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Achieving Maintainable Cross-Platform Performance in the Particle-in-Cell Accelerator Modeling Code Synergia using Kokkos

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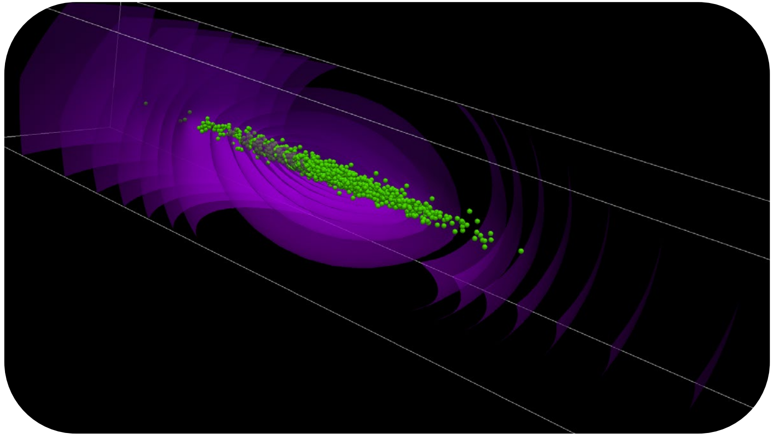
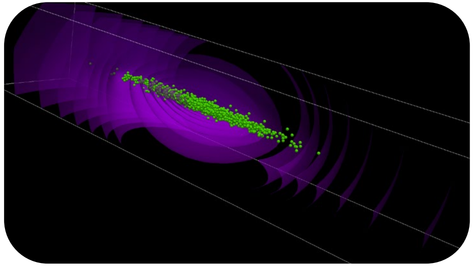
Synergia
Particle Accelerator
Modeling Framework



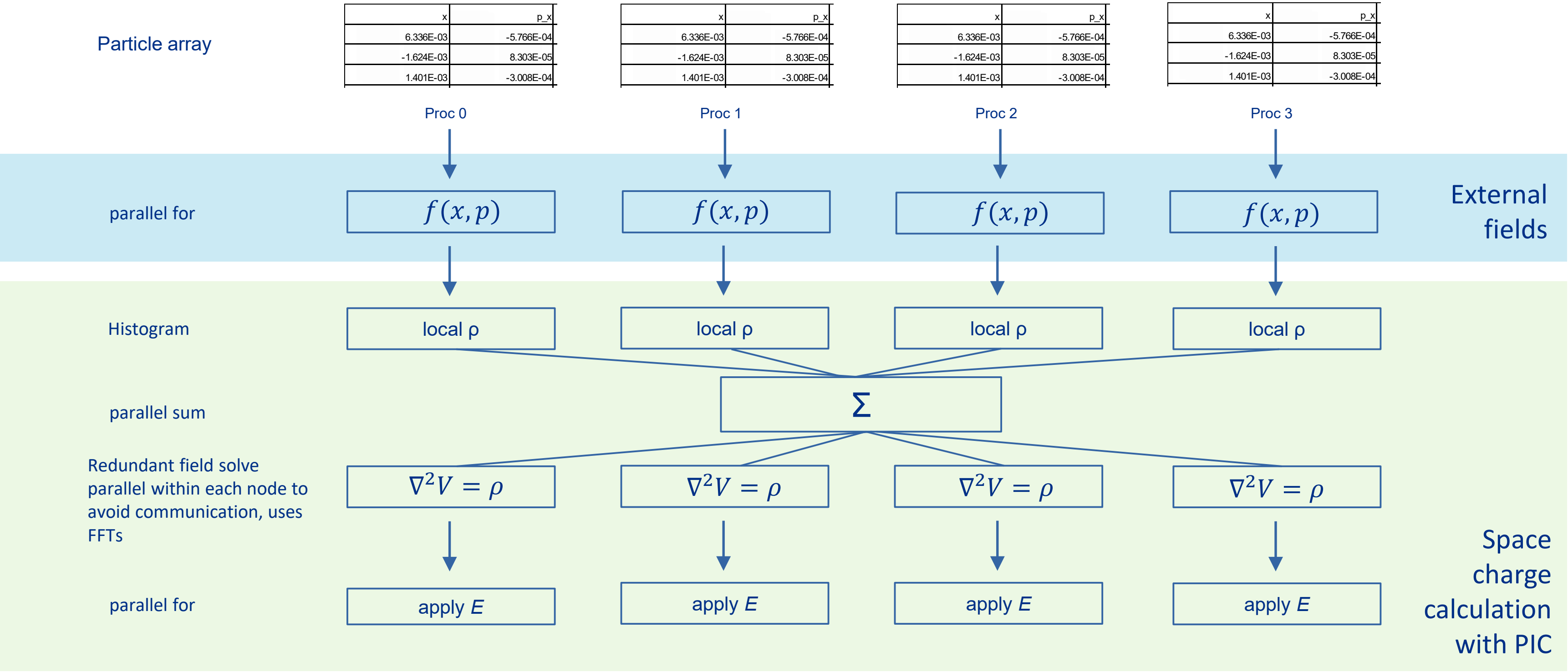
- Beam dynamics simulation and modeling package for particle accelerators
  - Beam optics from external fields
  - Internal fields calculation (space charge with particle-in-cell)
  - Beam-beam interactions, wakefield simulations, etc.

Synergia Modeling Framework



- C++ library with Python wrappers
  - Most simulations are written in Python and import modules to perform the heavy calculation. Main processing loop is in C++.
- Uses MPI parallel processing to scale to large problems.
- Runs on desktop/laptop, small/medium clusters, supercomputers.
  - Small problems can be run on small systems (number of particles, size of accelerator, etc.)
  - Code scales well for large problems on large systems.

Synergia computational ingredients



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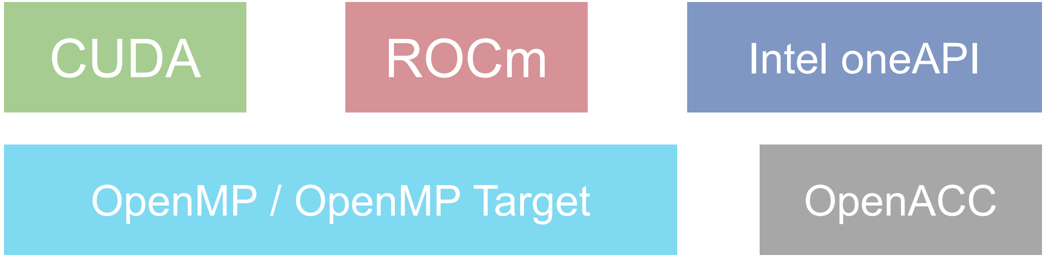
New Challenges in the Era of Exascale Computing

The bulk of computing power at the new large facilities is heavily shifting towards accelerators such as GPU or other co-processors

- Summit at OLCF: Power9 + Nvidia V100 GPU
- Frontier at OLCF: AMD EPYC CPU + AMD Radeon GPU
- Aurora at ALCF: Intel Xeon CPU + Intel Xe GPU
- Perlmutter at NERSC: AMD EPYC CPU + NVidia A100 GPU

Along with emerging parallel programming models and tools, oftentimes locked-in to specific hardware or platform



New Challenges in the Era of Exascale Computing

The application needs to adapt and make use of the accelerators

- Shifting the paradigm from CPU centric parallelization to a hybrid of CPU and accelerator parallelization

… and be portable

- Keep broad accessibility across computing platforms.
- Use “standard” languages and programming techniques as much as possible.
- Avoid architecture lock-in for code maintainability and execute-everywhere capability.
- Minimize architecture specific code and algorithms.
  - a previous CUDA specific Synergia version was unmaintainable and rotted into uselessness

… with high performance!

- Portability is not an excuse for poor performance

kokkos

- https://kokkos.org
- Part of the Exascale Computing Project
- C++ library maintained as an open-source repository on Github.

- Shared memory programming model that supports architecture specific backends, e.g., OpenMP or CUDA.
- Hardware agnostic: supports NVIDIA (now), AMD and Intel GPUs (promised)

- Provides abstractions for both parallel execution of code and data management
- Allows significant expressibility, particularly on GPUs

Kokkos Data Storage

- `Kokkos::View<T>` is a generic multi-dimensional data container
  - Allows the user to control “where” (memory spaces) the data resides,
  - and “how” (memory layout) the data are stored
    - E.g., `Kokkos::View<double**, CudaSpace, LayoutLeft>` is a 2d double array stored in the CUDA device memory with column major (left) layout.

- Managing the bulk of particle data with Kokkos::View<>
  - Resides in the device memory during its lifetime for fast accessing from computing kernels
  - has a host mirror and gets synced manually when necessary
    - For OpenMP threads backend, syncing between host and "device" has virtually no costs
  - Uses column major for both CPU and GPU backends, optimal for
    - CPU vectorization
    - GPU memory coalescing

Kokkos Parallel Dispatch

An example with drift propagation in Synergia with Kokkos

```
// simplified for demonstration ...
KOKKOS_INLINE_FUNCTION
double drift_unit(double px, double t)
{ return px * t; }

const size_t N = ...;
View<double*[6]> p("particles", N);
double t = ...;

// fill p with some numbers ...

parallel_for(N, [=](int i) {
     p(i,0) += drift_unit(p(i,1), t);
     p(i,2) += drift_unit(p(i,3), t);
});
```

- The same code can be compiled and run on both CPU (OpenMP) and GPU (CUDA, or other backends supported by Kokkos)
- 3 types of parallel dispatchers serve as the building blocks for more complicated algorithms
  - parallel_for()
  - parallel_reduce()
  - parallel_scan()

SIMD Vectorization with Kokkos

- Very limited vectorization support from Kokkos
  - Auto-vectorization with compiler directives, available with only Intel compilers in the OpenMP backend

- Yet being able to use vectorization on CPU is crucial to the performance

- Synergia has implemented a portable SIMD primitive with explicit vector types to work with Kokkos kernels
  - C++ templated class for a range of SIMD vector types
  - Uses Agner Fog's vectorclass (https://github.com/vectorclass) for x86/64 SSE/AVX/AVX512 intrinsic/types
  - Supports Quad Processing eXtension(QPX) for IBM Power CPUs
  - Compatible with GPU kernels (by falling back to single width data types)

SIMD Vectorization with Kokkos

```
template<class T>
struct Vec : public VecExpr<Vec<T>, T>
{
    T data;

    KOKKOS_INLINE_FUNCTION
    static constexpr int size();

    KOKKOS_INLINE_FUNCTION
    Vec(const double *p);

    KOKKOS_INLINE_FUNCTION
    void store(double *p);

    KOKKOS_INLINE_FUNCTION
    T & cal()       { return data; }

    KOKKOS_INLINE_FUNCTION
    T   cal() const { return data; }

    template <typename E>
    KOKKOS_INLINE_FUNCTION
    Vec(VecExpr<E, T> const& vec)
    : data(static_cast<E const&>(vec).cal()) { }
};
```

- The template class Vec<T> can be instantiated with vector types that has basic operators (+-*/, etc) overloaded
  - SSE: Vec<Vec2d>
  - AVX: Vec<Vec4d>
  - AVX512: Vec<Vec8d>
  - On GPU it is just Vec<double>

- VecExpr<E, T> is an expression template where expressions are evaluated only as needed. It …
  - avoids the need for creating temporaries
  - avoids the need for multiple loops in evaluating vectors

SIMD Vectorization with Kokkos

```
template<class T>
KOKKOS_INLINE_FUNCTION
T drift_unit(T px, double t)
{ return px * t; }

// Vec4d is the avx type from vector class
using gsv = Vec<Vec4d>;

parallel_for(N, [=](int i) {
      int idx = i * gsv::size();

      gsv p0(&p(idx,0));
      gsv p1(&p(idx,1));

      p0 += drift_unit(p1, t);

      p0.store(&p(idx,0));
});
```

- The same drift method written in SIMD primitive
- drift_unit() is now a function template to work with various vector types
- Particle data is still a double array (as opposed to a vector typed array)
  - Extra load() and store() to construct and writeback the vectors around the calculation
  - Allows flexible control over whether to use vector calculation (not all algorithms are suitable for vectorization)

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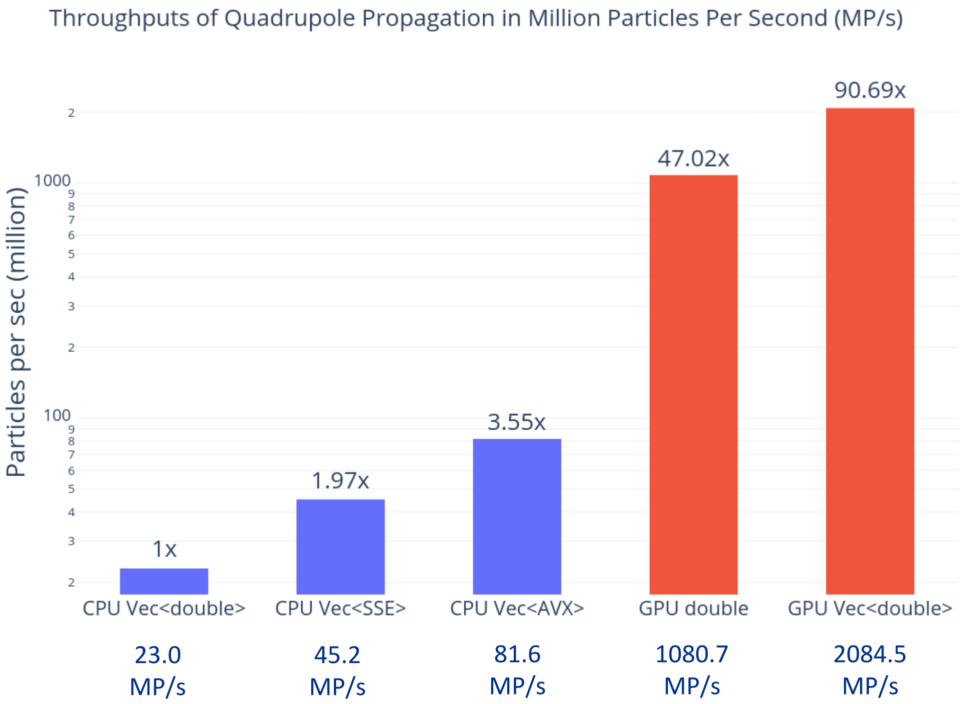
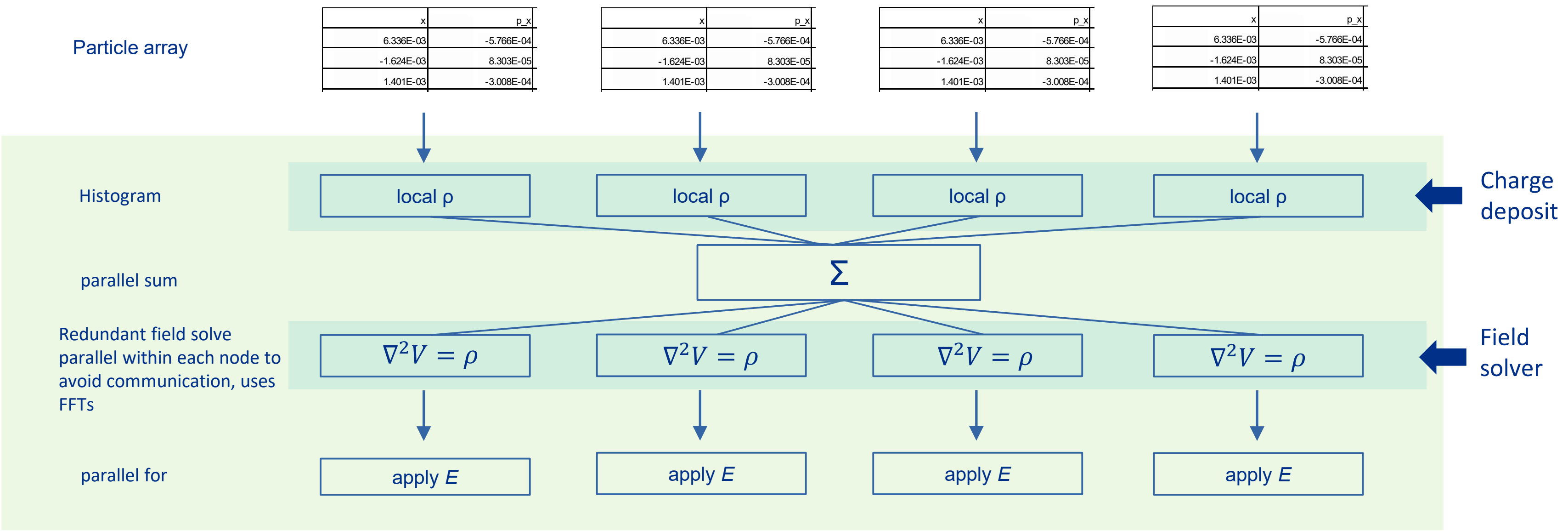
Performance Comparison of Unified Computing Kernels

- Intel Xeon 6248
  - 20 cores / 40 threads @ 3.90GHz turbo
  - SSE4.2 / AVX / AVX2 / AVX512
  - Max throughput @ 81.6 MP/s
  - 81.8 MP/s for pure OpenMP implementation
  - 2x and 3.5x for SSE and AVX vectorization
- Nvidia Volta V100 GPU
  - 84 SM / 5120 CUDA cores
  - Max throughput @ 2084.5 MP/s
  - Using expression templates has nearly doubled the throughputs on GPUs!
- Nvidia Ampere A100 GPU
  - Max throughputs @ 2876.8 MP/s
  - ~40% increases vs V100



Space Charge



Parallel Charge Deposit in Shared-memory

- Two approaches:
  - Data duplication is often faster on the host, but too memory expensive on GPUs
  - Atomics are faster on GPUs, but slow on the host

```
View<double**, LayoutLeft> p;
View<double***> grid;
ScatterView<double***> sv(grid);

parallel_for(N, [=](int i) {
     auto access = sv.access();

     auto [ix, iy, iz] = get_indices(
          p(i,0), p(i,2), p(i,4));

     access(ix, iy, iz) += charge;
     access(ix+1, iy, iz) += charge;
     ...
});

contribute(grid, sv);
```

- Kokkos::ScatterView<> does duplication on the host backend, and atomics on GPUs
- As of the latest Kokkos version (3.3.1), ScatterView still has some performance issues on OpenMP backend
- Synergia has manually implemented the data duplication histogram on the OpenMP code path

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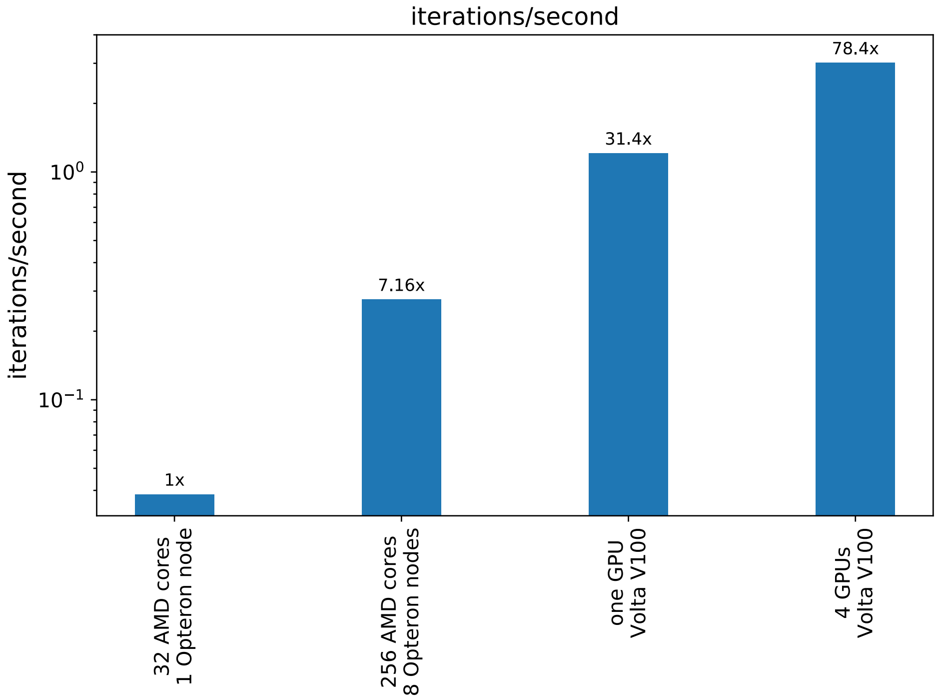
Field Solver

- The 2D and 3D open boundary conditions space charge solver in Synergia uses the convolution method to solve the field

- Needs a portable FFT method for the solver to be truly portable
  - Provides unified FFT interfaces for 2d/3d R2C/C2R DFTs, 3d DST/DCT, etc.
  - Handles device/host data movement, memory padding, and data alignments automatically
  - Calls FFTW on host
  - Calls CUFFT on CUDA backend
  - Needs to be extended for AMD GPUs and Intel GPUs

Benchmark accelerator simulation results

- Overall performance comparison
  - Real world particle accelerator simulations
  - 4M particles, 3D space charge @ 64x64x128 grid size
- 1 or 8 AMD 32 core Opteron nodes
- Power9 + Nvidia V100 GPUs
  - 1 - 4 GPUs per node
  - Similar to Summit nodes



Conclusion

- It is possible to achieve portable performance with a unified codebase
  - Shifts the burden of hardware specific implementations/optimizations to the third-party libraries and people with expertise, so we can focus on the algorithms of our specific problems
  - A portable and unified codebase is much more maintainable than multiple hardware specific code branches

- Caveats
  - Took a year of work to migrate the code from mostly OpenMP parallelization to Kokkos
  - Even though the code can be hardware agnostic, doesn’t mean the developers should also ignore the differences in underlying hardware – some algorithms and data structures are not suitable for GPUs and the memory model, therefore needs to be redesigned
  - Still some device-specific code was necessary

Acknowledgment

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