

Ernst Hairer
Christian Lubich
Gerhard Wanner

Geometric Numerical Integration

Structure-Preserving Algorithms
for Ordinary Differential Equations

Second Edition

With 146 Figures

 Springer

Table of Contents

I.	Examples and Numerical Experiments	1
I.1	First Problems and Methods	1
I.1.1	The Lotka–Volterra Model	1
I.1.2	First Numerical Methods	3
I.1.3	The Pendulum as a Hamiltonian System	4
I.1.4	The Störmer–Verlet Scheme	7
I.2	The Kepler Problem and the Outer Solar System	8
I.2.1	Angular Momentum and Kepler’s Second Law	9
I.2.2	Exact Integration of the Kepler Problem	10
I.2.3	Numerical Integration of the Kepler Problem	12
I.2.4	The Outer Solar System	13
I.3	The Hénon–Heiles Model	15
I.4	Molecular Dynamics	18
I.5	Highly Oscillatory Problems	21
I.5.1	A Fermi–Pasta–Ulam Problem	21
I.5.2	Application of Classical Integrators	23
I.6	Exercises	24
II.	Numerical Integrators	27
II.1	Runge–Kutta and Collocation Methods	27
II.1.1	Runge–Kutta Methods	28
II.1.2	Collocation Methods	30
II.1.3	Gauss and Lobatto Collocation	34
II.1.4	Discontinuous Collocation Methods	35
II.2	Partitioned Runge–Kutta Methods	38
II.2.1	Definition and First Examples	38
II.2.2	Lobatto IIIA–IIIB Pairs	40
II.2.3	Nyström Methods	41
II.3	The Adjoint of a Method	42
II.4	Composition Methods	43
II.5	Splitting Methods	47
II.6	Exercises	50

III.	Order Conditions, Trees and B-Series	51
III.1	Runge–Kutta Order Conditions and B-Series	51
III.1.1	Derivation of the Order Conditions	51
III.1.2	B-Series	56
III.1.3	Composition of Methods	59
III.1.4	Composition of B-Series	61
III.1.5	The Butcher Group	64
III.2	Order Conditions for Partitioned Runge–Kutta Methods	66
III.2.1	Bi-Coloured Trees and P-Series	66
III.2.2	Order Conditions for Partitioned Runge–Kutta Methods	68
III.2.3	Order Conditions for Nyström Methods	69
III.3	Order Conditions for Composition Methods	71
III.3.1	Introduction	71
III.3.2	The General Case	73
III.3.3	Reduction of the Order Conditions	75
III.3.4	Order Conditions for Splitting Methods	80
III.4	The Baker–Campbell–Hausdorff Formula	83
III.4.1	Derivative of the Exponential and Its Inverse	83
III.4.2	The BCH Formula	84
III.5	Order Conditions via the BCH Formula	87
III.5.1	Calculus of Lie Derivatives	87
III.5.2	Lie Brackets and Commutativity	89
III.5.3	Splitting Methods	91
III.5.4	Composition Methods	92
III.6	Exercises	95
IV.	Conservation of First Integrals and Methods on Manifolds	97
IV.1	Examples of First Integrals	97
IV.2	Quadratic Invariants	101
IV.2.1	Runge–Kutta Methods	101
IV.2.2	Partitioned Runge–Kutta Methods	102
IV.2.3	Nyström Methods	104
IV.3	Polynomial Invariants	105
IV.3.1	The Determinant as a First Integral	105
IV.3.2	Isospectral Flows	107
IV.4	Projection Methods	109
IV.5	Numerical Methods Based on Local Coordinates	113
IV.5.1	Manifolds and the Tangent Space	114
IV.5.2	Differential Equations on Manifolds	115
IV.5.3	Numerical Integrators on Manifolds	116
IV.6	Differential Equations on Lie Groups	118
IV.7	Methods Based on the Magnus Series Expansion	121
IV.8	Lie Group Methods	123
IV.8.1	Crouch–Grossman Methods	124
IV.8.2	Munthe–Kaas Methods	125

IV.8.3	Further Coordinate Mappings	128
IV.9	Geometric Numerical Integration Meets Geometric Numerical Linear Algebra	131
IV.9.1	Numerical Integration on the Stiefel Manifold	131
IV.9.2	Differential Equations on the Grassmann Manifold	135
IV.9.3	Dynamical Low-Rank Approximation	137
IV.10	Exercises	139
V.	Symmetric Integration and Reversibility	143
V.1	Reversible Differential Equations and Maps	143
V.2	Symmetric Runge–Kutta Methods	146
V.2.1	Collocation and Runge–Kutta Methods	146
V.2.2	Partitioned Runge–Kutta Methods	148
V.3	Symmetric Composition Methods	149
V.3.1	Symmetric Composition of First Order Methods	150
V.3.2	Symmetric Composition of Symmetric Methods	154
V.3.3	Effective Order and Processing Methods	158
V.4	Symmetric Methods on Manifolds	161
V.4.1	Symmetric Projection	161
V.4.2	Symmetric Methods Based on Local Coordinates	166
V.5	Energy – Momentum Methods and Discrete Gradients	171
V.6	Exercises	176
VI.	Symplectic Integration of Hamiltonian Systems	179
VI.1	Hamiltonian Systems	180
VI.1.1	Lagrange’s Equations	180
VI.1.2	Hamilton’s Canonical Equations	181
VI.2	Symplectic Transformations	182
VI.3	First Examples of Symplectic Integrators	187
VI.4	Symplectic Runge–Kutta Methods	191
VI.4.1	Criterion of Symplecticity	191
VI.4.2	Connection Between Symplectic and Symmetric Methods	194
VI.5	Generating Functions	195
VI.5.1	Existence of Generating Functions	195
VI.5.2	Generating Function for Symplectic Runge–Kutta Methods	198
VI.5.3	The Hamilton–Jacobi Partial Differential Equation	200
VI.5.4	Methods Based on Generating Functions	203
VI.6	Variational Integrators	204
VI.6.1	Hamilton’s Principle	204
VI.6.2	Discretization of Hamilton’s Principle	206
VI.6.3	Symplectic Partitioned Runge–Kutta Methods Revisited	208
VI.6.4	Noether’s Theorem	210

VI.7	Characterization of Symplectic Methods	212
VI.7.1	B-Series Methods Conserving Quadratic First Integrals	212
VI.7.2	Characterization of Symplectic P-Series (and B-Series)	217
VI.7.3	Irreducible Runge–Kutta Methods	220
VI.7.4	Characterization of Irreducible Symplectic Methods	222
VI.8	Conjugate Symplecticity	222
VI.8.1	Examples and Order Conditions	223
VI.8.2	Near Conservation of Quadratic First Integrals	225
VI.9	Volume Preservation	227
VI.10	Exercises	233
VII.	Non-Canonical Hamiltonian Systems	237
VII.1	Constrained Mechanical Systems	237
VII.1.1	Introduction and Examples	237
VII.1.2	Hamiltonian Formulation	239
VII.1.3	A Symplectic First Order Method	242
VII.1.4	SHAKE and RATTLE	245
VII.1.5	The Lobatto IIIA - IIIB Pair	247
VII.1.6	Splitting Methods	252
VII.2	Poisson Systems	254
VII.2.1	Canonical Poisson Structure	254
VII.2.2	General Poisson Structures	256
VII.2.3	Hamiltonian Systems on Symplectic Submanifolds	258
VII.3	The Darboux–Lie Theorem	261
VII.3.1	Commutativity of Poisson Flows and Lie Brackets	261
VII.3.2	Simultaneous Linear Partial Differential Equations	262
VII.3.3	Coordinate Changes and the Darboux–Lie Theorem	265
VII.4	Poisson Integrators	268
VII.4.1	Poisson Maps and Symplectic Maps	268
VII.4.2	Poisson Integrators	270
VII.4.3	Integrators Based on the Darboux–Lie Theorem	272
VII.5	Rigid Body Dynamics and Lie–Poisson Systems	274
VII.5.1	History of the Euler Equations	275
VII.5.2	Hamiltonian Formulation of Rigid Body Motion	278
VII.5.3	Rigid Body Integrators	280
VII.5.4	Lie–Poisson Systems	286
VII.5.5	Lie–Poisson Reduction	289
VII.6	Reduced Models of Quantum Dynamics	293
VII.6.1	Hamiltonian Structure of the Schrödinger Equation	293
VII.6.2	The Dirac–Frenkel Variational Principle	295
VII.6.3	Gaussian Wavepacket Dynamics	296
VII.6.4	A Splitting Integrator for Gaussian Wavepackets	298
VII.7	Exercises	301

VIII. Structure-Preserving Implementation	303
VIII.1 Dangers of Using Standard Step Size Control	303
VIII.2 Time Transformations	306
VIII.2.1 Symplectic Integration	306
VIII.2.2 Reversible Integration	309
VIII.3 Structure-Preserving Step Size Control	310
VIII.3.1 Proportional, Reversible Controllers	310
VIII.3.2 Integrating, Reversible Controllers	314
VIII.4 Multiple Time Stepping	316
VIII.4.1 Fast-Slow Splitting: the Impulse Method	317
VIII.4.2 Averaged Forces	319
VIII.5 Reducing Rounding Errors	322
VIII.6 Implementation of Implicit Methods	325
VIII.6.1 Starting Approximations	326
VIII.6.2 Fixed-Point Versus Newton Iteration	330
VIII.7 Exercises	335
IX. Backward Error Analysis and Structure Preservation	337
IX.1 Modified Differential Equation – Examples	337
IX.2 Modified Equations of Symmetric Methods	342
IX.3 Modified Equations of Symplectic Methods	343
IX.3.1 Existence of a Local Modified Hamiltonian	343
IX.3.2 Existence of a Global Modified Hamiltonian	344
IX.3.3 Poisson Integrators	347
IX.4 Modified Equations of Splitting Methods	348
IX.5 Modified Equations of Methods on Manifolds	350
IX.5.1 Methods on Manifolds and First Integrals	350
IX.5.2 Constrained Hamiltonian Systems	352
IX.5.3 Lie–Poisson Integrators	354
IX.6 Modified Equations for Variable Step Sizes	356
IX.7 Rigorous Estimates – Local Error	358
IX.7.1 Estimation of the Derivatives of the Numerical Solution	360
IX.7.2 Estimation of the Coefficients of the Modified Equation	362
IX.7.3 Choice of N and the Estimation of the Local Error	364
IX.8 Long-Time Energy Conservation	366
IX.9 Modified Equation in Terms of Trees	369
IX.9.1 B-Series of the Modified Equation	369
IX.9.2 Elementary Hamiltonians	373
IX.9.3 Modified Hamiltonian	375
IX.9.4 First Integrals Close to the Hamiltonian	375
IX.9.5 Energy Conservation: Examples and Counter-Examples	379
IX.10 Extension to Partitioned Systems	381
IX.10.1 P-Series of the Modified Equation	381
IX.10.2 Elementary Hamiltonians	384
IX.11 Exercises	386

X.	Hamiltonian Perturbation Theory and Symplectic Integrators	389
X.1	Completely Integrable Hamiltonian Systems	390
X.1.1	Local Integration by Quadrature	390
X.1.2	Completely Integrable Systems	393
X.1.3	Action-Angle Variables	397
X.1.4	Conditionally Periodic Flows	399
X.1.5	The Toda Lattice – an Integrable System	402
X.2	Transformations in the Perturbation Theory for Integrable Systems	404
X.2.1	The Basic Scheme of Classical Perturbation Theory	405
X.2.2	Lindstedt–Poincaré Series	406
X.2.3	Kolmogorov’s Iteration	410
X.2.4	Birkhoff Normalization Near an Invariant Torus	412
X.3	Linear Error Growth and Near-Preservation of First Integrals	413
X.4	Near-Invariant Tori on Exponentially Long Times	417
X.4.1	Estimates of Perturbation Series	417
X.4.2	Near-Invariant Tori of Perturbed Integrable Systems	421
X.4.3	Near-Invariant Tori of Symplectic Integrators	422
X.5	Kolmogorov’s Theorem on Invariant Tori	423
X.5.1	Kolmogorov’s Theorem	423
X.5.2	KAM Tori under Symplectic Discretization	428
X.6	Invariant Tori of Symplectic Maps	430
X.6.1	A KAM Theorem for Symplectic Near-Identity Maps	431
X.6.2	Invariant Tori of Symplectic Integrators	433
X.6.3	Strongly Non-Resonant Step Sizes	433
X.7	Exercises	434
XI.	Reversible Perturbation Theory and Symmetric Integrators	437
XI.1	Integrable Reversible Systems	437
XI.2	Transformations in Reversible Perturbation Theory	442
XI.2.1	The Basic Scheme of Reversible Perturbation Theory	443
XI.2.2	Reversible Perturbation Series	444
XI.2.3	Reversible KAM Theory	445
XI.2.4	Reversible Birkhoff-Type Normalization	447
XI.3	Linear Error Growth and Near-Preservation of First Integrals	448
XI.4	Invariant Tori under Reversible Discretization	451
XI.4.1	Near-Invariant Tori over Exponentially Long Times	451
XI.4.2	A KAM Theorem for Reversible Near-Identity Maps	451
XI.5	Exercises	453
XII.	Dissipatively Perturbed Hamiltonian and Reversible Systems	455
XII.1	Numerical Experiments with Van der Pol’s Equation	455
XII.2	Averaging Transformations	458
XII.2.1	The Basic Scheme of Averaging	458
XII.2.2	Perturbation Series	459

XII.3	Attractive Invariant Manifolds	460
XII.4	Weakly Attractive Invariant Tori of Perturbed Integrable Systems	464
XII.5	Weakly Attractive Invariant Tori of Numerical Integrators	465
	XII.5.1 Modified Equations of Perturbed Differential Equations	466
	XII.5.2 Symplectic Methods	467
	XII.5.3 Symmetric Methods	469
XII.6	Exercises	469
XIII.	Oscillatory Differential Equations with Constant High Frequencies .	471
XIII.1	Towards Longer Time Steps in Solving Oscillatory Equations of Motion	471
	XIII.1.1 The Störmer–Verlet Method vs. Multiple Time Scales .	472
	XIII.1.2 Gautschi's and Deufhard's Trigonometric Methods ...	473
	XIII.1.3 The Impulse Method	475
	XIII.1.4 The Mollified Impulse Method	476
	XIII.1.5 Gautschi's Method Revisited	477
	XIII.1.6 Two-Force Methods	478
XIII.2	A Nonlinear Model Problem and Numerical Phenomena	478
	XIII.2.1 Time Scales in the Fermi–Pasta–Ulam Problem	479
	XIII.2.2 Numerical Methods	481
	XIII.2.3 Accuracy Comparisons	482
	XIII.2.4 Energy Exchange between Stiff Components	483
	XIII.2.5 Near-Conservation of Total and Oscillatory Energy ...	484
XIII.3	Principal Terms of the Modulated Fourier Expansion	486
	XIII.3.1 Decomposition of the Exact Solution	486
	XIII.3.2 Decomposition of the Numerical Solution	488
XIII.4	Accuracy and Slow Exchange	490
	XIII.4.1 Convergence Properties on Bounded Time Intervals ...	490
	XIII.4.2 Intra-Oscillatory and Oscillatory–Smooth Exchanges ..	494
XIII.5	Modulated Fourier Expansions	496
	XIII.5.1 Expansion of the Exact Solution	496
	XIII.5.2 Expansion of the Numerical Solution	498
	XIII.5.3 Expansion of the Velocity Approximation	502
XIII.6	Almost-Invariants of the Modulated Fourier Expansions	503
	XIII.6.1 The Hamiltonian of the Modulated Fourier Expansion .	503
	XIII.6.2 A Formal Invariant Close to the Oscillatory Energy ...	505
	XIII.6.3 Almost-Invariants of the Numerical Method	507
XIII.7	Long-Time Near-Conservation of Total and Oscillatory Energy .	510
XIII.8	Energy Behaviour of the Störmer–Verlet Method	513
XIII.9	Systems with Several Constant Frequencies	516
	XIII.9.1 Oscillatory Energies and Resonances	517
	XIII.9.2 Multi-Frequency Modulated Fourier Expansions	519
	XIII.9.3 Almost-Invariants of the Modulation System	521
	XIII.9.4 Long-Time Near-Conservation of Total and Oscillatory Energies	524

XIII.10 Systems with Non-Constant Mass Matrix	526
XIII.11 Exercises	529
XIV. Oscillatory Differential Equations with Varying High Frequencies ..	531
XIV.1 Linear Systems with Time-Dependent Skew-Hermitian Matrix ..	531
XIV.1.1 Adiabatic Transformation and Adiabatic Invariants	531
XIV.1.2 Adiabatic Integrators	536
XIV.2 Mechanical Systems with Time-Dependent Frequencies	539
XIV.2.1 Canonical Transformation to Adiabatic Variables	540
XIV.2.2 Adiabatic Integrators	547
XIV.2.3 Error Analysis of the Impulse Method	550
XIV.2.4 Error Analysis of the Mollified Impulse Method	554
XIV.3 Mechanical Systems with Solution-Dependent Frequencies	555
XIV.3.1 Constraining Potentials	555
XIV.3.2 Transformation to Adiabatic Variables	558
XIV.3.3 Integrators in Adiabatic Variables	563
XIV.3.4 Analysis of Multiple Time-Stepping Methods	564
XIV.4 Exercises	564
XV. Dynamics of Multistep Methods	567
XV.1 Numerical Methods and Experiments	567
XV.1.1 Linear Multistep Methods	567
XV.1.2 Multistep Methods for Second Order Equations	569
XV.1.3 Partitioned Multistep Methods	572
XV.2 The Underlying One-Step Method	573
XV.2.1 Strictly Stable Multistep methods	573
XV.2.2 Formal Analysis for Weakly Stable Methods	575
XV.3 Backward Error Analysis	576
XV.3.1 Modified Equation for Smooth Numerical Solutions ..	576
XV.3.2 Parasitic Modified Equations	579
XV.4 Can Multistep Methods be Symplectic?	585
XV.4.1 Non-Symplecticity of the Underlying One-Step Method	585
XV.4.2 Symplecticity in the Higher-Dimensional Phase Space	587
XV.4.3 Modified Hamiltonian of Multistep Methods	589
XV.4.4 Modified Quadratic First Integrals	591
XV.5 Long-Term Stability	592
XV.5.1 Role of Growth Parameters	592
XV.5.2 Hamiltonian of the Full Modified System	594
XV.5.3 Long-Time Bounds for Parasitic Solution Components	596
XV.6 Explanation of the Long-Time Behaviour	600
XV.6.1 Conservation of Energy and Angular Momentum	600
XV.6.2 Linear Error Growth for Integrable Systems	601
XV.7 Practical Considerations	602
XV.7.1 Numerical Instabilities and Resonances	602
XV.7.2 Extension to Variable Step Sizes	605

XV.8	Multi-Value or General Linear Methods	609
XV.8.1	Underlying One-Step Method and Backward Error Analysis	609
XV.8.2	Symplecticity and Symmetry	611
XV.8.3	Growth Parameters	614
XV.9	Exercises	615
Bibliography		617
Index		637