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!
OVERVIEW

- Quarks & gluons
- Lattice QCD basics
- LQCD community software
- QUDA
- Experience with LQCD on Juwels GPUs
QUANTUM-CHROMODYNAMICS (QCD)

1 Å = 100,000 fm
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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)

- Gluons
  - Spin
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  - Color anti-charge (R B G)
In the proton are:

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- Quantum fluctuations
LONELY ELECTRONS, BUT NO LONELY QUARKS
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\[ e^+ e^- \]

\[ q \bar{q} \]
LONELY ELECTRONS, BUT NO LONELY QUARKS

\[ e^+ \quad e^- \]

\[ q \bar{q} \quad q \bar{q} \]

“Color-confinement”
QUANTUM FLUCTUATIONS ARE IMPORTANT!

\[2 \times M_{\text{up}} + M_{\text{down}} = 2 \times (2.2 \text{ MeV}) + (4.7 \text{ MeV}) \approx 9 \text{ MeV}\]

But...

\[M_{\text{proton}} = 938 \text{ MeV}\]

To understand properties of hadrons, we must take quantum fluctuations into effect.
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To understand properties of hadrons, we must take quantum fluctuations into effect.
WHAT CAN WE HOPE TO CALCULATE?

Properties of hadrons
- mass
- internal structure
- decay probabilities

Existence of un-observed states

BIG QUESTION:

$$\text{experiment} - \text{theory} = 0$$
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BIG QUESTION:
Does \{\text{experiment}\} − \{\text{theory}\} = 0
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BIG QUESTION:

Does

\[ \{\text{experiment}\} - \{\text{theory}\} \neq 0 \]

Physics beyond the Standard Model?
QCD ACTION

In the continuum:

\[ S_{\text{QCD}} = \int d^4x \frac{1}{4} F^a_{\mu\nu} F^a_{\mu\nu} + \sum_f \int d^4x \overline{\psi}_f(x) (i\gamma_\mu D_\mu - m_f) \psi_f(x) = S_G + S_F \]
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Depend on gluon fields.
QCD ACTION

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Fermionic part – depends on quark fields \( \psi, \overline{\psi} \)
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Fermionic part – depends on quark fields \( \psi, \bar{\psi} \)

We calculate physical quantities by “path-integral” formulism:

\[ \langle \mathcal{O} \rangle = \frac{\int D[\bar{\psi}, \psi] D[A] \mathcal{O} e^{-iS[\bar{\psi}\psi A]}}{\int D[\bar{\psi}, \psi] D[A] e^{-iS[\bar{\psi}\psi A]}} \]
LQCD BASICS

Perform non-perturbative calculation for a universe that

- is finite in size (with some boundary conditions)
- is discrete (Lattice!)
- has imaginary time $t \rightarrow it$
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$$\langle O \rangle = \frac{\int \mathcal{D}[\bar{\psi}, \psi] \mathcal{D}[A] O e^{-S[\bar{\psi}\psi A]}}{\int \mathcal{D}[\bar{\psi}, \psi] \mathcal{D}[A] e^{-S[\bar{\psi}\psi A]}}$$
LQCD BASICS

Perform non-perturbative calculation for a universe that

- is finite in size (with some boundary conditions)
- is discrete (Lattice!)
- has imaginary time* \( t \rightarrow i t \)

\[
\langle O \rangle = \frac{\int \mathcal{D} [\bar{\psi}, \psi] \mathcal{D} [A] O e^{-S[\bar{\psi}\psi A]}}{\int \mathcal{D} [\bar{\psi}, \psi] \mathcal{D} [A] e^{-S[\bar{\psi}\psi A]}}
\]

*Necessary mathematical trick — allows calculation of some quantities.
Quark fields $\phi(x)$ live on lattice sites. They are 3 (or 3×4)-component, complex:

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

Gauge fields $U_{\mu}(x)$ live on links: 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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QCD ON THE LATTICE

- Quark fields $\phi(x)$ live on lattice sites
  3 (or $3 \times 4$)-component, complex:
  $$\phi(x) = \begin{pmatrix} \phi_0 \\ \phi_1 \\ \phi_2 \end{pmatrix}$$

- Gauge fields $U_\mu(x) = \exp(i\text{ag}A(x))$
  live on links: $(3 \times 3)$-component, complex
  $$U_\mu(x) = \begin{pmatrix} U_{00} & U_{01} & U_{02} \\ U_{10} & U_{11} & U_{12} \\ U_{20} & U_{21} & U_{22} \end{pmatrix}$$
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.:

\[ S_F = \sum_f \sum_{xy} \phi^f_x \left( \gamma_\mu D_\mu + m_f \right)_{xy} \phi^f_y \]
THE FERMION MATRIX

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"fermion matrix", \( M[U] \)

\[ M_{xy}[U] = \sum_{\mu=0}^3 \frac{1}{2a} \left( U_\mu(x) \delta_{x+a\mu,y} - U_{-\mu}(x) \delta_{x-a\mu,y} \right) + \delta_{xy}m \]
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- Very large (dim\( \sim \) 10^7—10^8), sparse
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- Very large (dim\( \sim \) 10^7—10^8), sparse
- Major steps in LQCD workflow require solving \( \phi_x = M^{-1}_{xy} \psi_y \)
Generate an ensemble of \textit{lattice gauge configurations} with statistical weight

\[ e^{-\tilde{S}[U]} = \det M[U] e^{-S_g[U]} \]
Generate an ensemble of lattice gauge configurations with statistical weight

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

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

\[ \langle O \rangle = \frac{1}{Z} \int D[\psi, \bar{\psi}, A] O(\psi, \bar{\psi}, A) e^{-iS_{QCD}[\psi, \bar{\psi}, A]} \]
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 \( i \)
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 integral calculation of expectation value

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

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

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\[ \langle O \rangle = \frac{1}{Z} \int D[\bar{\psi}, \psi, A] O(\bar{\psi}, \psi, A) e^{-iS_{\text{QCD}}[\bar{\psi}, \psi, A]} \]
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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QDP-JIT  QDP++  QIO
  QMP

← I/O
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- QUDA
- QDP-JIT
- QDP++
- QIO
- QMP

← Solvers
LQCD community software

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<table>
<thead>
<tr>
<th>QUDA</th>
<th>QPHIX</th>
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<td>QDP-JIT</td>
<td>QDP++</td>
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Stack of codes and libraries designed to provide common functionality, optimized for a wide range of HPC architecture.

QLUA
QUDA
QPHIX
QDP-JIT
QDP++
QIO
QMP

← Simulation codes
LQCD community software

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

Simulation codes

QLUA | CPS |
-----|-----|
QUDA | QPHIX|
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← Simulation codes
INSTALLED SOFTWARE

On JUWELS, Chroma is installed with:

<table>
<thead>
<tr>
<th>MPI</th>
<th>QDP</th>
<th>Solver</th>
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<tbody>
<tr>
<td>MVAPICH2</td>
<td>qdp-jit</td>
<td>QUDA</td>
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<tr>
<td>MVAPICH2</td>
<td>qdpxx</td>
<td>QUDA</td>
</tr>
<tr>
<td>PS-MPI</td>
<td>qdp-jit</td>
<td>QUDA</td>
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<td>QUDA</td>
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<tr>
<td>PS-MPI</td>
<td>qdpxx</td>
<td>QPHIX (AVX512)</td>
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On JURECA, Chroma is installed with:

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<tbody>
<tr>
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- Load Stages/Devel-2019a stages to test
- Request activation of features, other simulation codes, complaints → Eric
- or request installation scripts from Mathias, Eric
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 → 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
32^3 \times 64 \text{ lattices}

**Graph**: Double precision GFLOPs vs. number of nodes for QUDA inverter (juwels GPUs) and QPHIX inverter (jureca KNLs).
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 community 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-tuning placement of calculation elements on optimal hardware in an heterogeneous system.
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- Focus on fine-tuning placement of calculation elements on optimal hardware in an heterogeneous system.
- *Stay healthy!*