

Build and Benchmark Automation of libNEGF

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Introduction

- libNEGF [4] is enhanced and expanded in cooperation with CNR.
- Project aim: simulate solar cells with realistic defects for prototyping.

JUBE

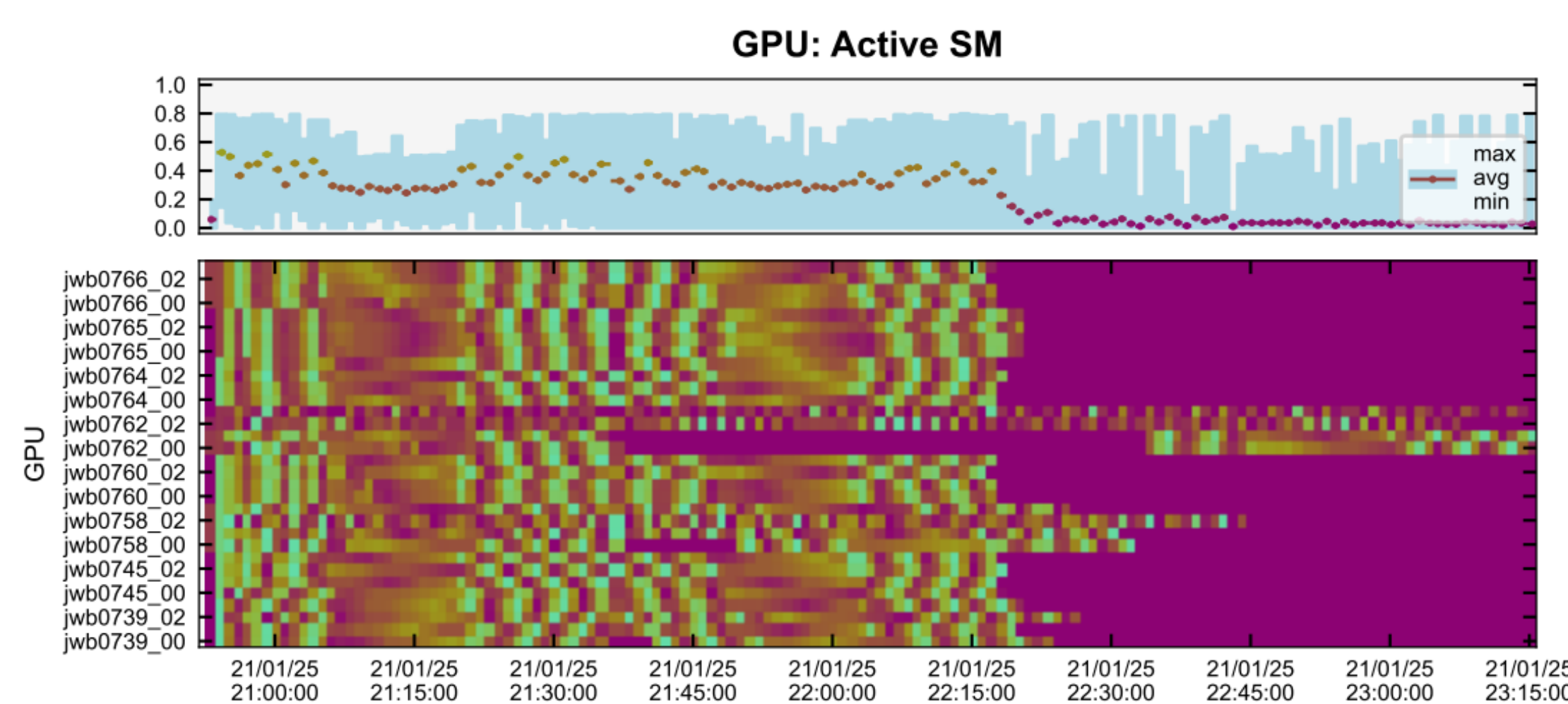
- With CI operational, JUBE was introduced to libNEGF [1, 2].
- Benchmarking data is posted to dedicated, monthly GitLab issues.
- As of today, there are thirteen issues with data about hundreds of runs.

Continuous Integration

- Continuous integration (CI) was set up.
- Every pushed change is built and tested in different environments.
- CI unconverged bugs, e. g., bugs in the C bindings of libNEGF.

Linux distribution	Rocky Linux 9, Debian 12
MPI implementation	MPICH, OpenMPI
Compute device	CPU, GPU (CUDA)

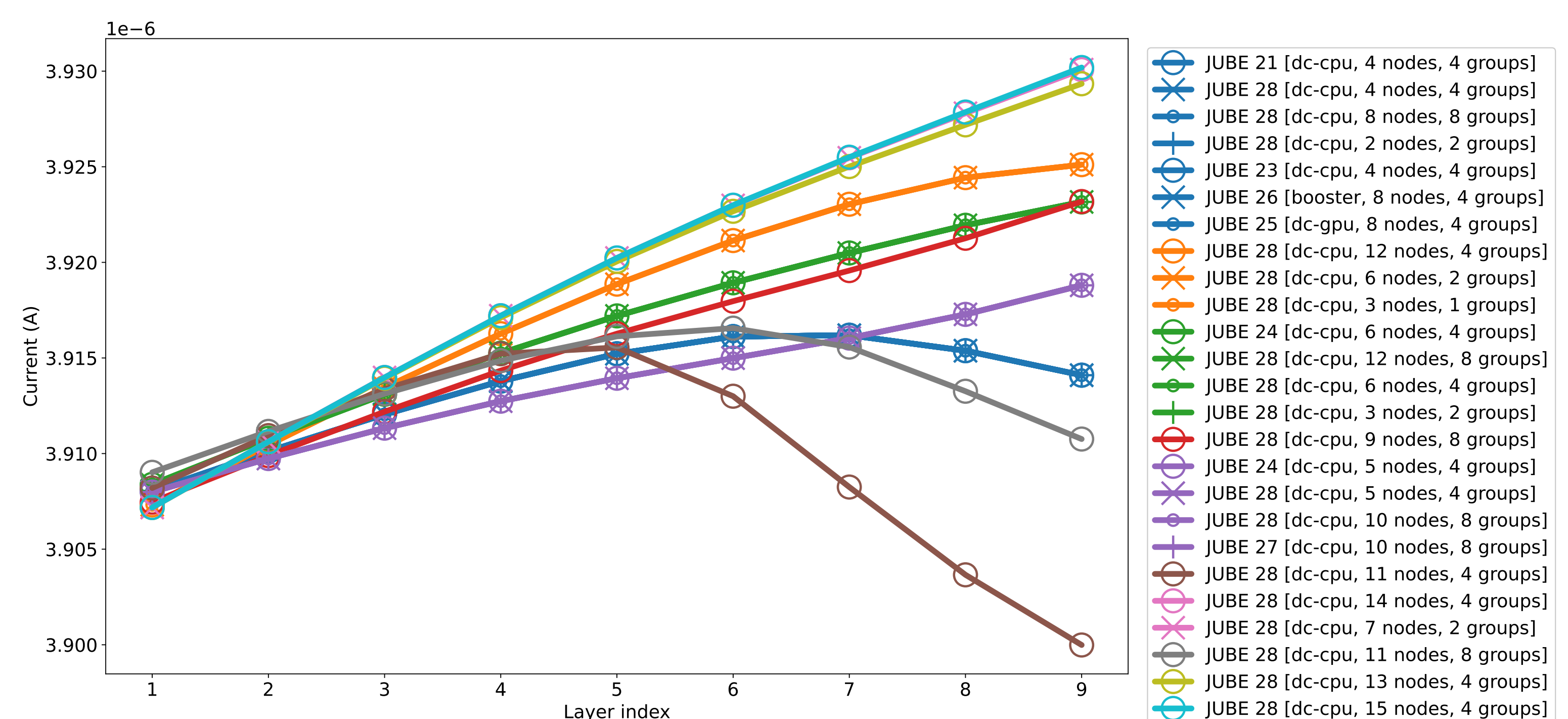
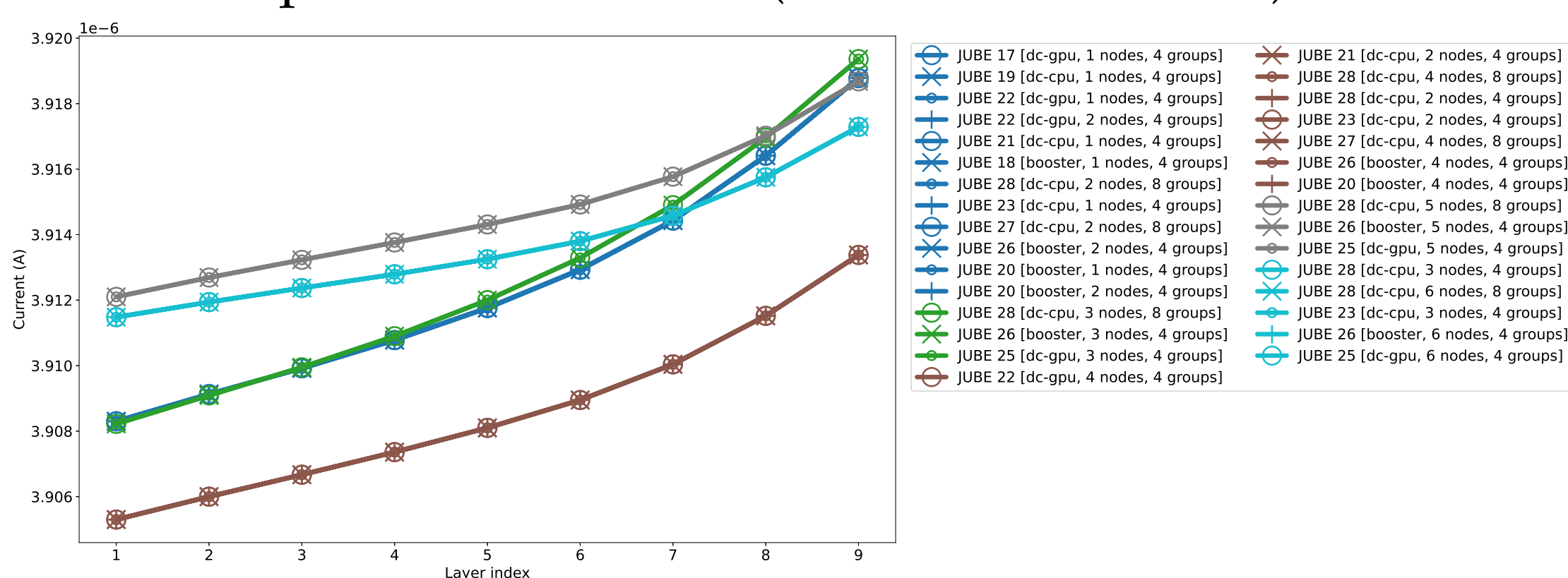
Tracking rare Performance Issues



- The project accumulated a large dataset of JUBE runs allowing to tackle seemingly random performance issues.
- The main symptom of the problem on JUWELS Booster shown left were idling nodes (purple) with the job reliably running into time-outs.
- Cause: quirks of JUWELS Booster hardware/software interaction.
- Problem resolved with the aid of LLview [3], JSC SC support.

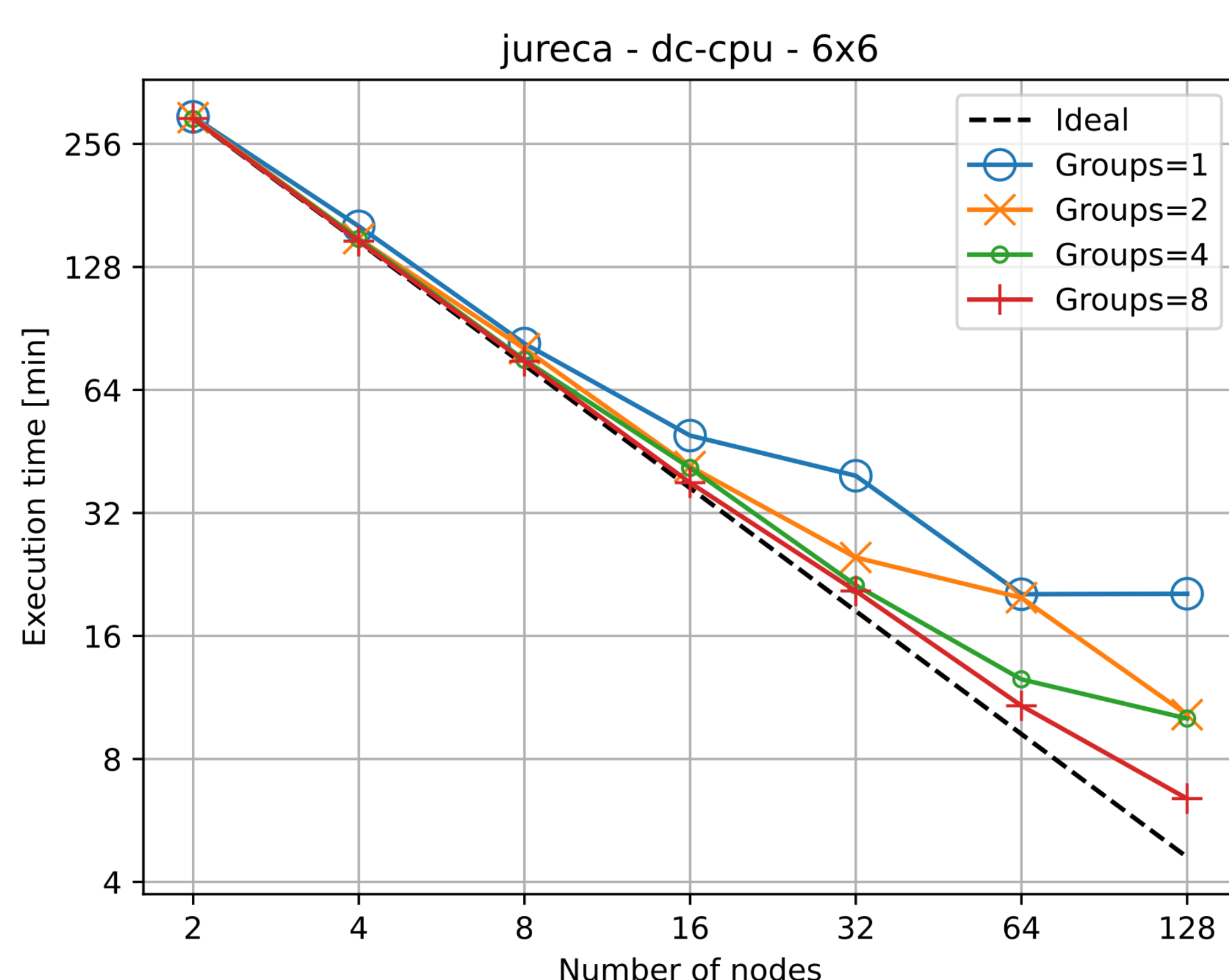
Diagnosing Bugs with More Runs

- With easier benchmarking, project members ran jobs with a greater variety of settings uncovering bugs in the process.
- Example: electric current depends on the node count with up to 1 % difference (far above tolerance).



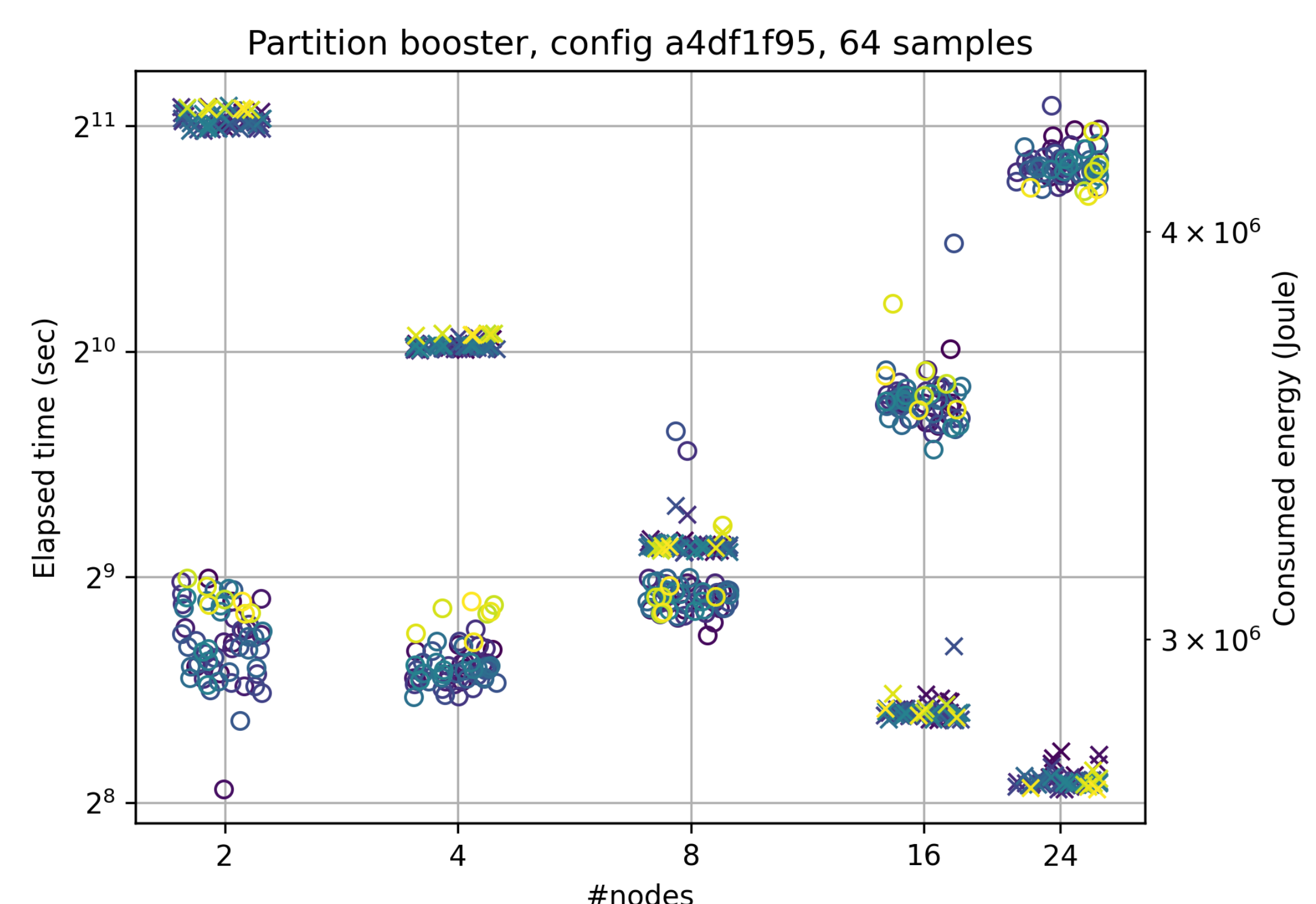
Analyzing Scaling

Based on the uniform format of JUBE benchmarking data, the project was able to implement a tool for analyzing scaling properties.



Continuous Benchmarking

- Continuous benchmarking (CB) launched in June 2025.
- Easy JSC set-up: Jacamar CI runners, GitLab pipeline schedules, JUBE
- Example: performance impact Sep'25 JUWELS Booster update (yellow)

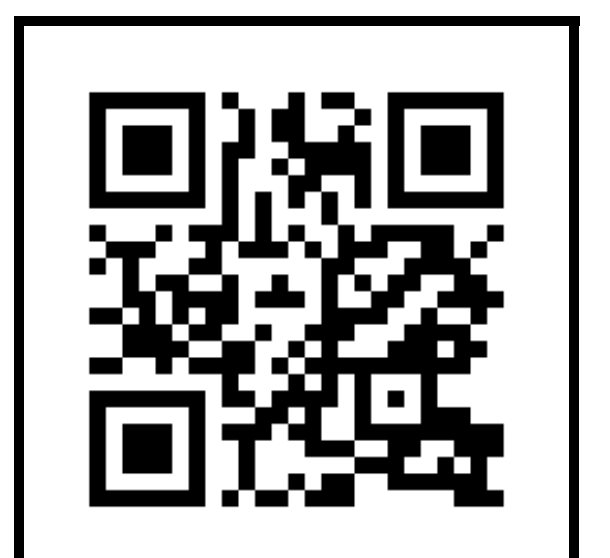


References

- [1] T. Breuer et al. *JUBE*. 2024. DOI: 10.5281/zenodo.7534372.
- [2] C. Conrads. "A CI/CB Setup for a Quantum Transport Code." *ISC High Performance 2025*. 2025. DOI: 10.34734/FZJ-2025-02874.
- [3] W. Frings et al. *LLview: User-level Monitoring in Computational Grids and e-Science Infrastructures*. 2007. HDL: 11858/00-001M-0000-0013-B103-7.
- [4] A. Pecchia et al. "Non-equilibrium Green's functions in density functional tight binding: method and applications." *In: New Journal of Physics* 10.6 (2008). DOI: 10.1088/1367-2630/10/6/065022.

Staying in Touch

- libNEGF: <https://github.com/libnegf/libnegf>
- My research group: SDL Quantum Materials
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EoCoE website

This project has received funding from the European High Performance Computing Joint Undertaking under grant agreement n°101144014.