SPEEDING UP SCIENCE THROUGH PARAMETRIC OPTIMIZATION ON HPC CLUSTERS

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OUR RESEARCH AT GSI

Parametric Optimization for Quantum Physics
Problem: Lattice Quantum Chromodynamics (QCD) simulations are computationally expensive

Goal: Effective quantum field theories for QCD

Method: Transformation to effective degrees of freedom in terms of unknown parameters (LEC)

Challenge: How to determine the LECs efficiently through optimization?
THE GENEVA
OPTIMIZATION LIBRARY

Large-scale Parametric Optimization in Distributed Environments
PARAMETRIC OPTIMIZATION WITH GENEVA

- Open-source framework in C++ for parametric optimization
- Focus on distributed execution: grids, clouds, clusters
- Used at GSI for QCD research
- Recently: MPI Consumer for distributed execution on HPC clusters: https://doi.org/10.1007/s41781-023-00098-6
- Today's Presentation: Performance of MPI Consumer

github.com/gemfony/geneva
gemfony.eu
PARALLELIZATION IN GENEVA

Graphic taken from our paper: https://doi.org/10.1007/s41781-023-00098-6
PERFORMANCE OF THE MPI CONSUMER

Comparison with Boost.Asio and Boost.Beast Consumers
On a Single 128-core Machine
BOOST.ASIO CONSUMER

• LIMITED SCALABILITY
• TYPICALLY AT GSI: 5+ SEC EVALUATION TIME
BOOST.BEAST CONSUMER WITH 64 THREADS
IMPROVED SCALABILITY
MPI VS. BEAST

- IMPROVEMENTS FOR ALL RELEVANT WORKLOADS
MPI CONSUMER PERFORMANCE

On GSI's Green IT Cube HPC Cluster

Photo: G.Otto, Image rights: GSI Helmholtzzentrum für Schwerionenforschung GmbH
GSI's green IT cube:
- >400 nodes
- 56-256 cores and 128GB-1TB RAM each
- Slurm workload manager

Test setup:
- 400 distributed clients
- Mean over 10 measurements
- \text{\textasciitilde} Compare results with results on multicore machine

TESTS ON HPC CLUSTER
DIFFERENCE OF 128-CORE MACHINE AND CLUSTER

MEASUREMENTS ARE REPRODUCIBLE ON CLUSTER WITH MINIMAL ERROR
Geneva optimization library handles large-scale problems

Better user experience for HPC because of MPI Consumer

MPI Consumer system design to be published in *Computing and Software for Big Science*:
[https://doi.org/10.1007/s41781-023-00098-6](https://doi.org/10.1007/s41781-023-00098-6)

Improved Scalability:
Even more efficient than ASIO/BEAST Consumers
FUTURE WORK

- MPI Consumer to be brought in production on GSI’s Green IT Cube cluster with 1000+ clients
- More optimization algorithms and metrics for Geneva optimization library
- Paper about performance evaluation in Proceedings of Science (PoS)
BACKUP SLIDES
MPI CONSUMER SCALABILITY
SERVER WITH 64 THREADS RUNNING ON 128-CORE MACHINE
MPI COMPARED WITH BOOST.ASIO CONSUMER

RELATIVE IMPROVEMENT
BENEFIT OF ASYNC CLIENT REQUESTS

Relative Improvement

Detailed explanation in our previous publication:
https://doi.org/10.1007/s41781-023-00098-6
IMPACT OF THREAD POOL SIZE

SYSTEM EFFICIENCY

Detailed explanation in our publication:
https://doi.org/10.1007/s41781-023-00098-6
MEAN ABSOLUTE ERROR ON 128-CORE MACHINE

- 10 MEASUREMENTS PER DATA POINT
- 400 CLIENTS
MEAN ABSOLUTE ERROR HPC CLUSTER

- 10 MEASUREMENTS PER DATA POINT
- 400 CLIENTS