# Jan Brandejs

Computational Scientist with 8+ years of experience optimizing massively parallel algorithms for state-of-the-art supercomputers. Specialized in designing scalable, distributed tensor contraction engines on GPUs—the foundational technology of modern AI. Passionate about accelerating discovery in Quantum Physics and Chemistry by bridging the gap between research challenges and cutting-edge, scalable computing solutions.

## 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 inc.
- I architected and developed a multiplatform PDF signing app. Angular+Java server.

## 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.

## Leadership, Community & Service

11/2025 PC member
Invited member of the **Programme Committee** Algorithms & Performance. Selecting contributions. ISC High Performance 2026. *Hamburg, Germany.*

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.*

2021-2024
**Teaching**: Technical University Liberec. Lecturer: Introduction to Quantum Mechanics.

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

## 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.*

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

## Technical Skills

HPC **C++, MPI, OpenMP,** CUDA, SYCL, OpenACC, Python (NumPy, SciPy).

AI & Machine Learning TensorFlow, PyTorch; Computer Vision; Foundational knowledge of Generative AI & LLM architectures (Transformers)

Systems & Tools EuroHPC-class systems (LUMI, Frontier, Summit, Karolina); GPU Profiling & Optimization (Omniperf, HPCToolkit); Schedulers (Slurm); Containerization (Docker, Singularity).

## Top 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.*

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.

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.

## 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.

**Languages**

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