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Carl T Kelley

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14. ABSTRACT
The PI and his students design, analyze, and implement novel algorithms for model calibration including method for noisy and ill-conditioned nonlinear least squares problems, reduced order models (such as POD and sparse interpolation), and methods based on Bayesian analysis which are part of uncertainty quantification. We also work on simulation methods such as flow in the vadose zone, non-Darcy flow models, linear and nonlinear solvers, pseudo-transient continuation, and preconditioning.

15. SUBJECT TERMS
Model calibration, nonlinear least squares, uncertainty quantification, ground water

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a. REPORT	b. ABSTRACT	c. THIS PAGE			Carl Kelley
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Report Title

Final Report: Algorithms for Model Calibration of Ground Water Simulators

ABSTRACT

The PI and his students design, analyze, and implement novel algorithms for model calibration including method for noisy and ill-conditioned nonlinear least squares problems, reduced order models (such as POD and sparse interpolation), and methods based on Bayesian analysis which are part of uncertainty quantification. We also work on simulation methods such as flow in the vadose zone, non-Darcy flow models, linear and nonlinear solvers, pseudo-transient continuation, and preconditioning.

Enter List of papers submitted or published that acknowledge ARO support from the start of the project to the date of this printing. List the papers, including journal references, in the following categories:

(a) Papers published in peer-reviewed journals (N/A for none)

Received		Paper
05/01/2013	6.00	Alex Toth, C. T. Kelley. Convergence Analysis of Anderson Acceleration, SIAM J Numer Anal, (05 2013): 0. doi:
06/02/2012	4.00	Cass T. Miller, Clint N. Dawson, Matthew W. Farthing, Thomas Y. Hou, Jingfang Huang, Christopher E. Kees, C.T. Kelley, Hans Petter Langtangen. Numerical Simulation of Water Resources Problems: Models, Methods, and Trends, Advances in Water Resources, (5 2012): 0. doi: 10.1016/j.advwatres.2012.05.008
07/05/2012	5.00	David Mokrauer, C. T. Kelley. Sparse interpolatory reduced-order models for simulation of light-induced molecular transformations, Optimization Methods and Software, (07 2012): 0. doi: 10.1080/10556788.2012.693928
07/13/2014	12.00	James Nance, Elena Jakubikova, C. Tim Kelley. Reaction Path Following with Sparse Interpolation, Journal of Chemical Theory and Computation, (07 2014): 0. doi: 10.1021/ct5004669
TOTAL:	**4**	

Number of Papers published in peer-reviewed journals:

(b) Papers published in non-peer-reviewed journals (N/A for none)

Received		Paper
TOTAL:		

Number of Papers published in non peer-reviewed journals:

(c) Presentations

Anna Meade Fregosi,
``Uncertainty Quantification for Heat Transport in the Shallow Subsurface",
Copper Mountain Conference on Iterative Methods, April 6-11, 2014.
Copper Mountain, CO. (with C. Winton, A. Hines, O. J. Eslinger, C. T. Kelley).

Deena Hannon Giffen,
``Simulating Non-Dilute Transport in Porous Media Using a TCAT-Based Model",
Copper Mountain Conference on Iterative Methods, April 6-11, 2014
Copper Mountain, CO. (with C. T. Kelley, P. Schultz, C. T. Miller, W. G. Gray)

James Nance, ``Following Molecular Reaction Paths with Sparse Interpolatory
Surrogate Models",
Copper Mountain Conference on Iterative Methods, April 6-11, 2014
Copper Mountain, CO. (with C. T. Kelley and E. Jakubikova)

Deena Hannon Giffen,
Computational Methdos in Water Resources, June 9â€”13, 2014, Stuttgart,
Germany. (with C. T. Kelley, P. Schultz, C. T. Miller, W. G. Gray)

C. T. Kelley, Implicit filtering and hidden constraints, July 22, 2014.
Sandia National Laboratory, Albuquerque, NM.

C. T. Kelley, Newton-krylov method for problems with embedded monte carlo simulations,
July 9, 2014.
SIAM 2014 Annual Meeting, Minisymposium on Advances in Krylov and
Extended Krylov Subspace Methods, Chicago, IL.

C. T. Kelley, Anderson acceleration, May 16, 2014 2014.
SIAM Student Chapter, Hong Kong Polytechnic University, Hong Kong,
China.

C. T. Kelley, Implicit filtering and imaging, May 13, 2014 2014.
SIAM Conference on Imaging, Hong Kong, China.

C. T. Kelley, ``Derivative-Free Optimization of Functions with
Embedded Monte Carlo Simulations",
Copper Mountain Conference on Iterative Methods, April 6-11, 2014,
Copper Mountain, CO.

C. T. Kelley, Calibration of a novel density-dependent flow model with implicit
filtering, Dec 16--18 2013.
Second Conference on Engineering and Computational Mathematics, Hong
Kong Polytechnic University, Hong Kong, China.

C. T. Kelley, Pseudo-transient continuation, October 2013.
Outstanding Alumni Colloquium, Purdue University.

Deena Hannoun, ``Simulating Non-Dilute Transport in Porous Media Using a Tcat-Based Model", SIAM Geosciences Meeting, Padova, Italy. June 2013. (with C. T. Kelley, P. Birak, C. T. Miller, W. G. Gray)

Anna Meade, ``Uncertainty Quantification for Transport Problems in the Shallow Subsurface", SIAM Geosciences Meeting, Padova, Italy. June 2013. (with C. T. Kelley, O. J. Eslinger)

C. T. Kelley, ``Newtonâ€™s Method for Monte Carlo Based Residuals", CUNY Applied Mathematics Symposium, New York, NY. April 25, 2013

C. T. Kelley, ``Newtonâ€™s Method for Monte Carlo Based Residuals", 12th International Symposium on Distributed Computing and Applications to Business, Engineering and Science, London, England, Sept 2â€”4, 2013. Keynote address.

C. T. Kelley,``Newtonâ€™s Method for Monte Carlo Based Residuals", University of Trier, Trier, Germany, June 14, 2013.

C. T. Kelley,``Randomized nonlinear equations in neutronics", Sept 7, 2012. Purdue University Applied Mathematics Seminar, West

Lafayette, IN.

C. T. Kelley,``Randomized nonlinear equations in neutronics", October 19â€“22, 2012. Eleventh International Symposium on Distributed Computing and Applications to Business, Engineering and Science, Guilin, China.

C. T. Kelley and D. Mokrauer,
"Sparse interpolatory reduced-order models for simulation of
light-induced molecular transformations",
8th International Conference on Numerical Optimization and Numerical
Linear Algebra, Xiamen, China,
November, 2011.

C. T. Kelley and D. Mokrauer,
"Interpolatory Reduced Order Models for Molecular Dynamics",
Minisymposium on Reduced-Order Models, SIAM Conference on
Uncertainty Quantification, Raleigh, NC.,
April 4, 2012

D. Hannoun, C. T. Kelley, C. T. Miller, W. G. Gray
"Simulating Non-Dilute Transport in Porous Media Using a
TCAT-based Model",
Computational Methods in Water Resources, XIX,
Urbana-Champaign, IL, June 19, 2012

C. Winton, C. T. Kelley, S. E. Howington, J. Pettway, O. J. Eslinger,
J. Hensley,
"Analysis of Accuracy in Formation of Reduced Order Model",
Computational Methods in Water Resources, XIX,
Urbana-Champaign, IL, June 19, 2012

C. T. Kelley and D. Mokrauer,
"Interpolatory Reduced Order Models for Molecular Dynamics",
International Symposium on Mathematical Programming, Berlin,
Germany, Aug 22, 2012.

Number of Presentations: 22.00

Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received	Paper

TOTAL:

Number of Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received	Paper

TOTAL:

Number of Peer-Reviewed Conference Proceeding publications (other than abstracts):

(d) Manuscripts

Received		Paper
01/01/2012	3.00	C. T. Miller , C. N. Dawson , M. W. Farthing, T. Y. Hou , J. Huang , C. E. Kees , C. T. Kelley, H. P. Langtangen. Numerical Simulation of Water Resources Problems: Models, Methods, and Trends, Advances in Water Resources (12 2011)
03/04/2014	9.00	James Nance, Elena Jakubikova, C. T. Kelley. Reaction Path Following with Sparse Interpolation, J. Chem. Th. Comp. (01 2014)
03/04/2014	10.00	Xiaojun Chen, C. T. Kelley. SAMPLING METHODS FOR OBJECTIVE FUNCTIONS WITH EMBEDDED MONTE CARLO SIMULATIONS, SIAM J of Optimization (02 2014)
05/07/2014	11.00	Owen J. Eslinger, Corey Winton, Jerrell R. Ballard, Jr., Stacy E. Howington, Anna Fregosi, Kimberly Ward, C. T. Kelley. Estimating Sampling Distributions of Apparent Thermal Diffusivityfor Partially Saturated Soils, IEEE Transactions on Geoscience and Remote Sensing (05 2014)
07/23/2013	7.00	Jeffrey Willert, C. T. Kelley, D. A. Knoll, H. Park. Hybrid Deterministic/Monte Carlo Neutronics, SIAM Journal on Scientific Computing (06 2012)
07/23/2013	8.00	J. Willert, X. Chen, C. T. Kelley. Newton's Method for Monte Carlo-Based Residuals, SIAM J Numer Anal (01 2013)
11/20/2014	13.00	Anna Fregosi, C. T. Kelley, Ralph Smith, James Nance, Owen J. Eslinger, Corey Winton, Jerrell R. Ballard, David Lease. Bayesian Model Calibration, Verification and Prediction Techniques for a Thermal Problem Arising inSoil Characterization, SIAM J Uncertainty Quantification (11 2014)
11/23/2011	1.00	C. T. Kelley, L-Z. Liao. Explicit Pseudo-Transient Continuation, Pacific Journal of Optimization (11 2011)
12/21/2011	2.00	David Mokrauer, C. T. Kelley. Sparse Interpolatory Reduced-Order Models for Simulation of Light-Induced Molecular Transformations, Optimization Methods and Software (12 2011)
TOTAL:	**9**	

Number of Manuscripts:

Books

Received Book

TOTAL:

Received Book Chapter

TOTAL:

Patents Submitted

Patents Awarded

Awards

Reelected Chair, SIAM Board of Trustees
Reappointed, Editor-in-Chief, SIAM Review
Outstanding Alumni Award, Department of Mathematics, Purdue University

Graduate Students

NAME	PERCENT_SUPPORTED	Discipline
Anna Fregosi	0.40	
Corey Winton	0.00	
FTE Equivalent:	**0.40**	
Total Number:	**2**	

Names of Post Doctorates

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Names of Faculty Supported

NAME	PERCENT_SUPPORTED	National Academy Member
Carl T Kelley	0.12	No
FTE Equivalent:	**0.12**	
Total Number:	**1**	

Names of Under Graduate students supported

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Student Metrics

This section only applies to graduating undergraduates supported by this agreement in this reporting period

The number of undergraduates funded by this agreement who graduated during this period: 0.00

The number of undergraduates funded by this agreement who graduated during this period with a degree in science, mathematics, engineering, or technology fields:..... 0.00

The number of undergraduates funded by your agreement who graduated during this period and will continue to pursue a graduate or Ph.D. degree in science, mathematics, engineering, or technology fields:..... 0.00

Number of graduating undergraduates who achieved a 3.5 GPA to 4.0 (4.0 max scale):..... 0.00

Number of graduating undergraduates funded by a DoD funded Center of Excellence grant for Education, Research and Engineering:..... 0.00

The number of undergraduates funded by your agreement who graduated during this period and intend to work for the Department of Defense 0.00

The number of undergraduates funded by your agreement who graduated during this period and will receive scholarships or fellowships for further studies in science, mathematics, engineering or technology fields: 0.00

Names of Personnel receiving masters degrees

NAME
Total Number:

Names of personnel receiving PHDs

NAME	
Corey Winton	
Total Number:	**1**

Names of other research staff

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Sub Contractors (DD882)

Inventions (DD882)

Scientific Progress

see attachment

Technology Transfer

We collaborate with a group at the Information Technology Laboratory (ITL) at the US Engineer Research and Development Center (ERDC) on applying our results to thermal inverse problems in the near-surface vadose zone. The group at ITL includes Corey Winton, a student of the PI who was supported by a previous ARO grant. Our other collaborators at ITL are Owen Eslinger, Amanda Hines, and Jeff Hensley. Our collaborators at CHL are Stacy Howington, Charles Berger, Matthew Farthing, Jackie Pettway, and Chris Kees.

Final Report for Army Research Office grant
W911NF-11-1-0367
Algorithms for Model Calibration of Ground Water Simulators
Reporting period: 9/16/11 – 09/15/14

1. Forward. The objectives of this project are to

- design, analyze, and implement novel algorithms for model calibration including:
  - methods for noisy and ill-conditioned nonlinear least squares problems,
  - reduced order models (such as POD and sparse interpolation), and
  - methods based on Bayesian analysis which are part of uncertainty quantification.
- simulation methods such as:
  - flow in the vadose zone and non-Darcy flow models,
  - linear solvers and preconditioning methods for those solvers, and
  - nonlinear solvers, especially pseudo-transient continuation.

The primary focus of this project is model calibration. The secondary objectives are continuations of previous ARO-funded projects. However, reduced order models for unsaturated flow may become important in the current work we do with ERDC.

We collaborate with a group at the Information Technology Laboratory (ITL) at the US Engineer Research and Development Center (ERDC) on applying our results to thermal inverse problems in the near-surface vadose zone. The group at ITL includes Corey Winton, a student of the PI who was supported by a previous ARO grant. Our other collaborators at ITL are Owen Eslinger, Amanda Hines, and Jeff Hensley. Our collaborators at CHL are Stacy Howington, Charles Berger, Matthew Farthing, Jackie Pettway, and Chris Kees.

1.1. Students. This project supports Anna (Meade) Fregosi, a Ph. D. student. Fregosi spent the summers of 2011 and 2012 at ERDC working on model calibration and thermal inverse problems in the subsurface. We have two paperssubmitted and one in preparation on this work and Fregosi will take her preliminary oral exam in January 2015. Corey Winton graduated in December 2012 and is now working at ERDC. Winton was supported from a previous ARO project and was stationed at ERDC when he finished his degree.

2. Problems Studied. In this project we have worked on

- thermal inverse problems in soil with Fregosi and the group at ITL,
- algorithms and solvers with Kees and Farthing from CHL,
- reduced order models for model calibration and inverse problems with Winton and the group at ITL,
- pseudo-transient continuation theory,
- accelerators for fixed-point iteration,
- non-Darcy flow models in a separate, but related, project, and
- solvers for nonlinear equations and optimization problems with low-accuracy/random residuals.

3. Results. In this period seven papers [2–4, 6, 11, 15, 17] have been submitted and five [7–10, 18] have appeared.

The PI and his students have given twenty-two presentations based on our work.

3.1. Solvers. We were invited to include many of our results from the past several years in a substantial review article [8]. That paper covered a broad range of issues in simulation. Kees and Farthing from ERDC were two of the many other authors of that paper.

Pseudo-transient continuation is a way to integrate time-dependent equations to steady state without having to capture transient behavior which is not of interest. This has been of use to ERDC [14] in surface water flow codes, and is a very important method in combustion computations. In [7] we analyze an explicit form of this algorithm.

We are also investigating Anderson acceleration, also known as Pulay mixing [1, 12, 13]. This is a method for accelerating fixed point iteration when Jacobian information is either not available or too expensive to compute and store. The method has recently been applied to subsurface flow simulations [16].

Anderson acceleration builds a new iterate from a linear combination of prior residuals, computing the coefficients by minimizing a linear residual. In the minimal storage case Anderson is identical to fixed point iteration. In [15] we report on the first convergence analysis for Anderson acceleration and show that the norm in which the linear residual is minimized can make a significant difference in the performance of the solver.

We have also investigated the performance of solvers when the nonlinear residual, Jacobian, and Jacobian-vector products are computed with a Monte Carlo simulation. This situation differs from the textbook case [5] in that one does not have errors, but variances. This difference causes significant changes, both in theory and in practice, from the standard case. We have submitted one paper on this [17] and one has been accepted [18].

These two lines of work have potential applications to hydrology and subsurface remediation. Anderson acceleration is a natural method for multi-physics coupling (for example subsurface flow, chemistry, and heat transfer) when the individual physics codes cannot be combined into a single package for which one can compute a Jacobian. Residuals with poor accuracy due to internal Monte Carlo simulations are not rare, and will become more common as high-performance computers become larger and fault-tolerance becomes more important. Monte Carlo simulations are naturally fault-tolerant, but are also much less accurate than conventional simulations and interact with the solvers in very different ways than deterministic simulations do.

3.2. Model Calibration. One paper on reduced order models [10] has appeared in print and another has been submitted [11]. Fregosi has made good progress and we have completed two paper in collaboration with ERDC staff. The first of these [3] takes a conventional nonlinear least squares approach. The second [4] compares various approaches to Bayesian inference and uncertainty quantification. A third, and final paper, will be on the variably saturated case. When the work on that paper is complete, Fregosi will graduate. The PI and Fregosi visited ERDC in May of 2014.

3.3. Work in Progress. Fregosi has completed her work on the saturated case [4] follow up our first paper with Eslinger. The problem is a thermal inverse problem (determine soil properties from temperature measurements) in the upper 30cm of the subsurface for several regions of the Earth. ERDC took data in field studies and we are using this resource in our work. The first two papers [4],on the constant saturation case, which covers some, but not

all of the data. The final part of Fregosi's work will be on the variably saturated cases.

We continue to work on non-Darcy flow models with a group at the University of North Carolina and a student Deena Hannoun, who is supported by an NSF grant. That modeling questions for that project took longer to resolve that we expected, but we now have good fits to data and the paper is almost ready to submit. That work should leverage the NSF support to inform model design for this project. Deena Giffen, the NSF-supported student on the project, will interview at ERDC in December.

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