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

Optimal MODIFIED CONTINUOUS Galerkin CFD, First Edition. A. J. Baker.

Companion Website: www.wiley.com/go/baker/GalerkinCFD

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

$$\text{conservation of mass:}\quad \mathrm{d}M = 0, M = \Sigma m_i \tag{1.1}$$

$$\text{Newton's second law:}\quad \mathrm{d}\mathbf{P} = \Sigma\mathbf{F}, \mathbf{P} = M\mathbf{V} \tag{1.2}$$

$$\text{thermodynamics, first law:}\quad \mathrm{d}E = \mathrm{d}Q - \mathrm{d}W \tag{1.3}$$

$$\text{thermodynamic process:}\quad \mathrm{d}S \geq 0 \tag{1.4}$$

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 V that

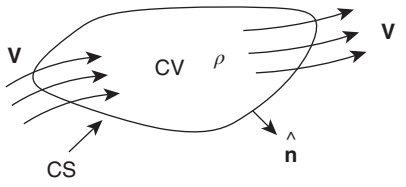

Figure 1.1 Control volume for Reynolds transport theorem

a *density* function ρ can be defined

$$\rho(\boldsymbol{x}, t) = \lim_{\mathrm{V}\to 0} \frac{1}{\mathrm{V}} \sum_i m_i \tag{1.5}$$

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*

$$\mathrm{d}() \Rightarrow \mathrm{D}() \equiv \frac{\partial}{\partial t} \int_{cv} (\,\cdot\,)\mathrm{d}\tau + \oint_{cs} (\,\cdot\,)\mathbf{V} \cdot \hat{\mathbf{n}}\ \mathrm{d}\sigma \tag{1.6}$$

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

$$\mathrm{D}M = \frac{\partial}{\partial t} \int_{\mathrm{cv}} \rho \mathrm{d}\tau + \oint_{\mathrm{cs}} \rho \mathbf{V} \cdot \hat{\mathbf{n}}\ \mathrm{d}\sigma = 0 \tag{1.7}$$

$$\mathrm{D}\mathbf{P} \Rightarrow \frac{\partial}{\partial t} \int_{\mathrm{cv}} \rho \mathbf{V} \mathrm{d}\tau + \oint_{\mathrm{cs}} \mathbf{V} \rho \mathbf{V} \cdot \hat{\mathbf{n}}\ \mathrm{d}\sigma = \int_{\mathrm{cv}} \rho \mathbf{B} \mathrm{d}\tau + \int_{\mathrm{cs}} \mathbf{T} \mathrm{d}\sigma \tag{1.8}$$

$$\mathrm{D}E \Rightarrow \frac{\partial}{\partial t} \int_{\mathrm{cv}} \rho e \mathrm{d}\tau + \oint_{\mathrm{cs}} (e + p/\rho)\rho\, \mathbf{V} \cdot \hat{\mathbf{n}}\ \mathrm{d}\sigma = \int_{\mathrm{cv}} s \mathrm{d}\tau + \int_{\mathrm{cs}} (W - \mathbf{q} \cdot \hat{\mathbf{n}}) \mathrm{d}\sigma \tag{1.9}$$

Note the eulerian "filling in" of the right hand sides for D**P** and DE with $\sum \mathbf{F} \Rightarrow$ body forces **B** + surface tractions **T**, and $\mathrm{d}Q - \mathrm{d}W \Rightarrow$ heat added s, bounding surface heat efflux $\mathbf{q} \cdot \hat{\mathbf{n}}$ 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)

$$\oint_{\mathrm{cs}} \rho \mathbf{V} \cdot \hat{\mathbf{n}}\ \mathrm{d}\sigma = \int_{\mathrm{cv}} \nabla \cdot \rho\, \mathbf{V} \mathrm{d}\tau \tag{1.10}$$

where ∇ 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 D*M*, D**P** and D*E* morph to the *nonlinear* PDE system

$$\mathrm{D}M\text{:}\quad \frac{\partial \rho}{\partial t} + \nabla \cdot \rho \mathbf{u} = 0 \tag{1.11}$$

$$\mathrm{D}\mathbf{P}\text{:}\quad \frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot \rho \mathbf{u}\mathbf{u} = \rho \mathbf{g} + \nabla \mathbf{T} \tag{1.12}$$

$$\mathrm{D}E\text{:}\quad \frac{\partial \rho e}{\partial t} + \nabla \cdot (\rho e + p)\mathbf{u} = s - \nabla \cdot \mathbf{q} \tag{1.13}$$

Herein the velocity vector label **V** in the preceding equations is replaced with the more conventional symbol **u**.

It remains to simplify (1.11–1.13) for constant density ρ_0 and to identify *constitutive closure* for traction vector **T** and heat flux vector **q**. For laminar flow **T** contains pressure and a fluid viscosity hypothesis involving the Stokes strain rate tensor. For constant density ρ_0 and multiplied through by ∇ the resultant vector statement is

$$\nabla \mathbf{T} = -\nabla p + \nabla \bullet \mu \nabla \mathbf{u} \tag{1.14}$$

where p is pressure and μ is fluid absolute viscosity. The Fourier conduction hypothesis for heat flux vector **q** is

$$\nabla \cdot \mathbf{q} = -\nabla \bullet k \nabla T \tag{1.15}$$

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

$$\mathrm{D}M\text{:}\quad \nabla \cdot \mathbf{u} = 0 \tag{1.16}$$

$$\mathrm{D}\mathbf{P}\text{:}\quad \frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot \mathbf{u}\mathbf{u} + \rho_0 \nabla p - \nabla \cdot \nu \nabla \mathbf{u} + (\rho/\rho_0)\mathbf{g} = 0 \tag{1.17}$$

$$\mathrm{D}E\text{:}\quad \frac{\partial T}{\partial t} + \nabla \cdot \mathbf{u}T - \nabla \cdot \kappa \nabla T - s/\rho_0 c_p = 0 \tag{1.18}$$

In (1.17), $\nu = \mu/\rho_0$ is fluid kinematic viscosity with density assumed as the constant ρ_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 τ, L, and U, respectively, with the (potential) temperature scale definition $\Theta = (T - \mathrm{T}_{\min})/(\mathrm{T}_{\max} - \mathrm{T}_{\min})$. Then implementing the Boussinesq buoyancy model for the gravity body

force, the *non*-D incompressible NS PDE system for thermal-laminar flow with mass transport is

$$\mathrm{D}M: \quad \nabla \cdot \mathbf{u} = 0 \tag{1.19}$$

$$\mathrm{D}\mathbf{P}: \quad \mathrm{St}\frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot \mathbf{u}\mathbf{u} + \nabla P - \frac{1}{\mathrm{Re}}\nabla \cdot \nabla \mathbf{u} + \frac{\mathrm{Gr}}{\mathrm{Re}^2}\Theta\, \widehat{\mathbf{g}} = 0 \tag{1.20}$$

$$\mathrm{D}E: \quad \mathrm{St}\frac{\partial \Theta}{\partial t} + \nabla \cdot \mathbf{u}\Theta - \frac{1}{\mathrm{RePr}}\nabla \cdot \nabla \Theta - s_\Theta = 0 \tag{1.21}$$

$$\mathrm{D}Y: \quad \mathrm{St}\frac{\partial Y}{\partial t} + \nabla \cdot \mathbf{u}Y - \frac{1}{\mathrm{ReSc}}\nabla \cdot \nabla Y - s_Y = 0 \tag{1.22}$$

The unknowns in PDE system (1.19–1.22) are the non-D velocity vector $\mathbf{u}$, kinematic pressure P, temperature Θ and mass fraction Y. No special notation emphasizes that these are non-D, which will always be the case. These variables as a group are hereinafter referenced as the NS PDE system *state variable* symbolized as the column matrix $\{q(\mathbf{x},t)\} = \{\mathbf{u}, P, \Theta, Y\}^T$.

The definitions for Stanton, Reynolds, Grashoff, Prandtl and Schmidt numbers are conventional as $\mathrm{St} \equiv \tau \mathrm{U/L}$, $\mathrm{Re} \equiv \mathrm{UL}/\nu$, $\mathrm{Gr} \equiv \mathrm{g}\beta\Delta\mathrm{TL}^3/\nu^2$, $\mathrm{Pr} \equiv \rho_0 \nu c_p/k$ and $\mathrm{Sc} \equiv \mathrm{D}/\nu$, where D is the binary diffusion coefficient. Additionally $\Delta\mathrm{T} \equiv (\mathrm{T}_{\max} - \mathrm{T}_{\min})$, $\beta \equiv 1/\mathrm{T}_{\mathrm{abs}}$ and $P \equiv p/\rho_0$. St is defined unity, $\tau \equiv \mathrm{L/U}$, except when addressing flowfields exhibiting harmonic oscillation, and the Peclet number $\mathrm{Pe} \equiv \mathrm{RePr}$ is the common replacement in D*E*.

1.3 Navier–Stokes PDE System Manipulations

The NS PDE system (1.19–1.22) is universally accepted as an accurate descriptor of fluid-thermal phenomena for all Reynolds numbers Re. However, it is also universally recognized that for $\mathrm{Re} \geq O(\sim\mathrm{E}{+}04)$, where $O(\bullet)$ signifies *order*, the resultant NS flowfields will be characterized as *turbulent*.

The CFD simulation procedure that addresses the expressed NS PDE system for all Re is called *direct numerical simulation* (DNS). Even with massive computer resources the DNS approach to solution of practical NS problem statements is contraindicated, cf. Dubois *et al*. (1999). The DNS approach is not addressed herein, although these algorithms do enjoy an identical weak form theoretical basis.

Instead, generating computational simulation algorithms for NS PDE statements for practical Re requires manipulations of (1.19–1.22). In the CFD community, the operation of *time averaging* generates the Reynolds-averaged NS (RaNS) PDE system. The alternative is *spatial filtering* via convolution with a filter function that produces the large eddy simulation (LES) NS PDE system. A union of the two has been termed *very large eddy simulation* (VLES), or a RaNS-LES hybrid termed *detached eddy simulation* (DES).

In each instance the mathematical manipulations introduce *a priori* unknown variables into the resultant PDE system *state variable* due to the *nonlinear* convection terms in (1.20–1.22). Time averaging resolves $\{q(\mathbf{x},t)\}=\{\mathbf{u}, p, \Theta, Y\}^T$ into the time-independent steady component and the fluctuation (in time) thereabout. In tensor index notation the resolution statement for velocity vector $\mathbf{u}$ is

$$\mathbf{u}(\mathbf{x},t) \Rightarrow u_i(x_k,t) \equiv \overline{u}_i(x_k) + u_i'(x_k,t) \tag{1.23}$$

Time averaging the convection term in (1.20) produces

$$\overline{u_j u_i} = \overline{u}_j \overline{u}_i + \overline{u'_j u'_i} \tag{1.24}$$

that is, the tensor product of time averaged velocity plus the time average of the tensor product of velocity fluctuations about the steady average.

The second term in (1.24) is called the RaNS *Reynolds stress tensor*, a model for which must be constructed to close the RaNS PDE system state variable. Similar operations on D*E* and D*Y* produce mean convection term products plus the fluctuating product *Reynolds vectors*

$$\overline{u_j \Theta} = \overline{u}_j \overline{\Theta} + \overline{u'_j \Theta'} \quad \text{and} \quad \overline{u_j Y} = \overline{u}_j \overline{Y} + \overline{u'_j Y'} \tag{1.25}$$

which must also be modeled to achieve closure.

The specifics of RaNS closure model development are derived in Chapter 4, then further detailed in Chapters 8 and Appendix B. It is sufficient here to note RaNS closure models emulate the force-flux form of the Stokes and Fourier fluid-dependent constitutive closures (1.14–1.15). The correlation coefficient becomes a *turbulent eddy viscosity, υ^t, extended* to turbulent heat/mass flux vector closure via turbulent Pr and Sc number assumptions.

The non-D turbulent eddy viscosity defines the *turbulent Reynolds number*

$$\mathrm{Re}^t \equiv \nu^t / \nu \tag{1.26}$$

and the non-D RaNS PDE system alternative to laminar NS PDEs (1.19–1.22), assuming unit Stanton number is

$$\mathrm{D}M: \quad \nabla \cdot \overline{\mathbf{u}} = 0 \tag{1.27}$$

$$\mathrm{D}\mathbf{P}: \quad \frac{\partial \overline{\mathbf{u}}}{\partial t} + \nabla \cdot \overline{\mathbf{u}}\overline{\mathbf{u}} + \nabla \overline{P} - \frac{1}{\mathrm{Re}} \nabla \cdot \left[(1 + \mathrm{Re}^t) \nabla \overline{\mathbf{u}} \right] + \frac{\mathrm{Gr}}{\mathrm{Re}^2} \overline{\Theta} = 0 \tag{1.28}$$

$$\mathrm{D}E: \quad \frac{\partial \overline{\Theta}}{\partial t} + \nabla \cdot \overline{\mathbf{u}} \overline{\Theta} - \frac{1}{\mathrm{Re}} \nabla \cdot \left[\left(\frac{1}{\mathrm{Pr}} + \frac{\mathrm{Re}^t}{\mathrm{Pr}^t} \right) \nabla \overline{\Theta} \right] - \overline{s}_\Theta = 0 \tag{1.29}$$

$$\mathrm{D}Y: \quad \frac{\partial \overline{Y}}{\partial t} + \nabla \cdot \overline{\mathbf{u}} \overline{Y} - \frac{1}{\mathrm{Re}} \nabla \cdot \left[\left(\frac{1}{\mathrm{Sc}} + \frac{\mathrm{Re}^t}{\mathrm{Sc}^t} \right) \nabla \overline{Y} \right] - \overline{s}_Y = 0 \tag{1.30}$$

The time averaging alternative of spatial filtering employs the mathematical operation of *convolution*. In one dimension for velocity scalar component u the space filtered velocity definition is

$$\overline{u}(x,t) \equiv \int_{-\infty}^{\infty} g(y)\, u(x-y,t) dy \tag{1.31}$$

where $g(y)$ denotes the filter function. The filtered velocity remains time dependent, and in n dimensions the CFD literature notation for spatial filtering

$$\overline{u}_i(x_j,t) \equiv g_\delta{}^* u_i(x_j,t) \tag{1.32}$$

is symbolized by * with δ denoting the *measure* (diameter) of the filter function g.

Spatial filtering the NS PDE system (1.19–1.22) produces the LES PDE system addressed in Chapter 9. Following convolution, Fourier transformation and deconvolution spatial filtering of the convection term in (1.20) generates the *a priori* unknown *stress tensor quadruple*

$$\overline{u_j u_i} = \overline{\overline{u}_j \overline{u}_i} + \overline{u'_j \overline{u}_i} + \overline{\overline{u}_j u'_i} + \overline{u'_j u'_i} \tag{1.33}$$

Generating closure models for the LES PDE system typically involves consequential approximations in (1.33). For example, adding and subtracting the filtered velocity tensor product in (1.33) produces the *triple decomposition* approximation

$$\overline{u_j u_i} = \overline{u}_j \overline{u}_i + \underbrace{\left(\overline{\overline{u}_j \overline{u}_i} - \overline{u}_j \overline{u}_i\right)}_{L_{ij}} + \underbrace{\left(\overline{\overline{u}_j u'_i} + \overline{u'_j \overline{u}_i}\right)}_{C_{ij}} + \underbrace{\overline{u'_j u'_i}}_{R_{ij}} \tag{1.34}$$

for L_{ij} termed the *Leonard stress*, C_{ij} the *cross stress* and R_{ij} the *Reynolds subfilter scale* tensors.

LES theory states that the latter accounts for energetic dissipation at the *unresolved scale threshold*, the spatial scale defined by filter measure δ. This is the LES theory equivalent of viscous dissipation in the unfiltered NS system at molecular scale. The legacy published *subgrid scale* (SGS) tensor models again are of force-flux mathematical form, (1.27–1.30), with many variations, Piomelli (1999). As with time averaging, spatial filtering the NS D*E* and D*Y* PDEs generates the companion unknown filtered thermal and mass *vector quadruples*.

An NS PDE system manipulation particularly pertinent to aerodynamics CFD applications alters the steady form of (1.19–1.22) assuming the velocity vector field is *unidirectional*. The end results are the famous *boundary layer* (BL) PDE system, and the *n*-dimensional generalization *parabolic Navier–Stokes* (PNS) PDE system. Both systems possess initial-value character in the direction of dominant flow. Importantly, both have largely supported development and validation of Reynolds stress tensor/vector closure models for the RaNS PDE system. The compressible turbulent PNS (PRaNS) PDE system is applicable to hypersonic external shock layer aerothermodynamics, detailed in Appendix B.

1.4 Weak Form Overview

The incompressible NS PDEs, also the model closed BL, PNS, RaNS and LES PDE systems, are elliptic boundary value (EBV) with selective initial-value character. Weak form theory is a *thoroughly formal process* for constructing approximate solutions to I-EBV/EBV PDE systems. The mathematical *hooker* in these PDEs is that each contains the *differential constraint* of D*M*, (1.19), which requires that the velocity field be *divergence-free*. This is *the* fundamental theoretical issue in identifying PDE systems with boundary conditions (BCs) that are well-posed, fully detailed in subsequent chapters.

The fundamental axiom of weak form theory is that one *indeed* seeks to construct an *approximate solution*. By very definition, a PDE solution is a *function* of space (and time perhaps) distributed continuously and smoothly, or possessing a finite number of finite discontinuities, over the PDE domain and on its boundaries. Thereby, the *prime requirement* for a weak form CFD algorithm is to clearly identify *the* candidate approximate solution.

This is *completely distinct* from historical FD/FV CFD approaches which generate a union of *stencils* via Taylor series approximations to PDE derivatives rather than stating the sought-for solution.

So, the starting point for a weak form construction is to identify a set of functions, called the *trial space*, endowed with properties appropriate for supporting an approximate solution. With certified existence of a trial space, the following questions come to mind:

- How good (accurate) an approximate solution can be supported by the selected trial space?
- How does the trial space supporting a finite element (FE) approximation differ from that for a finite difference (FD) scheme or a finite volume (FV) integral construction?
- Can these trial spaces be identical, and, if not, what are the distinguishing issues?
- Bottom line: is the *error* in the approximation related to a specific trial space selection?

Weak form theory possesses an elegant formalism for defining approximate solution error, developed in thoroughness in the next few chapters. The premier realization is that *approximation error* is a function(!) distributed over the PDE domain and its boundaries, as are the approximate *and* the exact NS solutions, with the latter of course never known. The key precept of weak form theory is to establish an integral *constraint on error* which requires definition of another set of functions termed the *test space*, against which the approximation error can be "tested." In English:

weak form theory formalizes the ingredients of
approximate solution construction in terms
of a trial space, a test space and the rendering
of the resultant approximation error an extremum
in an appropriate integral measure called a norm

Weak form theory practice is no more complicated than implementing this statement. Thereby, one must immediately enquire whether there exists an *optimal* test space, such that the approximation *error is the smallest* possible for *any* trial space selection. Again weak form theory provides the answer:

Weak form theory predicts the approximation
error is extremized, in practice minimized, when
the trial and test spaces contain the identical
members, which is termed the Galerkin criterion

Weak form theoretical musings always occur in the *continuum* and fully utilize calculus and vector field theory for generality with precision. Of pertinence, the weak form continuum construction holds for the PDE + BCs analytical solution as well as *any* approximation! Once the theory statement is formed, the remaining decision is trial space selection, hence identical test space, for error extremization. The key trial space requirement is for members to possess differentiability sufficient to enable integrals of their PDE derivatives to exist. This is really no problem, so the completion issue is forming the integrals that the weak form generates.

The continuum trial space contains functions spanning the global extent of the PDE domain. Finding suitable functions that one can integrate is nigh impossible (*the* challenge in DNS), hence the solution is to *discretize* the PDE domain and its boundaries, and hence identify much smaller *subsets* of the global trial (and test) space. Underlying is interpolation theory with net result a *discrete approximation trial space basis*. Trial space bases possess support *only* in the *generic* discretization cell, the *union* (non-overlapping sum) of which constitutes the computational mesh. This process admits full geometric generality, accurate evaluation of weak form integrals and a rigorous path to progressively more accurate formulations. Of ultimate importance is that it supports *analytical* formation of nonlinear algebraic matrix statements *amenable to computing*.

Summarizing, weak form theory involves *clear* organization of the sequence of decisions required for *approximate solution error extremization*, prior to definition of any specific discrete trial space basis. Thus, any given discrete solution methodology, specifically FE, FD or FV, becomes clearly identifiable among its peers by the sequence of decisions exposed in the weak formulation process. This text develops the subject in thoroughness, across a broad spectrum of fluid-thermal NS and manipulated NS PDE systems for which an *optimal performance* CFD algorithm is sought.

1.5 A Brief History of Finite Element CFD

Finite difference methods in CFD were first reported in the late 1920s, Courant *et al*. (1928), with fundamental theoretical developments emerging from the Courant Institute following World War II, Lax (1954), Lax and Wendroff (1960). Thereafter, many contributions to CFD emerged from the Los Alamos Scientific Laboratory (LASL), Amsden and Harlow (1970), Harlow (1971), coincident with the Imperial College team's development of the "SIMPLE" algorithm, Gosman *et al*. (1969). The NASA Ames Research Center (ARC) picked up the lead on compressible aerodynamics CFD, MacCormack (1969), Beam and Warming (1976), with timing coincident with CFD maturing to an international research topic with hundreds of contributors.

The progenitor of weak form theory is the *finite element method* developed in practice in the late 1950s by aeronautical engineers to analyze aircraft structural components. Exploratory musings preceded this; for example Hrenikoff (1941) developed an elasticity solution for torsion problems based on triangles, Courant (1943) developed a variational formulation for problems in vibrations. Turner *et al*. (1956) first derived the *stiffness matrix* for truss and beam analysis, and Clough (1960) coined the term *finite element*. Argyris (1963) published the first monograph detailing a precise mathematical foundation for the engineer's newly emerging finite element analysis capability.

The finite element method's first application to the non-structural problem of unsteady heat conduction required convolution, Zienkiewicz and Cheung (1965). A formal addressing of the wider problem class in nonlinear mechanics followed, Oden (1972). As finite element structural theory and methodology matured, the *mechanistic* engineering precepts became replaced by a rich mathematical basis founded in the variational calculus and Rayleigh–Ritz methods, Rayleigh (1877), Ritz (1909). This classic theory base for finite element structural analyses grew rapidly, including many fundamental contributions, Babuska and Aziz (1972), Ciarlet and Raviart (1972), Aubin (1972), Lions and Magenes (1972), Strang and Fix (1973) and Oden and Reddy (1976).

The direct extension of classic variational mechanics to CFD algorithm construction for fluid/thermal descriptions is not possible. The impediment is the conservation principle eulerian reference frame, which renders momentum conservation D**P** explicitly nonlinear. For this reason, at least, pioneering CFD procedures employed replacement of derivatives by divided differences, that is, *finite differences*, Richtmyer and Morton (1967), Roache (1972).

The FD successor *finite volume* CFD developments involved direct integration of each PDE over cells of a domain discretization, followed by the divergence theorem which exposed cell face fluxes. These were evaluated via finite difference quotients coupled with an approximate enforcement for D*M*, Patankar (1980). The *particle-in-cell* method, Evans and Harlow (1957), also employed a cell flux concept and used pseudo-lagrangian particle distributions for approximate satisfaction of the D*M* constraint.

Most FD/FV quotient-based CFD algorithms were discovered recoverable as specific criteria selections within the *discrete weighted residuals* (WR) framework, with Finlayson (1972) the pioneering exposition. In WR theory, approximation error was constrained by requiring local integrals containing "weights" to vanish. Within the class, the *collocation* method weights were the Dirac delta, which exactly reproduced classic FD quotients. A *finite volume* algorithm was retrieved for a constant weight. Generalizing the weights to functions, and defining them identical to the discrete trial space basis reproduced the *Galerkin* method, named after the (non-discrete, non-CFD) procedure of B.G. Galerkin (1915). Finally, defining the weights to be the PDE operator itself reproduced the *least squares* method.

Pioneering FE CFD algorithms employed various WR criteria. Oden (1969, 1972) was among the first to derive the basic theoretical analog for the NS PDE system. Using a Galerkin WR FE formulation, Baker (1971, 1973, 1974) reported two-dimensional compressible and incompressible flow simulations with recirculation regions. Olson (1972) detailed a pseudo-variational (hence Galerkin) FE algorithm for the streamfunction biharmonic PDE equivalent of the two-dimensional NS PDE system.

Lynn (1974) used the least squares criterion for an FE laminar boundary layer flow algorithm that retained a symmetric matrix structure. Popinski and Baker (1974) published an FE Galerkin WR algorithm for laminar boundary layer flow and reported accuracy and convergence in an appropriate norm, including direct comparisons with the Crank–Nicolson (1947) FD algorithm. Chung and Chiou (1976) published an FE Galerkin WR algorithm for compressible laminar boundary layer development behind an impinging shock. Connor and Brebbia (1974) authored *Finite Element Techniques for Fluid Flow*, the first monograph for a restricted problem class. Then followed *The Finite Element Method for Engineers*, Huebner (1975), with limited FE Galerkin WR content, and *Finite Element Simulation in Surface and Subsurface Hydrology*, Pinder and Gray (1977), with content restricted to the title category.

From the mid 1970s through the 1980s burgeoning interest in weak form FE CFD algorithm research and applications sparked annual international conferences. This resulted in the Wiley conference monograph series *Finite Elements in Fluids*, with Gallagher, Oden and Zienkiewicz principal editors, Gallagher *et al*. (1975–1988). Publication of FE discrete CFD algorithms for NS systems moved to textbooks. *Finite Element Computational Fluid Mechanics*, Baker (1983), was the first topical treatise to specifically include asymptotic convergence theory validation for RaNS systems. (Therein *weak form* never appeared, owing to the author's opinion that engineers didn't do weak things!)

Fletcher (1984) authored *Computational Galerkin Methods* containing a handful of NS solutions. With a sharp mathematical focus, but containing applications restricted to very small Reynolds number, Gunzburger (1989) published *Finite Element Methods for Viscous Incompressible Flows*. Similarly, Pironneau (1989) published *Finite Element Methods for Fluids*, an exceptionally formal mathematical treatise which included laminar flow benchmark problem validation data. Coincident with PC capability maturation, Baker and Pepper (1991) authored *Finite Elements* 1–2–3 which included a 5¼ inch floppy disc containing Fortran code.

It's quite alarming looking into these early texts and viewing solution graphics computed on *incredibly coarse* meshes! Much larger scale PC computing emerged in the 1990s, as the FE CFD textbook litany moved forward. First prize for size (over 1000 pages!) goes to Gresho and Sani (1998) for *Incompressible Flow and the Finite Element Method*, which contained incredible mathematical detail for laminar isothermal incompressible flows only! Reddy and Gartling (2001) published *The Finite Element Method in Heat Transfer and Fluid Dynamics*, with applications to low-Re non-Newtonian fluids.

Chung (2002) followed with *Computational Fluid Dynamics*, also scaling in at over 1000 pages, covering a broad spectrum in FD/FV CFD theory and practice but with a very limited FE content. Donea and Huerta (2003) followed with *Finite Element Methods for Flow Problems*, with validations restricted to two-dimensional laminar NS benchmarks. Recently, *Finite Elements* ⇔ *Computational Engineering Sciences*, Baker (2012), details introductory coverage of weak form theory broadly applied to heat transfer, structural mechanics, vibrations, fluid mechanics and heat/mass transport. Text content assimilation includes still/dynamic color graphics and academic course organization support at www.wiley.com/go/baker/finite. Hands-on PC computing is Matlab- and COMSOL-enabled with focus generation of *a posteriori* data validating asymptotic convergence theory, error estimation, the impact of *non-smooth* data and design optimization.

1.6 A Brief Summary

So, does the CFD community need another textbook on weak form FE-implemented algorithms? I believe the answer is yes, as the broad duplication of historical, small Re constructions reported can now be replaced by a single comprehensive weak form theory text with precise attention to performance estimation and *validation*. This current knowledge base is applicable across the complete spectrum of NS, BL, PNS, RaNS, LES and PRaNS PDE systems.

Weak form theory, of necessity *linear*, predicts that the solution associated with the stationary coordinate of the Galerkin criterion is *optimal*. Its failure to address dispersive error instability and phase accuracy compromising issues associated with pioneering Galerkin NS constructions is now fully resolved. Via weak form manipulations based on limiting independent coordinate-derived Taylor series, differential term additions to the *classic text* NS PDE statements generate *modified* (*m*PDE) systems. The analysis framework ultimately leads to a precise theory recovering essentially *all* prior FD/FV/FE constructions, but most importantly theoretical prediction of an *optimal* construction.

Hence, CFD algorithms for all NS, BL, PNS, RaNS, LES and PRaNS *m*PDE systems herein are based on this theoretically sound *optimal modified continuous Galerkin weak*

form CFD theory. The key required *confirmation* of this assertion, as detailed herein, is that linear weak form theory *is* the *accurate predictor* of nonlinear NS PDE/*m*PDE CFD algorithm performance. Had this not occurred, this text would not have been written!

To summarize, weak form theory enables removal of essentially all elements of *mystery* surrounding algorithm constructions in NS fluid-thermal CFD. Comparison to legacy and/or current discrete CFD formulations is direct, simply by selecting the non-Galerkin, non-augmented PDE weak form criteria appropriate to reproducing that algorithm. This text is the culmination of the author's decades-held premise that the (multiple) hundreds of published CFD algorithms do not produce a corresponding number of *linearly independent* constructions! That the cogent approach to the subject can shed light uniformly across the spectrum was my academic research objective. This text is the result, hopefully written in a manner making the exposé enjoyable and rewarding. *Bon voyage*!

References

Amsden, A. and Harlow, F. (1970). "The SMAC Method: A Numerical Technique for Calculating Incompressible Fluid Flow," Univ. Calif. LASL Technical Report LA-4370.

Argyris, J.H. (1963). *Recent Advances in Matrix Methods of Structural Analysis*, Pergamon Press, Elmsford, NY.

Aubin, J.P. (1972). *Approximation of Elliptic Boundary Value Problems*, Wiley-Interscience, New York.

Babuska, I. and Aziz, A.K. (1972). "Lectures on the Mathematical Foundations of the Finite Element Method," in A.K. Aziz (ed.), *Mathematical Foundations of the Finite Element Method with Applications to Partial Differential Eqns*, Academic, NY, pp. 1–345.

Baker, A.J. (1971). "A Finite Element Computational Theory for the Mechanics and Thermodynamics of a Viscous Compressible Multi-Species Fluid," Bell Aerospace Research Rpt. 9500–920200.

Baker, A.J. (1973). "Finite Element Solution Algorithm for Viscous Incompressible Fluid Dynamics," *J. Numerical Methods Engineering*, V6, pp. 89–101.

Baker, A.J. (1974). "A Finite Element Algorithm for the Navier–Stokes Equations," NASA Technical Report CR-2391.

Baker, A.J. (1983). *Finite Element Computational Fluid Mechanics*, Hemisphere/McGraw-Hill, New York.

Baker, A.J. and Pepper, D.W. (1991). *Finite Elements* 1–2–3, McGraw-Hill, New York.

Baker, A.J. (2012). *Finite Elements ⇔ Computational Engineering Sciences*, John Wiley and Sons, London.

Beam, R. and Warming. R. (1976). "An Implicit Finite-Difference Algorithm for Hyperbolic Systems in Conservation Law Form," *J. Computational Physics* V22, pp. 87–110.

Chung, T.J. and Chiou, J.N. (1976). "Analysis of Unsteady Compressible Boundary Layer Flow Via Finite Elements," *Computers & Fluids*, V4, pp. 1–12.

Chung, T.J. (2002). *Computational Fluid Dynamics*, Cambridge University Press, UK.

Ciarlet, P.G. and Raviart, P.A. (1972). "General Lagrange and Hermite Interpolation in R^n with Applications to the Finite Element Method," *Arch. Rat. Mech. Anal.*, V46, pp. 177–199.

Clough, R.W. (1960). "The Finite Element Method in Plane Stress Analysis," *Proc. 2nd Conf. Electronic Computation*, Amer. Soc. Civil Engineers, Pittsburgh, PA, pp. 345–378.

Connor, J.J. and Brebbia, C.A. (1974). *Finite Element Techniques for Fluid Flow*, Newnes-Butterworths, UK.

Courant, R., Friedrichs, K. and Lewy, H. (1928). "Uber die Partiellen Differenzengleichungen der Mathematischen Physik," *Mathematische Annalen*, V100, pp. 32–74.

Courant, R. (1943). "Variational Methods for Solution of Problems of Equilibrium and Vibrations," *Bull. Amer. Math. Soc.*, V49, pp. 1–23.

Crank, J. and Nicolson, P. (1947). "A Practical Method for Numerical Evaluation of Solutions of Partial Differential Equations of Heat-Conduction Type," *Proc. Cambridge Philosophical Soc.*, V43, p. 50.

Donea, J. and Huerta, A. (2003). *Finite Element Methods for Flow Problems*, Wiley, West Sussex.

Dubois, T., Jauberteau, F. and Temam, R. (1999). *Dynamic Multilevel Methods and the Numerical Simulation of Turbulence*, Cambridge University Press, London.

Evans, M.E. and Harlow, F.H. (1957). "The Particle-in-Cell Method for Hydrodynamic Calculations," Univ. Calif., LASL Technical Report. LA-2139.

Finlayson, B.A. (1972). *The Method of Weighted Residuals and Variational Principles*, Academic, New York.
Fletcher, C.A.J. (1984). *Computational Galerkin Methods*, Springer-Verlag, Berlin.
Gallagher, R.H, Oden, J.T. and Zienkiewicz, O.C. (1975 –1988). Principal Editors. *Finite Elements in Fluids*, Volumes 1–7, Wiley Interscience, London.
Galerkin, B.G. (1915). "Series Occurring in Some Problems of Elastic Stability of Rods and Plates," *Eng. Bull.*, V19, pp. 897–908.
Gosman, A., Pun, W., Runchal, A., Spalding, D. and Wolfshtein, M. (1969). *Heat and Mass Transfer in Recirculating Flows*, Academic, London.
Gresho, P.M. and Sani, R.L. (1998). *Incompressible Flow and the Finite Element Method; Advection-Diffusion and Isothermal Laminar Flow*, Wiley, England.
Gunzburger, M.D. (1989). *Finite Element Methods for Viscous Incompressible Flows*, Academic, New York.
Harlow, F. (1971). "Fluid Dynamics – a LASL Monograph," Univ. Calif., LASL Technical Report LA-4700.
Hrenikoff, A. (1941). "Solution of Problems in Elasticity by the Frame Work Method." *J. Appl. Mechanics, ASME Trans.*, V8, pp. 169–175.
Huebner, K.H. (1975). *The Finite Element Method for Engineers*, Wiley, New York.
Lions, J.L. and Magenes, E. (1972). "Non-Homogeneous Boundary-Value Problems and Applications, Vol. I," (Trans., 1963 French edition by P. Kenneth), Springer-Verlag, Germany.
Lax, P. (1954). Weak Solutions of Nonlinear Hyperbolic Equations and their Numerical Computation," *Comm. Pure & Appl. Math*, V7, p. 159.
Lax, P. and Wendroff, B. (1960). Systems of Conservation Laws," *Comm. Pure & Applied Math*, V13, pp. 217–237.
Lynn, P.O. (1974). "Least Squares Finite Element Analysis of Laminar Boundary Layers," *J. Numerical Methods Engineer*, V8, p. 865.
MacCormack, R. (1969). "The Effect of Viscosity in Hypervelocity Impact Cratering," AIAA Technical Paper 69–354.
Oden, J.T. (1969). "Finite Element Applications in Fluid Dynamics," ASCE, *J. Engr. Mechanics Div.*, V95, EM3, pp. 821–826.
Oden, J.T. (1972). *Finite Elements of Nonlinear Continua*, McGraw-Hill, New York.
Oden, J.T. and Reddy, J.N. (1976). *Introduction to the Mathematical Theory of Finite Elements*, Wiley, New York.
Olson, M.E. (1972). "Formulation of a Variational Principle-Finite Element Method for Viscous Flows," *Proc. Variational Methods Engineering*, Southampton University, pp. 5.27–5.38.
Patankar, S.V. (1980). *Numerical Heat Transfer and Fluid Flow*, Hemisphere, Washington, DC.
Pinder, G.F. and Gray, W.G. (1977). *Finite Element Simulation in Surface and Subsurface Hydrology*, Academic, New York.
Piomelli, U. (1999). "Large Eddy Simulation: Achievements and Challenges," *Prog. Aerospace Sciences*, V35, pp. 335–362.
Pironneau, O. (1989). *Finite Element Methods for Fluids*, Wiley, Paris.
Popinski, Z. and Baker, A.J. (1974). "An Implicit Finite Element Algorithm for the Boundary Layer Equations," *J. Computational Physics*, V21, p. 55.
Rayleigh, J.W.S. (1877). *Theory of Sound*, 1st Edition Revised (1945), Dover, New York.
Reddy, J.N. and Gartling, D.K. (2001). *The Finite Element Method in Heat Transfer and Fluid Dynamics*, CRC Press, Boca Raton.
Richtmyer, R.D. and Morton, K.W. (1967). *Difference Methods of Initial-Value Problems*, 2nd Edition, Interscience, New York.
Ritz, W. (1909). "Uber Eine Neue Methode zur Losung Gewisser Variations-Probleme der Mathematischen Physik," *J. Reine Angew. Math.*, V135, p. 1.
Roache, P.J. (1972). *Computational Fluid Mechanics*, Hermosa Press, Albuquerque, NM.
Strang, G. and Fix, G.J. (1973). *An Analysis of the Finite Element Method*, Prentice Hall, Englewood Cliffs, NJ.
Turner, M., Clough, R., Martin, H. and Topp, L. (1956). "Stiffness and Deflection Analysis of Complex Structures," *J. Aeronautical Sciences*, V23(9), pp. 805–823.
Zienkiewicz, O.C. and Cheung, Y.K. (1965). "Finite Elements in the Solution of Field Problems," *The Engineer*, pp. 507–510.