David A. Kopriva

## Implementing Spectral Methods for Partial Differential Equations

Algorithms for Scientists and Engineers



## Contents

Pref	ace		vii				
Part	I	Approximating Functions, Derivatives and Integrals					
1	Spec	tral Approximation	3				
	1.1	Preamble: Series Solution of PDEs	3				
	1.2	The Fourier Basis Functions and Fourier Series	4				
	1.3	Series Truncation	6				
	1.4	Modal vs. Nodal Approximation	11				
	1.5	Discrete Orthogonality and Quadrature	11				
	1.6	Fourier Interpolation	14				
		1.6.1 Direct Computation of the Fourier Interpolation	17				
		1.6.2 Error of the Fourier Interpolation	19				
	1.7	The Derivative of the Fourier Interpolant	21				
	1.8	Polynomial Basis Functions	23				
		1.8.1 The Legendre Polynomials	24				
		1.8.2 The Chebyshev Polynomials	25				
	1.9	Polynomial Series	26				
	1.10	Polynomial Series Truncation	28				
		1.10.1 Derivatives of Truncated Series	30				
	1.11	Polynomial Quadrature	31				
	1.12	Orthogonal Polynomial Interpolation	35				
2	Algo	rithms for Periodic Functions	39				
	2.1	How to Compute the Discrete Fourier Transform	39				
		2.1.1 Fourier Transforms of Complex Sequences	40				
		2.1.2 Fourier Transforms of Real Sequences	43				
		2.1.3 The Fourier Transform in Two Space Variables	48				
	2.2	The Real Fourier Transform	50				
	2.3	How to Evaluate the Fourier Interpolation Derivative by FFT	53				
	2.4	How to Compute Derivatives by Matrix Multiplication	54				
3	Algo	rithms for Non-Periodic Functions					
	3.1	How to Compute the Legendre and Chebyshev Polynomials	59				
	3.2	How to Compute the Gauss Quadrature Nodes and Weights	62				
		3.2.1 Legendre Gauss Quadrature	62				
		3.2.2 Legendre Gauss-Lobatto Quadrature	64				
		3.2.3 Chebyshev Gauss Quadratures	67				
	3.3	How to Evaluate Chebyshev Interpolants via the FFT	67				
	5.5	3.3.1 The Fast Chebyshev Transform	68				
	3.4	How to Evaluate Polynomial Interpolants in Lagrange Form	73				
	5.4	now to Evaluate i orynomial merpolants in Eagrange i offit	, ,				

## Contents

	3.5	How to Evaluate Polynomial Derivatives	78
		3.5.1 Direct Evaluation of the Derivative	
		3.5.2 Evaluation of Derivatives by Matrix Multiplication	
		3.5.4 Evaluation by Transform Methods	
		3.5.5 Performance of Various Polynomial Derivative Algorithms	84
Par	t II	Approximating Solutions of PDEs	
	0		01
4		vey of Spectral Approximations	
	4.1	The Fourier Collocation Method	
		4.1.1 How to Implement the Fourier Collocation Method	
		4.1.2 Benchmark Solution	
	4.2	The Fourier Galerkin Method	
		4.2.1 How to Implement the Fourier Galerkin Method	103
		4.2.2 Benchmark Solution	
	4.3	Nonlinear and Product Terms	
		4.3.1 The Galerkin Approximation	
		4.3.2 How to Compute the Convolution Sum	
		4.3.3 The Collocation Approximation	
	4.4	Polynomial Collocation Methods	
		4.4.1 Approximation of the Diffusion Equation	
		4.4.2 How to Implement the Methods	
		4.4.3 Benchmark Solution	
		4.4.4 Approximation of Scalar Advection	
	4.5	The Legendre Galerkin Method	123
		4.5.1 How to Implement the Method	. 127
	4.6	The Nodal Continuous Galerkin Method	129
		4.6.1 How to Implement the Method	
		4.6.2 Benchmark Solution	
	4.7	The Nodal Discontinuous Galerkin Method	
	1.7	4.7.1 How to Implement the Method	
		4.7.1 How to implement the method	
	4.0		
	4.8	Summary and Some Broad Generalizations	144
5	Spe	ctral Approximation on the Square	149
		Approximation of Functions in Multiple Space Dimensions	
	5.2	Potential Problems on the Square	
	0.2	5.2.1 The Collocation Approximation	
	5.2		
	5.3	Approximation of Time Dependent Advection-Diffusion	
		5.3.1 The Collocation Approximation	
		5.3.2 The Nodal Galerkin Approximation	
		5.3.3 Time Integration	
		5.3.4 How to Implement the Approximations	. 193
		5.3.5 Benchmark Solution: Advection and Diffusion of a Spot	
		in a Uniform Flow	200

x

Contents
----------

x	1
~	•

	5.4	Appro	ximation of Wave Propagation Problems	202
		5.4.1	The Nodal Discontinuous Galerkin Approximation	204
		5.4.2	How to Implement the Nodal Discontinuous Galerkin	
			Approximation	212
		5.4.3	Benchmark Solution: Plane Wave Propagation	
		5.4.4	Benchmark Solution: Propagation of a Circular Sound Wave	
6	Trai	nsforma	tion Methods from Square to Non-Square Geometries	223
	6.1	Mappi	ngs and Coordinate Transformations	223
		6.1.1	Mapping a Straight Sided Quadrilateral	224
		6.1.2	How to Approximate Curved Boundaries	225
		6.1.3	How to Map the Reference Square to a Curved-Sided	
			Quadrilateral	229
	6.2	Transfe	ormation of Equations under Mappings	
		6.2.1	Two-Dimensional Forms	
	6.3	How to	Approximate the Metric Terms	
	6.4		Compute the Metric Terms	
7	Spec	ectral Methods in Non-Square Geometries		
	7.1	Steady	Potentials in a Quadrilateral Domain	247
		7.1.1	The Collocation Approximation	247
		7.1.2	The Nodal Galerkin Approximation	252
		7.1.3	Solution of the Linear Systems	254
		7.1.4	Benchmark Solution: Potential in Non-Square Domains	
		7.1.5	Benchmark Solution: Incompressible Flow over a Circular	
			Obstacle	261
	7.2	Steady	Potentials in an Annulus	
		7.2.1	Benchmark Solution: Potential in an Annulus with a Source	
	7.3	Advect	ion and Diffusion in Quadrilateral Domains	
		7.3.1	Transformation of the Advection-Diffusion Equation	
		7.3.2	The Collocation Approximation	
		7.3.3	The Nodal Galerkin Approximation	
		7.3.4	How to Implement the Approximations	
		7.3.5	Benchmark Solution: Advection and Diffusion	275
		7.5.5	in a Non-Square Geometry	276
		7.3.6	Benchmark Solution: Advection and Diffusion	270
		7.5.0	of a Pollutant in a Curved Channel	277
	7.4	Conser	vation Laws in Quadrilateral Domains	
	7.4	7.4.1	The Nodal Discontinuous Galerkin Approximation	
		7.4.2	How to Implement the Nodal Discontinuous Galerkin	200
		1.4.2	Approximation	282
		712	Benchmark Solution: Acoustic Scattering off a Cylinder	
		7.4.3	Denominark Solution: Acoustic Scattering on a Cymider	285
8	Snec	tral Ele	ment Methods	293
U	8.1 Spectral Element Methods in One Space Dimension			
	0.1	8.1.1	The Continuous Galerkin Spectral Element Method	
		0,1.1	The Conditions Suferkin Speedur Element Method	

Contents

		8.1.2	How to Implement the Continuous Galerkin Spectral Element Method	301
		8.1.3	Benchmark Solution: Cooling of a Temperature Spot	. 305
		8.1.4 8.1.5	The Discontinuous Galerkin Spectral Element Method How to Implement the Discontinuous Galerkin Spectral	
			Element Method	. 310
	_	8.1.6	Benchmark Solution: Wave Propagation and Reflection	
	8.2		wo-Dimensional Mesh and Its Specification	
		8.2.1	How to Construct a Two-Dimensional Mesh	
	0.0	8.2.2	Benchmark Solution: A Spectral Element Mesh for a Disk	
	8.3		pectral Element Method in Two Space Dimensions	
		8.3.1	How to Implement the Spectral Element Method	. 331
		8.3.2	Benchmark Solution: Steady Temperatures in a Long	240
	0.4	T1 D	Cylindrical Rod	
	8.4		iscontinuous Galerkin Spectral Element Method	. 341
		8.4.1	How to Implement the Discontinuous Galerkin Spectral	212
		8.4.2	Element Method	. 343
		ð.4. <i>2</i>	in a Circular Domain	. 344
		8.4.3	Benchmark Solution: Transmission and Reflection from	. 544
		0.4.3	a Material Interface	. 347
A	Pseu	idocodo	e Conventions	. 355
B	Floa	nting Po	oint Arithmetic	. 359
С	Basi	ic Linea	ar Algebra Subroutines (BLAS)	. 361
D	Line	ear Solv	vers	. 363
	D.1	Direct	Solvers	
		D.1.1	Tri-Diagonal Solver	
		D.1.2	LU Factorization	
	D.2	Iterati	ve Solvers	. 368
E	Data Structures			
	E.1		d Lists	
		E.1.1	Example: Elements that Share a Node	
	E.2	Hash '	-	
		E.2.1	Example: Avoiding Duplicate Edges in a Mesh	
Ref	ferenc	es.		. 385
Ind	lex of	Algorif	thms	. 387
Suł	ject ]	ndex .		. 389

xii