

# Contents

## Preface — v

<b>1</b>	<b>The basic properties of Richardson extrapolation — 1</b>
1.1	The introduction of an initial value problem for systems of ODEs — 3
1.2	Numerical treatment of initial value problems for systems of ODEs — 6
1.3	An introduction to Richardson extrapolation — 8
1.4	Accuracy of Richardson extrapolation — 9
1.5	Evaluation of the error — 10
1.6	Major drawbacks and advantages of Richardson extrapolation — 11
1.7	Two implementations of Richardson extrapolation — 17
1.8	Obtaining higher accuracy — 20
1.9	General conclusions related to Chapter 1 — 21
1.10	Topics for further research — 22
<b>2</b>	<b>Richardson extrapolation for explicit Runge–Kutta methods — 23</b>
2.1	Stability function of one-step methods for solving systems of ODEs — 25
2.2	Stability polynomials of explicit Runge–Kutta methods — 30
2.3	Using Richardson extrapolation together with the scalar test problem — 31
2.4	Impact of Richardson extrapolation on absolute stability properties — 32
2.4.1	Stability regions related to the first-order one-stage explicit Runge–Kutta method — 34
2.4.2	Stability regions related to the second-order two-stage explicit Runge–Kutta methods — 35
2.4.3	Stability regions related to third-order three-stage explicit Runge–Kutta methods — 36
2.4.4	Stability regions related to fourth-order four-stage explicit Runge–Kutta methods — 38
2.4.5	On the use of complex arithmetic in the program for drawing the plots — 39
2.5	Preparation of appropriate numerical examples — 39
2.5.1	Numerical example with a large real eigenvalue — 40
2.5.2	Numerical example with large complex eigenvalues — 40
2.5.3	A nonlinear numerical example — 42
2.6	Organization of the computations — 44
2.7	Particular numerical methods used in the experiments — 45
2.8	Numerical results — 46

2.9	The development of methods with enhanced absolute stability properties —	<b>55</b>
2.9.1	The derivation of two classes of numerical methods with good stability properties —	<b>56</b>
2.9.2	Selecting particular numerical methods for Case 1: $p = 3$ and $m = 4$ —	<b>60</b>
2.9.3	Selecting particular numerical methods for Case 2: $p = 4$ and $m = 6$ —	<b>62</b>
2.9.4	Possibilities for further improvement of the results —	<b>68</b>
2.10	General conclusions related to Chapter 2 —	<b>72</b>
2.11	Topics for further research —	<b>74</b>
<b>3</b>	<b>Linear multistep and predictor-corrector methods —</b>	<b>75</b>
3.1	Linear multistep methods for solving systems of ODEs —	<b>77</b>
3.1.1	Order conditions —	<b>78</b>
3.1.2	Basic definitions —	<b>78</b>
3.1.3	Attainable order of linear multistep methods —	<b>80</b>
3.1.4	Drawbacks and advantages of linear multistep methods —	<b>80</b>
3.1.5	Frequently used linear multistep methods —	<b>82</b>
3.2	Variation of the time-step size for linear multistep methods —	<b>83</b>
3.2.1	Calculation of the coefficients of an LM VSVFM —	<b>84</b>
3.2.2	Zero-stability properties of an LM VSVFM —	<b>85</b>
3.3	Absolute stability of the linear multistep methods —	<b>86</b>
3.4	Difficulties related to the implementation of Richardson extrapolation —	<b>90</b>
3.5	Introduction of some predictor-corrector schemes —	<b>91</b>
3.6	Local error estimation —	<b>93</b>
3.7	Absolute stability of predictor-corrector schemes —	<b>98</b>
3.8	The application of several different correctors —	<b>102</b>
3.8.1	An example from the field of environmental modelling —	<b>103</b>
3.8.2	Some absolute stability considerations related to environmental modelling —	<b>105</b>
3.8.3	Numerical experiments —	<b>108</b>
3.9	A-stability of the linear multistep methods —	<b>110</b>
3.10	Coefficients of some popular linear multistep methods —	<b>111</b>
3.11	General conclusions related to Chapter 3 —	<b>111</b>
3.12	Topics for further research —	<b>117</b>
<b>4</b>	<b>Richardson extrapolation for some implicit methods —</b>	<b>119</b>
4.1	Description of the class of $\theta$ -methods —	<b>120</b>
4.2	Stability properties of the $\theta$ -methods —	<b>122</b>
4.3	Combining the $\theta$ -method with Richardson extrapolation —	<b>126</b>

4.4	Stability of Richardson extrapolation combined with $\theta$ -method —	127
4.5	The problem with implicitness —	134
4.5.1	Application of the classical Newton iterative method —	135
4.5.2	Application of the modified Newton iterative method —	138
4.5.3	Achieving better efficiency by keeping an old decomposition of the Jacobian matrix —	139
4.5.4	Selecting stopping criteria —	140
4.5.5	Richardson extrapolation and the Newton method —	144
4.6	Numerical experiments —	146
4.6.1	Atmospheric chemical scheme —	146
4.6.2	Organization of the computations —	149
4.6.3	Achieving second-order accuracy —	152
4.6.4	Comparison of the $\theta$ -method with $\theta = 0.75$ and the backward Euler formula —	153
4.6.5	Comparing the computing times needed to obtain the prescribed accuracy —	154
4.6.6	Using the trapezoidal rule in the computations —	157
4.7	Using implicit Runge–Kutta methods —	159
4.7.1	Fully implicit Runge Kutta methods —	159
4.7.2	Diagonally implicit Runge–Kutta methods —	160
4.7.3	Evaluating the reduction of the computational cost when DIRK methods are used —	161
4.7.4	Applying Richardson extrapolation for fully implicit Runge–Kutta methods —	163
4.7.5	Applying Richardson extrapolation for diagonally implicit Runge–Kutta methods —	166
4.7.6	Stability results related to active Richardson extrapolation —	167
4.7.7	Numerical experiments —	170
4.8	General conclusions related to Chapter 4 —	178
4.9	Topics for further research —	179
5	<b>Richardson extrapolation for splitting techniques —</b>	<b>181</b>
5.1	Richardson extrapolation for sequential splitting —	181
5.2	Derivation of the stability function for the sequential splitting procedure —	183
5.3	Stability properties of the sequential splitting procedure —	186
5.4	Some numerical experiments —	192
5.4.1	Splitting the atmospheric chemical scheme —	193
5.4.2	Organization of the computations —	193
5.4.3	Results obtained when the backward Euler formula is used —	195
5.4.4	Results obtained when the $\theta$ -method with $\theta = 0.75$ is used —	195
5.4.5	Results obtained when the trapezoidal rule is used —	197

5.4.6	Some conclusions from the numerical experiments —	<b>197</b>
5.5	Marchuk–Strang splitting procedure —	<b>198</b>
5.5.1	Some introductory remarks —	<b>198</b>
5.5.2	The Marchuk–Strang splitting procedure and Richardson extrapolation —	<b>200</b>
5.5.3	Stability function of the combined numerical method —	<b>201</b>
5.5.4	Selection of an appropriate class of Runge–Kutta methods —	<b>203</b>
5.5.5	Absolute stability regions of the combined numerical methods —	<b>205</b>
5.5.6	Some numerical results —	<b>207</b>
5.5.7	Concluding remarks —	<b>213</b>
5.6	General conclusions related to Chapter 5 —	<b>213</b>
5.7	Topics for further research —	<b>214</b>
<b>6</b>	<b>Richardson extrapolation for advection problems —</b>	<b>215</b>
6.1	The one-dimensional advection problem —	<b>216</b>
6.2	Combining the advection problem with Richardson extrapolation —	<b>218</b>
6.3	Implementation of Richardson extrapolation —	<b>220</b>
6.4	Order of accuracy of the combined numerical method —	<b>221</b>
6.5	Three numerical examples —	<b>225</b>
6.5.1	Organization of the computations —	<b>225</b>
6.5.2	Construction of a test problem with steep gradients of the unknown function —	<b>227</b>
6.5.3	Construction of an oscillatory test problem —	<b>230</b>
6.5.4	Construction of a test problem with discontinuous derivatives of the unknown function —	<b>231</b>
6.5.5	Comparison of the four implementations of Richardson extrapolation —	<b>233</b>
6.6	Multi-dimensional advection problem —	<b>235</b>
6.6.1	Introduction of the multi-dimensional advection equation —	<b>235</b>
6.6.2	Expanding the unknown function in Taylor series —	<b>236</b>
6.6.3	Three special cases —	<b>241</b>
6.6.4	Designing a second-order numerical method for multi-dimensional advection —	<b>243</b>
6.6.5	Application of Richardson extrapolation —	<b>244</b>
6.7	General conclusions related to Chapter 6 —	<b>255</b>
6.8	Topics for further research —	<b>256</b>
<b>7</b>	<b>Richardson extrapolation for some other problems —</b>	<b>257</b>
7.1	Acceleration of the speed of convergence for sequences of real numbers —	<b>258</b>
7.1.1	Improving the accuracy in calculations related to the number $\pi$ —	<b>259</b>

7.1.2	Definitions related to the convergence rate of some iterative processes — 259
7.1.3	The Aitken scheme and Steffensen's improvement — 261
7.1.4	Richardson extrapolation for sequences of real numbers: An example — 264
7.2	Application of Richardson extrapolation to numerical integration — 268
7.3	General conclusions related to Chapter 7 — 271
7.4	Topics for further research — 271

**8 General conclusions — 277**

**References — 279**

**List of abbreviations — 287**

**Author index — 289**

**Subject index — 291**