Optimal MODIFIED CONTINUOUS Galerkin CFD
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Professor Emeritus
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Yogi Berra is quoted,
“If you come to a fork in the road take it.”
With Mary Ellen’s agreement,
following this guidance
I found myself at the
dawning of weak form CFD
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Preface

Fluid dynamics, with heat/mass transport, is the engineering sciences discipline wherein explicit nonlinearity fundamentally challenges analytical theorization. Prior to digital computer emergence, hence computational fluid dynamics (CFD), the subject of this text, the regularly revised monograph Boundary Layer Theory, Schlichting (1951, 1955, 1960, 1968, 1979) archived Navier–Stokes (NS) knowledge analytical progress. Updates focused on advances in characterizing turbulence, the continuum phenomenon permeating genuine fluid dynamics. The classic companion for NS simplified to the hyperbolic form, which omits viscous-turbulent phenomena while admitting non-smooth solutions, is Courant et al. (1928).

The analytical subject of CFD is rigorously addressed herein via what has matured as optimal modified continuous Galerkin weak form theory. The predecessor burst onto the CFD scene in the early 1970s disguised as the weighted-residuals finite element (FE) alternative to finite difference (FD) CFD. Weighted-residuals obvious connections to variational calculus prompted mathematical formalization, whence emerged continuum weak form theory. It is this theory, discretely implemented, herein validated precisely pertinent to nonlinear(!) NS, and time averaged and space filtered alternatives, elliptic boundary value (EBV) partial differential equation (PDE) systems.

Pioneering weighted-residuals CFD solutions proved reasonable compared with expectation and comparative data. Reasonable was soon replaced with rigor, first via laminar and turbulent boundary layer (BL) a posteriori data which validated linear weak form theory-predicted optimal performance within the discrete peer group, Soliman and Baker (1981a,b). Thus matured NS weak form theorization in continuum form, whence discrete implementation became a post-theory decision. As thoroughly detailed herein, the FE trial space basis choice is validated optimal in classic and weak form theory-identified norms. Further, this decision uniquely retains calculus and vector field theory supporting computable form generation precision.

Text focus is derivation and thorough quantitative assessment of optimal modified continuous Galerkin CFD algorithms for incompressible laminar-thermal NS plus the manipulations for turbulent and transitional flow prediction. Optimality accrues to continuum alteration of classic text NS PDE statements via rigorously derived nonlinear differential terms. Referenced as modified PDE (mPDE) theory, wide ranging a posteriori data quantitatively validate the theory-generated dispersive/anti-dispersive operands annihilate significant order discrete approximation error in space and time, leading to monotone solution prediction without an artificial diffusion operator.
Weak formulations in the computational engineering sciences, especially fluid dynamics, have a storied history of international contributions. Your author’s early 1970s participation culminated in leaving the Bell Aerospace principal research scientist position in 1975 to initiate the University of Tennessee (UT) Engineering Science graduate program focusing in weak form CFD. UT CFD Laboratory, formed in 1982, fostered collaboration among aerospace research technical colleagues, graduate students, commercial industry and the UT Joint Institute for Computational Science (JICS), upon its founding in 1993.

As successor to the 1983 text *Finite Element Computational Fluid Mechanics*, this book organizes the ensuing three decades of research generating theory advances leading to rigorous, efficient, optimal performance Galerkin CFD algorithm identification. The book is organized into 10 chapters, Chapter 1 introducing the subject content in perspective with an historical overview. Since postgraduate level mathematics are involved, Chapter 2 provides pertinent subject content overview to assist the reader in gaining the appropriate analytical dexterity. Chapters 3 and 4 document weak interaction aerodynamics, the union of potential flow NS with Reynolds-ordered BL theory, laminar and time averaged turbulent, with extension to parabolic NS (PNS) with PNS-ordered full Reynolds stress tensor algebraic closure. Linearity of the potential EBV enables a thoroughly formal derivation of continuum weak form theory via bilinear forms. Content concludes with optimal algorithm identification with an isentropic (weak) shock validation. An Appendix extends the theory to a Reynolds-ordered turbulent hypersonic shock layer aerothermodynamics formulation (PRaNS).

Chapter 5 presents a thorough derivation of mPDE theory generating the weak form optimal performance modified Galerkin algorithm, in time for linear through cubic trial space bases, and in space for optimally efficient linear basis. Theory assertion of optimality within the discrete peer group is quantitatively verified/validated. Chapter 6 validates the algorithm for laminar-thermal NS PDE system arranged to well-posed using vector field theory. Chapter 7 complements content with algorithm validation for the classic state variable laminar-thermal NS system, rendered well-posed via pressure projection theory with a genuine pressure weak formulation pertinent to multiply-connected domains. Content derives/validates a Galerkin theory for radiosity theory replacing Stephan–Boltzmann, also an ALE algorithm for thermo-solid-fluid interaction with melting and solidification.

Chapter 8 directly extends Chapter 7 content to time averaged NS (RaNS) for single Reynolds stress tensor closure models, standard deviatoric and full Reynolds stress model (RSM). Chapter 9 addresses space filtered NS (LES) with focus the Reynolds stress quadruple formally generated by filtering. Manipulations rendering RaNS and LES EBV statements identical lead to closure summary via subgrid stress (SGS) tensor modeling. The alternative completely model-free closure (arLES) for the full tensor quadruple is derived via union of rational LES (RLES) and mPDE theories. Thus is generated an $O(1, \delta^2, \delta^3)$ member state variable for gaussian filter uniform measure $\delta$ a priori defining unresolved scale threshold. Extended to bounded domains, arLES EBV system including boundary convolution error (BCE) integrals is rendered well-posed via derivation of non-homogeneous Dirichlet BCs for the complete state variable. The arLES theory is validated applicable $\forall \text{Re}$, generates $\delta$-ordered resolved-unresolved scale diagnostic a posteriori data, and confirms model-free prediction of laminar-turbulent wall attached resolved scale velocity transition.

Chapter 10 collates text content under the US National Academy of Sciences (NAS) large scale computing identification “Verification, Validation, Uncertainly Quantification”
Observed in context is replacement of legacy CFD algorithm numerical diffusion formulations with proven mPDE operand superior performance. More fundamental is the ∀Re model-free arLES theory specific responses to NAS-cited requirements:

- error quantification
- a posteriori error estimation
- error bounding
- spectral content accuracy extremization
- phase selective dispersion error annihilation
- monotone solution generation
- error extremization optimal mesh quantification
- mesh resolution inadequacy measure
- efficient optimal radiosity theory with error bound

which in summary address in completeness VVUQ.

Your author must acknowledge that the content of this text is the result of collaborative activities conducted over three decades under the umbrella of the UT CFD Lab, especially that resulting from PhD research. Content herein is originally published in the dissertations of Doctors Soliman (1978), Kim (1987), Noronha (1988), Iannelli (1991), Freels (1992), Williams (1993), Roy (1994), Wong (1995), Zhang (1995), Chaffin (1997), Kolesnikov (2000), Barton (2000), Chambers (2000), Grubert (2006), Sahu (2006) and Sekachev (2013), the last one completed in the third year of my retirement. During 1977–2006 the UT CFD Lab research code enabling weak form theorization transition to a posteriori data generation was the brainchild of Mr Joe Orzechowski, the maturation of a CFD technical association initiated in 1971 at Bell Aerospace. The unsteady fully 3-D a posteriori data validating arLES theory was generated using the open source, massively parallel PICMSS (Parallel Interoperable Computational Mechanics Systems Simulator) platform, a CFD Lab collaborative development led by Dr Kwai Wong, Research Scientist at JICS.

Teams get the job done – this text is proof positive.

A. J. Baker
Knoxville, TN
November 2013
About the Author

A. J. Baker, PhD, PE, left commercial aerospace research to join The University of Tennessee College of Engineering in 1975, with the goal to initiate a graduate academic research program in the exciting new field of CFD. Now Professor Emeritus and Director Emeritus of the University’s CFD Laboratory (http://cfdlab.utk.edu), his professional career started in 1958 as a mechanical engineer with Union Carbide Corp. He departed after five years to enter graduate school full time to “learn what a computer was and could do.” A summer 1967 digital analyst internship with Bell Aerospace Company led to the 1968 technical report “A Numerical Solution Technique for a Class of Two-Dimensional Problems in Fluid Dynamics Formulated via Discrete Elements,” a pioneering expose in the fledgling field of finite-element (FE) CFD. Finishing his (plasma physics topic) dissertation in 1970, he joined Bell Aerospace as Principal Research Scientist to pursue fulltime FE CFD theorization. NASA Langley Research Center stints led to summer appointments at their Institute for Computer Applications in Science and Engineering (ICASE), which in turn led to a 1974–1975 visiting professorship at Old Dominion University. He transitioned directly to UT and in the process founded Computational Mechanics Consultants, Inc., with two Bell Aerospace colleagues, with the mission to convert FE CFD theory academic research progress into computing practice.
Notations

\[ a \] expansion coefficient; speed of sound; characteristics coefficient
\[ A \] plane area; 1-D FE matrix prefix; coefficient
\[ AD \] approximate deconvolution
\[ ADBC \] approximate deconvolution boundary condition algorithm
\[ AF \] approximate factorization algorithm
\[ ALE \] arbitrary-lagrangian-eulerian algorithm
\[ [A] \] factored global matrix, RLES theory auxiliary problem matrix operator
\[ arLES \] essentially analytic LES closure theory
\[ b \] coefficient; boundary condition subscript
\[ \{b\} \] global data matrix
\[ B \] 2-D FE matrix prefix
\[ B(\bullet) \] bilinear form
\[ \mathbf{B} \] body force
\[ BC \] boundary condition
\[ BCE \] boundary commutation error integral
\[ BHE \] borehole heat exchanger
\[ \text{BiSec} \] bisected borehole heat exchanger
\[ BL \] boundary layer
\[ c \] coefficient; specific heat
\[ \mathbf{c} \] phase velocity vector
\[ C \] 3-D matrix prefix; coefficient; chord; Courant number \( \equiv \frac{U\Delta t}{\Delta x} \)
\[ C_{ij} \] cross stress tensor
\[ C_p \] aerodynamic pressure coefficient, \( \equiv \frac{p}{\rho u^2/2} \)
\[ C_S \] Smagorinsky constant, its generalization
\[ CFD \] computational fluid dynamics
\[ CFL \] Courant number
\[ C_f \] skin friction coefficient
\[ CF/2 \] boundary layer skin friction coefficient
\[ CNFD \] Crank–Nicolson finite difference
\[ CS \] control surface
\[ CV \] control volume
\[ d(\bullet) \] ordinary derivative, differential element
\[ d \] coefficient; FE matrix basis degree label, RSM distance; characteristics coefficient
\[ D \] binary diffusion coefficient; diagonal matrix
<table>
<thead>
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<th>Symbol</th>
<th>Definition</th>
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<tr>
<td>$D$</td>
<td>dimensionality, non-D diffusion coefficient $\equiv \Delta t/\rho h^2$</td>
</tr>
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<td>$D(\bullet)$</td>
<td>differential definition</td>
</tr>
<tr>
<td>$D(\bullet)$</td>
<td>substantial derivative</td>
</tr>
<tr>
<td>$D^m(\bullet)$</td>
<td>modified substantial derivative</td>
</tr>
<tr>
<td>DES</td>
<td>detached eddy simulation</td>
</tr>
<tr>
<td>DE</td>
<td>conservation of energy PDE</td>
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<tr>
<td>DG</td>
<td>discontinuous Galerkin weak form theory</td>
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<tr>
<td>DM</td>
<td>conservation of mass PDE</td>
</tr>
<tr>
<td>DP</td>
<td>conservation of momentum PDE</td>
</tr>
<tr>
<td>DY</td>
<td>conservation of species mass fraction PDE</td>
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<tr>
<td>$\mathbf{D}(\mathbf{u}, P)$</td>
<td>NS full stress tensor, $\equiv -\nabla P + (2/Re)\nabla \cdot \mathbf{S}(\mathbf{u})$</td>
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<tr>
<td>diag[$\bullet$]</td>
<td>diagonal matrix</td>
</tr>
<tr>
<td>[DIFF]</td>
<td>laplacian diffusion matrix</td>
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<tr>
<td>DNS</td>
<td>direct numerical simulation</td>
</tr>
<tr>
<td>$e$</td>
<td>specific internal energy; element-dependent (subscript)</td>
</tr>
<tr>
<td>$e^N$</td>
<td>error</td>
</tr>
<tr>
<td>$e^h$</td>
<td>continuum approximation error</td>
</tr>
<tr>
<td>$e_{ijk}$</td>
<td>alternating tensor</td>
</tr>
<tr>
<td>$e_{KL}$</td>
<td>curl alternator on $n = 2$</td>
</tr>
<tr>
<td>EBV</td>
<td>elliptic boundary value</td>
</tr>
<tr>
<td>$Ec$</td>
<td>Eckert number</td>
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<tr>
<td>$eta_{ji}$</td>
<td>coordinate transformation data</td>
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<tr>
<td>$E$</td>
<td>thermal energy; energy semi-norm (subscript)</td>
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<tr>
<td>$f_j$</td>
<td>flux vector</td>
</tr>
<tr>
<td>$f_n$</td>
<td>normal flux</td>
</tr>
<tr>
<td>$f(\bullet)$</td>
<td>function of the argument</td>
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<tr>
<td>$f(vf, \epsilon)$</td>
<td>radiation view factor</td>
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<tr>
<td>$F(\bullet)$</td>
<td>Fourier transform</td>
</tr>
<tr>
<td>${F}$</td>
<td>weak form terminal algebraic statement</td>
</tr>
<tr>
<td>$F(k \rightarrow i)$</td>
<td>Lambert’s cosine law viewfactor</td>
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<tr>
<td>FD</td>
<td>finite difference</td>
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<tr>
<td>FE</td>
<td>finite element</td>
</tr>
<tr>
<td>FV</td>
<td>finite volume</td>
</tr>
<tr>
<td>$f$</td>
<td>efflux vector on $\partial \Omega$</td>
</tr>
<tr>
<td>$F$</td>
<td>applied force</td>
</tr>
<tr>
<td>$g$</td>
<td>gravity magnitude; amplification factor; spatial filter function; characteristics enthalpy ratio</td>
</tr>
<tr>
<td>$g$</td>
<td>gravity</td>
</tr>
<tr>
<td>Gr</td>
<td>Grashoff number $\equiv g \beta \Delta TL^3/\nu^2$</td>
</tr>
<tr>
<td>$G_{k\rightarrow i}$</td>
<td>Gebhart viewfactor</td>
</tr>
<tr>
<td>GHP</td>
<td>ground source heat pump</td>
</tr>
<tr>
<td>GLS</td>
<td>Galerkin least squares algorithm</td>
</tr>
<tr>
<td>GWS</td>
<td>Galerkin weak statement</td>
</tr>
<tr>
<td>$h$</td>
<td>mesh measure; discrete (superscript), heat transfer coefficient</td>
</tr>
<tr>
<td>H</td>
<td>boundary layer shape factor</td>
</tr>
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</table>
\( H \) Gauss quadrature weight; Hilbert space
\( H.O.T. \) truncated Taylor series higher order terms
\( i \) summation index; mesh node
\( \hat{i} \) unit vector parallel to \( x \)
\( I \) discrete matrix summation index, identity matrix
\( i ff \) if and only if
\( I-EBV \) initial-elliptic boundary value
\( J \) discrete matrix summation index
\( [J] \) coordinate transformation jacobian
\( [JAC] \) matrix statement jacobian
\( k \) thermal conductivity; basis degree; index; diffusion coefficient
\( k_{ij} \) element of the \([\text{DIFF}]\) matrix
\( \overline{k} \) average value of conductivity
\( \mathbf{k} \) unit vector parallel to \( z \)
\( K \) discrete matrix summation index
\( \ell \) element length; summation index
\( \ell(\cdot) \) differential operator on \( \partial \Omega \)
\( L \) reference length scale
\( L \) discrete matrix summation index
\( \mathcal{L}(\cdot) \) differential operator on \( \Omega \)
\( L_{ij} \) Leonard stress tensor
\( \text{LES} \) large eddy simulation, convolved Navier–Stokes PDEs
\( m \) non-D wavenumber \( \equiv \kappa h \), integer
\( [m] \) mass matrix
\( m_i \) point mass; discrete matrix summation index
\( M \) particle system mass; domain matrix prefix; elements in \( \Omega^h \)
\( M_i \) molecular mass
\( [M] \) \( \text{mPDE} \) theory altered mass matrix
\( \text{Ma} \) Mach number
\( m\text{GWS} \) optimal modified Galerkin weak form
\( m\text{PDE} \) modified partial differential equation
\( m\text{ODE} \) modified ordinary differential equation
\( \text{MLT} \) mixing length theory
\( n \) index; normal subscript; dimension of domain \( \Omega \); integer
\( n-D \) \( n \)-dimensional, \( 1 \leq n \leq 3 \)
\( \mathbf{n} \) outward pointing unit vector normal to \( \partial \Omega \)
\( N \) Neumann BC matrix prefix
\( N \) summation termination; approximation (superscript)
\( \text{NC} \) natural coordinate basis
\( \text{NWM} \) near wall modeling LES BCs
\( \text{NWR} \) near wall resolution LES algorithm
\( \text{NS} \) Navier–Stokes
\( \{N_k\} \) finite element basis of degree \( k \)
\( O(\bullet) \) order of argument (\( \bullet \))
Notations

\( p \) pressure
\( P \) kinematic pressure
\( P \) Gauss quadrature order
\( P \) linear momentum
\( \text{Pa} \) placeholder for non-D groups \( \text{Re}, \text{Pr}, \text{Gr}, \text{Ec} \)
\( \{P\} \) intermediate computed matrix
\( \text{PDE} \) partial differential equation
\( \text{Pe} \) Peclet number \( = \text{RePr} \)
\( \text{PNS} \) parabolic Navier–Stokes
\( \text{PRaNS} \) hypersonic parabolic Reynolds-averaged Navier–Stokes
\( \text{Pr} \) Prandtl number \( \equiv \rho_0 \nu c_p / k \)
\( \text{pr} \) non-uniform mesh progression ratio
\( q \) generalized dependent variable
\( Q \) discretized dependent variable; heat added
\( \{Q\} \) nodal coefficient column matrix
\( r \) reference state subscript; radius
\( R \) perfect gas constant, temperature degrees Rankine
\( \mathcal{R} \) radiosity
\( R \) universal gas constant
\( R_{ij} \) Reynolds subfilter scale tensor
\( \text{RaNS} \) Reynolds-averaged Navier–Stokes
\( \text{Re} \) Reynolds number \( \equiv UL/\nu \)
\( \text{Re}' \) turbulent Reynolds number \( \equiv \nu'/\nu \)
\( \text{Re}^* \) compressible turbulent BL similarity coordinate \( = \rho u_\tau y / \mu \)
\( \mathcal{R}^n \) euclidean space of dimension \( n \)
\( \text{RSM} \) Reynolds stress model
\( \{\text{RES}\} \) weak form terminal matrix statement residual
\( s \) source term on \( \Omega \); heat added
\( s \) unit vector tangent to \( \partial \Omega \)
\( S \) entropy
\( \bar{\mathbf{S}} \) filtered Stokes tensor dyadic
\( S_e \) matrix assembly operator
\( S_{i,j,k} \) stencil assembly operator
\( \{S\} \) computational matrix
\( \text{Sc} \) Schmidt number \( \equiv D/\nu \)
\( \text{SFS}_{ij} \) subfilter scale tensor
\( \text{SGS}_{ij} \) subgrid scale tensor
\( \text{St} \) Stanton number \( \equiv \tau U/L \)
\( \text{SUPG} \) Streamline upwind Petrov Galerkin
\( \text{sym} \) symmetric
\( t \) time; turbulent (superscript)
\( T \) temperature
\( T(z) \) BHE conduit temperature distribution
\( \text{TE} \) Taylor series truncation error
\( \text{TG} \) Taylor Galerkin algorithm
TP tensor product basis
T surface traction vector
$T^N$ continuum approximate temperature solution
TWS Taylor weak statement
$\mathbf{u}$ displacement vector; velocity vector
$u$ velocity $x$ component; speed
$\overline{u_j}$ time averaged NS Reynolds stress tensor
$\overline{u_j}$ Favre time averaged velocity
$U$ reference velocity scale
UQ uncertainty quantification
$U$ discretized speed nodal value
$v$ velocity $y$ component
$\mathbf{v}_g(\kappa)$ group velocity, $\equiv \nabla_k \omega$
$v_j$ LES theory scalar state variable closure vector
V volume
VBV verification, benchmarking, validation
VVUQ verification, validation, uncertainty quantification
$\mathbf{V}$ velocity
VLES very large eddy simulation
$w$ weight function; fin thickness; velocity $z$ component
$W$ weight; work done by system
WF weak form
WR weighted residuals
WS weak statement
$x, x_i$ cartesian coordinate, coordinate system $1 \leq i \leq n$
$\bar{x}$ transformed local coordinate
$X$ discrete cartesian coordinate
$y$ displacement; cartesian coordinate
$y^+$ incompressible turbulent BL similarity coordinate $= u_e y/\nu$
$Y$ mass fraction; discrete cartesian coordinate
$z$ cartesian coordinate
$Z$ thickness ratio; discrete cartesian coordinate
$\nabla$ gradient differential operator
$\nabla^2$ laplacian operator
$d(\cdot)/dx$ ordinary derivative
$\partial(\cdot)/\partial x$ partial derivative
(·) scalar (number)
{·} column matrix
{·}T row matrix
[·] square matrix
$\text{diag}[\cdot]$ diagonal square matrix
$\|\cdot\|$ norm
$\cup$ union (non-overlapping sum)
$\cap$ intersection
det [·] matrix determinant
$\forall$ denotes “for all”
\( \in \) inclusion
\( \subset \) belongs to
\( \ast \) complex conjugate multiplication
\( \otimes \) matrix tensor product
\( \alpha \) coefficient, thermal diffusivity ratio
\( \beta \) absolute temperature; coefficient
\( \gamma \) specific heat ratio, coefficient, gaussian filter shape factor
\( \delta \) boundary layer thickness, coefficient, spatial filter measure, bow shock standoff distance
\( \delta^* \) boundary layer displacement thickness
\( \delta_{ij} \) Kronecker delta
\( \Delta \) discrete increment
\( \epsilon \) isotropic dissipation function, emissivity
\( \epsilon_{ij} \) cartesian alternator
\( \phi \) velocity potential function
\( \phi(\cdot) \) trial space function
\( \Phi \) potential function
\( \Phi_p(x) \) test space
\( \Psi_\alpha(x) \) trial space
\( \Psi \) vector streamfunction
\( \psi \) streamfunction scalar component
\( \eta \) transform space, wave vector angle
\( \eta_i \) tensor product coordinate system
\( \kappa \) thermal diffusivity, Karman constant = 0.435
\( \kappa^T \) turbulent thermal diffusivity
\( \kappa \) wavenumber vector
\( \kappa_{efb} \) element of a square matrix
\( \lambda \) Lagrange multiplier, wavelength, Lame’ parameter
\( \mu \) absolute viscosity
\( \nu \) kinematic viscosity
\( \nu' \) kinematic eddy viscosity
\( \pi \) pi (3.1415926 . . .)
\( \Theta \) TS implicitness factor, BL momentum thickness
\( \Theta \) potential temperature \( \equiv (T - T_{min})/(T_{max} - T_{min}) \)
\( \rho \) density
\( \sigma \) Stefan-Boltzmann coefficient = 5.67 E-08 w/m²K⁴
\( d\sigma \) differential element on \( \partial \Omega \)
\( \tau \) time scale
\( \tau_{ij} \) Reynolds stress tensor
\( \tau_{ij}^D \) deviatoric Reynolds stress tensor
\( \omega \) frequency, Van Driest damping function, vorticity scalar
\( \Omega \) vorticity vector
\( \Omega \) domain of differential equation
\( \Omega_e \) finite element domain
\( \Omega^h \) discretization of \( \Omega \)
\( \partial \Omega \) boundary of \( \Omega \)
\( \zeta_\alpha \) natural coordinate system
1

Introduction

1.1 About This Book

This text is the successor to *Finite Element Computational Fluid Mechanics* published in 1983. It thoroughly organizes and documents the subsequent three decades of progress in *weak form* theory derivation of *optimal performance* CFD algorithms for the infamous Navier–Stokes (NS) *nonlinear* partial differential equation (PDE) systems. The text content addresses the complete range of NS and *filtered* NS (for addressing turbulence) PDE systems in the incompressible fluid-thermal sciences. Appendix B extends subject NS content to a weak form algorithm addressing hypersonic shock layer aerothermodynamics.

As perspective color and dynamic computer graphics are support *imperatives* for CFD *a posteriori* data assimilation, and hence interpretation, www.wiley.com/go/baker/GalerkinCFD renders available the full color graphics content absent herein. The website also contains detailed academic course lecture content at advanced graduate levels in support of outreach and theory exposure/implementation.

Weak form theory is the mathematically *elegant* process for generating *approximate solutions* to nonlinear NS PDE systems. Theoretical formalities are always conducted in the *continuum*, and *only* after such musings are completed are space and time discretization decisions made. This final step is a *matter of choice*, with a *finite element* (FE) spatial semi-discretization retaining use of calculus and vector field theory throughout conversion to terminal *computable form*. This choice enables implementing weak form theory precision into an *optimal* performance compute engine, eliminating any need for *heurism*.

The text tenor assumes that the reader remembers some calculus and is adequately versed in fluid mechanics and heat and mass transport at a post-baccalaureate level. It further assumes that this individual is neither comfortable with nor adept at formal mathematical manipulations. Therefore, text fluid mechanics subject exposure sequentially enables *just-in-time* exposure to essential mathematical concepts and methodology, in progressively addressing more detailed NS PDE systems and closure formulations.

Potential flow enables elementary weak form theory exposure, with subsequent theorization modifications becoming progressively more involved in addressing NS pathological nonlinearity. The exposure process is sequentially supported by *a posteriori* data from
precisely designed computational experiments, enabling *quantitative validation* of theory predictions of *accuracy, convergence, stability* and *error estimation/distribution* which, in concert, lead to confirmation of *optimal mesh* solution existence.

Text content firmly quantifies the practice preference for an FE semi-discrete spatial implementation. The apparent simplicity of finite volume (FV) and finite difference (FD) discretizations engendered the FV/FD commercial CFD code legacy practice. However, as documented herein, FV/FD spatial discretizations constitute non-Galerkin weak form decisions leading to nonlinear *schemes* via *heuristic* arguments. This is totally obviated in converting FE algorithms to computable syntax using calculus and vector field theory. This aspect hopefully further prompts the reader’s interest in acquiring knowledge of these elegant *practice* aspects, such that assimilating FE constructs proves to be worth the effort.

The progression within each chapter, hence throughout the text, sequentially addresses more detailed fluid/thermal NS PDE systems, each chapter building on prior material. The elegant uniformity of weak form theory facilitates this approach with mathematical formalities *never* requiring an *ad hoc* scheme decision. In his reflections on teaching the finite element method Bruce Irons is quoted, “Most people, mathematicians apart, abhor *abstraction*.” Booker T. Washington concurred, “An ounce of application is worth a ton of abstraction.” These precepts guide the development and exposition strategies in this text, with abstraction *never* taking precedence over developing a firm engineering-based theoretical exposure.

Summarizing, *modified continuous* Galerkin weak formulations for fluid/thermal sciences CFD generate practical computational algorithms fully validated as *optimal* in performance as predicted by a rich theory. Conception and practice goals always lead to the theoretical exposition, to convince the reader that its comprehension is a worthwhile goal, paying the requisite dividend.

### 1.2 The Navier–Stokes Conservation Principles System

Computational fluid-thermal system simulation involves seeking a *solution* to the *nonlinear* PDE systems generated from the basic conservation observations in engineering mechanics. In the lagrangian (point mass) perspective, these principles state

\[
\begin{align*}
\text{conservation of mass:} & \quad dM = 0, M = \Sigma m_i \\
\text{Newton’s second law:} & \quad d\mathbf{P} = \Sigma \mathbf{F}, \mathbf{P} = MV \\
\text{thermodynamics, first law:} & \quad dE = dQ - dW \\
\text{thermodynamic process:} & \quad dS \geq 0
\end{align*}
\]

In (1.1) \( m_i \) denotes a point mass, \( M \) is total mass of a particle system, \( \mathbf{V} \) is velocity of that system and \( \mathbf{F} \) denotes applied (external) forces. Equations (1.3–1.4) are statements of the first and second law of thermodynamics where \( E \) is system total energy, \( Q \) is heat added, \( W \) is work done by the system and \( S \) is entropy.

Practical CFD applications almost never involve addressing the conservation principles in lagrangian form. Instead, the transition to the *continuum* (eulerian) description is made, wherein one assumes that there exist so many mass points per characteristic volume \( \mathbf{V} \) that
a density function $\rho$ can be defined

$$\rho(x, t) = \lim_{V \to 0} \frac{1}{V} \sum_{i} m_i$$

(1.5)

One then identifies a control volume $CV$, with bounding control surface $CS$, Figure 1.1, and transforms the conservation principles from lagrangian to eulerian viewpoint via Reynolds transport theorem

$$\frac{d()}{dt} \approx D() \equiv \frac{\partial}{\partial t} \int_{cv} \rho d\tau + \int_{cs} (\cdot ) V \cdot n d\sigma$$

(1.6)

Thus is produced a precise mathematical statement of the conservation principles for continuum descriptions as a system of integro-differential equations

$$DM = \frac{\partial}{\partial t} \int_{cv} \rho d\tau + \int_{cs} \rho V \cdot \hat{n} d\sigma = 0$$

(1.7)

$$DP \Rightarrow \frac{\partial}{\partial t} \int_{cv} \rho V d\tau + \int_{cs} \rho V \cdot \hat{n} d\sigma = \int_{cv} \rho B d\tau + \int_{cs} T d\sigma$$

(1.8)

$$DE \Rightarrow \frac{\partial}{\partial t} \int_{cv} \rho e d\tau + \int_{cs} (e + p/\rho) \rho V \cdot \hat{n} d\sigma = \int_{cv} s d\tau + \int_{cs} (W - q \cdot \hat{n}) d\sigma$$

(1.9)

Note the eulerian “filling in” of the right hand sides for $DP$ and $DE$ with $\sum F \Rightarrow$ body forces $B +$ surface tractions $T$, and $dQ - dW \Rightarrow$ heat added $s$, bounding surface heat efflux $q \cdot \hat{n}$ and work done $W$.

From (1.7–1.9), one easily develops the PDE statements of direct use for CFD formulations by assuming that the control volume $CV$ is stationary, followed by invoking the divergence theorem for the identified surface integrals. For example for (1.7)

$$\int_{cs} \rho V \cdot \hat{n} d\sigma = \int_{cv} \nabla \cdot \rho V d\tau$$

(1.10)

where $\nabla$ is the gradient (vector) differential operator.

Via the divergence theorem the integro-differential equation system (1.7–1.9) is uniformly re-expressed as integrals vanishing identically on the CV. Such expressions can
hold in general if and only if (iff) the integrand vanishes identically, whereupon DM, DP and DE morph to the nonlinear PDE system

\[ DM: \frac{\partial \rho}{\partial t} + \nabla \cdot \rho \mathbf{u} = 0 \]  \hspace{1cm} (1.11)

\[ DP: \frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot \rho \mathbf{u} \mathbf{u} = \rho \mathbf{g} + \nabla \mathbf{T} \]  \hspace{1cm} (1.12)

\[ DE: \frac{\partial p e}{\partial t} + \nabla \cdot (p e + p) \mathbf{u} = s - \nabla \cdot \mathbf{q} \]  \hspace{1cm} (1.13)

Herein the velocity vector label \( \mathbf{V} \) in the preceding equations is replaced with the more conventional symbol \( \mathbf{u} \).

It remains to simplify (1.11–1.13) for constant density \( \rho_0 \) and to identify constitutive closure for traction vector \( \mathbf{T} \) and heat flux vector \( \mathbf{q} \). For laminar flow \( \mathbf{T} \) contains pressure and a fluid viscosity hypothesis involving the Stokes strain rate tensor. For constant density \( \rho_0 \) and multiplied through by \( \nabla \) the resultant vector statement is

\[
\nabla \mathbf{T} = -\nabla p + \nabla \cdot \mu \nabla \mathbf{u}
\]  \hspace{1cm} (1.14)

where \( p \) is pressure and \( \mu \) is fluid absolute viscosity. The Fourier conduction hypothesis for heat flux vector \( \mathbf{q} \) is

\[
\nabla \cdot \mathbf{q} = -\nabla \cdot k \nabla T
\]  \hspace{1cm} (1.15)

where \( k \) is fluid thermal conductivity and \( T \) is temperature.

Substituting these closure models and enforcing that density and specific heat are assumed constant converts (1.11–1.13) to the very familiar textbook appearance of Navier–Stokes. Herein the homogeneous form preference leads to the subject incompressible NS PDE system

\[ DM: \nabla \cdot \mathbf{u} = 0 \]  \hspace{1cm} (1.16)

\[ DP: \frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot \mathbf{u} \mathbf{u} + \rho_0 \nabla p - \nabla \cdot \nu \nabla \mathbf{u} + (p/\rho_0)\mathbf{g} = 0 \]  \hspace{1cm} (1.17)

\[ DE: \frac{\partial T}{\partial t} + \nabla \cdot \mathbf{u} T - \nabla \cdot \kappa \nabla T - s/\rho_0 c_p = 0 \]  \hspace{1cm} (1.18)

In (1.17), \( \nu = \mu/\rho_0 \) is fluid kinematic viscosity with density assumed as the constant \( \rho_0 \) except for thermally induced impact in the gravity body force term in (1.17). Finally, in (1.18) \( \kappa = k/\rho c_p \) is fluid thermal diffusivity.

Thermo-fluid system performance is thus characterized by a balance between unsteadiness and convective and diffusive processes. This identification is precisely established by non-dimensionalizing (1.16–1.18). The reference time, length and velocity scales are \( \tau \), \( L \), and \( U \), respectively, with the (potential) temperature scale definition \( \Theta = (T - T_{\text{min}})/(T_{\text{max}} - T_{\text{min}}) \). Then implementing the Boussinesq buoyancy model for the gravity body