Jan Brandejs

Interdisciplinary Computational Scientist with 8+ years of experience architecting high-performance computing (HPC) solutions. My expertise lies in designing scalable, distributed tensor engines for GPUs—the computational core of both modern AI/Large Language Models and next-generation quantum simulations.

Project Spotlight: Tensor Lib Architecture for Science & LLMs

02/2025 certificate

- I was awarded the Marie Curie Fellowship **Seal of Excellence** with a 91% score.
- I architected a novel HPC tensor library for both fundamental science and **Large Language Model** (LLM) applications, targeting optimization for **Grace-Hopper** architecture.
- Group theory-based problem encapsulation, graph theory-based load balancing.

Work Experience

04/2022 - present
Postdoc **researcher in computational science**/theoretical chemistry
Prof. Trond Saue, *Laboratoire de Chimie et Physique Quantiques,* CNRS, Toulouse.
I architected and developed a novel tensor toolchain for an Advanced ERC grant:

- Enabled automatic optimization of tensor expressions in Coupled cluster method.
- **Distributed memory tensor contractions on GPUs**, excellent weak scaling.

01/2021 - 12/2021
fellowship+mobility grant. Prof. Örs Legeza, *Wigner RCP,* Budapest, Hungary.

- I implemented high-performance **Tree Tensor** Network State method, C++.

10/2018 - 12/2020
HPC **C++** developer, **MOLMPS** package, part of my PhD, *J.Heyrovsky Inst.* Prague.

- The first **MPI parallelization** of DMRG for chemists efficient to over 100 nodes.
- One of the three core developers.

01/2015 - 12/2018
Founding Software Developer, *SignoSoft,* Prague. signosoft.com. Part-time.

- Using **Recurrent Neural Networks**, I built the first machine learning-based car insurance recommender for VIG AG.
- I architected and developed a multiplatform PDF signing app. Angular+Java server.

Selected Publications & Conferences

10/2025
invited participant; NVIDIA Atomistic Simulation Summit 2025. *Santa Clara, USA*.

07/2025 paper
J. Brandejs, J. Pototschnig, T. Saue: Generating coupled cluster code for modern **distributed memory tensor software**; JCTC, vol. 21, 15, 7320–7334

06/2025 paper
P. Sehlstedt, J. Brandejs, P. Bientinesi, et al.: **Software Landscape** for DMRG; arXiv:2506.12629. Shortlisted in 'good reviews' by Prof. Tomotoshi Nishino.

06/2025 talk & award
Best poster prize, talk, **'customer' session**: TAPP - the BLAS for tensors. Recognized for presenting novel techniques at Reusable libraries in quantum chemistry 2025 conference. *Helsinki, Finland*; led a hands-on session for HPC developers, demonstrating a commitment to enabling the scientific software community.

11/2024 **Best poster nomination**. SC24 conference. *Atlanta, GA, USA.*

10/2024 paper *J. Visnak, J. Brandejs, M. Mate, L. Visscher, et al.*: **DMRG-tailored coupled cluster method** in the 4c-relativistic domain; JCTC, vol. 20 (20), p.8862–8875

06/2024 invited talk **Generating coupled cluster code** for modern distributed memory tensor software. JCS8 Theoretical Chemistry Symposium. *Hokkaido University, Japan*.

12/2023 paper *O. Demel, J. Brandejs, J. Lang, et al.*: Hilbert space **multireference coupled cluster tailored** by matrix product states; J. Chem. Phys., vol. 159, p.224115.

10/2023 contributed talk, 7th Users' Conference, IT4Innovations **(PRACE)**. *Ostrava, Czechia*.

01/2021 paper *J. Brabec, J. Brandejs, K. Kowalski, et al.*: **Massively parallel** quantum chemical density matrix renormalization group method; JCC, vol. 42, p. 534-544, 2021.

05/2020 paper *J. Brandejs, et al.*: Toward DMRG-tailored coupled cluster method in the **4c-relativistic domain**; J. Chem. Phys., vol. 152 (17), 2020.

04/2020 paper *J. Lang, A. Antalík, L. Veis, J. Brandejs, et al.*: **Near-Linear Scaling** in DMRG-Based Tailored Coupled Clusters; JCTC, vol. 16 (5), p. 3028–3040, 2020.

05/2019 paper *J. Brandejs, et al.*: **Quantum information-based analysis** of electron-deficient bonds; J. Chem. Phys., vol. 150, p 204117, 2019.

10/2018 paper *L. Veis, J. Brandejs, J. Pittner*: **Strongly correlated systems** and the DMRG method in quantum chemistry; Chemické listy, vol. 10, 2018, p. 655-666

Scientific Leadership, Teaching & Service

2021-2024 lecturer **Teaching**: Technical University Liberec. Lecturer: Introduction to Quantum Mechanics. Teacher's assistant: Physics for mechanical engineering, Physics for architects

09/2025 main organizer 2nd Toulouse Tensor Workshop. *Toulouse, France*. I envagelized and negotatied community standard interfaces and benchmarks for operations on tensors with known structure.

05/2024 main organizer CECAM Workshop on **Tensor Contraction Library Standardization**. *Toulouse, France*. I co-founded and led the workshop. Now leading an international **working group** to develop Reference implementation with scientists and experts from NVIDIA, AMD, Intel.

2023-2025 MaProLab: I established a project-based **Machine learning** course for Talnet network.

2022-present Pioneered a weekly online **python course** for children of Ukraine war refugees. *PeopleInNeed.*

2019-2021 International Young Physicist Tournament. National team Supervisor & prep course organizer.

Education

10/2016 - 03/2022 **PhD** in Theoretical Physics, *Charles University, Prague, Czech Republic*. **Tensor Network**-based Methods for Strongly Correlated Molecular Quantum Mechanics.

03/2020 - 06/2020 **Erasmus traineeship**. Topic: Relativistic DMRG in MATLAB and C++. *Wigner Research Center for Physics, Budapest, Hungary.* Group of Örs Legeza.

10/2014 - 09/2016 Theoretical Physics, *Charles University, Faculty of Mathematics and Physics*. master's degree. Optimizing quantum simulations and the DMRG method.

09/2015 - 12/2015 Master's exchange program. ***McGill University***, *Montreal, Canada*.

10/2011 - 06/2014 General Physics, *Charles University, Faculty of Mathematics and Physics*. bachelor's degree. Topic: **Quantum computing** in manybody physics.

Training

07/2024 Gray Scott school. **CUDA, SYCL, OpenACC, C++20**, Fortran 2018. *Toulouse.*

11/2023 LUMI hackathon. GPU profiling-Omniperf, compiling **OpenMPI**. onsite, *Krakow.*

06 & 10/2023 2 Frontier hackathons. **Profiling multi-GPU** ExaTENSOR with HPCToolkit. Debugging OpenMP+MPI code. I proved a bug in Cray MPICH: Meetings with HPE stilll ongoing.

11/2022 TREX HPC Training 2022. **StarPU**. *CALMIP, University of Toulouse, France.*

06/2022 **Deep learning with TensorFlow**. *iFORM BALMA, Toulouse, France.*

09/2019 Fundamentals of **Deep Learning for Computer Vision**. NVIDIA Deep L. Institute

11/2018 **Advanced OpenMP Programming**. *PRACE, Ostrava, Czechia.*

2017-2018 **Academic Writing in English**: 3-semester course. *Czech Academy of Sciences.*

11/2017 **Tensor Network School** 2017. *Ghent University, Belgium.*

Languages

Czech native
English proficient user *(C1/C2)*
French independent user *(B1/B2)*
Italian pre-intermediate