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Finite elements on accelerators: an experience using FEniCSx and SYCL

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In this presentation, we are going to talk about our experience implementing the finite element method on different architectures and accelerators using the FEniCSx libraries and the SYCL programming model. Our main focus is on performance portability, we would like the FEM program to get consistent performance on a wide variety of platforms, instead of being very efficient on a single one.

SYCL is a modern kernel-based parallel programming model that allows for one code to be written which can run in multiple types of computational devices (eg CPUs and GPUs). A kernel describes a single operation, that can be instantiated many times and applied to different input data (eg cell-wise matrix assembly). This kernel-based model matches nicely with the new FEniCS data-centric design: DOLFINx generates data to operate in parallel (geometry, topology, and dofmaps) and FFCx generates efficient code that can be used as part of the parallel kernels.

We will discuss how different ways of expressing parallelism can affect the performance we ultimately achieve, for instance, we consider different global assembly strategies and data structures. We will also discuss how carefully arranging memory transfer and allocations can reduce latency and increase throughput in different accelerators. Finally, we will show some performance results of simplified finite element simulations on different architectures, ranging from Intel and AMD CPUs to NVIDIA GPUs.

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Finite elements on accelerators

An experience using FEniCSx and SYCL

Igor Baratta Chris Richardson Garth Wells

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What's Performance Portability? And why do we care about it?

An application is performance portable if it:

 Achieves reasonable level of performance

 Requires minimal platform specific code



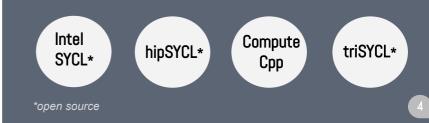
Programming Model



SYCL is a high-level single source parallel programming model, that can target a range of heterogeneous platforms:

- uses completely standard C++;
- both host CPU and device code can be written in the same C++ source file;
- open standard coordinated by the Khronos group.

SYCL implementations:



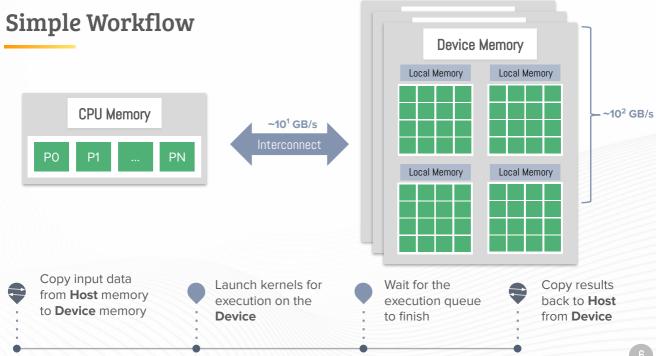
```
cl::sycl::queue q{cl::sycl::gpu selector()};
```

```
int N = 100;
auto a = cl::sycl::malloc_device<double>(N, q);
auto b = cl::sycl::malloc_shared<double>(N, q);
auto e = q.fill(a, 3.0, N);
```

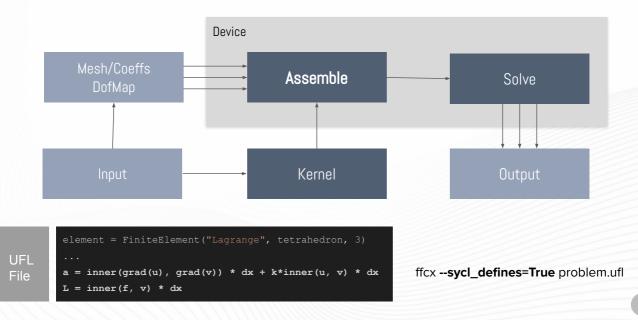
```
q.parallel_for(cl::sycl::range<l>(N), e,
[=](cl::sycl::id<1> Id) {
    int i = Id.get(0);
    b[i] = 2 * a[i];
});
```

```
q.wait();
```

```
for (int i = 0; i < N; i++)
  assert(b[i] == 6.);</pre>
```



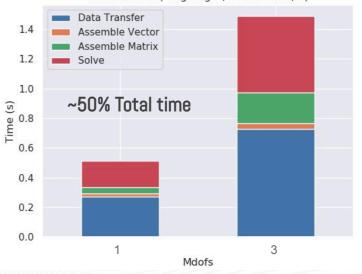
An idealised modular Finite Element worflow



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Data Transfer to Computation Ratio - P1

FiniteElement("Lagrange", tetrahedron, 1)



Data Transfer to Computation Ratio - P3

FiniteElement("Lagrange", tetrahedron, 3)



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Matrix Assembly

For each cell:

01 Gather cell coordinates and coefficients

02 Compute element matrix

03 Update global CSR matrix

Global assembly strategies:

- Binary Search*
- Lookup Table*
- Two Stage

* atomic operations

```
uto kernel = [=](cl::sycl::id<1> ID)
    const int i = ID.get(0);
    ...
    double Ae [ndofs * nofs]:
```

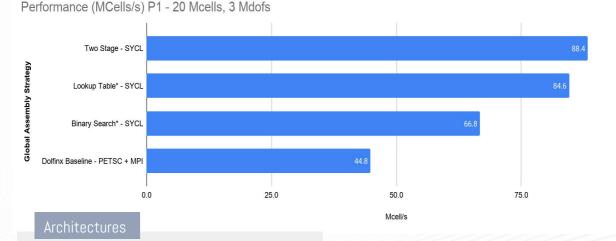
```
// Gather cell coordinates and coefficients
for (std::size_t j = 0; j < 4; ++j)</pre>
```

```
const std::size_t dmi = x_coor[i * 4 + j];
for (int k = 0; k < gdim; ++k)
  cell_geom[j * gdim + k] = x[dmi * gdim + k];
```

```
// Compute element matrix
tabulate_cell_a(Ae, coeffs, cell_geom);
```

```
// Update global matrix - Binary Search
for (int j = 0; j < ndofs; j++)
for (int k = 0; k < ndofs; k++)
{
    int ind = dofs[offset + k];
    int pos = find(indices, first, last, ind);
    atomic_ref atomic_A(data[pos]);
    atomic_A += Ae[j * ndofs + k];
}</pre>
```

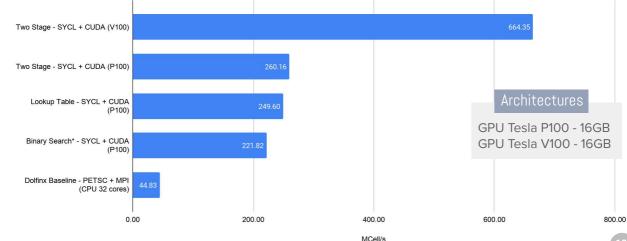
Matrix Assembly - CPU Performance



2 x Intel Xeon Skylake 6142 processors, 2.6GHz 16-core Theoretical peak performance: 2.7 TFlop/s. 192GB RAM 100.0

Matrix Assembly - GPU Performance

Performance (in Mcell/s) of assembling a CSR matrix for the Helmholtz problem on a GPU. FiniteElement('Lagrange', tetrahedron, 1)

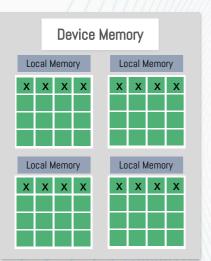


Matrix Assembly - GPU Performance

Performance (in Mcell/s) of assembling a CSR matrix for the Helmholtz problem on a GPU. FiniteElement('Lagrange', tetrahedron, 1)



Low Achieved Occupancy



Achieved Occupancy: ~25% The occupancy limited by register usage.

Solution:

Use shared memory for precomputed tables.

Each thread block (work-group) has shared memory visible to all threads (work-item) of the block.

	Occupancy	MCell/s
1st Version	25%	664 MCell/s
Shared Memory	63%	1660 MCell/s
Reference CUDA ¹	*	1627 MCells/s

[1] James Trotter - High-performance finite element computations - Performance modelling, optimisation, GPU acceleration & automated code generation - Phd Thesis 2021.

Thank you!

The code and reproducibility instructions can be found at <u>https://github.com/Excalibur-SLE/dolfinx.sycl</u>



You can reach me via e-mail: ia397@cam.ac.uk

Future/Ongoing Work

Different problems, and meshes

Linear Elasticity, Maxwell's equations Profiling in a wider range of devices

AMD GPU, A64FX

Multi-GPU

MPI-based distributed memory computations

Code transformation

Improve generated code