WP1: “TH” tasks
1.4 1.5 1.6

Michelangelo Mangano, CERN TH
Andreas Jüttner, CERN TH

Task 1.4: Tensor Networks for Quantum Systems

year	goals	deliverable	resources
1	Benchmark execution performance of quantum circuit simulations using tensor networks and state-vector techniques.	Setup quantum simulation techniques on classical hardware for the IT infrastructure described in 1.2 Develop a tensor network algorithm for quantum simulations with more than 37 qubits.	1 LD+support for collaborations (visits, etc)
2	Compare the performance of tensor networks and state-vector simulations on large qubit systems.	Develop and deploy quantum circuit simulations for large systems, up to O(100) qubits, using tensor networks and state-vector techniques.	same
3	Benchmark the performance of quantum machine learning models to classical AI counterpart.	Develop quantum machine learning models for trigger applications with the possibility of deployment on large systems.	same
4	Achieve efficient and reliable quantum machine learning models for supervised and unsupervised learning.	Publish a study of the quantum machine learning foundations: from model building to efficient optimizers.	same
5	Determine to which extent FPGAs are beneficial for quantum circuit simulation in comparison to CPUs and GPUs.	Prototype of tensor network and state-vector simulators on FPGA using hls4ml.	same

Note:

- **LD** applications received, review committee formed, short-list formed, further input from external experts being collected, deadline of Febr 26. Expect offer out by early March

Task 1.5: New computing strategies for data modeling and interpretation

1.5 (a):

- porting and optimization of current event-generation codes and higher-order perturbative calculations to state-of-the-art and future hardware architectures, particularly GPUs
- development of ML/AI strategies to accelerate and improve the efficiency of phase-space sampling and the estimation of matrix elements driving the events' unweighting;
- AI-driven modeling of the non-perturbative aspects of pp collisions, eg underlying event, the hadronization and the multi-parameter tuning of shower-evolution algorithms;
- Advanced HPC tools, in addition to NNs already exploited, to accelerate ancillary tasks such as the global fitting of PDFs
- Further work, of direct impact on the trigger studies, may include the optimization of theoretically robust clustering algorithms portable to FPGAs.

1.5 (b):

- development of software and algorithms for efficiently exploiting next-generation computer architectures (e.g., NVidia Grace Hopper) for use in LQFT simulations on extreme-scaling low-latency/high-bandwidth accelerator-based clusters.

Task 1.5 (a): Event generators acceleration

Tasks and deliverables: as outlined in previous slide, distributed across the years depending on priorities and progress, as assessed during regular Workshops, interactions with experiments and with MC developers community, relying also on ongoing activities in the context of the LHC MC WG. Specific projects under discussion with MCnet management

Resources:

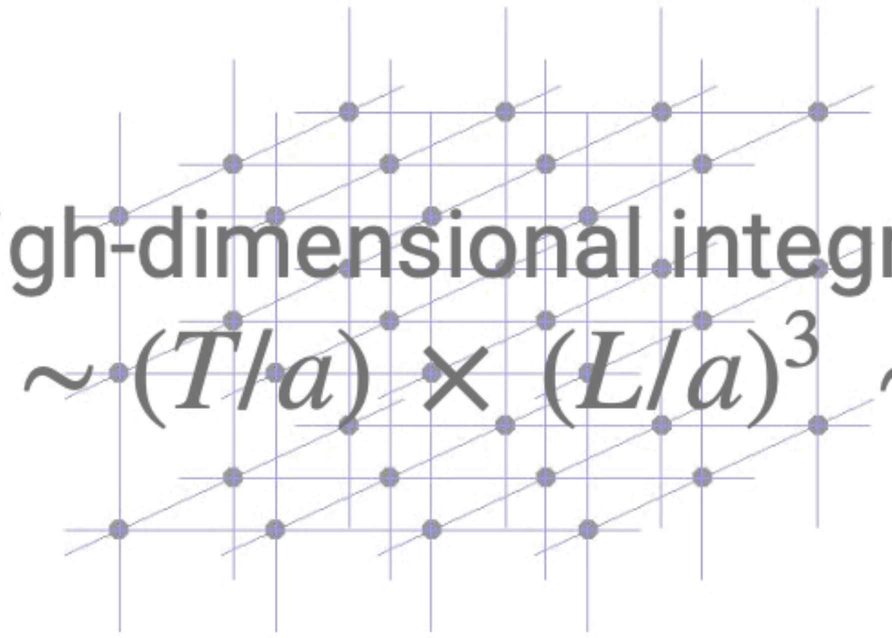
- 1 Quest and 1-2 Origins, jointly supported with Task 1.7, assigned to collaborate in IT in the context of ongoing Madgraph2GPU project
- Support for short/long term visits of colleagues from MC developers community

Lattice QCD

Nonperturbative contributions to precision physics (α_S, $g-2$, B-physics MEs, PDFs, …)

$$\langle 0|O|0\rangle \quad = \quad \frac{1}{Z}\int \mathcal{D}[U,\psi,\bar{\psi}]Oe^{-S_{\text{lat}}[U,\psi,\bar{\psi}]}$$

- discretise 4d space time
- sparse problem (next-neighbour)
- ideally suited for extreme-parallelism



high-dimensional integral:

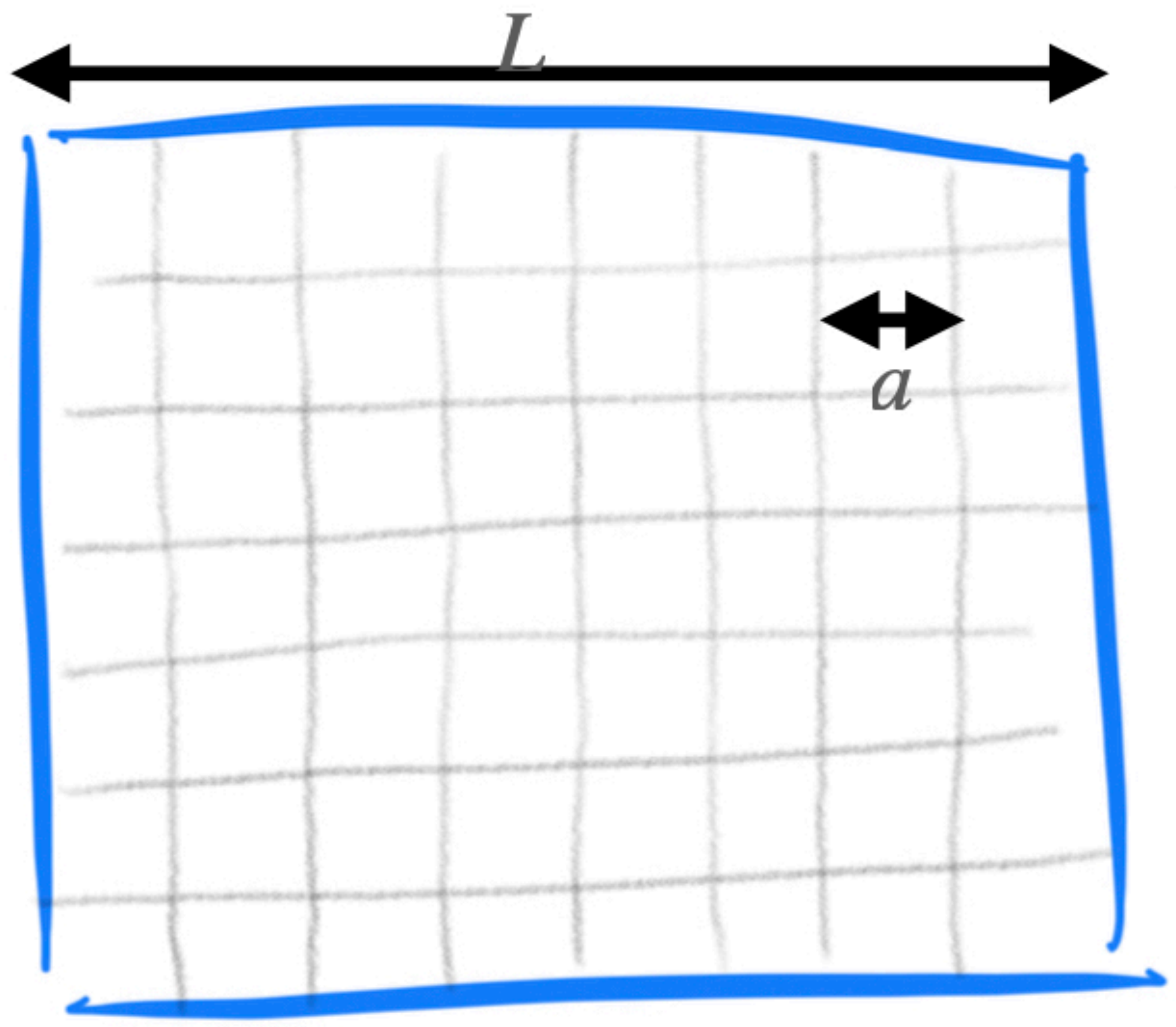
$$N_{\text{sim}} \sim (T/a) \times (L/a)^3 \sim 10^9$$

Two core computational steps:

- generate field configurations (Hamiltonian Monte Carlo)
- compute quark propagators (Krylov-space solvers)

Lattice QCD

$\frac{1}{L} \ll$



$\ll \frac{1}{a}$

Bigger lattice → control finite-volume effects

smaller lattice spacing → control cutoff effects

Larger lattice size limited by memory/computing power

Smaller lattice spacings in addition is theoretically hard (critical slowing down)

in any case: Physics + Machine ↔ algorithm development
Focus of WP 1.5

Example HPC environment

DiRAC Tursa @ Edinburgh

- 6 CPU nodes
- 114 GPU nodes each with 4x NVIDIA A100-40
- 64 GPU nodes each with 4x NVIDIA A100-80
- GPU Nodes: 1,024 GB per node
- CPU Nodes: 256 GB per node
- 4xMellanox 200 Gbit/s HDR IB per node with a fat tree topology

Typical production job-size 1-16nodes but scaling can go beyond

Benchmark code used for various procurements exists
https://github.com/paboyle/Grid

Expertise and input for WP1.1

Task 1.5 (b): Lattice HPC algorithms

year	goals	deliverable	res's
1	Provide benchmarking support with lattice QFT codes guiding hardware procurement and commissioning for HPC hardware.	- Organization of community Workshops - Develop LQFT benchmarking software tailored to hardware infrastructure procured under 1.1. - Share expertise on parallelism and accelerator-based algorithms with TH/IT/CMS/ATLAS	1 TH LD
2	- Devise and execute hardware commissioning upon delivery & installation. - Port code and optimize LQFT simulation performance for new hardware that is being procured.	- sign-off of new HPC cluster assuming new hardware performing to specs - show optimised parallel scaling performance of LQFT codes on new hardware	same
3	- Optimise LQFT simulation algorithms for procured and future hardware. - Improve LQFT simulation algorithm performance in large-volume and investigate variance-reduction techniques for hadronic matrix elements.	- Show LQFT code-performance improvement. - Improvements of signal-to-noise ratio in hadronic matrix elements	same
4	- Develop variance-reduction techniques for hadronic matrix elements in LQFT in large volume and combine with spectral-reconstruction techniques.	- Improvements of signal-to-noise ratio in hadronic matrix element and study of systematics in spectral reconstruction	same
5	-Develop understanding of viability of spectral reconstruction techniques.	- application of LQFT to spectral-reconstruction problems.	same

Note:

- **LD** applications received, review committee formed, short-list formed, further input from external experts being collected, deadline of end-Febr. Expect decision by early March

Task 1.6: New Physics scenarios and SM properties as trigger benchmarks

- In collaboration with the experiments, develop benchmarks to evaluate the enhanced sensitivity of NGTs to New Physics scenarios and on the determination of fundamental SM properties (eg Higgs couplings)
- Will propose concrete BSM models, as well as model-independent anomaly searches. In addition, will determine to which extent the next-generation triggers improve the precision of the determination of SM parameters.
- These concrete physics targets will allow for a robust performance assessment, validation and optimization of NGTs.
- As a spin-off of the required simulation activities, expect algorithmic improvements of event-generation codes

year	goals	deliverable	resources
2	Defining clear NP observables of specific relevance to new triggers, with a clear understanding of performance of current triggers	- Development of New Physics benchmark scenarios with exotic detector signatures - Evaluation of the current sensitivity based on the current triggers	1 TH fellow
3	Liaise across the project to determine planned next generation trigger performance.	- Development of SM benchmarks - Cooperation with ATLAS/CMS experimentalistsand evaluation of the improved performance on the benchmarks	same
4	Benchmark new trigger performance.	- Model-independent anomaly search and assessment of the new trigger performance - Comparison of current and next-generation triggers on precision SM measurements (eg Higgs boson couplings)	same

Note: fellow to be selected during 2024 Fall round. Start date no later than Fall 2025

Contacts

- Temporary overall coordinator for tasks 1.4, 1.5a and 1.6: michelangelo.mangano@cern.ch
    - will be replaced for task 1.4 by the appointed LD
- Temporary contact for the lattice component of Task 1.5: andreas.juttner@cern.ch
    - may be replaced for task 1.5b by the appointed LD