Dr. Robert J. B. Kalescky

Résumé, May 2025

Principal Scientist
Adjunct Professor of Data Science
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Professional Summary

Computational scientist with over a decade of experience in high-performance computing (HPC), quantum chemistry, molecular dynamics, and machine learning-driven simulations. Proven leadership in academic research computing infrastructure, parallelization, and performance optimization. Recognized for impactful interdisciplinary work and awarded for innovative computational strategies. Seeking to transition to an industry R&D role to apply deep computational expertise in solving complex, real-world challenges.

Core Competencies

- High-Performance Computing (HPC), Parallel and Distributed Algorithms
- Quantum Chemistry and Molecular Dynamics Method Development and Simulations
- Machine Learning for Scientific and Data-Driven Modeling
- Scientific Application Development, Optimization, and Scaling using Best Practices
- Project Management, Interdisciplinary Collaboration, Research Consulting

Technologies

Languages	Python, C, C++, Fortran, Rust
Parallelism	MPI, (Open|NV)SHMEM, NCCL, CUDA, OpenMP/OpenACC, KOKKOS, RAJA
Libraries	Armadillo, Eigen, PyTorch, PyG, GPyTorch, RAPIDS, HPC SDK
Tools	Git, Linux, Slurm, Kubernetes, Docker, Apptainer/Singularity, Enroot, Nix
Molecular Modelling	Gaussian, CFOUR, PySCF, DFTB+, LAMMPS, Charmm, OpenMM

Experience

Principal Scientist — May 2024 to May 2025
O'Donnell Data Science and Research Computing Institute
Southern Methodist University, Dallas, Texas

- Directed and developed strategic initiatives and funding opportunities for research computing across disciplines.
- Developed scalable and efficient applications and workflows for chemical simulations and data-intensive machine-learning.

HPC Applications Scientist — May 2015 to May 2024
Office of Information Technology: Research and Data Science Services & Center for Research Computing
Southern Methodist University, Dallas, Texas

- Provided consulting on performance, parallelization, GPU acceleration, and HPC adoption; supported research groups with code migration and optimization across HPC clusters; and mentored faculty and students in computational best practices.
- Instrumental in the procurement, integration, and optimization of ManeFrame II, NVIDIA DGX SuperPOD, and M3 clusters.
- Designed and led HPC and data science courses, workshops, and training sessions for advanced users and researchers.
- SMU President's Award for Innovation (2020) for contributions to computational strategies in COVID-19 campus response.

Education

Doctor of Philosophy in Chemistry — August 2009 to May 2014
Southern Methodist University, Dallas, Texas
Description of the Strength of Chemical Bonds Utilizing Local Vibrational Modes

Master of Science in Chemistry — August 2007 to May 2009
University of Texas at Dallas, Dallas, Texas
Area Per Ligand as a Function of Nanoparticle Radius: A Theoretical and Computer Simulation Approach

Bachelor of Science in Chemical Engineering, Minors in Mathematics and Chemistry — August 2001 to May 2006
Texas Tech University, Lubbock, Texas
Prairie Grass Ethanol Production Pilot Plant Facility and Optimization