MSA SEMINAR: GPUS

Topics and Talks

- **Today (5 May):**
  Scaling Lattice QCD on many GPU Nodes of JUWELS (Eric Gregory, JSC, and Mathias Wagner, NVIDIA)
- Next (19 May):
  Plasma Physics with PIConGPU – Lessons learned from 10 years of living with the HPC hardware zoo (Michael Bussmann, HZDR)

→ https://fz-juelich.de/ias/jsc/msa-seminar

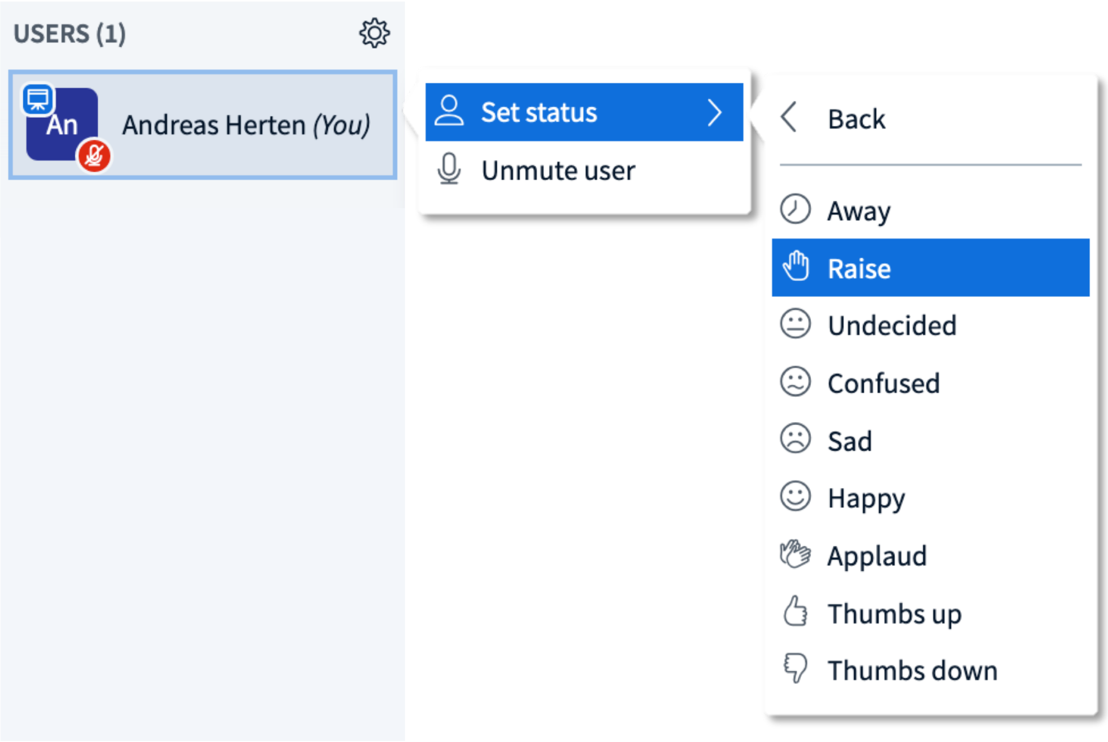
→ https://fz-juelich.de/ias/jsc/msa-seminar-slides

- After that:
  - ParFlow
  - GROMACS
  - Deep Brain
  - *JUWELS Booster*

ONLINE WEBINAR SETUP

Topics and Talks

- Webcams disabled to preserve bandwidth
- Questions welcome
  - During talk: As messages in chat
  - After talk: Everyone will be able to unmute themselves and ask;
    indicate by raising hand to be called
- *This is new for us, feedback welcome!*



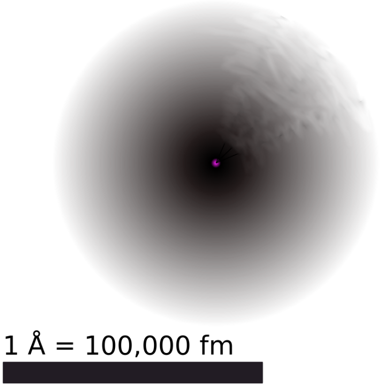
LATTICE QCD ON JUWELS GPUS

May 5, 2020 | Eric B. Gregory | JSC

OVERVIEW

- Quarks & gluons
- Lattice QCD basics
- LQCD community software
- *QUDA*
- Experience with LQCD on Juwels GPUs

QUANTUM-CHROMODYNAMICS (QCD)



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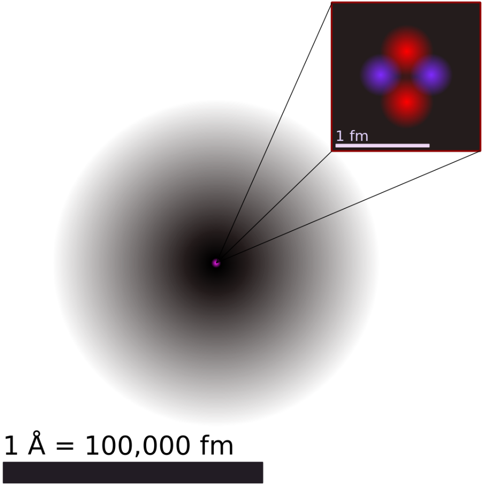
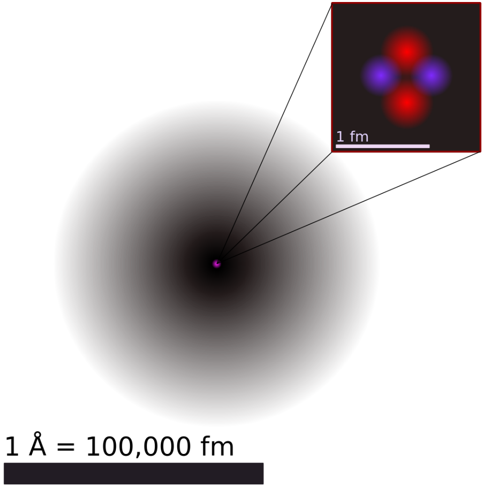
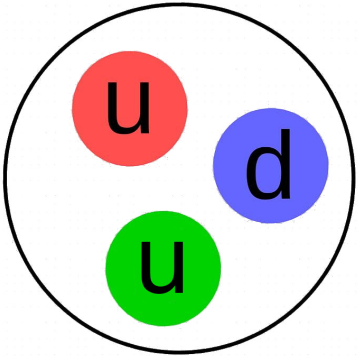


QCD





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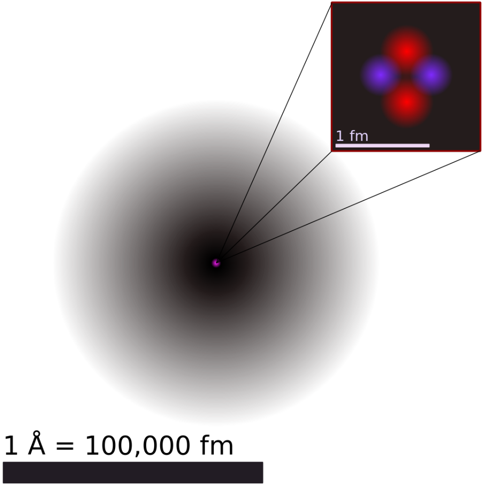
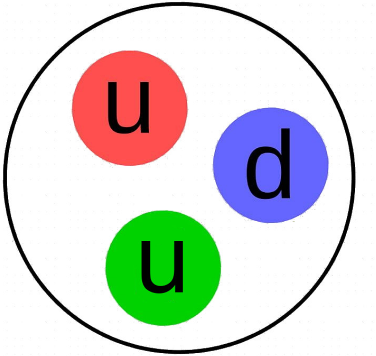
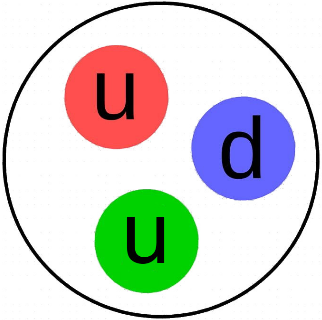




Proton is a *hadron*, a particle made of quarks bound together by the strong force.

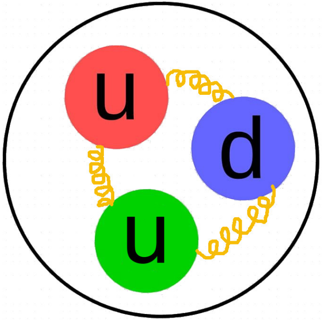
QCD



In the proton are:

- Quarks
  - Spin
  - Electric charge $+\frac{2}{3}/-\frac{1}{3}$
  - Color charge (R B G)

QCD



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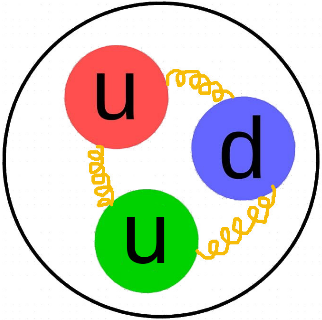

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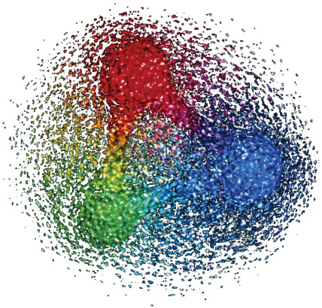

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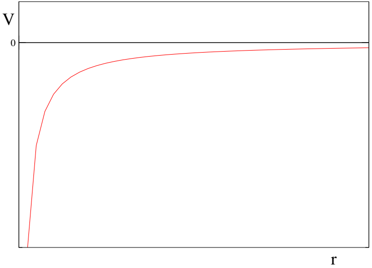
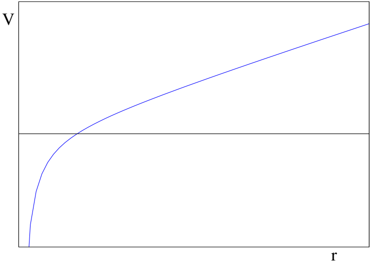
- Quantum fluctuations

LONELY ELECTRONS, BUT NO LONELY QUARKS





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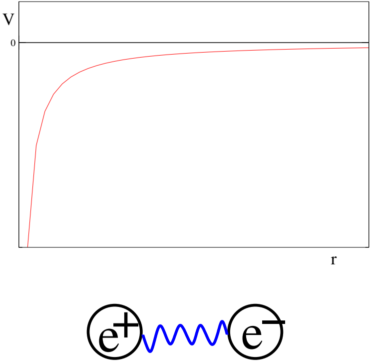

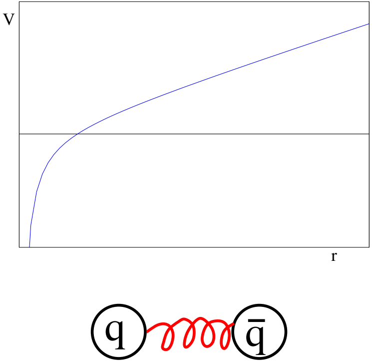

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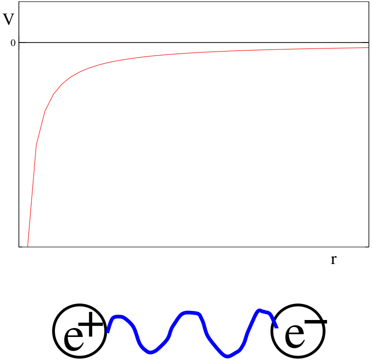

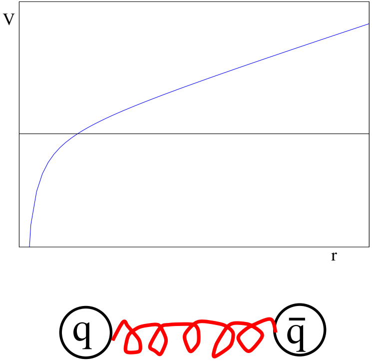

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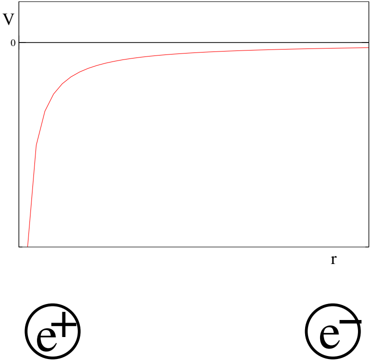

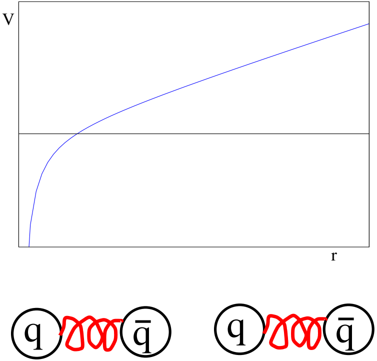

“Color-confinement”

QUANTUM FLUCTUATIONS ARE IMPORTANT!

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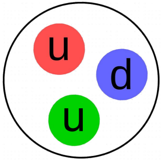

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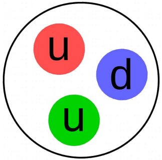

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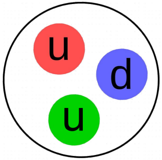

$$
\begin{array}{llll}
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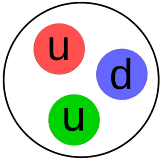

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But ...

$$M_{\text{proton}} = 938\ \text{MeV}$$

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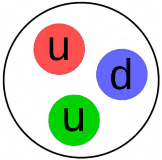

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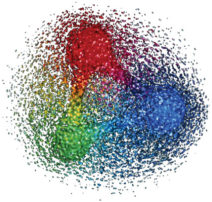

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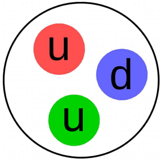

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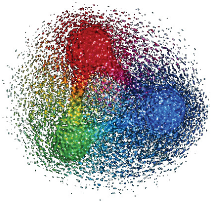

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To understand properties of hadrons, we must take quantum fluctuations into effect.

WHAT CAN WE HOPE TO CALCULATE?

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- **Properties of hadrons**
  - **mass**
  - **internal structure**
  - **decay probabilities**
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JÜLICH Forschungszentrum

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- **BIG QUESTION:**

  Does

$$\{\text{experiment}\} - \{\text{theory}\} \stackrel{?}{=} 0$$

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Physics beyond the Standard Model?

QCD ACTION

In the continuum:

$$S_{\mathrm{QCD}} = \int d^4x \frac{1}{4} F^a_{\mu\nu} F^a_{\mu\nu} + \sum_f \int d^4x \overline{\psi}_f(x) \left(i\gamma_\mu D_\mu - m_f\right) \psi_f(x) = S_G + S_F$$

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Depend on gluon fields.

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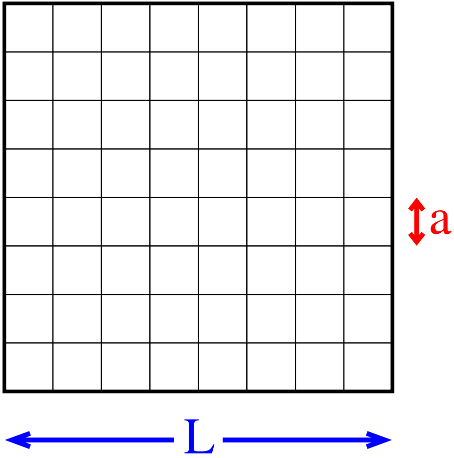
We calculate physical quantities by "path-integral" formulism:

$$\langle \mathcal{O} \rangle = \frac{\int \mathcal{D}\left[\overline{\psi}, \psi\right] \mathcal{D}[A]\, \mathcal{O} \mathrm{e}^{-iS[\overline{\psi}\psi A]}}{\int \mathcal{D}\left[\overline{\psi}, \psi\right] \mathcal{D}[A]\, \mathrm{e}^{-iS[\overline{\psi}\psi A]}}$$

LQCD BASICS

Perform non-perturbative calculation for a universe that

- is finite in size (with some boundary conditions)
- is discrete (Lattice!)
- has imaginary time $t \longrightarrow it$



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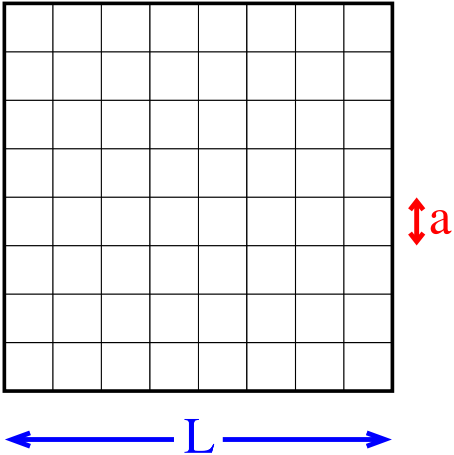

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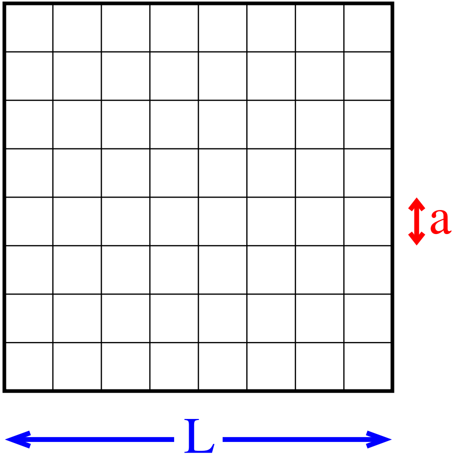

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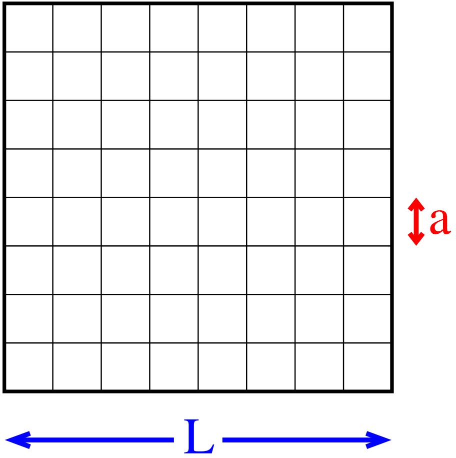
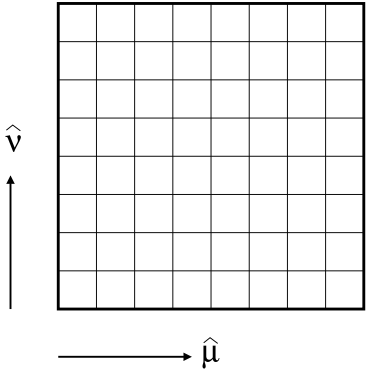
*Necessary mathematical trick — allows calculation of *some* quantities.



QCD ON THE LATTICE



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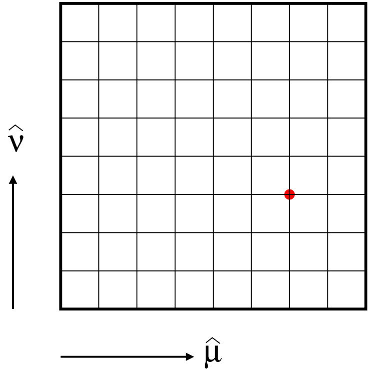
- Quark fields $\phi(x)$ live on lattice sites
  3 (or 3×4)-component, complex:

$$\phi(x) = \begin{pmatrix} \phi_0 \\ \phi_1 \\ \phi_2 \end{pmatrix}$$



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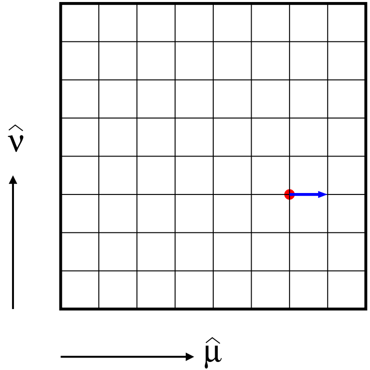
- Gauge fields $U_\mu(x) = \exp(iagA(x))$
  live on links: (3×3)-component, complex

$$U_\mu(x) = \begin{pmatrix} U_{00} & U_{01} & U_{02} \\ U_{10} & U_{11} & U_{12} \\ U_{20} & U_{21} & U_{22} \end{pmatrix}$$



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THE FERMION MATRIX

The continuum action term

$$S_F = \sum_f \int d^4x \overline{\psi}_f(x) \left(i\gamma_\mu D_\mu - m_f\right) \psi_f(x)$$

contains derivative which are discretized, e.g.:

$$S_F = \sum_f \sum_{xy} \overline{\phi}^f_x \left(\gamma_\mu D_\mu + m_f\right)_{xy} \phi^f_y$$

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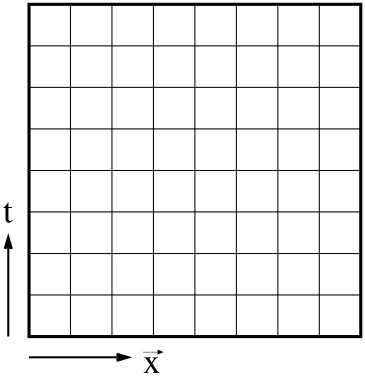
- Very large (dim$\sim 10^7$—10^8), sparse
- Major steps in LQCD workflow require solving $\phi_x = M_{xy}^{-1}\psi_y$

LQCD WORKFLOW

- Generate an ensemble of *lattice gauge configurations* with statistical weight

$$e^{-\tilde{S}[U]} = \det M[U] e^{-S_g[U]}$$



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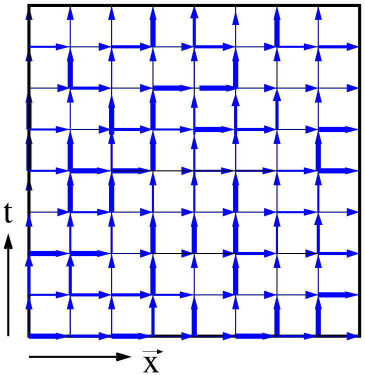

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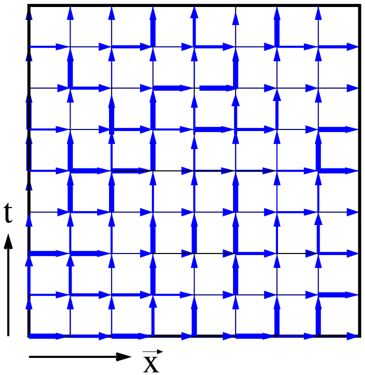

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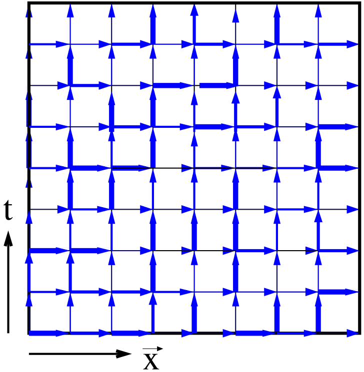
- Average of measurements is Euclidean path intergral calculation of expectation value

$$\langle \mathcal{O} \rangle = \frac{1}{N} \sum_i^N \mathcal{O}_i \exp\left[-\tilde{S}_{\mathrm{Euc}}\left\{U_i\right\}\right]$$



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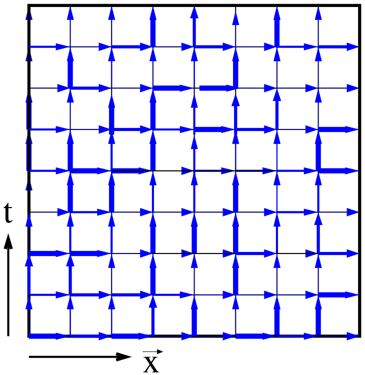
LQCD WORKFLOW

- Generate an ensemble of *lattice gauge configurations* with statistical weight

$$e^{-\tilde{S}[U]} = \det M[U] e^{-S_g[U]}$$

- measure some operator $\mathcal{O}_i$ on each configuration i
- Average of measurements is Euclidean path intergral calculation of expectation value

$$\langle \mathcal{O} \rangle = \frac{1}{N} \sum_i^N \mathcal{O}_i \exp\left[-\tilde{S}_{\mathrm{Euc}}\left\{U_i\right\}\right]$$



In the limits $N \longrightarrow \infty$, $L \longrightarrow \infty$, $a \longrightarrow 0$ this is equivalent to the path integral:

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int \mathcal{D}[\overline{\psi}, \psi, A] \mathcal{O}(\overline{\psi}, \psi, A) e^{-iS_{\mathrm{QCD}}[\overline{\psi}, \psi, A]}$$

LQCD community software

Stack of codes and libraries designed to provide common functionality, optimized for a wide range of HPC architecture.

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QMP

⟵ Message passing

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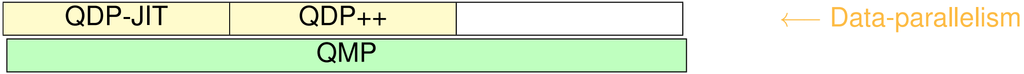

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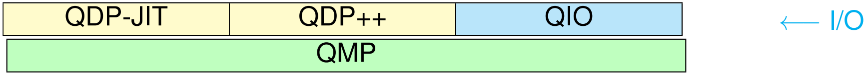

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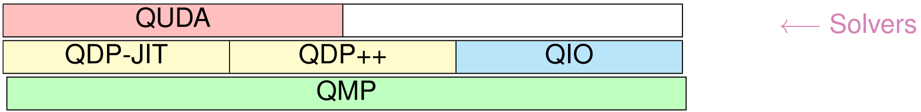

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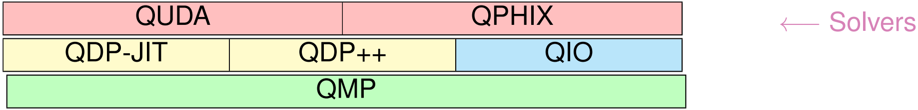

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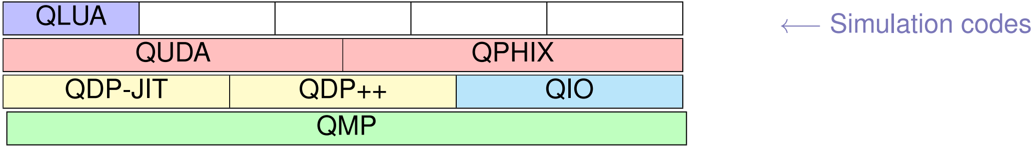

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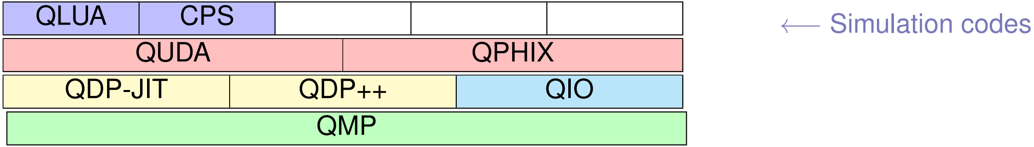

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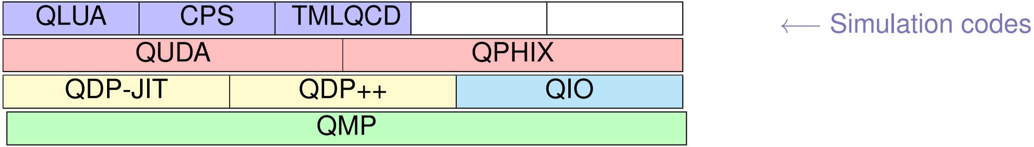

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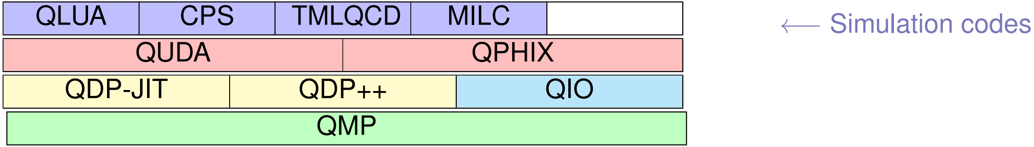

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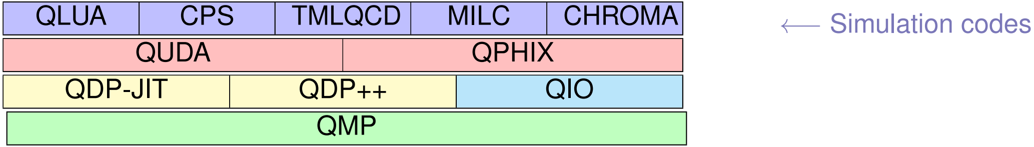

INSTALLED SOFTWARE

On JUWELS, Chroma is installed with:

MPI	QDP	Solver
MVAPICH2	qdp-jit	QUDA
MVAPICH2	qdpxx	QUDA
PS-MPI	qdp-jit	QUDA
PS-MPI	qdpxx	QUDA
PS-MPI	qdpxx	QPHIX (AVX512)

On JURECA, Chroma is installed with:

MPI	QDP	Solver
PS-MPI	qdpxx	QPHIX (AVX2)
PS-MPI	qdpxx	QPHIX (AVX512)

- Load `Stages/Devel-2019a` stages to test
- Request activation of features, other simulation codes, complaints $\longrightarrow$ Eric
- or request installation scripts from Mathias, Eric

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MODULAR SUPERCOMPUTING

In development:
QMOD library
interface designed for

- LQCD task-parallelism across different architectures
- exchange of lattice data structures between separate communicators
- lattice field I/O $\longrightarrow$ intercommunicator data exchange

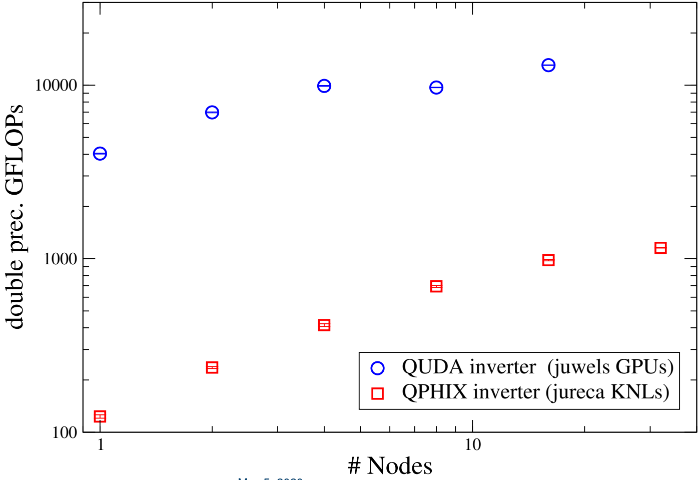
Example application: group of nodes of one architecture solves quark matrix system, passes solutions (propagators) to a separate hardware group which begins assembling them into multi-nucleon correlation functions.

And now to Mathias...

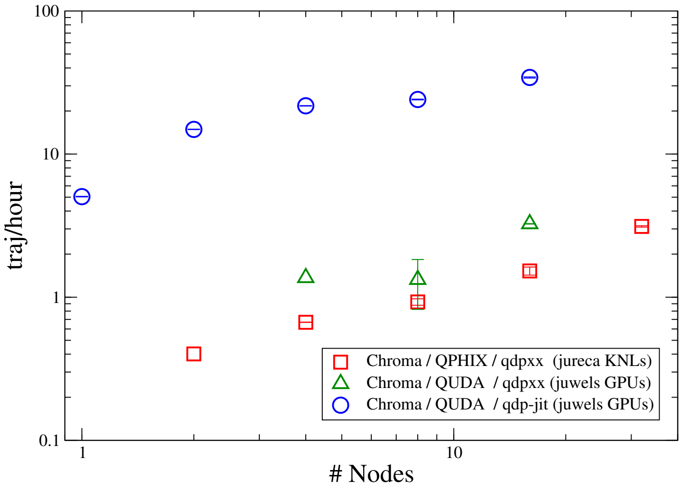
Some results and experiences

SOLVER STRONG SCALING COMPARISON

$32^3 \times 64$ lattices



HMC THROUGH-PUT COMPARISON



SPECTROSCOPY EXPERIENCE

Determine hadron masses

- Use QUDA solver
- pass solutions of $y = M^{-1}x$, to Chroma's generic "hadron-spectroscopy" routine
- solution vectors are joined in a element-wise products — "contractions" — similar to scalar product

Problem:

- contractions are *Memory intensive!!!* — did not fit on 4 nodes of GPU memory

Solution:

- Compile CHROMA with QUDA, but `qdpxx`, rather than `qdp-jit`
- Contractions remain on CPU
- $\sim 3\times$ as much memory on host as in the associated 4 GPUs

CONCLUSIONS

- Lattice QCD commmunity software maps physics problems to hardware in an optimized yet flexible way.
- QUDA solver library makes Juwels GPU nodes ideal platform for LQCD
- Solver performance on Juwels GPU node $\sim 60\times$ faster than KNL node.
- Focus on fine-tunining placement of calculation elements on optimal hardware in an heterogeneous system.

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- Focus on fine-tunining placement of calculation elements on optimal hardware in an heterogeneous system.
- *Stay healthy!*