Bimal **Gaudel**

C++ Systems · Numerical Libraries · Tensor Algebra & Scientific Computing

Blacksburg, VA, USA

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Summary

Led the development of **SeQuant**, a tensor-algebra framework with a compiler-style pipeline. It takes a symbolic quantum-chemistry derivation and runs it as numerical code at supercomputer scale — work that took researchers months now takes days.

Open to

Systems and runtime roles, numerical and simulation libraries, scientific software R&D, and HPC research-software / postdoc roles. Open to relocation.

Focus

Modern C++ (17/20/23), Template metaprogramming, Distributed-memory parallelism, Numerical & tensor libraries, Optimizing compiler pipelines, Graph-theoretic transforms

Experience

Lead Developer, SeQuant — Blacksburg, VA

Virginia Tech — Research Associate — 2018 – 2025

Developed a runtime that optimizes symbolic tensor expressions for automated efficient evaluation.

Selected Projects

SeQuant — ValeevGroup/SeQuant

Designed and led the implementation of an embedded DSL, a graph-canonicalized IR, a cost-based optimizer, an interpreter, and a transpiler.

- SeQuant expressions double as the AST in idiomatic C++. Node identity in the IR comes from tensor-network graph canonicalization, making common-subexpression elimination work across separate equations.
- Contraction ordering is cost-based — e.g. subset dynamic programming over tensor networks, scored by flop and memory counts. The interpreter evaluates the IR with memoization keyed on canonical identity and memory-aware cache eviction.
- Backend interface is extensible: TiledArray, BTAS, and TAPP backends ship with SeQuant, and the IR also lowers to C++/Python for downstream tensor compilers like TACO.

TiledArray — ValeevGroup/TiledArray

Contributing developer on the massively-parallel block-sparse distributed tensor framework. Extended its operation basis to support tensor-of-tensor data structures, enabling block-wise compression and PNO-like local-correlation methods.

Education

PhD, Theoretical & Computational Chemistry — Blacksburg, VA

Virginia Tech — 2018 – 2025

Dissertation: *Automated implementation of advanced electronic structure methods*.

Selected Publications

Gaudel, B., Adam, R. G., Melekamburath, A., Masteran, C., Teke, N., Besharatnik, A., Köhn, A., & Valeev, E. F. (2026). SeQuant framework for symbolic and numerical tensor algebra. I. Core capabilities. *Journal of Chemical Physics*, *164*(14), 142502. https://doi.org/10.1063/5.0311913

Masteran, C., Gaudel, B., & Valeev, E. F. (2025). Toward a Balanced Description of Ground and Excited States with Transcorrelated F12 Methods. *Journal of Chemical Theory and Computation*, *21*(20), 10329–10339. https://doi.org/10.1021/acs.jctc.5c01434

Masteran, C., Kumar, A., Teke, N., Gaudel, B., Yanai, T., & Valeev, E. F. (2023). Comment on "Canonical Transcorrelated Theory with Projected Slater-Type Geminals" [J. Chem. Phys. 136, 084107 (2012)]. *Journal of Chemical Physics*, *158*(5), 57101. https://doi.org/10.1063/5.0135257

Powell, S. R., Surjuse, K. A., Gaudel, B., & Valeev, E. F. (2025). Slimmer Geminals for Accurate F12 Electronic Structure Models. *Journal of Chemical Theory and Computation*, *21*(18), 8833–8842. https://doi.org/10.1021/acs.jctc.5c00971

Teke, N. K., Melekamburath, A., Gaudel, B., & Valeev, E. F. (2024). "Best" Iterative Coupled-Cluster Triples Model? More Evidence for 3CC. *Journal of Physical Chemistry a*, *128*(45), 9819–9828. https://doi.org/10.1021/acs.jpca.4c04667