

Contents

1. Introduction	7
1.1 Why Do We Need Meshfree Particle Methods ?	7
1.2 Preliminary	12
1.2.1 Notation	12
1.2.2 Partition of Unity	14
1.2.3 Window Function and Mollifier	15
1.2.4 Hilbert Space	16
1.2.5 Variational Weak Formulation	18
1.2.6 Galerkin Methods	19
1.2.7 Time-stepping Algorithms	20
1.2.8 Voronoi Diagram and Delaunay Tessellation	22
2. Smoothed Particle Hydrodynamics (SPH)	25
2.1 SPH Interpolation	26
2.1.1 Delta Function	26
2.1.2 SPH Averaging Operator	26
2.1.3 Kernel Functions	28
2.1.4 Choice of Smoothing Length h	30
2.2 Approximation Theory of SPH	31
2.2.1 SPH Approximation Rules	31
2.2.2 SPH Approximations of Derivatives (Gradients)	33
2.3 Discrete Smooth Particle Hydrodynamics	36
2.3.1 Conservation Laws in Continuum Mechanics	36
2.3.2 SPH Continuity Equation	37
2.3.3 SPH Momentum Equation	38
2.3.4 SPH Energy Equation	39
2.3.5 SPH Artificial Viscosity	39
2.3.6 Time Integration of SPH Conservation Laws	42
2.3.7 SPH Constitutive Update	43
2.4 Invariant Properties of SPH Equations	44
2.4.1 Galilean Invariance	44
2.4.2 Conservation of Mass	45
2.4.3 Conservation of Linear Momentum	45
2.4.4 Conservation of Angular Momentum	46

2.4.5	Conservation of Mechanical Energy	47
2.4.6	Variational SPH Formulation	47
2.5	Corrective SPH and Other Improvements on SPH	50
2.5.1	Enforcing the Essential Boundary Condition	50
2.5.2	Tensile Instability	52
2.5.3	SPH Interpolation Error	55
2.5.4	Correction Function (RKPM)	56
2.5.5	Moving Least Square Hydrodynamics (MLSPH)	61
2.5.6	Johnson-Beissel Correction	62
2.5.7	Randles-Libersky Correction	63
2.5.8	Krongauz-Belytschko Correction	63
2.5.9	Chen-Beraun Correction	64
2.6	Remarks	65
	Exercises	66
3.	Meshfree Galerkin Methods	68
3.1	Moving Least Square Reproducing Kernel Interpolant	68
3.1.1	Polynomial Reproducing Property	72
3.1.2	The Shepard Interpolant	74
3.1.3	Interpolating Moving Least Square Interpolant	75
3.1.4	Orthogonal Basis for the Local Approximation	79
3.1.5	Examples of RKPM Kernel Function	80
3.1.6	Conservation Properties of RKPM Interpolant	88
3.1.7	One-dimensional Model Problem	91
3.1.8	Program Description	94
3.2	Meshfree Wavelet Interpolant	96
3.2.1	Variation in a Theme: Generalized Moving Least Square Reproducing Kernel	96
3.2.2	Interpolation Formulas	101
3.2.3	Hierarchical Partition of Unity and Hierarchical Basis ..	103
3.3	MLS Interpolant and Diffuse Element Method	109
3.3.1	Diffuse Element Method	109
3.3.2	Evaluate the Derivative of MLS Interpolant	109
3.4	Element-free Galerkin Method (EFGM)	111
3.4.1	Lagrangian Multiplier Method	111
3.4.2	Penalty Method	113
3.4.3	Nitsche's Method	114
3.4.4	Transform Method	116
3.4.5	Boundary Singular Kernel Method	120
3.4.6	Coupled Finite Element and Particle Approach	121
3.5	H-P Clouds Method	123
3.6	The Partition of Unity Method (PUM)	125
3.6.1	Examples of Partition of Unity	126
3.6.2	Examples of PUM Interpolants	127
3.7	Meshfree Quadrature and Finite Sphere Method	128

3.7.1	Cubature on Annular Sectors in \mathbb{R}^2	132
3.8	Meshfree Local Petrov-Galerkin (MLPG) Method	133
3.9	Finite Point Method	135
3.10	Meshfree Local Boundary Integral Equation	137
3.11	Meshfree Quadrature and Nodal Integration	138
4.	Approximation Theory of Meshfree Interpolants	142
4.1	Requirements and Properties of Meshfree Discretization	142
4.1.1	Regularity of Particle Distributions	143
4.1.2	Bounds on Shape Functions and Their Derivatives	152
4.2	Completeness and Consistency of Meshfree Interpolants	154
4.2.1	p-th Order Consistency Condition	155
4.2.2	Differential Consistency Conditions	157
4.3	Meshfree Interpolation Error Estimate	160
4.3.1	Local Interpolation Estimate	160
4.4	Convergence of Meshfree Galerkin Procedures	165
4.4.1	The Neumann Boundary Value Problem (BVP)	165
4.4.2	The Dirichlet Boundary Value Problem	169
4.4.3	Numerical Examples	172
4.5	Approximation Theory of Meshfree Wavelet Functions	177
4.5.1	The Generalized Consistency Conditions	177
4.5.2	Interpolation Estimate	181
5.	Applications	187
5.1	Explicit Meshfree Computations in Large Deformation	187
5.2	Meshfree Simulation of Large Deformation	192
5.2.1	Simulations of Large Deformation of Thin Shell Structures	192
5.2.2	J_2 Hypoelastic-plastic Material at Finite Strain	194
5.2.3	Hemispheric Shell under Concentrated Loads	196
5.2.4	Crash Test of a Boxbeam	198
5.3	Simulations of Strain Localization	201
5.3.1	Model Problems	201
5.3.2	Mesh-alignment Sensitivity	201
5.3.3	Meshfree Techniques for Simulations of Strain Localization	205
5.3.4	Adaptive Procedures	210
5.4	Simulations of Dynamics Shearband Propagation	215
5.4.1	Thermal-viscoplastic Model	217
5.4.2	Constitutive Modeling in Post-bifurcation Phase	221
5.4.3	Numerical Examples	223
5.4.4	Case I: Intermediate Speed Impact ($V = 30$ m/s)	224
5.4.5	Case II: High Speed Impact ($V = 33$ m/s)	228
5.5	Simulations of Crack Growth	228
5.5.1	Visibility Condition	228

5.5.2	Crack Surface Representation and Particle Splitting Algorithm	231
5.5.3	Parametric Visibility Condition	233
5.5.4	Reproducing Enrichment Technique	238
5.6	Meshfree Contact Algorithm	241
5.6.1	Contact Detection Algorithm	241
5.6.2	Examples of Contact Simulations	247
5.7	Meshfree Simulations of Fluid Dynamics	249
5.7.1	Meshfree Stabilization Method	249
5.7.2	Multiscale Simulation of Fluid Flows	255
5.8	Implicit RKPM Formulation	258
5.8.1	The Governing Equations	258
5.8.2	Essential Boundary Conditions	260
5.8.3	Discretization of the Weak Form	263
5.8.4	Time Integration Scheme	264
5.8.5	Communication Structure	266
5.8.6	Partitioning Schemes	268
5.8.7	Outline of Procedures	268
5.9	Numerical Examples of Meshfree Simulations	269
5.9.1	Simple 3-D Flow Past a Circular Cylinder	269
5.9.2	3-D Flow past a Building	270
6.	Reproducing Kernel Element Method (RKEM)	276
6.1	Introduction	276
6.2	Reproducing Kernel Element Interpolant	278
6.2.1	Global Partition Polynomials	278
6.2.2	Some Properties	283
6.2.3	Error Analysis of the Method with Linear Reproducing Property	288
6.2.4	Numerical Examples	291
6.3	Globally Conforming I^m/C^n Hierarchies	299
6.4	Globally Conforming I^m/C^n Hierarchy I	300
6.4.1	1D I^2/C^n Interpolation	304
6.4.2	2D I^0/C^n Quadrilateral Element	305
6.4.3	Globally Compatible Q12P1I1 Quadrilateral Element	308
6.4.4	Globally Compatible Q16P2I2 Quadrilateral Element	310
6.4.5	Smooth I^0/C^n Triangle Element	311
6.4.6	Globally Compatible T9P1I1 Triangle Element	313
6.4.7	Globally Compatible T18P2I2 Triangle Element	315
6.5	Globally Conforming I^m/C^n Hierarchy II	317
6.5.1	Construction	317
6.5.2	1D Example: An $I^1/C^4/P^3$ Interpolant	320
6.5.3	2D Example I: Compatible Gallagher Element	322
6.5.4	2D Example II: $T12P3I(4/3)$ Triangle Element	323
6.5.5	2D Example III: Q12P3I1 Quadrilateral Element	326

6.6	Numerical Examples	328
6.6.1	Equilateral Triangular Plate	328
6.6.2	Clamped Circular Plate	331
7.	Molecular Dynamics and Multiscale Methods	333
7.1	Classical Molecular Dynamics	333
7.1.1	Lagrangian Equations of Motion	334
7.1.2	Hamiltonian Equations of Motion	336
7.1.3	Interatomic Potentials	338
7.1.4	Two-body (pair) Potentials	339
7.1.5	Energetic Link between MD and Quantum Mechanics ..	343
7.2	Ab initio Methods	346
7.2.1	Density Functional Theory	349
7.2.2	Ab initio Molecular Dynamics	350
7.2.3	Tight Binding Method	351
7.2.4	Numerical Examples	352
7.3	Coupling between MD and FEM	355
7.3.1	MAAD	355
7.3.2	MD/FE Coupling - 1D Example	357
7.3.3	Quasicontinuum Method and Cauchy-Born Rule	365
7.3.4	Cauchy-Born Numerical Examples	370
7.3.5	Multi-scale Algorithms	373
7.3.6	Generalized Langevin Equation	376
7.3.7	Multiscale Boundary Conditions	379
7.4	Introduction to Bridging Scale Method	385
7.4.1	Multiscale Equations of Motion	388
7.4.2	Langevin Equation for Bridging Scale	390
7.4.3	Staggered Time Integration Algorithm	395
7.4.4	Bridging Scale Numerical Examples	396
7.5	Applications	398
7.5.1	Two-dimensional Wave Propagation	400
7.5.2	Dynamic Crack Propagation in Two Dimensions	405
7.5.3	Simulations of Nanocarbon Tubes	413
8.	Immersed Meshfree/Finite Element Method and Applica-	
	tions	422
8.1	Introduction	422
8.2	Formulations of Immersed Finite Element Method	423
8.3	Computational Algorithm	426
8.4	Application to Biological Systems	427
8.4.1	Three Rigid Spheres Falling in a Tube	428
8.4.2	20 Soft Spheres Falling in a Channel	429
8.4.3	Fluid-flexible Structure Interaction	429
8.4.4	IFEM Coupled with Protein Molecular Dynamics	432
8.4.5	Cell-cell Interaction and Shear Rate Effects	434

8.4.6	Micro- and Capillary Vessels	435
8.4.7	Adhesion of Monocytes to Endothelial Cells	437
8.4.8	Flexible Valve-viscous Fluid Interaction	439
9.	Other Meshfree Methods	440
9.1	Natural Element Method	440
9.1.1	Construction of Natural Neighbor	440
9.1.2	Natural Neighbor Interpolation	441
9.2	Meshfree Finite Difference Methods	443
9.3	Vortex-in-cell Methods	446
9.4	Material Point Method (Particle-in-cell Method)	448
9.5	Lattice Boltzmann Method	449
	References	453
10.	Program Listings	479



<http://www.springer.com/978-3-540-22256-9>

Meshfree Particle Methods

Li, S.; Liu, W.K.

2004, IV, 502 p., Hardcover

ISBN: 978-3-540-22256-9