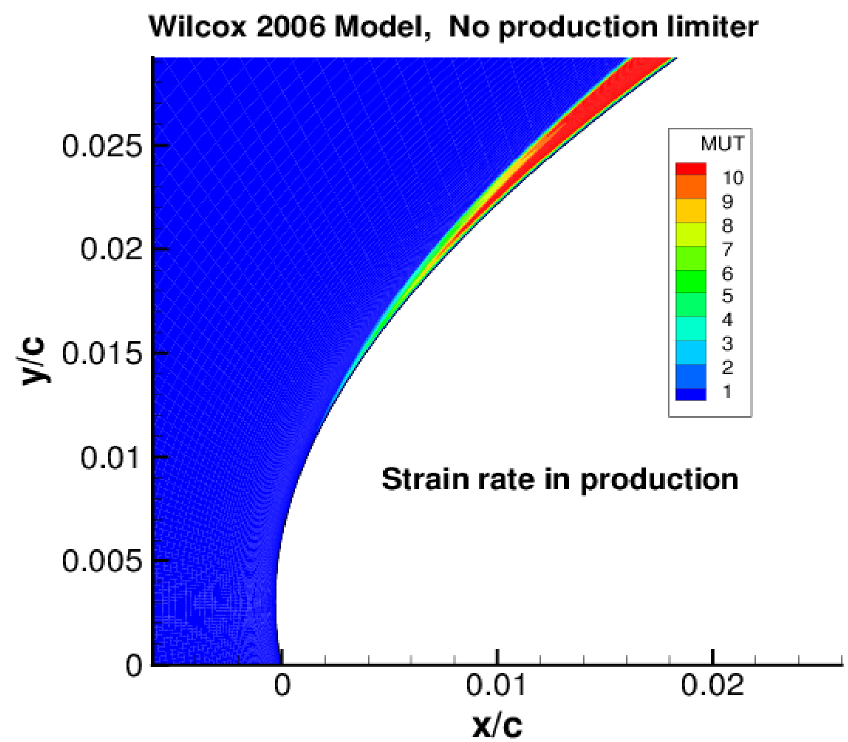
High Angle of Attack (α)

$\alpha = 13.87^o$, $M = 0.09$, $Re = 1.52 \times 10^6$

Lower and Upper LE Region, 2006 Wilcox Model



(a) No production limiter



(b) No production limiter

Navier-Stokes (N-S) Equations

- Mathematical foundation
  - Need to solve: Problem of well-posedness, regularity, and global existence
  - Progress made for particular cases.
  - Problem in general **remains unsolved**
- Transport equations for turbulence models
  - Form is similar to that for N-S equations.
  - Mathematical foundation is not established.
- Thus, we do not know a priori for the transport equations
  - If a solution exist
  - Possibly, there are multiple solutions
- Existence of a realistic solution to the transport equations depends only on **numerical demonstrations**.

Mathematical Formulation for Turbulent Flow Problems

- Issues
  - Often, complete descriptions of continuous and discrete problems are not given
  - BCs are not always stated, and often are only approximate
  - Sometimes, a boundary-value problem is not even be solved for each iteration (e.g., wall BC for ω equation).
- There is usually neglect of a proper study of the mathematical properties of transport equations
  - This is even true when mean flow and turbulence model equations are weakly coupled.
  - Exception has been with the Spalart-Allmaras (SA) model.
- Even without mathematical questions, additional numerical difficulties can occur
  - When considering two or more transport equations (i.e., PDE related to length scale equation used)
  - Increased stiffness of system of equations

Mathematical Formulation for Turbulent Flow Problems

- Thus, the reliability of using such models on a routine basis for industrial application can be problematic.

Conjecture 1 *The construction of a reliable and efficient algorithm for solving the transport equations of a turbulence model, either weakly or strongly coupled to the Reynolds average N-S (RANS) equations, is highly unlikely, in general, without complete mathematical and numerical analysis of the system or systems of equations.*

Another View of Turbulence Modeling

- Generally, we consider turbulence modeling a direct problem
  - Model parameters determined by comparing solutions and data for range of problems.
  - Solve RANS equations with given turbulence model
- One can consider turbulence modeling an inverse problem, as suggested by S. Langer [Habilitation, 2017].
  - Then, we have a parameter identification problem
  - Reconstruct the eddy viscosity from given data
- Indicators that inverse problem is ill-posed
  - More than one turbulence model of a given type gives essentially same surface C_p and C_f values.
  - Small perturbation in C_p variation can yield different solution and μ_t.
- Such observations suggest that turbulence modeling by its mathematical nature is an ill-posed problem.

Developing of Turbulence Models

- Developers of turbulence models
  - Again, generally give little attention to solving equations of model
  - Difficulties arise due to both stiffness issues and source terms
- Need to consider two factors in modeling of turbulence
  - Ultimately, the success of model depends on heuristics of model.
  - Models with more than one equation are not based upon first principles derivations.
- Consider a two-equation model
  - One equation is turbulence kinetic energy (TKE) equation derived from first princples.
  - Second equation is used to give a length scale; it is **kludged up** (as Peter Bradshaw might say)
    * Form of equation based on that of TKE equation
    * Example: equation for turbulence dissipation rate (ω)
    * Eddy viscosity is $\mu_t = \rho k/\omega$.

Developing of Turbulence Models

- The two factors previously given suggest that there is flexibility in changing model to make amenable to solving equations.
- The essential requirements for changing model
  - Must maintain integrity of model.
  - Must verify the modified model for standard test cases used to calibrate parameters of model.

Strong Solution Algorithms

- Assume RANS and transport equations are weakly coupled.

- Numerical algorithms for both RANS and transport equations
  - Should both belong to the class of strong solution algorithms
  - Would like algorithms to be the same to allow eventually a strongly coupled solver
  - Must be highly implicit: L-stability is desired to solve stiff systems.
  - Algorithm must be unconditionally stable in linear sense, including BCs.
  - Fluid dynamics equations highly nonlinear in general $\longrightarrow$ desirable to have nonlinear stability
  - Same stability properties should apply to solvers for mean flow and transport equation.

Stiffness Issues Concerning Transport Equations

- No generally accepted mathematical definition of stiffness.
- Some examples of stiff systems:
  - Linear constant coefficient system with large stiffness ratio
  - Stability requirements rather than accuracy restrict stepsize
- Two fundamental sources of stiffness
  - Systems of PDEs themselves
    - Large condition number (stiffness number) for compressible Euler or Navier-Stokes equations as $M \to 0$
    - Source terms of turbulence modeling equations create stiff systems.
  - Discrete resolution of viscous terms using stretched grids results in stability determining stepsize.
- Stiff ODEs require strongly implicit schemes for an effective solution algorithm.

Positivity and Realizability

- Need for Positivity Preserving Scheme
  - Requirement of positivity for thermodynamic variables of mean flow equations
  - For two-equation model (e.g., $k - \omega$ model of Wilcox),
    - Need to ensure positivity of k and ω
    - Eddy viscosity $\mu_t = \rho k/\omega > 0$
  - For full RSM, dependent variables include Reynolds stresses
    - Need to ensure positivity of normal Reynolds stresses and ω
    - Realizability conditions: $\overline{\rho u_i'' u_i''} \geq 0$, $(\overline{\rho u_i'' u_j''})^2 \leq \overline{\rho u_i'' u_i''}\ \overline{\rho u_j'' u_j''}$
- For turbulence models, there are 3 methods used to ensure positivity of dependent variables.
  - Explicitly enforce positivity
  - Replace k, ω with $\ln(k)$, $\ln(\omega)$ (Ilinca and Pelletier, [IJTS 1999])
    - Need wall function since k vanishes at solid wall boundary
    - Approach can experience difficulties with upper bound on μ_t.

Positivity and Realizability

- Replace ω with $\ln(\omega)$ (Bassi et al, [Comput Fluids, 2005])
  - Limiting k
  - Imposing lower bound on ω using realizability conditions
    - Positive normal Reynolds stresses
    - Satisfying Schwarz inequality for Reynolds shear stresses.
- Construct M-matrix (Mor-Yossef [JCP 2006])
  - A semi-positive matrix with positive eigenvalues
  - Used to approximate Jacobian of transport equations
  - A non-singular M-matrix has convergent regular splitting and positive inverse.
  - These properties guarantee
    - Unconditional linear stability
    - Positivity of dependent variables in turbulence equations
  - Note: M-matrix approach does not appear to have a counterpart for mean flow equations.

Linear and Nonlinear Stability

- Linear stability
  - Local mode analysis (Fourier transform of linear equations)
  - For initial-boundary value (IBV) problems, it is beneficial to consider **energy stability**.
    - Allows variable coefficents
    - Includes boundary conditions
- Eigensystem analysis for IBV problems
- With Krylov method, using Arnoldi algorithms, one can determine stability behavior of actual discrete problem being solved (Langer [JCP 2014]).

Linear and Nonlinear Stability

- Nonlinear stability
  - Generally not included in constructing numerical algorithms
  - Nonlinearity can have significant effects such as producing spurious oscillations, occurring in
    * Under-resolved regions
    * Neighborhood of discontinuities such as shock waves
- For this purpose, we consider entropy stability.
- Entropy stability guarantees that the thermodynamic entropy is bounded for all time in L_2 under two conditions (Carpenter et al. [AIAA 2013]).
  - $\rho, T > 0$
  - Boundary data results in a well-posed problem and preserves entropy estimate.
- To construct entropy stable scheme, a convex function is required.

Linear and Nonlinear Stability

- Entropy function
  - Mathematical function
  - Negative of thermodynamic entropy of gas dynamics
- Global conservation of entropy is derived from transforming (contracting) N-S equations using
  - Entropy function and
  - Integrating over the domain
- By mimicking each term of this equation discretely, we can obtain a semi-discrete entropy estimate.
- Using procedure of Tadmor [Acta Numerica, 2003] called comparison of arguments, conditions that guarantee entropy stability can be established.
- Considering entropy stability for algorithm to solve transport equations of turbulence model requires
  - Appropriate entropy function
  - Again, proving well-posedness for discrete problems

Summary: Solution Algorithms

- Basic elements
  - Implicit scheme
    - Required for stiff equations (L-stability)
    - Point and line relaxation to invert implicit operator
    - Parallelizability
  - Multigrid or emulator
    - Scheme with good smoothing properties
    - Multistage framework for scheme to enhance eigenvalue clustering
- A class of strong algorithms
  - Basic elements
  - Minimized inconsistencies: implicit operator and residual function
  - Newton-Krylov methods
    - Effective preconditioner
    - Multigrid in linear solver

Summary: Solution Algorithms

- Enhanced robustness with Adaptive Algorithms
  - Local measures of stability and resolution
  - Enriched local resolution
  - Variable order of discretization
  - Additional local relaxation due to high residuals
  - Modification of algorithm parameters
  - Modified local relaxation strategy
- Ensure positivity
- Contruct schemes with entropy (nonlinear) stability