

# the ExaLAT project

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# aims

*... to redesign high priority simulation codes and algorithms to fully harness the power of future supercomputers, keeping UK research and development at the forefront of high-performance simulation science...*

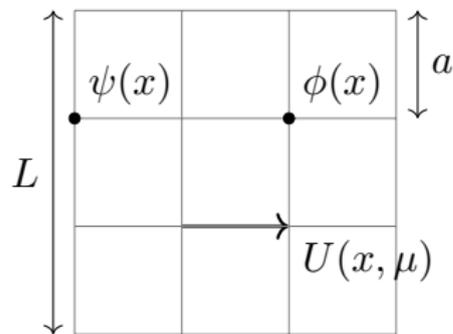
- **hardware:** future supercomputers
- **science:** scientific goals with 10-100x increase in resources
- **benchmark:** identify simulation codes/algorithms and bottlenecks
- **algorithms:** migration, co-design, separation of concerns
- **data:** volume of data, curation of data
- **training:** develop a portfolio, new challenges/opportunities
- **people:** role of RSEs, career path

# towards Exascale machines

## a few examples

- Piz Daint (CSCS - Switzerland) – 25 Pflops  
Intel Xeon + P100 NVIDIA GPUs + Cray Aries network
- JEWELS BOOSTER (Jülich - Germany) – 85 Pflops  
AMD Rome + 3,744 A100 NVIDIA GPUs + Infiniband 200 Gbit/s
- LUMI (Kajaani - Finland) – 552 Pflops  
AMD Epyc + AMD Instinct GPUs + Cray Slingshot 200 Gbit/s

# qft on a lattice



$$Z = \int \mathcal{D}U \mathcal{D}\psi \mathcal{D}\bar{\psi} \mathcal{D}\phi e^{-S[U, \psi, \bar{\psi}, \phi]}$$

couplings at the scale  $\mu = a^{-1}$ :  $g, am, \dots$

MonteCarlo evaluation of interesting observables: control  
stat and sys errors

# lqft action

$$S = \int d^D x \bar{\psi}(x) D \psi(x) \longrightarrow S_L = a^D \sum_{x,y} \bar{\psi}_{x\alpha}^a \left[ D_{x\alpha,y\beta}^{ab} \psi_{y\beta}^b \right]$$

$D_{xy}$  is a sparse matrix:

$$D_{xy} = \frac{1}{2a} \sum_{\mu} \gamma_{\mu} \left( U(x, \mu) \delta_{x+\mu,y} - U(x - \mu, \mu)^{\dagger} \delta_{x-\mu,y} \right)$$

where

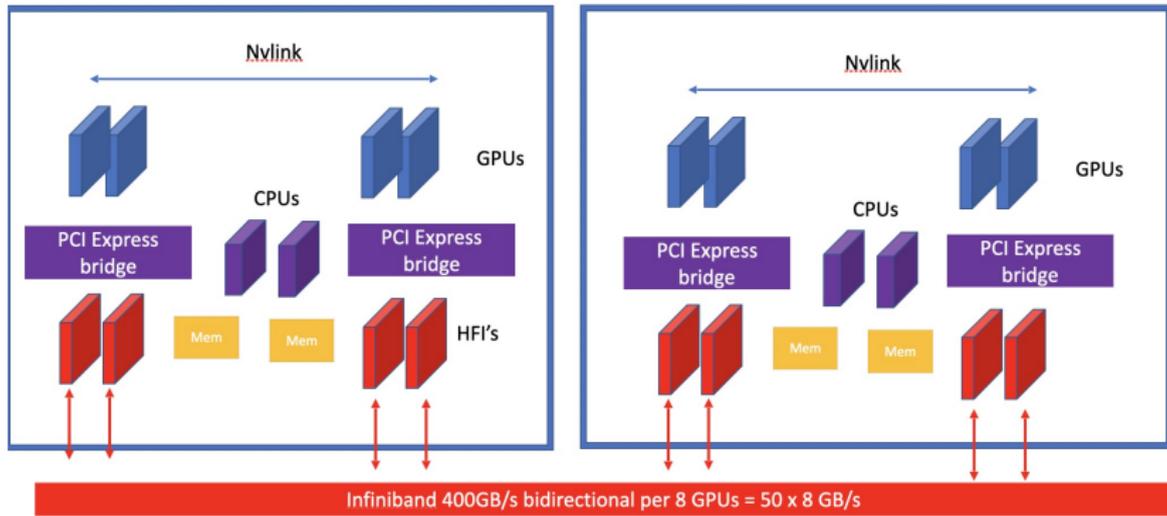
$$U(x, \mu) \in \text{SU}(3)$$

for  $64^3 \times 128$  lattice:  $\sim 100$  GB

one application of  $D$  is 50 GFlop

**Measured:** 200GB/s for 8 GPUs (Juelich zero-copy put)

**Promised:** Improved result – **expect** 340GB/s but **not proven** – *headroom for code optimisation*



# science opportunities

- light quarks: radiative corrections, rare decays, hadronic scattering
- heavy quarks:  $1/a > m_b$  precision HQ physics
- finite temperature QCD
- BSM strongly interacting theories – composite Higgs
- holographic models of cosmology: NP regime of 3d qft
- these projects require  $O(10)$  Pflops\*yr

# benchmarks

meeting 08/09/2020

- identify a set of standard codes that are relevant for the Lattice Field Theory Programme and extract representative benchmarks that will be maintained as a part of the project
- adapt the benchmarks to the most relevant architectures, as they become available
- ensure that the benchmarks remain relevant by implementing all the algorithmic improvements that become available in the lifetime of the project
- identify figures of merit and key performance indicators on current architectures that can be used to characterise performance on the upcoming architectures

# algorithms

meeting 19/08/2020

- support the community effort to identify innovative algorithms and methodologies that are best suited to exploit the parallelism necessary to reach efficient Exascale computing usage
- investigate novel algorithms developed in complementary research fields (data science, big data) that can have a positive impact in our research field
- identify the possibility of a joint coding effort to extend some of the most widely spread community simulation platforms towards better compliance with the Exascale candidate hardware
- contribute to the identification of coding paradigms that have the potential of exploiting hardware efficient usage while preserving portability of the codes

# data curation

meeting 19/08/2020

- tap into HEP experiments know-how
- Rucio/irods for data management, “data lakes”?
- it is **hoped** that containers will facilitate reproducibility and portability
- workflows/databases, new code designed with data curation in mind
- data needs to be available to international collaborators
- opportunity for joint activities between the two WGs

# training

meeting 22/07/2020

- develop new material – survey the existing material...
- training of a cohort of scientists/professionals
- organise one (TWO) schools, one hackathon
  - 15-16/02/2021: GPU programming
  - 01-05/03/2021: executable binariesfeedback from the schools very important
- work in collaboration with other WGs

# schools and registration

- Schools:

GPU coding for lattice practitioners (15-16.02.2021)

[link to gpu](#)

A pedestrian introduction to executable binaries (01-05.03.2021)

[link to binaries](#)

- Registration:

[link to gpu](#)

[link to binaries](#)

# people

- people are *central* to all these activities
- RSE are engaged in all aspects of the ExaLAT Programme
- RSE can engage with MSc and/or industry
- how do we sustain these people? (job description, career path)