Report on ACH-VTT activities

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Members:

- Fredric Granberg
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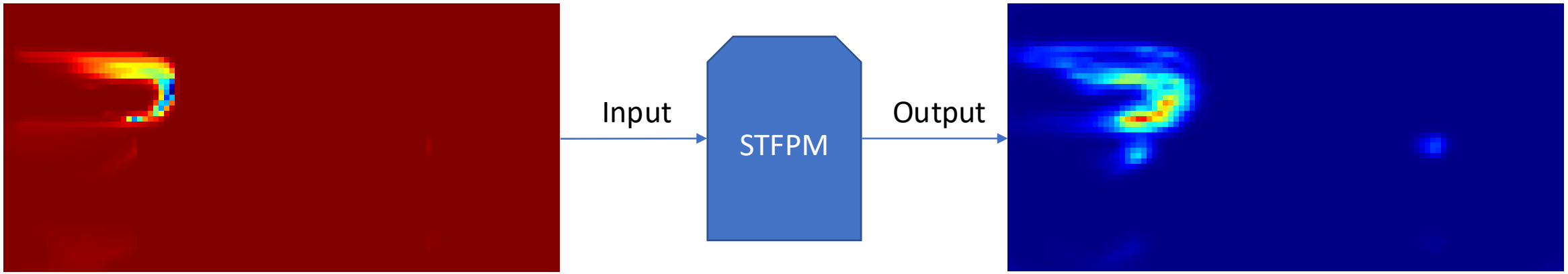
- Keijo Heljanko
- Aaro Järvinen
- Jan Åström
- Laurent Chôné
- Oskar Lappi
- Bruno Cattelan
- Daniel Jordan
- Emil Amnell
- Ville-Markus Yli-Suutala

Funders and Collaborators

Anomaly Detection

Using Student-Teacher Feature Pyramid Matching method for automated anomaly detection and localization

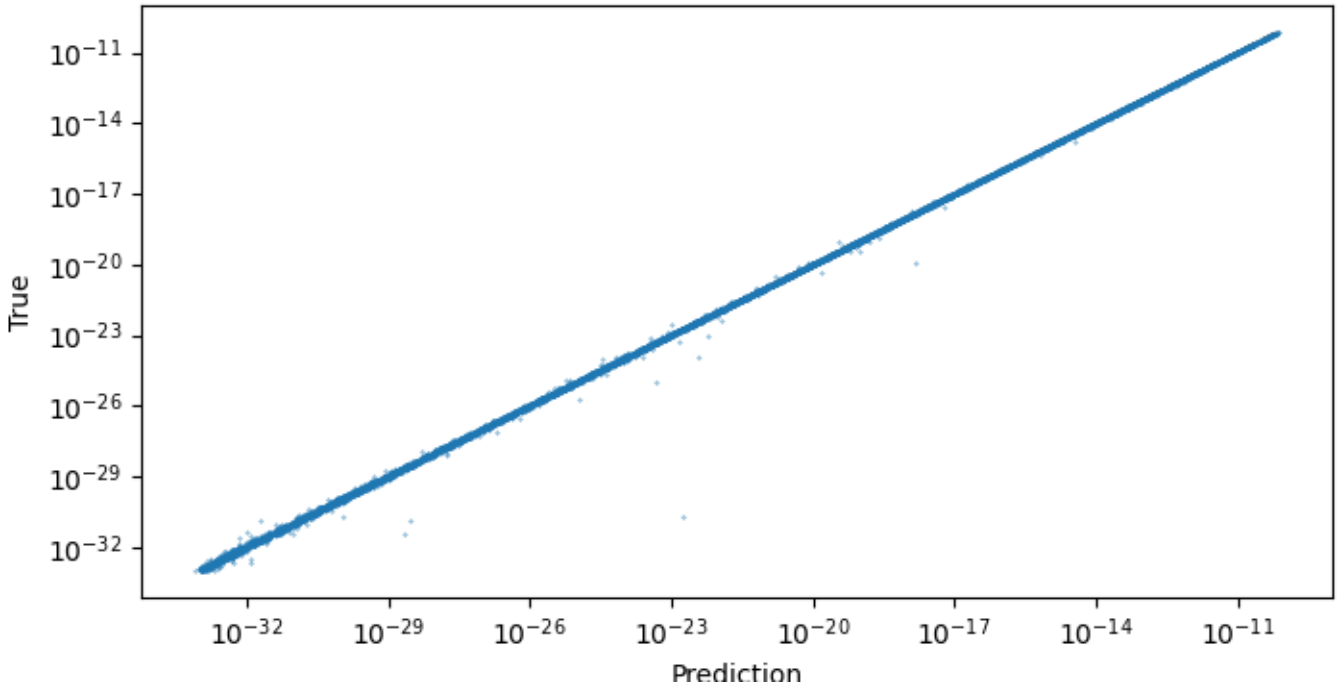


Simulation Grid as Image

Anomaly Map as Image

Dreicer Runaway

Improving existing results of previous work to estimate the Dreicer runaway generation rate in a plasma with heavy impurities



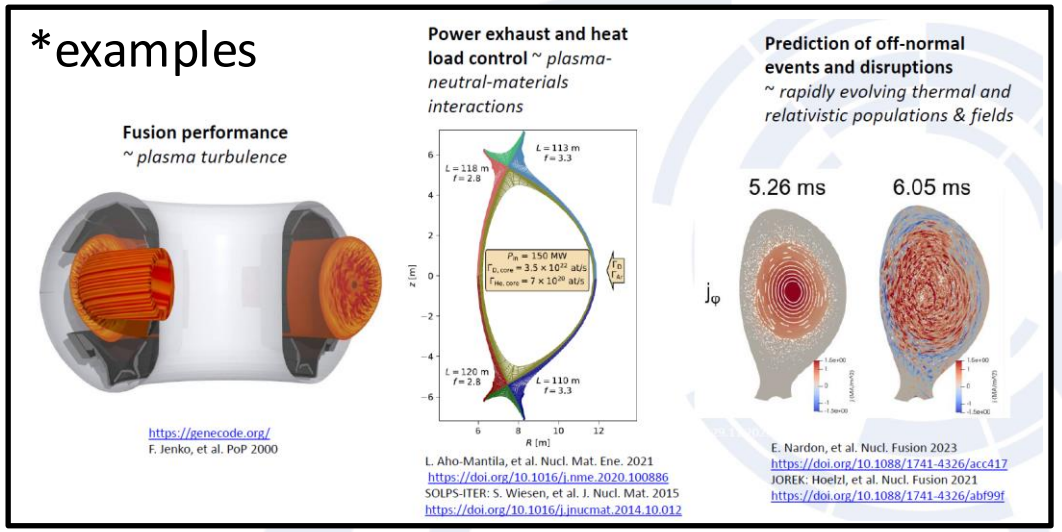
Cases:

- No Impurity
- Ne,
- Ar,
- He
- B
- C
- N
- O
- Fe
- Be
- W
- Kr
- Xe
- Mix

Computational models with uncertain parameters are ubiquitous in fusion energy research*

Given limited resources (CPUh / human time), how to optimally quantify the uncertainties?

E.g. in large-scale model validation or scenario prediction applications

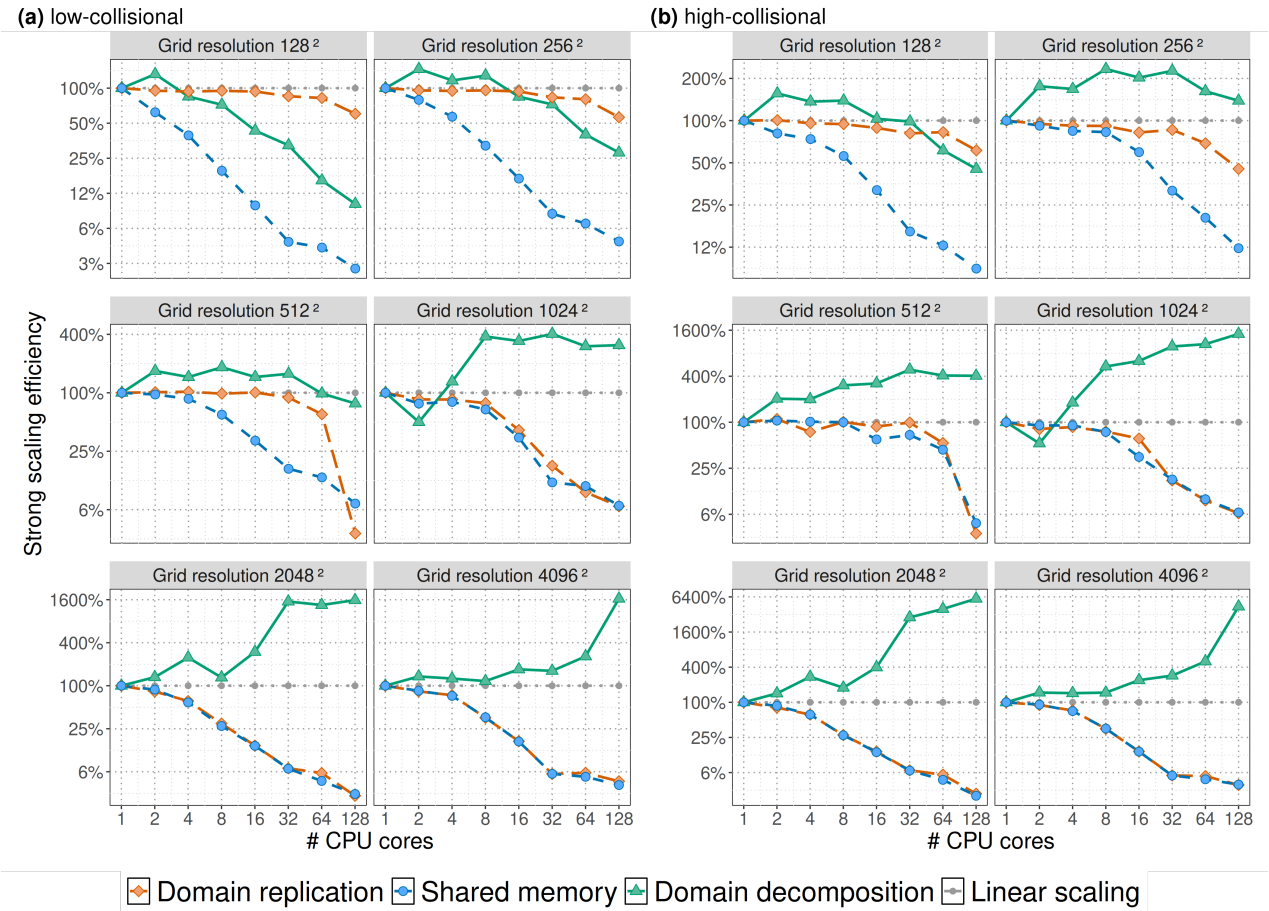


- Simulation-based inference (SBI) algorithms have emerged to address the need for statistical inference with complex simulators [Cranmer, PNAS 2020 https://www.pnas.org/doi/epdf/10.1073/pnas.1912789117]
- **The ACH-VTT team has investigated application of various SBI methods for application with complex simulators connected to the EUROfusion TSVVs: Bayesian Optimization, Neural Likelihood/Posterior, Sparse-grid methods.**

➢ Bayesian Optimization for validation of runaway electron simulations, A.E. Järvinen JPP 2022, https://doi.org/10.1017/S0022377822001210]
➢ Webinar on Bayesian optimization for validation of computationally demanding models in fusion https://indico.euro-fusion.org/event/3042/
➢ Efficient uncertainty quantification in plasma micro-instability simulations with mode transitions, D. Jordan, EPS 2025
➢ Bayesian optimization for efficient parameter space coverage with computationally demanding simulations in fusion energy applications, A.E. Järvinen, IAEA Fusion AI Workshop 2023, https://conferences.iaea.org/event/335/contributions/28998/
➢ Simulation-based inference for validation of computationally demanding models in fusion energy applications, A.E. Järvinen, ICDDPS5 2024
➢ Towards scalable large-scale model validation with data science, A.E. Järvinen, AAPPS-DPP 2025
➢ Bayesian likelihood-free inference for effective uncertainty quantification in plasma physics simulators, E. Amnell, MSc Thesis 2025
➢ Framework actively developed and available at https://github.com/DIGIfusion/enchanted-surrogates

Domain decomposition scalability results

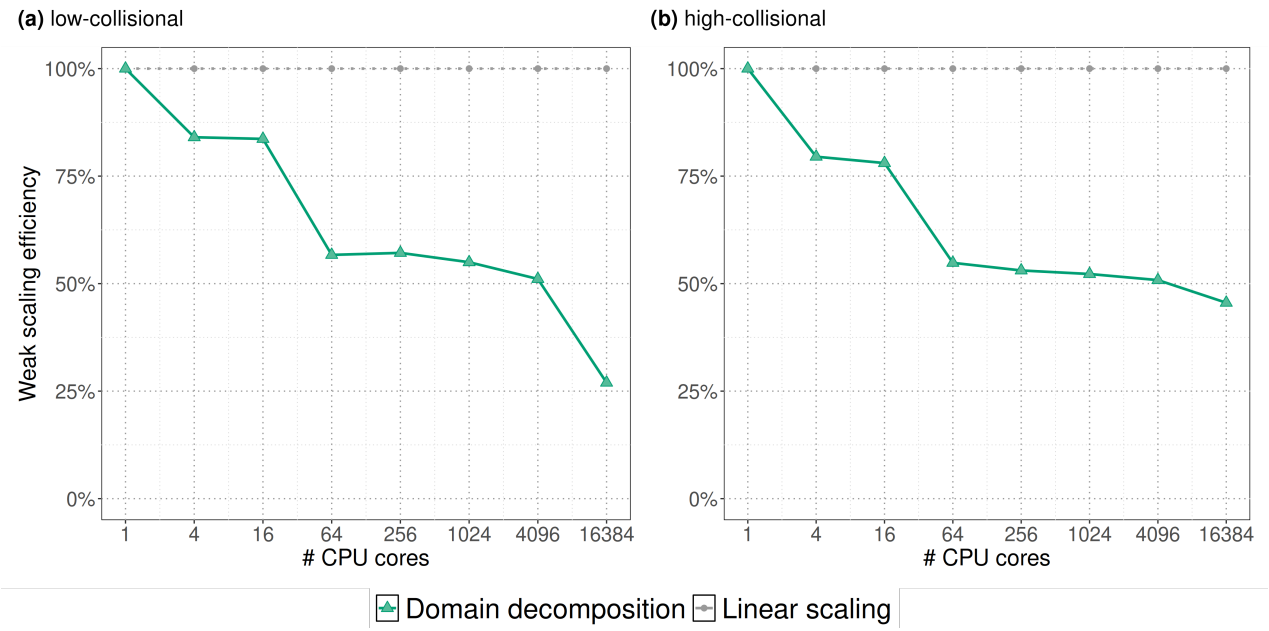
Eiron, a reduced version of EIRENE has been used to show advantage of domain decomposition (DD) compared to existing EIRENE parallelization



In the above log-log figure, strong scaling efficiency is shown across grid resolutions and collision regimes. DD strong scaling is superlinear.

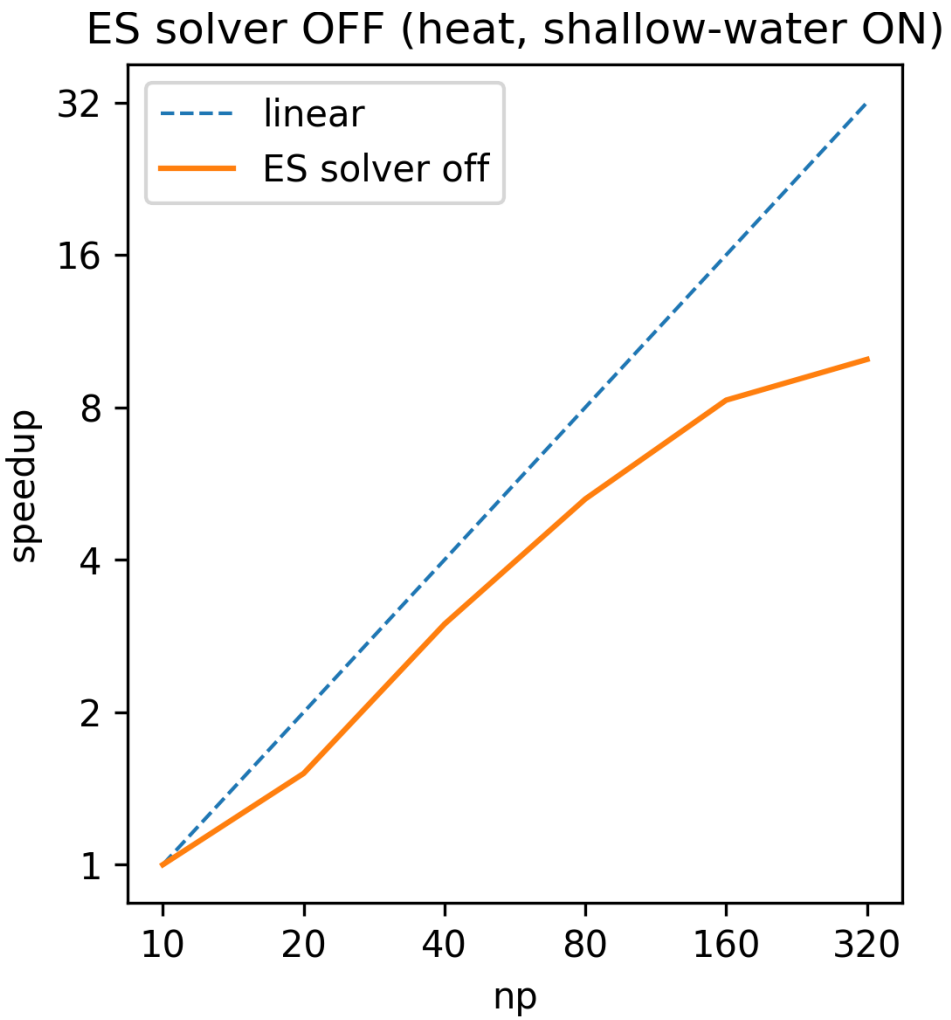
Domain decomposition scalability results

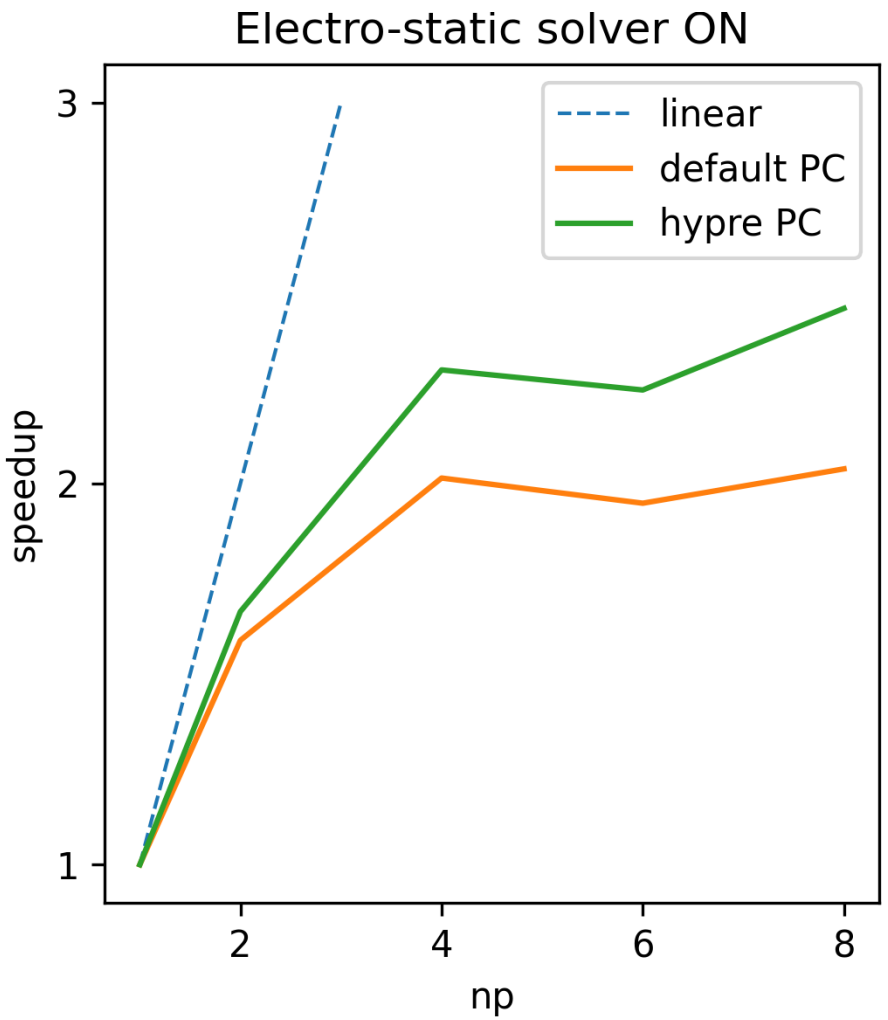
The weak scaling is also good, at 16384 CPU cores it is around 50% for high-collisional cases, 25% for low-collisional cases.



More results in a paper titled *Scalable Domain-decomposed Monte Carlo Neutral Transport for Nuclear Fusion*, by Lappi et al., submitted to the Journal of Computational Physics. It is available on the pin board.

- Checkpointing/restart and MPI parallel features added to Memento
- ES solver MPI scaling hampered by limited PC options through AMReX Fortran interface





- Kokkos port of fix electron stopping for LAMMPS
- tabGAP GPU enabled with Kokkos, neighbor list sorting to improve cache use