NILS WENTZELL

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Research scientist and library developer focused on high-performance numerical software: algorithm development, API design, performance engineering, and cross-language library design in modern C++ (C++23/26) and Python. Lead developer of TRIQS, an open-source software stack for quantum many-body simulation, used by research groups worldwide (900+ citations to its founding papers, 500+ GitHub stars across its repositories): reusable C++ core libraries (nda, h5, mpi), a central framework, and 25+ domain applications. Deep HPC experience (multi-node MPI, OpenMP, SIMD, GPU-accelerated libraries); publications in PRX, PNAS, and Nature Communications.

Experience

Flatiron Institute
Simons Foundation
2018–present

Research Scientist (2023–present) · Associate Data Scientist (2018–2023),
Center for Computational Quantum Physics

- Lead developer of the TRIQS software stack (30+ repositories), owning technical direction, code review, and release coordination involving up to 15 developers:
  - Modernized the stack across the 2.x–3.x series: shipped the Python 3 migration, decomposed the monolith into standalone C++ libraries (nda, h5, mpi, itertools), built CI/CD running LLVM sanitizers, and packaged for conda-forge, Docker, Debian, and EasyBuild.
  - Shipped the 4.0 major release (2026): 25 synchronized application releases and the ecosystem-wide port to clair/c2py, a Clang/LLVM-based C++/Python binding generator.
- Software lead of nda, a C++23 N-dimensional array library used across the Flatiron Institute: authored the GPU foundation (device/unified-memory model; cuBLAS, cuSOLVER, cuTENSOR, MAGMA backends).
- Drive the development of continuous-time quantum Monte Carlo (CTQMC) impurity solvers, spanning implementation, algorithmic improvements, and performance optimization:
  - Designed a self-tuning sampling controller: online autocorrelation estimation, adaptive measurement spacing, automatic warmup detection.
  - Co-developed the inchworm solver; devised its importance-sampling schemes: proximity-biased operator insertions, order reweighting.
  - Generalized the low-rank determinant updates to batched, arbitrary-rank insertions and removals.
  - Delivered 2–50× CPU speedups in the rate-limiting higher-order correlation-function measurements.
- Co-developing TRIQS/DiagMC, a lattice diagrammatic Monte Carlo solver: reworked its determinant recursion; implemented and benchmarked physical response-function measurements.
- Algorithmic development and implementation of vertex-based quantum embedding schemes: TRILEX (PRX 2021, PRB 2021) and eMBEX (PRR 2024).
- Designed the solver API and Julia/Python interop for a tensor-network solver on ITensorNetworks.jl.
- Founded the TRIQS Summer School (50+ students); co-organize the TRIQS Community Meetings (100+ participants) and previously the institute-wide Sciware seminars; lead a working group on agentic coding for scientific software; supervise postdoctoral fellows; serve on hiring and computing committees.

CEA Saclay
2016–2018

Postdoctoral Researcher, Institut de Physique Théorique

- Joined the TRIQS core team: co-authored the 2.0 release; wrote the TRIQS/CTINT impurity solver from scratch, deriving its higher-order correlation-function estimators.
- Devised a compression scheme for the high-frequency asymptotics of higher-order correlation functions, now adopted across fRG and DMFT codes (PRB 2020).

U Vienna &
TU Vienna
2012–2016

Doctoral Researcher in Theoretical Condensed Matter Physics

- Authored fRGdyn, a C++ functional renormalization group code; developed correlated starting points for the method (PRB 2015) and algorithmic improvements for parquet-equation solvers (PRB 2016).

Education

PhD
2012–2016

Physics, University of Tübingen, Germany *[cum laude]*

- Thesis: Functional renormalization group beyond the perturbative regime.

M.Sc. & B.Sc.
2006–2012

Physics, RWTH Aachen University, Germany *[M.Sc. grade 1.1; 1.0 = best]*

- Studienstiftung des deutschen Volkes scholarship.

Skills

Programming

- Modern C++: 15+ yrs, C++23/26; concepts, ranges, compile-time & generic programming
- Python: 12+ yrs, NumPy/SciPy, Jupyter
- Library & API design; C++/Python bindings, Python/C API

HPC & Performance

- Parallelism: multi-node MPI, OpenMP; Slurm, Linux
- Libraries: BLAS/LAPACK, HDF5, FFTW, FINUFFT; GPU (cuBLAS, cuSOLVER, cuTENSOR, MAGMA)
- Optimization: profiling-driven (gperftools), SIMD vectorization, allocation strategies (stack-first, small-buffer), memory-access restructuring

Toolchain & Infrastructure

- Build & test: git/GitHub, CMake, GoogleTest
- CI/CD: GitHub Actions, Jenkins
- Packaging: Docker, conda-forge, Debian, EasyBuild
- Documentation: Sphinx, Doxygen
- Debugging & tooling: LLVM, sanitizers, LLDB
- Agentic coding: 1+ yr, Claude Code, Codex

Many-Body Methods

- Quantum embedding: DMFT & extensions, DFT+DMFT
- Impurity solvers: CTQMC, exact diagonalization, tensor networks
- Lattice diagrammatic Monte Carlo, Bethe–Salpeter & parquet equations, functional renormalization group, response-function calculations

Numerics

- Numerical linear algebra: matrix factorizations, eigendecomposition, low-rank matrix updates
- Compressed representations of correlation functions: asymptotics, orthogonal polynomials, low-rank/DLR, symmetry reduction
- Fourier transforms: FFT & nonuniform FFT (NUFFT)
- Markov chain Monte Carlo & statistical error analysis

Languages

- German (native), English (fluent), French (basic)

Selected Software Projects

- **TRIQS** (github.com/TRIQS/triqs) — lead developer; central framework of the TRIQS software stack.
- **nda** (github.com/TRIQS/nda) — software lead; C++23 N-dimensional array library; authored its GPU foundation.
- **clair/c2py** (github.com/flatironinstitute/clair) — co-developer; C++/Python binding generator, successor to cpp2py.
- **ctint** (github.com/TRIQS/ctint) — author; interaction-expansion CTQMC impurity solver.
- **h5, mpi, itertools** (github.com/TRIQS) — primary author; C++ utility libraries (HDF5 I/O, MPI, range adaptors).

Selected Publications

- T. Schäfer, **N. Wentzell**, *et al.* (26 authors), "Tracking the Footprints of Spin Fluctuations: A Multi-Method, Multi-Messenger Study of the Two-Dimensional Hubbard Model", Phys. Rev. X **11**, 011058 (2021)
- P. Cha, **N. Wentzell**, O. Parcollet, A. Georges, and E.-A. Kim, "Linear resistivity and Sachdev-Ye-Kitaev (SYK) spin liquid behavior in a quantum critical metal with spin-1/2 fermions", Proc. Natl. Acad. Sci. U.S.A. **117**, 18341 (2020)
- H. Suzuki, …, **N. Wentzell**, *et al.* (16 authors), "Distinct spin and orbital dynamics in Sr_2RuO_4", Nat. Commun. **14**, 7042 (2023)
- **N. Wentzell**, G. Li, A. Tagliavini, *et al.* (8 authors), "High-frequency asymptotics of the vertex function: diagrammatic parametrization and algorithmic implementation", Phys. Rev. B **102**, 085106 (2020)
- J. Vučičević, J. Kokalj, R. Žitko, **N. Wentzell**, D. Tanasković, and J. Mravlje, "Conductivity in the square lattice Hubbard model at high temperatures: importance of vertex corrections", Phys. Rev. Lett. **123**, 036601 (2019)

23 journal articles total (1 PRX, 1 PNAS, 1 Nat. Commun., 1 PRL, 12 PRB, 3 Phys. Rev. Res., 1 Comput. Phys. Commun., 2 J. Open Source Softw., 1 SciPost Phys. Codebases) · 1,200+ citations · h-index 15 (Google Scholar, Aug. 2026)

Selected Talks, Teaching & Community

- TRIQS Summer Schools (founder & tutorials, 2023, 2025); TRIQS Community Meetings (co-organizer, 2017–2019, 2022–2026)
- TRIQS tutorials: International Summer School on Computational Quantum Materials, Sherbrooke (2018, 2022, 2024, 2026); Simons Many-Electron Summer School, Stony Brook (2017, 2022); Arnold Sommerfeld School (2017)
- Modern C++ lectures & 2-day C++ bootcamp, Flatiron Institute; debugging & sanitizer talks, Simons Summer School
- C++ conferences: C++Now (2019), CppCon (2023, 2025; 2026 upcoming)
- NVIDIA DLI training: Fundamentals of Accelerated Computing with Modern CUDA C++ (full-day, 2025)