

Contents

1	Matrix-Variation-of-Constants Formula	1
1.1	Multi-frequency and Multidimensional Problems	1
1.2	Matrix-Variation-of-Constants Formula	3
1.3	Towards Classical Runge-Kutta-Nyström Schemes	8
1.4	Towards ARKN Schemes and ERKN Integrators	9
1.4.1	ARKN Schemes	9
1.4.2	ERKN Integrators	10
1.5	Towards Two-Step Multidimensional ERKN Methods	11
1.6	Towards AAVF Methods for Multi-frequency Oscillatory Hamiltonian Systems	13
1.7	Towards Filon-Type Methods for Multi-frequency Highly Oscillatory Systems	14
1.8	Towards ERKN Methods for General Second-Order Oscillatory Systems	16
1.9	Towards High-Order Explicit Schemes for Hamiltonian Nonlinear Wave Equations	17
1.10	Conclusions and Discussions	18
	References	20
2	Improved Störmer–Verlet Formulae with Applications	23
2.1	Motivation	23
2.2	Two Improved Störmer–Verlet Formulae	26
2.2.1	Improved Störmer–Verlet Formula 1	26
2.2.2	Improved Störmer–Verlet Formula 2	29
2.3	Stability and Phase Properties	31
2.4	Applications	33
2.4.1	Application 1: Time-Independent Schrödinger Equations	34
2.4.2	Application 2: Non-linear Wave Equations	35
2.4.3	Application 3: Orbital Problems	37
2.4.4	Application 4: Fermi–Pasta–Ulam Problem	40

2.5	Coupled Conditions for Explicit Symplectic and Symmetric Multi-frequency ERKN Integrators for Multi-frequency Oscillatory Hamiltonian Systems	42
2.5.1	Towards Coupled Conditions for Explicit Symplectic and Symmetric Multi-frequency ERKN Integrators	43
2.5.2	The Analysis of Combined Conditions for SSMERKN Integrators for Multi-frequency and Multidimensional Oscillatory Hamiltonian Systems	44
2.6	Conclusions and Discussions	48
	References	49
3	Improved Filon-Type Asymptotic Methods for Highly Oscillatory Differential Equations	53
3.1	Motivation	53
3.2	Improved Filon-Type Asymptotic Methods.	54
3.2.1	Oscillatory Linear Systems	56
3.2.2	Oscillatory Nonlinear Systems	59
3.3	Practical Methods and Numerical Experiments	61
3.4	Conclusions and Discussions	66
	References	67
4	Efficient Energy-Preserving Integrators for Multi-frequency Oscillatory Hamiltonian Systems	69
4.1	Motivation	69
4.2	Preliminaries	71
4.3	The Derivation of the AAVF Formula	73
4.4	Some Properties of the AAVF Formula	77
4.4.1	Stability and Phase Properties	77
4.4.2	Other Properties	79
4.5	Some Integrators Based on AAVF Formula	83
4.6	Numerical Experiments	87
4.7	Conclusions	91
	References	92
5	An Extended Discrete Gradient Formula for Multi-frequency Oscillatory Hamiltonian Systems	95
5.1	Motivation	95
5.2	Preliminaries	98
5.3	An Extended Discrete Gradient Formula Based on ERKN Integrators	100
5.4	Convergence of the Fixed-Point Iteration for the Implicit Scheme	104

5.5	Numerical Experiments	109
5.6	Conclusions	114
	References.	114
6	Trigonometric Fourier Collocation Methods for Multi-frequency Oscillatory Systems.	117
6.1	Motivation	117
6.2	Local Fourier Expansion	120
6.3	Formulation of TFC Methods	121
6.3.1	The Calculation of I_{1j} , I_{2j}	122
6.3.2	Discretization	124
6.3.3	The TFC Methods.	125
6.4	Properties of the TFC Methods.	128
6.4.1	The Order	129
6.4.2	The Order of Energy Preservation and Quadratic Invariant Preservation	130
6.4.3	Convergence Analysis of the Iteration	133
6.4.4	Stability and Phase Properties	135
6.5	Numerical Experiments	137
6.6	Conclusions and Discussions	146
	References.	146
7	Error Bounds for Explicit ERKN Integrators for Multi-frequency Oscillatory Systems.	149
7.1	Motivation	149
7.2	Preliminaries for Explicit ERKN Integrators	150
7.2.1	Explicit ERKN Integrators and Order Conditions	152
7.2.2	Stability and Phase Properties.	154
7.3	Preliminary Error Analysis	155
7.3.1	Three Elementary Assumptions and a Gronwall's Lemma.	155
7.3.2	Residuals of ERKN Integrators.	156
7.4	Error Bounds	159
7.5	An Explicit Third Order Integrator with Minimal Dispersion Error and Dissipation Error	166
7.6	Numerical Experiments	169
7.7	Conclusions	173
	References.	173
8	Error Analysis of Explicit TSERKN Methods for Highly Oscillatory Systems.	175
8.1	Motivation	175
8.2	The Formulation of the New Method.	176
8.3	Error Analysis	183

8.4	Stability and Phase Properties	186
8.5	Numerical Experiments	188
8.6	Conclusions	191
	References.	192
9	Highly Accurate Explicit Symplectic ERKN Methods for Multi-frequency Oscillatory Hamiltonian Systems	193
9.1	Motivation	193
9.2	Preliminaries	194
9.3	Explicit Symplectic ERKN Methods of Order Five with Some Small Residuals	196
9.4	Numerical Experiments	204
9.5	Conclusions and Discussions	208
	References.	208
10	Multidimensional ARKN Methods for General Multi-frequency Oscillatory Second-Order IVPs.	211
10.1	Motivation	211
10.2	Multidimensional ARKN Methods and the Corresponding Order Conditions	212
10.3	ARKN Methods for General Multi-frequency and Multidimensional Oscillatory Systems	214
10.3.1	Construction of Multidimensional ARKN Methods	215
10.3.2	Stability and Phase Properties of Multidimensional ARKN Methods	220
10.4	Numerical Experiments	222
10.5	Conclusions and Discussions	225
	References.	227
11	A Simplified Nyström-Tree Theory for ERKN Integrators Solving Oscillatory Systems.	229
11.1	Motivation	229
11.2	ERKN Methods and Related Issues.	231
11.3	Higher Order Derivatives of Vector-Valued Functions	233
11.3.1	Taylor Series of Vector-Valued Functions	233
11.3.2	Kronecker Inner Product	234
11.3.3	The Higher Order Derivatives and Kronecker Inner Product	235
11.3.4	A Definition Associated with the Elementary Differentials	236
11.4	The Set of Simplified Special Extended Nyström Trees	238
11.4.1	Tree Set SSENT and Related Mappings.	238
11.4.2	The Set SSENT and the Set of Classical SN-Trees	242
11.4.3	The Set SSENT and the Set SENT	245

11.5	B-series and Order Conditions	246
11.5.1	B-series	247
11.5.2	Order Conditions	249
11.6	Conclusions and Discussions	251
	References.	252
12	General Local Energy-Preserving Integrators for Multi-symplectic Hamiltonian PDEs	255
12.1	Motivation	255
12.2	Multi-symplectic PDEs and Energy-Preserving Continuous Runge–Kutta Methods	256
12.3	Construction of Local Energy-Preserving Algorithms for Hamiltonian PDEs	258
12.3.1	Pseudospectral Spatial Discretization	258
12.3.2	Gauss-Legendre Collocation Spatial Discretization.	264
12.4	Local Energy-Preserving Schemes for Coupled Nonlinear Schrödinger Equations	268
12.5	Local Energy-Preserving Schemes for 2D Nonlinear Schrödinger Equations	272
12.6	Numerical Experiments for Coupled Nonlinear Schrödingers Equations.	275
12.7	Numerical Experiments for 2D Nonlinear Schrödinger Equations.	284
12.8	Conclusions	289
	References.	290
	Conference Photo (Appendix).	293
	Index	295