

Yang Cao

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Education University of California, Santa Barbara, Santa Barbara, CA
Ph.D. in Computer Science, March 2003
Dissertation title: "Sensitivity Analysis and Condition Estimation of Computational Models"

Tsinghua University, Beijing, P. R. China
M.S. in Mathematics, June 1998

Tsinghua University, Beijing, P. R. China
B.S. in Mathematics, June 1993

Research Interest Stochastic simulation of biochemical systems

Multiscale algorithms and softwares

Sensitivity and uncertainty analysis, robustness in biological system

Error and condition estimation for computational systems

Numerical methods for ODE/DAE systems

Professional Experience **University of California, Santa Barbara, Santa Barbara, CA (2003-present).** I have been working as a postgraduate researcher in the Department of Computer science associated with Professor Linda Petzold. My research is focused on algorithms and softwares for efficient stochastic simulation of biochemical systems. We studied stiffness in stochastic biochemical simulation, proposed multi-scale simulation algorithms for stochastic simulation, discussed efficient implementation and error measurement of algorithms and developed the software **StochKit**. We applied our software to biochemical models for the study of circadian rhythm, heat shock response of E. Coli and Prokaryotic gene expression.

University of California, Santa Barbara, Santa Barbara, CA (1998-2003)

I worked as a research assistant in the Department of Computer science associated with Professor Linda Petzold. My research was focused on the sensitivity and error analysis of three computational models: linear system, matrix equations, and differential-algebraic systems. We proposed the theory of adjoint sensitivity analysis for differential-algebraic equations and a posteriori error estimation method for general computational model. The adjoint method was implemented in the software DASPK3.0. The a posteriori error estimation method for ODEs has been used by our collaborator from LLNL.

Mentor Graphics, Wilsonville, Oregon (2000), I worked as a software engineer in an intern program. I helped to improve the efficiency and accuracy of MachTA, a circuit simulation software by Mentor Graphics.

Tsinghua University, Beijing, P. R. China (1993-1998), I worked first as a teaching assistant (1993-94), and later as an instructor (1994-97), and then as a lecturer (1997-98) in the department of mathematics. As a TA, I was in charge of the discussion session in the course "Optimization and its Engineering Application". As an instructor and a lecturer, I taught two courses in different semesters: Fortran language and basic numerical analysis (one semester), C language (two semesters and one summer session course). During this time, my research was focused on efficient algorithms for solving differential-algebraic equations.

Software Developed	DASPKAdjoint, the adjoint sensitivity solver for DASPK3.0. StochKit, a stochastic simulation toolkit for chemically reacting systems.
Membership	SIAM
Publications	See attached
References	See attached

List of Publications

Journal Papers

(most papers can be downloaded from <http://www.cs.ucsb.edu/~ycao>)

1. Y. Cao, L. Petzold, Accuracy limitations and the measurement of errors in the stochastic simulation of chemically reacting systems, submitted, *J. Comput. Phys.*, 2004.
2. Y. Cao, L. Petzold, M. Rathinam, D. Gillespie, The numerical stability of leaping methods for stochastic simulation of chemically reacting systems, *J. Chem. Phys.*, 121(24), 12169-12178, 2004.
3. R. Gunawan, Y. Cao, L. Petzold, F. Doyle III, Sensitivity analysis of discrete stochastic systems, submitted, *Biophys. J.*, 2004.
4. Y. Cao, D. Gillespie and L. Petzold, The slow-scale stochastic simulation algorithm, *J. Chem. Phys.*, 122(1), 014116, 2005.
5. M. Rathinam, L. Petzold, Y. Cao, D. Gillespie, Consistency and stability of tau leaping schemes for chemical reaction systems, submitted to *SIAM Multiscale Modeling and Simulation*, 2004.
6. Y. Cao, L. Petzold, D. Gillespie, Multiscale stochastic simulation algorithm with stochastic partial equilibrium assumption for chemically reacting systems, accepted, *J. Comput. Phys.*, 2004.
7. Y. Cao, H. Li and L. Petzold, Efficient formulation of the stochastic simulation algorithm for chemically reacting systems, *J. Chem. Phys.*, 121(9), 4059-4067, 2004.
8. Y. Cao and L. Petzold, A posteriori error estimation and global error control for ordinary differential equations by the adjoint method, accepted, *SIAM J. Scientific Computing*, 2004.
9. Y. Cao and L. Petzold, An error estimate for matrix equations, *Applied Numerical Mathematics*, 50, 395-407, 2004.

10. M. Rathinam, L. Petzold, Y. Cao, D. Gillespie, Stiffness in stochastic chemically reacting systems: The implicit tau-leaping method, *J. Chem. Phys.*, 119, 12784-94, 2003.
11. Y. Cao and L. Petzold, A subspace error estimate for linear systems, *SIAM J. Mat. Anal. Appl.*, 24, 787-801, 2003.
12. Y. Cao, S. Li, L. Petzold and R. Serban, Adjoint sensitivity analysis for differential-algebraic equations: the adjoint DAE system and its numerical solution, *SIAM J. Sci. Comput.*, 24, 1076–1089, 2002.
13. Y. Cao, S. Li and L. Petzold, Adjoint sensitivity analysis for differential-algebraic equations: algorithms and software, *J. Comp. Appl. Math.*, 149, 171–191, 2002.
14. Y. Cao, Q. Li, Multistep discretization of index 3 DAEs. *Journal of Computational Mathematics, ICMSEC Chinese Acad. Sci*, 18, 325-36, 2000.
15. Y. Cao, Q. Li, Predictor-corrector formula for solving index-2 differential-algebraic equations. *Mathematica Numerica Sinica*, 21, 65-74, 1999.
16. Y. Cao and Q. Li, Highest order multistep formula for solving index-2 differential algebraic equations, *BIT*, 38, 663-673, 1998.
17. Y. Cao and Q. Li, A-stable explicit nonlinear Runge-Kutta methods, *Tsinghua Science & Technoloty*, 3, 1227-1232, 1998.
18. Y. Cao and Q. Li, Nonlinear Runge-Kutta methods for solving differential-algebraic equations. *Chinese J. Numer. Math. Appl.* 20, 75–85, 1998.

Conference Papers, Posters and Presentations

1. Y. Cao and L. Petzold, Measurement of error in stochastic simulation: when the mean and the variance are not enough, to be presented at the 4th SIAM conference on Computational Science and Engineering, Feb, 2005.
2. Y. Cao, S. Lampoudi, H. Li and L. Petzold, A software package for discrete stochastic simulation of chemically reacting systems, to be presented at the 4th SIAM conference on Computational Science and Engineering, Feb, 2005.

3. Y. Cao, H. Li and L. Petzold, Efficient formulation of the stochastic simulation algorithm for chemically reacting systems, the 5th International Conference on Systems Biology, October, 2004 (poster).
4. R. Gunawan, Y. Cao, S. Lampoudi, L. Petzold and F. Doyle III, Stochastic sensitivity analysis of a circadian gene network, the 5th International Conference on Systems Biology, Heidelberg, Germany, October, 2004 (poster).
5. Y. Cao, L. Petzold, D. Gillespie, Towards the multiscale simulation of biochemical systems, the workshop of U.S. Army Research Office, Institute for Collaborative Biotechnologies site visit, UCSB, July, 2003 (poster).
6. L. Petzold, Y. Cao, S. Li and R. Serban, Adaptive numerical methods for sensitivity analysis of differential-algebraic equations and partial differential equations, Proceedings, Workshop on Modeling and Simulation in Chemical Engineering, Coimbra, Portugal, 2003.
7. L. Petzold, R. Serban, S. Li, S. Raha and Y. Cao, sensitivity analysis and design optimization of differential-algebraic equation systems, Proc. NATO Advanced Research Workshop on Computational Aspects of Nonlinear Structural Systems with Large Rigid Body Motion, 2001.
8. Y. Cao, S. Li and L. Petzold, Adjoint sensitivity analysis for DAE systems, NSF-KDI/IGPP Workshop 2000 on Accurate Simulation and Modelling of Physical Systems, San Diego, 2000 (poster).