# Dan Lu

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| **Contact Information** | Computational Sciences and Engineering Division<br>Oak Ridge National Laboratory<br>P.O. Box 2008 MS 6301<br>Oak Ridge, TN 37831-6301 | Office: Building 4500N, F107<br>Email: lud1@ornl.gov<br>Cell Phone: (850) 591-3598<br>Homepage: http://www.ornl.gov/~dgk |

**Research Interests**

– Uncertainty quantification and risk assessment in environmental sciences

– Numerical simulation of groundwater flow and contaminant reactive transport

– Computational methods and algorithms for inverse modeling

– Hierarchical Bayesian inferences and statistical methods

– Mathematical and computational analysis for efficient forward modeling

– Design of experiments for cost-effective data collection

**Education**

**Ph.D. in Computational Hydrology** — Apr. 2012
Florida State University, Tallahassee, FL
Advisor: Professor Ming Ye
Dissertation title: *Assessment of parametric and model uncertainty in groundwater modeling*

**M.S. in Hydrology and Water Resources** — Jun. 2007
China University of Geosciences, Beijing, China
Advisor: Professor Wenpeng Li
Thesis title: *Using GIS and remote sensing techniques to analyze soil salinization in Yanqi Basin*

**B.S. in Environmental Engineering** — Jun. 2004
Hebei University of Geosciences, Shijiazhuang, China

**Research Experience**

**Research Scientist** — Oct. 2016 – Present
Oak Ridge National Laboratory

**Postdoctoral Research Associate** — Dec. 2013 – Sep. 2016
Oak Ridge National Laboratory

**Postdoctoral Research Associate** — May 2012 – May 2013
U.S. Geological Survey, Menlo Park, CA

**Graduate Research Assistant** — Aug. 2007 – Apr. 2012
Department of Scientific Computing
Florida State University

**Internship Researcher** — Jul. 2010 – Dec. 2010
U.S. Geological Survey, Boulder, CO

JOURNAL ARTICLES
(PUBLISHED)

Mo, S., **D. Lu**, X. Shi, G. Zhang, M. Ye, J. Wu, and J. Wu, *A Taylor expansion-based adaptive design strategy for global surrogate modeling with applications in groundwater modeling*, **Water Resources Research**, to appear.

**Lu, D.**, D. Ricciuto, A. Walker, C. Safta, and W. Munger, *Bayesian calibration of terrestrial ecosystem models: a study of advanced Markov chain Monte Carlo Methods*, **Biogeosciences**, 14, 4295–4314, 2017.

Xi, M., **D. Lu**, D. Gui, Z. Qi, and G. Zhang, *Calibration of an agricultural-hydrological model (RZWQM2) using surrogate global optimization*, **Journal of Hydrology**, 544, 456–466, 2017.

**Lu, D.**, G. Zhang, C. Webster, and C. Barbier, *An improved multilevel Monte Carlo method for estimating probability distribution functions in stochastic oil reservoir simulations*, **Water Resources Research**, 52, 9642–9660, 2016.
(This work was reported in *The BAKKEN Magazine in 2015* [online version].)

Liu, P., A. S. Elshall, M. Ye, P. Beerli, X. Zeng, **D. Lu**, and Y. Tao, *Evaluating marginal likelihood with thermodynamic integration method and comparison with several other numerical methods*, **Water Resources Research**, 52, doi:10.1002/2014WR016718, 2016.

Hill, M. C., D. Kavetski, M. Clark, M. Ye, M. Arabi, **D. Lu**, L. Foglia, and S. Mehl, *Practical use of computationally frugal model analysis methods*, **Ground Water**, 54, 159–170, 2015.

**Lu, D.**, M. Ye, and G. P. Curtis, *Maximum likelihood Bayesian model averaging and its predictive analysis for groundwater reactive transport models*, **Journal of Hydrology**, 529(3), 1859–1873, 2015.

**Lu, D.**, M. Ye, M. C. Hill, E. P. Poeter, and G. P. Curtis, *A computer program for uncertainty analysis integrating regression and bayesian methods*, **Environmental Modeling & Software**, 60, 41–56, 2014.

Zhang, G., **D. Lu**, M. Ye, M. Gunzburger, and C. Webster, *An adaptive sparse-grid high-order stochastic collocation method of Bayesian inference in groundwater reactive transport modeling*, **Water Resources Research**, 49(10), 6871–6892, 2013.

**Lu, D.**, M. Ye, P. D. Meyer, G. P. Curtis, X. Shi, X. Niu, and S. B. Yabusaki, *Effects of error covariance structure on estimation of model averaging weights and predictive performance*, **Water Resources Research**, 49(9), 6029–6047, 2013.

Hill, M. C., D. Kavetski, M. Clark, M. Ye, and **D. Lu**, *Uncertainty Quantification for Environmental Models*, **SIAM News**, 45(9), 2012.

**Lu, D.**, M. C. Hill, and M. Ye, *Analysis of regression confidence intervals and Bayesian credible intervals for uncertainty quantification*, **Water Resources Research**, 48(9), W09521, 2012.
(This paper was selected as *Editor's Highlight* entitled new insights into faster computation of uncertainties)

**Lu, D.**, M. Ye, S. P. Neuman, and L. Xue, *Multimodel Bayesian analysis of data-*

*worth applied to unsaturated fractured tuffs*, **Advances in Water Resources**, 35, 69–82, 2012.

Neuman, S. P., L. Xue, M. Ye, and **D. Lu**, *Bayesian analysis of data-worth considering model and parameter uncertainties*, **Advances in Water Resources**, 36, 75–85, 2012. (*Top 10 Cited Paper* in 2012-2013 of Advances in Water Resources [Certificate])

**Lu, D.**, M. Ye, and S. P. Neuman, *Dependence of Bayesian model selection criteria and Fisher information matrix on sample size*, **Mathematical Geoscience**, 43, 971–993, 2011.

Ye, M., **D. Lu**, S. P. Neuman, and P. D. Meyer, *Comment on "Inverse groundwater modeling for hydraulic conductivity estimation using Bayesian model averaging and variance window" by Frank T.-C. Tsai and Xiaobao Li*, **Water Resources Research**, 46, W02801, 2010.

JOURNAL ARTICLES (IN PROCESS)

**Lu, D.**, D. Ricciuto, M. Stoyanov, and L. Gu, *Calibration of a land model using surrogate based global optimization*, **Journal of Advances in Modeling Earth Systems**, under review.

**Lu, D.**, D. Ricciuto, and K. Evans, *An efficient Bayesian data-worth analysis using a multilevel Monte Carlo method*, **Advances in Water Resources**, under review.

REFEREED CONFERENCE PUBLICATIONS

Zhang, G., **D. Lu**, M. Ye, M. Gunzburger, and C. Webster, *An efficient surrogate modeling approach in Bayesian uncertainty analysis*, 11th International Conference of Numerical Analysis and Applied Mathematics, 1558, 898–901, 2013.

Ye, M., **D. Lu**, S. P. Neuman, and L. Xue , *Multimodel Bayesian analysis of data-worth applied to unsaturated fractured tuffs*, International Conference on Groundwater: Our Source of Security in an Uncertain Future, Pretoria, South Africa, 2011.

**Lu, D.**, M. C. Hill, and M. Ye, *Analysis of regression and Bayesian predictive uncertainty measures*, MODFLOW and More 2011 Conference, Golden, CO, 2011.

Neuman, S. P., L. Xue, M. Ye, and **D. Lu**, *Multimodel assessment of the worth of data under uncertainty*, Water Management Symposium, Phoenix, AZ, 2011.

Ye, M., **D. Lu**, G. Miller, G. P. Curtis, P. D. Meyer, and S. B. Yabusaki, *Assessment of predictive uncertainty in coupled groundwater reactive transport modeling*, Conference on Goldschmidt – Earth, Energy and Environment, Knoxville, TN, 2010.

TECHNICAL REPORTS

Barbier, C., **D. Lu**, N. Collier, F. Curtis, C. G. Webster, and Y. Polsky, *High performance computing simulations for shale gas formation flow transport and uncertainty quantification analysis*, ORNL Technical Report, ORNL/TM-2015/543, 2015.

SOFTWARE DEVELOPMENT

**UCODE_2014**: A Computer Code for Sensitivity Analysis, Model Calibration, and Uncertainty Evaluation

Sponsor: U.S. Geological Survey

Developers: Eileen P. Poeter, Mary C. Hill, **Dan Lu**, and Steffen Mehl

Webpage: http://igwmc.mines.edu/freeware/ucode/

Description: UCODE_2014 is one of a set of inverse modeling codes supported by the U.S. Geological Survey. UCODE_2014 was developed for models in which the number of parameters is less than the number of observations. It can be used with existing process models to perform sensitivity analysis, data needs assessment, model calibration, prediction and uncertainty quantification.

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| LECTURES IN SHORT COURSES | MODFLOW, with the GIS-based GUI FREEWAT and Calibration and Uncertainty Quantification Using UCODE, Colorado School of Mines, Golden, CO, 2017. |
| | Groundwater Model Calibration Using OSTRICH: with Presentation of Additional Capabilities Available using PEST, PEST++ and UCODE-2014, Colorado School of Mines, Golden, CO, 2015. |
| ORAL PRESENTATIONS | *Quantum Behaved Particle Swarm Optimization for Parameter Estimation in Terrestrial Ecosystem Models*, 2017 ESS PI Meeting, Washington D. C., 2017. |
| | *Calibration of the Community Land Model (CLM4.5) using surrogate based global optimization*, 49th American Geophysics Union Annual Meeting, San Francisco, CA, 2016. |
| | *A Systematic Bayesian Framework for Uncertainty Quantification in Environmental Modeling*, Earth System Modeling Workshop, Oak Ridge National Laboratory, TN, 2015. |
| | *Multilevel Monte Carlo Method with Application to Uncertainty Quantification in Oil Reservoir Simulation*, 47th American Geophysics Union Annual Meeting, San Francisco, CA, 2014. |
| | *Assessment of Predictive Performance of Bayesian Model Averaging in Groundwater Reactive Transport Models*, 2014 SIAM Conference on Uncertainty Quantification, Savannah, GA, 2014. |
| | *Maximum Likelihood Bayesian Model Averaging of Groundwater Reactive Transport Models*, 2014 SIAM SEAS Annual Meeting, Melbourne, FL, 2014. |
| | *Integration of Markov Chain Monte Carlo Simulation into UCODE for Bayesian Uncertainty Analysis*, Geological Society of America Annual Meeting, Charlotte, NC, 2012. |
| | *Effects of Temporal Error Correlation on Quantification of Predictive Uncertainty in Groundwater Reactive Transport Modeling*, annual PI meeting of the Subsurface Biogeochemical Research Program of the Department of Energy, Washington D.C., 2012. |
| | *Effects of Temporal Residual Correlation on Model Weights*, 44th American Geophysics Union Annual Meeting, San Francisco, CA, 2011. |
| | *Multimodel Bayesian Analysis of Data-Worth Applied to Unsaturated Fractured Tuffs*, Geosciences Applications Opening Workshops on Uncertainty Quantification, Research Triangle Park, NC, 2011. |

*Analysis of Predictive Uncertainty Measures of Regression and Bayesian*, 2011 MOD-FLOW and More Meeting, Golden, CO, 2011.

*A Controlled Experiment for Investigating Prediction Accuracy and Prediction Uncertainty in Groundwater Flow Modeling*, 43th American Geophysics Union Annual Meeting, San Francisco, CA, 2010.

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| HONORS AND AWARDS | Student travel fellowship to the annual PI meeting of the subsurface biogeochemical research program of the Department of Energy, 2012. |
| | Statistical and Applied Mathematical Sciences Institute (SAMSI) travel award to the geosciences applications opening workshops on uncertainty quantification, 2011 |
| REVIEWER FOR JOURNALS | Water Resources Research |
| | Stochastic Environmental Research and Risk Assessment |
| | Environmental Modeling & Software |
| | Analytical Chemistry |
| | Journal of Hydrology |
| | Hydrogeology Journal |
| | Hydrological Processes |
| | Biogeosciences |
| | Geoscientific Model Development |
| SERVIES | Guest Editor of a Special Issue in Geofluids |
| MEMBERSHIPS | American Geophysical Union (AGU) |
| | Geologic Society of America (GSA) |
| | Society for Industrial and Applied Mathematics (SIAM) |
| | Chinese American Water Resources Association (CAWRA) |