Professor Dr. Theodore E. Simos, Academician

List of Publications

1/10/2016

Research Papers

A. DOCTORAL DISSERTATION

D1. Theodore E. Simos, Numerical Solution Of Ordinary Differential Equations with Periodical Solution, Doctoral Dissertation, National Technical University Of Athens, 1990.

B. REVIEW PAPERS - MONOGRAPHS

R1. T.E. Simos and P.S. Williams, On finite difference methods for the solution of the Schrödinger equation, *Computers & Chemistry,* 23, 513-554(1999).

R2. J. Vigo-Aguiar and T.E. Simos, Review of multistep methods for the numerical solution of the radial Schrödinger equation, INT J QUANTUM CHEM 103 (3): 278-290 JUN 5 2005

R3. T.E. Simos, Atomic Structure Computations in **Chemical Modelling: Applications and Theory**, **Vol 1** *(Editor: A. Hinchliffe, UMIST)*, pp. 38-142, The Royal Society of Chemistry, 2000. **(after invitation)**.

R4. T.E. Simos, Numerical Methods for 1D, 2D and 3D Differential Equatrions Arising in Chemical Problems in **Chemical Modelling: Applications and Theory, Vol 2** *(Editor: A. Hinchliffe, UMIST)*, pp. 170-270, The Royal Society of Chemistry, 2002. **(after invitation)**.

R5 T.E. Simos, Numerical Methods in Chemistry in **Chemical Modelling: Applications and Theory, Vol 3** *(Editor: A. Hinchliffe, UMIST)*, pp. 271-378, The Royal Society of Chemistry, 2004. **(after invitation)**.

R6 T.E. Simos, Numerical Methods in Chemistry in **Chemical Modelling: Applications and Theory, Vol 4** *(Editor: A. Hinchliffe, The University of Manchester)*, pp. 161-244, The Royal Society of Chemistry, 2006. **(after invitation)**.

R7 T.E. Simos, Numerical Methods in Chemistry in **Chemical Modelling: Applications and Theory, Vol 5** *(Editor: A. Hinchliffe, The University of Manchester)*, in press, The Royal Society of Chemistry, 2008. **(after invitation)**.

R8 T.E. Simos, Numerical Methods in Chemistry in **Chemical Modelling: Applications and Theory, Vol 6** *(Editor: Michael Springborg, Universitaet des Saarlandes)*, in press, The Royal Society of Chemistry, pp. 210-509, 2009. **(after invitation)**.

R9. Z.A. Anastassi and T.E. Simos, Numerical Methods for the Efficient Solution of Problems in Quantum Mechanics, **Physics Reports**, **482-483**, 1-240(2009).

R10. T.E. Simos, Numerical Methods in Chemistry in **Chemical Modelling: Applications and Theory, Vol 7** *(Editor: Michael Springborg, Universitaet des Saarlandes)*, The Royal Society of Chemistry, 2010, pp. 261-338, 2010, **(after invitation)**.

R11. Z. Kalogiratou, Th. Monovasilis, G. Psihoyios, T.E. Simos, Runge–Kutta type methods with special properties for the numerical integration of ordinary differential equations, Physics Reports, Volume: 536 Issue: 3 Pages: 75-146 Published: MAR 20 2014

C. PAPERS AND TECHNICAL REPORTS

P1. G. Papageorgiou, T. Kalvouridis and Th. Simos: An application of the scaled Runge-Kutta algorithms to some problems of celestial mechanics, Astrophysics and Space Science 137, 129-138(1987).

P2. T. Kalvouridis, G. Papageorgiou and Th. Simos: A comparison of numerical integration methods in the equatorial magnetic-binary problem, Astrophysics and Space Science 139, 21-35(1987).

P3. G. Papageorgiou, Th. Simos and Ch. Tsitouras: Some new Runge-Kutta methods with interpolation properties and their application to the magnetic-binary problem, Celestial Mechanics 44, 167-177(1988).

P4. Th. Simos, T. Kalvouridis and G. Papageorgiou: Application of high order Runge-Kutta methods in the magnetic-binary problem, Astrophysics and Space Science 147, 271-285(1988).

P5. T. Kalvouridis, G. Papageorgiou and Th. Simos: On the integration of the magnetic-binary problem by Explicit-Runge-Kutta methods, Technical Report 1/1988, Department of Mathematics, National Technical University of Athens.

P6. C.D. Papageorgiou, A.D. Raptis and T.E. Simos: An algorithm for the solution of the eigenvalue Schrödinger equation, Journal of Computational Physics, 88, 477-483(1990).

P7. C.D. Papageorgiou, A.D. Raptis and T.E. Simos: A method for computing phase shifts for scattering, Journal of Computational and Applied Mathematics, 29, 61-67(1990).

P8. J.R. Cash, A.D. Raptis and T.E. Simos: A fortran program for the numerical integration of the one-dimensional Schrödinger equation using exponential and Bessel fitting methods, Computer Physics Communications 56, 391-407(1990).

P9. T.E. Simos: A four-step method for the numerical solution of the Schrödinger equation, Journal of Computational and Applied Mathematics, 30, 251-255(1990).

P10. J.R. Cash, A.D. Raptis and T.E. Simos: A sixth order exponentially-fitted method for the numerical solution of the radial Schrödinger equation, Journal of Computational Physics 91, 413-423(1990).

P11. T.E. Simos and A.D. Raptis: Numerov-type methods with minimal phase-lag for the numerical integration of the one-dimensional Schrödinger equation, Computing, 45, 175-181(1990).

P12. T.E. Simos: A two-step method with phase-lag of order infinity for the numerical integration of second order periodic initial-value problems, International Journal of Computer Mathematics, 39, 135-140(1991).

P13. T.E. Simos: Some new four-step exponential fitting methods for the numerical solution of the radial Schrödinger equation, IMA Journal of Numerical Analysis, 11, 347-356(1991).

P14. A.C. Allison, A.D. Raptis and T.E. Simos: An eighth order formula for the numerical integration of the one-dimensional Schrödinger equation, Journal of Computational Physics, 97, 240-248(1991).

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P23. T.E. Simos: High - order methods with minimal phase-lag for the numerical integration of the special second order initial value problem and their application to the one-dimensional Schrödinger equation, Computer Physics Communications, 74, 63-66(1993).

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