
**The COMPUTATIONAL
ENGINEERING
SCIENCES**

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The COMPUTATIONAL ENGINEERING SCIENCES

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FOREWORD

The computer revolution has profoundly impacted how engineers and scientist conduct their professional activities. In the early 1960s, a computer fully occupied and amply heated (!) a space the size of a classroom. The PC was introduced in the mid-1970s as a “toy.” Yet by the millennia, Linux clusters of cheap gigahertz-gigabyte PCs can execute truly large scale computational simulations. Indeed, the “desktop Cray,” fantasized in ~1980, is here and is truly inexpensive!

The companion maturation of theory and practice in the computational engineering sciences has been an evolutionary (not revolutionary!) process. It remains highly fragmented by discipline, even though computational fluid dynamics (CFD) and computational structural mechanics (CSM) emerged simultaneously from the research laboratory in the late 1950s. The former relied on finite difference (FD) methods to convert theory to computable form. Conversely, the latter’s classical *virtual work* foundation enabled a calculus-based finite element (FE) theory implementation of the underlying variational principle extremum. Finally, in chemical engineering collocation methods were developed for process simulations, and at first glance these underlying theories appear absolutely “linearly independent.”

Research now completed has proven that practically all developments supporting the *computational engineering sciences* can be formulated from the *extremum* of the mathematician’s *weak form theory* termed a *weak statement* (WS). The weak form process enables *theorization* to be completed in the *continuum*, using calculus, vector field theory and modern approximation concepts. When finished, the discretized implementation of the theory extremum can be formed using FE, FD and/or finite volume (FV) procedures. The FE discrete implementation is typically guaranteed *optimal* in its performance, i.e., accuracy, asymptotic convergence rate, etc. Furthermore, FE methodology leads to *precise constructions* since the formal integral-differential calculus is used, rather than difference algebra, to generate the algebraic statement amenable to computing.

This text develops discrete FE implementation of WS theory for a diverse set of problem statements in the *computational engineering sciences*. Unique to these developments, the resulting FE *algorithms* are immediately rendered *computable* via a transparent, object-oriented programming syntax. The engineering science problem classes developed herein include

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- heat conduction,
- structural mechanics,
- mechanical vibrations,
- heat transfer, with convection and radiation,
- fluid mechanics, and
- heat and/or mass convective transport.

The text is organized into eleven chapters. Following an introduction, and some very pertinent overview material, a *tutorial* in elementary heat conduction clearly illustrates all element matrix constructs, the “famous” assembly algorithm and the concept of error estimation and measurement. Subsequent chapter pairs develop expository one-dimensional, then general n -dimensional, FE WS implementations in each continuum mechanics category. The sequence of developments serves to illustrate, examine and generalize the available theoretical error estimates, introducing in the process the concept of a *norm*. In moving to the convection-diffusion problem class, a sequence of Taylor series manipulations leads to a *modified* conservation principle form, still written in the *continuum*, the focus of which is to understand, hence moderate the action of *phase lag* and *dispersive error* mechanisms.

Incisive computer experiments complement each development, with principle focus to gain a firm usable understanding of approximation error mechanisms as associated with data non-smoothness, problem non-linearity, stability, dispersion error and boundary conditions, as impacted by the selected FE basis degree. The n -dimensional computer experiments focus more on design and validation issues, hence refinements for error nuances associated with non-convex boundaries, phase lag, and artificial *numerical diffusion*. An intervening brief chapter clearly identifies the connections between FD, FV and FE discrete implementations for a Poisson equation in 1- and n -dimensions.

Engineers are clearly of the opinion that “theory is fine, but show me the numbers!” which requires theory conversion to “code.” Since the FE implemented WS theory is so highly organized, the algorithm statement for any discipline ends up constituted of six, and *only* six, types of data to convert theory to practice. Capitalizing on *object-oriented* concepts, these six data types are organized in a *template* such that the “computing” statement, including explicit non-linearity, is unambiguously expressible. Templates for expository analyses employ Matlab as the *problem solving environment* (PSE), with the computer lab

solutions enabled via the DVD-included *toolbox*. The more comprehensive computer experiments employ script files for COMSOL, formerly FEMLAB, a commercial FE-based discipline-driven PSE.

In summary, this text fully develops modern FE discrete algorithms for the computational engineering sciences with applications aimed to available and emergent PSEs. Its organization and content has benefited from a decade and a half of teaching the material, and the resultant academic courses are now online at the UT CFD Laboratory (cfdlab.utk.edu/Internet). This text fully obsoletes the predecessor 1991 text *Finite Elements* 1-2-3, sold with a “spaghetti” Fortran PC code on a 5.25 inch floppy disk. The included DVD contains all computer exercise m-files and script files, the Matlab toolbox and select (time-dependent) color graphics of highly informative heat and mass transport verification and benchmark problem executions. It also contains select lectures, generated by the author on these subjects, amenable to video-streaming on your PC.

Many colleagues and graduate students have contributed to creation and refinement of the text content. I owe a deep debt of gratitude to my Computational Mechanics Corp. co-founders Paul Manhardt, who invented the template concept, and Joe Orzechowski, who designed assimilation of templates into reliable computational syntax for mainly CFD problems. The dissertations of Drs. Jin Kim, Subrata Roy, David Chaffin and Alexy Kolesnikov each contributed to the improved theoretical and practical understanding of FE algorithm performance nuances presented herein. Drs. Zac Chambers, Marcel Grubert and Sunil Sahu, along with Messrs. Mike Taylor and Shawn Ericson, have each contributed significantly to the polishing of these fundamental underlying precepts to pedagogical acceptability.

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a	expansion coefficient
A	plane area; one-dimensional FE matrix prefix; coefficient
$[A]$	factored global matrix
b	coefficient; boundary condition subscript; body force component
$\{b\}$	global data (load) matrix
B	two-dimensional FE matrix prefix
\mathbf{B}	body force
c	coefficient; specific heat
C	three-dimensional FE matrix prefix; source constant
d	coefficient; FE matrix indicator
D	diagonal matrix
$[DIFF]$	global diffusion matrix
e	element-dependent; unit vector component
$e(\cdot)$	error
e^N	approximation error
e^h	discrete approximation error
eta_{ji}	coordinate transformation data
E	energy seminorm (subscript), elastic modulus
\mathbf{E}	Hooke's law matrix
\mathbf{F}	applied force
f	flux magnitude on $\partial\Omega$
g	gravity magnitude
\mathbf{g}	gravity
G	elastic shear modulus
GWS	Galerkin weak statement
h	discretization (superscript), convective heat transfer coefficient
H	Gauss quadrature weight; Hilbert space
$[HBC]$	global convection matrix
i	summation index; mesh node
$\hat{\mathbf{i}}$	unit vector parallel to x
I	moment of inertia; element matrix summation index
j	summation index, mesh node
$\hat{\mathbf{j}}$	unit vector parallel to y
J	template summation index
$[J]$	coordinate transformation jacobian
$[JAC]$	matrix statement jacobian
k_{ij}	element of the $[DIFF]$ matrix
k	thermal conductivity; basis degree; index; diffusion coefficient

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\bar{k}	average value of conductivity
κ	thermal diffusivity
$\hat{\mathbf{k}}$	unit vector parallel to z
K	template matrix summation index
ℓ	element length; summation index
$\ell(\cdot)$	differential operator on $\partial\Omega$
L	one-dimensional domain span
$\mathcal{L}(\cdot)$	differential operator on Ω
m	integer
m_i	point mass
M	elements in Ω^h ; moment; matrix prefix; particle system mass
n	index; normal subscript; dimension of domain Ω ; integers
$\hat{\mathbf{n}}$	outward pointing unit vector normal to $\partial\Omega$
N	summation termination; approximation (superscript)
$\{N_k\}$	finite element basis of degree k
p	load (data); pressure
P	discretized nodal load; Gauss quadrature order
$\{P\}$	computational matrix
q	generalized dependent variable
Q	discretized dependent variable; heat added
$\{Q\}$	nodal coefficient column matrix
r	reference state subscript; radius
R	nodal radial coordinate
\mathfrak{R}^n	Euclidean space
$\{\text{RES}\}$	global matrix statement residual
s	source term on Ω ; heat added
\mathbf{s}	unit vector tangent to $\partial\Omega$
S	finite element assembly operator; entropy
$\{S\}$	computational matrix
t	time
T	temperature
\mathbf{T}	surface traction vector
T^N	approximate temperature solution
TWS	Taylor weak statement
\mathbf{u}	displacement vector; velocity vector
u	velocity x component; speed
U	discretized speed nodal value
[UVEL]	global fluid convection matrix

NOTATION v

v	velocity y component
V	shear force; volume; discrete nodal value
\mathbf{V}	velocity
w	weight function; fin thickness; velocity z component
W	weight; work done by system
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	discrete cartesian coordinate
z	cartesian coordinate
Z	thickness ratio; discrete cartesian coordinate
(\cdot)	scalar (number)
$\{\cdot\}$	column matrix
$\{\cdot\}^T$	row matrix
$[\cdot]$	square matrix
$\ \cdot\ $	norm
\cup	union (non-overlapping sum)
\cap	intersection
$\det [\cdot]$	matrix determinant
sym	symmetric
α	coefficient
β	coefficient
γ	coefficient
δ_{ij}	Kronecker delta
Δ	discrete increment
ε	normal strain
ϕ	electric potential, flow potential
$\phi(\cdot)$	trial space function; potential function
Φ	potential function
$\Phi_\beta(\mathbf{x})$	test space
$\Psi_\alpha(\mathbf{x})$	trial space
γ	shear strain
η	transform space
η_i	tensor product coordinate system
$\kappa_{\alpha\beta}$	element of a square matrix

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λ	Lamé parameter
μ	Lamé parameter
ν	Poisson ratio
$O(\cdot)$	order of (truncation error)
π	pi (3.1415926...)
θ	time integration implicitness factor
ρ	density
$d\sigma$	differential element on $\partial\Omega$
τ	normal stress
ω	frequency
Ω	domain of differential equation
Ω_e	finite element domain
Ω^h	discretization of Ω
$\partial\Omega$	boundary of Ω
ζ_α	natural coordinate system
$d(\cdot)/dx$	ordinary derivative
$\partial(\cdot)/\partial x$	partial derivative
∇	vector derivative
∇^2	laplacian derivative