Weiße, Andrea Y.; **Huisinga, Wilhelm**

Error-controlled global sensitivity analysis of ordinary differential equations. (English)

Zbl 1252.65017
J. Comput. Phys. 230, No. 17, 6824-6842 (2011).

Summary: We propose a novel strategy for global sensitivity analysis of ordinary differential equations. It is based on an error-controlled solution of the partial differential equation (PDE) that describes the evolution of the probability density function associated with the input uncertainty/variability. The density yields a more accurate estimate of the output uncertainty/variability, where not only some observables (such as mean and variance), but, also, structural properties (e.g., skewness, heavy tails, bi-modality) can be resolved up to a selected accuracy.

For the adaptive solution of the PDE Cauchy problem, we use the Rothe method with multiplicative error correction, which was originally developed for the solution of parabolic PDEs. We show that, unlike in parabolic problems, conservation properties necessitate a coupling of temporal and spatial accuracy to avoid accumulation of spatial approximation errors over time. We provide convergence conditions for the numerical scheme and suggest an implementation using approximate approximations for spatial discretization to efficiently resolve the coupling of temporal and spatial accuracy. The performance of the method is studied by means of low-dimensional case studies. The favorable properties of the spatial discretization technique suggest that this may be the starting point for an error-controlled sensitivity analysis in higher dimensions.

MSC:

65C30 Numerical solutions to stochastic differential and integral equations
35R60 PDEs with randomness, stochastic partial differential equations
60H15 Stochastic partial differential equations (aspects of stochastic analysis)
60H35 Computational methods for stochastic equations (aspects of stochastic analysis)
65M20 Method of lines for initial value and initial-boundary value problems involving PDEs
65M15 Error bounds for initial value and initial-boundary value problems involving PDEs

Keywords:

random initial conditions; global sensitivity analysis; Cauchy problem; error control/adaptivity; Rothe method; approximate approximations; numerical examples; convergence

Software:

Matlab

Full Text: DOI

References:

[1] Barton, H.A.; Chiu, W.A.; Setzer, R.W.; Andersen, M.E.; Bailer, A.J.; Bois, F.Y.; DeWoskin, R.S.; Hays, S.; Johanson, G.; Jones, N.; Loizou, G.; MacPhail, R.C.; Portier, C.J.; Spendiff, M.; Tan, Y., Characterizing uncertainty and variability in physiologically based pharmacokinetic models: state of the science and needs for research and implementation, Toxicol. sci., 99, 395-402, (2007)

[2] Blower, S.M.; Dowlatabadi, H., Sensitivity and uncertainty analysis of complex models of disease transmission: an HIV model, as an example, Int. stat. rev., 62, 229-243, (1994) · Zbl 0825.62860

[3] Ingalls, B.P.; Sauro, H.M., Sensitivity analysis of stoichiometric networks: an extension of metabolic control analysis to non-steady state trajectories, J. theor. biol., 222, 23-36, (2003)

[4] Krewski, D.; Wang, Y.; Bartlett, S.; Krishnan, K., Uncertainty, variability, and sensitivity analysis in physiological pharmacokinetic models, J. biopharm. stat., 5, 245-271, (1995) · Zbl 0907.62127

[5] Deuflhard, P.; Bornemann, F.A., Scientific computing with ordinary differential equations, (2002), Springer · Zbl 1001.65071

[6] Hairer, E.; Nørsett, S.; Wanner, G., Solving ordinary differential equations I. nonstiff problems, (1987), Springer Berlin · Zbl 0638.65058

[7] Hammersley, J.M.; Handscomb, D.C., Monte Carlo methods, (1964), Methuen, John Wiley \& Sons London, New York · Zbl 0121.35503

[8] Helton, J.C.; Davis, F.J., Latin hypercube sampling and the propagation of uncertainty in analyses of complex systems, Reliab. eng. syst. saf., 81, 23-69, (2003)

[9] Marino, S.; Hogue, I.B.; Ray, C.J.; Kirschner, D.E., A methodology for performing global uncertainty and sensitivity analysis in systems biology, J. theor. biol., 254, 178-196, (2008) · Zbl 1400.92013

[10] ()

[11] Robert, C.P.; Casella, G., Monte Carlo statistical methods, (2004), Springer New York · Zbl 1096.62003

[12] Fang, S.; Gertner, G.Z.; Shinkareva, S.; Wang, G.; Anderson, A., Improved generalized Fourier amplitude sensitivity test (FAST) for model assessment, Stat. comput., 13, 221-226, (2003)

[13] Hill, W.J.; Hunter, W.G., A review of response surface methodology: a literature survey, Technometrics, 8, 571-590, (1966)

[14] ()

[15] Costanza, V.; Seinfeld, J.H., Stochastic sensitivity analysis in chemical kinetics, J. chem. phys., 74, 3852-3858, (1981)

[16] Rabitz, H.; Kramer, M.; Dacol, D., Sensitivity analysis in chemical kinetics, Ann. rev. phys. chem., 34, 419-461, (1983)

[17] Turányi, T., Sensitivity analysis of complex kinetic systems tools. and applications, J. math. chem., 5, 203-248, (1990)

[18] Grossmann, C.; Roos, H.-G., Numerical treatment of partial differential equations, (2007), Springer Berlin-Heidelberg

[19] Bornemann, F.A., An adaptive multilevel approach to parabolic equations, Impact comput. sci. eng., 3, 93-122, (1991) · Zbl 0735.65066

[20] F.A. Bornemann, An adaptive multilevel approach to parabolic equations in two space dimensions, Ph.D. Thesis, Freie Universität Berlin, 1991.

[21] Kröner, D., Numerical schemes for conservation laws, (1997), Wiley \& Sons Chichester · Zbl 0872.76001

[22] LeVeque, R.J., Finite volume methods for hyperbolic problems, Cambridge texts in applied mathematics, (2004), Cambridge University Press

[23] Horenko, I.; Lorenz, S.; Schütte, C.; Huisinga, W., Adaptive approach for non-linear sensitivity analysis of reaction kinetics, J. comput. chem., 26, 941-948, (2005)

[24] Alspach, D.L.; Sorenson, H.W., Nonlinear Bayesian estimation using Gaussian sum approximations, IEEE T. automat. contr., AC-17, 439-448, (1972) · Zbl 0264.93023

[25] Maz'ya, V.; Schmidt, G., Approximate approximations, (2007), American Mathematical Society · Zbl 1119.41015

[26] Bungartz, H.-J.; Griebel, M., Sparse grids, Acta numer., 13, 147-269, (2004) · Zbl 1122.65405

[27] Zenger, C., Sparse grids, (), 241-251 · Zbl 0763.65091

[28] Fasshauer, G.E., Meshfree approximation methods with MATLAB, (2007), World Scientific Publishing Co. Pte Ltd. · Zbl 1123.65001

[29] Liu, G.R.; Gu, Y.T., An introduction to meshfree methods and their programming, (2005), Springer · Zbl 1109.74371

[30] Arnold, V.I., Ordinary differential equations, (2006), Springer Berlin

[31] Lasota, A.; Mackey, M.C., Chaos, fractals, and noise, stochastic aspects of dynamics, (1994), Springer · Zbl 0784.58005

[32] K. Rektorys, Numerical and theoretical treating of evolution problems by the method of discretization in time, in: M. Zlámal, J. Vosmanský (Eds.), Equadiff 6, Proceedings of the International Conference on Differential Equations and Their Applications, pp. 71-84. · Zbl 0613.65122

[33] Brenner, P.; Thomée, V., On rational approximation of semigroups, SIAM J. numer. anal., 16, 683-694, (1979) · Zbl 0413.41011

[34] Lang, J., Adaptive multilevel solution of nonlinear parabolic PDE systems, (2001), Springer

[35] Maz'ya, V., Approximate approximations, (), 77-104, · Zbl 0827.65083

[36] V. Maz'ya, A new approximation method and its applications to the calculation of volume potentials. Boundary point method, 3. DFG-Kollquium des DFG-Forschungsschwerpunktes "Randelementmethoden", 1991.

[37] Fasshauer, G.E., Toward approximate moving least squares approximation with irregularly spaced centers, Comput. meth. appl. mech. eng., 193, 1231-1243, (2004) · Zbl 1060.65041

[38] Ivanov, T.; Maz'ya, V.; Schmidt, G., Boundary layer approximate approximations and cubature of potentials in domains, Adv. comput. math., 10, 311-342, (1999) · Zbl 0935.65128

[39] Lanzara, F.; Maz'ya, V.; Schmidt, G., Approximate approximations from scattered data, J. approx. theor., 145, 141-170, (2007) · Zbl 1119.41015

[40] A.Y. Weiße, Global sensitivity analysis of ordinary differential equations: adaptive density propagation using approximate approximations, Ph.D. Thesis, Freie Universität Berlin, 2009.

[41] Cornish-Bowden, A., Fundamentals of enzyme kinetics, (2004), Portland Press

[42] Keener, J.; Sneyd, J., Mathematical physiology, (2001), Springer · Zbl 0913.92009