A. J. BAKER

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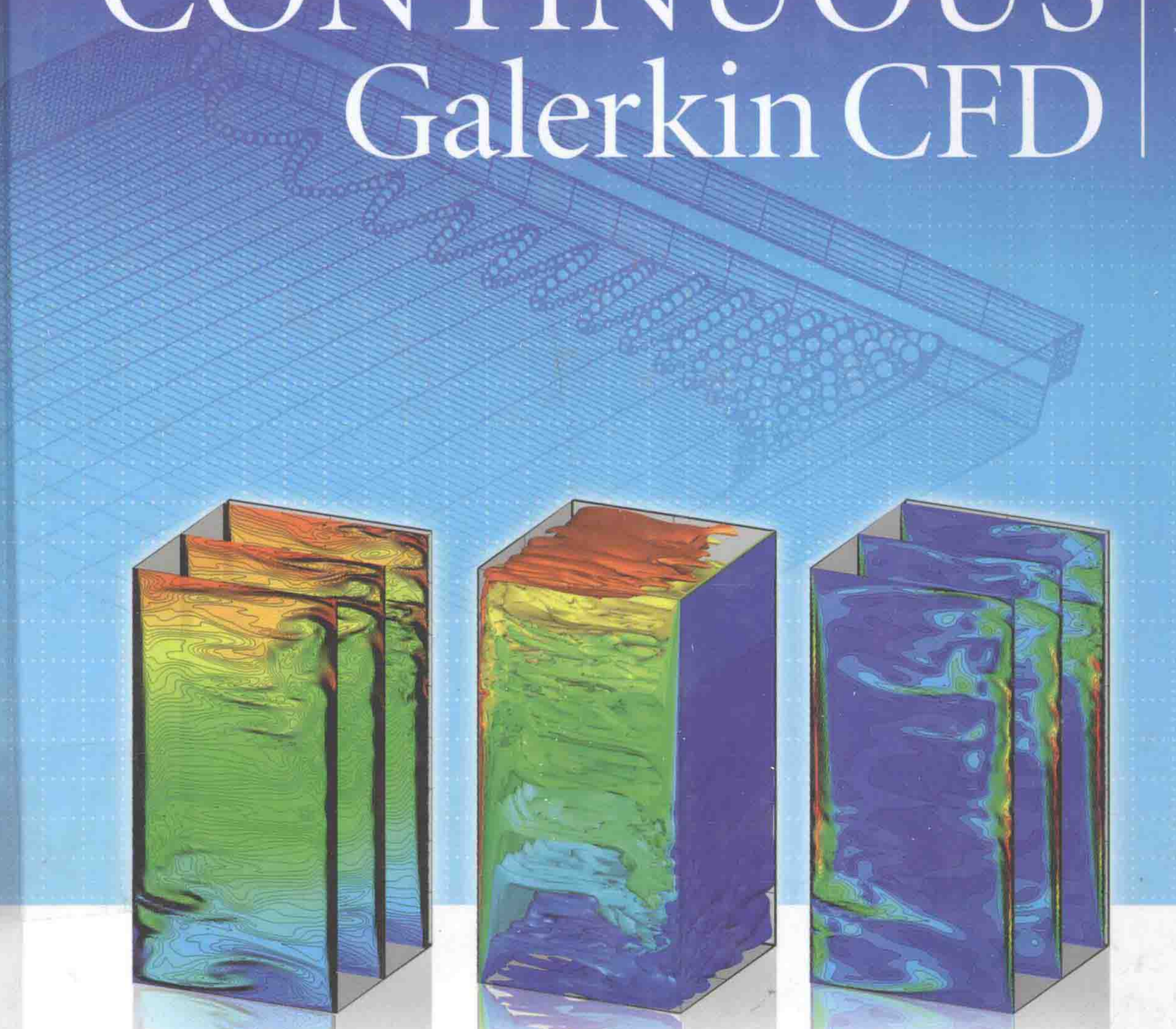

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Yogi Berra is quoted,
"If you come to a fork in the road take it."
With Mary Ellen's agreement,
following this guidance
I found myself at the
dawning of weak form CFD

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 *m*odified PDE (*m*PDE) 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 *m*PDE 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 (*ar*LES) for the full tensor quadruple is derived via union of rational LES (RLES) and *m*PDE theories. Thus is generated an $O(1, \delta^2, \delta^3)$ member state variable for gaussian filter uniform measure δ *a priori* defining unresolved scale threshold. Extended to bounded domains, *ar*LES 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 *ar*LES theory is validated applicable $\forall$ Re, generates δ-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"

(VVUQ). Observed in context is replacement of legacy CFD algorithm numerical diffusion formulations with proven *m*PDE operand superior performance. More fundamental is the ∀Re model-free *ar*LES 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 *ar*LES 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(•)	bilinear form
B	body force
BC	boundary condition
BCE	boundary commutation error integral
BHE	borehole heat exchanger
BiSec	bisected borehole heat exchanger
BL	boundary layer
c	coefficient; specific heat
c	phase velocity vector
C	3-D matrix prefix; coefficient; chord; Courant number $\equiv U\Delta t/\Delta x$
C_{ij}	cross stress tensor
C_p	aerodynamic pressure coefficient, $= p/\rho u^2/2$
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(•)	ordinary derivative, differential element
d	coefficient; FE matrix basis degree label, RSM distance; characteristics coefficient
D	binary diffusion coefficient; diagonal matrix

D	dimensionality, non-D diffusion coefficient $\equiv \Delta t/\mathrm{Pa}h^2$
$D(\bullet)$	differential definition
$\mathrm{D}(\bullet)$	substantial derivative
$\mathrm{D}^{\mathrm{m}}(\bullet)$	modified substantial derivative
DES	detached eddy simulation
DE	conservation of energy PDE
DG	discontinuous Galerkin weak form theory
DM	conservation of mass PDE
D$\mathbf{P}$	conservation of momentum PDE
DY	conservation of species mass fraction PDE
$\mathbf{D}(\mathbf{u}, P)$	NS full stress tensor, $\equiv -\nabla P + (2/\mathrm{Re})\nabla \cdot \mathbf{S}(\mathbf{u})$
diag[•]	diagonal matrix
[DIFF]	laplacian diffusion matrix
DNS	direct numerical simulation
e	specific internal energy; element-dependent (subscript)
$e(\cdot)$	error
e^N	continuum approximation error
e^h	discrete approximation error
e_{ijk}	alternating tensor
e_{KL}	curl alternator on $n=2$
EBV	elliptic boundary value
Ec	Eckert number
eta_{ji}	coordinate transformation data
E	thermal energy; energy semi-norm (subscript)
f_j	flux vector
f_n	normal flux
$f(\bullet)$	function of the argument
$f(\mathrm{vf}, \epsilon)$	radiation *view factor*
$F(\bullet)$	Fourier transform
{F}	weak form terminal algebraic statement
$F(k \rightarrow i)$	Lambert's cosine law viewfactor
FD	finite difference
FE	finite element
FV	finite volume
$\mathbf{f}$	efflux vector on $\partial\Omega$
$\mathbf{F}$	applied force
g	gravity magnitude; amplification factor; spatial filter function; characteristics enthalpy ratio
$\mathbf{g}$	gravity
Gr	Grashoff number $\equiv \mathrm{g}\beta\Delta \mathrm{TL}^3/\nu^2$
$G_{k\rightarrow i}$	Gebhart viewfactor
GHP	ground source heat pump
GLS	Galerkin least squares algorithm
GWS	Galerkin weak statement
h	mesh measure; discrete (superscript), heat transfer coefficient
H	boundary layer shape factor

H	Gauss quadrature weight; Hilbert space
$H.O.T.$	truncated Taylor series higher order terms
i	summation index; mesh node
$\hat{\mathbf{i}}$	unit vector parallel to x
I	discrete matrix summation index, identity matrix
iff	if and only if
I-EBV	initial-elliptic boundary value
j	summation index, mesh node
$\hat{\mathbf{j}}$	unit vector parallel to y
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 [DIFF] matrix
$\bar{k}$	average value of conductivity
$\hat{\mathbf{k}}$	unit vector parallel to z
K	discrete matrix summation index
ℓ	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 Ω
L_{ij}	Leonard stress tensor
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 Ω^h
M_i	molecular mass
[M]	*m*PDE theory altered mass matrix
Ma	Mach number
*m*GWS	optimal modified Galerkin weak form
*m*PDE	modified partial differential equation
*m*ODE	modified ordinary differential equation
MLT	mixing length theory
n	index; normal subscript; dimension of domain Ω; integer
n-D	n-dimensional, $1 \leq n \leq 3$
$\hat{\mathbf{n}}$	outward pointing unit vector normal to $\partial\Omega$
N	Neumann BC matrix prefix
N	summation termination; approximation (superscript)
NC	natural coordinate basis
NWM	near wall modeling LES BCs
NWR	near wall resolution LES algorithm
NS	Navier–Stokes
$\{N_k\}$	finite element basis of degree k
$O(\bullet)$	order of argument $(\bullet)$

p	pressure
P	kinematic pressure
P	Gauss quadrature order
$\mathbf{P}$	linear momentum
Pa	placeholder for non-D groups Re, Pr, Gr, Ec
$\{P\}$	intermediate computed matrix
PDE	partial differential equation
Pe	Peclet number = RePr
PNS	parabolic Navier–Stokes
PRaNS	hypersonic parabolic Reynolds-averaged Navier–Stokes
Pr	Prandtl number $\equiv \rho_0 \nu c_p / k$
pr	non-uniform mesh progression ratio
q	generalized dependent variable
$\mathbf{q}$	heat flux vector
Q	discretized dependent variable; heat added
$\{Q\}$	nodal coefficient column matrix
r	reference state subscript; radius
R	perfect gas constant, temperature degrees Rankine
R	radiosity
$\mathcal{R}$	universal gas constant
R_{ij}	Reynolds subfilter scale tensor
RaNS	Reynolds-averaged Navier–Stokes
Re	Reynolds number $\equiv$ UL/ν
Re^t	turbulent Reynolds number $\equiv \nu^t / \nu$
Re$^+$	compressible turbulent BL similarity coordinate $= \rho u_\tau y / \mu$
$\Re^n$	euclidean space of dimension n
RSM	Reynolds stress model
{RES}	weak form terminal matrix statement residual
s	source term on Ω; heat added
$\mathbf{s}$	unit vector tangent to $\partial\Omega$
S	entropy
$\overline{\mathbf{S}}$	filtered Stokes tensor dyadic
S_e	matrix assembly operator
$S_{i,j,k}$	stencil assembly operator
{S}	computational matrix
Sc	Schmidt number $\equiv$ D/ν
SFS$_{ij}$	subfilter scale tensor
SGS$_{ij}$	subgrid scale tensor
St	Stanton number $\equiv \tau$U/L
SUPG	Streamline upwind Petrov Galerkin
sym	symmetric
t	time; turbulent (superscript)
T	temperature
$\overline{T}(z)$	BHE conduit temperature distribution
TE	Taylor series truncation error
TG	Taylor Galerkin algorithm

TP	tensor product basis
T	surface traction vector
T^N	continuum approximate temperature solution
TWS	Taylor weak statement
u	displacement vector; velocity vector
u	velocity x component; speed
$\overline{u_i'u_j'}$	time averaged NS Reynolds stress tensor
$\tilde{u}_j$	Favre time averaged velocity
U	reference velocity scale
UQ	uncertainty quantification
U	discretized speed nodal value
v	velocity y component
$\mathbf{v}_g(\boldsymbol{\kappa})$	group velocity, $\equiv \nabla_\kappa \omega$
v_j	LES theory scalar state variable closure vector
V	volume
VBV	verification, benchmarking, validation
VVUQ	verification, validation, uncertainty quantification
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 $= u_\tau y/\nu$
Y	mass fraction; discrete cartesian coordinate
z	cartesian coordinate
Z	thickness ratio; discrete cartesian coordinate
∇	gradient differential operator
∇^2	laplacian operator
$\mathrm{d}(\cdot)/\mathrm{d}x$	ordinary derivative
$\partial(\cdot)/\partial x$	partial derivative
$(\cdot)$	scalar (number)
$\{\cdot\}$	column matrix
$\{\cdot\}^T$	row matrix
$[\cdot]$	square matrix
$\mathrm{diag}[\cdot]$	diagonal square matrix
$\lVert\cdot\rVert$	norm
$\cup$	union (non-overlapping sum)
$\cap$	intersection
$\det\,[\cdot]$	matrix determinant
$\forall$	denotes "for all"

$\in$	inclusion
$\subset$	belongs to
$*$	complex conjugate multiplication
$\otimes$	matrix tensor product
α	coefficient, thermal diffusivity ratio
β	absolute temperature; coefficient
γ	specific heat ratio, coefficient, gaussian filter shape factor
δ	boundary layer thickness, coefficient, spatial filter measure, bow shock standoff distance
δ^*	boundary layer displacement thickness
δ_{ij}	Kronecker delta
Δ	discrete increment
ϵ	isotropic dissipation function. emissivity
ϵ_{ij}	cartesian alternator
ϕ	velocity potential function
$\phi(\cdot)$	trial space function
Φ	potential function
$\Phi_{\beta}(\mathbf{x})$	test space
$\Psi_{\alpha}(\mathbf{x})$	trial space
$\boldsymbol{\Psi}$	vector streamfunction
ψ	streamfunction scalar component
η	transform space, wave vector angle
η_i	tensor product coordinate system
κ	thermal diffusivity, Karman constant = 0.435
κ^T	turbulent thermal diffusivity
$\boldsymbol{\kappa}$	wavenumber vector
$\boldsymbol{\kappa}_{\alpha\beta}$	element of a square matrix
λ	Lagrange multiplier, wavelength, Lame' parameter
μ	absolute viscosity
ν	kinematic viscosity
ν^t	kinematic eddy viscosity
π	pi (3.1415926. . .)
θ	TS implicitness factor, BL momentum thickness
Θ	potential temperature $\equiv (T - T_{min})/(T_{max} - T_{min})$
ρ	density
σ	Stefan-Boltzmann coefficient = 5.67 E-08 w/m^2K^4
$d\sigma$	differential element on $\partial\Omega$
τ	time scale
τ_{ij}	Reynolds stress tensor
τ_{ij}^D	deviatoric Reynolds stress tensor
ω	frequency, Van Driest damping function, vorticity scalar
$\boldsymbol{\Omega}$	vorticity vector
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

Contents