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A CFD laboratory archive supporting the academic process

Shawn Ericson

To the Graduate Council:

I am submitting herewith a thesis written by Shawn Ericson entitled "A CFD laboratory archive supporting the academic process." I have examined the final electronic copy of this thesis for form and content and recommend that it be accepted in partial fulfillment of the requirements for the degree of Master of Science, with a major in Engineering Science.

A. J. Baker, Major Professor

We have read this thesis and recommend its acceptance:

Joe Iannelli, Masood Parang

Accepted for the Council:
Carolyn R. Hodges

Vice Provost and Dean of the Graduate School

(Original signatures are on file with official student records.)

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Interim Vice Provost and
Dean of The Graduate School

A CFD Laboratory Archive Supporting the Academic Process

A Thesis

Presented for the

Master of Science

Degree

The University of Tennessee, Knoxville

Shawn Ericson

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Abstract

The high level of complexity and non-linearity in modeling and simulation of fluid-thermal systems leads to uncertainty in the computational results. In response, the CFD technical community has developed a method of test involving verification, benchmark, and validation concepts to assist in assessing, hence understanding, the impact of error and uncertainty. As each computational model is unique, the use of validation and verification is paramount to obtaining credibility in solutions. Therefore it should be a key issue in the education process in computational fluid dynamics (CFD). A student taking CFD academic course work can benefit from an archive of associated computational results. Herein, these models include boundary layer flow, turbulence closure modeling, and applications to full Navier-Stokes statements. Of paramount importance are the issues of false diffusion, mass conservation, non-linear iteration technique, linear algebra, accuracy and asymptotic convergence. The starting point for each model is the incompressible flow Navier-Stokes equations.

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List of Symbols

A_j	kinetic flux vector jacobian
Ar	Archimedes number
c_p	specific heat
C_v, C_ε, C_k	model constants
E	wall rougness factor
E_{ij}	mean flow strain rate tensor
f_v, f_k, f_ε	Lam-Bremhorst viscosity, TKE and ε dissipations functions
f_j, f_j^v	kinematic and dissipative flux vector
g_i	gravity acceleration unit vector
Gr	Grashoff Number
i,j,k	spatial direction subscript
JAC	jacobian matrix
k	turbulent kinetic energy
k_+	log-law region turbulent kinetic energy
k_c	thermal conductivity
L	a length scale
M	mass matrix
n	time step variable
$\mathbf{n}_i$	boundary outward pointing normal
N_k	trial space basis function
P	kinematic pressure (p/ρ)
p	iteration variable
Pa	dissipative parameter
Pe	Peclet Number
Pr, Pr^t	laminar and turbulent Prandtl Number

q	state variable
Q_α	state variable approximation coefficients
Re, Re^t	laminar and turbulent Reynolds number
RES	descretized residual
R_y, Re_T	Lam-Bremhorst Reynolds numbers
s	general source term
s_θ	non-dimensionalized energy source term
T	temperature
u_τ	shear velocity
u,v,w	velocity resolution scalar components for u_i, $(1 \le i \le 3)$.
u^+	log-law region velocity
y^+	log-law region distance from wall

Greek Symbols

$\alpha, \beta, \gamma, \mu$	TWS formulation linear combination coefficients
β_o	Coefficient of thermal expansion
δ_{ij}	Kronecker delta
ε	isotropic dissipation
ε_+	log-law region isotropic dissipation
ϕ	pressure correction potential function
Φ_α	test function
κ	Karman constant
μ_o	viscosity
ν, ν^t	kinematic and turbulent viscosity
Θ	potential temperature
θ	implicitness

ρ	density
ω	vorticity function
Ψ	3-D stream vector
ψ	k scalar component of Ψ
Ψ_α	trial function

Chapter 1. Introduction

The high level of complexity and non-linearity in modeling and simulation of fluid-thermal systems leads to uncertainty in the computational results. In response, the CFD technical community has developed a test method involving verification ,benchmark, and validation concepts to assist in assessing, hence understanding, the impact of error and uncertainty.

Modeling and simulation can be viewed as the combination of three phases: the conceptual model, the computerized model, and reality [1]. Verification precisely assesses the conceptual model by comparing the computational solution to an exact analytical solution. This facilitates incisive characterization of computational error mechanisms such as spatial and temporal discretization error, iterative convergence error and programming error. Mesh and temporal refinement studies are components of a verification study.

Benchmark testing involves the comparison of the CFD solution to "other numerical solutions of 'accepted known accuracy'" [2]. Benchmark computational solutions always involve non-linearity and have proven through history to have consistent results.

Validation involves comparison of the computerized model to reality. The endpoint of validation compares a computational solution to experimental data. A well stated difference between verification and validation is , "verification provides evidence that the model is solved right" and "validation ... provides evidence that the right model is solved"[1].

As a point of interest, note that verification, benchmark, and validation do not provide an absolute measure of error in a computational or conceptual model, but rather "should be viewed as historical statements, i.e., reproducible evidence that a model has achieved a given level of accuracy in the solution of specified problems"[1].

As each computational model is unique, the use of validation and verification is paramount to obtaining credibility in solutions. Therefore it should be a key issue in the education process of computational fluid dynamics (CFD). A student taking CFD academic course work can benefit from an archive of verification and validation models. These models should include, at the least, boundary layer flow, turbulence closure modeling, and thermal convection for Navier-Stokes statements. Of paramount importance are the issues of false diffusion, mass conservation, non-linear iteration technique, linear algebra, accuracy and asymptotic convergence. The starting point for each model is the incompressible flow Navier-Stokes equations.

Chapter 2. Fluid-Thermal Systems Statement

2.1 - The Navier-Stokes Equation System

The differential equation system characterizing fluid-thermal systems analysis stems from the transformation to the Eulerian viewpoint of the conservation principles of mass, momentum, and energy. The general forms for flows at vanishingly small Mach number, i.e. incomressible, is

$$\frac{\partial u_i}{\partial x_j} = 0 \qquad \text{continuity}$$

$$\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} + \frac{1}{\rho}\frac{\partial p}{\partial x_i} - \nu \frac{\partial^2 u_i}{\partial x_j^2} + \beta_o (T - T_o) g_i = 0 \qquad \text{momentum}$$

$$\frac{\partial T}{\partial t} + u_j \frac{\partial T}{\partial x_j} - \left(\frac{k_c}{\rho c_p}\right) \frac{\partial^2 T}{\partial x_j^2} - s_\theta = 0 \qquad \text{energy}$$

Note: constant properties assumption is consistent with low Mach number flow, for which the energy source due to viscous dissipation is negligible ($\Phi = 0$). Further, the Boussinesq approximation has been made for bouyancy body force.

For non-dimensionalization the following variables and parameters are defined,

u, v, w = velocity resolution scalar components for u_i, $(1 \leq i \leq 3)$
P = kinematic pressure (p/ρ_o)
Θ = potential temperature
g_i = gravity acceleration unit vector
s_θ = non-dimensionalized energy source term (if present)
ρ_o = reference density
ν_o = reference kinematic viscosity
L = a length scale
$Re = UL/\nu$
$Gr = g\beta L^3 \Delta T/\nu$
$Pe = \rho c_p UL/k_c = RePr$

The non-dimensionalized continuity, momentum, and energy equation set, commonly termed the Navier-Stokes equations, takes the form,

$$\frac{\partial u_j}{\partial x_j} = 0 \qquad \text{continuity}$$

$$\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} + \frac{\partial P}{\partial x_i} - \frac{1}{Re}\frac{\partial^2 u_i}{\partial x_j^2} + \frac{Gr}{Re^2}\Theta g_i = 0 \qquad \text{momentum}$$

$$\frac{\partial \Theta}{\partial t} + u_j \frac{\partial \Theta}{\partial x_j} - \frac{1}{Pe}\frac{\partial^2 \Theta}{\partial x_j^2} - s_\theta = 0 \qquad \text{energy}$$

The apparent similarity between the momentum and energy equations, which will extend to turbulence closure models, allows a general form for the conservation law system as,

$$\frac{\partial q}{\partial t} + \frac{\partial}{\partial x_j}(f_j - f^v_j) - s = 0$$

where $f_j = f_j(u_j,q,P)$ is the kinetic flux vector and $f^v_j = \frac{1}{Pa}\frac{\partial q}{\partial x_j}$ is the dissipative flux vector.

Here, q is the state variable $q(x,t) = \{u,v,w,\Theta,k,\varepsilon,...\}$ and Pa is the associated q-dependent non-D parameter, e.g. Re, Pe. Continuity must still be satisfied while suitable boundary and initial conditions are required for a well posed problem statement.

2.2 - Conservation of Mass

2.2.1 - Introduction

An absolutely key issue in conceptualizing an incompressible Navier-Stokes (INS) solution algorithm is enforcing the constraint of conserving mass. There exist several approaches, with applicability dependent on the distinct flow-geometry situations.

2.2.2 - A Taylor Series on V

For 2-D (or 3-D) incompressible laminar and/or turbulent steady boundary layer flow, Reynolds ordering confirms that the y-momentum equation yields that pressure is a function only of the x coordinate spanning the dominant flow direction. This leaves the x-momentum and energy equations to solve as initial value problems in x and boundary value in y. The resultant construction to conserve mass is the direct solution for v via initial-value integration of the continuity equation in the y-direction. The appropriate Taylor series is,

$$V_{j+1} = V_j + \Delta y \left.\frac{\partial v}{\partial y}\right|_{j+1/2} + O(\Delta y^3)$$

where Δy = length of the finite element (l_e) and the gradient is evaluated at the midpoint to maintain 2nd order accuracy. From the continuity equation,

$$\frac{\partial v}{\partial y} = -\frac{\partial u}{\partial x}.$$

Substituting into the Taylor series, $V_{j+1} = V_j - l_e \left.\frac{\partial u}{\partial x}\right|_{j+1/2} + O(\Delta y^3)$

The gradient $\partial u/\partial x$ evaluated at $j + 1/2$ constitutes data which has to be formed from the u-momentum solution. In the discretized implementation, the u velocity gradient is represented as $(UP_{j+1} + UP_j)/2$, where UP denotes "u prime". It is evaluated at $j+1/2$ by averaging the nodal values at j and $j + 1$. The nodal values of UP are determined via a second order accurate finite difference recursion on x.

2.2.3 - Dependent Variable Transformation

For incompressible flows, $\nabla \bullet \mathbf{u} = 0$ guarantees that $\mathbf{u} = \nabla \times \Psi$ where Ψ is the (3-D) stream vector. Simplifying to two-dimensional flows, $\mathbf{u} = \nabla \times \psi \mathbf{k}$, hence only the **k** scalar component of Ψ is required. Taking the curl of the momentum equation eliminates pressure and yields the vorticity transport equation for the **k** component, $\omega = \nabla \times \mathbf{u} \bullet \mathbf{k}$.

Then,

$$\nabla \times L(u_i) = L(\omega) = \frac{\partial \omega}{\partial t} + \nabla \times \psi \mathbf{k} \bullet \nabla \omega - \frac{1}{Re} \nabla^2 \omega + \frac{Gr}{Re^2} \nabla \times \Theta \mathbf{g} = 0 \qquad \text{(vorticity transport)}$$

The resultant vorticity-streamfunction Navier-Stokes conservation law form is completed via the kinematic definitions yielding $L(\psi) = -\nabla^2 \psi - \omega = 0$.

2.2.4 - Iterative Approximation

An approximate way to conserve mass employs an iterative strategy [2]. The legacy construction begins with an explicit time Taylor series on the velocity vector u_i. But the Taylor series does not enforce the divergence freeness of the velocity vector. So an approximated velocity, u_i^*, is assumed and an explicit time Taylor series is written for it as well. Taking the difference defines the error as [2],

$$u_i^{n+1} - u_i^* = \Delta t \left(\frac{\partial u_i}{\partial t} - \frac{\partial u_i^*}{\partial t} \right) + \frac{\Delta t^2}{2} \left(\frac{\partial^2 u_i}{\partial t^2} - \frac{\partial^2 u_i^*}{\partial t^2} \right) + O(\Delta t^3)$$

$$= \Delta t\left(\frac{\partial P}{\partial x_i} - \frac{\partial P^*}{\partial x_j}\right) + \frac{\Delta t^2}{2}\frac{\partial}{\partial x_i}\left(\frac{\partial P}{\partial t} - \frac{\partial P^*}{\partial t}\right) + O(\Delta t^3)$$

noting that the velocity at the previous time is identical to the approximation, $u_i^n = u_i^*$ at any time t_n. Since the pressure field is independent of time in an incompressible fluid (changes in pressure occur instantaneously), and the curl of the pressure gradient vanishes, the difference between (any) computed and the exact velocity is curl free. Therefore, this difference can be precisely represented as the gradient of a scalar potential, i.e. $u_i^{n+1} - u_i^* = \partial\phi/\partial x_i$.

The fundamental problem with this formulation is that pressure changes occur instantaneously, which is not recognized in the explicit Taylor series. Therefore an implicit algorithm formulation is required. Following the above procedure for θ - time integration including turbulence and the bouyancy body force, the velocity field error is [2],

$$u_i^{n+1} - u_i^n = -\theta\Delta t\left(\frac{\partial(u_i u_j)}{\partial x_j} - \frac{\partial}{\partial x_j}\left(\frac{1+Re^t}{Re}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)\right) + \frac{\partial P}{\partial x_i} + Ar\,\Theta g_i\right)^{n+1}$$

$$-(1-\theta)\,\Delta t\left(\frac{\partial(u_i u_j)}{\partial x_j} - \frac{\partial}{\partial x_j}\left(\frac{1+Re^t}{Re}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)\right) + \frac{\partial P}{\partial x_i} + Ar\,\Theta g_i\right)^{n} + H.O.T.$$

which can no longer be related to a potential function because $\mathrm{curl}(u_i^{n+1} - u_i^n) \neq 0$.

The necessary correction is an implicit iterative procedure. Assuming that at convergence the p+1 iterate approximates the correct velocity, the error can again be related to a potential function,

$$(u_i^* - u_i)\Big|_{n+1}^{p+1} = \frac{-\partial\phi}{\partial x_i}\Big|_{n+1}^{p+1}$$

Substituting this into the implicit Taylor series and neglecting 2nd order and higher derivatives, and noting that the bouyancy term scales the expression by a constant, then

$$P\Big|_{n+1}^{p} = P^*\Big|_{n+1}^{p} + \frac{1}{\theta\Delta t}\,\phi\Big|_{n+1}^{p+1}$$

But this has two implementation flaws. First the iteration index of ϕ at p+1 and pressure at p are backwards. In addition, the exact pressure at iterate p is not known. So a computable strategy is required as detailed in [2]. The action of the pressure at time n+1 is calculated assuming the pressure at time n is known, modified by the accumulation of ϕ over the iterations at t_{n+1} as,

$$P^*\Big|_{n+1}^{p} = P_n + \frac{1}{\theta\Delta t}\,\Sigma\phi^{\alpha+1}\Big|_{n+1} \qquad \text{for } 0 \le \alpha \le p$$

Since ϕ is known following each iteration, then the kinematic action of the pressure can be approximately enforced at time n+1 via P*.

Forming the divergence of the potential definition provides the appropriate differential equation. Noting that the divergence of the correct solution is zero, then, $L(\phi) = \nabla^2\phi + \nabla \bullet u^* = 0$. The Neumann boundary condtion is given by $(u_i^{n+1} - u_i^*)\mathbf{n}_i = (\partial\phi/\partial x_i)\,\mathbf{n}_i$.

2.3 - Pressure

The several ways to enforce the continuity constraint have been identified. For 2-D boundary layer flow, dP/dx becomes known data, the simplest enforcement.

In the vorticity-streamfunction formulation the pressure term was eliminated by virtue of the momentum equation curl operation. A post-processing determination of pressure accrues to forming the divergence of the laminar flow momentum equation. Doing so produces the Poisson equation [2],

$$L(p) = \frac{1}{\rho}\nabla^2 p - \frac{\partial u_i}{\partial x_j}\frac{\partial u_j}{\partial x_i} - \frac{Gr}{Re^2}\frac{\partial\Theta\delta_{gj}}{\partial x_j} = 0$$

where the velocity components and temperature distributions are known data since this is a post-process.

This "pressure Poisson" equation becomes well posed upon determination of the enclosing boundary conditions. This is found by dotting the momentum equation with the unit normal. For steady flow, with no slip at the wall and significantly large Reynolds number, the pressure gradient on a viscous wall boundary is vanishingly small. Conversely, at a through flow boundary, a Neumann -type boundary integral must be evaluated.

Note that the "pressure action" calculation using the summation of phi is just a computational mechanism for approximating the kinematic effect of pressure. This does not represent the genuine pressure. Pressure for the phi algorithm is post-processed as in the omega-psi algorithm, except it must be computed at each time step.

2.4 - Turbulence Closure Models

Creating a model for turbulence in the momentum equation introduces the Reynolds stress tensor $(\overline{u_i u_j})$, the time- or volume-averaged product of velocity component fluctuations. The addition of this unknown requires a defining equation.

For Reynolds averaged 2-D incompressible boundary layer flow, Reynolds ordering determines the sole significant term is the Reynolds shear stress $\overline{u'v'}$. Mixing length theory (MLT) assumes this term is proportional to the mean flow strain rate, i.e. $\overline{u'v'} \equiv - \nu^t \, \partial u/\partial y$. Here the turbulent eddy viscosity, ν^t, is a property of the flow, as opposed to the kinematic viscosity, $\nu = \mu_o/\rho$, which is a property of the fluid. Two constituitive models for the calculation of ν^t form "CFD standards".

2.4.1 - Mixing Length Theory (MLT)

The turbulent eddy viscosity is defined via introduction of a "mixing length, l_m", and a time scale, yielding $\nu^t \equiv (\omega l_m)^2 |\partial u/\partial y|$. The correction for the original MLT model very close to the wall is the van Driest damping function, $\omega \equiv 1 - e^{-y/A}$ [4]. The mixing length is defined over the boundary layer, δ, as

$$l_m \equiv \begin{cases} \kappa y & 0 \le y \le \lambda\delta/\kappa \\ \lambda\delta & y > \lambda\delta/\kappa \end{cases} \quad [3].$$

where $\kappa = 0.435$is the Karman constant and $\lambda = 0.09$.

2.4.2 - Turbulent Kinetic Energy (TKE)

The definition of eddy viscosity in the TKE closure model is $\nu^t \equiv C_\nu k^2/\varepsilon$. The turbulent kinetic energy is defined as $k \equiv (\overline{u'u'} + \overline{v'v'} + \overline{w'w'})/2$, and the isotropic dissipation function definition is ,

$$\varepsilon = \nu \overline{\frac{\partial u_i}{\partial x_j} \frac{\partial u_i}{\partial x_j}}.$$

For 2-D boundary layer flow, the additional differential equations required for closure are then [3, pp178-180],

$$L(k) = u\frac{\partial k}{\partial x} + v\frac{\partial k}{\partial y} - \frac{\partial}{\partial y}\left(\frac{\nu^t}{C_\nu}\frac{\partial k}{\partial y}\right) - \nu^t\left(\frac{\partial u}{\partial y}\right)^2 + \varepsilon = 0$$

$$L(\varepsilon) = u\frac{\partial \varepsilon}{\partial x} + v\frac{\partial \varepsilon}{\partial y} - \frac{\partial}{\partial y}\left(\frac{\nu^t}{C_\varepsilon}\frac{\partial \varepsilon}{\partial y}\right) - C_\varepsilon \varepsilon k^{-1} \nu^t \left(\frac{\partial u}{\partial y}\right)^2 + C_\varepsilon^2 \varepsilon^2 k^{-1} = 0$$

where all variables are Reynolds averaged. These 2 parabolic equations each require 2 boundary conditions in y and an initial condition in x. At the surface [3, p180],

$$u(x,0) = v(x,0) = 0$$
$$k(x,0) = 0$$

and ε takes on a large value.

Vanishing derivatives $\frac{\partial u}{\partial y} = \frac{\partial k}{\partial y} = \frac{\partial \varepsilon}{\partial y} = 0$ are the appropriate freestream definition.

Like MLT theory, problems arise near the wall where k vanishes and the dissipation increases to "infinity". Lam and Bremhorst [11] developed a low turbulence Reynolds number model that addresses this issue. Turbulent viscosity and the kinetic energy and isotropic dissipation equation source terms are damped as a function of select Reynolds numbers as

$$f_v = (1 - e^{-0.165R_y})^2 (1 + 20.5/Re_T)$$

$$f_k = 1 + (0.05/f_v)^3$$

and $f_\varepsilon = 1 - e^{-2Re_T}$

where R_y and Re_T are a Reynolds numbers based on distance (y) from the wall.

2.4.3 - TKE Closure for Full Navier-Stokes

Chapter 2.1 introduced the generalized differential equation for incompressible Navier-Stokes as,

$$L(q) = \frac{\partial q}{\partial t} + \frac{\partial}{\partial x_j}(f_j - f^v_j) - s = 0 \quad \text{for} \quad q = \{u, v, w, \Theta, k, \varepsilon, ...\}.$$

Closure for the full Reynolds-averaged Navier-Stokes equations [6, Ch. 28] for turbulent flow is,

$$f^v_j = \left\{ \begin{array}{l} \frac{1}{Re}(1 + Re^t)\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3}\frac{\partial u_k}{\partial x_k}\delta_{ij}\right) - \frac{1}{3}k\delta_{ij} \\ \frac{1}{Re}\left(\frac{Re}{Pr} + \frac{Re^t}{Pr^t}\right)\frac{\partial \Theta}{\partial x_j} \\ \frac{1}{Re}\left(1 + \frac{Re^t}{C_k}\right)\frac{\partial k}{\partial x_j} \\ \frac{1}{Re}\left(1 + \frac{Re^t}{C_\varepsilon}\right)\frac{\partial \varepsilon}{\partial x_j} \end{array} \right\}, \quad s = \left\{ \begin{array}{l} \frac{Gr}{Re^2}\Theta \bar{g}_i \\ s_\theta \\ -\nu^t E_{ij}\frac{\partial u_i}{\partial x_j} + \varepsilon \\ -C_\varepsilon^1 \frac{\varepsilon}{\kappa} \nu^t E_{ij}\frac{\partial u_i}{\partial x_j} + C_\varepsilon^2 \frac{\varepsilon}{\kappa}\varepsilon \end{array} \right\}$$

where $E_{ij} \equiv (\partial u_i/\partial x_j + \partial u_j/\partial x_i)$ is the mean flow strain rate tensor.

The wall boundary conditions for full NS turbulent flow simulations typically replaces the meshing demands of a low Re^t closure model with the "law-of-the-wall" turbulent boundary layer correlation (Cole's law). In local similarity variables, Cole's law is $u^+ = \ln(y^+E)/\kappa$ + constant, which is valid in the "log-law" region $50 < y^+ < 1200$. The parameter E is the wall roughness factor and κ is the Karman constant. Here, $y^+ = u_\tau y/\nu$ is a Reynolds number, u_τ is the shear velocity, and $u^+ \equiv \bar{u}/u_\tau$, hence the equation is non-linear. Local ordering of the source terms in the TKE PDE leads to $k_+ = u_\tau^2/\sqrt{C_\nu}$, $\varepsilon_+ = |u_\tau|^3/\kappa y$, and $\nu^t = \kappa y u_\tau$, which provide BCs for the TKE closure model at the first node off the wall. Typically, k and ε profiles are fixed at the inflow, and are assumed to have vanishing derivatives at outflow, which yields the required well-posed EBV problem.

Chapter 3. The Weak Form and Linear Algebra

3.1 - The Galerkin Weak Statement

The extremum of the mathematicians weak form is the weak statement which generalizes the predecessor, Method of Weighted Residuals, discrete process by requiring the state variable approximation to be orthogonal to the test function set in the continuum. The developed Navier-Stokes equations are in the generalized form,

$$\frac{\partial u_i}{\partial x_j} = 0$$

$$\frac{\partial q}{\partial t} + u_j\frac{\partial q}{\partial x_j} - \frac{\partial f_j^v}{\partial x_j} - s(q) = 0$$ where the state variable $q = \{u, v, \omega, \Theta, k, \varepsilon, \psi, \phi, P, \ldots\}$.

Assume the solution, q, can be approximated and call it q^N. The weak statement formulation requires identification of the trial function (set) $\Psi_\alpha(\mathbf{x})$ supporting q^N. The specific form for the approximation is typically $q^N(\mathbf{x},t) \equiv \Sigma\Psi_\alpha(\mathbf{x})Q_\alpha(t)$, where $\Psi_\alpha(\mathbf{x})$ is the set of trial functions implementing the choice of spatial interpolation. Q_α is then the time-dependent set of coefficients to be determined (numerically) for the approximation.

The weak statement requires the available measure of the error in q^N be made orthogonal to a set of test functions, i.e. $WS = \int_\Omega \Phi_\beta L(q^N)d\tau \equiv 0$, where $\Phi_\beta(\mathbf{x})$ is the test function set. Utilizing the Green-Gauss form of the divergence theorem on the dissipative flux vector term yields

$$WS = \int_\Omega \Phi_\beta\left(\frac{\partial q}{\partial t} + u_j\frac{\partial q}{\partial x_j} - \frac{\partial f_j^v}{\partial x_j} + s(q)\ d\tau\right) = 0$$

$$= \int_\Omega\left(\Phi_\beta \frac{\partial q^N}{\partial t} + \Phi_\beta u_j\frac{\partial q^N}{\partial x_j} + \frac{\partial \Phi_\beta}{\partial x_j} f_j^v - \Phi_\beta s(q^N)\right)d\tau - \int_\sigma \Phi_\beta f_j^v n_j d\sigma = 0$$

The weak statement construction solution is optimally accurate (for linear elliptic boundary value problems) upon selection of the Galerkin criteria, i.e., the test and trial function sets are identical, $\Phi_\alpha = \Psi_\alpha$. The finite element implementation then implements $\Psi_\alpha(\mathbf{x})$ via a set of trial space basis functions and on each element $q_e(\mathbf{x}) \equiv \{N_k\}^T\{Q\}_e$. Then, $q^N \equiv q^h = \cup_e q_e$, that is, the approximated solution is defined as the discretized solution constituted as the non-overlapping sum of solutions over all finite elements of the domain discretization. Substituting $q_e(\mathbf{x})$ the Galerkin Weak Statement (GWS) finite element implementation yields

$$GWS = \int_\Omega \left(\{N_k\}\frac{\partial\{Q\}}{\partial t}^T\{N_k\} + \{N_k\}u_j\frac{\partial\{N_k\}}{\partial x_j}^T\{Q\} + \frac{\partial\{N_k\}}{\partial x_j}(f_j^v)_e - \{N_k\}s_e \right) d\tau - \int_\sigma \{N_k\}(f_j^v)_e n_j\, d\sigma \equiv 0$$

and the state variable dependence in $(f_j^v)_e$ is implemented via q_e.

3.2 - The Taylor Weak Statement

The issue of stability is of primary concern when the physical diffusion level becomes very small, i.e. Pa >>1. To combat this problem an artificial diffusion mechanism has traditionally been introduced. It is now becoming recognized that this artificial diffusion may not be so artificial, but rather can recover to an extent accuracy that is lost in the discretizing process [5]. For this reason it will be called numerical diffusion herein.

To formulate the numerical diffusion term appropriate to L(q), recall the basic NS equation in terms of the kinetic and dissipative flux vectors, $\partial q/\partial t + \partial (f_j - f_j^v)/\partial x_j - s(q) = 0$, where the state variable $q = \{u, v, \Theta, k\ \varepsilon, ...\}$. The theoretical formulation neglects the stabilizing contribution from f_j^v and discards the source term. Then $\partial q/\partial t + A_j \partial q/\partial x_j = 0$ which identifies the kinetic flux vector jacobian $A_j = \partial f_j/\partial q$. Writing an explicit time Taylor series on q,

$$q^{n+1} = q^n + \Delta t\frac{\partial q}{\partial t} + \frac{\Delta t^2}{2}\frac{\partial^2 q}{\partial t^2} + \frac{\Delta t^3}{6}\frac{\partial^3 q}{\partial t^3} + \text{truncation error}$$

then substituting from the previous equation and recognizing $\partial q/\partial t = -\partial f_j/\partial x_j$,

$$q^{n+1} = q^n - \Delta t\left(\frac{\partial q}{\partial t}\right) - \frac{\Delta t^2}{2}\frac{\partial}{\partial t}\left(\frac{\partial f_j}{\partial x_j}\right) - \frac{\Delta t^3}{6}\frac{\partial^2}{\partial t^2}\left(\frac{\partial f_j}{\partial x_j}\right) + \text{truncation error}$$

Consider the 2nd order term

$$-\frac{\Delta t^2}{2}\frac{\partial}{\partial t}\frac{\partial f_j}{\partial x_j} = -\frac{\partial}{\partial x_j}\left(\frac{\partial f_j}{\partial q}\frac{\partial q}{\partial t}\right) = -\frac{\partial}{\partial x_j}\left(\frac{\partial f_j}{\partial q}\left(-\frac{\partial f_k}{\partial x_k}\right)\right) = -\frac{\partial}{\partial x_j}\left(\frac{\partial f_j}{\partial q}A_k\frac{\partial q}{\partial x_k}\right)$$

Choosing a linear combination yields,

$$\frac{\partial}{\partial x_j}\left(\alpha\frac{\partial f_j}{\partial q}\frac{\partial q}{\partial t} + \beta\frac{\partial f_j}{\partial q}\frac{\partial f_k}{\partial x_k}\right) = \frac{\partial}{\partial x_j}\left(A_j\left(\alpha\frac{\partial q}{\partial t} + \beta A_k\frac{\partial q}{\partial x_k}\right)\right)$$

Similarly for the 3rd order term,

$$\frac{\partial^2}{\partial t^2}\frac{\partial f_j}{\partial x_j} = \frac{\partial}{\partial x_j}\left(A_j\left(\frac{\partial}{\partial x_i}A_i\left(\gamma\frac{\partial q}{\partial t} + \mu A_k\frac{\partial q}{\partial x_k}\right)\right)\right)$$

Plugging these expressions back into the time Taylor series and taking the limit as $\Delta t \to \varepsilon > 0$, then keeping only the β term and returning to the full parent NS equation yields,

$$\frac{\partial q}{\partial t} + \frac{\partial}{\partial x_j}(f_j - f^v_j) - s - \frac{\beta\Delta t}{2}\frac{\partial}{\partial x_j}\left(A_jA_i\frac{\partial q}{\partial x_i}\right) = 0, \quad \text{where } A_jA_i \cong u_ju_i \text{ for INS.}$$

The Taylor-series modified equation then replaces the original NS equation in the weak statement with,

$$L^m(q) = L(q) - \frac{\partial}{\partial x_j}\left(\frac{\beta\Delta t}{2}u_ju_i\frac{\partial q}{\partial x_i}\right) = 0$$

For steady flow, the discrete time scale Δt has been locally expressed as $(h/|u|)_e$, where h_e is a measure of the mesh and $|u|_e$ is a local speed. Letting $B = \beta/2$, an alternate form for $L^m(q)$ is

$$L^m(q) = L(q) - Bh_e\frac{\partial}{\partial x_j}\left(u_j\mathbf{u}_i\frac{\partial q}{\partial x_j}\right) \quad \text{where } \mathbf{u}_i \text{ is the unit vector.}$$

The Galerkin WS written on $L^m(q)$ rather than $L(q)$ is termed the "Taylor Weak Statement (TWS)".

3.3 - Integration in Time

Since $q^N = \Sigma_\alpha \Psi_\alpha(\mathbf{x})Q_\alpha(t)$, hence the Q_α are a function of time only, any GWS or TWS construction produces the matrix ordinary differential equation system,

$$\text{TWS} = [M]\frac{\partial\{Q\}}{\partial t} + \{RES\} = \{0\}, \text{ where } \{RES\} \text{ contains all but the time term in } L^m(q).$$

The TWS thus provides the derivative for a Taylor series in time. Taking a linear combination of the implicit and explicit derivatives, $Q_{n+1} = Q_n + \Delta t\,(\theta Q'_{n+1} + (1-\theta)Q'_n) + \text{H.O.T.}$, where Q' is the first derivative of Q w.r.t. time and $0 \le \theta \le 1.0$. Then TWS + θTS yields $\{FQ\} = [M](\{Q\}_{n+1} - \{Q\}_n) + \Delta t(\theta\{RES\}_{n+1} + (1-\theta)\{RES\}_n) = 0$, a large order non-linear algebraic equation system.

3.4 - The Newton Statement, Approximations

Since few non-linear algebraic equation solutions are available, most practical non-linear systems require an iterative procedure. For $\{FQ\} = [M]\{Q^{n+1} - Q^{n}\} + \Delta t\{RES\}_{n+\theta} = \{0\}$ the Newton algorithm is, $[JAC]\{\delta Q\}^{p+1} = -\{FQ\}^{p}$, where p is at the iteration index and the jacobian definition is $[JAC] \equiv \partial\{FQ\}/\partial\{Q\}$. The iterate definition is $\{\delta Q\} = \{Q_{n+1}{}^{p+1} - Q_{n+1}{}^{p}\}$. For $\{Q\} = \{U,V,T\}$, say in the case of coupled 2-D momentum and energy, the Newton jacobian takes the form

$$[JAC] = \begin{bmatrix} JUU & JUV & JUT \\ JVU & JVV & JVT \\ JTU & JTV & JTT \end{bmatrix} \quad \text{, where } JUU = \partial F(U)/\partial U \text{, etc.}$$

A quasi-Newton jacobian is a simplified form of the Newton jacobian. For example, if the bouyancy body force in the momentum equation is small, then the 3 equations for u and v momentum and energy can be decoupled via the assumption that $JUT = JVT = JTU = JTV \approx 0$. The quasi-Newton iteration then employs

$$[JAC] = \begin{bmatrix} JUU & JUV & 0 \\ JVU & JVV & 0 \\ 0 & 0 & JTT \end{bmatrix}$$

which can be reduced to a 2x2 matrix statement with $[JTT]\{\delta T\}^{p+1} = -\{F(T)\}^{p}$ solved separately.

3.5 - Template Form

Implementation of a weak statement (GWS, TWS) via a finite element construction is assisted by a template form generalizing the "coding" process. The template object-oriented concept recognizes existence of six distinct data structure types as

WS $\Rightarrow$ (global scalar data) (element averaged data) (element distributed data) (metric data) (FE matrix) (variable or element data).

As an example consider the TWS for a steady problem using element-averaged velocity, a distributed source and vanishing derivatives on the boundary. The template form of the TWS on the generic element domain Ω_e is,

$$WS = (\,)(UI)(\,)(\eta_{ij})(M20J)(Q) + (Pa^{-1})(\,)(\,)(\eta_{ij}\eta_{ik};-1)(M2JK)(Q)$$

$$+ (B)(UIUJA)(\,)(\eta_{li}\eta_{mj};-1/n)(M2LM)(Q) - (\,)(\,)(\,)(1)(M200)(SRC),$$

where n is the problem dimension. The eta terms (η_{ij}) come from the differentiation of the finite element basis with respect to the element natural coordinate system. In 1 dimension this has historically been called zeta, in 2 or more dimensions the general expression is eta. By the chain rule, then, differentiation of the intrinsic coordinate with respect to the Cartesian global coordinates yields, in 2-dimensions,

$$\int_\Omega \frac{1}{Pa}\frac{\partial \Psi_\beta}{\partial x_i}\frac{\partial q^N}{\partial x_i}\,d\tau = \int_\Omega \frac{1}{Pa}\frac{\partial\{N\}}{\partial x_i}\frac{\partial\{N\}}{\partial x_i}\,d\tau\,\{Q\} = \int_\Omega \frac{1}{Pa\,DET^2}\frac{\partial\{N\}}{\partial \eta_j}\frac{\partial\{N\}}{\partial \eta_k}\left(\frac{\partial \eta_j}{\partial x_i}\frac{\partial \eta_k}{\partial x_i}\right)d\eta_e\,\{Q\}$$

$$= (Pa^{-1})(\,)(\,)(\eta_{ij}\eta_{ik};-1)(B2JK)(Q).$$

The FE matrices [M...] include the description of the action of derivatives of the bases. A convention has M becoming A, B or C for 1,2 or 3-dimensions, respectively. The M20J is a matrix formed by 2 bases with the second differentiated once. Likewise, M2JK is a matrix with both bases differentiated once. The first derivative of a basis contains a measure of the element in the denominator, e.g. l_e^{-1} in 1-D. Integrating two first derivatives over the domain leaves l_e^{-1}. Hence the -1 with the diffusion term of the template in 1-D. A one-dimensional unsteady Taylor weak statement for the example is then,

$$TWS + \theta TS = (\,)(\,)(\,)(0;1)(A200)(Q_{n+1}-Q_n)$$

$$+ (\theta,\Delta t)(U1)(\,)(1;0)(A201)(Q_{n+1}) + (1-\theta,\Delta t)(U1)(\,)(1;0)(A201)(Q_n)$$

$$+ (\theta,\Delta t,Pa^{-1})(\,)(\,)(11;-1)(A211)(Q_{n+1}) + (1-\theta,\Delta t,Pa^{-1})(\,)(\,)(11;-1)(A211)(Q_n)$$

$$+ (\theta,\Delta t,B)(U1U1A)(\,)(11;0)(A211)(Q_{n+1}) + (1-\theta,\Delta t,B)(U1U1A)(\,)(11;0)(A211)(Q_n)$$

$$+ (\Delta t)(\,)(\,)(0;1)(A200)(SRC).$$

Chapter 4. Verification, Benchmark, and Validation Archive

This verification, benchmark and validation archive leads the student through a staged exposure to CFD. Following is a list of the model INS problems (see compact disc in Appendix) that aid in defining and comprehending the solution process in CFD for these, and related, simulations.

- A Navier-Stokes Problem
- Axisymmetric Heat Conduction with Convection
- Two-Dimensional Boundary Layer Flow
- Two-Dimensional Driven Cavity
- Thermal Cavity, Omega-Psi Algorithm
- Thermal Cavity, Pressure Projection
- Laminar and Turbulent Duct Flow
- Linear Convection-Diffusion, Stability

The archive begins with a representative student-generated Navier-Stokes class problem to give the reader a practical example by describing some possible assumptions and complications associated with it.

For the 1-dimensional unsteady axisymmetric heat conduction problem, the energy equation only is addressed. The key point addressed is that non-smooth data can produce solution oscillations on inadequate discretizations. Mesh adaption resolves this and time stepping (truncation error) must be considered as well. Time implicitness and the finite volume algorithm comparison complete the exercise.

Two-dimensional steady boundary layer flow is a classical fluid mechanics class. It exemplifies approaches to continuity satisfaction and turbulence closure modeling. Mesh refinement performance confirms asymptotic convergence theory and two turbulence models are introduced and implemented. For laminar flow, an exact solution for flat plate BL flow is available via the Blasius similarity solution.

The transformed variable approach for rigorous mass conservation is illustrated via the two-dimensional isothermal driven cavity benchmark. Vorticity and the stream function are defined which automatically conserves mass and handles pressure in a elegant manner. The driven cavity has boundary condition singularities that produce large local gradients. As the Reynolds number increases it becomes more difficult to produce a smooth solution. Mesh refinement techniques, estimates of "the best mesh" and numerical diffusion are thus introduced.

The thermal cavity benchmark introduces the bouyancy body force into the momentum equation. Temperature becomes the driving force via natural convection rather than an imposed velocity. The thermal cavity is devoid of boundary singularities, though complications still arise as the diffusion coefficient is decreased. Then, as before, the implications of mesh refinement are examined. With the momentum and energy equation coupled, Newton and quasi-Newton iteration introduces analysis of linear algebra versus computer speed performance.

The thermal cavity is re-examined using an approximate method of mass conservation. Performance of the iterative pressure projection method is compared to the variable transformation algorithm. Mass is conserved via a potential, introducing new variables, i.e., phi and sum-phi. The action of this correction and the interplay between phi, sum-phi and pressure are examined, along with stability and various quasi-Newton jacobian iteration performances.

A 2-D laminar duct flow simulation gives an opportunity to study the action of phi and sum phi given inflow and outflow boundary conditions. The ability to conserve mass in laminar versus turbulent flow is established and stability issues prove the need for numerical diffusion. The turbulent duct flow problem uses a "law-of-the-wall" model since detail close to the wall requires excessive meshing.

The 1-D steady Peclet problem is a good model for testing stability and monotonicity where the exact solution is known. Stabiliy is tested by altering mesh resolution in the vicinity of the sharp break in conjunction with numerical diffusion for various values of the genuine diffusion coefficient, Peclet.

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Appendix

See attached CD ROM for Appendix material.

The CD in the Appendix is the Laboratory archive, intended for use in a web based course. This CD is best viewed on a pc with a 17" monitor in a Netscape web browser, though other browsers should work adequately. Simply insert the CD in the CD ROM drive and wait. If the main page does not load automatically it can be opened via a file manager. The main page is in the root CD directory and is named "index.html".

Vita

Shawn Ericson was born in Quantico, Virginia in 1969. After graduating from Tennessee Technological University in 1993 he worked for MagneTek, Gordonsville, a division of Century Electric in Gordonsville, Tennessee. Later, as a Product Engineer at Howmet Casting Support, in Morristown, Tennessee, he discovered a desire to study computational fluid dynamics, which brought him to the University of Tennessee in 1999.