Christopher Thiele

Department of Computational and Applied Mathematics Rice University, Houston, TX christopher.thiele92@gmail.com

Personal profile

I am a graduate student in computational and applied mathematics at Rice University. My work focuses on iterative linear solvers, particularly multigrid methods, and their parallel implementation. I have experience in the development of large-scale numerical simulations, mostly in the context of hydrocarbon recovery.

Education

Aug. 2016-present Graduate studies at the department for Computational and

Applied Mathematics at Rice University, Houston, TX

Intended degree: PhD

MA degree awarded in May 2018

Oct. 2014–Jul. 2016 Master of Science at University of Kaiserslautern,

Kaiserslautern, Germany

Major: Mathematics
Minor: Computer science

Master's degree was completed at Rice University.

Oct. 2011–Sep. 2014 Bachelor of Science at University of Kaiserslautern,

Kaiserslautern, Germany

Major: Mathematics Minor: Computer science

Practical experience

May 2020–Jul. 2020 Internship at Shell Technology Center Houston (STCH), Houston, TX (remotely)

• Machine learning techniques in content-based image retrieval for pore images

May 2019–Aug. 2019 Internship at Shell Technology Center Houston (STCH), Houston, TX

- Evaluation of second-order optimization methods for machine learning applications
- Implementation in Python using TensorFlow

May 2018–Aug. 2018

Internship at Shell Technology Center Houston (STCH), Houston, TX

- Evaluation of GPU-based iterative solvers (Krylov, multigrid) in a pore-scale fluid simulation software
- Implementation in C++ using MPI, OpenMP, Trilinos, AMGX

May 2017-Aug. 2017

Internship at Shell Technology Center Houston (STCH), Houston, TX

- Improvement of software quality, performance, and scalability of a pore-scale fluid simulation software
- Implementation in C++ using MPI, OpenMP, Trilinos
- Performance analysis using Intel VTune and ITAC

Dec. 2015-Jul. 2016

Research Assistant at Fraunhofer Institute for Industrial Mathematics (ITWM), Kaiserslautern, Germany

- Implementation of hybrid parallel sparse matrix-vector product and conjugate gradient solver
- Implementation in C++ using GPI2 (PGAS) and POSIX threads

Aug. 2015-Nov. 2015

Associate Research Mathematician at Brunel Energy GmbH, Bremen, Germany

- Performance analysis of a large-scale fluid simulation software
- Development of an iterative linear solver algorithm for discontinuous Galerkin discretizations
- Evaluation of parallel linear algebra frameworks
- Implementation in C++ using MPI, OpenMP, Trilinos, and GPI2

Apr. 2014–Jul. 2015

Research Assistant at Fraunhofer Institute for Industrial Mathematics (ITWM), Kaiserslautern, Germany

- Finite difference methods for Poisson and Helmholtz problems with absorbing boundary conditions
- Implementation in C++ using PETSc, prototyping with MATLAB

Oct. 2013–Apr. 2014

Internship at Fraunhofer Institute for Industrial Mathematics (ITWM), Kaiserslautern, Germany

- Introduction to parallel programming models and analysis of performance and scalability
- Parallel implementation of basic linear algebra operations in C++ using MPI, GPI2, POSIX threads, and OpenMP

Publications in peer-reviewed journals

- C. Liu, F. Frank, C. Thiele, F.O. Alpak, S. Berg, W. Chapman, and B. Riviere. An efficient numerical algorithm for solving viscosity contrast Cahn–Hilliard–Navier–Stokes system in porous media. *Journal of Computational Physics*, 2020.
- C. Thiele, M. Araya-Polo, F.O. Alpak, B. Riviere, and F. Frank. Inexact hierarchical scale separation: A two-scale approach for linear systems from discontinuous Galerkin discretizations. Computers & Mathematics with Applications, 2017.

Publications in conference proceedings and workshops

- C. Thiele, M. Araya-Polo, and D. Hohl. Deep learning with a stochastic quasi-Gauss-Newton method. Workshop "Beyond First Order Methods in ML Systems," Thirty-seventh International Conference on Machine Learning (ICML), 2020.
- C. Thiele, M. Araya-Polo, F.O. Alpak, B. Riviere, and D. Hohl. Weak scalability analysis of GPGPU-based iterative solvers in a two-phase pore-scale flow simulator. *Fourth EAGE Workshop on High Performance Computing for Upstream*, 2019.
- **C. Thiele**, M. Araya-Polo, F.O. Alpak, B. Riviere. Distributed parallel hybrid CPU-GPGPU implementation of the phase-field method for accelerated high-accuracy simulations of pore-scale two-phase flow. *SPE Reservoir Simulation Conference*, 2019.
- C. Thiele, M. Araya-Polo, F.O. Alpak, B. Riviere, F. Frank. Inexact hierarchical scale separation: An efficient linear solver for discontinuous Galerkin discretizations. *SPE Reservoir Simulation Conference*, 2017.
- C. Thiele, M. Araya-Polo, D. Stoyanov, F. Frank, F.O. Alpak. Asynchronous hybrid parallel SpMV in an industrial application. *International Conference on Computational Science and Computational Intelligence*, 2016.

Preprints

- C. Thiele, M. Araya-Polo, D. Hohl. Deep neural network learning with second-order optimizers a practical study with a stochastic quasi-Gauss–Newton method. arXiv preprint arXiv:2004.03040, 2020.
- M. Grossman, C. Thiele, M. Araya-Polo, F. Frank, F.O. Alpak, V. Sarkar. A survey of sparse matrix-vector multiplication performance on large matrices. arXiv preprint arXiv:1608.00636, 2016.

Talks

Hybrid-parallel multigrid preconditioners in a pore-scale flow simulation. Rice Oil & Gas HPC Conference, Mar. 2–4, 2020, Houston, TX, USA.

p-Multigrid with partial smoothing – an efficient preconditioner for discontinuous Galerkin methods with modal bases. Finite Element Rodeo, Feb. 28–29, 2020, Waco, TX, USA.

p-Multigrid methods for discontinuous Galerkin discretizations with modal bases. Friedrich-Alexander-Universität Erlangen-Nürnberg, Dec. 19, 2019, Erlangen, Germany. (Invited talk)

Distributed parallel hybrid CPU-GPGPU implementation of the phase-field method for accelerated high-accuracy simulations of pore-scale two-phase flow. SPE Reservoir Simulation Conference, Apr. 10–11, 2019, Galveston, TX, USA.

Hierarchical scale separation: A multi-scale solver for linear systems in modal discontinuous Galerkin discretizations. Finite Element Rodeo, Mar. 1–2, 2019, Austin, TX, USA.

Improving scalability and performance of linear system solves in pore-scale simulations. Rice Oil & Gas HPC Conference. Mar. 15–16, 2017, Rice University, Houston, TX, USA.

Asynchronous hybrid parallel SpMV in an industrial application. *International Conference on Computational Science and Computational Intelligence, Dec.* 15–17, 2016, Las Vegas, NV, USA.

Posters

- C. Thiele, M. Araya-Polo, F.O. Alpak, B. Riviere. Hierarchical scale separation: A linear solver based on block relaxation and multigrid. *Rice Oil & Gas HPC Conference, Mar.* 4–6, 2019, Houston, TX, USA.
- C. Thiele, M. Araya-Polo, F.O. Alpak, B. Riviere, F. Frank. Inexact hierarchical scale separation: An efficient linear solver for discontinuous Galerkin discretizations. SPE Reservoir Simulation Conference, Feb. 20–22, 2017, Montgomery, TX, USA.

Theses

Inexact hierarchical scale separation for linear systems in modal discontinuous Galerkin discretizations. MA thesis, April 2018, Rice University, Houston, TX, USA.

Finite-Differenzen-Approximation der zweidimensionalen Helmholtz-Gleichung (Finite difference approximation of the two-dimensional Helmholtz equation). BS thesis, September 2014, University of Kaiserslautern, Kaiserslautern, Germany.

Participation in conferences and workshops

If a talk or poster presentation is indicated, please refer to the respective section for details.

Workshop "Beyond First Order Methods in ML Systems," Thirty-seventh International Conference on Machine Learning (ICML). Jul. 17, 2020.

Rice Oil & Gas HPC Conference. Mar. 2-4, 2020, Houston, TX, USA. (Talk)

SPE Reservoir Simulation Conference. Apr. 10–11, 2019, Galveston, TX, USA. (Talk)

SIAM Conference on Mathematical & Computational Issues in the Geosciences (GS19). Mar. 11–14, 2019, Houston, TX, USA.

Rice Oil & Gas HPC Conference. Mar. 4-6, 2019, Houston, TX, USA. (Poster)

Finite Element Rodeo. Mar. 1-2, 2019, Austin, TX, USA. (Talk)

International Conference for High Performance Computing, Networking, Storage, and Analysis (SC18). Nov. 11–16, 2018, Dallas, TX, USA.

Rice Oil & Gas HPC Conference. Mar. 12–13, 2018, Houston, TX, USA.

Rice Oil & Gas HPC Conference. Mar. 15–16, 2017, Houston, TX, USA. (Talk)

Finite Element Rodeo. Mar. 3-4, 2017, Houston, TX, USA.

SPE Reservoir Simulation Conference. Feb. 20–22, 2017, Montgomery, TX, USA. (Poster)

International Conference on Computational Science and Computational Intelligence. Dec. 15–17, 2016, Las Vegas, NV, USA. (Talk)

International Conference for High Performance Computing, Networking, Storage, and Analysis (SC15). Nov. 15–20, 2015, Austin, TX, USA.

Sparse Solvers for Exascale: From Building Blocks to Applications. Mar. 23–25, 2015, Greifswald, Germany.

Awards

Alan Weiser Memorial Travel Award. Rice University, Department of Computational and Applied Mathematics, 2019.

Ken Kennedy Institute for Information Technology Shell Graduate Fellowship. Rice University, Ken Kennedy Institute for Information Technology, 2018.