SC2011

International Conference on Scientific Computing

A Conference to celebrate the 70th birthday of
Claude Brezinski and *Sebastiano Seatzu*
and the 20th anniversary of the Springer journal
Numerical Algorithms

S. Margherita di Pula, Cagliari, Italy
October 10-14, 2011

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- Michela Redivo-Zaglia, University of Padova, Italy
- Giuseppe Rodriguez, University of Cagliari, Italy

Scientific Program

- **Plenary Speakers**
  - **Mark J. Ablowitz**, University of Colorado at Boulder, U.S.A.
  - **Michele Benzi**, Emory University, U.S.A.
  - **Daniel Bessis**, Texas Southern University, Houston, U.S.A.
  - **Philippe G. Ciarlet**, City University of Hong Kong
  - **Lothar Reichel**, Kent State University, U.S.A.
- **Special Sessions**
  1. **Approximation Theory**
     Organized by Giuseppe Mastroianni and Wiesław Pleśniak
  2. **Extrapolation and Convergence Acceleration**
     Organized by Claude Brezinski and Ernst Joachim Weniger
  3. **Inverse Problems and Regularization**
     Organized by Martin Hanke and Per Christian Hansen
  4. **Iterative Methods for Linear Systems**
     Organized by Zhong-Zhi Bai and Hassane Sadok
  5. **Nonlinear Evolution Equations**
     Organized by Tuncay Aktosun and Sebastiano Seatzu
  6. **Optimization and Management Science**
     Organized by Marcos Raydan and Paola Zuddas
  7. **Orthogonal Polynomials and Quadrature**
     Organized by Adhemar Bultheel and Walter Gautschi
  8. **Padé Approximation and Continued Fractions**
     Organized by Bernd Beckermann and Annie Cuyt
  9. **Partial Differential Equations**
     Organized by Carsten Carstensen and Alfio Quarteroni
  10. **Structured Linear Algebra**
      Organized by Dario Bini and Marc Van Barel
  11. **History of Computational Mathematics**
      Organized by Michela Redivo-Zaglia and Giuseppe Rodriguez
- **General Session**
- **Poster Session**

List of Participants

1. **Lamia Abbas** (lamia.abbas@insa-rouen.fr)
   Département de Génie Mathématiques, INSA de ROUEN, Saint Etienne du Rouvray, France.

2. **Kuniyoshi Abe** (abe@gifu.shotoku.ac.jp)
   Faculty of Economics and Information, Gifu Shotoku University, Gifu, Japan.

3. **Mark J. Ablowitz** (mark.ablowitz@colorado.edu)
   Department of Applied Mathematics, University of Colorado, Boulder, USA.

4. **Lidia Aceto** (l.aceto@dma.unipi.it)
   Department of Applied Mathematics, University of Pisa, Italy.

5. **Kensuke Aihara** (j1411701@ed.tus.ac.jp)
   Department of Mathematical Science for Information Sciences, Graduate School of Science, Tokyo University of Science, Japan.

6. **Alessandra Aimi** (alessandra.aimi@unipr.it)
   Department of Mathematics, University of Parma, Italy.

7. **Tuncay Aktosun** (aktosun@uta.edu)
   Department of Mathematics, University of Texas at Arlington, USA.

8. **Guido Ala** (guido.ala@unipa.it)
   Dipartimento di Ingegneria Elettrica, Elettronica e delle Telecomunicazioni, Università di Palermo, Italy.

9. **Eman Salem Al-Aidarous** (ealaidarous@kau.edu.sa)
   Department of Mathematics, King Abdulaziz University, Jeddah, Saudi Arabia.

10. **Sergio Amat** (sergio.amat@upct.es)
    Dpto. de Matemática Aplicada y Estadística, Universidad Politécnica de Cartagena, Spain.

11. **Roberto Andreani** (andreani@ime.unicamp.br)
    Department of Applied Mathematics, State University of Campinas, São Paulo, Brazil.

12. **Alexander I. Aptekarev** (aptekaa@keldysh.ru)
    Department of Mathematics, Keldysh Institute of Applied Mathematics RAS, Moscow, Russian Federation.

13. **Antonio Aricò** (arico@unica.it)
    Department of Mathematics and Computer Science, University of Cagliari, Italy.

14. **Zhong-Zhi Bai** (bzz@lsec.cc.ac.cn)
    Institute of Computational Mathematics, Chinese Academy of Sciences, Beijing, China.

15. **Mariateresa Basile** (mariateresa.basile@unina.it)
Dipartimento di Matematica e Applicazioni, University of Naples Federico II, Italy.

16. **Bernhard Beckermann** (bbecker@math.univ-lille1.fr)
UFR Mathématiques, Laboratoire Painlevé UMR 8524, Université des Sciences et Technologies de Lille, Villeneuve d'Ascq, France.

17. **Skander Belhaj** (skander_belhaj@yahoo.fr)
Department of Quantitative Methods, University of Jendouba, Tunisia.

18. **Stefania Bellavia** (stefania.bellavia@unifi.it)
Dipartimento di Energetica, Università di Firenze, Italy.

19. **Michele Benzi** (benzi@mathcs.emory.edu)
Department of Mathematics and Computer Science, Emory University, Atlanta, GA, USA.

20. **Luca Bergamaschi** (berga@dmsa.unipd.it)
Dipartimento di Metodi e Modelli Matematici per le Scienze Applicate, University of Padova, Italy.

21. **Jean-Paul Berrut** (jean-paul.berrut@unifr.ch)
Département de Mathématiques, Université de Fribourg, Switzerland.

22. **Daniele Bertaccini** (bertaccini@mat.uniroma2.it)
Dipartimento di Matematica, Università di Roma Tor Vergata, Italy.

23. **Daniel J. Bessis** (dbessis@comcast.net)
Department of Physics, Texas Southern University, Houston Texas, USA.

24. **Dario Andrea Bini** (bini@dm.unipi.it)
Dipartimento di Matematica, Università di Pisa, Italy.

25. **Hans-Peter Blatt** (hans.blatt@ku-eichstaett.de)
Mathematisch-Geographische Fakultaet, Katholische Universitaet Eichstätt-Ingolstadt, Eichstaett, Germany.

26. **Daniele Boffi** (daniele.boffi@unipv.it)
Dipartimento di Matematica, Università di Pavia, Italy.

27. **Francesca Bonadei** (francesca.bonadei@springer.com)
Springer, Milan, Italy.

28. **Riccardo Borghi** (borghi@uniroma3.it)
Dipartimento di Elettronica Applicata, Università degli Studi Roma Tre, Italy.

29. **Abderrahman Bouhamidi** (a.bouhamidi@lmpa.univ-littoral.fr)
LMPA, Université du Littoral Côte d'Opale, Calais, France.

30. **Claude Brezinski** (claude.brezinski@univ-lille1.fr)
    Université des Sciences et Technologies de Lille, France.

31. **Paola Brianzi** (brianzi@dima.unige.it)
    Dipartimento di Matematica, Università di Genova, Italy.

32. **Adhemar Bultheel** (adhemar.bultheel@cs.kuleuven.be)
    Department of Computer Science, K.U. Leuven, Heverlee, Belgium.

33. **Maria Rosaria Capobianco** (mariarosaria.capobianco@cnr.it)
    Istituto per le Applicazioni del Calcolo, CNR–National Research Council of Italy, Napoli, Italy.

34. **Carsten Carstensen** (cc@mathematik.hu-berlin.de)
    Department of Mathematics, Humboldt-Universität zu Berlin, Germany.

35. **Kenier Castillo** (kcastill@math.uc3m.es)
    Departamanto de Matematicás, Universidad Carlos III de Madrid, Leganés, Spain.

36. **Roberto Cavoretto** (roberto.cavoretto@unito.it)
    Dipartimento di Matematica, Università di Torino, Italy.

37. **Raymond Honfu Chan** (rchan@math.cuhk.edu.hk)
    Department of Mathematics, The Chinese University of Hong Kong, Shatin, Hong Kong.

38. **Philippe G. Ciarlet** (mapgc@cityu.edu.hk)
    Department of Mathematics, City University of Hong Kong, Kowloon, Hong Kong.

39. **Dajana Conte** (dajconte@unisa.it)
    Dipartimento di Matematica, Università di Salerno, Italy.

40. **Pietro Contu** (contu@interfree.it)
    Dipartimento di Matematica e Informatica, Università degli Studi di Cagliari, Italy.

41. **Ronald Cools** (ronald.cools@cs.kuleuven.be)
    Department of Computer Science, K.U. Leuven, Heverlee, Belgium.

42. **Francesco Aldo Costabile** (costabil@unical.it)
    Dipartimento di Matematica, Università della Calabria, Rende (CS), Italy.

43. **Cathleen Marie Craviotto** (cathleen.craviotto@unco.edu)
    Department of Mathematical Sciences, University of Northern Colorado, Greeley, CO, USA.

44. **Ana Luisa Custódio** (alcustodio@fct.unl.pt)
    Department of Mathematics, New University of Lisbon, Portugal.

45. **Annie Cuyt** (annie.cuyt@ua.ac.be)
    Department of Mathematics and Computer Science, Universiteit Antwerpen, Belgium.

46. **Ljiljana Cvetkovic** (lila@dmi.uns.ac.rs)
Department of Mathematics and Informatics, Faculty of Science, Novi Sad, Serbia.

47. **Pasqua D'Ambra** (pasqua.dambra@cnr.it)
Istituto di Calcolo e Reti ad Alte Prestazioni (ICAR) del CNR, Napoli, Italy.

48. **Raffaele D'Ambrosio** (rdambrosio@unisa.it)
Department of Mathematics, University of Salerno, Fisciano (SA), Italy.

49. **Valentina De Simone** (valentina.desimone@unina2.it)
Dipartimento di Matematica, Seconda Università di Napoli, Caserta, Italy.

50. **Karl Deckers** (karl.deckers@cs.kuleuven.be)
Department of Computer Science, K.U. Leuven, Belgium.

51. **Antonio Degasperis** (antonio.degasperis@roma1.infn.it)
Department of Physics, Sapienza University of Rome, Italy.

52. **Gianna Maria Del Corso** (delcorso@di.unipi.it)
Department of Computer Science, University of Pisa, Italy.

53. **Francesco Dell'Accio** (fdellacc@unical.it)
Dipartimento di Matematica, Università della Calabria, Rende (CS), Italy.

54. **Francesco Demontis** (fdemontis@unica.it)
Dipartimento di Matematica e Informatica, University of Cagliari, Italy.

55. **Jean Guy Dhombres** (Jean.Dhombres@damesme.cnrs.fr)
Centre Koyré, EHESS, Paris, France.

56. **Fabio Di Benedetto** (dibenede@dima.unige.it)
Dipartimento di Matematica, Università di Genova, Italy.

57. **Daniela Di Serafino** (daniela.diserafino@unina2.it)
Dipartimento di Matematica, Seconda Università di Napoli, Caserta, Italy.

58. **Filomena Di Tommaso** (ditommaso@mat.unical.it)
Dipartimento di Matematica, Università della Calabria, Rende (Cs), Italy.

59. **Marco Donatelli** (marco.donatelli@uninsubria.it)
Department of Physics and Mathematics, University of Insubria, Como, Italy.

60. **Froilán M. Dopico** (dopico@math.uc3m.es)
Departamento de Matemática, Universidad Carlos III de Madrid, Leganés, Spain.

61. **André Draux** (andre.draux@insa-rouen.fr)
Génie Mathématique, INSA de ROUEN, Saint-Étienne-du-Rouvray, France.

62. **Vladimir Druskin** (druskin1@slb.com)
Schlumberger-Doll Research, Cambridge, MA, USA.

63. **Yuli Eidelman** (eideyu@post.tau.ac.il)
Department of Mathematics, Tel-Aviv University, Israel.

64. **Terje Oskar Espelid** (Terje.Espelid@math.uib.no)
Department of Mathematics, University of Bergen, Norway.

65. **Claudio Estatico** (claudio.estatico@uninsubria.it)
Department of Physics and Mathematics, University of Insubria, Como, Italy.

66. **Caterina Fenu** (kate.fenu@gmail.com)
Dipartimento di Matematica, Università degli Studi di Cagliari, Italy.

67. **Paraskevi Fika** (pfika@math.uoa.gr)
Department of Mathematics, University of Athens, Greece.

68. **Luca Formaggia** (luca.formaggia@polimi.it)
Dipartimento di Matematica, MOX - Politecnico di Milano, Italy.

69. **Massimo Fornasier** (massimo.fornasier@ma.tum.de)
Department of Mathematics, Technical University of Munich, Germany.

70. **Miguel Ángel Fortes** (mafortes@ugr.es)
Department of Applied Mathematics, University of Granada, Spain.

71. **Giorgio Fotia** (Giorgio.Fotia@crs4.it)
CRS4 Bioinformatica, Pula (CA), Italy.

72. **Elisa Francomano** (e.francomano@unipa.it)
Dipartimento di Ingegneria Chimica, Gestionale, Informatica e Meccanica, Università degli studi di Palermo, Italy.

73. **Ana Friedlander** (friedlan@ime.unicamp.br)
Department of Applied Mathematics, State University of Campinas, São Paulo, Brazil.

74. **Marco Frontini** (marco.frontini@polimi.it)
Dipartimento di Matematica, Politecnico di Milano, Italy.

75. **Seiji Fujino** (fujino@cc.kyushu-u.ac.jp)
Research Institute for Information Technology, Kyushu University, Fukuoka, Japan.

76. **Akiko Fukuda** (afukuda@rs.tus.ac.jp)
Department of Mathematical Information Science, Tokyo University of Science, Japan.

77. **Efstratios Gallopoulos** (stratis@ceid.upatras.gr)
Department of Computer Engineering & Informatics, University of Patras, Greece.

78. **Martin Jakob Gander** (martin.gander@unige.ch)
Department of Mathematics, University of Geneva, Switzerland.

79. **Ubaldo García-Palomares** (ubaldo@det.uvigo.es)
Departamento de Ingeniería Telemática, Universidade de Vigo, Spain.

80. **Roberto Garrappa** (garrappa@dm.uniba.it)
Dipartimento di Matematica, Università degli Studi di Bari, Italy.

81. **Lucia Gastaldi** (lucia.gastaldi@ing.unibs.it)
Dipartimento di Matematica, Università di Brescia, Italy.

82. **Walter Gautschi** (wgautschi@purdue.edu)
Department of Computer Sciences, Purdue University, West Lafayette, USA.

83. **Marco Gaviano** (gaviano@unica.it)
Dipartimento di Matematica e Informatica, Università di Cagliari, Italy.

84. **Silvia Gazzola** (gazzola@math.unipd.it)
Dipartimento di Matematica Pura e Applicata, Università degli Studi di Padova, Italy.

85. **Luca Gemignani** (gemignan@dm.unipi.it)
Department of Mathematics, University of Pisa, Italy.

86. **Tomáš Gergelits** (gergelits.tomas@seznam.cz)
Institue of Computer Science, Czech Academy of Sciences, Prague, Czech Republic.

87. **Jacek Gilewicz** (gjacek@hotmail.com)
Centre de Physique Theorique, Marseille, France.

88. **Maria Italia Gualtieri** (gualtieri@mat.unical.it)
Dipartimento di Matematica, Università della Calabria, Rende (CS), Italy.

89. **Martin Hermann Gutknecht** (mhg@math.ethz.ch)
Seminar for Applied Mathematics, ETH Zurich, Switzerland.

90. **Uno Hämarik** (uno.hamarik@ut.ee)
Department of Mathematics and Informatics, University of Tartu, Estonia.

91. **Carola Hammer** (carola.hammer@wi.tum.de)
Chair of Management Accounting and Control, Technical University Munich, Germany.

92. **Martin Hanke** (hanke@mathematik.uni-mainz.de)
Institut fur Mathematik, University of Mainz, Germany.

93. **Per Christian Hansen** (pch@imm.dtu.dk)
DTU Informatics, Technical University of Denmark, Lyngby, Denmark.

94. **Ken Hayami** (hayami@nii.ac.jp)
National Institute of Informatics, Tokyo, Japan.

95. **Jiří Horáček** (jiho@matfyz.cz)
Institute of Theroetical Physics, Charles University in Prague, Czech Republic.

96. **Xing-Biao Hu** (hxb@lsec.cc.ac.cn)
LSEC, Institute of Computational Mathematics, AMSS, Chinese Academy of Sciences, Beijing, China.

97. **Bruno Iannazzo** (bruno.iannazzo@dipmat.unipg.it)
Dipartimento di Matematica e Informatica, Università di Perugia, Italy.

98. **Emiko Ishiwata** (ishiwata@rs.kagu.tus.ac.jp)
Department of Mathematical Information Science, Tokyo University of Science, Japan.

99. **Timur Zinferovich Ismagilov** (timurismagilov@yahoo.com)
Department of Information Technology, Novosibirsk State University, Russia.

100. **Masashi Iwasaki** (imasa@kpu.ac.jp)
Department of Life and Environmental Science, Kyoto Prefectural University, Japan.

101. **Khalide Jbilou** (jbilou@lmpa.univ-littoral.fr)
LMPA, Université du Littoral Côte d'Opale, Calais, France.

102. **Valery Alexandrovich Kalyagin** (vkalyagin@hse.ru)
Department of Applied Mathematics and Informatics, National Research University Higher School of Economics, Nizhny Novgorod, Russia.

103. **Urve Kangro** (urve.kangro@ut.ee)
Department of Mathematics and Computer Science, University of Tartu, Estonia.

104. **Anna Karapiperi** (akarapi@math.uoa.gr)
Department of Mathematics, University of Athens, Greece.

105. **Martin Klaus** (klaus@math.vt.edu)
Department of Mathematics, Virginia Polytechnic Institute and State University, Blacksburg, USA.

106. **Boris Konopeltchenko** (Boris.Konopeltchenko@le.infn.it)
Department of Physics, University of Salento, Lecce, Italy.

107. **Nataša Krejić** (natasak@uns.ac.rs)
Department of Mathematics and Informatics, University of Novi Sad, Serbia.

108. **Maria V. Kulikova** (Kulikova.Maria@yahoo.com)
CEMAT (Centro de Matemática e Aplicações), Instituto Superior Técnico, Lisboa, Portugal.

109. **Gennady Kulikov** (gkulikov@math.ist.utl.pt)
CEMAT (Centro de Matemática e Aplicações), Instituto Superior Técnico, Lisboa, Portugal.

110. **Lahcen Laayouni** (l.laayouni@aui.ma)
School of Science and Engineering, Al Akhawayn University, Ifrane, Morocco.

111. **George Labahn** (glabahn@uwaterloo.ca)
Cheriton School of Computer Science, University of Waterloo, Ontario, Canada.

112. **Paola Lamberti** (paola.lamberti@unito.it)
Department of Mathematics, University of Torino, Torino, Italy.

113. **Elisabeth Larsson** (Elisabeth.Larsson@it.uu.se)
Department of Information Technology, Scientific Computing, Uppsala University, Sweden.

114. **Hervé Le Ferrand** (leferran@u-bourgogne.fr)
Institut de Mathématiques de Bourgogne, Dijon, France.

115. **Wen-shin Lee** (wen-shin.lee@ua.ac.be)
Department of Mathematics and Computer Science, Universiteit Antwerpen, Belgium.

116. **Flavia Lenti** (flavialenti@libero.it)
Dipartimento per le Tecnologie, Università di Napoli, Italy.

117. **Elie Leopold** (Leopold.E@free.fr)
Département de Mathematiques, USTV La Garde (Toulon) - CPT (Marseille), France.

118. **Daniela Lera** (lera@unica.it)
Dipartimento di Matematica e Informatica, Università degli Studi di Cagliari, Italy.

119. **Pedro Lima** (plima@math.ist.utl.pt)
Dep. Matematica /CEMAT, Instituto Superior Técnico, Lisboa, Portugal.

120. **Elizabeth Loew** (Elizabeth.Loew@springer.com)
Springer, New York, USA.

121. **Elisabetta Longo** (longo@mat.unical.it)
Department of Mathematics, University of Calabria, Rende (CS), Italy.

122. **Lisa Lorentzen** (lisa@math.ntnu.no)
Department of Mathematics, Norwegian University of Science and Technology, Trondheim, Norway.

123. **Ana Filipa Soares Loureiro** (anafsl@fc.up.pt)
Department of Mathematics, CMUP, University of Porto, Portugal.

124. **Fabio Maggio** (maggio@crs4.it)
CRS4 Bioinformatica, Pula (CA), Italy.

125. **Giorgio Domenico Mantica** (giorgio@uninsubria.it)
Department of Physics and Mathematics, Center for non-linear and complex systems, Como, Italy.

126. **Francisco José Marcellán Español** (pacomarc@ing.uc3m.es)
Departamanto de Matemáticas, Universidad Carlos III de Madrid, Leganés, Spain.

127. **Pascal Maroni** (maroni@ann.jussieu.fr)
Laboratoire Jacques-Louis Lions, Université de Paris VI (Pierre et Marie Curie), France.

128. **David Royce Martin** (dmarti49@kent.edu)
Department of Mathematical Sciences, Kent State University, Warren, Ohio, USA.

129. **José Mario Martínez** (martinez@ime.unicamp.br)
Department of Applied Mathematics, State University of Campinas, São Paulo, Brazil.

130. **Gunnar Martinsson** (martinss@colorado.edu)
Department of Applied Mathematics, University of Colorado at Boulder, CO, USA.

131. **Giuseppe Mastroianni** (giuseppe.mastroianni@unibas.it)
Dipartimento di Matematica e Informatica, Università della Basilicata, Potenza, Italy.

132. **Nicola Mastronardi** (n.mastronardi@ba.iac.cnr.it)
Consiglio Nazionale delle Ricerche, Istituto per le Applicazioni del Calcolo, Bari, Italy.

133. **Peter Mathé** (mathe@wias-berlin.de)
Weierstrass Institute for applied Analysis and Stochastics, Berlin, Germany.

134. **Ana Matos** (Ana.Matos@univ-lille1.fr)
UFR Mathématiques, Laboratoire Painlevé UMR 8524, Université des Sciences et Technologies de Lille, Villeneuve d'Ascq, France.

135. **Marie-Laurence Mazure** (mazure@imag.fr)
Laboratoire Jean Kuntzmann, University Joseph Fourier, Grenoble, France.

136. **Eleonora Messina** (eleonora.messina@unina.it)
Dipartimento di Matematica e Applicazioni, University of Naples, Italy.

137. **Gérard Meurant** (gerard.meurant@gmail.com)
CEA, Paris, France.

138. **Jean-Claude Miellou** (jmiellou@gmail.com)
Département de Mathématique, Université de Franche-Comté, France.

139. **Gradimir V. Milovanović** (gvm@megatrend.edu.rs)
Faculty of Computer Sciences, Megatrend University, Belgrade, Serbia.

140. **Marilena Mitrouli** (mmitroul@math.uoa.gr)
Department of Mathematics, University of Athens, Greece.

141. **Charles Moore** (cnmoore@math.ksu.edu)
Department of Mathematics, Kansas State University, Manhattan, KS, USA.

142. **Yoshiaki Muroya** (ymuroya@waseda.jp)
Department of Mathematics, Waseda University, Tokyo, Japan.

143. **James Nagy** (nagy@mathcs.emory.edu)
Department of Mathematics and Computer Science, Emory University, Atlanta, GA, USA.

144. **Silvia Noschese** (noschese@mat.uniroma1.it)
Dipartimento di Matematica, Università di Roma La Sapienza, Italy.

145. **Sotiris E. Notaris** (notaris@math.uoa.gr)
Department of Mathematics, University of Athens, Greece.

146. **Vedran Novaković** (venovako@fsb.hr)
Faculty of Mechanical Engineering and Naval Architecture, University of Zagreb, Croatia.

147. **Paolo Novati** (novati@math.unipd.it)
Department of Pure and Applied Mathematics, University of Padova, Italy.

148. **Donatella Occorsio** (donatella.occorsio@unibas.it)
Dipartimento di Matematica ed Informatica, Università della Basilicata, Potenza, Italy.

149. **Dai Okada** (j1410606@ed.kagu.tus.ac.jp)
Department of Mathematical Science for Information Sciences, Graduate school of Science, Tokyo University of Science, Japan.

150. **Saulo Pomponet Oliveira** (saulopo@ufpr.br)
Department of Mathematics, Universidade Federal do Parana, Brazil.

151. **Giovanni Ortenzi** (giovanni.ortenzi@unimib.it)
Department of Mathematics and Applications, University of Milano Bicocca, Italy.

152. **Naoki Osada** (osada@cis.twcu.ac.jp)
Department of Information and Sciences, Tokyo Woman's Christian University, Japan.

153. **Beatrice Paternoster** (beapat@unisa.it)
Dipartimento di Matematica, University of Salerno, Fisciano (SA), Italy.

154. **Aleksandar V. Pejčev** (apejcev@mas.bg.ac.rs)
Department of Mathematics, University of Beograd, Faculty of Mechanical Engineering, Belgrade, Serbia.

155. **Teresa E. Pérez** (tperez@ugr.es)
Department of Applied Mathematics, University of Granada, Spain.

156. **Miguel Piñar** (mpinar@ugr.es)
Department of Applied Mathematics, University of Granada, Spain.

157. **Paolo Pintus** (paolo.pintus@sssup.it)
Scuola Superiore Sant'Anna, Pisa, Italy.

158. **Olivier Pironneau** (olivier.pironneau@upmc.fr)
Laboratoire Jacques-Louis Lions, University of Paris VI (Pierre et Marie Curie), France.

159. **Wiesław Pleśniak** (Wieslaw.Plesniak@im.uj.edu.pl)
Faculty of Mathematics and Informatics, Jagiellonian University, Kraków, Poland.

160. **Bor Plestenjak** (bor.plestenjak@fmf.uni-lj.si)
Department of Mathematics, University of Ljubljana / IMFM, Slovenia.

161. **Marina Popolizio** (marina.popolizio@unisalento.it)
Dipartimento di Matematica, Università del Salento, Lecce, Italy.

162. **Miroslav Pranić** (pranic77m@yahoo.com)
Department of Mathematics and Informatics, University of Banja Luka, Bosnia and Herzegovina.

163. **Barbara Prinari** (bprinari@uccs.edu)
Dipartimento di Fisica and Sezione INFN, Università del Salento, Italy and Department of Mathematics, University of Colorado at Colorado Springs, USA.

164. **Alfio Quarteroni** (alfio.quarteroni@epfl.ch)
EPFL, MATHICSE CMCS, Lausanne, Switzerland and MOX-Politecnico di Milano, Italy.

165. **Francesca Rapetti** (frapetti@unice.fr)
Department of Mathematics, Université de Nice Sophia-Antipolis, France.

166. **Marcos Raydan** (mraydan@usb.ve)
Departamanto de Cómputo Cientifico y Estadística, Universidad Simón Bolívar, Caracas, Venezuela.

167. **Michela Redivo-Zaglia** (Michela.RedivoZaglia@unipd.it)
Department of Pure and Applied Mathematics, University of Padova, Italy.

168. **Lothar Reichel** (reichel@math.kent.edu)
Department of Mathematics, Kent State University, USA.

169. **Sara Remogna** (sara.remogna@unito.it)
Dipartimento di Matematica, Università di Torino, Italy.

170. **Maria João Rodrigues** (mjsrodri@fc.up.pt)
Departamento de Matemática, Faculdade de Ciências - Universidade do Porto, Porto, Portugal.

171. **Giuseppe Rodriguez** (rodriguez@unica.it)
Dipartimento di Matematica e Informatica, University of Cagliari, Cagliari, Italy.

172. **Miguel L. Rodríguez** (miguelrg@ugr.es)
Department of Applied Mathematics, University of Granada, Spain.

173. **Jose E. Roman** (jroman@dsic.upv.es)
Departamento de Sistemes Informàtics i Computació, Universitat Politècnica de València, Spain.

174. **Miroslav Rozloznik** (miro@cs.cas.cz)
Institute of Computer Science, Czech Academy of Sciences, Prague, Czech Republic.

175. **Maria Grazia Russo** (mariagrazia.russo@unibas.it)
Dipartimento di Matematica e Informatica, Università della Basilicata, Potenza, Italy.

176. **Maria Rosaria Russo** (mrrusso@math.unipd.it)
Dipartimento di Matematica Pura ed Applicata, Università di Padova, Italy.

177. **Paul Sablonnière** (Paul.Sablonniere@insa-rennes.fr)
Centre de Mathématiques, Rennes, France.

178. **Paul Sacks** (psacks@iastate.edu)
Department of Mathematics, Iowa State University, Ames, IA, USA.

179. **Hassane Sadok** (sadok@lmpa.univ-littoral.fr)
LMPA, Université du Littoral Côte d'Opale, Calais, France.

180. **Hassan Safouhi** (hsafouhi@ualberta.ca)
Campus Saint-Jean, University of Alberta, Edmonton, Canada.

181. **Ahmed Salam** (salam@lmpa.univ-littoral.fr)
LMPA, Université du Littoral Côte d'Opale, Calais, France.

182. **Oliver Salazar Celis** (oliver.salazarcelis@ua.ac.be)
Department of Mathematics & Computer Science, Universiteit Antwerpen, Belgium.

183. **Paolo M. Santini** (paolo.santini@roma1.infn.it)
Department of Physics, University of Roma La Sapienza, Italy.

184. **Cornelia Schiebold** (Cornelia.Schiebold@miun.se)
Department of Natural Sciences, Engineering, and Mathematics, Mid Sweden University, Sundsvall, Sweden.

185. **Sebastiano Seatzu** (seatzu@unica.it)
Dipartimento di Matematica e Informatica, University of Cagliari, Italy.

186. **Matous Sedlacek** (sedlacek@in.tum.de)
Institut für Informatik, Technische Universität München, Germany.

187. **Stefano Serra-Capizzano** (s.serracapizzano@uninsubria.it)
Dipartimento di Fisica e Matematica, Università dell'Insubria, Como, Italy.

188. **Fiorella Sgallari** (sgallari@dm.unibo.it)
Department of Mathematics-CIRAM, University of Bologna, Italy.

189. **Markus Siegle** (markus.siegle@unibw.de)
Department of Computer Science, University of the German Armed Forces Munich, Neubiberg, Germany.

190. **Samuli Siltanen** (samuli.siltanen@helsinki.fi)
Department of Mathematics and Statistics, University of Helsinki, Finland.

191. **Sanja Singer** (ssinger@fsb.hr)
Faculty of Mechanical Engineering and Naval Architecture, University of Zagreb, Croatia.

192. **Ian Hugh Sloan** (i.sloan@unsw.edu.au)
Department of Mathematics, University of New South Wales, Sydney, NSW, Australia.

193. **Alvise Sommariva** (alvise@math.unipd.it)
Department of Pure and Applied Mathematics, University of Padova, Italy.

194. **Gabriele Steidl** (steidl@mathematik.uni-kl.de)
Department of Mathematics, University of Kaiserslautern, Germany.

195. **Zdeněk Strakoš** (strakos@karlin.mff.cuni.cz)
Department of Numerical Mathematics, Charles University, Prague, Czech Republic.

196. **Zbigniew S. Szewczak** (zssz@mat.uni.torun.pl)
Faculty of Mathematics and Computer Science, Nicolaus Copernicus University, Toruń, Poland.

197. **Woula Themistoclakis** (wt@na.iac.cnr.it)
IAC Institute for Computational Applications, CNR National Research Council, Napoli, Italy.

198. **Dominique Tournès** (dominique.tournes@univ-reunion.fr)
Mathematics and Computer Science Laboratory, University of La Reunion, Sainte-Clotilde, France.

199. **Lloyd Nicholas Trefethen** (trefethen@maths.ox.ac.uk)
Mathematical Institute, Oxford University, United Kingdom.

200. **Juan Carlos Trillo** (jc.trillo@upct.es)
Department of Applied Mathematics and Statistics, Universidad Politécnica de Cartagena, Spain.

201. **Gennadi Vainikko** (gennadi.vainikko@ut.ee)
Department of Mathematics and Informatics, University of Tartu, Estonia.

202. **Walter Van Assche** (walter@wis.kuleuven.be)
Department of Mathematics, Katholieke Universiteit Leuven, Heverlee, Belgium.

203. **Marc Van Barel** (marc.vanbarel@cs.kuleuven.be)
Department of Computer Science, Katholieke Universiteit Leuven, Heverlee, Belgium.

204. **Marnix Van Daele** (Marnix.VanDaele@ugent.be)
Applied Mathematics and Computer Science, Ghent University, Belgium.

205. **Cornelis van der Mee** (cornelis@krein.unica.it)
Dipartimento di Matematica e Informatica, Università di Cagliari, Italy.

206. **Raf Vandebril** (raf.vandebril@cs.kuleuven.be)
Department of Computer Science, K.U. Leuven, Heverlee, Belgium.

207. **Ravi Varadhan** (rvaradhan@jhmi.edu)
School of Medicine, Johns Hopkins University, Baltimore, USA.

208. **Antonia Vecchio** (antonia.vecchio@cnr.it)
IAC - Napoli, Consiglio Nazionale delle Ricerche, Naples, Italy.

209. **Andreas Veeser** (andreas.veeser@unimi.it)
Dipartimento di Matematica, Università degli Studi di Milano, Italy.

210. **Federica Vitale** (federica.vitale@le.infn.it)
Dipartimento di Fisica and Sezione INFN, Università del Salento, Lecce, Italy.

211. **Lina von Sydow** (lina@it.uu.se)
Department of Information Technology, Uppsala University, Sweden.

212. **Ernst Joachim Weniger** (joachim.weniger@chemie.uni-regensburg.de)
Institut für Physikalische und Theoretische Chemie, Universität Regensburg, Germany.

213. **Olof Bertil Widlund** (widlund@cims.nyu.edu)
Courant Institute, New York, NY, USA.

214. **Franck Wielonsky** (wielonsk@cmi.univ-mrs.fr)
Laboratoire LATP, Université de Provence Aux-Marseille I, Marseille, France.

215. **Joshua Willis** (josh.willis@acu.edu)
Department of Physics, Abilene Christian University, TX, USA.

216. **Joab Ron Winkler** (j.winkler@dcs.shef.ac.uk)
Department of Computer Science, Sheffield University, United Kingdom.

217. **Pawel Woźny** (Pawel.Wozny@ii.uni.wroc.pl)
Institute of Computer Science, University of Wroclaw, Poland.

218. **Yu-Jiang Wu** (myjaw@lzu.edu.cn)
School of Mathematics and Statistics, Lanzhou University, China.

219. **Irem Yaman** (irem.yaman@ua.ac.be)
Department of Mathematics and Computer Science, Universiteit Antwerpen, Belgium.

220. **Ning Yang** (yangningbit@hotmail.com)
Department of Computer Science, University of Sheffield, United Kingdom.

221. **Gaetano Zanghirati** (g.zanghirati@unife.it)
Department of Mathematics, University of Ferrara, Italy.

222. **Bing Zheng** (bzheng@lzu.edu.cn)
School of Mathematics and Statistics, Lanzhou University, China.

223. **Paola Zuddas** (zuddas@unica.it)
Dipartimento di Ingegneria del Territorio, University of Cagliari, Italy.

Abstracts

General Session **155**

Keynote Speakers

NONLINEAR WAVES: FROM OCEANS TO "OPTICAL GRAPHENE"

M. J. Ablowitz
Department of Applied Mathematics
University of Colorado
Boulder, CO 80309, USA
mark.ablowitz@colorado.edu

The study of localized waves has a long history dating back to the discoveries in the 1800s describing water waves in shallow water. In both fluid dynamics and nonlinear optics there has been considerable interest in various aspects of localized waves. This lecture will discuss a novel formulation of water and interfacial waves and some of their properties and nonlinear waves in photonic lattices including honeycomb lattices where novel discrete nonlinear systems can be derived. Honeycomb lattices appear widely in physics, a notable case being graphene.

APPROXIMATION OF MATRIX FUNCTIONS ARISING IN THE ANALYSIS OF COMPLEX NETWORKS

M. Benzi
Department of Mathematics and Computer Science
Emory University
Atlanta, Georgia, USA
benzi@mathcs.emory.edu

Following recent work of Estrada, Hatano, Higham and coworkers I will describe some new techniques for the analysis of complex networks using matrix functions. Examples include notions like subgraph centrality, communicability, Estrada index, and other measures that can be expressed in terms of the exponential of the adjacency matrix of the underlying graph, as well as other matrix functions. Computational techniques for bounding and estimating quantities of interest for large networks will be discussed and illustrated by numerical examples.

UNIVERSAL ANALYTIC PROPERTIES OF NOISE

L. Perotti, **D. Bessis**
Department of Physics
Texas Southern University
Houston, TX 77004, USA
dbessis@comcast.net

We propose a new method in the spectral analysis of noisy time-series data for damped oscillators. From the Jacobi three terms recursive relation for the denominators of the Padé approximations built on the well-known Z-transform of an infinite time series, we build a Hilbert space operator, a J-operator, where each bound state (inside the unit circle in the complex plane) is simply associated with one damped oscillator while the essential spectrum of the J-operator, which lies on the unit circle itself, is shown to represent the noise.

Signal and noise are thus clearly separated in the complex plane. For a finite time series of length 2N, the J-operator is replaced by a finite order J-matrix J_N, having N eigenvalues which are time reversal covariant. Different classes of input noise, such as blank (white and uniform), gaussian and pink, are discussed in detail, the J-matrix formalism allowing us to efficiently calculate hundreds of poles of the Z-transform. Evidence of a universal behavior in the final statistical distribution of the associated poles and zeros of the Z-transform is shown. In particular, the poles and zeros tend, when the length of the time series goes to infinity, to a uniform angular distribution on the unit circle.

Therefore at finite order, the roots of unity in the complex plane *appear to be noise attractors.* We show that the Z-transform presents the exceptional feature of allowing *lossless undersampling* and how to make use of this property. A few basic examples are given to suggest the power of the proposed method.

SHELL MODELS: OLD AND NEW

P. G. Ciarlet
City University of Hong Kong
MAPGC@cityu.edu.hk

Intrinsic methods in elasticity have been introduced in a landmark series of papers by Wei-Zhang Chien in 1944. During the last two decades, Professor Wojciech Pietraszkiewicz and his group have achieved major advances in their analysis from the mechanical and engineering viewpoints, as well as in their actual numerical implementation. However, it was only in 2005 that their mathematical analysis began to be carried out in earnest, first for three-dimensional elasticity and more recently for elastic shells, by the author and his group. This presentation, which is intended for a general audience, will briefly review and discuss various problems as yet unresolved when this approach is applied to shell structures. In the classical approach, the main mathematical challenge is to establish that the associated energy has a minimizer. In the linear case, this is achieved through a "Korn inequality on a surface", which guarantees the positive-definiteness of the associated energy. In the nonlinear case, the problem remains basically open for Koiter's model, which is one of the most commonly used nonlinear models in numerical simulations. In the intrinsic approach, the main challenges lie not only in the mathematical analysis, but in effect in the modeling itself. Since the new unknowns are the change of metric and change of curvature tensor fields (instead of the displacement field in the classical approach), the Gauss and Codazzi-Mainardi compatibility equations conditions (or other equivalent equations) must be satisfied by these new unknowns, in order that they indeed correspond to a displacement of the middle surface of the shell. Another challenge is to adequately express boundary conditions in terms of these new unknowns. We will briefly review the existence theorems that has been recently obtained in the linear case. Besides, we will give in particular an explicit form of the compatibility conditions, as well as an explicit "Cesaro-Volterra integral formula on a surface" for reconstructing a displacement field from the knowledge of these new unknowns.

RATIONAL LANCZOS METHODS FOR THE APPROXIMATION OF MATRIX FUNCTIONS

L. Reichel
Department of Mathematical Sciences
Kent State University
Kent, OH 44242, USA
reichel@math.kent.edu

The need to evaluate expressions of the form $f(A)v$ and $v^T f(A)v$, where A is a large, sparse or structured, invertible symmetric matrix, v is a vector, and f is a nonlinear function, arises in many applications. The extended Krylov subspace method can be an attractive scheme for computing approximations of such expressions. This method projects the approximation problem onto an extended Krylov subspace

$$\mathcal{K}^{\ell,m}(A,v) = \text{span}\{A^{-\ell+1}v,\ldots,A^{-1}v,v,Av,\ldots,A^{m-1}v\}$$

of fairly small dimension, and then solves the small projected approximation problems so obtained. Orthonormal bases for extended Krylov subspaces can be generated with short recursion formulas, which can be derived using properties of Laurent polynomials. We will discuss the structure of the projections of the matrices A and A^{-1} onto $\mathcal{K}^{\ell,m}(A,v)$. This structure helps us derive efficient algorithms and relate projections of $v^T f(A)v$ to rational Gauss-type quadrature rules. The talk presents joint work with C. Jagels.

1. Special Session on Approximation Theory

APPLICATIONS OF LINEAR BARYCENTRIC RATIONAL INTERPOLATION AT EQUISPACED NODES

J.-P. Berrut
Département de Mathématiques
Université de Fribourg
Pérolles, 1700 Fribourg, Suisse
jean-paul.berrut@unifr.ch

Efficient linear and infinitely smooth approximation of functions from equidistant samples is a fascinating problem, at least since Runge showed in 1901 that it is not delivered by the interpolating polynomial.

In 1988, I suggested to substitute linear rational for polynomial interpolation by replacing the denominator 1 with a polynomial depending on the nodes, though not on the interpolated function. Unfortunately the so-obtained interpolant converges merely as the square of the mesh size. In 2007, Floater and Hormann have given for every integer a denominator that yields convergence of that prescribed order.

In the present talk I shall present the corresponding interpolant to those not familiar with it, before describing some of its applications, e.g., to differentiation, integration or the solution of boundary value problems. This is joint work with Georges Klein and Michael Floater.

GROWTH AND VALUE DISTRIBUTION OF RATIONAL APPROXIMANTS

H.-P. Blatt
Mathematisch-Geographische Fakultaet
Katholische Universitaet Eichstaett-Ingolstadt
85071 Eichstaett, Germany
hans.blatt@ku-eichstaett.de

We investigate the growth and the distribution of a-values, $a \in \overline{\mathbb{C}}$, of rational approximants r_n to a function f on a compact set E in $\mathbb{C}$, where $r_n = r_{n,m_n}$ is a rational function with numerator degree $\leq n$ and denominator degree $\leq m_n$, as $n \to \infty$. Three different situations are considered:

(1) f is meromorphic on E and $\{r_n\}_{n\in\mathbb{N}}$ is a sequence of maximally convergent rational functions to f on E. Examples are best approximants and Padé approximants.

(2) E is a continuum, f continuous on E and $\{r_n\}_{n\in\mathbb{N}}$ converges geometrically to f on E.

(3) $f \in C[-1,1]$, but f is not holomorphic on $[-1,1]$ and $\{r_{n,m_n}\}_{n\in\mathbb{N}}$ is a sequence of rational best approximants in the upper half of the Walsh table, i.e.,

$$m_n \leq cn \text{ and } 0 \leq c < 1.$$

WEIGHTED POLYNOMIAL APPROXIMATION

G. Mastroianni,
Department of Mathematics and Computer Science
University of Basilicata
V.le dell'Ateneo Lucano 10, Potenza, Italy
giuseppe.mastroianni@unibas.it

The approximation of functions having singularities at the endpoints of the definition domain (one-dimensional, bounded and/or unbounded) naturally leads to the weighted polynomial approximation.

In this talk I want to discuss about some recent results concerning the exponential weights: polynomial inequalities, best approximation estimates, Fourier sums and Lagrange interpolation.

INTERLACING PROPERTIES OF GENERALIZED LAGUERRE ZEROS AND SOME APPLICATIONS

D. Occorsio
Department of Mathematics and Computer Science
University of Basilicata
V.le dell'Ateneo Lucano 10, Potenza, Italy
donatella.occorsio@unibas.it

Let $w(x) = e^{-x^\beta}x^\alpha$, $\alpha > -1$, $\beta > \frac{1}{2}$ be a Generalized Laguerre weight, and denote by $\{p_m(w)\}$ the corresponding sequence of orthonormal polynomials. Setting $\bar{w}(x) = xw(x)$, let $\{p_m(\bar{w})\}$ the sequence of orthonormal polynomials corresponding to $\bar{w}$. We prove that the polynomial $Q_{2m+1} = p_{m+1}(w)p_m(\bar{w})$ has simple zeros and that they are also well distributed in some sense.

In view of this property we propose two different applications: the *extended interpolation polynomial* $L_{2m+2}(w, \bar{w}, f)$, defined as the Lagrange polynomial interpolating a given function f at the zeros of Q_{2m+1} and on additional knots, estimating the Lebesgue constants in some weighted spaces. Moreover, we propose a method to approximate the Hilbert transform on the real positive semiaxis by a suitable Lagrange interpolating polynomial.

POLYNOMIAL INEQUALITIES ON SUBANALYTIC SETS

W. Pleśniak
Institute of Mathematics
Jagiellonian University
Łojasiewicza 6, 30-348 Kraków, Poland
Wieslaw.Plesniak@im.uj.edu.pl

The classical inequalities like those of Bernstein, Markov or Jackson are crucial in the approximation of functions. They are well understood in the one-dimensional setting. Their multivariate versions require, however, application of essentially stronger methods. A satisfactory theory of such inequalities has been developed due to applications of both pluripotential methods based on the Bedford-Taylor theory of the complex Monge-Ampère operator and the Gabrielov-Hironaka-Łojasiewicz subanalytic geometry. The application of the latter theory to approximation problems has unexpectedly yielded very effective tools that permit one to overcome difficulties related to the geometry of multidimensional sets (e.g. cuspidal sets problems). The goal of my talk is to present some of the most spectacular results obtained by such an approach.

MEAN CONVERGENCE OF EXTENDED LAGRANGE INTERPOLATION ON UNBOUNDED INTERVALS

D. Occorsio and **M. G. Russo**,
Department of Mathematics and Computer Science
University of Basilicata
V.le dell'Ateneo Lucano 10, Potenza, Italy
mariagrazia.russo@unibas.it

In [1] it was proved that if $w(x) = e^{-x^\beta}x^\gamma$, $\gamma \geq -1$, $\beta > \frac{1}{2}$, is a generalized Laguerre weight and $\bar{w}(x) = xw(x)$, then the zeros of the orthonormal polynomial $p_{m+1}(w)$ interlace with those of $p_m(\bar{w})$. Hence it is possible to consider an extended Lagrange interpolation process based on the zeros of $p_{m+1}(w)p_m(\bar{w})$. In this talk the named interpolation is considered in L^p weighted norm. Necessary and sufficient conditions on the involved weights functions are stated in order to obtain the convergence of the process and the boundedness of the Lagrange operator in subspaces of Sobolev type. Analogous results are discussed concerning the real line and the weights of Markov-Sonin type $w_\beta(x) = e^{-x^2}|x|^\beta$, $\beta > -1$.

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POLYNOMIAL APPROXIMATION ON SPHERES – GENERALISING DE LA VALLÉE POUSSIN

I. H. Sloan
School of Mathematics and Statistics
University of New South Wales
Sydney, Australia
i.sloan@unsw.edu.au

For trigonometric polynomial approximation on a circle, the de la Vallée Poussin construction has two notable properties as the polynomial degree goes to infinity: it yields uniform convergence for all continuous functions; yet it also exhibits arbitrarily fast convergence for smooth functions. It is allowed to have both properties because it is a uniformly bounded but not positive projection onto the trigonometric polynomial space. In this talk I present a generalisation of the de la Vallée construction to higher dimensional spheres. Such a generalisation seems to be not presently known.

COMPUTING FEKETE AND LEBESGUE POINTS: SIMPLEX, SQUARE, DISK

M. Briani, **A. Sommariva**, and M. Vianello
Department of Pure and Applied Mathematics
University of Padova
Via Trieste 63, Padova, Italy
alvise@math.unipd.it

The main purpose of our work is to provide Fekete and Lebesgue points on three basic bidimensional compact sets, the simplex, the square, and the disk, by solving numerically the corresponding large-scale nonlinear optimization problems up to degree $n = 18$. Our results reach and often improve those previously known [1], [3]. In the case of the simplex, due to their relevance in developing spectral and high-order methods for PDEs [2] we have also computed interpolation sets that have an assigned distribution on the sides (Legendre-Gauss-Lobatto side nodes), which appear to be better than those previously known. Concerning the square, besides Fekete and Lebesgue points, we have computed some new sets that generalize the Padua points and improve their already good quality. Very little seems to be known about Fekete and Lebesgue points for the disk, and we hope that our computational results could put some insight into this topic.

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ROBUST RATIONAL INTERPOLATION AND LEAST-SQUARES

L. N. Trefethen, P. Gonnet, and R. Pachón
Mathematical Institute
University of Oxford
24-29 St. Giles, Oxford OX1 3LB, UK
trefethen@maths.ox.ac.uk

Approximating functions or data by polynomials is an everyday tool, starting with Taylor series. Approximating by rational functions can be much more powerful, but also much more troublesome. In different contexts rational approximations may fail to exist, fail to be unique, or depend discontinuously on the data. Some approximations show forests of seemingly meaningless pole-zero pairs or "Froissart doublets", and when these artifacts should not be there in theory, they often appear in practice because of rounding errors on the computer. Yet for some applications, like extrapolation of sequences and series, rational approximations are indispensable.

In joint work with Pedro Gonnet and Ricardo Pachon we have developed a method to get around most of these problems in rational interpolation and least-squares fitting, based on the singular value decomposition. The talk will show many examples of the performance of our "ratdisk" code, as well as generalizations for Pade approximation and extrapolation of sequences and series.

2. Special Session on Extrapolation and Convergence Acceleration

ANALYSIS OF THE CONVERGENCE FEATURES OF THE δ TRANSFORMATION FOR A CLASS OF FACTORIALLY DIVERGING ASYMPTOTIC SERIES

R. Borghi and E. J. Weniger
Dipartimento di Elettronica Applicata
Università degli Studi "Roma Tre"
Roma, Italy
borghi@uniroma3.it

An analysis of the convergence features of the sequence obtained by applying the δ transformation [1, Eq. (8.4-4)] on the partial sums of the following class of asymptotic series:

$$\sum_{k=0}^{\infty} (-1)^k z^k \Gamma(k+q+1),$$

is presented. In particular, on using the inverse factorial representation of the converging factor of the series found in Ref. [2, Eq. (52)], together with the recently reviewed treatment of factorial series [3], an asymptotic analysis of the convergence speed of the transformation, in the limit of large values of the transformation order, is provided for $z > 0$ and $q \in (-1, 1)$.

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PFAFFIAN AND ITS APPLICATION TO SEQUENCE TRANSFORMATIONS AND CORRESPONDING CONVERGENCE ACCELERATION ALGORITHMS

X. B. Hu
LSEC, Institute of Computational Math.
AMSS, CAS, China
hxb@lsec.cc.ac.cn

Pfaffians are closely related to determinants. They are usually defined by the property that the square of a pfaffian is the determinant of an antisymmetric matrix. It is known that determinants have played an important role in the construction of sequence transformations and their corresponding convergence acceleration algorithms. In this talk, I will give some examples to show that pfaffians may be applied to construction of sequence transformations and their corresponding convergence acceleration algorithms.

SOME ASPECTS OF THE INTEGRABLE DISCRETE LOTKA-VOLTERRA SYSTEM

M. Iwasaki and Y. Nakamura
Department of Informatics and Environmental Science
Kyoto Prefectural University
Kyoto 606-8522, Japan
imasa@kpu.ac.jp

The integrable Lotka-Volterra (LV) system [2] is known as a dynamical systems which gives a mathematical description of food chain structure. The discrete LV system (dLV) system [1] is derived from a skillful time-discretization of the LV system.

In this talk, we mainly discuss an application of the dLV system to computing matrix singular values. We also review the positivity of dLV variables through considering orthogonal polynomials, and deeply investigate the asymptotic behavior with the help of center manifold theory. In order to accelerate the convergence rate, we explain how to introduce the shift of origin from the viewpoint of matrix theory. Some examples are given for numerically confirming that the computed singular values are high relative accurate. Additionally, we describe an interesting relationship between the dLV system and the well-known Fibonacci sequence.

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FOURIER SERIES AND ACCELERATION METHODS

C. N. Moore
Department of Mathematics
Kansas State University
Manhattan, Kansas, U.S.A.
cnmoore@math.ksu.edu

For a function f which is integrable on $[-\pi, \pi]$, we consider the partial sums of its Fourier series

$$S_n f(x) := \sum_{k=-n}^{n} \hat{f}(k) e^{ikx}.$$

We transform the sequence of partial sums using the δ^2 and the Lubkin transforms to obtain respectively the sequences of functions

$$T_n f(x) := \frac{S_{n+1}f(x)S_{n-1}f(x) - (S_n f(x))^2}{S_{n+1}f(x) + S_{n-1}f(x) - 2S_n f(x)}$$

(where we set $T_n f(x) = S_n f(x)$ if the denominator of the fraction is zero) and

$$S_n^* f(x) := S_n f(x) + \frac{(S_{n+1}f(x) - S_n f(x))(1 - \rho_{n+1}f(x))}{1 - 2\rho_{n+1}f(x) + \rho_n f(x)\rho_{n+1}f(x)}.$$

where $\rho_n f(x) = (S_{n+1}f(x) - S_n f(x))/(S_n f(x) - S_{n-1}f(x))$.

Both of these transforms fail to accelerate convergence in general: For functions which are smooth, except for a single jump discontinuity, both transforms diverge on a dense set. We also construct Hölder continuous functions, analytic on the interior of the unit disk, for which the transformed sequences fail to converge at every point. We discuss iterations of these transforms and the epsilon algorithm.

MULTISTEP ε–ALGORITHM AND SHANKS' TRANSFORMATION BY HIROTA'S METHOD

C. Brezinski, Y. He, X.-B. Hu,
M. Redivo-Zaglia and J.-Q. Sun
Department of Pure and Applied Mathematics
University of Padova, Italy
Michela.RedivoZaglia@unipd.it

In this paper, we propose a multistep extension of the Shanks' sequence transformation [2, 3]. It is defined as a ratio of determinants. Then, we show that this transformation can be recursively implemented by a multistep extension of the ε–algorithm of Wynn [4]. Some of their properties are specified. These results are obtained by using the Hirota's bilinear method [1], a procedure quite useful in the solution of nonlinear partial differential and difference equations.

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A COMPARATIVE NUMERICAL STUDY OF EXTRAPOLATION METHODS, SEQUENCE TRANSFORMATIONS AND STEEPEST DESCENT METHODS IN NUMERICAL INTEGRATION

R. M. Slevinsky and **H. Safouhi**
Mathematical Section, Campus Saint-Jean
University of Alberta
8406, 91 Street, Edmonton (AB), Canada T6C 4G9
hsafouhi@ualberta.ca

With the advent of computers and scientific computing, there has been a push to develop more accurate and efficient techniques in computing challenging problems in applied mathematics. In the numerical evaluation of infinite-range integrals, three general methods have come to the forefront. These methods are known as extrapolation methods, sequence transformations and steepest descent methods.

In extrapolation methods, through numerical quadrature or otherwise, one computes a sequence of approximations to the infinite-range integral and uses analytical properties of the integrand to then extrapolate on this sequence to obtain an approximation for the integral. In sequence transformations, one derives the asymptotic series expansion of the integral and, whether convergent or divergent, one applies transformations to the asymptotic series hoping to approximate the limit or antilimit of the series with a relatively small number of terms. In the steepest descent methods, a deformation of the path of integration is used to transform oscillations or irregular exponential behaviour into linear exponential decay. On the deformed contour, a Gauss-Laguerre-type quadrature is used to approximate the integral.

In this work, we put these three general methods to the test on five prototypical infinite-range integrals exhibiting oscillatory, logarithmic and exponential properties or combinations thereof. On the bases of accuracy, efficiency, simplicity, and reliability, we compare and contrast the three general methods for the evaluation of infinite-range integrals.

THE REMARKABLE EFFECTIVENESS OF A NEW CLASS OF EXTRAPOLATION TECHNIQUES FOR ACCELERATING MONOTONE ALGORITHMS IN STATISTICAL MODELING

R. Varadhan
Johns Hopkins University
Baltimore, MD, USA
rvaradhan@jhmi.edu

Maximum likelihood estimation (MLE) plays a central role in statistical inference. Expectation maximization (EM) algorithm is a very popular computational approach for MLE. A more general approach to MLE is the minorize-maximize (MM) algorithm. The EM algorithm may be viewed as a special case of the MM algorithm. A major reason for the popularity of MM algorithms is that they are monotone, i.e. they always head uphill in terms of the likleihood function. MM algorithm is locally linearly convergent. MM algorithms are globally convergent under rather weak regularity conditions. However, in many applications the linear rate of convergence is painfully slow. We recently developed a new classes of iterative scheme called the squared iterative methods (SQUAREM), to accelerate the convergence of MM (Varadhan and Roland 2008). By viewing SQUAREM as continuations of MM, we showed that fast and globally-convergent schemes can be obtained. SQUAREM is especially attractive in high-dimensional problems, when compared to numerical accelerators such as quasi-Newton and conjugate gradient methods, due to its simplicity and minimal storage requirements. We present several examples of the remarkable effectiveness of SQUAREM for accelerating the MM algorithm in high-dimensional problems(multi-dimensional scaling, genetic admixture, PET imaging, and movie ratings). We also discuss some approaches for handling parameter constraints including projection onto feasible region and backtracking of steplength.

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EXTENSIONS OF PADÉ-TYPE APPROXIMANTS

E. J. Weniger
Institut für Physikalische und Theoretische Chemie
Universität Regensburg
D-93040 Regensburg, Germany
joachim.weniger@chemie.uni-regensburg.de

A Padé approximant $[l/m]_f(z)$ to a function $f(z)$ is the ratio of two polynomials $P^{[l/m]}(z) = p_0 + p_1 z + \cdots + p_l z^l$ and $Q^{[l/m]}(z) = 1 + q_1 z + \cdots + q_m z^m$. The polynomial coefficients can be determined via the *accuracy-through-order* relationship $Q^{[l/m]}(z) f(z) - P^{[l/m]}(z) = \mathrm{O}(z^{l+m+1})$ as $z \to 0$.

It is normally highly advantageous that for the computation of $[l/m]_f(z)$ only the numerical values of the partial sums $f_n(z) = \sum_{\nu=0}^{n} \gamma_\nu z^\nu$ with $0 \leq n \leq l+m$ of the (formal) power series for $f(z)$ have to be known. No additional information is necessary. But this also means that there is no obvious way of incorporating additional information about f or the index dependence of the partial sums $f_n(z)$ into the transformation process, although such an information may be available.

As a remedy, Brezinski [J. Approx. Theory, 25 (1979), pp. 295 – 317] proposed so-called *Padé-type* approximants $(l/m)_f(z) = \mathcal{U}^{(l/m)}(z)/\mathcal{V}^{(l/m)}(z)$, which are also ratios of two polynomials. But now, it is assumed that the coefficients of the the denominator polynomial are known. Thus, only the coefficients of the numerator polynomial have to be determined via the modified *accuracy-through-order* relationship $\mathcal{V}^{(l/m)}(z) f(z) - \mathcal{U}^{(l/m)}(z) = \mathrm{O}(z^{l+1})$ as $z \to \infty$.

The zero's of the denominator polynomial correspond to the poles of a Padé-type approximant. Unfortunately, there are not too many non-trivial functions whose pole structure is fully understood. Accordingly, indirect approaches for the choice of the denominator polynomials of Padé-type approximant have to be pursued.

This talk first discusses certain Levin-type transformations, which are known to be very powerful convergence acceleration and summation techniques and which are actually special Padé-type approximants [E. J. Weniger, J. Math. Phys., 45 (2004), pp. 1209 – 1246, Section VI]. Then, some examples from special function theory are discussed which show how denominator polynomials can be chosen by utilizing knowledge about the location of the cuts of the function.

3. Special Session on Inverse Problems and Regularization

A VARIATIONAL APPROACH FOR EXACT HISTOGRAM SPECIFICATION

R. Chan, M. Nikolova, and Y.-W. Wen
Department of Mathematics
The Chinese University of Hong Kong
Shatin, NT, Hong Kong
rchan@math.cuhk.edu.hk

We focus on exact histogram specification when the input image is quantified. The goal is to transform this input image into an output image whose histogram is exactly the same as a prescribed one. In order to match the prescribed histogram, pixels with the same intensity level in the input image will have to be assigned to different intensity levels in the output image. An approach to classify pixels with the same intensity value is to construct a strict ordering on all pixel values by using auxiliary attributes. Local average intensities and wavelet coefficients have been used by the past as the second attribute. However, these methods cannot enable strict-ordering without degrading the image. In this paper, we propose a variational approach to establish an image preserving strict-ordering of the pixel values. We show that strict-ordering is achieved with probability one. Our method is image preserving in the sense that it reduces the quantization noise in the input quantified image. Numerical results show that our method gives better quality images than the preexisting methods.

AN ITERATIVE MULTIGRID REGULARIZATION METHOD FOR TOEPLITZ DISCRETE ILL-POSED PROBLEMS

M. Donatelli
Department of Physics and Mathematics
University of Insubria
Via Valleggio 11 - 22100 Como, Italy
marco.donatelli@uninsubria.it

Iterative regularization multigrid methods have been successful applied to signal/image deblurring problems. When zero-Dirichlet boundary conditions are imposed the deblurring has a Toeplitz structure and it is potentially full. A crucial task of a multilevel strategy is to preserve the Toeplitz structure at the coarse levels which can be exploited to obtain fast computations. The smoother has to be an iterative regularization method. The grid transfer operator should preserve the regularization property of the smoother.

In this talk we improve the iterative multigrid method proposed in [1] introducing a wavelet soft-thresholding denoising post-smoother. Such post-smoother preserves the edges and avoids the noise amplification that is the cause of the semi-convergence of iterative regularization methods. The resulting iterative multigrid method stabilizes the iteration so that and imprecise (over) estimate of the stopping iteration does not have a deleterious effect on the computed solution.

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ITERATIVE REGULARIZATION FOR NONLINEAR IMAGING IN BANACH SPACES

C. Estatico, P. Brianzi, F. Di Benedetto,
M. Pastorino, A. Randazzo and G. Rodriguez
Dep. of Physics and Mathematics
University of Insubria, Como, Italy.
claudio.estatico@uninsubria.it

Several regularization methods for inverse problems have been firstly and deeply analyzed in the context of the Hilbert space L^2. Unfortunately, regularization methods in Hilbert spaces usually show over-smoothness, which is a drawback in all the practical imaging applications, where the true solutions have natural discontinuities.

More recently, some regularization methods have been introduced and investigated in the context of more general Banach spaces. Due to the geometrical properties of Banach spaces, these new regularization methods allow us to obtain solutions endowed with lower over-smoothness, which results, as instance, in a better localization and restoration of the edges in image deblurring.

In this talk, we consider the nonlinear operator equation $F(x) = y$, where $F : X \longrightarrow Y$ is a nonlinear and ill-posed operator between the two Banach spaces X, Y, and $x \in X$ is the "cause" to be found of some known "effects" $y \in Y$. In particular, we analyze an iterative method for the minimization of the functional $\Phi(x) = \frac{1}{p}||F(x) - y||_Y^p$, where $Y = L^p$ is the Banach space of p-th power Lebesgue integrable functions, with $1 < p < +\infty$.

The proposed iterative algorithm in the framework of L^p is a nonlinear generalization of the simple Landweber method for nonlinear equations in L^2. The algorithm is applied to a nonlinear inverse scattering problem where the dielectric distributions x (i.e., the image to restore) of a $2D$ domain have to be recovered by means of its scattered microwave field y (i.e., the known data) outside the domain. We will show how the new computational results in Banach spaces well outperform classical "Hilbertian regularization".

A FAMILY OF RULES FOR PARAMETER CHOICE IN TIKHONOV REGULARIZATION OF ILL-POSED PROBLEMS WITH INEXACT NOISE LEVEL

U. Hämarik, R. Palm and T. Raus
Faculty of Mathematics and Informatics
University of Tartu
J. Liivi 2, 50409 Tartu, Estonia
uno.hamarik@ut.ee

We consider the equation $Au = f, f \in \mathcal{R}(A)$, where $A \in \mathcal{L}(H,F)$ and H, F are real Hilbert spaces. We suppose that instead of f we have an approximation $\tilde{f} \in F$ and inexact noise level δ. We consider the case where δ may be a serious overestimation with $\|\tilde{f} - f\| \leq \delta$, but also the case of possible underestimation of the noise level: for example, it may be known only that with high probability $\delta/\|y - y_*\| \in [1/10, 10]$. We consider choice of the regularization parameter α in the Tikhonov method $u_\alpha = (\alpha I + A^*A)^{-1}A^*\tilde{f}$.

To guarantee convergence of u_α, the choice of α must use the noise level. Classical rules for parameter choice as the discrepancy principle, monotone error rule and the balancing principle are unstable with respect to the inaccuracies of the noise level: they fail in case of underestimated noise level and give large error of u_α already at very moderate overestimation of the noise level. We propose for choice of $\alpha = \alpha(\delta)$ the following family of rules.

Define $B_\alpha = \sqrt{\alpha}(\alpha I + AA^*)^{-1/2}$, $D_\alpha = \alpha^{-1}AA^*B_\alpha^2$. Fix the parameters q, k, l such that $3/2 \leq q < \infty$, $l \geq 0$, $k \geq l/q$. Choose $\alpha = \alpha(\delta)$ as the largest solution of the equation

$$\frac{(1+\alpha\|A\|^{-2})^{((k+s_0)q-l)/(2q-2)}\|D_\alpha^k B_\alpha(Au_\alpha - \tilde{f})\|^{q/(q-1)}}{\|D_\alpha^l B_\alpha^{2q-2}(Au_\alpha - \tilde{f})\|^{1/(q-1)}} = b\delta,$$

where b is constant large enough and $s_0 = 0$ if $k = l/q$, $s_0 = 1/2$ if $k > l/q$.

We will analyze the quasi-optimality and the stability of these rules. The advantages of some rules of this family over classical rules in case of the over- or underestimated noise level with $\delta/\|\tilde{f} - f\| \in [1/64, 64]$ are demonstrated on extensive numerical experiments in test problems of P.C. Hansen and from paper C. Brezinski, G. Rodriguez and S. Seatzu.

CONJUGATE GRADIENT ITERATION UNDER WHITE NOISE

P. Mathé
Weierstrass Institute for applied Analysis and Stochastics
Mohrenstrasse 39, D-10117 Berlin, Germany
mathe@wias-berlin.de

Conjugate gradient iteration for ill-posed problems in Hilbert space, say given by an operator equation

$$y^\delta = Ax + \delta\xi,$$

where $A\colon X \to Y$ acts between Hilbert spaces, is well known to yield regularization if it is stopped according to the discrepancy principle. The seminal work in this direction is [2]. This presumes that the data y^δ are noisy, but the noise is bounded in the original norm of Y. If, instead, we assume that the noise ξ is white noise, i.e., it is centered and has identity covariance operator, then the data y^δ will not belong to Y (a.s.), and hence the discrepancy is not well defined.

Based on previous work [1] we propose a modified discrepancy principle and we show that order optimal regularization can be achieved. These modifications concern both, the norm in which the discrepancy is evaluated and an emergency stop, which guarantees that the iteration stops even if the data at hand behave badly.

This modified discrepancy principle also works for linear regularization of statistical ill-posed problems.

This is joint work with G. Blanchard, Potsdam University.

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A NONLINEAR INVERSE PROBLEM IN POLYENERGETIC TOMOSYNTHESIS IMAGE RECONSTRUCTION

J. Nagy
Mathematics and Computer Science
Emory University
Atlanta, GA, 30322, USA
nagy@mathcs.emory.edu

Tomosynthesis imaging is a limited angle tomography approach that uses conventional x-ray systems to obtain 3-dimensional image reconstructions. Most breast tomosynthesis image reconstruction algorithms use a simplified, but incorrect assumption that the source x-ray beam is comprised of photons with a constant energy; that is, the x-ray beam is assumed to be monoenergetic. We consider mathematical models that use the physically correct, and hence more accurate, assumption that the x-ray beam is polyenergetic. The image reconstruction problem requires solving the nonlinear inverse problem

$$\boldsymbol{b} = \exp(\boldsymbol{R}\boldsymbol{\mathcal{M}})\boldsymbol{\rho} + \boldsymbol{\eta}\,,$$

where $\boldsymbol{b}$ is known measured projection data, $\boldsymbol{R}$ is a known *ray trace* matrix, $\boldsymbol{\rho}$ is a known vector that contains information about the source x-ray energy, $\boldsymbol{\eta}$ is a vector that represents unknown additive noise, and $\boldsymbol{\mathcal{M}}$ is an unknown matrix, where each entry $\mu_{i,j}$ is the attenuation coefficient for voxel i and x-ray energy level j. The exponentiation is done element wise on the entries of the matrix $\boldsymbol{R}\boldsymbol{\mathcal{M}}$.

The image reconstruction problem requires computing an approximation of $\boldsymbol{\mathcal{M}}$. In this talk we describe how this model arises from the physics of the x-ray tomosynthesis system, discuss computational approaches to compute approximations of $\boldsymbol{\mathcal{M}}$, and consider applications for breast imaging.

This is joint work with Veronica Bustamante, Steve Feng and Ioannis Sechopoulos, Emory University, and Julianne Chung, University of Texas at Arlington.

ALTERNATING KRYLOV SUBSPACE IMAGE RESTORATION METHODS

S. Morigi, J. Orlando, L. Reichel and **F. Sgallari**,
Department of Mathematics-CIRAM
University of Bologna
Via Saragozza 8 - 40123 Bologna, Italy
sgallari@dm.unibo.it

Alternating methods for image deblurring and denoising have recently received considerable attention. The simplest of these methods are two-way methods that restore contaminated images by alternating between deblurring and denoising. This talk discusses Krylov subspace-based two-way alternating iterative methods that allow the application of regularization operators different from the identity in both the deblurring and the denoising steps. Numerical examples show that this can improve the quality of the computed restorations. The methods are particularly attractive when matrix-vector products with a discrete blurring operator and its transpose can be evaluated rapidly, but the structure of these operators does not allow inexpensive diagonalization.

ELECTRICAL IMPEDANCE IMAGING USING NONLINEAR FOURIER TRANSFORM

S. Siltanen
Department of Mathematics and Statistics
University of Helsinki
PO Box 68, 00014 Helsinki, Finland
peaker@email.addr

The aim of electrical impedance tomography (EIT) is to reconstruct the inner structure of an unknown body from voltage-to-current measurements performed at the boundary of the body. EIT has applications in medical imaging, nondestructive testing, underground prospecting and process monitoring. The imaging task of EIT is nonlinear and an ill-posed inverse problem. A non-iterative EIT imaging algorithm is presented, based on the use of a nonlinear Fourier transform. Regularization of the method is provided by nonlinear low-pass filtering, where the cutoff frequency is explicitly determined from the noise amplitude in the measured data. Numerical examples are presented, suggesting that the method can be used for imaging the heart and lungs of a living patient.

QUADRATURE ERRORS, DISCREPANCIES AND VARIATIONAL DITHERING

G. Steidl
Department of Mathematics
University of Kaiserslautern
E. Schrödinger Str, 67653 Kaiserslautern, Germany
steidl@mathematik.uni-kl.de

The stippling technique places black dots such that their density gives the impression of tone. This is the first paper that relates the distribution of stippling dots to the classical mathematical question of finding 'optimal' nodes for quadrature rules. More precisely, we consider quadrature error functionals on reproducing kernel Hilbert spaces (RKHSs) with respect to the quadrature nodes and suggest to use optimal distributions of these nodes as stippling dot positions. Interestingly, in special cases, our quadrature errors coincide with discrepancy functionals and with recently proposed attraction-repulsion functionals. Our framework enables us to consider point distributions not only in R^2 but also on the torus T^2 and the sphere S^2. For a large number of dots the computation of their distribution is a serious challenge and requires fast algorithms. To this end, we work in RKHSs of bandlimited functions, where the quadrature error can be replaced by a least squares functional. We apply a nonlinear conjugate gradient (CG) method on manifolds to compute a minimizer of this functional and show that each step can be efficiently realized by nonequispaced fast Fourier transforms. We present numerical stippling results on S^2.

This is joint work with M. Gräf and D. Potts, University of Chemnitz, Germany.

CORDIAL VOLTERRA INTEGRAL EQUATIONS OF THE FIRST KIND

G. Vainikko
Institute of Mathematics
University of Tartu
J. Liivi 2, 50409 Tartu, Estonia
gennadi.vainikko@ut.ee

Consider the equation $V_\varphi u = f$, where $(V_\varphi u)(t) = \int_0^t t^{-1}\varphi(t^{-1}s)u(s)ds$, $0 < t \le T$, $\varphi \in L^1(0,1)$. The spectrum of V_φ as an operator in the space $C^m = C^m[0,T]$ is described in [1]. This enables to establish criteria for the existence and boundedness of the inverse V_φ^{-1} as an operator from C^{m+k} to C^m, $m \ge 0$, $k \ge 1$. In some cases, $\|V_\varphi^{-1}\|$ can be effectively estimated, e.g.:

Theorem 1. *Let $\varphi \in L^1(0,1)$, $\widehat{\varphi}(0) := \int_0^1 \varphi(x)dx > 0$, $x\varphi' \in L^1(0,1)$, and let $x\varphi'(x) + \alpha\varphi(x) \ge 0$ $(0 < x < 1)$ for an $\alpha < 1$. Then $V_\varphi^{-1} \in \mathcal{L}(C^{m+1}, C^m)$ exists, and*

$$\|V_\varphi^{-1} f\|_{C^m} \le \frac{1}{(1-\alpha)\widehat{\varphi}(0)} \|tf' + (1-\alpha)f\|_{C^m} \text{ for } f \in C^{m+1},\ m \ge 0.$$

The claim remains to be true if condition $x\varphi' \in L^1(0,1)$ is relaxed to the form $x\varphi' \in L^1(0,1-\varepsilon)$ for any $\varepsilon > 0$, and $\lim\limits_{x\to 1} \varphi(x) = \infty$, $\lim\limits_{x\to 1}(1-x)\varphi(x) = 0$.

More complete results are obtained using the weighted spaces

$$C_\star^{m,r} = \left\{ u \in C^m(0,T] : \lim_{t\to 0} t^{k-r} u^{(k)}(t) \text{ exists for } k = 0,1,...,m \right\},$$

$$\|u\|_{C_\star^{m,r}} = \max_{0\le k\le m} \sup_{0<t\le T} t^{k-r}|u^{(k)}(t)|, \quad m \ge 0, \quad r \in \mathbf{R}.$$

The power functions t^p, $p \ge r$, are eigenfunctions of V_φ in $C_\star^{m,r}$, $m \ge 0$. This enables to design approximate and exact solvers of equation $V_\varphi u = f$.

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4. Special Session on Iterative Methods for Linear Systems

PRECONDITIONING AND ITERATIVE METHODS FOR COMPLEX LINEAR SYSTEMS

Z.-Z. Bai
State Key Laboratory of Scientific/Engineering Computing
Institute of Computational Mathematics
and Scientific/Engineering Computing
Academy of Mathematics and Systems Science
Chinese Academy of Sciences
P.O. Box 2719, Beijing 100190, P.R.China
Email: bzz@lsec.cc.ac.cn

For a class of complex symmetric systems of linear equations, by modifying the *Hermitian and skew-Hermitian splitting* (**HSS**) iteration method and making use of the special structure of the coefficient matrix, we have designed a class of matrix splitting iteration schemes, which is unconditional convergent for any initial guess. We have then discussed real equivalent reformulations of these matrix splitting iteration schemes applied them to solve and precondition the saddle-point linear systems arising from the Galerkin finite-element discretizations of the distributed control problems.

This talk is based on joint works with Michele Benzi and Fang Chen [1, 2].

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DEFLATION BASED PRECONDITIONING OF LINEAR SYSTEMS OF EQUATIONS

M. H. Gutknecht
Seminar for Applied Mathematics, ETH Zurich
CH-8092 Zurich, Switzerland
mhg@math.ethz.ch

For most real-world problems Krylov space solvers only converge in a reasonable number of iterations if a suitable preconditioning technique is applied. This is particularly true for problems where the linear operator has eigenvalues of small absolute value — a situation that is very common in practice. One suitable technique for dealing with such problems is to identify an approximately invariant subspace $\mathcal{Z}$ that belongs to the set of these small eigenvalues. By using an orthogonal projection along $\mathcal{Z}$ the Krylov solver can then be applied only to the orthogonal complement by restricting the operator accordingly. The basis constructed implicitly or explicitly by this restricted operator should then be augmented by a set of basis vectors for $\mathcal{Z}$. There are various ways to handle and implement this approach. They differ not only algorithmically and numerically, but sometimes also mathematically. Some keywords associated with such methods are '(spectral) deflation', 'augmented basis', 'recycling Krylov subspaces', and 'singular preconditioning'.

While we quickly also review the 'symmetric case', where the linear system is Hermitian (or real and symmetric), we are mostly interested in the 'non-symmetric case', where our main message is that the orthogonal projection should be replaced by a suitable oblique projection, so that when its nullspace is invariant, so is its range. For details, see [1].

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INNER-ITERATION GMRES METHODS FOR UNDERDETERMINED LEAST SQUARES PROBLEMS

K. Morikuni and **K. Hayami**
National Institute of Informatics, Tokyo, Japan
hayami@nii.ac.jp

Consider the underdetermined least squares problem

$$\min_{\boldsymbol{x}\in\mathbf{R}^n} \|\boldsymbol{b} - A\boldsymbol{x}\|_2, \tag{1}$$

where $A \in \mathbf{R}^{m\times n}$, $\boldsymbol{b} \in \mathbf{R}^m$, and $m < n$.

We can precondition (1) from the right as

$$\min_{\boldsymbol{u}\in\mathbf{R}^n} \|AB\boldsymbol{u} - \boldsymbol{b}\|_2, \quad \boldsymbol{x} = B\boldsymbol{u} \tag{2}$$

or from the left as

$$\min_{\boldsymbol{x}\in\mathbf{R}^n} \|B\boldsymbol{b} - BA\boldsymbol{x}\|_2 \tag{3}$$

by using a preconditioner $B \in \mathbf{R}^{n\times m}$ [2].

However, when solving inconsistent systems ($\boldsymbol{b} \notin \mathcal{R}(A)$), the effective condition number becomes dangerously large[1], and GMRES for (2) will breakdown numerically before it determines a least squares solution.

On the other hand, (3) is consistent when $\mathcal{R}(B^T) = \mathcal{R}(A)$. Thus, GMRES can numerically determine a least squares solution for (1) even when $m < n$ and $\boldsymbol{b} \notin \mathcal{R}(A)$. To form such a preconditioner B, we propose using inner-iteration preconditioners, which do not require a preconditioning matrix and can save memory. Numerical experiments illustrate that the methods are efficient and robust for large ill-conditioned and rank-deficient problems.

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BLOCK ARNOLDI-BASED METHODS FOR LARGE SCALE DISCRETE-TIME ALGEBRAIC RICCATI EQUATIONS

K. Jbilou
L.M.P.A.
Université du Littoral Côte d'Opale
50 rue F. Buisson BP699, F-62228 Calais Cedex, France
jbilou@lmpa.univ-littoral.fr

Algebraic Riccati equations (discrete-time or continuous-time) play a fundamental role in many problems in control theory. They arise in linear-quadratic regulator problems, H_∞ or H_2-control, model reduction problems and many others. In this talk we propose numerical methods for large discrete-time algebraic Riccati equations (DARE).

We present block projection methods that allow us to compute low rank approximations to the d-stabilizing solution. We project the initial problem onto a block or onto an extended block Krylov subspace, generated by the pair (A, C) and we obtain a low dimensional DARE that is solved by a standard algorithm such as the Schur method. We present the two methods and give new theoretical results such as upper bounds for the norm of the error. We will also present the Newton method associated with the block Arnoldi algorithm used for solving, at each Newton's iteration, the obtained Stein matrix equation.

THE COMPUTATION OF ISOTROPIC VECTORS

G. Meurant
http://gerard.meurant.pagesperso-orange.fr/
Paris, France
gerard.meurant@gmail.com

We show how to compute isotropic vectors for matrices with real or complex entries. These are unit vectors b satisfying $b^*Ab = 0$ where the $*$ denotes the conjugate transpose. For real matrices, the algorithm uses only the eigenvectors of the symmetric part of A corresponding to the extreme eigenvalues. For complex matrices, we first use the eigenvalues and eigenvectors of the Hermitian matrix $K = (A - A^*)/2i$. This works in many cases. In case of failure, we use the eigenvectors of the Hermitian part H or a combination of eigenvectors of H and K. We give some numerical experiments comparing our algorithm with those proposed in [2] and [1]. In many cases our algorithm use only one computation of eigenvectors whence the other algorithms use at least two computations of eigenvectors.

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A NEW APPROACH TO CONJUGATE GRADIENT AND GMRES CONVERGENCE

H. Sadok
L.M.P.A
Université du Littoral Côte d'Opale
50 rue F. Buisson BP699, F-62228 Calais Cedex, France
sadok@lmpa.univ-littoral.fr

Known as one of the best iterative methods for solving symmetric positive definite linear systems, CG generates as FOM an Hessenberg matrix which is symmetric then triangular. This specific structure may be really helpful to understand how does behave the convergence of the conjugate gradient method and its study gives an interesting alternative to Chebyshev polynomials. The talk deals about some new bounds on residual norms and error A-norms using essentially the condition number.

GMRES is one of the most widely used iterative methods for the solution of linear system of equations, with a large real or complex nonsingular matrix. Convergence properties of GMRES are discussed by many authors. But most convergence results are obtained as a polynomial approximation problem.

We will show that bounding the norm of the residual vectors determined by GMRES in terms of the eigenvalues of the matrix, is a difficult constrained optimization problem. We therefore focus on diagonalizable matrices and in the particular case where the matrix is we will show how to derive a bound of the norm of the residual by solving a constrained optimization problem using Lagrange multipliers.

MATCHING MOMENTS AND KRYLOV SUBSPACE METHODS

J. Liesen and **Z. Strakoš**
Department of Mathematics
Charles University
Sokolovska 83, Prague, Czech Republic
strakos@karlin.mff.cuni.cz

Matching moments is inherently linked with numerical quadrature, continued fractions and orthogonal polynomials. The concept of moments arose with the work of Chebyshev, Markov and Stieltjes in the second half of the 19th century; the related numerical quadrature with Gauss in 1814, with further founding contributions due to Jacobi, Christoffel, Markov, Stieltjes and many others. The related fundamental concept of continued fractions can essentially be rooted back to Euclid and other ancient mathematicians; see the thorough descriptions given by Brezinski in several books, papers and essays. Stieltjes published in 1894 his analytic theory of continued fractions with an impact in forming foundations of functional analysis by Hilbert in 1906 - 1912, as well as in forming mathematical foundations of quantum mechanics by von Neumann in 1927 - 1932.

The original work of Krylov from 1931 refers to the work of Jacobi from 1846. Its algebraic formulation, with using what we now call the Krylov sequence, was given by Gantmacher in 1934. In modern computational mathematics, sciences and engineering, many ideas behind Krylov subspace methods and matching moments model reduction (in approximation of large scale dynamical systems and elsewhere) resemble the classical concepts mentioned above. Surprisingly, several important works which made these links transparent remained almost unknown; see, in particular, the work of Vorobyev from 1958 which would be without its popularization by Brezinski essentially forgotten.

In agreement with the views presented by Brezinski, Golub and Meurant, we consider viewing relevant matrix computations as matching moments inspirational and useful. We will demonstrate this on several examples. In particular, we will address the question of cost evaluation and numerical stability in Krylov subspace iterations.

PRECONDITIONED MULTIPARAMETER AND NEWTON-MULTIPARAMETER ITERATIVE METHODS FOR SYSTEMS OF EQUATIONS

Y.-J. Wu and Y. Wang
School of Mathematics and Statistics
Lanzhou University
Lanzhou 730000, China
myjaw@lzu.edu.cn

We propose, in this article, three types of modified multiparameter iterative schemes which lay the foundation for us to successively establish preconditioned multiparameter iterative methods for the solution of systems of linear equations and preconditioned Newton-multiparameter iterative methods for the solution of systems of nonlinear equations. Based on the matrix version of Kantorovich inequality, we obtain successfully the proof of convergence of the preconditioned multiparameter and the preconditioned Newton-multiparameter iterative methods. Incremental unknowns preconditioners are used. Inexact Newton techniques are also applied while computing. Numerical results from examples confirm the efficiency of our new methods.

DISTINCT PRECONDITIONED HSS ITERATION METHOD FOR NON-HERMITIAN POSITIVE DEFINITE LINEAR SYSTEMS

B. Zheng and S.-X. Miao
School of Mathematics and Statistics
Lanzhou University
Lanzhou, 730000, People's Republic of China
bzheng@lzu.edu.cn

We introduce and analyze a distinct PHSS (DPHSS) method for solving the large sparse non-Hermitian positive definite system of linear equations, in which two linear subsystems with different preconditioners are solved at each iteration. The convergence properties of the DPHSS method are studied and the optimal parameter for an upper bound of the the contraction factor of the DPHSS method is derived. Numerical experiments are performed with different examples.

5. Special Session on Nonlinear Evolution Equations

EXACT SOLUTIONS TO INTEGRABLE NONLINEAR EVOLUTION EQUATIONS

T. Aktosun, F. Demontis, and C. van der Mee
Department of Mathematics
University of Texas at Arlington
Arlington, Texas 76019, USA
aktosun@uta.edu

A review is presented for the method of constructing explicit solutions to integrable evolution equations in terms of a matrix triplet. The construction is based on solving the associated Marchenko integral equations explicitly by representing their kernels in terms of a matrix triplet, using matrix exponentials, and exploiting the separability of those kernels. Once an explicit formula is obtained for the relevant integrable evolution equation, it is usually possible to independently verify that the formula does indeed satisfy the corresponding nonlinear evolution equation. Such exact solutions can alternatively be written explicitly as algebraic combinations of exponential, trigonometric, and polynomial functions of the spatial and temporal coordinates. The method is illustrated with some explicit examples.

INTEGRABILITY AND SOLVABILITY OF NONLOCAL WAVE INTERACTION MODELS

A. Degasperis, and J.P. Borgna, M.F. De Leo, D. Rial
Department of Physics
Sapienza University of Rome
Piazzale Aldo Moro 2, 00185 Roma, Italy
antonio.degasperis@roma1.infn.it

A general class of integrable nonlinear multi-component wave interaction equations is discussed to the purpose of showing that Lax integrability does not imply solvability of the initial value problem by means of the direct and inverse spectral methods. A simple system in this class, with applicative relevance to nonlinear optics, is discussed as a prototype model. Conservation laws and special solutions are displayed as an expansion of the content of the paper [1].

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EXACT SOLUTIONS TO THE FOCUSING DISCRETE NONLINEAR SCHRÖDINGER EQUATION

F. Demontis and C. van der Mee
Department of Mathematics and Informatics
University of Cagliari
Viale Merello 92, 09121 Cagliari, Italy
fdemontis@unica.it

In this talk, by using the Inverse Scattering Transform (IST), we derive explicit solutions of the discrete nonlinear Schrödinger equation (IDNLS):

$$i\frac{d}{d\tau}\mathbf{u}_n = \mathbf{u}_{n+1} - 2\mathbf{u}_n + \mathbf{u}_{n-1} + \mathbf{u}_{n+1}\mathbf{u}_n^\dagger\mathbf{u}_n + \mathbf{u}_n\mathbf{u}_n^\dagger\mathbf{u}_{n-1}\,, \tag{4}$$

where n is an integer and $\mathbf{u}_n$ is an $N \times M$ matrix function depending on time τ. More precisely, the IST associates (1) to the following discrete Zakharov-Shabat system,

$$\mathbf{v}_{n+1} = \begin{pmatrix} zI_N & \mathbf{u}_n \\ \mathbf{u}_n^\dagger & z^{-1}I_M \end{pmatrix}\mathbf{v}_n \tag{5}$$

where z is the (complex) spectral parameter.

We get the explicit solutions for (1) announced above by applying the Marchenko method to solve the inverse problem associated with (2). In fact, representing the kernel of the Marchenko equation as

$$CA^{-(n+j+1)}e^{i\tau(A-A^{-1})^2}B,$$

where (A, B, C) is a matrix triplet such that the $p \times p$ matrix A has only eigenvalues of modulus larger than one, while B and C have sizes, respectively, $p \times N$ and $M \times p$, the Marchenko equation can be solved explicitly by separation of variables. The class of solutions obtained contains the N-soliton and the breather solutions as special cases, as well as the so-called multipole soliton solutions.

SPECTRAL PROPERTIES OF THE LAX OPERATOR FOR THE MATRIX NONLINEAR SCHRÖDINGER SYSTEM

M. Klaus
Department of Mathematics
Virginia Polytechnic Institute and State University
Blacksburg, VA 24061, USA
klaus@math.vt.edu

We discuss spectral properties of the AKNS system associated with the matrix nonlinear Schrödinger system. In particular we consider systems whose coefficients have nontrivial asymptotics. We discuss the location and existence of eigenvalues and we obtain some new results that generalize earlier ones for systems whose coefficients decay at infinity.

QUASICLASSICAL DA RIOS SYSTEM AND GRADIENT CATASTROPHE FOR VORTEX FILAMENT MOTION

B. Konopelchenko
Department of Physics
University of Salento
73100 Lecce, Italy
konopel@le.infn.it

Quasiclassical Da Rios (or dispersionless focusing NLS system) describe motion of vortex filament with slow varying curvature and torsion. It is shown that the points of gradient catastrophe for this system correspond to the fluttering points of filament at which the local behaviour of the corresponding curve is drastically different from that of normal points. Concrete examples of such behaviour are discussed.

COUPLED MAXWELL-BLOCH EQUATIONS WITH INHOMOGENEOUS BROADENING FOR A 3-LEVEL SYSTEM

S. Chakravarty, **B. Prinari** and M. J. Ablowitz
Department of Physics and Sezione INFN
University of Salento
bprinari@uccs.edu

The phenomenon that describes the effect of a coherent medium response to an incident electric field, to which the medium is totally transparent and which undergoes lossless propagation, is known as self-induced transparency (SIT). SIT was first discovered by McCall and Hahn (1969) in the case of non-degenerate two-level atoms. Special solutions for the two-level system were found by Lamb (1971), while the initial value problem for the propagation of a pulse through a resonant two-level optical medium was solved by Inverse Scattering Transform (IST) in [1, 2].

It is possible to formulate the SIT equations in the framework of the IST also in the case of a three-level system, as in [3]. While the associated scattering problem is the same as for the coupled nonlinear Schrödinger equation, the time evolution depends on asymptotic values of the material polarizability envelopes and is highly non-trivial.

This talk will address the solution of the initial value problem for the SIT equations for three level systems, for generic preparation of the medium, and describe its soliton interactions.

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NUMERICAL SOLUTION OF INVERSE SCATTERING PROBLEMS AND APPLICATION TO NONLINEAR EVOLUTION EQUATIONS

P. Sacks
Department of Mathematics
Iowa State University
Ames, IA 50011, USA
psacks@iastate.edu

Some particular numerical methods for solution of inverse scattering problems on the line, such as ones connected to the Zakharov-Shabat system, will be discussed. Corresponding examples of solving evolution equations by the inverse scattering transform will be given.

COMMUTING VECTOR FIELDS AND INTEGRABLE PDES OF HYDRODYNAMIC TYPE

S. V. Manakov and **P. M. Santini**
Department of Physics
University of Roma "La Sapienza"
Piazz.le A. Moro 2, 00185 Roma, Italy
paolo.santini@roma1.infn.it

Using a recently developed Inverse Spectral Transform for commuting multidimensional vector fields [1], we have been able to solve the Cauchy problem for physically relevant PDEs, like the heavenly equation of Plebansky [1], relevant in General Relativity, the dispersionless Kadomtsev - Petviashvili (dKP) equation [2], describing the propagation of weakly nonlinear and quasi one dimensional waves in the absence of dispersion and dissipation, and the 2D dispersionless Toda (2DDT) equation [3], describing integrable Einstein - Weyl metrics and ideal Hele - Shaw flows. In addition, the associated nonlinear Riemann - Hilbert inverse problem has turned out to be a powerful tool to study the longtime behavior of solutions, to construct classes of exact implicit solutions and to study in great detail the gradient catastrophe of multidimensional waves, like in the case of the dKP and 2DDT equations.

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RECURSION OPERATORS AND HIERARCHIES OF NONCOMMUTATIVE KDV-TYPE EQUATIONS

C. Schiebold
Department of Natural Sciences, Engineering, and Mathematics,
Mid Sweden University
S-85170 Sundsvall, Sweden
cornelia.schiebold@miun.se

We explain an operator theoretic approach to construct simultaneous solutions to all equations of the noncommutative counterparts to the potential KdV, KdV and mKdV hierarchies. One of the main technical issues will be to take advantage of the recursive construction of these hierarchies. In an excursion, we will address general structural properties of the underlying recursion operator of the noncommutative KdV equation. In the applications part, we will discuss both the classical scalar hierarchies (countable nonlinear superposition) and matrix hierarchies (generalized multisoliton solutions).

Large parts of the talk are based on recent joint work in [1], [2] with Sandra Carillo, Roma 1.

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NOVEL FORMULATION OF DISCRETE INTEGRABLE NONLINEAR SCHRÖDINGER EQUATIONS

C. van der Mee
Dipartimento di Matematica e Informatica
Università di Cagliari
Viale Merello 92, 09123 Cagliari, Italy
cornelis@krein.unica.it

Discretizations of matrix nonlinear Schrödinger equations have the problem that the natural finite difference discretization of the matrix NLS equation leads to a nonlinear equation whose integrability is not obvious. This has led to the development of an inverse scattering transform scheme where the (focusing) discrete NLS solution $\boldsymbol{u}_n(t)$ is required to let $\boldsymbol{u}_n(t)\boldsymbol{u}_n(t)^\dagger$ and $\boldsymbol{u}_n(t)^\dagger\boldsymbol{u}_n(t)$ be nonzero multiples of the identity matrix, thus preventing a proper discretization of the Manakov system.

In this talk we explore various remedies. One is to discretize every single step in the IST, but in this case the nonlinear evolution problem might be difficult to formulate (although integrability is guaranteed). The other option is to apply central differencing (and not one-sided differencing as Ablowitz-Ladik did) in the matrix Zakharov-Shabat system, develop the direct and inverse scattering theory of the resulting system

$$iJ\frac{u_{n+1}-u_{n-1}}{2h} = [\lambda I_{N+M} + U_n]u_n,$$

stick in time factors, and apply the usual matrix triplet method to develop explicit discrete NLS solutions. Again we have to hope knowing the nonlinear evolution system. Here we attempt finding suitable Lax pairs.

6. Special Session on Optimization and Management Science

CONSTANT POSITIVE GENERATORS: A NEW CONSTRAINT QUALIFICATION

R. Andreani, G. Haeser, P. J. S. Silva, M. L. Schuverdt
University of State of Campinas
Rua Sérgio Buarque de Holanda, 651, Brazil
andreani@ime.unicamp.br

We present a new constraint qualification that extends the relaxed constant rank constraint qualification. We relax the assumption that the rank of all subsets of gradients of active inequality constraints and equalities constraints must remain constant, to a single subset of such gradients which is easily computed. Our new constraint qualification also extends the relaxed constant positive linear dependence condition recently proposed and ensures the convergence of penalty based methods, like the augmented Lagrangian, and of a sequential quadratic programming algorithm.

PRECONDITIONER UPDATES FOR SEQUENCES OF SYMMETRIC POSITIVE DEFINITE LINEAR SYSTEMS ARISING IN OPTIMIZATION

S. Bellavia, V. De Simone, D. di Serafino and B. Morini
Dipartimento di Energetica
Università degli Studi di Firenze, Italy
stefania.bellavia@unifi.it

We consider sequences of large and sparse linear systems of the form

$$(A + D_j)x_j = b_j, \qquad j = 1, \ldots, m,$$

where A is a symmetric positive definite matrix and D_j are positive definite diagonal matrices. The solution of such sequences often arises in optimization, e.g. in trust-region and regularization subproblems, in Levenberg-Marquadt approaches, in affine scaling methods for quadratic programming, and in nonlinear least-squares. Our interest is in the case where the systems are solved by using Krylov methods with preconditioning techniques.

The spectral properties of the matrices of the sequence may considerably differ. Therefore, it may be inappropriate to use a frozen preconditioner for all the systems. We are interested in forming an efficient preconditioner for each system of the sequence without recomputing the preconditioner from scratch, in order to reduce the overall computational cost.

In this talk, we discuss techniques to update an incomplete LDL^T factorization of the matrix A. The proposed procedures, extending previous work on shifted systems [1], are cheap and easy to implement. A theoretical justification of our approach is presented along with numerical experiments illustrating its performance.

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DIRECT MULTISEARCH: A NEW DFO APPROACH FOR MULTIPLE OBJECTIVE FUNCTIONS

A. L. Custódio, J. F. A. Madeira, A. I. F. Vaz and L. N. Vicente
New University of Lisbon
Department of Mathematics, FCT-UNL,
Quinta da Torre, 2829-516 Caparica, Portugal
alcustodio@fct.unl.pt

Direct MultiSearch (DMS) is a novel derivative-free algorithm for multiobjective optimization, which does not aggregate any of the objective functions. Inspired by the search/poll paradigm of direct-search, DMS uses the concept of Pareto dominance to maintain a list of nondominated points, from which the new poll centers are chosen. The aim is to generate as many points in the Pareto frontier as possible from the polling procedure itself, while keeping the whole framework general to accommodate other disseminating strategies, in particular when using the (here also) optional search step.

We provide a convergence analysis for the algorithm and report computational results, which show that our methodology has an impressive capability of generating the whole Pareto frontier even without using a search step.

BILEVEL OPTIMIZATION PROBLEMS VIA INEXACT RESTORATION

A. Friedlander
Department of Applied Mathematics
State University of Campinas
Campinas, São Paulo, Brazil
friedlan@ime.unicamp.br

We discuss different approaches for solving bilevel optimization problems. There are many theoretical issues such as specifical optimality conditions and constraint qualifications and we analize their relationship with practical algorithms. Inexact Restoration methods are one of the techniques proposed for bilevel problems. We present some theoretical results concerning these methods and some practical algorithms developed based in these technique.

NUMERICAL TESTS ON A NEW STRATEGY FOR PARALLEL DERIVATIVE FREE OPTIMIZATION

Ub. M. García-Palomares, I. García, and P. Rodríguez
Departamento of Ingeniería Telemática
Universidad de Vigo
Lagoas, Marcosende s/n, 36310 Vigo, Spain
ubaldo@det.uvigo.es

We present numerical tests on a new paradigm for solving derivative free optimization problems in a multiprocessor environment. The exchange of information among processors is realized whenever a point that belong to a sequence of quasi-minimal points is detected. This concept was coined by [1] for unconstrained optimization and later adapted to bound constraint optimization by [2]. The computing time needed for solving benchmarking problems is clearly superior to those given by state of the art packages for unconstrained and bound constrained problems.

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MODELING LONG-TERM IMPACTS OF THE EUROPEAN EMISSION TRADE SYSTEM

C. Hammer
Chair of Management Accounting and Control
Technical University Munich
Arcisstrasse 21, 80333 Munich, Germany
Carola.Hammer@wi.tum.de

This study deals with regulatory instruments, but focuses especially on the Emission Trade System (ETS) designed by the United Nations Framework Convention on Climate Change and introduced by the European Union in 2005. It is in our interest to forecast the effects of the ETS on different indicators with economic importance (e.g. emission abatement, power price, import dependency, supply security, efficiency increase) and its costs up to the year 2020. Therefore we use an optimization model, in which we consider the regulation framework, the market parameters and technical constraints for the German energy market as well as an endogenous price for emission allowances, running times of plants and capacity enlargements. After solving the model with linear programming in different scenarios we find, that the ETS has strong impacts on production decisions, but low interest rates offered by the market inventive program are more effective in long-term decisions like plant investments.

A LINE SEARCH METHOD WITH VARIABLE SAMPLE SIZE

N. Krejić and N. Krklec
Department of Mathematics and Informatics
University of Novi Sad
Trg Dositeja Obradovića 4, Novi Sad, Serbia
natasak@uns.ac.rs

Minimization of uncostrained objective function in the form of mathematical expectation is considered. Sample Average Approximation - SAA method transforms the expectation objective function into a real-valued deterministic function using large sample in each iteration and thus deals with deterministic function minimization. The main drawback of this approach is its cost. A large sample of the random variable that defines the expectation must be taken in order to get reasonably good approximation and thus the sample average approximation method assumes very large number of functional evaluations. We will present a line search strategy that uses variable sample size and thus makes the process significantly cheaper. Two measures of progress - lack of precision and functional decrease are calculated at each iteration. Based on this two measures a new sample size is determined. The rule we will present allows us to increase or decrease the sample size in each iteration until we reach some neighborhood of the solution. After that the maximal sample size is used so the variable sample size strategy generates the solution of the same quality as SAA method but with significantly smaller number of functional evaluations.

REMARKS ON CONSTRAINED OPTIMIZATION

J. M. Martínez
Department of Applied Mathematics
State University of Campinas
Campinas, São Paulo, Brazil
martinez@ime.unicamp.br

Optimization is the art of finding the lowest possible value of a given function on some domain. Its importance comes from the great variety of direct applications. Solving optimization problems requires efficient and robust software. Global optimization is very hard, however, modern efficient software should incorporate global optimization tools. Software performance depends on stopping criteria. Good theory is necessary to understand the behavior of algorithms when they do not converge to a solution. According to it we decide the application of global optimization tools. KKT-optimizers should be integrated to Global-optimizers and to engineers. Modeling is a part of the optimization task.

STOCHASTIC MODELLING TECHNIQUES MEET PRACTICAL NEEDS

M. Siegle
University of the German Armed Forces Munich
Dept. of Computer Science
D-85577 Neubiberg, Germany
markus.siegle@unibw.de

Stochastic modelling and analysis is a well-established discipline which focuses on the evaluation of quantitative measures of systems, such as performance, dependability, or energy consumption. A wide range of sophisticated modelling methods and analysis algorithms has been developed in this area, many of which have been implemented in available software tools. Even though these methods and tools are extremely powerful, they often reach their limits when facing the needs of real-world systems, due to the following reason: Scalable parallel or distributed systems with a high degree of concurrency lead to models with extremely large state spaces, which renders most state-space-based analysis techniques intractable.

Among the techniques addressing this problem, the so-called “symbolic” approach, which relies on the use of decision diagrams as its basic data structure, has shown to be very effective. Starting from a formal model specification (expressed, for example, in the language of queueing networks, stochastic Petri nets or stochastic process algebra), a compact symbolic representation of the underlying labelled Markov chain is generated automatically. All subsequent steps of analysis can be performed in an efficient manner based on this representation. This includes preprocessing steps, such as reachability analysis and the elimination of vanishing states, but also different forms of numerical analysis and the computation of the measures of interest. Iterative methods for calculating the vector of steady-state or transient probabilities can be realised efficiently, while being much more space-efficient than solutions relying, on sparse representations. The key to success with this symbolic approach lies in the proper exploitation of the system’s compositional structure, which is reflected in the structure of the decision diagram, leading to its compactness and efficiency of manipulation.

7. Special Session on Orthogonal Polynomials and Quadrature

QUADRATURE ON THE POSITIVE REAL LINE WITH QUASI AND PSEUDO ORTHOGONAL RATIONAL FUNCTIONS

A. Bultheel, P. González-Vera, E. Hendriksen, and O. Njåstad
Department of Computer Science
K.U. Leuven
Celestijnenlaan 200A, box 2402
Heverlee, Belgium
adhemar.bultheel@cs.kuleuven.be

We consider a positive measure on $[0,\infty)$ and a sequence of nested spaces $\mathcal{L}_0 \subset \mathcal{L}_1 \subset \mathcal{L}_1 \cdots$ or rational functions with prescribed poles in $[-\infty,0]$. Let $\varphi_k \in \mathcal{L}_k$ be the associated sequence of orthogonal rational functions. The zeros of φ_n can be used as the nodes of a rational Gauss quadrature formula that is exact for all functions in $\mathcal{L}_n \cdot \mathcal{L}_{n-1}$, a space of dimension $2n$. Quasi- and pseudo-orthogonal functions are functions in $\mathcal{L}_n$ that are orthogonal to some subspace of $\mathcal{L}_{n-1}$. Both of them are generated from φ_n and φ_{n-1} and depend on a real parameter τ. Their zeros can be used as the nodes of a rational Gauss-Radau quadrature formula where one node is fixed in advance and the others are chosen to maximize the subspace of $\mathcal{L}_n \cdot \mathcal{L}_{n-1}$ where the quadrature is exact. The parameter τ is used to fix a node at a pre-assigned point. The space where the quadratures are exact have dimension $2n-1$ in both cases but it is in $\mathcal{L}_{n-1} \cdot \mathcal{L}_{n-1}$ in the quasi-orthogonal case and it is in $\mathcal{L}_n \cdot \mathcal{L}_{n-2}$ in the pseudo-orthogonal case. Although the quasi and the pseudo orthogonal rational functions and their zeros have very similar properties theoretically, the pseudo orthogonal rational functions are computationally much less favorable as compared to the quasi orthogonal rational functions if we want to compute the nodes and weights via a generalized eigenvalue problem.

FROM OPTIMAL CUBATURE FORMULAE TO CHEBYSHEV LATTICES: A WAY TOWARDS GENERALISED CLENSHAW-CURTIS QUADRATURE

R. Cools and K. Poppe
Dept. of Computer Science
K.U. Leuven
Celestijnenlaan 200A, B-3001 Heverlee, Belgium
Ronald.Cools@cs.kuleuven.be

A landmark paper for cubature formulae in two dimensions is [1]. It used the ideal-theoretical approach to construct cubature formulae of arbitrary degrees attaining Möller's lower bound and pointed the direction towards a multivariate extension of Clenshaw-Curtis quadrature. To develop this idea, we introduced Chebyshev lattices [2]. This is a framework for cubature with the Chebyshev weight function. In combination with hyperinterpolation theory, this can be used to construct multivariate Chebyshev approximations and interpolating cubature rules. These rules extends the idea of Clenshaw-Curtis quadrature, including the efficient implementations that use the fast Fourier transform (FFT), to higher dimensions. Our framework includes Morrow-Patterson rules as well as other (near-)optimal point sets in two dimensions (such as Padua points). Higher dimensional point sets due to Noskov and Godzina also fit into this framework.

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ASYMPTOTICS FOR CHRISTOFFEL FUNCTIONS BASED ON ORTHOGONAL RATIONAL FUNCTIONS

K. Deckers
Department of Computer Science
K.U. Leuven
Heverlee, Belgium
karl.deckers@cs.kuleuven.be

Suppose the rational functions $\{\varphi_j\}$, with poles in $\{\alpha_1, \ldots, \alpha_j\} \subset (\mathbb{C} \cup \{\infty\}) \setminus [-1,1]$, form an orthonormal system with respect to a positive bounded Borel measure μ on $I := [-1,1]$, satisfying the Erdős-Turán condition $\mu' > 0$ a.e. on I, and let the associated Christoffel functions be given by $\lambda_n(x) = [\sum_{j=0}^{n-1} |\varphi_j(x)|^2]^{-1}$. Assuming the sequence $\{n\lambda_n(x)\}_{n>0}$ converges for certain $x \in I$, and the poles are all real and bounded away from I, in [2, Appendix A.2] the author obtained an expression for the limit function $k(x) = \lim_{n\to\infty} n\lambda_n(x)$. The actual convergence, however, has only been proved for the special case of the Chebyshev weight functions $\frac{d\mu(t)}{dt} = (1+t)^a(1-t)^b$, where $a, b \in \{\pm\frac{1}{2}\}$, and for every $x \in I$ in [2, Chapter 9.7]. In this contribution we will prove convergence for arbitrary complex poles bounded away from I, and weight functions of the form $\frac{d\mu(t)}{dt} = g(t)\prod_{i=1}^{k} |t-t_i|^{\nu_i}$, where $-1 \leqslant t_1 < \ldots < t_i < \ldots < t_k \leqslant 1$, $\nu_i > -1$, $0 < C_1 \leqslant g(t) \leqslant C_2 < \infty$ for every $t \in I$, and $g(t)$ is continuous in a neighbourhood of $x \in I$.

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N-COHERENT PAIRS OF MEASURES

F. Marcellán
Departamento de Matemáticas
Universidad Carlos III de Madrid
Avenida de la Universidad 30, 28911 Leganés, Spain
pacomarc@ing.uc3m.es

Let us introduce the Sobolev type inner product $\langle f, g\rangle = \langle f, g\rangle_1 + \lambda\langle f', g'\rangle_2$ where $\lambda > 0$ and

$$\langle f, g\rangle_1 = \int_{-1}^{1} f(x)g(x)(1-x)^{\alpha}(1+x)^{\beta}dx,$$

$$\langle f, g\rangle_2 = \int_{-1}^{1} f(x)g(x)\frac{(1-x)^{\alpha+1}(1+x)^{\beta+1}}{\prod_{k=1}^{M}|x-\xi_k|^{N_k+1}}dx + \sum_{k=1}^{M}\sum_{i=0}^{N_k} M_{k,i}f^{(i)}(\xi_k)g^{(i)}(\xi_k),$$

with $\alpha, \beta > -1$, $|\xi_k| > 1$, and $M_{k,i} > 0$, for all k, i. A Mehler-Heine type formula, the inner strong asymptotics on $(-1, 1)$ as well as some estimates for the polynomials orthogonal with respect to the above Sobolev inner product are obtained. Necessary conditions for the norm convergence of Fourier expansions in terms of such Sobolev orthogonal polynomials are given (see [1]).

Some extensions of these results for other classical measures are analyzed.

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MULTIPLE ORTHOGONAL POLYNOMIALS AND GENERALIZED QUADRATURE FORMULAE

G. V. Milovanović
Faculty of Computer Sciences
Megatrend University
Bulevar Umetnosti 29, 11070 Beograd, Serbia
gvm@megatrend.edu.rs

There are several applications of multiple orthogonal polynomial, which are also known as Hermite-Padé polynomials (cf. Aptekarev [1]). Some interesting properties of these polynomials were investigated by Van Assche [2] and Van Assche and Coussement [3].

An application of multiple orthogonal polynomials to Borges quadratures (1994) was given by Milovanović and Stanić (2003).

In this lecture we consider a class of generalized quadrature formulae of Birkhoff-Young type for analytic functions in the complex plane and give a direct connection with multiple orthogonal polynomials. Precisely, we give a characterization of such generalized quadratures in terms of multiple orthogonal polynomials and prove the existence and uniqueness of these quadratures. Finally, a method for constructing such kind of quadratures and some numerical examples are given.

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THE ERROR NORM OF QUADRATURE FORMULAE

S. E. Notaris
Department of Mathematics
University of Athens
Panepistemiopolis, 15784 Athens, Greece
notaris@math.uoa.gr

In certain spaces of analytic functions the error term of a quadrature formula is a continuous linear functional. We give a survey of the methods used in order to compute or estimate the norm of the error functional. The results, some of which are fairly recent, cover, among others, interpolatory, Gaussian and Kronrod formulae.

CONTINUOUS SOBOLEV ORTHOGONAL POLYNOMIALS ON THE UNIT BALL

T. E. Pérez and M. A. Piñar
Departamento de Matemática Aplicada
Universidad de Granada
18071 Granada, Spain
tperez@ugr.es

Sobolev orthogonal polynomials in several variables are defined via inner products involving derivation tools such as gradients. Such a kind of polynomials appears for the first time in [2] in a problem related to dwell time for polishing tools in fabricating optical surfaces.

The Sobolev modification of standard multivariate measures by adding another measure involving gradients is studied. We emphasize the particular case when both measures are classical measures on the unit ball.

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ORTHOGONAL POLYNOMIALS ON A BI-LATTICE

W. Van Assche
Katholieke Universiteit Leuven
Walter.VanAssche@wis.kuleuven.be

We investigate generalizations of the Charlier and the Meixner polynomials on the lattice $\mathbb{N}$ and on the shifted lattice $\mathbb{N}+1-\beta$. We combine both lattices to obtain the bi-lattice $\mathbb{N}\cup(\mathbb{N}+1-\beta)$ and show that the orthogonal polynomials on this bi-lattice have recurrence coefficients which satisfy a non-linear system of recurrence relations, which we can identify as a limiting case of an asymmetric discrete Painlevé equation. The asymptotic behavior of the recurrence coefficients is very sensitive to the initial conditions, which are in terms of modified Bessel functions and confluent hypergeometric functions. This is joint work with Christophe Smet.

PROPERTIES AND APPLICATIONS OF CONSTRAINED DUAL BERNSTEIN POLYNOMIALS

S. Lewanowicz, and **P. Woźny**
Institute of Computer Science
University of Wrocław
ul. Joliot-Curie 15, 50-383 Wrocław, Poland
Pawel.Wozny@ii.uni.wroc.pl

Constrained dual Bernstein polynomials $D_i^{(n,k,l)}(x;\alpha,\beta) \in \Pi_n^{(k,l)}$ $(i = k, k+1, \ldots, n-l;\ 0 \leq k+l \leq n)$ are defined so that

$$\int_0^1 (1-x)^\alpha x^\beta D_i^{(n,k,l)}(x;\alpha,\beta) B_j^n(x) dx = \delta_{ij} \qquad (k \leq i,j \leq n-l),$$

where $\alpha, \beta > -1$, and

$$B_j^n(x) := \binom{n}{j} x^j (1-x)^{n-j} \qquad (j = 0, 1, \ldots, n)$$

are basis Bernstein polynomials. Here $\Pi_n^{(k,l)}$ denotes the space of all polynomials of degree n, whose derivatives of order $\leq k-1$ at $t = 0$, as well as derivatives of order $\leq l-1$ at $t = 1$, vanish.

Polynomials $D_i^{(n,k,l)}(x;\alpha,\beta)$ are closely related to some families of orthogonal polynomials, namely shifted Jacobi and Hahn polynomials. We show many properties of constrained dual Bernstein polynomials, as well as quantities related to them. Using these results, we propose efficient algorithms of solving some approximation problems which appear in computer aided geometric design.

8. Special Session on Padé Approximation and Continued Fractions

STRONG ASYMPTOTICS OF NUTTALL-STAHL POLYNOMIALS

A. I. Aptekarev and M. Yattselev
Keldysh Institute of Applied Mathematics RAS,
Miusskaya Square 4, Moscow 125047, Russia
aptekaa@keldysh.ru

Given a germ of an analytic function

$$f(z) = \sum_{k=0}^{\infty} \frac{c_k}{z^{k+1}}$$

which has the analytic continuation along any path in the complex plane which does not go through a finite set of points $f \in \mathcal{A}(\overline{\mathbb{C}} \setminus A), \quad \sharp A < \infty$. Nuttall has put forward the important relation between the *maximal* domain of holomorphicity for the analytic function f and the domain of convergence of the diagonal Padé approximants. The Padé approximants, which are single valued rational functions, approximate a holomorphic branch of the analytic function in the domain of their convergence. At the same time most of the poles of the rational approximants tend to the boundary of the domain of convergence and the support of their limiting distribution models the cuts which make the function f single valued. Nuttall has conjectured (and proved for many important special cases) that these cuts have a minimal logarithmic capacity among all cuts converting the function to a single valued branch. Thus the domain of convergence corresponds to the *maximal* (in the sense of *minimal* boundary) domain of holomorphicity for the analytic function $f \in \mathcal{A}(\overline{\mathbb{C}} \setminus A)$. The complete proof of Nuttall's conjecture (even in a more general setting where the set A has logarithmic capacity 0) was obtained by Stahl. We obtain strong asymptotics for denominators of the diagonal Pade-Approximants for this problem in rather general settings. Our restrictions are that A is a finite set of branch points of f which have the algebro-logarithmic character and which placed at generic positions. The last restriction means that we exclude from our consideration some degenerated "constellations" of the branch points.

SYMBOLIC-NUMERIC INTEGRATION, MULTIVARIATE ORTHOGONALITY AND PADÉ APPROXIMATION

A. Cuyt
Universiteit Antwerpen,
Department of Mathematics and Computer Science
Middelheimlaan 1, B-2020 Antwerpen, Belgium
annie.cuyt@ua.ac.be

Moving from one to more dimensions with polynomial-based numerical techniques leaves room for a lot of different approaches and choices. We focus here on rational approximation, orthogonal polynomials and integration rules, three very related concepts.

In one variable there is a close connection between orthogonal polynomials, Gaussian quadrature rules and Padé approximation. An m-point Gaussian quadrature formula for the integral

$$I(z) = \int_{-1}^{1} \frac{1}{1-tz}\, dt$$

can be viewed as the $[m-1/m]$ Padé approximant for the function

$$f(z) = \sum_{i=0}^{\infty} \left(\int_{-1}^{1} t^i\, dt \right) z^i$$

where the nodes and weights of the Gaussian quadrature formula are obtained from the orthogonal polynomial $V_m(z)$ satisfying

$$\int_{-1}^{1} z^i V_m(z)\, dz = 0, \qquad i = 0, \ldots, m-1.$$

We show that this close connection can be preserved in several variables when starting from spherical orthogonal polynomials. We obtain Gaussian cubature rules with symbolic nodes and numeric weights which can be used to integrate parameterized families of functions. The spherical orthogonal polynomials are also related to the homogeneous Padé approximants introduced a few decades ago.

APPROXIMATION OF SMOOTH FUNCTIONS BY WEIGHTED MEANS OF N-POINT PADÉ APPROXIMANTS

J. Gilewicz and R. Jedynak
Centre de Physique Theorique, CNRS
Cedex 09 Marseille, France
gjacek@hotmail.com

We suggest to explore the properties of two-sided estimates of Stieltjes functions s by two neighboroud N-point Padé approximants (NPA) p_1 and p_2 to obtain a good approximation of Stieltjes-like functions, in particular: convexes functions. The idea consists in a calculation of a set of $N-1$ rational parameters a_i which optimize in each interval $[x_i, x_{i+1}]$ the approximation $a_i p_1 + (1-a_i)p_2$ of knowing Stieltjes function s and then, to use these parameters to compute the expressions $a_i f_1 + (1-a_i)f_2$, where f_1 and f_2 are two NPA of a certain smooth function f. Few numerical examples show the efficiency of this experimental method to approximate the non-Stieltjes smooth functions.

ON VECTOR CONTINUED FRACTIONS ASSOCIATED WITH NIKISHIN SYSTEMS

V. A Kalyagin and M. V. Sokolov
Department of Applied Mathematics and Informatics
Higher School of Economics
Bolshaya Pecherskaya 25/12, Nizhny Novgorod, 603155 RUSSIA
vkalyagin@hse.ru

Vector continued fractions are a useful tools in the investigation of simultaneous rational approximations (Hermite-Padé approximations) and multiple orthogonal polynomials. An algorithm of vector continued fraction representation for a system of holomorphic functions can be considered as an algorithm of calculation of recurrence coefficients for the associated multiple orthogonal polynomials. Nikishin systems appear as a wide class of systems of holomorphic functions with a common support of generating measures. From the recurrence coefficients point of view any Nikishin system with the same support of generating measures is a compact perturbation of the system with periodic recurrence coefficients (see [1]). In this paper we study periodic vector continued fractions associated with Nikishin systems. Our main results are: transformation of the vector continued fraction to the Stieltjes type fraction, calculation of the generating measures of Nikishin system on the base of this transformation, investigation of the Stieltjes type vector continued fractions associated with Nikishin systems. This work is partly supported by RFFI grant 10-01-00682.

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ORDER BASES: COMPUTATION AND USES IN COMPUTER ALGEBRA

G. Labahn
Cheriton School of Computer Science
University of Waterloo
Waterloo, Ontario, Canada
glabahn@uwaterloo.ca

Let $\mathbf{F} \in \mathbf{K}[[x]]^{m \times n}$ be a matrix of power series over a field $\mathbf{K}$. Then a vector $\mathbf{p} \in \mathbf{K}[x]^{n \times 1}$ of polynomials gives an *order* σ approximation of $\mathbf{F}$, if

$$\mathbf{F} \cdot \mathbf{p} \equiv \mathbf{0} \bmod x^{\sigma},$$

that is, the first σ terms of $\mathbf{F} \cdot \mathbf{p}$ are zero. Examples of such problems include Padé, Hermite-Padé, Simultaneous-Padé approximants and their vector and matrix generalizations. The set of all such order $(\mathbf{F}, \sigma)$ approximations forms a module over $\mathbf{K}[x]$. An *order basis* - or minimal approximant basis or σ-basis - is a basis of this module having a type of minimal degree property.

In this talk we will describe how to efficiently compute order bases in exact arithmetic environments. This includes the case where coefficient growth is an issue (and so bit complexity is needed) along with the case when one uses only the complexity of the arithmetic operations. Finally, we describe the use of order bases in the area of computer algebra. This includes normal form computation for matrix polynomials and fast polynomial matrix arithmetic.

CONVERGENCE OF RANDOM CONTINUED FRACTIONS

L. Lorentzen
Department of Mathematics
Norwegian University of Science and Technology
7491 Trondheim, Norway
lisa@math.ntnu.no

Let $\mu(z)$ be a probability measure on the complex plane $\mathbb{C}$ minus the origin, where

- the expectation $\mathbb{E}\{\ln(1+|z|)\} < \infty$, and
- the support $\operatorname{supp} \mu$ contains more than one point.

Let $K(a_n/1)$ be a continued fraction whose elements a_n are picked randomly from $\mathbb{C} \setminus \{0\}$ according to this measure.

We address the question: under what conditions on μ will $K(a_n/1)$ converge with probability 1?

We shall see that there are some mild sufficient conditions with surprising consequences.

SMOOTHING THE GIBBS PHENOMENON USING PADÉ-HERMITE APPROXIMANTS

B. Beckermann, V. Kaliagyn, **A. Matos**, and F. Wielonsky
UFR de Mathématiques
Université de Lille 1
59655 Villeneuve d'Ascq Cedex, France
Ana.Matos@univ-lille1.fr

The aim of this talk is to propose a method to reduce the Gibbs phenomenon exhibited by the partial Fourier sums of a periodic function f, defined on $[-\pi, \pi]$, discontinuous at 0. Let g_2 denote the series such that $f(t) = \Re(g_2(e^{it}))$. Then, the goal is to approach g_2 on the unit circle (and more precisely its real part). It is typical that the singularity of the function f, located at 0 say, corresponds to a logarithmic singularity for g_2, then located at 1, and that this function g_2 is analytic in the complex plane, with a branch cut that can be taken as the interval $[1, \infty)$. Defining $g_1(z) = \log(1 - z)$, we may consider the problem of determining polynomials p_0, p_1, p_2 such that

$$p_0(z) + p_1(z)g_1(z) + p_2(z)g_2(z) = O(z^{n_0+n_1+n_2+2}) \quad (z \to 0)$$

where n_j denotes the degree of p_j, $j = 0, 1, 2$. We can then propose the *Hermite-Padé approximant*

$$\Pi_{\vec{n}}(z) = -\frac{p_0(z) + p_1(z)g_1(z)}{p_2(z)}, \tag{6}$$

to approximate g_2.

We obtain rates of convergence of sequences of Hermite–Padé approximants for a class of functions known as *Nikishin systems*. Our theoretical findings and numerical experiments confirm that particular sequences of Hermite-Padé approximants (diagonal and row sequences, as well as linear HP approximants) are more efficient than the more elementary Padé approximants, particularly around the discontinuity of the goal function f.

BERNSTEIN–SZEGŐ POLYNOMIALS ON THE TRIANGLE

A. M. Delgado, R. Orive, and **M. A. Piñar**
Department of Applied Mathematics
University of Granada
18071 Granada, Spain
mpinar@ugr.es

In this work we consider the extension of the one variable Bernstein–Szegő theory for orthogonal polynomials on the real line (see [3]) to bivariate measures supported on the triangle. A similar problem for measures supported in the square was studied in [1].

Following essentially [2] the orthogonal polynomials and the corresponding kernel functions are constructed. Finally, some asymptotic results concerning the Christoffel functions are obtained.

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EQUILIBRIUM PROBLEMS FOR VECTOR POTENTIALS

B. Beckermann, V. Kalyagin, A. C. Matos, **F. Wielonsky**
Laboratoire LATP - UMR CNRS 6632
Université de Provence
CMI 39 Rue Joliot Curie
F-13453 Marseille Cedex 20, FRANCE
wielonsky@cmi.univ-mrs.fr

The study of vector equilibrium problems in logarithmic potential theory is an important tool in the investigation of many questions in approximation theory, e.g. like those involving multiple orthogonal polynomials, with numerous applications in numerical or applied mathematics. In this talk, we consider the problem of minimizing the logarithmic energy of vector potentials associated to a d-tuple of positive measures supported on closed subsets of the complex plane. Existence and uniqueness of a solution, and its characterization in terms of variational equations, are obtained under assumptions on the interaction matrix that are weaker than the usual ones. Moreover, we assume that the masses of the measures vary in a compact subset of $\mathbb{R}_+^d$.

We will also review a few examples taken from the recent literature that are related to our results.

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RADIALLY ORTHOGONAL MULTIVARIATE BASIS FUNCTIONS

I. Yaman, A.Cuyt
Universiteit Antwerpen
Dept WIS-INF
Middelheimlaan 1, B-2020 Antwerpen, Belgium
irem.yaman@ua.ac.be

It is well-known that radial basis functions provide a practical way to interpolate large scattered datasets. It is equally well-known that the interpolation matrix may be singular or ill-conditioned for some of the basis functions. We establish a connection with spherical orthogonal polynomials $V_m(z), X = (x_1, \ldots, x_d) = (\xi_1 z, \ldots, \xi_d z), ||(\xi_1, \ldots, \xi_d)||_p = 1$, defined on the unit hyperball (in different norms) by

$$\int \ldots \int_{||X||_p \leq 1} w(|z|) \left(\sum_{k=1}^{d} x_k \xi_k \right)^i V_m \left(\sum_{k=1}^{d} x_k \xi_k \right) \, dX = 0, \; i = 0, \ldots, m-1.$$

Because of the orthogonality of these multivariate basis functions, the interpolation matrix is better conditioned. Also small Lebesgue constants are obtained. We show how the multivariate spherical orthogonal polynomials can be used in:

- collocation methods, to compute a multivariate analytic model representing the European call option price (and its Greeks) as obtained from the Black-Scholes differential equation,
- CAGD, where we show that a fully orthogonal multivariate basis set can be obtained with orthogonality between different basis functions of the same total degree which, in a multivariate setting, is termed mutual orthogonality,
- data fitting, illustrating the radial usage of the orthogonal basis functions, where the variable is the signed distance function, versus the cartesian usage, where the variable is a linear combination of the cartesian coordinates.

9. Special Session on Partial Differential Equations

SOME REMARKS ON EIGENVALUE APPROXIMATION ARISING FROM PARTIAL DIFFERENTIAL EQUATIONS

D. Boffi
Dipartimento di Matematica "F. Casorati"
Università degli Studi di Pavia
Via Ferrata 1, I-27100 Pavia, Italy
daniele.boffi@unipv.it

The aim of this talk is to review some topics related to the approximation of eigenvalues and eigenfunctions arising from partial differential equations, which have been the object of two recent surveys [1, 2].

We will discuss in particular the Hodge–Laplace eigenvalue problem in the framework of differential forms. After recalling the main issues concerning its analysis, we focus on some numerical examples with a particular interest in multiple eigensolutions. We will show how a double eigenvalue can be associated to eigenfunctions with different regularity; in this case, there are two discrete eigenvalues converging towards the common limit with different orders, which depend on the smoothness of the corresponding eigenfunctions.

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A POSTERIORI ENERGY NORM ERROR ESTIMATION FOR 2ND-ORDER PARTIAL DIFFERENTIAL EQUATIONS

C. Carstensen*
Department of Mathematics
Humboldt-Universiät zu Berlin
Germany
cc@math.hu-berlin.de

Five classes of up to 13 a posteriori error estimators compete in three second-order model cases, namely the conforming and non-conforming first-order approximation of the Poisson-Problem plus some conforming obstacle problem. Since it is the natural first step, the error is estimated in the energy norm exclusively. The competition allows merely guaranteed error control and excludes the question of the best error guess. The former a posteriori error estimators apply to the obstacle problem as well and lead to surprisingly accurate guaranteed upper error bounds. This approach allows an extension to more general boundary conditions and a discussion of efficiency for the affine benchmark examples. The Luce-Wohlmuth and the least-square error estimators win the competition in several computational benchmark problems. Novel equilibration of nonconsistency residuals and novel conforming averaging error estimators win the competition for Crouzeix-Raviart nonconforming finite element methods. Our numerical results provide sufficient evidence that guaranteed error control in the energy norm is indeed possible with efficiency indices between one and two.

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NUMERICAL MODELLING FOR GEOSCIENCE APPLICATIONS

L. Formaggia, E. Miglio, A. Scotti, A. Fumagalli
Department of Mathematics
Politecnico di Milano
Piazza Leonardo da Vinci 32, Milano, Italy
luca.formaggia@polimi.it

The study of geological evolution and subsurface tranport is a critical issue for several important applications, from oil recovery to CO2 sequestration, identification of nuclear waste sites and soil remediation.

It is also a challenge for numerical simulations. The problems involved are of multiphysic nature and often lead to large scale problems. Another important aspect is the uncertainty of soil properties and of boundary data.

In this talk we will present some recent results concerning the simulation of geological evolution and flow in fractured porous media, focusing on the open mathematical issues and numerical challenges.

DOMAIN DECOMPOSITION METHODS FOR TOTAL VARIATION MINIMIZATION

M. Fornasier
Department of Mathematics
Technical University of Munich
Boltzmanstr. 3, Garching, Germany
massimo.fornasier@ma.tum.de

Domain decomposition methods are well-known techniques to address a very large scale problem by splitting it into smaller scale sub-problems. The theory of such methods is fully clarified when the energy minimized by the method is either smooth and strictly convex or splits additively with respect to the decomposition. Otherwise counterexamples to convergence exist. In this talk we present a convergent overlapping domain decomposition method for energy functionals with total variation terms, which are nonsmooth and do not split additively. We state several open problems, such as the rate of convergence and scalability with respect to the mesh size. We conclude the talk by showing an extension of the proposed algorithm to a multiscale (wavelet) subspace correction method. We present a counterexample to convergence in a specific case and preconditioning effects in other cases related to certain image deblurring problems.

LOCAL MASS CONSERVATION FOR THE FINITE ELEMENT IMMERSE BOUNDARY METHOD

L. Gastaldi
Dipartimento di Matematica
Università di Brescia
Via Valotti 9, 25133 Brescia, Italy
lucia.gastaldi@ing.unibs.it

The aim of this talk is to discuss the performances of different finite elements in the space discretization of the Finite Element Immersed Boundary Method. In this exploration we will analyze two popular solution spaces: *Hood-Taylor* and *Bercovier-Pironneau* (P1-iso-P2). Immersed boundary solution is characterized by pressure discontinuities at fluid structure interface. Due to such a discontinuity a natural enrichment choice is to add piecewise constant functions to the pressure space. Results show that $P_1 + P_0$ pressure spaces are a significant cure for the well known "boundary leakage" affecting IBM. We refer to[4] for a review on the original IBM and to [1, 2, 3] for its finite element discretization. Convergence analysis is performed, showing how the discontinuity in the pressure is affecting the convergence rate for our finite element approximation.

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POD FOR COMPLEX BLACK-SCHOLES EQUATIONS

O. Pironneau
Laboratoire J.-L. Lions
University of Paris VI
Boite 187, Place Jussieu, F-75252 Paris 05
Olivier.Pironneau@upmc.fr

In financial engineering in banks at least the Black-Scholes equations are solved very many times each day and so any numerical speed-up is welcome. To compute several financial options with local volatilities or/and jumps, we introduce a one dimensional Galerkin basis for solving the parabolic partial integro-differential equations which arise from an Itô calculus when the random evolution of the underlying asset is driven by a Wiener process, or a Lévy process or more generally, a time-inhomogeneous jump-diffusion process.

The choice of the basis of functions is driven by the 3 main constraints: the numerical efficiency in the computation of the basis, the suitable global shape so as to be a complete basis with correct asymptotic behavior at infinity and the capacity to compute all the correlation matrices with analytical formulas. Elementary solutions of the Black-Scholes equation with constant volatilities fit these 3 criteria.

A convergence proof is given and numerical tests are performed on calls with non constant volatilities such as CEV and Lévy processes with Merton's kernel because analytical solutions are known for these. The basis is tried also for calibration of a local volatilities.

The method is a Proper Orthogonalization Decomposition very similar to those used for the heat equations; however here the basis is known in closed form.

The method is very fast but hampered by the bad condition numbers of the linear systems and so it is limited to no more than 40 basis beyond which the systems are numerically unsolvable.

It can be extended to two dimensional problems such as basket option and stochastic volatility models and we will show good numerical results but again unless a better numerical solver is found - and perhaps it will have been found by October 2011 - the method is limited by the size of the matrices that the SVD solvers can handle.

RELIABLE REDUCED BASIS METHOD FOR EFFICIENT GEOMETRICAL PARAMETRIZATIONS

A. Quarteroni, T. Lassila, A. Manzoni, G. Rozza
EPFL, MATHICSE CMCS
alfio.quarteroni@epfl.ch

In the last decades optimal control and shape optimization problems have gained an increasing importance in many engineering fields and especially in structural mechanics and in thermo-fluid dynamics. The problems we consider involve the study of a system modelled by parametric PDEs and the evaluation of functionals depending on the field variables, such as velocity, pressure, drag forces, temperature, energy, wall shear stress or vorticity. Especially in the field of shape optimization and parameter estimation, where the recursive evaluation of the solution is required for many possible configurations, the computational costs can easily become unacceptably high. Nevertheless, the evaluation of an input/output relationship of the system plays a central role: a set of input parameters identifies a particular configuration of the system and they may represent design and/or geometrical variables, while the outputs may be expressed as functionals of the field variables associated with PDEs. The rapid and reliable evaluation of many input/output relationships typically would require great computational expense, and therefore strategies to reduce the computational time and effort are needed. Among model order reduction strategies, reduced basis method represents a promising tool for the simulation of flow in parametrized geometries, for shape optimization or sensitivity analysis. An implementation of the reduced basis method is presented by considering different shape or domain parametrizations: from simple affine and non-affine maps, to more flexible techniques, such as free-form deformations or radial basis functions. In order to develop efficient numerical schemes for inverse problems related with shape variation such as shape optimization, fluid-structure interaction, shape analysis through parameter identification, we combine a suitable low-dimensional parametrization of the geometry (yielding a geometrical complexity reduction) with reduced basis methods (yielding a reduction of computational complexity). The analysis will focus on the general properties and performance of the reduced basis method: several examples will highlight its special suitability for the analysis of flows in parametrized geometries with a special interest in cardiovascular problems.

DISPERSION ANALYSIS OF SPECTRAL ELEMENT METHODS ON TRIANGLES FOR ELASTIC WAVE PROPAGATION

I. Mazzieri and **F. Rapetti**
Dept. Mathematics
Univ. de Nice & CNRS
frapetti@unice.fr

The need for geometric flexibility is especially important in computational seismology when dealing with complex wave phenomena, such as the scattering by rough topographies of the Earth and sea bottom surfaces, or the seismic response of sedimentary basins with complex structures and fault geometries. Today, such flexibility can be achieved by the recently developed triangular/tetrahedral spectral element method (TSEM); see [2, 3], and therein references. In this paper the stability and grid dispersion of the TSEM for elastic wave propagation [1], are explored and compared with those of the classical spectral elements on quadrangular grids (QSEM) [4].

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SHARP CONSTANT-FREE A POSTERIORI ERROR BOUNDS FOR OBSTACLE PROBLEMS

A. Veeser
Dipartimento di Matematica
Università degli Studi di Milano
Via Saldini 50, 20133 Milano, Italy
andreas.veeser@mat.unimi.it

The presence of obstacles in a boundary value problem entails a nonlinear dependence of the solution on the problem data. We review the main features of this dependence and discuss the ensuing difficulties for a posteriori error estimation. We derive a posteriori upper bounds for the error of the linear finite element solution. They enjoy the following properties:

- They are constant-free, or guaranteed, in that they do not involve any constant which is not explicitly known or difficult to estimate sharply.
- They are essentially insensitive to perturbations of the problem data that do not affect the error of the finite element solution.
- They are complemented by lower bounds (which, as without obstacles, involve constants and oscillations terms).

Consequently, these upper bounds quantify rather precisely the error of a given approximate solution and may be used to direct and to stop safely and efficiently an adaptive iteration.

DOMAIN DECOMPOSITION ALGORITHMS FOR H(CURL) PROBLEMS

O. B. Widlund
Courant Institute
251 Mercer Street, New York, NY 10012, USA
widlund@cims.nyu.edu

In this talk, we will discuss recent progress on developing domain decomposition algorithms for problems formulated in H(curl) and approximated by low order edge elements. We are focusing on self-adjoint positive definite model problems and are, in particular, interested in developing algorithms with a performance which is insensitive to large changes in the material properties.

All this work is carried out with Dr. Clark Dohrmann of the Sandia National Laboratories, Albuquerque, New Mexico.

A first technical report has appeared late last year, [1]. In that paper, condition number bounds of the form $C(1+\log(H/h))^2$ were developed for problems in two dimensions. Here, C is a constant which is independent of the number of subdomains into which the given domain has been partitioned. This bound is also independent of arbitrary jumps in the two coefficients across the interface between the subdomains and it is also valid for quite irregular subdomain boundaries.

The goal of our work, now in progress, is to extend these results, to the extent possible, to the three dimensional case.

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10. Special Session on Structured Linear Algebra

AN ERROR ANALYSIS FOR RATIONAL GALERKIN PROJECTION APPLIED TO THE SYLVESTER EQUATION

B. Beckermann
Department of Mathematics
University of Lille
Labo Painlevé UMR 8524, 59655 Villeneuve d'Ascq, France
bbecker@math.univ-lille1.fr

In this talk we suggest a new formula for the residual of Galerkin projection onto rational Krylov spaces applied to a Sylvester equation, and establish a relation to three different underlying extremal problems for rational functions. These extremal problems enable us to compare the size of the residual for the above method with that obtained by ADI. In addition, we may deduce several new a priori error estimates for Galerkin projection onto rational Krylov spaces, both for the Sylvester and for the Lyapunov equation.

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RECOVERY OF EIGENVECTORS OF MATRIX POLYNOMIALS FROM GENERALIZED FIEDLER LINEARIZATIONS

F. M. Dopico, M. I. Bueno and F. De Terán
Department of Mathematics, Universidad Carlos III de Madrid
Avenida de la Universidad 30, 28911, Leganés, Spain
and
Department of Mathematics, University of California
Santa Barbara, CA 93106, USA
dopico@math.uc3m.es

A standard way to solve polynomial eigenvalue problems $P(\lambda)x = 0$ is to convert the matrix polynomial $P(\lambda)$ into a matrix pencil that preserves its elementary divisors and, therefore, its eigenvalues. This process is known as linearization and is not unique, since there are infinitely many linearizations with widely varying properties associated with $P(\lambda)$. This freedom has motivated the recent development and analysis of new classes of linearizations that generalize the classical first and second Frobenius companion forms, with the goals of finding linearizations that retain whatever structures that $P(\lambda)$ might possess and/or of improving numerical properties, as conditioning or backward errors, with respect the companion forms. In this context, an important new class of linearizations is what we name generalized Fiedler linearizations, introduced in 2004 by Antoniou and Vologiannidis as an extension of certain linearizations introduced previously by Fiedler for scalar polynomials. On the other hand, the mere definition of linearization does not imply the existence of simple relationships between the eigenvectors, minimal indices, and minimal bases of $P(\lambda)$ and those of the linearization. So, given a class of linearizations, to provide easy recovery procedures for eigenvectors, minimal indices, and minimal bases of $P(\lambda)$ from those of the linearizations is essential for the usefulness of this class. In this paper we develop such recovery procedures for generalized Fiedler linearizations and pay special attention to structure preserving linearizations inside this class.

QUASISEPARABLE REPRESENTATIONS OF MATRICES AND DISCRETE SYSTEMS WITH BOUNDARY CONDITIONS

Y. Eidelman
Department of Mathematics
Tel-Aviv University
Ramat Aviv, Israel
eideyu@post.tau.ac.il

We say that a matrix has quasiseparable order (n_1, n_2) if its submatrices from the strictly lower triangular part are of rank n_1 at most and submatrices from the strictly upper triangular part are of rank n_2 at most. The quasiseparable order defines representations of strictly lower and upper parts of matrices which are called quasiseparable representations. For numerical reasons one can treat matrices with quasiseparable representations as matrices of the input output operators of linear discrete time-varying systems with boundary conditions. This reduction allows to obtain linear complexity algorithms for multiplication of a matrix by a vector, product of matrices and matrix inversion.

EFFICIENT NUMERICAL METHODS FOR THE POLYNOMIAL SPECTRAL FACTORIZATION

L. Gemignani
Department of Mathematics
University of Pisa
Largo B. Pontecorvo, 56127 Pisa, Italy
gemignan@dm.unipi.it

First in this talk we review efficient and accurate numerical methods for computing the polynomial spectral factorization. Then we discuss some extensions and applications of these methods for dealing with bivariate polynomials.

MEANS OF STRUCTURED MATRICES: PROPERTIES, APPLICATIONS AND ALGORITHMS

D. A. Bini and **B. Iannazzo**
Dipartimento di Matematica e Informatica
Università di Perugia
Via Vanvitelli 1, Perugia, Italy
bruno.iannazzo@dmi.unipg.it

Averaging matrices is a problem arising when one has to represent, through a single matrix, the results of several experiments made up by a set of many matrices. Besides the straightforward arithmetic mean, there are other types of means which are suitable for different problems: for positive definite matrices, good averages are obtained by the Karcher mean [1], which verifies all the properties required from a good definition of geometric mean.

In certain applications there is the need to compute means of positive definite matrices which have further structures. A noticeable example arises in radar signal processing, where the matrices to be averaged are correlation matrices, which are Toeplitz and positive definite [2]. Unfortunately, the Karcher mean of Toeplitz matrices is not Toeplitz.

We introduce the new concept of structured geometric mean and prove that it maintains the structure of the input matrices. We restate the properties of geometric mean in terms of the structure and show that most of them are satisfied by our definition. We discuss some applications in which structured means are required. Finally, we provide an iterative algorithm for computing the structured geometric mean and analyze its convergence properties.

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TRACKING THE DOMINANT SUBSPACE OF INDEFINITE MATRICES

N. Mastronardi and P. Van Dooren
Istituto per le Applicazioni del Calcolo, CNR
Via Amendola 122D, 70126 Bari, Italy
n.mastronardi@ba.iac.cnr.it

Indefinite symmetric matrices occur in many applications, such as optimization, partial differential equations and variational problems where they are linked to a so-called saddle point problem. In these applications one is often interested in computing an estimate of the dominant eigenspace of such matrices, in order to solve regularized least squares problems or compute preconditioners. In this talk we propose an incremental method to compute the UTU^T factorization of a symmetric indefinite matrix, where U is an orthogonal matrix and T is a symmetric anti–triangular one, i.e., a matrix having zero entries below the anti–diagonal.

We show that the latter factorization is a symmetric rank–revealing one [2]. Moreover, we describe an algorithm for computing an estimate of the dominant eigenbasis of such matrices based on low rank updates and downdates of indefinite matrices.

We show that the proposed algorithms are well–suited for large scale problems since they are efficient in terms of complexity as well as data management.

Some numerical experiments showing the behavior of the proposed algorithms are presented.

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TOEPLITZ OPERATORS WITH MATRIX-VALUED SYMBOLS AND SOME (UNEXPECTED) APPLICATIONS

S. Serra Capizzano
Dipartimento di Fisica e Matematica
Università dell'Insubria
Como, Italy
s.serracapizzano@uninsubria.it

We discuss the eigenvalue distribution in the Weyl sense of general matrix-sequences associated to a symbol. As a specific case we consider Toeplitz sequences generated by matrix-valued (non Hermitian) bounded functions. We show that the canonical distribution can be proved under mild assumptions on the spectral range of the given symbol. Finally some applications are introduced and discussed.

ORTHOGONAL FUNCTIONS AND MATRIX COMPUTATIONS

M. Van Barel
Department of Computer Science
Katholieke Universiteit Leuven
Celestijnenlaan 200A, B-3001 Leuven (Heverlee), Belgium
marc.vanbarel@cs.kuleuven.be

Orthogonal polynomials on the real line satisfy a three term recurrence relation. This relation can be written in matrix notation by using a tridiagonal matrix. Similarly, orthogonal polynomials on the unit circle satisfy a Szegő recurrence relation that corresponds to an (almost) unitary Hessenberg matrix. It turns out that orthogonal rational functions with prescribed poles satisfy a recurrence relation that corresponds to diagonal plus semiseparable matrices. This leads to efficient algorithms for computing the recurrence parameters for these orthogonal rational functions by solving corresponding linear algebra problems. In this talk we will study several of these connections between orthogonal functions and matrix computations and give some numerical examples illustrating the numerical behaviour of these algorithms.

CHASING BULGES OR ROTATIONS? A NEW FAMILY OF MATRICES ADMITTING LINEAR TIME QR-STEPS

R. Vandebril and D. Watkins
Department of Computer Science
K.U. Leuven, Belgium
and
Department of Mathematics
Washington State University, USA
raf.vandebril@cs.kuleuven.be

The QR-algorithm is a renowned method for computing all eigenvalues of an arbitrary matrix. A preliminary unitary similarity transformation to Hessenberg form is indispensable for keeping the computational complexity of the subsequent QR-steps under control. In this paper, a whole new family of matrices, sharing the major qualities of Hessenberg matrices, will be put forward. This gives rise to the development of innovative implicit QR-type algorithms, pursuing rotations instead of bulges.

The key idea is to benefit from the QR-factorization of the matrices involved. The prescribed order of rotations in the decomposition of the Q-factor uniquely characterizes several matrix types such as, for example, Hessenberg, inverse Hessenberg and CMV matrices. Loosening the fixed ordering of these rotations provides us the class of matrices under consideration.

Establishing a new implicit QR-type algorithm for these matrices requires a generalization of diverse well-established concepts. We consider: the preliminary unitary similarity transformation; a proof of uniqueness of this reduction; an explicit and implicit QR-type algorithm and; a convergence analysis of this novel method.

A detailed complexity analysis illustrates the competitiveness of the novel method with the traditional Hessenberg approach. The numerical experiments show comparable accuracy for a wide variety of matrix types, but discloses an intriguing difference between the average number of iterations before deflation can be applied.

11. Special Session on History of Computational Mathematics

EARLY RESEARCH ON MATRIX ITERATIONS: THE ITALIAN CONTRIBUTION

M. Benzi
Department of Mathematics and Computer Science,
Emory University,
Atlanta, Georgia, USA
benzi@mathcs.emory.edu

In this talk I will review some early work on iterative methods for solving linear systems by Italian mathematicians during the 1930s, with particular attention to the contributions of Lamberto Cesari (1910–1990) and Gianfranco Cimmino (1908–1989). I will also provide some background information on Italian applied mathematics and especially on Mauro Picone's *Istituto Nazionale per le Applicazioni del Calcolo*, where most of this early numerical work took place. Finally, I will illustrate the influence of Cimmino's work on modern and current research.

ANDRÉ LOUIS CHOLESKY: FAMILY, LIFE, AND WORK

C. Brezinski
U.F.R. de Mathématiques
University of Sciences and Technologies of Lille
59655 – Villeneuve d'Ascq cedex, France
claude.brezinski@univ-lille1.fr

André Louis Cholesky (1875–1918) is well know for his method for solving a system of equations with a symmetric positive definite matrix.

First, indications about his ancestors and his family will be given. Then, his biography will be presented. Finally, some of its achievements in topography and mathematics will be reviewed.

Cholesky's method was first published in 1924 by a fellow of him, the Commandant Benoit whose life will be shortly described.

The talk is illustrated by many photos and documents including his handwritten unpublished paper on his method, dated December 2, 1910.

How to evaluate the historical and epistemological role of practical computing methods for the fundamental theorem of algebra

J. G. Dhombres
Centre Koyré, EHESS, 27 rue Damesme, F-75013, Paris
Jean.Dhombres@damesme.cnrs.fr

By the end of the 18th century, many proofs had already been proposed for the fundamental theorem of algebra, by Euler, by d'Alembert (around 1750), by Lagrange, de Foncenex, and Laplace (around 1795). All such proofs, except d'Alembert's one, required the existence of "imaginary" quantities, and the proof was to reduce such quantities to complex numbers. In 1799, Gauss in his Dissertation thesis, proposed a proof inspired by d'Alembert, but requiring a rather difficult result on algebraic curves entering a bounded closed subset of the topological plane, more difficult in fact that the theorem to be proved. All such algebraic proofs were indirect ones, based as if it was obvious on the intermediate value theorem, which was then conceived as a computing result. In many papers of the time, there was a sort of antinomy between computing and what we may call commutative algebra. Using an idea of Legendre in number theory (in fact the maximum principle idea for holomorphic functions), Argand who was not known in the main mathematical circles in Paris, proposed in 1806 a direct and elementary proof, as well as his famous representation of imaginary quantities (this time such quantities indeed were complex numbers). There is a failure in the proof, and later Cauchy, using Argand's ideas, went back to an indirect proof. But the idea was maintained that there was something in Argand's proof, which was coming from computing methods and had an algorithmic flavour. An elementary but rather sophisticated proof by Kneser settled the situation in our in the middle of the 20th century. My aim is to discuss, on this concrete example, a sort of mentality of mathematicians concerning practical methods as opposed to theoretical ones.

EULER, LAGRANGE, RITZ, GALERKIN, COURANT, CLOUGH: ON THE ROAD TO THE FINITE ELEMENT METHOD

M. J. Gander, and G. Wanner
Department of Mathematics, University of Geneva
CP 64, 1211 Geneva 4, Switzerland
martin.gander@unige.ch

The finite element method has become indispensable for the numerical simulation of partial differential equations. But where does this method come from? How was it invented? I will show in my talk how everything started with Euler and Lagrange, and their discrete and continuous formulations of variational problems, which led to the highway of variational calculus. We will then see the fundamental contributions of the Swiss physicist and mathematician Walther Ritz in detail, and his method to compute Chladni figures. The development went further on a detour to Russia, to Timoshenko, Bubnov and Galerkin, who immediately realized the importance of Ritz' method, and used it to solve hard problems in science and engineering. The western world in contrast was at that time more interested in existence and uniqueness proofs around Hilbert and Courant. The value of Ritz' invention was only recognized much later by Courant, who presented the first finite element calculation we were able to find in an address to the AMS. The name Finite Element Method was finally coined by Ray Clough and collaborators at Boeing. The mathematical development of the finite element method was then however just to begin.

ALGEBRAIC CONTINUED FRACTIONS: THE CONTRIBUTION OF R. DE MONTESSUS DE BALLORE

H. Le Ferrand,
Institut de Mathématiques de Bourgogne,
Dijon, France
leferran@u-bourgogne.fr

During the year 1902, Robert de Montessus de Ballore (1870-1937) proved his famous theorem ([3]) on the convergence of Padé's approximants of meromorphic functions ([2]). Until 1909, Robert de Montessus published works on algebraic continued fractions. We investigate the circulation of this theorem and give other results proved by Robert de Montessus. First of all, the genesis of the theorem is explained thanks to letters and first drafts that we have recovered ([1]). These letters have been adressed to Robert de Montessus by differents mathematicians. Extracts of some letters and first drafts will be done in that paper. Particularly, Henri Padé and Robert de Montessus corresponded by letter during the years 1901-1902. In a second part, we deal with authors who mention the theorem.The theorem was rapidly cited by mathematicians like Nörlund and O. Perron. Let us mention that Robert de Montessus dealt with Probabilities at the same period. But, it is quite surprising that Robert did'nt take an interest in the metric theory of continued fractions as E. Borel did. Yet, Robert de Montessus and E. Borel were in correspondance.

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THE EARLY HISTORY OF CONVERGENCE ACCELERATION METHODS

N. Osada
Department of Information and Sciences,
Tokyo Woman's Christian University
2-6-1 Zempukuji, Suginami-ku, Tokyo, 167-8585 JAPAN
osada@cis.twcu.ac.jp

We consider the history of convergence acceleration methods before 1723. Taken up methods are as follows. Names in brackets are discoverers or provers.

1. Using the correction terms [Mādhava (c.1400), Isaac Newton (1676)]
2. Linear acceleration
   (i) the arithmetic weighted mean [Willebrord Snell (1621), Christiaan Huygens (1654)]
   (ii) the Richardson extrapolation [C. Huygens (1654)]
   (iii) the Euler transformation [I. Newton (1684), Jean Christophe Fatio de Duillier (before 1704)]
   (iv) the iterated Richardson extrapolation [Katahiro Takebe (before 1711)]
3. Nonlinear acceleration
   (i) the harmonic weighted mean [Nikolaus van Kues (before 1464), W. Snell (1621), C. Huygens (1654)]
   (ii) the Aitken Δ^2 process [Takakazu Seki (1680)]

We give an asymptotic error estimate for each taken up method and focus on the Aitken Δ^2 process by Takakazu Seki and the iterated Richardson extrapolation by Katahiro Takebe.

CALCULATING FIRING TABLES IN 18TH AND 19TH CENTURIES

D. Tournès
Mathematics and Computer Science Laboratory
University of La Réunion
Parc Technologique Universitaire
2 rue Joseph-Wetzell, F-97490 Sainte-Clotilde, France
dominique.tournes@univ-reunion.fr

In this talk, I would like to explore the various methods used during 18th and 19th centuries to numerically integrate the ballistic differential equation and to calculate firing tables for the needs of artillery.

Throughout this period, there has been an interesting interaction between analytic theory of differential equations, numerical and graphical techniques of integration, and empirical research by means of experimental measures. Mathematicians, ballisticians and artillerymen, although belonging to different milieus, collaborated and inspired themselves mutually. All this led however to a relative failure, both experimentally to find a good law of air resistance, and mathematically to find a simple solution of the ballistic equation.

Mathematical research on the ballistic equation has played nevertheless the role of a laboratory where the modern numerical analysis was able to develop. Mathematicians have indeed been able to test on this recalcitrant equation all possible approaches to calculate the solution of a differential equation. There is no doubt that these trials have helped to organize the domain into an autonomous discipline at the beginning of the 20th century.

General Session

LANDAU-KOLMOGOROV TYPE INEQUALITIES FOR THE HERMITE AND CLOSELY CONNECTED MEASURES

A. Draux and **L. Abbas**
Département de Génie Mathématiques
INSA de Rouen
Avenue de l'Université, BP 8, F-76801, France
lamia.abbas@insa-rouen.fr

Different types of polynomial inequalities have been studied since more one century. The first type is the so-called Markov-Bernstein inequalities (A. A. Markov in 1889 [5]). More recently other inequalities involving the L^2-norm for the Hermite measure were given (see Bojanov and Varma [2], Alves and Dimitrov [1]). Inequalities given in the previous papers are particular cases of the more general ones which can be obtained by using the variational method. The basis of our study can be found in the papers of Draux and Elhami ([3], [4]). In this talk we will present the Landau-Kolmogorv inequalities obtained in the case of Hermite and closely connected measures.

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A FAMILY OF P-STABLE LINEAR MULTISTEP METHODS FOR SECOND ORDER IVPS

L. Aceto, C. Magherini, and P. Ghelardoni
Department of Applied Mathematics
University of Pisa
Via Filippo Buonarroti 1/c, 56127 Pisa, Italy
l.aceto@dma.unipi.it

In the last years the study of the numerical solution of initial value problems (IVPs) for second order ODEs of special type given by

$$y''(x) = f(x,y)\,, \quad y(x_0) = y_0\,, \quad y'(x_0) = y'_0, \qquad x \in [x_0, X]\,, \tag{7}$$

having periodic and oscillatory solution, has attracted the interest of many authors. When the problem to be solved is *stiff,* namely when its solution is a combination of components with dominant short frequencies and components with large frequencies and small amplitudes, the use of schemes satisfying "good" stability properties is mandatory. Following the idea of Dahlquist, a rigorous definition of them was given by Lambert and Watson in [2] for Linear Multistep Methods (LMMs) which solve (7) in its original formulation. In such paper they established that the order of a P-stable LMM, used as Initial Value Method (IVM), cannot exceed two.
In this talk, it will be shown that the use of LMMs as Boundary Value Methods (BVMs) [1] may be successful in overcoming the barrier of Lambert and Watson. In particular, a family of P-stable BVMs, called PGSCMs and obtained as a generalization of the Störmer-Cowell schemes, will be presented.

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CONVERGENCE OF THE IDRSTAB METHOD USING THE RESIDUAL SMOOTHING TECHNIQUES

K. Aihara, K. Abe, and E. Ishiwata
Graduate School of Science
Tokyo University of Science
1-3 Kagurazaka, Shinjuku-ku, Tokyo 162-8601, Japan
j1411701@ed.tus.ac.jp

The IDRstab method [2] has been proposed for solving large nonsymmetric linear systems. IDRstab is more effective than both IDR(s) and BiCGstab(ℓ), but the residual norms still oscillate, and the convergence of recursively computed residual norms sometimes does not coincide with that of true residual norms by numerical errors on some model problems.

In this talk, we use the residual smoothing techniques presented in [3] to overcome these difficulties. Here, we apply the smoothing techniques to an alternative implementation of IDRstab noted in [2] to reduce the computational cost. Since it is known that the approximate solutions obtained by the smoothing algorithms are not more accurate than that of the non-smoothed one [1], we present a strategy to improve the accuracy of the approximate solutions by combining the smoothing techniques and the alternative implementation of IDRstab. Numerical experiments demonstrate the efficiency of our smoothed variant of IDRstab.

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ON AN EXPANSION METHOD FOR INVERTING NUMERICALLY A FIRST KIND FREDHOLM INTEGRAL EQUATION

E. Alaidarous and A. Salam
King Abdul Aziz University (KAU)
Department of Mathematics,
Girls Section, P.O. Box 80203, Jeddah 21589,
Kingdom of Saudi Arabia
ealaidarous@kau.edu.sa

In this talk, we deal with the numerical inversion of the first kind Fredholm integral equation $G^*(w) = \int_0^\infty k(w,\tau)H(\tau)d\tau$, where the kernel is given by $k(w,\tau) = \dfrac{iw}{\tau(1+iw\tau)}$. This inverse problem is widely known to be ill-conditioned. The complex modulus G^* is typically given as a discrete data measured experimentally in industrial Rheology context.

We use an expansion method based on a sequence of orthogonal polynomials with respect to a given weight function for computing approximations of the relaxation spectrum function H. Then numerical tests are given using the experimental data.

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ON A VARIATIONAL APPROXIMATION OF DAES

S. Amat, M.J. Legaz, and P. Pedregal
Departamento de Matemática Aplicada y Estadística
Universidad Politécnica de Cartagena
Paseo de Alfonso XIII 52, 30203 Cartagena (Murcia), Spain
sergio.amat@upct.es

This paper deals to the study and approximation of systems of differential-algebraic equations based on an analysis of a certain error functional. In seeking to minimize the error by using standard descent schemes, the procedure can never get stuck in local minima, but will always and steadily decrease the error until getting to the solution sought. Starting with an initial approximation to the solution, we improve it, adding the solution of some associated linear problems, in such a way that the error is significantly decreased. A variable step procedure is proposed in order to improve the implementation. Some numerical examples are presented to illustrate the main theoretical conclusions. Finally, we should mention that we have already explored in some previous papers this point of view [1], [2], [3]. However, the main hypothesis in these papers asks for some requirements that essentially rule out the application to singular problems.

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A NUMERICAL METHOD FOR A NONLINEAR INTEGRO-DIFFERENTIAL BOUNDARY VALUE PROBLEM

M. Basile, E. Messina, W. Themistoclakis, and A. Vecchio Dip. di Matematica e Appl.
Università di Napoli " Federico II "
Via Cintia, I-80126 Napoli, Italy
mariateresa.basile@unina.it

We design and analyse a numerical method for the solution of the following second order integro-differential boundary value problem,

$$\nu(y)g(y) = \int_0^\infty k(x)g(x)dx \left(D(y)g'(y)\right)' + p(y), \quad y \geq 0, \quad g'(0) = 0,\ g(+\infty) = 0,$$

which arises in the study of the kinetic theory of dusty plasmas.
First we provide those informations on the existence and other qualitative properties of the solution that will be essential in the numerical investigation. Then we propose a method which is based on the discretization of the differential and integral terms and on an iteration process to solve the resulting nonlinear system. Under suitable hypotheses we prove the convergence of the overall method. The peculiarity of this equation is that the coefficients of the differential terms depend on the integral of the unknown function. This influences both the choice of the discretization process and the approach for studying its convergence. We will show the characteristics of the method by means of some numerical simulations.

RELAXED MIXED CONSTRAINT PRECONDITIONERS FOR GENERALIZED SADDLE POINT LINEAR SYSTEMS

L. Bergamaschi and Á. Martínez
Dipartimento di Metodi e Modelli Matematici per le Scienze Applicate
Università di Padova
berga@dmsa.unipd.it

The solution of the (generalized) saddle point linear system of the form $\mathcal{A}\boldsymbol{x} = \boldsymbol{b}$, where $\mathcal{A} = \begin{bmatrix} A & B^\top \\ B & -C \end{bmatrix}$ and A is symmetric positive definite, C is symmetric semi-positive definite, and B a full-rank rectangular matrix, is encountered in many field such as e.g. constrained optimization, least squares, coupled consolidation problems and Navier-Stokes equations. Iterative solution is recommended against direct factorization methods due to the extremely large size of these systems. We propose here a development of the Mixed Constraint Preconditioners (MCP) introduced in [1] which is based on two preconditioners for A (P_A and $\widetilde{P_A}$) and a preconditioner (P_S) for a suitable Schur complement matrix $S = B\widetilde{P_A}^{-1}B^\top + C$. The family of Relaxed MCP is denoted by $\mathcal{M}^{-1}(\omega)$ where

$$\mathcal{M}(\omega) = \begin{bmatrix} I & 0 \\ BP_A^{-1} & I \end{bmatrix} \begin{bmatrix} P_A & 0 \\ 0 & -\omega P_S \end{bmatrix} \begin{bmatrix} I & P_A^{-1}B^\top \\ 0 & I \end{bmatrix}. \tag{8}$$

We perform a complete eigenanalysis of $\mathcal{M}^{-1}(\omega)\mathcal{A}$ showing that the optimal value of ω can be put in connection with the largest positive eigenvalues of $\tilde{A} = P_A^{-1}A$ and $\tilde{S} = P_S^{-1}S$. Numerical results on geomechanical coupled consolidation problems of size up to 2×10^6 unknowns show that proper choice of ω based on a cheap estimation of spectral radius of $\tilde{A}$ and $\tilde{S}$ may lead to a 70% CPU time saving with respect to the *naive* MCP.

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GLOBAL KRYLOV SUBSPACE METHODS FOR COMPUTING THE MESHLESS ELASTIC SPLINES

A. Bouhamidi
L.M.P.A
Université du Littoral Côte d'Opale
50 rue F. Buisson BP699, F-62228 Calais Cedex, France
bouhamidi@lmpa.univ-littoral.fr

Meshless elastic polyharmonic splines are useful for the approximation of vector fields from scattered data points without using any mesh nor grid [1, 2, 4]. They are based on a minimization of certain energy in an appropriate functional native space. A such energy is related to the strain tensor constraint and to the divergence of the vector field. The computation of such splines leads to a large linear system. In this talk, we will discuss how to transform a such linear system to a general Sylvester matrix equation [3]. So, we will use global Krylov subspace methods to compute approximations to the solution.

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QUADRATURE RULES FOR SINGULAR INTEGRALS ON UNBOUNDED INTERVALS

M. R. Capobianco and G. Criscuolo
CNR–National Research Council of Italy
I.A.C.–Sede Napoli
Via Pietro Castellino 111, 80131 Napoli, Italy
mariarosaria.capobianco@cnr.it

The importance of singular and hypersingular integral transforms, coming from their many applications, justifies some interest in their numerical approximation. The literature about the numerical evaluation of such integrals on bounded intervals is wide and quite satisfactory; instead only few papers deal with the numerical evaluation of such integral transforms on half-infinite intervals or on the real line. Here, we propose some quadrature formulas for integrals of this kind and we compare the new convergence and stability results with that in [1], [2]. Further, following the idea of [3], we construct another quadrature rule, characterized by the Möbius transformation and the Gauss-Jacobi quadrature formula. Also in this case we prove the convergence and the stability.

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SZEGŐ AND PARA-ORTHOGONAL POLYNOMIALS ON THE REAL LINE. ZEROS AND CANONICAL SPECTRAL TRANSFORMATIONS

K. Castillo, R. L. Lamblém, F. R. Rafaeli, and A. Sri Ranga
Department of Mathematics
Universidad Carlos III
Ave. Universidad 30, Leganés, Spain
kcastill@math.uc3m.es

We study polynomials which satisfy the same recurrence relation as the Szegő polynomials, however, with the restriction that the (reflection) coefficients in the recurrence are larger than one in modulus. Para-ortogonal polynomials that follows from these Szegő polynomials are also considered. With two particular choice of real values (positive and alternatively positive) for the reflection coefficients, zeros of the Szegő polynomials, para-orthogonal polynomials and associated quadrature rules are also studied. Finally, again for the two particular choice of real values for the reflection coefficients, interlacing properties of the Szegő polynomials and polynomials arising from canonical spectral transformations are obtained.

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COLLOCATION BASED NUMERICAL METHODS FOR VOLTERRA INTEGRO-DIFFERENTIAL EQUATIONS

A. Cardone, **D. Conte**, and B. Paternoster
Department of Mathematics, University of Salerno
via Ponte don Melillo, I-84084 Fisciano (Salerno), Italy
dajconte@unisa.it

We present multistep collocation based numerical methods for Volterra Integro-Differential Equations (VIDEs). Multistep collocation methods and several modifications have already been proposed for ordinary differential equations [3] and for Volterra integral equations [1, 2]. These methods allow to increase the uniform order of convergence with respect to classical one-step collocation methods, at the same computational cost. We extend the analysis of multistep collocation methods to VIDEs with the aim of combining high accuracy with good stability properties. We analyze the convergence properties of the constructed methods and carry out the numerical stability with respect to the basic test equation and to test equation with decomposable kernel. Moreover classes of A_0-stable methods are provided. Numerical experiments confirm theoretical expectations and make comparisons with the one-step collocation methods.

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FAST AND EFFECTIVE NUMERICAL METHODS FOR 2D PHOTONIC CRYSTALS

P. Contu,* C. van der Mee and S. Seatzu
Dipartimento di Matematica e Informatica
Università di Cagliari
viale Merello 92, 09123 Cagliari, Italy
contu22@interfree.it

In this article we develop two numerical methods to compute the band spectra of 2D photonic crystals without impurities, a finite difference frequency domain (FDFD) method and a finite element frequency domain (FEFD) method. Exploiting periodicity to identify discretization points differing by a period, the computational complexity of the algorithms is reduced significantly. Numerical results on the three test problems most considered in the literature are presented.

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APPLICATIONS OF PPC-FRACTIONS AND SZEGŐ POLYNOMIALS TO FREQUENCY ANALYSIS

C. Craviotto and W. B. Jones
Department of Mathematical Sciences,
University of Northern Colorado
Greeley, Colorado 80639 U.S.A.
cathleen.craviotto@unco.edu

The frequency analysis problem consists of determining unknown frequencies (possibly anharmonic) from a signal consisting of the superposition of sinusoidal waves using a sample of observed data at equal intervals of time. Much work has been published on the mathematical theory of positive Perron-Caratheodory continued fractions (PPC-fractions) and Szegő polynomials and their application to frequency analysis. This talk explores applications of this theory to specific examples of frequency analysis, illustrating the effectiveness of the method and its limitations.

HIGH-PERFORMANCE LARGE EDDY SIMULATION OF INCOMPRESSIBLE TURBULENT FLOWS

A. Aprovitola, **P. D'Ambra**, F.M. Denaro, D. di Serafino, and S. Filippone
ICAR-CNR
Naples, Italy
pasqua.dambra@cnr.it

Large Eddy Simulation (LES) of turbulent flows is based on the idea of directly computing the dynamics of the flow scales responsible for the energy transfer, while modeling the dynamics of the scales where dissipation takes place. Although LES has a reduced cost with respect to Direct Numerical Simulation, where all the scales are solved, it is a computationally expensive technique, and its application to realistic flows is a usual context for high-performance computing. In this talk, we focus on the design and development of a parallel LES code for wall-bounded incompressible turbulent flows. Starting from suitably filtered Navier-Stokes equations, a projection method is applied for decoupling the continuity and momentum equations. The discretization of the resulting equations leads to a numerical procedure that requires, at each time step, two main tasks: computation of convective and diffusive fluxes, and solution of large and sparse linear systems. Our software design methodology is based on a formulation of these tasks in terms of basic linear algebra operations involving sparse matrices, to use reliable and efficient open-source scientific software, such as PSBLAS [1] and MLD2P4 [2], for developing an effective simulation code.

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STABILITY ANALYSIS OF GENERAL LINEAR NYSTRÖM METHODS

R. D'Ambrosio, E. Esposito, and B. Paternoster
Dipartimento di Matematica
University of Salerno
via ponte don Melillo, 84084 Fisciano, Italy
rdambrosio@unisa.it

In this talk we investigate the linear stability properties of the new family of General Linear Nyström methods (GLNs), which is an extension of General Linear Methods to special second order ODEs $y'' = f(x,y)$. We present the extension of the classical notions of stability matrix, stability polynomial, stability and periodicity interval, A-stability and P-stability to the family of GLNs. We next focus our interest on the derivation of highly stable GLNs inheriting the same stability properties of highly stable numerical methods existing in literature, i.e. Runge-Kutta-Nyström methods based on indirect collocation on Gauss-Legendre points: this property, in analogy to a similar feature introduced for General Linear Methods solving first order ODEs, is called *Runge-Kutta-Nyström stability*. The stability properties of GLNs with Runge-Kutta-Nyström stability depend on a quadratic polynomial, which is exactly the stability polynomial of the best Runge-Kutta-Nyström assumed as reference. We also provide examples of GLNs with Runge-Kutta-Nyström stability.

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A UNIFICATION OF UNITARY SIMILARITY TRANSFORMS TO COMPRESSED REPRESENTATIONS

R. Vandebril and **G. M. Del Corso**
Department of Computer Science
University of Pisa
Largo Pontecorvo 3, Pisa, Italy
delcorso@di.unipi.it

A new framework for transforming arbitrary matrices to compressed representations is presented. The framework provides a generic way of transforming a matrix via unitary similarity transformations to e.g. Hessenberg, Hessenberg-like and combinations of both. The new algorithms are deduced, based on the QR-factorization of the original matrix. Based on manipulations with Givens transformations, all the algorithms consist of eliminating the correct set of Givens transformations, resulting in a matrix obeying the desired structural constraints.

Starting from this new reduction procedure we investigate further correspondences such as irreducibility, unicity of the reduction procedure and the link with (rational) Krylov methods.

The unitary similarity transform to Hessenberg-like form as presented here, differs significantly from the one presented in earlier works [1, 2]. Not only does it use less Givens transformations to obtain the desired structure, but also the convergence to rational Ritz values is not observed in the standard way.

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SCALABLE AMG PRECONDITIONERS FOR PDE-CONSTRAINED OPTIMIZATION PROBLEMS

A. Borzì, V. De Simone, and **D. di Serafino**
Dipartimento di Matematica
Seconda Università di Napoli
Caserta, Italy
daniela.diserafino@unina2.it

PDE-constrained optimization problems arise in many applications, such as optimal control, shape design, and parameter estimation. Their size and complexity demands for efficient numerical methods able to exploit high-performance computing resources. In this context, motivations for using multigrid methods [1] include their optimal convergence rates as well as the possibility of developing scalable implementations. We focus on parallel algebraic multigrid (AMG) preconditioners for the solution, through Krylov methods, of large-scale linear systems resulting from the discretization of the optimality conditions for distributed elliptic optimal control problems. We present AMG preconditioners based on Schwarz methods and a modification of the smoothed aggregation coarsening technique. This modification exploits the block structure of the matrix that results from ordering the unknowns so that the degrees of freedom corresponding to the same node of the discretization grid are consecutive. The aggregation and the prolongation and restriction operators are built by using only the entries of the blocks corresponding to the PDE constraint. This approach has been implemented within the framework of the parallel preconditioning package MLD2P4 [2]. Numerical experiments show the effectiveness of the preconditioners and their parallel efficiency.

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COMPLEMENTARY LIDSTONE INTERPOLATION ON SCATTERED DATA SETS

F.A. Costabile, F. Dell'Accio, and **F. Di Tommaso**
Dipartimento di Matematica
Università della Calabria
via P. Bucci 30A 87036 Rende (Cs), Italy
ditommaso@mat.unical.it

Recently we have introduced a new technique for combining classical bivariate Shepard operators with three point polynomial interpolation operators. This technique is based on the association, to each sample point V, of a triangle with a vertex in V and other ones in a neighborhood of V, to minimize the error of the three point polynomial interpolant. The combination inherits both degree of exactness and interpolation conditions, at each node V, of the polynomial interpolant, so that in [1] we succeed to extend Lidstone interpolation to scattered data sets by combining Shepard operators with the three point Lidstone interpolation polynomial [2]. Complementary Lidstone interpolation was recently introduced in [3] and drawn on by Agarwal, Pinelas and Wong. Complementary Lidstone interpolation naturally complements Lidstone interpolation. In this talk we generalize Complementary Lidstone interpolation to the case of bivariate scattered sample points. Numerical results are provided.

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FORMAL QD ALGORITHM AND MARKOV-BERNSTEIN INEQUALITIES

A. Draux
INSA de Rouen
Département de Génie Mathématique
Avenue de l'université, BP 8
F-76801 Saint-Étienne-du-Rouvray Cedex, FRANCE
andre.draux@insa-rouen.fr

Let $L^2(\Omega;\mu_m)$, $m = 0,1$, be Hilbert spaces of square integrable real functions on the open set $\Omega \subset \mathbb{R}$ for the positive Borel measures μ_m supported on Ω. The norm on this space is defined from the inner product

$$\| f \|_{L^2(\Omega;\mu_m)} = (\int_\Omega f(x)^2 d\mu_m)^{\frac{1}{2}}, \qquad \forall f \in L^2(\Omega;\mu_m), \quad m = 0,1.$$

Let $\mathcal{P}_n$ be the vector space of real polynomials in one variable of degree at most equal to n. A Markov-Bernstein inequality corresponds to

$$||p'||_{L^2(\Omega;\mu_1)} \leq M_n ||p||_{L^2(\Omega;\mu_0)}, \quad \forall p \in \mathcal{P}_n,$$

where p' is the derivative of p. The smallest possible value of M_n is called the constant of Markov-Bernstein. It is well known that this best constant is linked with the smallest eigenvalue $\alpha_{1,n}$ of a $n \times n$ positive definite symmetric matrix : $M_n = \frac{1}{\sqrt{\alpha_{1,n}}}$. It is exceptional to obtain the exact value of M_n. So, it remains the solution to produce formal lower and upper bounds of $\alpha_{1,n}$ in order to give the asymptotic behavior of this eigenvalue.

Our aim is to do a review of the use of formal different versions of the qd algorithm in such a way that some sequences of upper bounds are given for this smallest eigenvalue $\alpha_{1,n}$ in the case of the classical measures (Laguerre-Sonin, Jacobi) and partially in the case of the generalized Gegenbauer measure.

A problem is still open : to use such a formal algorithm for finding an upper bound of the smallest eigenvalue of a generalized eigenvalue problem $Ax = \lambda Bx$, where (in our case) A and B are $n \times n$ positive definite symmetric matrices.

OPTIMAL RATIONAL KRYLOV SUBSPACES FOR LARGE-SCALE DYNAMICAL SYSTEMS

V. Druskin, L. Knizhnerman, V. Simoncini, and M. Zaslavsky
Schlumberger-Doll Research
1 Hampshire st. Cambridge, MA 02139 USA
druskin1@slb.com

Ruhe's Rational Krylov Subspace is recognized as a powerful tool within Model Order Reduction techniques for linear dynamical systems. However, its success has been hindered by the lack of procedures, which would generate the sequence of shifts used to build the space with good approximation properties.

We begin with the first order passive problems $Au + u_t = 0, \quad u|_{t=0} = b$ for $0 \leq t < \infty$, where $u(t), \varphi \in \mathbf{R^N}$ and $A \in \mathbf{R^{N \times N}}$. We will solve this problem by projecting it onto the Rational Krylov Subspace (RKS). We first assume that the numerical range $W(A)$ is known and design a-priori algorithms of optimal shift generation. We consider this problem in the frequency domain and reduce it to the third Zolotaryov problem in complex plane.

Then we propose a recursive greedy algorithm for adaptive choice of shifts taking into account non-uniformity of the spectrum. The algorithm is based on an explicit formula for the residual in the frequency domain allowing adaptive shift optimization at negligible cost.

Finally, we extend the our approach from the first order problem to the solution of passive high and infinite order dynamical systems.

We illustrate obtained results with application to first order and fractional diffusion Maxwell's system.

EXTRAPOLATION OF OPERATOR MOMENTS, WITH APPLICATIONS TO LINEAR ALGEBRA PROBLEMS

C. Brezinski, **P. Fika**, and M. Mitrouli
Department of Mathematics
University of Athens
Panepistimiopolis, Athens, Greece
pfika@math.uoa.gr

Let A be a linear self-adjoint operator from H to H, where H is a real infinite dimensional Hilbert space with the inner product $(\cdot,\cdot)$. For positive powers of A, the Hilbert space H could be infinite dimensional, while, for negative powers it is always assumed to be a finite dimensional, and, in this case, A is also assumed to be invertible. Using the singular value decomposition for a compact linear self-adjoint operator A and its moments, we can define it's fractional powers by $A^\nu z = \sum_k \sigma_k^\nu (z, u_k) u_k$, and its fractional moments by $c_\nu(z) = (z, A^\nu z) = \sum_k \sigma_k^\nu \alpha_k^2(z)$, where $\alpha_k(z) = (z, u_k)$, for $\nu \in \mathbb{Q}$.

We will approximate $c_q(z)$ by interpolating or extrapolating, at the point $q \in \mathbb{Q}$, the $c_n(z)$'s for different values of the non-negative integer index n by a conveniently chosen function obtained by keeping only one or two terms in the preceding summations.

Estimates of the trace of A^q, for $q \in \mathbb{Q}$, and of the norm of the error when solving a system $Ax = f \in H$ will be given. For $q = -1$, other estimates of the trace of the inverse of a matrix could be found in [1, 2].

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MULTIRESOLUTION ANALYSIS FOR SURFACES

M. A. Fortes and M. L. Rodríguez
Department of Applied Mathematics
University of Granada
Facultad de Ciencias, C/ Severo Ochoa, s/n, Spain
miguelrg@ugr.es

Beam and Warming proved in [1] that the supercompact wavelets can exactly represent any piecewise polynomial function in one variable, generalizing the fact that Haar wavelet can exactly represent any piecewise constant function. Higher level of accuracy is attained by higher order polynomials of supercompact wavelets. Later, in [2], the authors developed an extension of the work [1] to the case of surfaces defined over uniform meshes of the domain of the surface. Such construction keeps the same advantages attained by [1] in relation with orthogonality, short support, approximation of surfaces with no border effects, detection of discontinuities, higher degree of accuracy and compressibility. The approach in [2] allows transfer information of a function between different resolution levels by means of reconstruction and decomposition algorithms stated in a multiresolution context.

Actually, we are working in generalizations of [2] in two different ways: First of all, we extend the multiresolution scheme for surfaces to the case of non-uniform meshes. On the other hand, we handle the problem of generalizing the multiresolution analysis with the aim of transfering other kinds of information, like derivative or integral values, curvatures,...between different resolution levels.

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A STUDY ON PRECONDITIONING SUITED FOR IDR(s)-RESIDUAL REDUCTION METHOD

S. Fujino and K. Murakami
Research Institute of Information Technology
Kyushu University
6-10-1, Hakozaki, Higashi-ku, Fukuoka, Japan
fujino@cc.kyushu-u.ac.jp

IDR(s)-based Residual Reduction (abbreviated as IDR(s)-R2) method [3] was proposed as one of iterative methods based on IDR theorem by P. Sonneveld and M. van Gijzen in 2008[2]. Since the iteration matrix is considered as one of preconditionings, we can choose flexibly preconditionings. This article estimates effectiveness of some preconditioning techniques for symmetric matrices applied to IDR(s)-R2 method. In particular, we focus on IC factorization with inverse-based dropping[1], and demonstrate its efficiency through numerical experiments.

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AN APPLICATION OF THE INTEGRABLE DISCRETE HUNGRY TODA EQUATION TO THE EIGENVALUE COMPUTATION

A. Fukuda, Y. Yamamoto, M. Iwasaki, E. Ishiwata, and Y. Nakamura
Department of Mathematical Information Science
Tokyo University of Science
Tokyo 162-8601, Japan
afukuda@rs.tus.ac.jp

The qd algorithm [1], for computing eigenvalues, has a close relationship with the integrable discrete Toda equation. It is known that the discrete Toda equation is extended to the discrete hungry Toda (dhToda) equation through the study of the box and ball system [2].

In this talk, we propose a new matrix eigenvalue algorithm in terms of the dhToda equation. We first show that a time evolution from n to $n+1$ of the dhToda equation corresponds to a similarity transformation of a totally nonnegative (TN) matrix. Here the TN matrix is a matrix with all nonnegative minors. We next reveal that the the dhToda variable has a periodical asymptotic behavior. As n becomes sufficiently large, the implicit equilibrium points are related to the eigenvalues of the TN matrix. Based on this property, we design a new algorithm, named the dhToda algorithm, for eigenvalues of the TN matrix. Numerical examples show that the dhToda algorithm is with high relative accuracy. We also describe some other properties of the algorithm.

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ON PROJECTION METHODS FOR ESTIMATING THE DIAGONAL OF A MATRIX INVERSE

C. Bekas, A. Curioni, **E. Gallopoulos**, and V. Kalantzis
CEID
University of Patras
Greece
stratis@ceid.upatras.gr

The estimation of the diagonal of the inverse of a symmetric matrix, A, is an important problem in many applications. Following the statistical estimation approach of Hutschinson, several methods for this task (e.g. [1, 3]) depend on presence of an effective method for computing $z^\top A^{-1} z$ for a suite of suitably selected vectors z. Recently, some of these techniques were combined with conjugate gradients, iterative refinement and parallel processing to produce a method that for large matrices gave substantially better performance than previous approaches ([2]). In this paper we propose solvers based on projections that exploit the multiple right-hand sides. We discuss the design of these algorithms and show that they further improve the performance of diagonal matrix inverse estimators.

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GENERALIZED EXPONENTIAL INTEGRATORS FOR FRACTIONAL DIFFERENTIAL EQUATIONS

R. Garrappa and M. Popolizio
Departimento di Matematica
Università degli Studi di Bari
Via E. Orabona n. 4 - 70125 Bari, Italy
garrappa@dm.uniba.it

Exponential integrators are powerful and well–established methods particularly suited for the time–integration of semilinear systems of ordinary differential equations (ODEs) with linear stiffness. By solving exactly the stiff term, exponential integrators allow to integrate the remaining non–stiff part of the system by means of explicit schemes without calling for severe restrictions on the step-size.

In this talk we discuss the generalization of exponential integrators to problems of non integer orders, namely fractional differential equations (FDEs), which are nowadays used in several areas, including biology, finance, physics and control theory, to model systems exhibiting anomalous dynamics [1].

The generalization of exponential integrators to FDEs presents some challenges: indeed, a more difficult function, specifically a Mittag-Leffler type function, has to be evaluated with matrix arguments; furthermore the presence of a persistent memory (a typical feature of FDEs) demands for different and more expensive techniques for the time–discretization [2].

In this talk we discuss the main computational issues and we present a class of exponential integrators for FDEs. Some results on accuracy and stability are also studied and we show, by means of some numerical experiments, the effectiveness of the proposed approach.

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NUMERICAL INTEGRATION OVER THE SQUARE IN THE PRESENCE OF ALGEBRAIC/LOGARITHMIC SINGULARITIES WITH AN APPLICATION TO AERODYNAMICS

W. Gautschi
Department of Computer Sciences
Purdue University
West Lafayette, IN 47907, USA
wgautschi@purdue.edu

A method based on one-dimensional Gaussian quadratures is developed for evaluating double integrals of the type indicated in the title. If the singularities occur only along the diagonal and the regular part of the integrand is a polynomial of total degree d, the method can be made exact by choosing the number of quadrature points larger than, or equal to, $1 + d/2$. Numerical examples are given as well as an application to a problem in aerodynamics.

ON THE CALCULATION OF RESONANCES BY MEANS OF ANALYTICAL CONTINUATION

J. Horáček
Institute of Theoretical physics
Charles University in Prague
V Holešovičkách 2, 180 00 Praha 8, Czech Republic
jiho@matfyz.cz

As is well known resonances play important roles in many processes in physics and chemistry. e.g., in dissociative attachment, associative detachment, vibrational excitation, etc., just to mention a few. For description of the above mentioned resonance processes an accurate knowledge of resonance energies and widths is required. To calculate these is however a complicated problem. There exist very efficient commercial programs for calculation of bound states but not an easy to apply method to calculate resonances. It is therefore natural to ask whether one could obtain some information on the resonance energies and widths using bound state energy calculations only. The answer is affirmative and one method following this idea was proposed already in seventieths in the field of nuclear physics. It works as follows: it is intuitively clear that if we modify the Hamiltonian in such a way so as to make the interaction between the colliding particles more attractive the bound states become more deeply bound. If the additional interaction is strong enough the resonances are eventually converted into bound states. One can calculate the bound state energy for various potential strength and then construct an analytic function by means of analytic continuation. Once the analytical expression is found, the resonance energy and width is determined by simply setting the additional potential strength to zero. Thus from a knowledge of bound state energies for only a slightly modified problem we can determine the resonance parameters. It is the purpose of this contribution to study the numerical performance of the process of analytical continuation on simple analytical models by means of the statistical Padé approximation. It is well known that the process of analytical continuation represents an ill-conditioned problem. It will be shown that the application of the Padé approximation nevertheless allows us to obtain very precise continued data provided the input data were accurate enough.

MODELLING PHOTONIC CRYSTAL DEVICES USING SECOND ORDER FINITE VOLUME METHOD

T. Z. Ismagilov
Department of Information Technology
Department of Mathematics and Mechanics
Novosibirsk State University
Pirogova 2, Novosibirsk, 630090, Russia
ismagilov@academ.org

A second order finite volume scheme is considered [1]. The scheme includes total field - scattered field formulation and a perfectly matched layer [2]. It was applied to evaluation of optical properties of photonic crystal waveguides [3]. Reflection and transmission coefficients were studied for a range of frequencies inside the photonic crystal bandgap for different configurations. Our results compare well with simplified analytic models from previous researchers [4].

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CONVERGENCE OF COLLOCATION METHOD WITH DELTA FUNCTIONS FOR INTEGRAL EQUATIONS OF FIRST KIND

U. Kangro
Department of Mathematics and Computer Science
University of Tartu
J. Liivi 2, Tartu 50409, ESTONIA
urve.kangro@ut.ee

We consider integral equations of type $\int_\gamma K(x,y)u(y)dS_y = f(x)$, $x \in \Gamma$, where γ and Γ are some closed disjoint curves or surfaces. Equations of this type arise when solving boundary value problems of elliptic partial differential equations by interior source methods. These methods generate the solution of the differential equation as an integral over a contour or a surface outside the closure of the (usually exterior) domain. Typically K has a singularity at $x = y$, and if Γ and γ are disjoint, the singularity is avoided. In fact, if Γ and γ are analytic, then the integral equation has an analytic kernel. Results about existence and uniqueness of the solution can often be obtained only in spaces of linear analytic functionals, and in general case, only density of the range of the integral operator can be proved.

We look for approximate solutions of the integral equation as linear combinations of Dirac's δ-functions. For the corresponding collocation method, in case of analytic data the convergence is exponential in the number of variables. If the boundary is only piecewise smooth, the convergence rate deteriorates to algebraic. To get a more robust method, one can choose on Γ more points than on γ, and solve the corresponding overdetermined system by least squares.

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EVALUATION OF MINORS FOR WEIGHING MATRICES $W(n, n-1)$ HAVING ZEROS ON THE DIAGONAL

A. Karapiperi, M. Mitrouli, and J. Seberry
Department of Mathematics
University of Athens
Panepistemiopolis 15784, Greece
akarapi@math.uoa.gr

A $(0, 1, -1)$ matrix $W = W(n, n-k)$, $k = 1, 2, \ldots$, of order n satisfying $W^T W = WW^T = (n-k)I_n$ is called a *weighing matrix of order n and weight $n-k$* or simply a *weighing matrix*. Every row and column of a $W(n, n-k)$ contains exactly k zeros.
The talk will be concentrated on the evaluation of minors for weighing matrices $W(n, n-1)$ with zeros on the diagonal. Theoretical proofs concerning their minors up to the order of $(n-3) \times (n-3)$ will be derived. A general theorem specifying the analytical form of any $(n-k) \times (n-k)$ minor will be developed.

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ARRAY SQUARE-ROOT APPROACH FOR THE MAXIMUM LIKELIHOOD ESTIMATION VIA ADAPTIVE KALMAN FILTERING METHODS

M. V. Kulikova
CEMAT (Centro de Matemática e Aplicações)
Instituto Superior Técnico, TU Lisbon
Av. Rovisco Pais 1, 1049-001 Lisboa, Portugal
Kulikova.Maria@yahoo.com

The maximum likelihood technique for identification of linear discrete-time stochastic systems incorporates optimization algorithms that may require calculation of the log likelihood gradient (known as a "score") and the Fisher information matrix (FIM). The gradient evaluation demands the determination of the sensitivities of the system state to unknown parameters. It leads to implementation of roughly $p + 1$ equivalent Kalman filters (KFs), where p is the dimension of the unknown system parameter vector.

Algorithms for the score and FIM calculation could be described and derived more compactly and simply by recasting the filtering problem in the so-called *array form*. Such algorithms do not propagate the Riccati recursion directly and, hence, are often much simpler to describe and implement (in software and hardware) than explicit sets of equations. They are becoming the method of choice in many applications.

Having been inspired by these and related problems, we construct a new square-root algorithm for the log-likelihood gradient evaluation. This avoids the use of the conventional KF with its inherent numerical instabilities and improves the robustness of computations against roundoff errors. Apart from the numerical advantages, the convenient array form allows for effective calculation method where the required "bank" of the filters is replaced by an augmented array to which the orthogonal transformations are applied.

A NEW APPROACH TO CONTROL THE GLOBAL ERROR OF NUMERICAL METHODS FOR DIFFERENTIAL EQUATIONS

G. Yu. Kulikov and R. Weiner
CEMAT (Centro de Matemática e Aplicações)
Instituto Superior Técnico, TU Lisbon
Av. Rovisco Pais, 1049-001 Lisboa, Portugal
gkulikov@math.ist.utl.pt

Recently, Kulikov presented the idea of double quasi-consistency, which facilitates global error estimation and control, considerably. More precisely, a local error control implemented in doubly quasi-consistent numerical methods plays a part of global error control at the same time. However, Kulikov studied only Nordsieck formulas and proved that there exists no doubly quasi-consistent scheme among those methods.

In this paper, we prove that the class of doubly quasi-consistent formulas is not empty and present the first example of such sort. This scheme belongs to the family of superconvergent explicit two-step peer methods constructed by Weiner et al. We present a sample of s-stage fixed-stepsize doubly quasi-consistent parallel explicit peer methods of order $s-1$ when $s=3$. Then, we discuss variable-stepsize explicit parallel peer methods grounded in the interpolation idea. Approximation, stability and convergence are studied in detail. In particular, we prove that some interpolation-type peer methods are stable on any variable mesh in practice. Double quasi-consistency is utilized to introduce an efficient global error estimation formula in the numerical methods under discussion. The main advantage of these new adaptive schemes is the capacity of producing numerical solutions for user-supplied accuracy conditions in automatic mode and almost at no extra cost. This means that a usual local error control mechanism monitors and regulates the global error at the same time because the true error of any doubly quasi-consistent numerical method is asymptotically equal to its local error. Numerical experiments support theoretical results of this paper and illustrate how the new global error control concept works in practice. We also conduct a comparison with explicit ODE solvers in MatLab.

ON THE PERFORMANCE OF THE ALGEBRAIC OPTIMIZED SCHWARZ PRECONDITIONING METHODS

L. Laayouni and D. B. Szyld
School of Science and Engineering Al Akhawayn University
Avenue Hassan II, 53000. P.O. Box 1630, Ifrane, Morocco
l.laayouni@aui.ma

The Algebraic Optimized Schwarz Methods (AOSM) have been introduced in [1]. These methods mimic in the algebraic form the well-known optimized Schwarz methods (OMS). The AOSM methods are based on the modification of the block matrices associated to the transmission conditions between sub-domains. The transmission blocks are replaced by modified blocks to improve the convergence of the corresponding methods. In the optimal case, the convergence can be achieved in two iterations. We are interested in how the algebraic optimized Schwarz methods, used as preconditioner solvers, perform in solving partial differential equations. We are also interested in their asymptotic behavior with respect to change in problems parameters. We will present different numerical simulations corresponding to different type of problems in two- and three-dimensions.

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A RADIAL BASIS FUNCTION BASED PARTITION OF UNITY METHOD FOR SOLVING PDE PROBLEMS

E. Larsson and A. Heryudono
Department of Information Technology
Uppsala University
Box 337, SE-751 05 Uppsala, Sweden
Elisabeth.Larsson@it.uu.se

Radial basis function (RBF) based approximation methods are interesting in the context of PDE solving due to their ease of implementation, their potentially spectral convergence rates, and their flexibility with respect to geometry. However, a persistent problem has been the severe ill-conditioning of the systems of equations that typically need to be solved. This ill-conditioning is partly related to the size of the system, but even more so to the shape parameter of the RBFs. As the shape parameter is decreased, the RBFs become increasingly flat, leading to a nearly linearly dependent basis. However, the nearly flat limit in many cases provide the best approximation properties. The recently developed RBF-QR method [1] provides numerically stable evaluations for the small shape parameter range in up to three space dimension. With the conditioning obstacle removed, the focus can be turned to more general computational issues such as computational cost and memory requirements. Instead of using a global RBF method resulting in a dense linear system, we propose a partition of unity approach with local RBF approximants. The locality reduces both memory usage and computational cost compared with the global method. We show that the RBF-QR algorithm is a key to success and provide both theoretical results and numerical experiments showing spectral convergence with respect to the local problem size and algebraic convergence with respect to the partition size.

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MULTIVARIATE PRONY'S METHOD

A. Cuyt and **W.-S. Lee**
Department of Mathematics and Computer Science
University of Antwerp
Middelheimlaan 1, 2020 Antwerpen, Belgium
wen-shin.lee@ua.ac.be

In 1795, Gaspard Riche de Prony presented a method for interpolating a sum of exponential functions. Closely related to Padé approximation, Prony's method has found applications in the shape from moments problem, spectral estimation, and lately sparse sampling of digital signals with finite rate of innovation.

The interesting connection between Prony's method and error-correcting codes has led to the development of symbolic-numeric sparse polynomial interpolation, which has also exploited a reformulation of Prony's method as a generalized eigenvalue problem and a link to Rutishauser's qd-algorithm.

Recall that a meromorphic function is a function analytic everywhere except at a set of isolated points that are called the poles of the function. Rutishauser's qd-algorithm can determine the poles of a meromorphic function from its Taylor expansion. In the multivariate case such poles form a set of solutions of the associated multivariate polynomial equations. The interdependence between the Taylor expansion and poles becomes less obvious because there can be various ways to order the multivariate Taylor coefficients.

Recent progress in the multivariate qd-algorithm expands our understanding in associating the convergence of multivariate poles to the different orderings of Taylor coefficients, among which a special case has been implemented in developing numerical multivariate polynomial factorization. Resorting to the link from qd to Padé leads us to a multivariate Prony's method, which intricately involves higher-order tensors and their decompositions.

PROPERTIES AND NUMERICAL RESULTS OF A PARALLEL ALGORITHM FOR GLOBAL OPTIMIZATION PROBLEMS

M. Gaviano and **D. Lera**
Dipartimento di Matematica e Informatica,
University of Cagliari, Italy
lera@unica.it

The problem of finding a global minimum of a real function on a set $S \subseteq \mathbb{R}^n$ occurs in many real world problems [2], [3]. Since its computational complexity is exponential, its solution can be a very expensive computational task. In this paper, we introduce a parallel algorithm that exploits the latest computers in the market equipped with more than one processor, and can be used in a clusters of computers. The algorithm belongs to the improvement of local minima algorithm family, and carries on local minimum searches iteratively but trying not to find an already found local optimizer [1]. Numerical experiments have been carried out on two computers equipped with four and six processors; fourteen configurations of the computing resources have been investigated. To evaluate the algorithm performances the *speedup* and the *efficiency* are reported for each configuration.

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NUMERICAL SOLUTION OF THE DENSITY PROFILE EQUATION FOR NON-NEWTONIAN FLUIDS

G. Hastermann, **P. Lima**, M.L. Morgado, and E. Weinmuller
CEMAT, Instituto Superior Técnico
Universidade Técnica de Lisboa
Av. Rovisco Pais, 1049-001 Lisboa, Portugal
plima@math.ist.utl.pt

We discuss the analytical properties and the numerical treatment of a nonlinear singular second order boundary value problem in ordinary differential equations, posed on an unbounded domain, which represents the density profile equation for the description of the formation of microscopic bubbles in a non-homogeneous non-newtonian fluid. First, we give an asymptotic analysis of the underlying equation and provide asymptotic expansions of the one-parameter families of solutions satisfying the boundary conditions at the singular points. Then, after the transformation of the problem into a new one, defined on a bounded interval, polynomial collocation is applied to solve the new problem. The results of the numerical simulation are presented and discussed.

In the present work, the analysis and computational methods proposed earlier for the case of newtonian fluids (see [1], [2]), are extended to the non-newtonian case.

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APPELL POLYNOMIALS OF SECOND KIND AND RELATED INTERPOLATION PROBLEM

F. A. Costabile, **E. Longo**, and R. Luceri
Department of Mathematics University of Calabria
Arcavacata di Rende, Italy
longo@mat.unical.it

Classical Appell polynomials are defined by differential equation $A_n' = nA_{n-1}$, $n \in \mathbb{N}$, where $n \in \mathbb{N}$ is the degree of polynomials $A_n(x)$. Now we define Appell polynomials of second kind the polynomials given by

$$\Delta \mathcal{A}_n = n\mathcal{A}_{n-1}, \quad n \in \mathbb{N} \tag{9}$$

where Δ is the classical difference operator: $\Delta f(x) = f(x+1) - f(x)$.
Well known examples are Bernoulli polynomials of second kind and Boole polynomials.
Let L be a linear functional on the space of real function defined in $[0,1]$. We look for a polynomial $P_n(f,x)$ of degree n such that

$$L\left(\Delta^k P_n\right) = L\left(\Delta^k f\right), \quad k = 0, ..., n. \tag{10}$$

We prove that this interpolation problem has the unique solution

$$P_n(f,x) = \sum_{k=0}^{n} \frac{L\left(\Delta^k f\right)}{k!} \mathcal{A}_n^L \tag{11}$$

where $\mathcal{A}_n^L$ is the class of Appell polynomials of second kind related to L.

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ON NONORTHOGONAL POLYNOMIALS GENERATED BY CLASSICAL FORMS

A. F. Loureiro and P. Maroni
Center of Mathematics
University of Porto
Rua do Campo Alegre, 687; 4169-007 Porto, Portugal
anafsl@fc.up.pt

A polynomial sequence generated by powers of certain first order differential operators will be under discussion. Despite their non-regular orthogonality, the corresponding canonical element of its dual sequence is a classical form of Hermite, Laguerre, Bessel and Jacobi. They will be thoroughly characterized.

HIGH-PERFORMANCE SPECTRAL-ELEMENT SIMULATION OF CARDIAC ELECTRICAL FUNCTION USING GPUS

G. Cuccuru, G. Fotia, and **F. Maggio**
CRS4 Bioinformatica
Pula (CA), Italy
maggio@crs4.it

Models of cardiac electrophysiology consist of a system of partial differential equations coupled with a system of ordinary differential equations representing cell membrane dynamics. Discretization with an average nodal spacing of 0.2 mm as required to prevent the onset of non-physical, spurious effects when these equations are solved numerically using finite element (FE), or finite difference (FD) methods generates a mesh with many millions of nodes, making whole heart simulation a demanding scientific computing problem. As an alternate choice, spectral-element method (SEM) can be adopted. SEM is designed to combine the good accuracy properties of pseudospectral techniques such as Legendre or Chebyshev methods with the geometrical flexibility of classical low-order FE methods. As a result, SEM is extremely efficient to model propagation phenomena on complex shapes using fewer mesh nodes than its FE equivalent (for the same level of accuracy).

Another issue is that current simulation software does not provide the required computational speed for practical applications. One reason for this is that little use is made of recent developments in hardware architecture for throughput-oriented computing and in the associated programming models, such as GPGPU (general purpose computation on GPUs).

Combining GPU programming with higher order discretization methods we developed a CUDA implementation of a spectral element code to perform the numerical simulation of cardiac action potential on a whole heart. We discuss the implementation and optimization of the code and compare it to an existing CPU based solver. We provide some examples that demonstrate the robustness of the method and the use of these numerical models, focusing specifically on some selected model problems.

COMPUTATION OF JACOBI MATRICES OF UNCOUNTABLE SYSTEMS OF ITERATED FUNCTIONS AND THE SOLUTION OF AN INVERSE PROBLEM

G. Mantica
Center for Nonlinear and Complex Systems
Department of Physics and Mathematics
University of Insubria
Via Valleggio 11, Como Italy
giorgio@uninsubria.it

Consider the random process in $\mathbf{R}$ given by $x_{n+1} = \delta(x_n - \beta) + \beta$, where $0 < \delta < 1$ is a real parameter and β is drawn randomly from a probability distribution $\sigma(\beta)$. Clearly, the points x are *attracted* towards the points β and, in the limit, their distribution converges to a measure μ. This latter is the invariant measure of a system of Iterated Functions (I.F.S.).

Usually in I.F.S. theory, the distribution $\sigma(\beta)$ is discrete and composed of a finite number of atoms. In this talk, we allow σ to be any compactly supported distribution. We describe a new technique for computing the Jacobi matrix of the measure μ, that is numerically stable for matrix orders as large as hundreds of thousands. The same theory can be reversed into an efficient technique for solving an inverse reconstruction problem, that requires to find σ from the knowledge of μ. This problem can be cast in the form of a generalized Gaussian integration problem. Introductory results to the new material presented here can be found in [1, 2].

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FAST DIRECT SOLVERS FOR ELLIPTIC PDES

P.G. Martinsson
Department of Applied Mathematics
University of Colorado at Boulder
Boulder, CO 80027, USA
martinss@colorado.edu

That the linear systems of algebraic equations arising upon the discretization of elliptic PDEs can be solved very rapidly is well-known, and many successful iterative solvers with linear complexity have been constructed (multigrid, Krylov methods, etc). More recently, it has been demonstrated that it is also often possible to directly compute an approximate inverse (or LU/Cholesky factorization) to the coefficient matrix in linear or close to linear time. The inverse is computed in a data-sparse format that exploits internal matrix structure such as rank-deficiencies in the off-diagonal blocks.

The talk will focus on methods relying on the *Hierarchically Semi-Separable (HSS)* matrix format to efficiently represent the solution operator to the PDE. This format is less versatile than the more popular $\mathcal{H}$ and $\mathcal{H}^2$ matrix formats, but typically results in very high performance in terms of speed and accuracy when it can be made to work. For problems on 1D domains such as a boundary integral equation (BIE) on a domain in the plane, the adaptation of the HSS format is straight-forward, and problems in higher dimensions can be handled via recursive domain decomposition techniques that reduce the dimensionality of the domain on which the compressed operator acts.

The talk will describe numerical examples in both two and three dimensions. Variable coefficient problems are handled via accelerated nested dissection methods, while constant coefficient problems are solved via the corresponding boundary integral equation formulations.

MINIMIZATION OF FUNCTIONALS ON THE SOLUTION OF A LARGE-SCALE ILL-POSED PROBLEM

E. Franchini, **D. Martin**, and L. Reichel
Department of Mathematical Sciences
Kent State University
Kent, OH 44242, USA
dmarti49@kent.edu

In this work we study the minimization of a linear functional defined on a set of approximate solutions of a discrete ill-posed problem. The primary application is computation of confidence intervals for components of the true solution. We exploit the technique introduced by Elden in 1990 ([1]), based on a parametric programming reformulation involving the solution of a sequence of quadratically constrained least squares problems. To minimize the number of matrix-vector products, we apply a numerical method based on Lanczos bidiagonalization and Gauss-type quadrature rules to solve the trust-region subproblems.

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POLYNOMIAL SPLINES AS EXAMPLES OF CHEBYSHEVIAN SPLINES

M.-L. Mazure
Laboratoire Jean Kuntzmann
Université Joseph Fourier
BP53, 38041 Grenoble Cedex 9, France
mazure@imag.fr

The results we present here concern geometrically continuous polynomial splines, in the sense that the left/right derivatives at the knots are linked by connection matrices. A classical sufficient condition for spaces of such splines to be suitable for either Approximation or Geometric Design is the total positivity of all their connection matrices (i.e., all their minors are non-negative) [1]. Their entries can then serve as shape parameters. As an example, they can be used in spline interpolation to make up for the Gibbs phenomenon.

We show how to obtain all the connection matrices leading to suitable spline spaces. The results in themselves are interesting in so far as they permit more efficient shape effects than total positivity. Even more interesting is the way we achieve them. They follow from considering polynomial splines as special instances of Chebyshevian splines and polynomial spaces on a closed bounded interval as special instance of Extented Chebyshev spaces [3, 2].

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ON THE GOOD PIVOTS OF HADAMARD MATRICES AND RELATED ISSUES

C. Kravvaritis and **M. Mitrouli**
Department of Mathematics
University of Athens
Panepistimiopolis, Athens, Greece
mmitroul@math.uoa.gr

We introduce for the first time the notion of *good pivot patterns* as follows. A pivot pattern $\{p_1, p_2, \ldots, p_n\}$ appearing after application of Gaussian Elimination (GE) with complete pivoting on a matrix of order n is called *good*, if its pivots satisfy $p_i p_{n-i+1} = n, \;\; i = 1, \ldots, n$. Clearly, good pivot patterns are of the form $\left\{ p_1, p_2, \ldots, p_{\frac{n}{2}}, \frac{n}{p_{\frac{n}{2}}}, \ldots, \frac{n}{p_2}, \frac{n}{p_1} \right\}$.

It is important to specify the possible existence of good pivot patterns appearing after application of GE on Completely Pivoted (CP) Hadamard matrices of various orders [2]. The appearance of this property confirms Cryer's conjecture [1] for all Hadamard matrices possessing good pivots and for those belonging to the same H-equivalence class, namely that their growth factor is equal to their order.

We shall prove that for every pivot p_k, $k = 2, \ldots, n$, of a CP Hadamard matrix H of order n it holds $p_k > 1$. Based on this fact, we take a small step towards the equality portion of Cryer's conjecture proving that if the pivots $\{p_1, p_2, \ldots, p_n\}$ of a CP Hadamard matrix H of order n are good, then its growth is equal to its order.

Hadamard matrices are the only matrices known so far that lead to good pivot patterns.

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ON A FORMAL SOLUTION FOR A DISCRETIZED SIRS EPIDEMIC MODEL

D. Okada, M. Sekiguchi, and E. Ishiwata
Graduate school of Science
Tokyo University of Science
1-3 Kagurazaka, Shinjuku-ku, Tokyo 162-8601, Japan
j1410606@ed.kagu.tus.ac.jp

To understand infection mechanisms, the stability of the solution for continuous epidemic models is often discussed. However, Acedo et al. [1] recently proposed a formal solution for a continuous SIRS model. We apply analytical approach by [1] to a discretized SIRS model. This analytical approach can not be applied to discretized model using traditional numerical schemes. Sekiguchi and Ishiwata [2] recently obtained a discretized SIRS model using the nonstandard discretization in [3] and also showed the sufficient conditions for global behaviors of the solution, which are corresponding to those of the original continuous model. Similarly, we derive a discretized SIRS model and, as in [1], we obtain a formal solution for this discretized model.

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SOME REMARKS ON THE ALTERNATE TRAPEZOIDAL QUADRATURE METHOD FOR FREDHOLM INTEGRAL EIGENVALUE PROBLEMS

S. P. Oliveira, A. C. da Rocha, and A. Ruiz de Zárate
Departamento de Matemática
Universidade Federal do Paraná
Curitiba-PR, Brazil
saulopo@ufpr.br

We consider a quadrature method based on the alternate trapezoidal quadrature for the eigenvalue problem given by the Fredholm integral equation of second kind. The understanding of the spectral properties of this quadrature method is of interest to the numerical computation of the periodic Hilbert transform and related operators without resorting to the spectral method. We prove that, for some convolution-type integral kernels, such a quadrature method always yields eigenvalues with double multiplicity. This could help to reduce the computational cost of the quadrature method by exploring the decoupling of the resulting discrete eigenvalue problem.

HAMILTONIAN MOTION OF ALGEBRAIC CURVES

B.G. Konopelchenko and **G. Ortenzi**
Department of Mathematics and Applications
University of Milano Bicocca
via Cozzi, 53, Italy
giovanni.ortenzi@unimib.it

In this talk we introduce the notion of Hamiltonian motion of algebraic curves [1]. This motion generates a deformation of the algebraic curve which is an interesting subclass of coisotropic deformations of algebraic varieties [2]. Such Hamiltonian deformations are related, in a large number of cases, to the integrability of suitable PDE systems. As an example we present the case of the elliptic curves and the relations with the motion of an inviscid vortex filament.

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GENERAL LINEAR NYSTRÖM METHODS

R. D'Ambrosio, E. Esposito, and **B. Paternoster**
Dipartimento di Matematica
University of Salerno
via ponte don Melillo, 84084 Fisciano, Italy
beapat@unisa.it

In this talk we describe the family of General Linear Nyström methods (GLNs), which provides the extension of the family of General Linear Methods for the numerical solution of first order Ordinary Differential Equations (ODEs) [1, 2] to special second order ODEs. The family of GLNs properly includes all the classical methods already considered in the literature for $y'' = f(x,y)$, such as linear multistep methods, Runge-Kutta-Nyström methods, two-step hybrid methods and two-step Runge-Kutta-Nyström methods as special cases. The family of methods we aim to consider is wider and more general with respect to the ones already considered in the literature: in fact, our new methods depend on more parameters which can be exploited, for instance, in order to provide a better balance between order of convergence and stability properties. At the same time, the theory of GLNs allows to provide an unifying approach for the analysis of the properties of convergence, consistency and stability. We present the re-formulation of the classical methods according to the new approach and the main results regarding consistency, zero-stability, convergence, order conditions and linear stability theory. Using GLNs theory, new examples of numerical methods for second order ODEs are introduced and discussed. The approach we will use is the natural extension of the General Linear Methods theory developed for first order ODEs [1, 2].

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NUMERICAL METHODS FOR NONLINEAR TWO-PARAMETER EIGENVALUE PROBLEMS

B. Plestenjak
Department of Mathematics
University of Ljubljana / IMFM
Jadranska 19, Slovenia
bor.plestenjak@fmf.uni-lj.si

In a nonlinear two-parameter eigenvalue problem (NMEP) we are searching for a pair (λ, μ) and nonzero vectors x_1, x_2, such that

$$\begin{aligned} F_1(\lambda,\mu)x_1 &= 0, \\ F_2(\lambda,\mu)x_2 &= 0, \end{aligned}$$

where $F_i : \mathbb{C}^2 \to \mathbb{C}^{n_i \times n_i}$ is a nonlinear operator for $i = 1,2$. In such case (λ, μ) is an eigenvalue and $x_1 \otimes x_2$ is the corresponding eigenvector. We assume that the problem is regular, i.e., $\det(F_i(\lambda,\mu)) \not\equiv 0$ for $i = 1,2$.

NMEP can be viewed as a generalization of the nonlinear eigenvalue problem (NEP) as well as a generalization of the algebraic two-parameter eigenvalue problem (MEP) of the form

$$\begin{aligned} (A_1 + \lambda B_1 + \mu C_1)x_1 &= 0, \\ (A_2 + \lambda B_2 + \mu C_2)x_2 &= 0, \end{aligned}$$

where A_i, B_i, C_i are $n_i \times n_i$ complex matrices. We will show that many numerical methods and theoretical results for NEP and MEP can be generalized to NMEP.

An example of a NMEP is a quadratic two-parameter eigenvalue problem (QMEP) which appears in the study of linear time-delay systems for the single delay case.

RESTARTED RATIONAL KRYLOV APPROXIMATIONS TO MATRIX FUNCTIONS

I. Moret and **M. Popolizio**
Department of Mathematics
University of Salento
Lecce, Italy
marina.popolizio@unisalento.it

Matrix functions are of great importance in lots of applications. This work deals with the numerical approximation of the action of matrix functions frequently occurring in the numerical solution of real life models. This issue is faced by means of rational Krylov methods and, for a wide class of matrices, error estimates are developed. In order to enhance the performance an adaptively restarted version is also proposed.
Numerical experiments related to important applications are presented to validate the theoretical results and to better explain the implementation aspects.

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RATIONAL GAUSS QUADRATURE

M. S. Pranić and L. Reichel
Department of Mathematics and Informatics
University of Banja Luka
M. Stojanovića 2, Banja Luka, Bosnia and Herzegovina
pranic77m@yahoo.com

We present three types of reccurence relations for orthogonal rational functions with arbitrary real and/or complex conjugate poles and their application to rational Gauss quadrature formulae. A matrix which has the same role for computation of rational Gauss quadrature as Jacobi matrix does for classical Gauss quadrature is now septadiagonal matrix (or pentadiagonal if we do not have complex poles) with 5×5 and/or 3×3 blocks along a diagonal.

LOCAL BASES FOR QUADRATIC DEFICIENT SPLINE SPACES ON CRISS-CROSS TRIANGULATIONS

C. Dagnino, P. Lamberti, and **S. Remogna**
Department of Mathematics
University of Torino
via C. Alberto 10, 10123 Torino, Italy
sara.remogna@unito.it

In many practical applications, piecewise polynomial surfaces need to be connected by using different smoothness degrees and, in the literature, tensor product spline surfaces of such a kind have been widely investigated. Several problems can arise with tensor product surfaces, for example this choice may cause oscillations far from the shape to be built. Therefore, in some cases spline surfaces of total degree are preferable (see e.g. [1, 2]).

In [2], the authors presented the idea of quadratic spline spaces $\mathcal{S}_2^{\mu}(\mathcal{T}_{mn})$ with smoothness $\mu = 0, 1$, on criss-cross triangulations $\mathcal{T}_{mn}$ of a rectangular domain, in order to construct NURBS surfaces. In this paper we continue the investigation of such spaces, introducing also the jump case, i.e. $\mu = -1$, with particular reference to the computation of their dimension and the construction and analysis of their local bases. Finally, we propose a computational procedure to construct such bases and we give some applications.

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A TAU METHOD FOR NONLINEAR DYNAMICAL SYSTEMS

M. J. Rodrigues and J. Matos
Faculdade de Ciências, Centro de Matemática
Universidade do Porto, Portugal
mjsrodri@fc.up.pt

Originally, the Tau method proposed by Lanczos was developed to approximate the solution of a linear ordinary differential equation. The operational version of the method, as in other methods of weighted residuals, or in other spectral methods, is based on solving a system of linear algebraic equations, obtained by imposing certain conditions for the minimization of the residual.

The generalization of the Tau method for solving nonlinear differential equations usually involves some kind of linearization of the problem and the subsequent use of the method's version for linear problems. In this work we propose an alternative technique by associating a nonlinear algebraic system to the nonlinear differential problem. We show that this system can be rearranged in order to allow resolution using forward substitution, and so avoiding the linearization of the given problem.

We present the application of an adaptive step by step version of this alternative nonlinear Tau method to several nonlinear dynamical systems problems, including to the Lorenz equations where we verify that the method is sufficiently stable to recover the known attractor.

STRATEGIES FOR SPECTRUM SLICING BASED ON RESTARTED LANCZOS METHODS

C. Campos, **J. E. Roman**
Instituto I3M
Universitat Politècnica de València
Camí de Vera s/n, 46022 València, Spain
jroman@dsic.upv.es

In the context of symmetric-definite generalized eigenvalue problems, $Ax = \lambda Bx$, it is often required to compute all eigenvalues contained in a prescribed interval. Research in this topic culminated with the paper by Grimes *et al.* [1], where a robust and efficient procedure is proposed. This technique, usually referred to as spectrum slicing, combines several ingredients: (1) unrestarted block Lanczos method with B-orthogonalization, (2) shift-and-invert spectral transformation, *i.e.*, to solve $(A - \sigma B)^{-1}Bx = \theta x$ for a given shift σ, (3) dynamic shift selection, and (4) use of inertia information to determine the number of eigenvalues in a given subinterval. Nowadays, robust Krylov methods are based on restarted variants such as the thick-restart Lanczos method [2]. We propose an updated spectrum slicing methodology that relies on such variants, and explore several strategies for shift selection, locking, enforcement of multiplicity, etc. Our aim is to provide an industrial-strength parallel implementation in SLEPc [3].

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SOLVING NONLINEAR EQUATIONS USING HERMITE INTERPOLATION BY POLYNOMIAL OR RATIONAL SPLINES

P. Sablonnière
INSA & IRMAR
Rennes, France
Paul.Sablonniere@insa-rennes.fr

We describe some new methods for the solution of nonlinear equations in one and two variables based on Hermite interpolation by polynomial or rational splines. In the univariate case, the method is an extension of Newton and secant methods. Numerical tests show that the convergence is cubic.
In the bivariate case, the solution of the system $f = g = 0$ is based on the approximation of functions f and g by convenient quadratic polynomial or rational spline approximants ϕ and ψ, followed by the solution of the system $\phi = \psi = 0$. Numerical examples will illustrate the method.

EQUIVALENCE BETWEEN MODIFIED SYMPLECTIC GRAM-SCHMIDT AND HOUSEHOLDER SR ALGORITHMS

A. Salam
L.M.P.A
Université du Littoral Côte d'Opale
50 rue F. Buisson BP699, F-62228 Calais Cedex, France
salam@lmpa.univ-littoral.fr

The symplectic Gram-Schmidt (SGS) orthogonalization process is a crutial procedure for some important structure-preserving methods in linear algebra. The algorithm perfoms a factorization $A = SR$, where the ordered columns of the matrix S form a symplectic basis of the range of A, and R is J-upper triangular. There exist two versions of SGS, the classical (CSGS) and the modified (MSGS). Both are equivalent in exact arithmetic, but have different numerical behaviors. In this paper, a numerical equivalence is showed between the MSGS algorithm and Householder SR algorithm applied to an embedded matrix obtained from A by adding two blocks of zeros in the middle and the bottom of the matrix A. The latter algorithm is based on transformations which are symplectic and rank-one modification of the identity (symplectic Householder transformations).

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MULTIVARIATE DATA FITTING WITH ERROR CONTROL

A. Cuyt and **O. Salazar Celis**
Department of Mathematics and Computer Science
University of Antwerp
Middelheimlaan 1, 2020 Antwerpen, Belgium
oliver.salazarcelis@ua.ac.be

We show how a newly developed multivariate data fitting technique enables to solve a variety of scientific computing problems in:

- filtering,
- queueing,
- networks,
- metamodelling,
- computational finance,
- computer graphics,
- antenna design,

and more.

We can capture linear as well as nonlinear phenomena because we use a generalized multivariate rational model.

The technique is a refinement of the basic ideas developed in [1] and interpolates interval data. Intervals allow to take the inherent data error in measurements and simulation into consideration, whilst guaranteeing an upper bound on the tolerated range of uncertainty. The latter is the main difference with a least squares technique which does as well as it can, but without respecting an imposed threshold on the approximation error. In applications where industry standards need to be guaranteed, the interval interpolation technique may be a valuable alternative.

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DATA BASED REGULARIZATION FOR DISCRETE ILL-POSED PROBLEMS

T. Huckle and **M. Sedlacek**
Department of Computer Science
Technische Universität München
Boltzmannstr. 3, D-85748 Garching, Germany
sedlacek@in.tum.de

We focus on the solution of discrete ill-posed problems to recover the original information from blurred signals in the presence of Gaussian white noise more accurately. For a certain class of blur operators and signals we develop a diagonal preconditioner to improve the reconstruction quality, both for direct and iterative regularization methods. In this respect, we incorporate the variation of the signal data during the construction of the preconditioner. For general blur operators and signals we present the impact of a piecewise reconstruction using a partitioning approach to improve the quality. Embedding both methods in an outer iteration may yield further improvement of the solution. In connection with iterative regularization methods we modify the stopping criterion and investigate two approaches to estimate the optimal number of iterations. Reconstructions of discrete ill-posed model problems, arising both from realistic applications and examples generated on our own, demonstrate the effect of the presented approaches. Regarding the stopping criteria, we provide comparison to standard tools known from literature which we moderatly adjust for certain problems.

KOGBETLIANTZ–LIKE METHOD FOR HYPERBOLIC SVD

S. Singer and V. Novaković
Faculty of Mechanical Engineering and Naval Architecture
University of Zagreb
Ivana Lučića 5, 10000 Zagreb, Croatia
ssinger@fsb.hr,venovako@fsb.hr

It is well–known that the hyperbolic Jacobi-like algorithm is an accurate algorithm for computation of the eigendecomposition of symmetric, but indefinite matrices. The first phase of the algorithm is the symmetric indefinite factorization, followed by the one-sided hyperbolic Jacobi-like orthogonalization of a matrix factor. The second phase could be replaced by the Kolgetliantz–like hyperbolic singular value decomposition (HSVD) of a matrix factor. In this talk we will present this algorithm, and compare it with the already known Jacobi HSVD algorithm.

POLYNOMIAL APPROXIMATION VIA DISCRETE DE LA VALLEE POUSSIN MEANS

W. Themistoclakis
CNR National Research Council
IAC Institute for Computational Applications "Mauro Picone"
via P. Castellino, 111, 80131 Naples, Italy
wt@na.iac.cnr.it

We deal with some polynomial quasi–projections defined starting from certain means of Fourier partial sums corresponding to a given system of orthogonal polynomial. In particular we discuss some applications to the weighted–L^1 polynomial approximation problem. The results we show are interesting in the case of non–smooth L^1 functions.

COMPARISON AMONG MULTIRESOLUTION SCHEMES WITH AND WITHOUT ERROR CONTROL STRATEGIES.

S. Amat, B. María Dolores, and **J. C. Trillo**
Department of Applied Mathematics and Statistics
Universidad Politécnica de Cartagena, Spain
jctrillo@upct.es

Multiresolution representations of data are widely used nowadays in several applications. Nonlinear methods are appropriate to deal with data containing singularities. The stability of nonlinear schemes is usually difficult to check. Thus, one can make use of error control algorithms to ensure it. Other approaches to study the stability of multiresolution schemes are studied in [2] and [1]. In [2] the authors compare Harten error control algorithms ([3]) with the syncronization strategy proposed by Sweldens ([4]). In [1] another possible modification of the Harten error control algorithms is proposed. In this work we analyze the advantages and disadvantages of the different approaches to control the error in comparison with the application of the schemes without any error control strategy.

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ADAPTIVE FILON METHODS FOR THE COMPUTATION OF HIGHLY OSCILLATORY INTEGRALS

V. Ledoux and **M. Van Daele**
Department of Applied Mathematics and Computer Science
Ghent University
Krijgslaan 281 - Building S9, B9000 Gent, Belgium
Marnix.VanDaele@ugent.be

First we revisit some important families of quadrature methods (Filon type methods and exponentially fitted methods) for highly oscillatory integrals, all sharing the remarkable property that their accuracy drastically improves as the frequency grows and we apply these methods to integrals of the form $\int_0^h f(x)e^{\mathrm{i}\omega x}dx, \omega > 0$. We also show that, for this type of problem, the methods are strongly related.

The EF rules depend upon frequency dependent nodes that start off at the Gauss nodes when the frequency is zero and end up at the Lobatto nodes when the frequency tends to infinity. This makes the rules well suited for small and very large frequencies. However, for a particular frequency of moderate size, the computation of the nodes is expensive (due to ill-conditioning and iteration).

On the other side, the Filon-type rules with (fixed, i.e. frequency independent) Lobatto nodes behave very well for large frequencies, but not so good for smaller frequencies, because Lobatto-type methods are of lower classical order than Gauss-type methods.

What we propose in this talk is a new type of quadrature rules with frequency dependent nodes, for which the evaluation for a particular value of the frequency is cheap, and which is suited for small as well as large frequencies. The ill-conditioning and the need for iteration is removed by the introduction of some S-shaped functions.

Finally a technique is proposed that can be used to produce accurate error estimates, allowing a successful practical implementation of the quadrature rules discussed.

ADAPTIVE, HIGH-ORDER METHODS TO PRICE OPTIONS

L. von Sydow
Department of Information Technology
Uppsala University
Box 337, 751 05, Uppsala, Sweden
lina@it.uu.se

We will present numerical option pricing with the use of finite differences. For option pricing problems where the option depends on several underlying assets (eg stocks) a high-dimensional PDE has to be solved. Due to this high-dimensionality standard methods will suffer from the "curse of dimensionality". To mitigate this curse we use adaptive techniques based on estimates of truncation errors. Hence, we place grid-points where they are most needed for accuracy reasons. In some cases we combine the adaptivity with high-order methods. We will show examples from both European options as well as options of American type. The latter type of options can be exercised at any time prior to the expiration date leading to an open boundary problem.

The whole procedure from discretization to the numerical solution of the linear system of equations that has to be solved each time-step will be presented.

SERIES ACCELERATION THROUGH PRECISE REMAINDER ASYMPTOTICS

J. L. Willis
Department of Physics
Abilene Christian University
Box 27963, Abilene, TX 79699
USA
josh.willis@acu.edu

Many modern series acceleration methods are built around an input of a sequence $\{s_n\}$ of partial sums of the series, and a remainder estimate ρ_n; they then proceed by extrapolating from the s_n and ρ_n a limit or antilimit of the sequence, based on the corrections to the remainder estimate assumed by the particular acceleration method. Generally, the remainder estimates are quite simple, at best correct to leading order, because precise forms for the remainders are usually not known. In this talk we show that whenever an asymptotic expansion for the ratio of the *terms* of the series is known in inverse powers of n, we can derive an asymptotic expansion $\rho_n \sim \omega_n \sum_k c_k/n^k$. Here the leading term ω_n may contain a power or factorial in n and can be determined analytically, but more importantly the asymptotic coefficients c_k can be explicitly computed to any desired order from the asymptotic expansion of the term ratio. We outline the derivation of this method and the circumstances under which it either accelerates the convergence or improves the divergence of an analytic series, and we give several examples of its application: to generalized hypergeometric functions, zeta functions, and some slowly convergent Fourier series. We thereby extend the results of [1], which considered only generalized hypergeometric series ${}_{q+1}F_q$.

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APPROXIMATE GREATEST COMMON DIVISORS OF BERNSTEIN POLYNOMIALS

N. Yang and **J. Winkler**
Department of Computer Science
The University of Sheffield
Regent Court, 211 Portobello, Sheffield S1 4DP, United Kingdom
j.winkler@dcs.shef.ac.uk

This paper considers the computation of the degree of an approximate greatest common divisor (AGCD) of two Bernstein basis polynomials $f(y)$ and $g(y)$. This computation is usually performed either by Euclid's algorithm, or by computing the singular value decomposition of the Sylvester resultant matrix $S(f,g)$, where $f = f(y)$ and $g = g(y)$, and determining the rank loss of this matrix. These methods give, however, poor results when $f(y)$ and $g(y)$ are corrupted by noise, which is the situation encountered in practical problems.

Two new methods for the computation of the degree of an AGCD of the inexact polynomials $f(y)$ and $g(y)$ are described, and computational results are presented when the greatest common divisor of the theoretically exact forms of $f(y)$ and $g(y)$ is of high degree. It is shown that the polynomials must be preprocessed by three operations before these methods are implemented. One of these preprocessing operations is the normalisation of the coefficients of $f(y)$ and $g(y)$, and it is shown that normalisation by the geometric means of their coefficients is superior to normalising by the 2-norms of their coefficients. The effect of the second preprocessing operation is the destruction of the Bernstein basis, that is, $f(y)$ and $g(y)$ are transformed to another basis. All computations are performed in the new basis, and the results obtained with this new basis are compared with the results obtained when the preprocessing operations are omitted, that is, the computations are performed in the Bernstein basis. It is shown that the inclusion of the preprocessing operations yields a considerable improvement in the computed results with respect to the results obtained when the computations are performed in the Bernstein basis, even when the theoretically exact forms of $f(y)$ and $g(y)$ have roots in the interval $[0,\ldots,1]$. A possible explanation for these improved results is considered.

PARJOINV: HIGH-PERFORMANCE SCIENTIFIC COMPUTING FOR MULTIDIMENSIONAL JOINT INVERSION

A. Giovannini, **G. Zanghirati**
Department of Mathematics
University of Ferrara
via Saragat 1, I-44122 Ferrara, Italy
g.zanghirati@unife.it

This talk deals with the study of a Tikhonov-like approach to the joint inversion of multidimensional data, based on an edge-preserving regularizer (M.D. Zhdanov *et al.*, 2004; E. Haber *et al.*, 1997), and its parallel implementation in an HPC software package. The package is built on top of the well known and widely used high-performance parallel libraries PETSc and TAO. The starting point is a joint work with G. Vignoli. Effective methods and efficient codes for a truly joint inversion have recently received increasing interest, because multiple types of observations of the same object can be used at once in a single procedure to recover an estimate of the object itself via non-invasive inspection (M.D. Jegen *et al.*, 2009; M. Meceira *et al.*, 2008; N. Linde *et al.*, 2008; L.A. Gallardo *et al.*, 2007, 2005; Dell'Aversana, 2007; D. Colombo *et al.*, 2007; G. Vignoli *et al.*, 2005). Indeed, jointly inverting different kind of data could allow to reduce both the ill-posedness of the data reconstruction problem and the total number of data to be collected, while still preserving the accuracy of the results. This is relevant to a large number of research and industrial fields such as Biology, Geophysics, Medicine and many others. Unfortunately, the study and the coding are more difficult than in the classical inversion. We discuss the current development of the software, which can use both first- and second-order methods to solve the underlying optimization problem. Finally, we report the preliminary results of a numerical experimentation that shows its potential for large-scale real-world applications.

Poster Session

ON THE REGULARIZATION OF GALERKIN BEM HYPERSINGULAR BILINEAR FORMS

A. Aimi, M. Diligenti, C. Guardasoni, and S. Panizzi
Department of Mathematics
University of Parma
Parco Area delle Scienze, 53/A, 43124 Parma, Italy
alessandra.aimi@unipr.it

We will discuss about the definition and regularization of bilinear forms related to Galerkin Boundary Element Methods for elliptic and hyperbolic problems, which involve double integrals with hypersingular kernels in space variables.
At first, starting from the classical definition of Hadamard Finite Part Integral, various characterizations of this type of integrals in one and two dimensions will be given, extending those recently presented in [2]. These characterizations are used to give a meaning to the so-called hypersingular bilinear form arising in the weak formulation of elliptic and hyperbolic problems with Neumann boundary conditions, rewritten in terms of hypersingular Boundary Integral Equations.
A unifying view of different regularization technique used in this context by mathematicians and engineers (see e.g. [3, 1]) will be given.

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APPROXIMATE INVERSION OF COMPLEX TRIANGULAR TOEPLITZ MATRICES

S. Belhaj
Department of Quantitative Methods
University of Jendouba
FSJEGJ, Tunisia
skander_belhaj@yahoo.fr

Let

$$T_n = lT_n\left[t_0, t_1, \ldots, t_{n-1}\right]$$

be a nonsingular lower triangular Toeplitz matrix with complex coefficients from the ring of $n \times n$ matrices over a field. The special structure of triangular Toeplitz matrices arise in a number of applications in scientific computing, signal and image processing. In this paper we consider the problem of a triangular Toeplitz matrice inversion. Explicitly, we propose an approximate algorithm of a $n \times n$ complex triangular Toeplitz matrice by using trigonometric polynomial interpolation [2, 4, 3] via two FFTs, one fast cosine transform (DCT) and one fast sine transform (DST) of $2n$-vectors. Moreover, our method can be used to improve the complexity of the approximate block diagonalization algorithm for complex Hankel matrices introduced in [1].

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NUMERICAL INTEGRATION ON SCATTERED DATA BY LOBACHEVSKY SPLINES

G. Allasia, **R. Cavoretto**, and A. De Rossi
Department of Mathematics
University of Turin
Via Carlo Alberto 10, 10123 Turin, Italy
roberto.cavoretto@unito.it

In this paper we investigate the problem of numerical integration on scattered data by a class of spline functions, called *Lobachevsky splines*. Thus, starting from the interpolation results given in [1, 2], we focus on the construction of new cubature formulas. The use of Lobachevsky splines takes advantages of their feature of being expressible in the multivariate setting as a product of univariate functions. Numerical results using Lobachevsky splines turn out to be interesting and promising, for both good accuracy and simplicity in computation. Finally, a comparison with radial basis functions (RBFs) [3, 4] confirms the goodness of the proposed approach.

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REGULARIZATION TECHNIQUES FOR GROUND CONDUCTIVITY DATA INVERSION

C. Fenu and G. Rodriguez
Department of Mathematics and Computer Science
University of Cagliari
Italy
kate.fenu@gmail.com

Electromagnetic induction measurements are often used for non-destructive investigation of soil properties, like the electrical conductivity and the magnetic permeability. Inversion of electromagnetic data allows one to theoretically determine the electromagnetic parameters of the subsurface, and so to ascertain the presence of particular substances and to identify their spatial position. These data are often measured by a ground conductivity meter, and two models can be found in the literature to describe its behaviour: a nonlinear model, arising from Maxwell equations, and a linear one, that may be used under suitable assumptions. The inverse problem is severely ill-conditioned in both cases, so regularization is needed. We computed the solution of the linear model by TSVD and Tikhonov regularization, whereas in the case of nonlinear model a Tikhonov-Newton methods has been implemented. Both the models will be described and we will present the results of numerical experiments in realistic applicative settings, for which experimental data are available.

AN IMPLICIT TIME DOMAIN MESHLESS FORMULATION FOR MAXWELL'S PDES

G. Ala and **E. Francomano**
DIEET, DICGIM
Università degli Studi di Palermo
viale delle Scienze, 90128 Palermo, Italy
e.francomano@unipa.it

A meshless particle approach based on an unconditionally stable time-domain method devoted to electromagnetic transient simulations, is presented. Maxwell's PDEs are solved by using a set of particles, arbitrarily placed in the problem domain [1]. An heavy limit in applying meshless formulation is usually in making use of an explicit finite difference scheme accounted for time stepping. In fact, as well as in the time domain grid schemes, the CFL-like relations strongly condition the performance of the numerical algorithm. In this paper, the meshless particle method is approached with an unconditionally stable time stepping scheme. A leapfrog alternating directions implicit finite difference algorithm [2] is taken into account. The computational tool is assessed and simulation results are discussed in order to validate the proposed approach.

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MICROWAVE RADIOMETRY PRODUCT GENERATION

F. Lenti, M. Migliaccio, F. Nunziata, and G. Rodriguez
Dipartimento per le Tecnologie
Università degli Studi di Napoli "Parthenope"
Napoli, Italy
flavialenti@libero.it

Microwave radiometers, such as the special sensor microwave imaged SSM/I, play a fundamental role in several remote sensing applications. A dense spatial and temporal coverage represents radiometers peculiarity to perform operational earth observation monitoring. Ocean surface wind speed, rain rate, integrated water vapor maps are routinely generated exploiting various radiometer channels. In order to apply such models we need to have measurements of the same resolution scale.

Unfortunately, due to the different electrical size of the antenna at different wavelengths, it is unavoidable that the channels are characterized by different spatial resolution. The preferred approach is to enhance the low resolution measurements up to that of the high resolution. The optimal methods to increase spatial resolution rely on an overlap of the adjacent antenna measurements gain functions. This information redundancy enables the resolution enhancement retrieval.

Mathematically, it is a linear inversion problem. The matrix which describes the model and depends on antenna gain, is undetermined and ill-conditioned. The system inversion causes noise amplification. Proper regularization techniques take into control noise amplification when the inversion is done.

Here, an inversion technique based on TSVD method for the 2-D case is described. The antenna gain is assumed separable (D.G. Long private communication). This inversion method is very attractive in terms of computational efficiency since the expansion coefficients depend only on the system configuration and not on measurements.

The study is conducted using synthetic microwave radiometer measurements. Radiometric measurements are simulated considering an hypothetical ideal sensor with a linear scanning configuration as the SSM/I.

MARKOV'S THEOREM AND PERTURBED RECURRENCE RELATIONS

E. Leopold
USTV (Phymat)
B.P.132 -83957 La Garde Cedex, France
and
CNRS (C.P.T)
Luminy, case 907, 13288 Marseille cedex 9, France
Leopold.E@free.fr

Let $j \geq 0$ be a fixed integer , $\{a_k\}_k$, $\{b_k\}_k$ be real sequences with $\forall k, b_k > 0$ and $N_{-1}(j,z) \equiv 0,\ N_0(j,z) \equiv 1,$

$$\forall k \geq 0,\ N_{k+1}(j,z) = (z - a_{k+j})N_k(j,z) - b_{k+j}N_{k-1}(j,z) \tag{1}$$

then we have the following classical result:

Theorem (Markov) If the sequence $\{a_k\}_k$ and $\{b_k\}_k$ are bounded then there exits an unique positive measure ν and a compact set $supp(\nu)$ in $\mathbf{R}$ such that

$$\forall z \in \mathbf{C} - supp(\nu) \quad \lim_{k\to\infty} \frac{N_{k-1}(1,z)}{N_k(z)} = c \int_{supp(\nu)} \frac{d\nu(x)}{z-x}$$

and this convergence is uniform on every compact subset of the complex plane that does not intersect $supp(\nu)$.
It is well known that the above result plays a fundamental role in the study of orthogonal polynomials, in the asymptotic behaviour of certain continous fractions and in many other types of numerical applications. Here, we give some new results about this Theorem when recurrence relation (1) is perturbed as well as its order. This work is the sequel of the paper [1].

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ERROR BOUNDS OF GAUSS-TYPE QUADRATURES WITH BERNSTEIN-SZEGŐ WEIGHTS

A. V. Pejčev and M. M. Spalević
Department of Mathematics
University of Beograd
Faculty of Mechanical Engineering
Kraljice Marije 16, 11120 Belgrade 35, Serbia
apejcev@mas.bg.ac.rs

The kernels $K_n(z) = K_n(z, w)$ in the remainder terms $R_n(f)$ of the Gauss-type quadrature formulas

$$\int_{-1}^{1} f(t)w(t)\,dt = G_n[f] + R_n(f), \quad G_n[f] = \sum_{\nu=1}^{n} \lambda_\nu f(\tau_\nu) \quad (n \in \mathbf{N})$$

for analytic functions inside elliptical contours $\mathcal{E}_\rho$ with foci at ∓ 1 and the sum of semi-axes $\rho > 1$, where w is a nonnegative and integrable weight function of Bernstein-Szegő type, are studied. The derivation of effective bounds for $|R_n(f)|$ is possible if good estimates for $\max_{z\in\mathcal{E}_\rho} |K_n(z)|$ are available, especially if we know the location of the extremal point $\eta \in \mathcal{E}_\rho$ at which $|K_n|$ attains its maximum. In such a case, instead of looking for upper bounds for $\max_{z\in\mathcal{E}_\rho} |K_n(z)|$ one can simply try to calculate $|K_n(\eta, w)|$. In the case under consideration the location on the elliptic contours where the modulus of the kernel attains its maximum value is investigated. This leads to effective bounds for $|R_n(f)|$.

MODELLING OF RING RESONATORS WITH MAGNETO-OPTIC MATERIALS USING THE FINITE ELEMENT METHOD

P. Pintus and F. Di Pasquale
Scuola Superiore Sant'Anna,
via Moruzzi 1, 56124 Pisa, Italy
paolo.pintus@sssup.it

In this work we consider the problem of the modal analysis for ring resonators realized with magneto-optic materials [1]. Considering the lossless case (including no radiation loss), we have implemented the finite element method in a cylindrical coordinate systems using the node-based formulation with second order shape functions. The penalty function [2] have been introduced to move out the spurious solutions and the final quadratic eigenvalue problem have been solved using the krylov method.

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GEOMETRIC DESIGN OF A DAM BY VARIATIONAL SPLINE APPROXIMATION

A. H. Delgado, M. Pasadas and **M. L. Rodríguez**
Department of Applied Mathematics
University of Granada
E.T.S. Civil Engeniering of Granada, Spain
miguelrg@ugr.es

Our aim is to study how to combine conditions of interpolation and approxima- tion in order to generate a surface. Our method is developed from a variational approach. As an application of the use of the proposed methodology, we have designed the walls (surfaces) of a dam with all the geometric calculations and their computerized processing.

TIKHONOV REGULARIZATION AND MATRIX FUNCTION EVALUATION

P. Novati and **M. R. Russo**
Department of Pure and Applied Mathematics
University of Padova
Via Trieste 63, 35121 Padova. Italy
mrrusso@math.unipd.it

We present a novel approach for solving ill-conditioned linear systems $Ax = b$ based on the computation of matrix functions. Starting from the Tikhonov regularized solution

$$x_\lambda = \arg\min_x \left(\|Ax - b\| + \lambda \|Hx\| \right)$$

where $\lambda > 0$ and H is the regularization matrix, we consider the relationship between x_λ and the exact solution of the system, that can be stated in terms of a suitable matrix function times a vector. We employ the standard Arnoldi method to compute this operation. The arising Krylov method seems to be competitive with the most powerful iterative solvers in terms of speed and accuracy, and the dependence on the regularization parameter λ is heavily reduced.

Numerical experiments on classical test problems and image restoration are presented.

DARK-DARK AND DARK-BRIGHT SOLITON INTERACTIONS IN THE TWO-COMPONENT DEFOCUSING NONLINEAR SCHRÖDINGER EQUATION

T. Klotz, G. Dean, B. Prinari and **F. Vitale**
Dip. di Fisica & Sezione INFN
University of Salento
Lecce, Italy
federica.vitale@le.infn.it

The subject of our investigation is the 2-component nonlinear Schrödinger equation in the normal dispersion regime (defocusing VNLS). Our research builds upon previous results [1, 2] where the Inverse Scattering Transform (IST) was developed to solve the initial value problem for VNLS under nonvanishing boundary conditions. We use the IST machinery to construct multisoliton solutions to the equation. Such solutions include dark-dark solitons, which have dark solitonic behavior in both components, as well as dark-bright soliton solutions, which have one dark and one bright component. In particular, we present the explicit expressions of one and two soliton solutions for all possible cases: two dark-dark solitons, two dark-bright solitons, and one dark-dark and one dark-bright soliton. We then compute the long-time asymptotic behavior of these solutions before and after any interactions and obtain the phase shifts associated to the interactions.

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Index of speakers

	09:00	09:30	10:00	10:30	11:00	11:30	12:00	12:30	13:00	16:00	16:30	17:00	17:30	18:00	18:30	19:00
Monday	opening	P. Ciarlet		S4.2	Coffee break	S4.7	S4.6	S4.4	Lunch	S4.8	S4.9	S4.3	Coffee break	S4.5	S4.1	
				S5.2		S5.8	S5.6	S5.7		S11.1	S11.5	S11.7		G47	G39	G29
				S7.4		S7.5	S7.6	S7.9		S7.1	S7.2	S7.3		S7.7	S7.8	
				G63		G67	G37	G68		G58	G3	G23		G52	G16	G7
Tuesday	M. Ablowitz		S10.7	S10.3		S10.9	S10.8	S10.5		S5.5	S5.4	S5.9		S5.3	S5.10	S5.1
			S9.6	S9.7		S9.10	S9.4	S9.5		S9.1	S9.2	S9.8		S9.9	S9.3	G44
			S6.1	S6.8		S6.3	S6.9	S6.5		G22	G38	G26		G10	G13	G62
			S11.2	S11.4		S11.3	S11.6	G66		G4	G6	G11		G30	G48	G64
Wednesday	M. Benzi		S3.1	S3.9		S3.3	S3.6	S3.7		Excursion						
			S1.9	S1.2		S1.7	S1.1	S1.5								
			S8.1	S8.3		S8.4	S8.6	S8.8								
			G18	G45		G54	G57	G59								
Thursday	L. Reichel		S10.2	S10.4		S10.1	S10.6	G46		G8	G20	G56		Poster session		
			S2.8	S2.1		S2.2	S2.5	S2.3		S2.4	S2.6	S2.7				
			S6.6	S6.7		S6.2	S6.4			G2	G5	G50				
			S1.3	S1.4		S1.6	S1.8	G27		G9	G42	G53		G49	G21	G31
Friday	D. Bessis		S3.5	S3.10		S3.8	S3.2	S3.4		G41	G12	G14				
			G1	G40		G24	G34	G25		G51	G60	G61				
			S8.7	S8.5		S8.2	S8.10	S8.9		G15	G55	G33				
			G17	G32		G35	G43	G65		G19	G28	G36				