# Índice general


**1. Introducción y objetivos** **7**

1.1. Objetivos . . . . . 7

1.2. Resumen del estado del arte . . . . . 8

1.2.1. Función exponencial . . . . . 10

1.2.1.1. Polinomios matriciales ortogonales . . . . . 11

1.2.1.2. Aproximaciones racionales . . . . . 13

1.2.1.3. Otros métodos . . . . . 15

1.2.2. Funciones seno y coseno . . . . . 16

1.2.2.1. Aproximantes de Padé . . . . . 17

1.2.2.2. Series de polinomios matriciales . . . . . 19

1.2.3. *Software* para el cálculo de funciones matriciales . . . . . 21

1.3. Organización de la tesis . . . . . 22

Bibliografía . . . . . 23

**2. Exponencial de una matriz** **27**

2.1. Introducción . . . . . 27

2.2. Efficient orthogonal matrix polynomial based method for computing matrix exponential . . . . . 29

2.2.1. Introduction . . . . . 29

2.2.2. Hermite matrix polynomial series expansions of matrix exponential . 30

2.2.3. Error analysis. . . . . 31

2.2.4. Numerical examples . . . . . 39

2.2.5. Conclusions . . . . . 44

2.3. Accurate matrix exponential computation to solve coupled differential models in Engineering . . . . . 46

2.3.1. Introduction . . . . . 46

2.3.2. Error analysis and algorithm . . . 47
2.3.2.1. Taylor matrix polynomial evaluation . . . 48
2.3.2.2. Scaling algorithm . . . 48
2.3.3. Numerical experiments and conclusions . . . 51
2.4. New scaling-squaring Taylor algorithms for computing the matrix exponential 54
2.4.1. Introduction . . . 54
2.4.2. State of the art . . . 55
2.4.2.1. Taylor and Padé series . . . 55
2.4.2.2. Details about Taylor series approximants . . . 55
2.4.2.3. Relations between the order and the computational effort . 56
2.4.2.4. Maximizing the order . . . 58
2.4.2.5. Estimating the total cost . . . 59
2.4.3. Proposed modifications . . . 60
2.4.3.1. Modification of the choices for order and scaling . . . 61
2.4.3.2. Neglecting higher-order terms of the Taylor polynomial . . . 63
2.4.4. Numerical experiments . . . 67
2.4.4.1. Case Study 1 . . . 67
2.4.4.2. Case Study 2 . . . 69
2.4.5. Conclusions . . . 71
2.5. Accurate and efficient matrix exponential computation . . . 72
2.5.1. Introduction . . . 72
2.5.2. Taylor Algorithm . . . 73
2.5.2.1. Roundoff error analysis . . . 75
2.5.2.2. Analysis of truncation error . . . 76
2.5.2.3. Scaling algorithm . . . 79
2.5.2.4. Calculation of initial scaling $s_0$ . . . 80
2.5.2.5. Scaling refinement . . . 81
2.5.2.6. New bounds for $\|g_{m+1}(2^s A)\|$ and $\|h_{m+1}(2^{-s} A)\|$ . . . 83
2.5.3. Numerical experiments and conclusions . . . 84
2.6. High perfomance computing of the matrix exponential . . . 89
2.6.1. Introduction . . . 89
2.6.2. Taylor algorithm . . . 90
2.6.3. Error analysis . . . 92
2.6.4. New Taylor algorithm . . . 93

2.6.4.1. New scaling algorithm . . . 93
2.6.4.2. Taylor algorithm . . . 96
2.6.5. Numerical experiments and conclusions . . . 98
2.6.6. Conclusions . . . 103
Bibliografía . . . 105

**3. Coseno y seno de una matriz** **109**
3.1. Introducción . . . 109
3.2. Computing matrix functions solving coupled differential models . . . 111
3.2.1. Introduction . . . 111
3.2.2. Hermite matrix polynomials series expansions of matrix sine and matrix cosine . . . 112
3.2.3. Accurate and error bounds for cosine and sine approximation. Algorithm 114
3.2.4. Numerical examples . . . 116
3.2.5. Conclusions . . . 119
3.3. Computing matrix functions arising in engineering models with orthogonal matrix polynomials . . . 122
3.3.1. Introduction . . . 122
3.3.2. Hermite matrix polynomial series expansions of matrix cosine. Error bound . . . 124
3.3.3. Algorithm . . . 125
3.3.4. Numerical examples. . . . 127
3.3.5. Conclusions. . . . 129
3.4. Efficient computation of the matrix cosine . . . 130
3.4.1. Introduction . . . 130
3.4.2. Matrix polynomial computation by Paterson-Stockmeyer's method . 131
3.4.3. General Algorithm . . . 132
3.4.4. Error analysis in exact arithmetic and practical considerations . . . 133
3.4.5. Scaling algorithm . . . 136
3.4.5.1. Initial value of the scaling parameter . . . 137
3.4.5.2. Refinement of the scaling parameter . . . 138
3.4.6. Rounding error analysis . . . 142
3.4.7. Numerical experiments . . . 143
3.4.8. Conclusions . . . 145
Bibliografía . . . 147

**4. Aplicaciones** **149**

4.1. Introducción . . . 149

4.2. Solving Initial Value Problems for Ordinary Differential Equations by two approaches: BDF and Piecewise-linearized Methods . . . 150

4.2.1. Introduction . . . 150

4.2.2. A BDF algorithm . . . 151

4.2.3. A piecewise-linearized approach for solving IVPs for ODEs . . . 154

4.2.3.1. Algorithms based on the scaling and squaring technique . . . 157

4.2.3.2. Algorithms not based on scale-squaring technique . . . 166

4.2.4. Experimental results . . . 170

4.2.4.1. Case study 1 (Chemical Akzo Nobel problem) . . . 171

4.2.4.2. Case study 2 (HIRES problem) . . . 174

4.2.4.3. Case study 3 . . . 176

4.2.4.4. Case study 4 . . . 178

4.2.4.5. Case study 5 (Medical Akzo Nobel problem) . . . 180

4.2.5. Conclusions and future work . . . 181

4.3. A Piecewise-linearized Algorithm based on Krylov Subspace for solving stiff ODEs . . . 183

4.3.1. Introduction . . . 183

4.3.2. A piecewise-linearized algorithm for solving ODEs based on the Krylov subspace approach . . . 184

4.3.3. Experimental results . . . 185

4.3.3.1. Case study 1 (the pollution problem [LdS98]) . . . 188

4.3.3.2. Case study 2 (the EMEP problem [LdS98]) . . . 188

4.3.3.3. Case study 3 (the Medical Akzo Nobel problem [LdS98]) . . . 190

4.3.3.4. Case study 4 (the Brusselator problem) [HW96, pp. 6] . . . 191

4.3.4. Conclusions and future work . . . 191

Bibliografía . . . 195

**5. Conclusiones** **197**