

In memory of Donato Trigiante

Contents

Foreword	xiii
Preface	xv
1 A primer on line integral methods	1
1.1 A general framework	1
1.2 Geometric integrators	4
1.3 Hamiltonian problems	9
1.3.1 Symplecticity	11
1.3.2 Integrable and nearly-integrable Hamiltonian systems	13
1.4 Symplectic methods	18
1.4.1 Symplectic Euler method	21
1.4.2 Störmer-Verlet method	22
1.4.3 Gauss-Legendre methods	23
1.5 s -Stage trapezoidal methods	27
1.6 Runge-Kutta line integral methods	32
1.6.1 Discrete line integral and collocation methods	32
1.6.2 Derivation of Runge-Kutta LIMs	33
1.6.3 What have we got?	36
1.6.4 Fundamental and silent stages	37
1.6.5 Hamiltonian Boundary Value Methods	39
1.6.6 Choice of the basis	44
2 Examples of Hamiltonian problems	51
2.1 Nonlinear pendulum	51
2.2 Cassini ovals	53
2.3 Hénon-Heiles problem	55
2.4 N -body problem	56
2.5 Kepler problem	59
2.6 Circular restricted three-body problem	66
2.6.1 Planar CRTBP	70
2.6.2 Hill's lunar problem	73
2.6.3 Optimal transfer trajectory	75
2.7 Fermi-Pasta-Ulam problem	76

2.8	Molecular dynamics	79
3	Analysis of Hamiltonian Boundary Value Methods (HB-VMs)	81
3.1	Derivation and analysis of the methods	82
3.1.1	Discretization	89
3.2	Runge-Kutta formulation	94
3.3	Properties of HBVMs	98
3.3.1	Isospectrality	98
3.3.2	Equivalence property for polynomial problems	99
3.3.3	A -stability	100
3.3.4	Symmetry	101
3.3.5	Link with collocation methods	104
3.4	Least square approximation and Fourier expansion	106
3.5	Related approaches	113
4	Implementing the methods and numerical illustrations	119
4.1	Fixed-point iterations	119
4.1.1	Estimating the local errors	121
4.1.2	The case of special second-order problems	121
4.2	Newton-like iterations	124
4.2.1	The case of special second-order problems	126
4.2.2	Matrix form of the discrete problems	127
4.3	Recovering round-off and iteration errors	128
4.4	Numerical illustrations	131
5	Hamiltonian Partial Differential Equations	147
5.1	The semilinear wave equation	147
5.2	Periodic boundary conditions	150
5.2.1	Higher-order space discretization	152
5.2.2	Fourier space expansion	153
5.2.3	Fourier-Galerkin space discretization	155
5.3	Nonperiodic boundary conditions	159
5.4	Numerical tests	163
5.5	The nonlinear Schrödinger equation	167
6	Extensions	173
6.1	Conserving multiple invariants	173
6.2	General conservative problems	181
6.3	EQUIP methods	186
6.4	Hamiltonian Boundary Value Problems	193

A Auxiliary Material	201
A.1 Legendre polynomials	201
A.2 Matlab software	204
Bibliography	207