BENCHMARKING PORTABLE STAGGERED FERMION KERNEL WRITTEN IN KOKKOS AND MPI

LATTICE 2023

31st July, 2023 | Simon Schlepphorst | Jülich Supercomputing Centre

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Staggered fermions

Quick recap

staggered fermionic action

$$S_F[\chi,\bar{\chi}] = a^4 \sum_{n\in\Lambda} \bar{\chi}(n) \left(\sum_{\mu=1}^{4} \eta_\mu(n) \frac{U_\mu(n)\chi(n+\hat{\mu}) - U_\mu^\dagger(n-\hat{\mu})\chi(n-\hat{\mu})}{2a} + m\chi(n) \right)$$

arithmetic intensity

$$I = \frac{570\,\mathrm{FLOP}}{792\,\mathrm{B}} = 0.72\,\mathrm{FLOP}/\mathrm{B}.$$

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C++ code

```
using complex_t = Kokkos::complex<float>;
using Site = Kokkos::View<complex_t ****[3];
using Link = Kokkos::View<complex_t ****[4][3][3];
```

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```
using BulkSpace_t = Kokkos::DefaultExecutionSpace;
using HaloSpace_t = Kokkos::DefaultExecutionSpace;

BulkSpace_t BulkExecSpace = BulkSpace_t();
HaloSpace_t HaloExecSpcae = HaloSpace_t();

Kokkos::fence(); // barrier for all execution spaces
HaloExecSpcae.fence(); //barrier for only one execution space
```

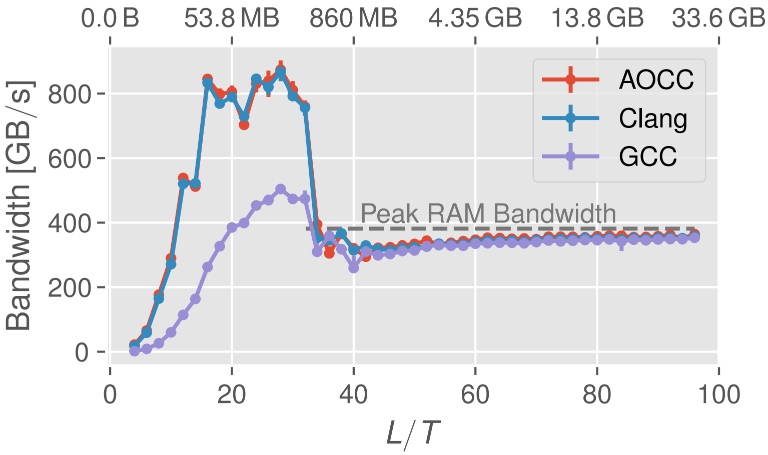
Kernel Algorithm

Kernel (Input: U_μ, χ_{in} Output: χ_{out})

$n \in \Lambda$
for $i \leftarrow 1, 2, 3$ **do**
  $t \leftarrow 0$
  for $j \leftarrow 1, 2, 3$ **do**
    for $\mu \leftarrow 1, 2, 3, 4$ **do**
      $t \leftarrow t + U_\mu(n)_{ij} * \chi_{\text{in}}(p(n + \hat{\mu}))_j$
      $t \leftarrow t - U_\mu(p(n - \hat{\mu}))_{ji} * \chi_{\text{in}}(p(n - \hat{\mu}))_j$
    end for
  end for
  $\chi_{\text{out},i} \leftarrow t$
end for

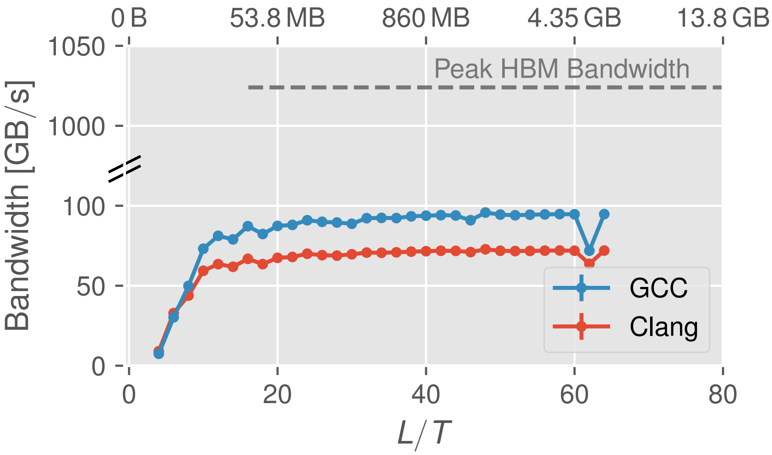
- $p()$ calculates the correct n according to periodic boundaries

AMD Ryzen 7742 (x86 CPU, Dual Socket)



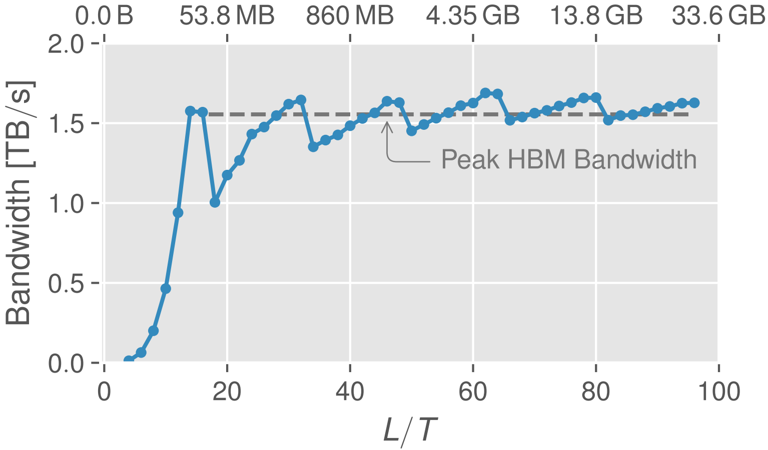
JURECA DC @ JSC, Kokkos 3.6, AOCC 3.2, Clang 13.0, GCC 11.2

Fujitsu A64FX (ARM CPU)



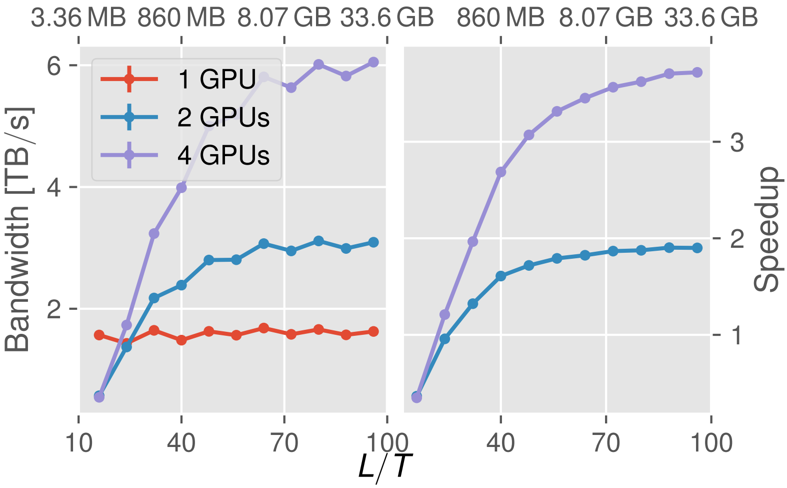
CTE-ARM @ BSC, Kokkos 3.6, GCC 11.1, Clang 14.0

Nvidia A100 (GPU)



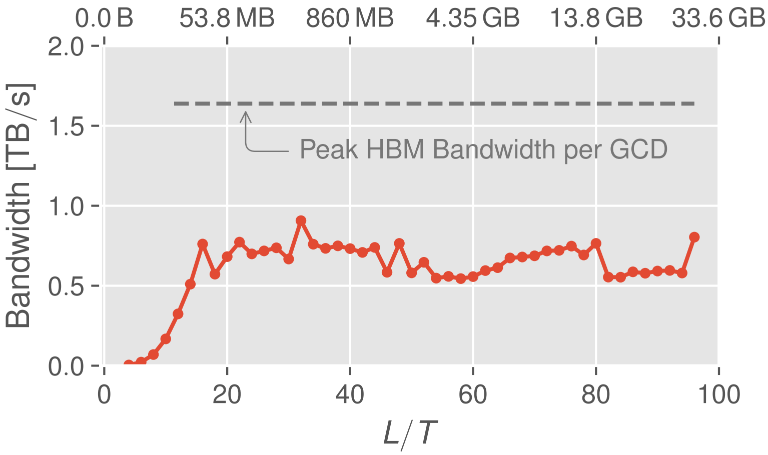
JURECA DC @ JSC, Kokkos 3.6, GCC 11.2, NVHPC 22.1, CUDA 11.5

Nvidia A100 (GPU) - Full node



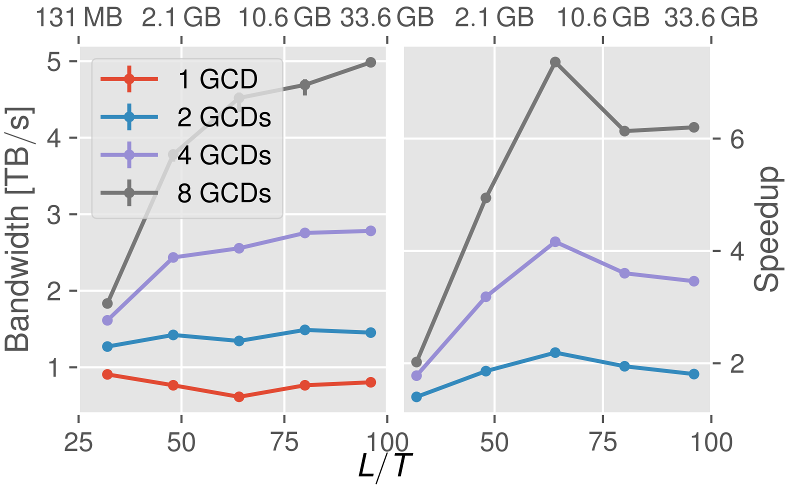
JURECA DC @ JSC, Kokkos 3.6, GCC 11.2, NVHPC 22.1, CUDA 11.5, PSMPI 5.5.0

AMD MI250 (GPU) - one Graphics Compute Die (GCD)



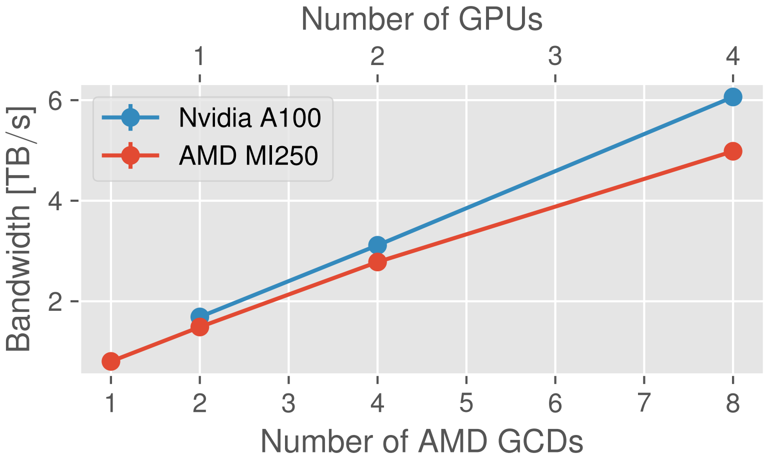
JURECA DC Evaluation Platform @ JSC, Kokkos 3.6, Clang 14.0, ROCm 5.2

AMD MI250 (GPU) - Full node

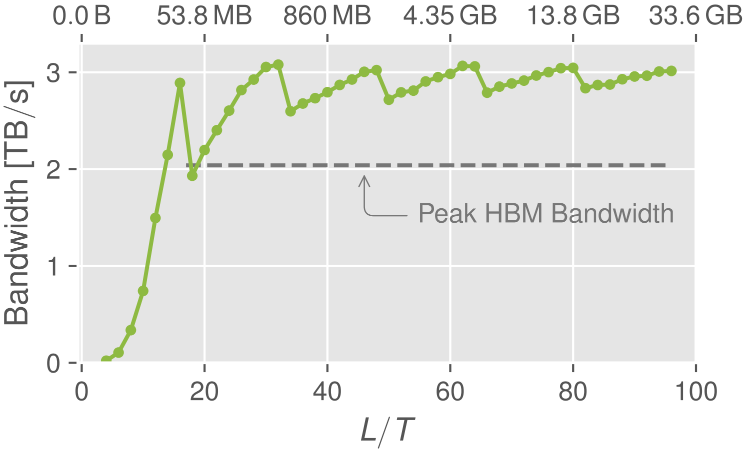


JURECA DC Evaluation Platform @ JSC, Kokkos 3.6, Clang 14.0, ROCm 5.2, OpenMPI 4.1.2

Nvidia A100 vs. AMD MI250 (GPU)

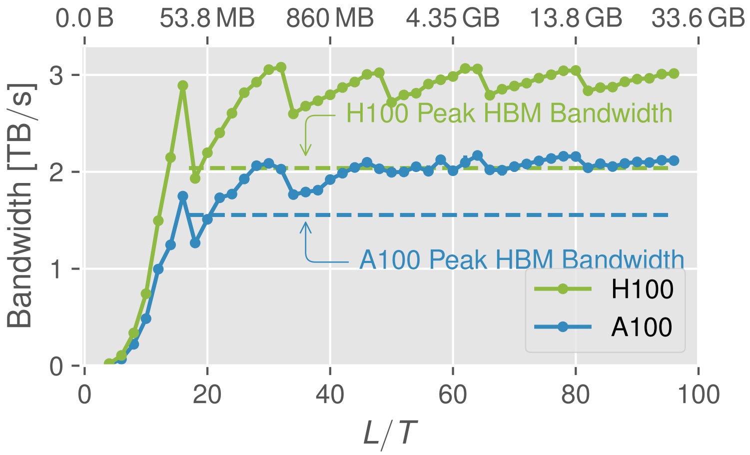


Nvidia H100 PCIe (GPU)



JURECA DC Evaluation Platform @ JSC, Kokkos 4.0, GCC 11.3, CUDA 12.0, LaunchBounds (384,1)

Nvidia H100 PCIe vs. Nvidia A100 (GPU)



JURECA DC Evaluation Platform @ JSC, Kokkos 4.0, GCC 11.3, CUDA 12.0, LaunchBounds (384,1)

END

Thank you for your attention!