Benchmarking and software sustainability at the exascale era

Preparing BigDFT for Aurora

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Motivation: Aurora

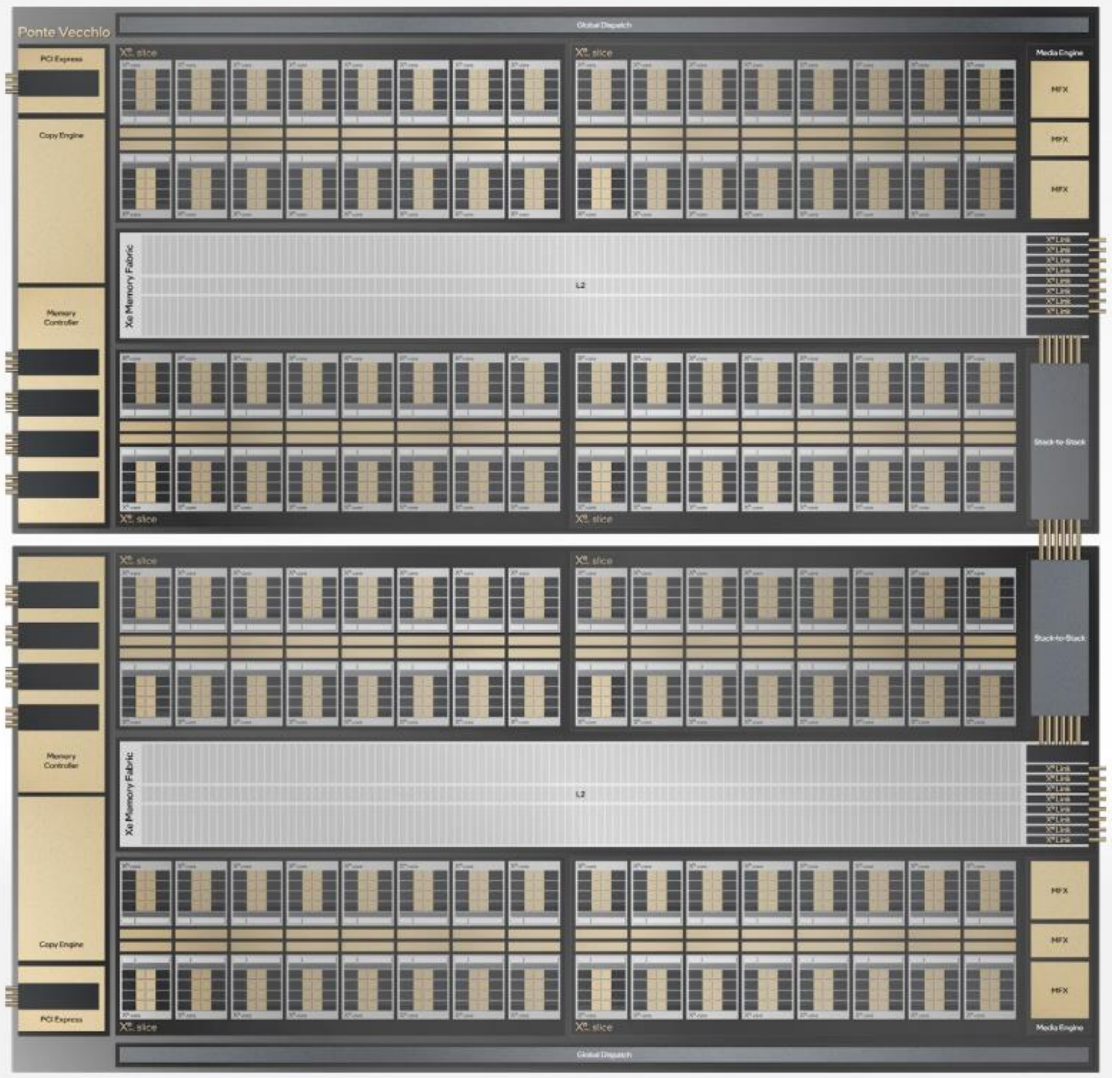
- Computer system at Argonne National Laboratory (ANL)
- >2 Exaflops FP64 theoretical peak performance
- 21,248 Intel Xeon CPU
- 63,744 Intel Data Center GPU

https://www.anl.gov/article/us-department-of-energys-incite-program-seeks-proposals-for-2024-to-advance-science-and-engineering, public domain

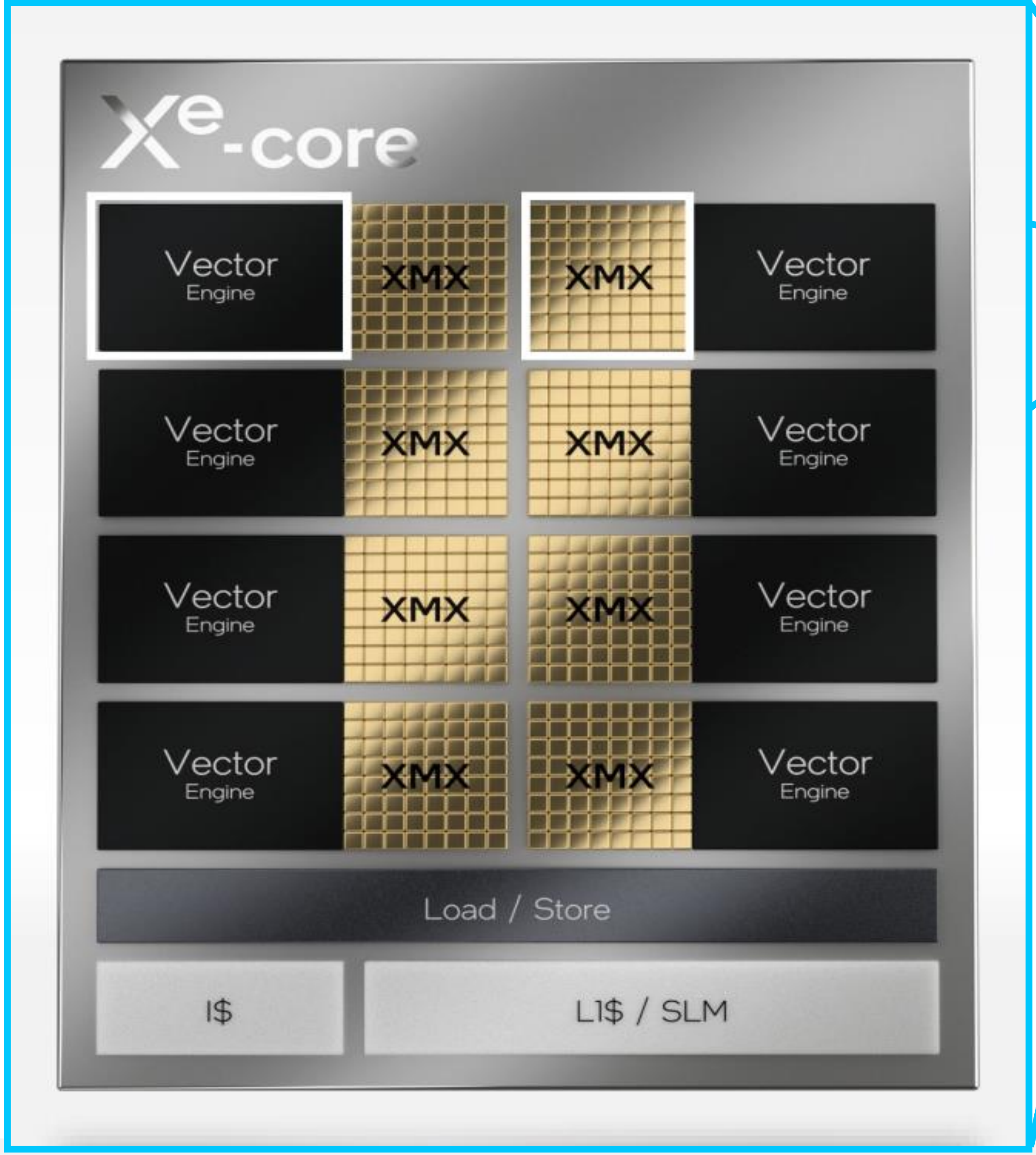
https://www.alcf.anl.gov/aurora

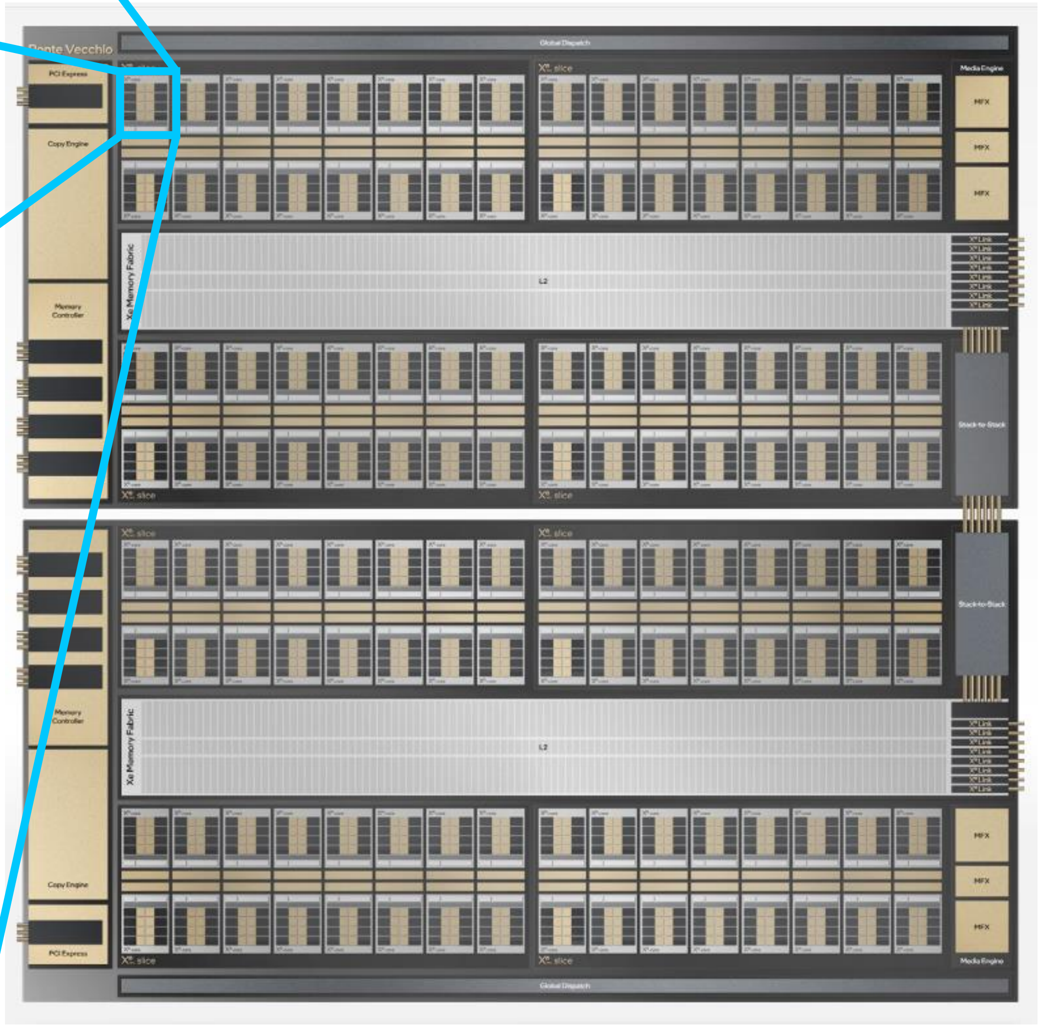
Intel Data Center GPU (PVC)

- 128GB HBM memory
- ~52 TFLOPS processing power (FP32 and FP64)
- TDP: 600W
- 2 Stacks



https://www.intel.com/content/www/us/en/docs/oneapi/optimization-guide-gpu/2023-2/intel-xe-gpu-architecture.html#XE-HPC-2-STACK-DATA-CENTER-GPU-MAX





https://www.intel.com/content/www/us/en/docs/oneapi/optimization-guide-gpu/2023-2/intel-xe-gpu-architecture.html#XE-HPC-2-STACK-DATA-CENTER-GPU-MAX

SYCL

- Standard by Khronos Group, initially released 2014
- Enables cross-platform single-source C++ code for heterogeneous and offload processors
- Implemented in Intel oneAPI DPC++
- Supported by several libraries (oneMKL, oneDNN, Kokkos, AMReX, etc.)

```cpp
#include <sycl/sycl.hpp>

int main(int argc, char ** argv)
{
    sycl::queue Q(sycl::gpu_selector_v);
    double *val_in =  sycl::malloc_shared<double>(32, Q);
    double *val_out = sycl::malloc_shared<double>(32, Q);

    Q.fill(val_in, 1.1, 32);

    Q.parallel_for(sycl::nd_range<1>(32, 32), [=](auto it)  {

        const int i = it.get_global_linear_id();

        val_out[i] = std::sqrt(val_in[i]);

    }).wait();

    sycl::free(val_in, Q);
    sycl::free(val_out, Q);

    return 0;
}
```

A simple SYCL example

BigDFT

- Code which implements Kohn-Sham Density Functional Theory (KS-DFT)
- Fortran code with C++, OpenCL, and CUDA
- “PBE0” functional GPU enabled (CUDA, OpenCL) since 2009
- CUDA implementation shown to scale to several thousand NVIDIA nodes

Laura E Ratcliff, A Degomme, José A Flores-Livas, Stefan Goedecker, and Luigi Genovese. 2018. Affordable and accurate large-scale hybrid-functional calculations on GPU-accelerated supercomputers. Journal of Physics: Condensed Matter 30, 9 (feb 2018), 095901. https://doi.org/10.1088/1361-648X/aaa8c9

Laura E Ratcliff, Luigi Genovese, Hyowon Park, Peter B Littlewood, and Alejandro Lopez-Bezanilla. 2021. “Exploring metastable states in UO2 using hybrid functionals and dynamical mean field theory”. Journal of Physics: Condensed Matter 34, 9 (dec 2021), 094003. https://doi.org/10.1088/1361-648X/ac3cf1

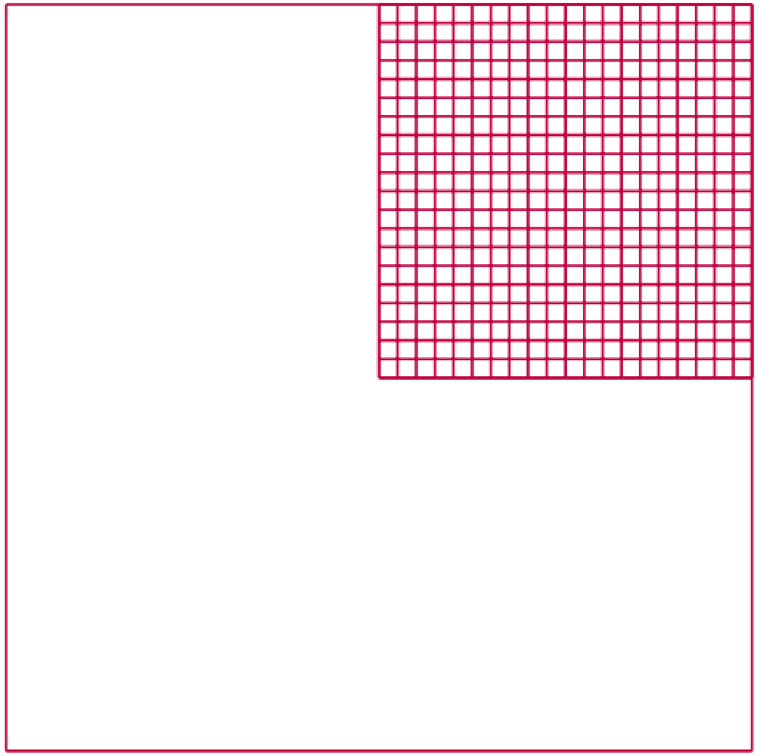
BigDFT – Fock operator evaluation

- Need to evaluate the Fock operator $$\left[\hat{D}_X\psi_i\right](\mathbf{r}) = \sum_j \underbrace{\int \mathrm{d}\mathbf{r}' \frac{\psi_j^*(\mathbf{r}')\psi_i(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}}_{V_{i,j}(\mathbf{r})}\psi_j(\mathbf{r})$$

1. Compute $\rho_{i,j}(\mathbf{r}) = \psi_j^*(\mathbf{r})\,\psi_i(\mathbf{r})$
2. Solve Poisson equation $\nabla^2 V_{i,j}(\mathbf{r}) = \rho_{i,j}(\mathbf{r})$
3. Multiply $V_{i,j}(\mathbf{r})$ with $\psi_j(\mathbf{r})$ to get Fock operator

BigDFT – Poisson Solver

- Uses convolution with Green function in Frequency Domain
- Performs convolution **as batched 1D FFTs**
- Can handle different boundary conditions
- Requires 0-padding in case of free boundary conditions



2D example of zero-padding

Nazim Dugan, Luigi Genovese, and Stefan Goedecker. 2013. A customized 3D GPU Poisson solver for free boundary conditions. Computer Physics Communications 184, 8 (2013), 1815–1820. https://doi.org/10.1016/j.cpc.2013.02.024

BigDFT – Poisson Solver

- Uses convolution with Green function in Frequency Domain
- Performs convolution **as batched 1D FFTs**
- Can handle different boundary conditions
- Requires 0-padding in case of free boundary conditions

```
if (<Boundary condition in x is free>)
    <zero-pad in x direction>
1DFFT_X(Ny*Nz, Sx) //real-to-complex FFT
if (<Boundary condition in y is free>)
    <zero-pad in y direction>
<transpose data>
1DFFT_Y((Sx/2+1)*Nz, Sy)
if (<Boundary condition in z is free>)
    <zero-pad in z direction>
<transpose data>
1DFFT_Z((Sx/2+1)*Sy, Sz)

<Convolution kernel multiplication>

inverse_1DFFT_Z((Sx/2+1)*Sy, Sz)
if (<Boundary condition in z is free>)
    <remove padding in z direction>
<inverse transpose>
inverse_1DFFT_Y((Sx/2+1)*Nz, Sy)
if (<Boundary condition in y is free>)
    <remove padding in y direction>
<inverse transpose>
inverse_1DFFT_X(Ny*Nz, Sx) //complex-to-real
if (<Boundary condition in z is free>)
    <remove padding in x direction>
```

Pseudo code of Poisson Solver in BigDFT

Nazim Dugan, Luigi Genovese, and Stefan Goedecker. 2013. A customized 3D GPU Poisson solver for free boundary conditions. Computer Physics Communications 184, 8 (2013), 1815–1820. https://doi.org/10.1016/j.cpc.2013.02.024

Porting BigDFT to SYCL – compatibility tool

- Existing accelerated code is CUDA and uses CuFFT
- We used Intel's DPC++ compatibility tool to automatically translate CUDA to SYCL
- We introduced an interface layer which chooses at runtime the CUDA or SYCL code
- oneMKL instead of CuFFT

```
//CUDA
__global__ void post_computation_kernel(int nx, int ny, int nz,
    double *rho, double *data1, int shift1, double *data2,
    int shift2, double hfac) {
    int tj = threadIdx.x;
    int td = blockDim.x;
    int blockData = (nx*ny*nz) / (gridDim.x*gridDim.y);
    int jj = (blockIdx.y*gridDim.x + blockIdx.x)*blockData;

    for (int k=0; k<blockData/td; k++) {
        int idx = jj + tj + k*td;
        data1[idx+shift1] = data1[idx+shift1] +
            hfac*rho[idx]*data2[idx+shift2];
    }
}

//SYCL
void post_computation_kernel(int nx, int ny, int nz,
    double *rho, double *data1, int shift1, double *data2,
    int shift2, double hfac, const sycl::nd_item<3> &item) {
    int tj = item.get_local_id(2);
    int td = item.get_local_range(2);
    int blockData = (nx*ny*nz) /
        (item.get_group_range(2)*item.get_group_range(1));
    int jj = (item.get_group(1)*item.get_group_range(2) +
        item.get_group(2))*blockData;

    for (int k=0; k<blockData/td; k++) {
        int idx = jj + tj + k*td;
        data1[idx+shift1] = data1[idx+shift1] +
            hfac*rho[idx]*data2[idx+shift2];
    }
}
```

CUDA kernel and automatically translated SYCL kernel.

https://www.intel.com/content/www/us/en/developer/tools/oneapi/dpc-compatibility-tool.html

Porting BigDFT to SYCL – BBFFT

- Goal: Further increasing SYCL performance on CPU
- Transposing and padding data is memory-bandwidth intensive and problematic on CPU
- Introduced double-batched FFT library

```
if (<Boundary condition in x is free>)
    <zero-pad in x direction>
1DFFT_X(Ny*Nz, Sx) //real-to-complex FFT
if (<Boundary condition in y is free>)
    <zero-pad in y direction>
<transpose data>
1DFFT_Y((Sx/2+1)*Nz, Sy)
if (<Boundary condition in z is free>)
    <zero-pad in z direction>
<transpose data>
1DFFT_Z((Sx/2+1)*Sy, Sz)

<Convolution kernel multiplication>

inverse_1DFFT_Z((Sx/2+1)*Sy, Sz)
if (<Boundary condition in z is free>)
    <remove padding in z direction>
<inverse transpose>
inverse_1DFFT_Y((Sx/2+1)*Nz, Sy)
if (<Boundary condition in y is free>)
    <remove padding in y direction>
<inverse transpose>
inverse_1DFFT_X(Ny*Nz, Sx) //complex-to-real
if (<Boundary condition in z is free>)
    <remove padding in x direction>
```

Remove additional memory accesses, where applicable

https://github.com/intel/double-batched-fft-library

Porting BigDFT to SYCL – BBFFT

- Bbfft allows zero-padding on-the-fly with callbacks
- Avoids transposing data due to double-batching
- In addition, utilize symmetries to half memory requirements for kernel
- Halved memory requirements
- More than halved computing time on 4^{th} generation Xeon CPU

```
if (<Boundary condition in x is free>)
    <set callback to add zeros>
1DFFT_X(Ny*Nz, Sx) //real-to-complex FFT
if (<Boundary condition in y is free>)
    <set callback to add zeros>
1DFFT_Y((Sx/2+1)*Nz, Sy)
if (<Boundary condition in z is free>)
    <set callback to add zeros>
1DFFT_Z((Sx/2+1)*Sy, Sz)

<Convolution kernel multiplication>

inverse_1DFFT_Z((Sx/2+1)*Sy, Sz)
inverse_1DFFT_Y((Sx/2+1)*Nz, Sy)
inverse_1DFFT_X(Ny*Nz, Sx) //complex-to-real
```

Pseudo code of Poisson Solver with bbfft in BigDFT

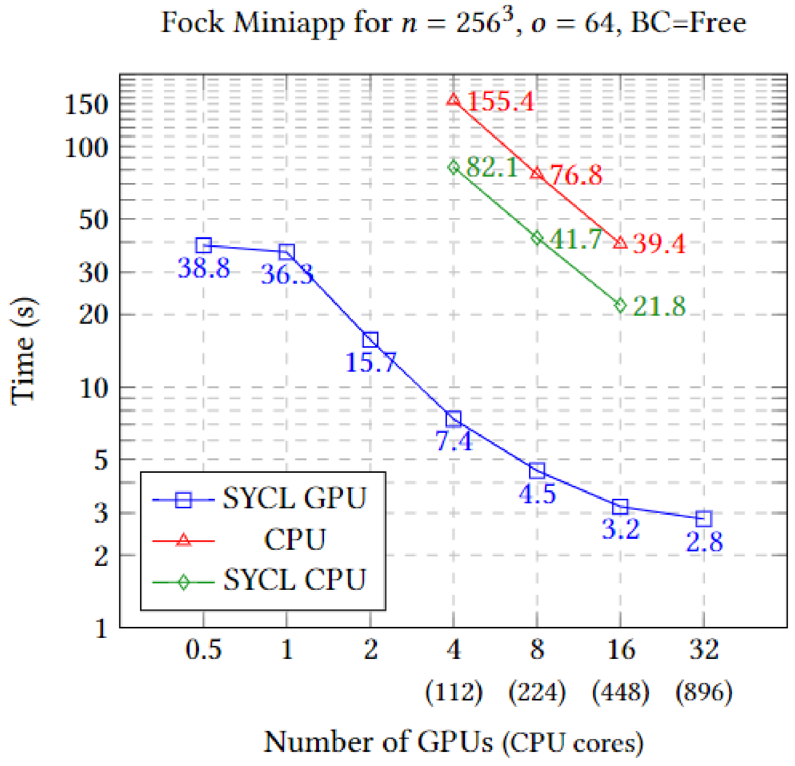
Benchmarking results – Test systems

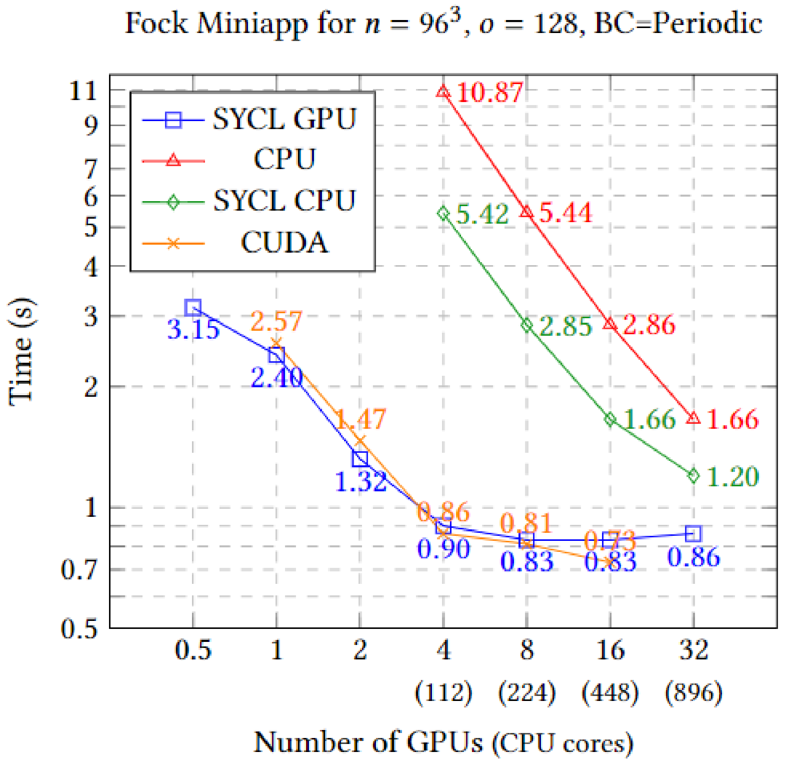
- PVC Test system: Florence
  - Lenovo SD650-I V3 servers with 2 Intel Xeon Platinum 8480+ Processors and 4 Intel Data Center GPU Max Series, 512 GB RAM
  - Each PVC is power-capped to 450 W
  - GPUs connected with XeLink
- NVIDIA Test system:
  - 2 Intel Xeon Platinum 8360Y Processors and 2 NVIDIA A100 40GB GPUs, 256 GB RAM
  - No NVLink
- Host code compiled with ifx, icx, icpx, intel oneAPI 2023.1
- Intel MPI 2021.9 in all cases

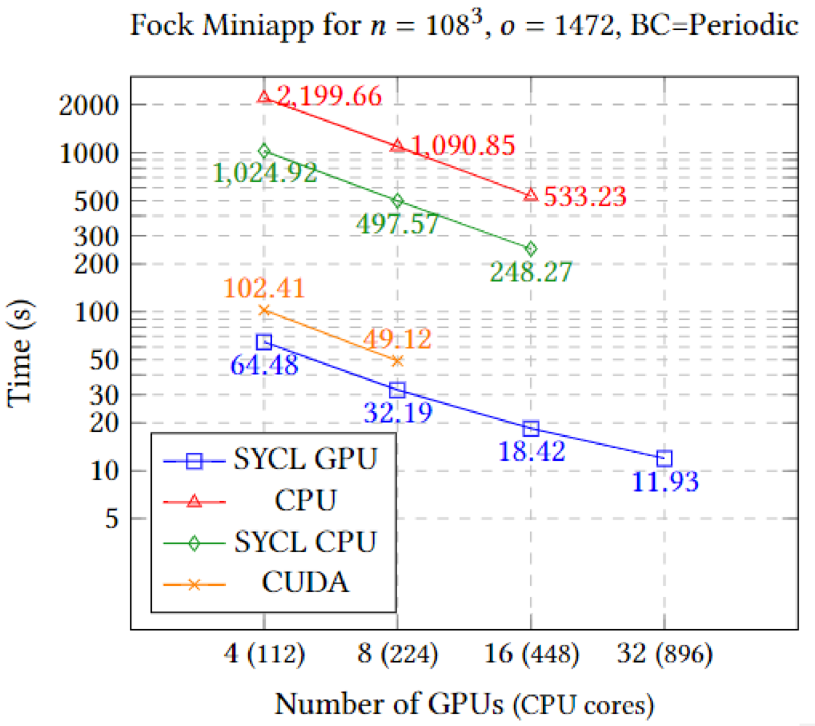
https://ark.intel.com/content/www/us/en/ark/products/231746/intel-xeon-platinum-8480-processor-105m-cache-2-00-ghz.html
https://www.intel.com/content/www/us/en/developer/articles/technical/intel-data-center-gpu-max-series-overview.html?wapkw=tuscany

Benchmarking results – Fock miniapp

- Fock miniapp is a small test code to evaluate performance and correctness of the Fock operator evaluation

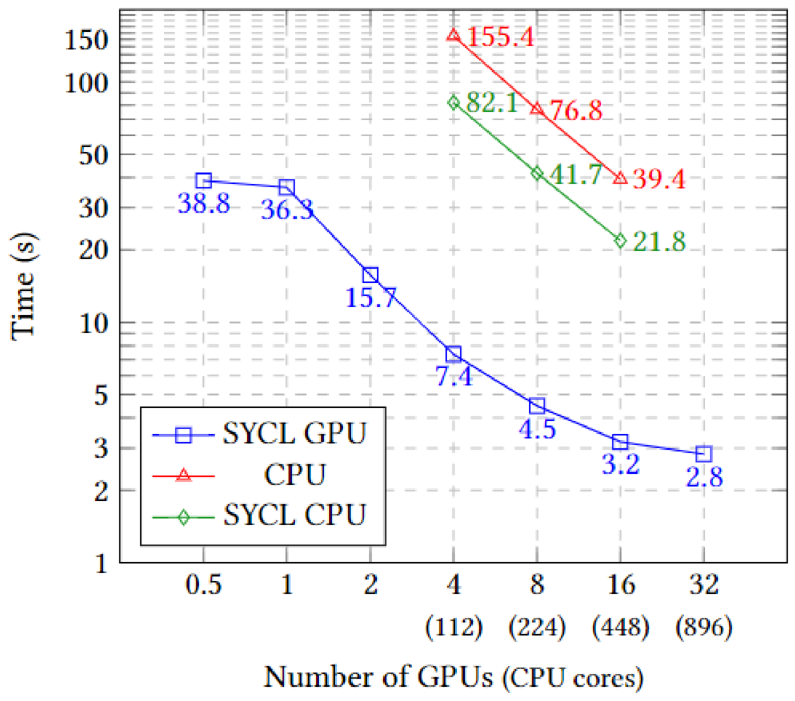




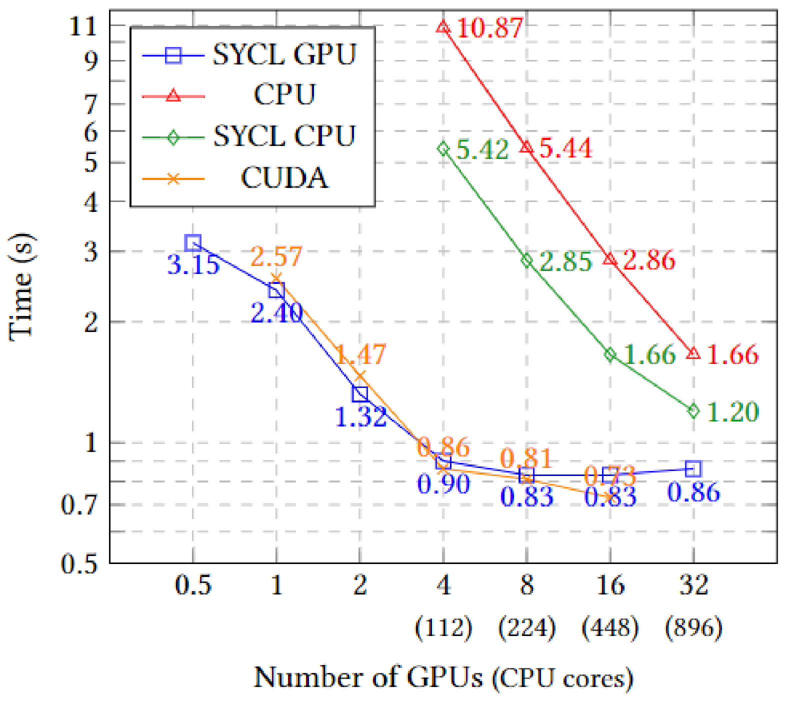


Benchmarking results – Fock miniapp

Fock Miniapp for $n = 256^3$, $o = 64$, BC=Free

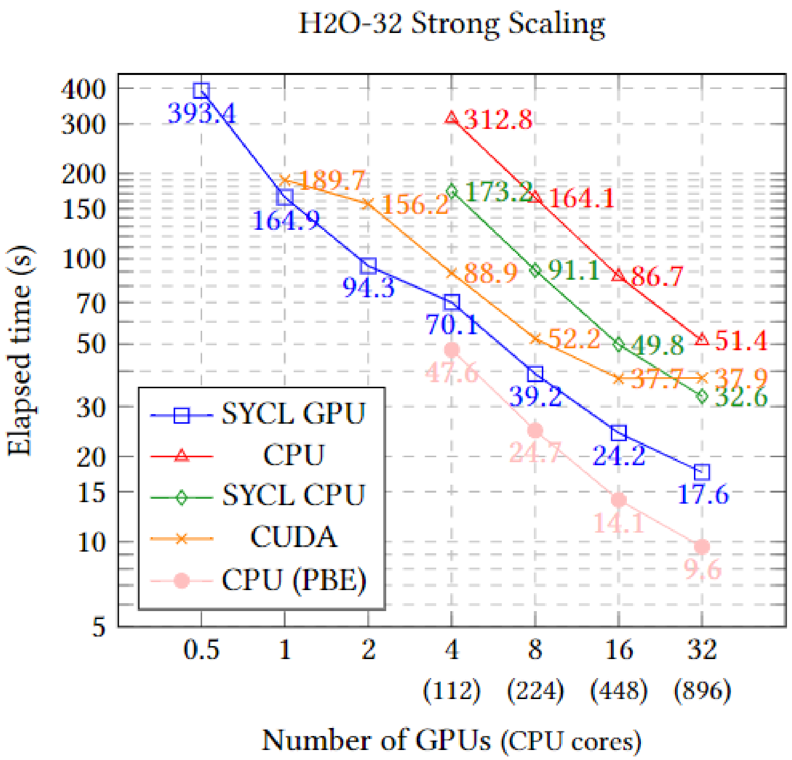


Fock Miniapp for $n = 96^3$, $o = 128$, BC=Periodic

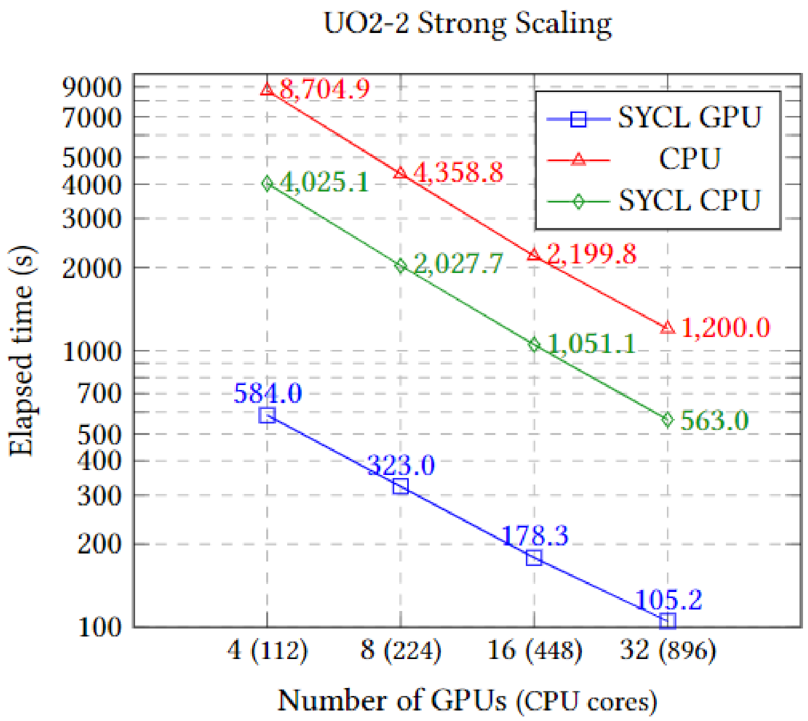


Case	Read (GB/s)		Write (GB/s)		Read+Write	
	L3	HBM	L3	HBM	L3	HBM
$n = 256^3$, $o = 64$	0.02	468	336	315	336	783
$n = 96^3$, $o = 128$	1172	66	1744	48	3516	114

Benchmarking results – Full App



32 H2O molecules. Performance delta between NVIDIA and Intel GPUs purely on the CPU side due to different processors



UO2 molecules with 1432 orbitals and a grid size of n=108x108x108.
Elapsed time is for 3 iterations.

Performance Portability

- Goal: Run SYCL code on all backends with great performance
  - Intel CPU
  - Intel GPU
  - AMD CPU
  - AMD GPU
  - NVIDIA GPU
- Problem: Lacking support from bbfft and oneMKL

Summary and Future Work

- Shown that CUDA to SYCL port is easy even in big projects
- Shown that SYCL+PVC performs and scales well, indicating readiness for Aurora
- Shown that SYCL+CPU is a viable alternative to existing Fortran+OMP implementation

- Continue working on AMD and NVIDIA support with our SYCL implementation
- Run large simulations on Aurora

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