Performance study of the CLUE algorithm with the alpaka library

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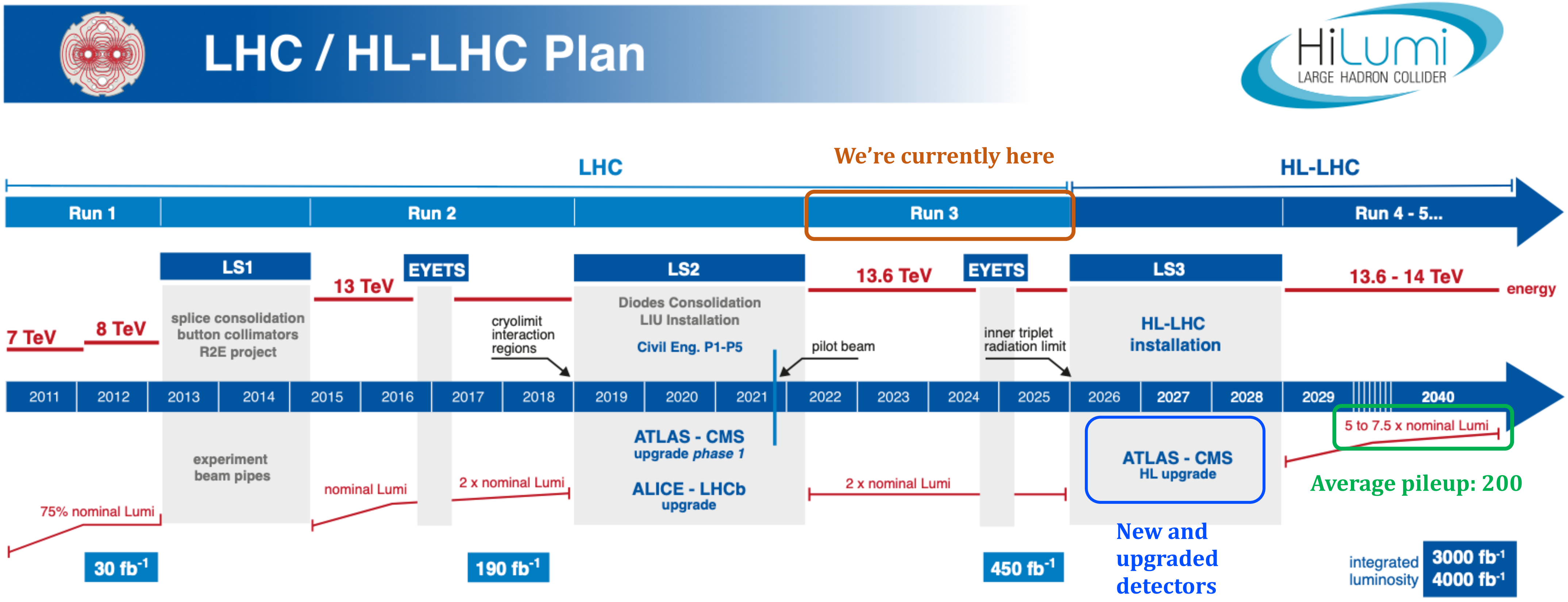
ACAT 2022

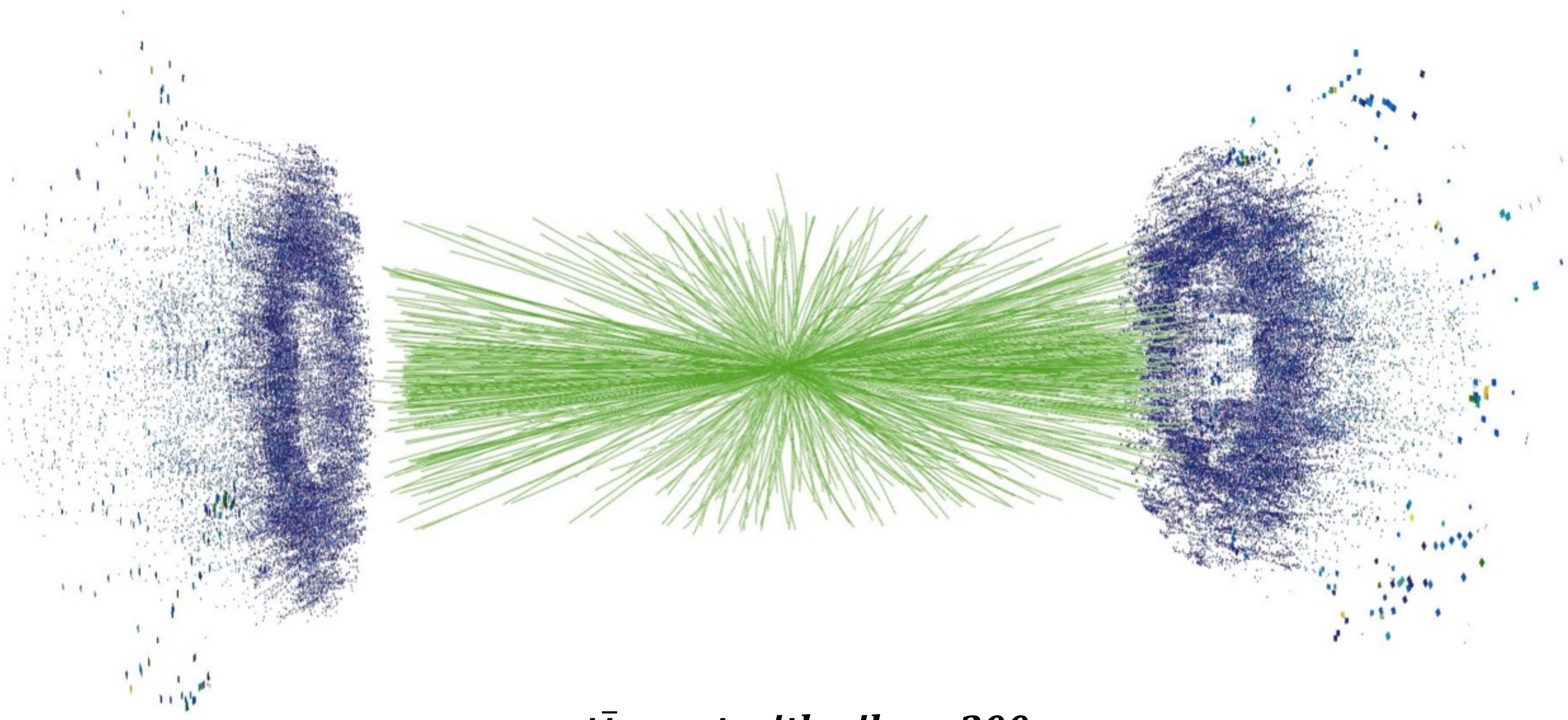
BARI

High Luminosity LHC

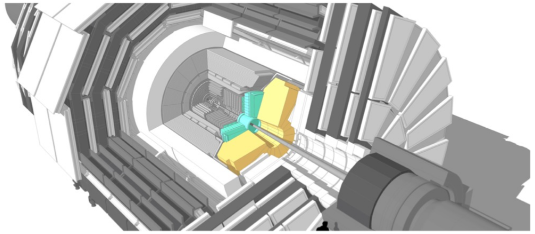


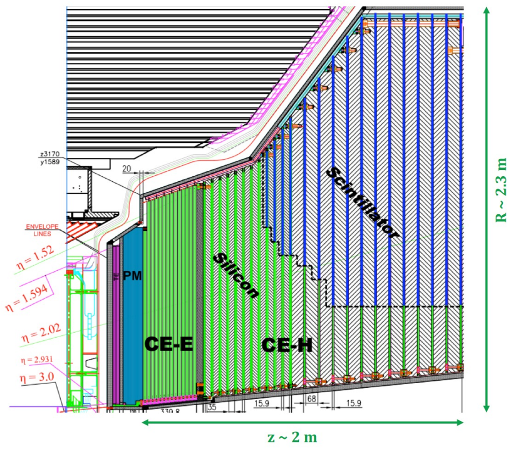
Discovering new physics and performing more accurate measurements due to the improved sensitivity level…

The CMS Phase-2 challenge



$t\bar{t}$ *event with pileup 200*





Future High Granularity Calorimeter for the CMS experiment

The software reconstruction challenge

Software reconstruction: digital signals in each detector must be processed to provide information about particles produced in the proton-proton collisions and successive decays and interaction with the absorber material.

- In the PU200 scenario, such a task becomes much **harder**
  - **Massive amount of computing resources** required
    - Advent of **heterogeneous computing**!

The heterogeneous computing scenario

Modern computing farms and data centers rely on ***heterogeneous architectures***

- CPU
- GPUs → ***hardware accelerators***

➢ ***HEP approach: offloading part of the reconstruction to GPUs for parallel execution***

❖ **Many vendors → many programming languages → many versions of the same code!!!**

NVIDIA CUDA · AMD ROCm · OpenCL

Performance portability with alpaka

- Performance portability libraries have become an interesting solution
  - Write code once
  - Compile for different backends
  - Execute on target platform
  - Not all the technologies provide close-to-native backend performance
- Portable code can be ***easily maintained*** and support new accelerators
- ***CMS choice for Run 3:*** alpaka

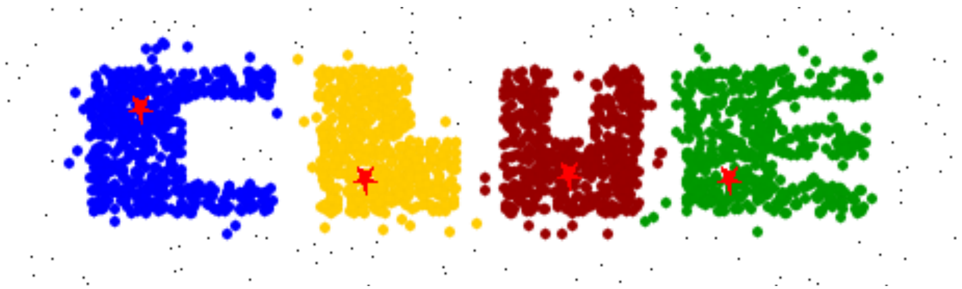
Alpaka

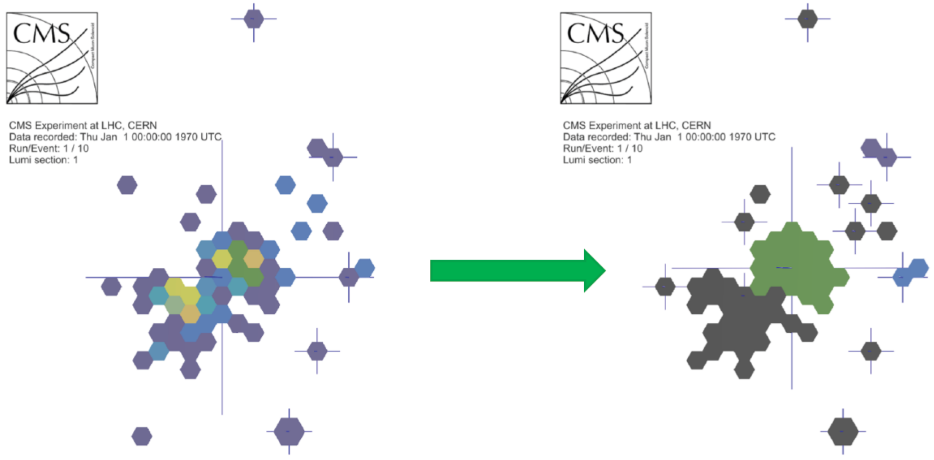
- **A**bstraction **L**ibrary for **Pa**rallel **K**ernel **A**cceleration
  - Developed and maintained at **HZDR** (Helmholtz-Zentrum-Dresden-Rossendorf) and **CASUS** (Center for Advanced Systems Understanding)
- C++ header-only library (*currently on C++17*)
- Supports a wide range of compilers (g++, clang, …)
- Several backends supported
  - CPU serial and parallel execution (std::thread or TBB)
  - NVIDIA GPU (CUDA)
  - AMD GPU (HIP/ROCm)
  - Intel GPU and FPGAs (SYCL) *under development*
- For more information, check **Jan Stephan's poster** "**Performance portability with alpaka**" on Thursday

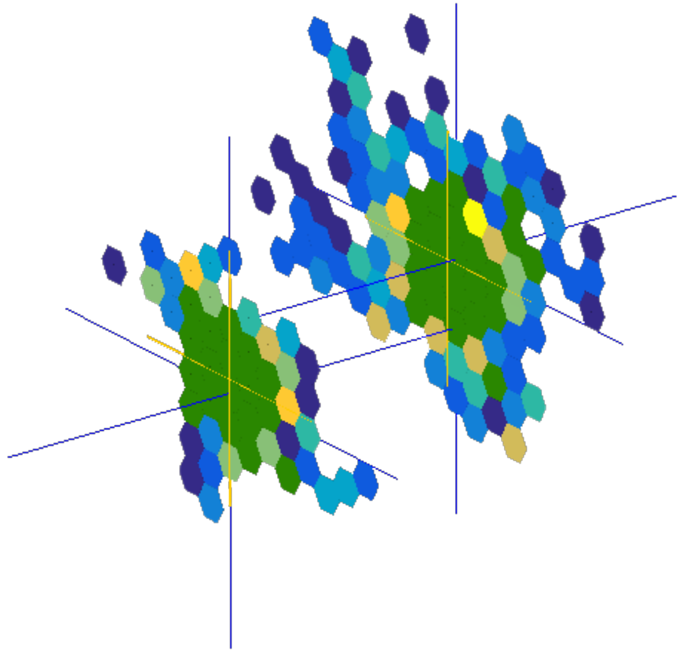
A real application: the CLUE algorithm

CLUstering of Energy (CLUE): fast 2D clustering algorithm developed for the future CMS-HGCAL detector

- Based on energy density
- Builds small clusters (~10 RecHits)
- **Fully ported to GPU (CUDA)**
- Uses a **tiled** data structure that fully exploits the detector granularity and allows fast querying of neighbor cells

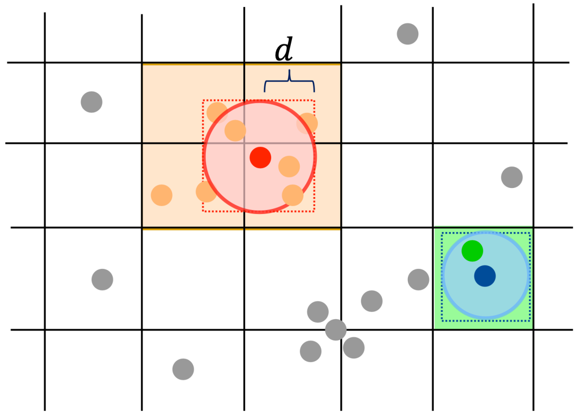






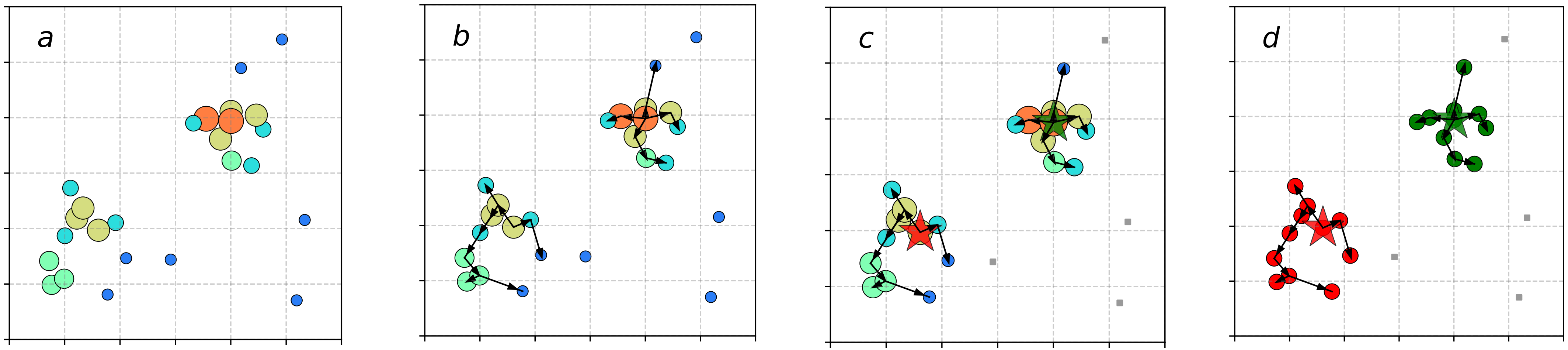
M. Rovere, Z. Chen, **A. Di Pilato**, F. Pantaleo, C. Seez, *CLUE: A Fast Parallel Clustering Algorithm for High Granularity Calorimeters in High Energy Physics*, Frontiers in Big Data, **3**, 2020.

CLUE procedure



Step 0: *arrange input data in "tiles" (spatial indexing)*
a. *calculate local energy density*
b. *find nearest higher and calculate its distance*
c. *find seeds and outliers*
d. *assign cluster indices*

Each of these steps can be written as a function (or kernel) and perform the same operation on each point



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Porting CLUE from CUDA to Alpaka - 1

```cpp
class CLUEAlgoCUDA {
public:
  // constructor
  CLUEAlgoCUDA() = delete;
  explicit CLUEAlgoCUDA(float const &dc, float const &rhoc, float const &outlierDeltaFactor, cudaStream_t stream)
      : d_points{stream}, dc_{dc}, rhoc_{rhoc}, outlierDeltaFactor_{outlierDeltaFactor}, stream_{stream} {
    init_device();
  }

  ~CLUEAlgoCUDA() = default;

  void makeClusters(PointsCloud const &host_pc);

  PointsCloudCUDA d_points;

  LayerTilesCUDA *hist_;
  cms::cuda::VecArray<int, maxNSeeds> *seeds_;
  cms::cuda::VecArray<int, maxNFollowers> *followers_;

private:
  float dc_;
  float rhoc_;
  float outlierDeltaFactor_;
  cudaStream_t stream_ = nullptr;
  cms::cuda::device::unique_ptr<LayerTilesCUDA[]> d_hist;
  cms::cuda::device::unique_ptr<cms::cuda::VecArray<int, maxNSeeds>> d_seeds;
  cms::cuda::device::unique_ptr<cms::cuda::VecArray<int, maxNFollowers>[]> d_followers;

  // private methods
  void init_device();

  void setup(PointsCloud const &host_pc);
};
```

```cpp
namespace ALPAKA_ACCELERATOR_NAMESPACE {

  class CLUEAlgoAlpaka {
  public:
    // constructor
    CLUEAlgoAlpaka() = delete;
    explicit CLUEAlgoAlpaka(float const &dc,
                            float const &rhoc,
                            float const &outlierDeltaFactor,
                            Queue stream,
                            uint32_t const &numberOfPoints)
        : d_points{stream, numberOfPoints},
          queue_{std::move(stream)},
          dc_{dc},
          rhoc_{rhoc},
          outlierDeltaFactor_{outlierDeltaFactor} {
      init_device();
    }

    ~CLUEAlgoAlpaka() = default;

    void makeClusters(PointsCloud const &host_pc);

    PointsCloudAlpaka d_points;

    LayerTilesAlpaka<Acc1D> *hist_;
    cms::alpakatools::VecArray<int, maxNSeeds> *seeds_;
    cms::alpakatools::VecArray<int, maxNFollowers> *followers_;

  private:
    Queue queue_;
    float dc_;
    float rhoc_;
    float outlierDeltaFactor_;

    std::optional<cms::alpakatools::device_buffer<Device, LayerTilesAlpaka<Acc1D>[]>> d_hist;
    std::optional<cms::alpakatools::device_buffer<Device, cms::alpakatools::VecArray<int, maxNSeeds>>> d_seeds;
    std::optional<cms::alpakatools::device_buffer<Device, cms::alpakatools::VecArray<int, maxNFollowers>[]>> d_followers;

    // private methods
    void init_device();

    void setup(PointsCloud const &host_pc);
  };
}  // namespace ALPAKA_ACCELERATOR_NAMESPACE
```

User-defined namespace that contain all the needed symbols (Platform , Device, Queue, BufferType)

Pointers to device memory passed to kernels

Executes the task (similar to cudaStream)

alpaka buffers don't have a default constructor

Porting CLUE from CUDA to Alpaka - 2

```
class PointsCloudCUDA {
public:
  PointsCloudCUDA() = delete;
  explicit PointsCloudCUDA(cudaStream_t stream, int nPoints)
      // input variables
      : x{cms::cuda::make_device_unique<float[]>(nPoints, stream)},
        y{cms::cuda::make_device_unique<float[]>(nPoints, stream)},
        layer{cms::cuda::make_device_unique<int[]>(nPoints, stream)},
        weight{cms::cuda::make_device_unique<float[]>(nPoints, stream)},
        // result variables
        rho{cms::cuda::make_device_unique<float[]>(nPoints, stream)},
        delta{cms::cuda::make_device_unique<float[]>(nPoints, stream)},
        nearestHigher{cms::cuda::make_device_unique<int[]>(nPoints, stream)},
        clusterIndex{cms::cuda::make_device_unique<int[]>(nPoints, stream)},
        isSeed{cms::cuda::make_device_unique<int[]>(nPoints, stream)},
        view_d{cms::cuda::make_device_unique<PointsCloudCUDAView>(stream)} {
    auto view_h = cms::cuda::make_host_unique<PointsCloudCUDAView>(stream);
    view_h->x = x.get();
    view_h->y = y.get();
    view_h->layer = layer.get();
    view_h->weight = weight.get();
    view_h->rho = rho.get();
    view_h->delta = delta.get();
    view_h->nearestHigher = nearestHigher.get();
    view_h->clusterIndex = clusterIndex.get();
    view_h->isSeed = isSeed.get();

    cudaMemcpyAsync(view_d.get(), view_h.get(), sizeof(PointsCloudCUDAView), cudaMemcpyHostToDevice, stream);
  }
```

```
namespace ALPAKA_ACCELERATOR_NAMESPACE {

  class PointsCloudAlpaka {
  public:
    PointsCloudAlpaka() = delete;
    explicit PointsCloudAlpaka(Queue stream, int nPoints)
        //input variables
        : x{cms::alpakatools::make_device_buffer<float[]>(stream, nPoints)},
          y{cms::alpakatools::make_device_buffer<float[]>(stream, nPoints)},
          layer{cms::alpakatools::make_device_buffer<int[]>(stream, nPoints)},
          weight{cms::alpakatools::make_device_buffer<float[]>(stream, nPoints)},
          //result variables
          rho{cms::alpakatools::make_device_buffer<float[]>(stream, nPoints)},
          delta{cms::alpakatools::make_device_buffer<float[]>(stream, nPoints)},
          nearestHigher{cms::alpakatools::make_device_buffer<int[]>(stream, nPoints)},
          clusterIndex{cms::alpakatools::make_device_buffer<int[]>(stream, nPoints)},
          isSeed{cms::alpakatools::make_device_buffer<int[]>(stream, nPoints)},
          view_d{cms::alpakatools::make_device_buffer<PointsCloudAlpakaView>(stream)} {
      auto view_h = cms::alpakatools::make_host_buffer<PointsCloudAlpakaView>(stream);
      view_h->x = x.data();
      view_h->y = y.data();
      view_h->layer = layer.data();
      view_h->weight = weight.data();
      view_h->rho = rho.data();
      view_h->delta = delta.data();
      view_h->nearestHigher = nearestHigher.data();
      view_h->clusterIndex = clusterIndex.data();
      view_h->isSeed = isSeed.data();

      alpaka::memcpy(stream, view_d, view_h);
    }
```

Allocate memory for alpaka buffers

Allocate memory for host view

Copy view from host to device

Porting CLUE from CUDA to Alpaka - 3

```
void KernelComputeHistogram(std::array<LayerTilesSerial, NLAYERS> &d_hist, PointsCloudSerial &points) {
  for (unsigned int i = 0; i < points.n; i++) {
    // push index of points into tiles
    d_hist[points.layer[i]].fill(points.x[i], points.y[i], i);
  }
};
```

CPU serial: loops over all the points

```
__global__ void kernel_compute_histogram(LayerTilesCUDA* d_hist, pointsView* d_points, int numberOfPoints) {
  int i = blockIdx.x * blockDim.x + threadIdx.x;
  if (i < numberOfPoints) {
    // push index of points into tiles
    d_hist[d_points->layer[i]].fill(d_points->x[i], d_points->y[i], i);
  }
} // kernel
```

GPU CUDA: each thread execute the same instruction with a different point

```
struct KernelComputeHistogram {
  template <typename TAcc>
  ALPAKA_FN_ACC void operator()(const TAcc &acc,
                                LayerTilesAlpaka<Acc1D> *d_hist,
                                pointsView *d_points,
                                uint32_t const &numberOfPoints) const {
    // push index of points into tiles
    cms::alpakatools::for_each_element_in_grid(
        acc, numberOfPoints, [&](uint32_t i) { d_hist[d_points->layer[i]].fill(d_points->x[i], d_points->y[i], i); });
  }
};
```

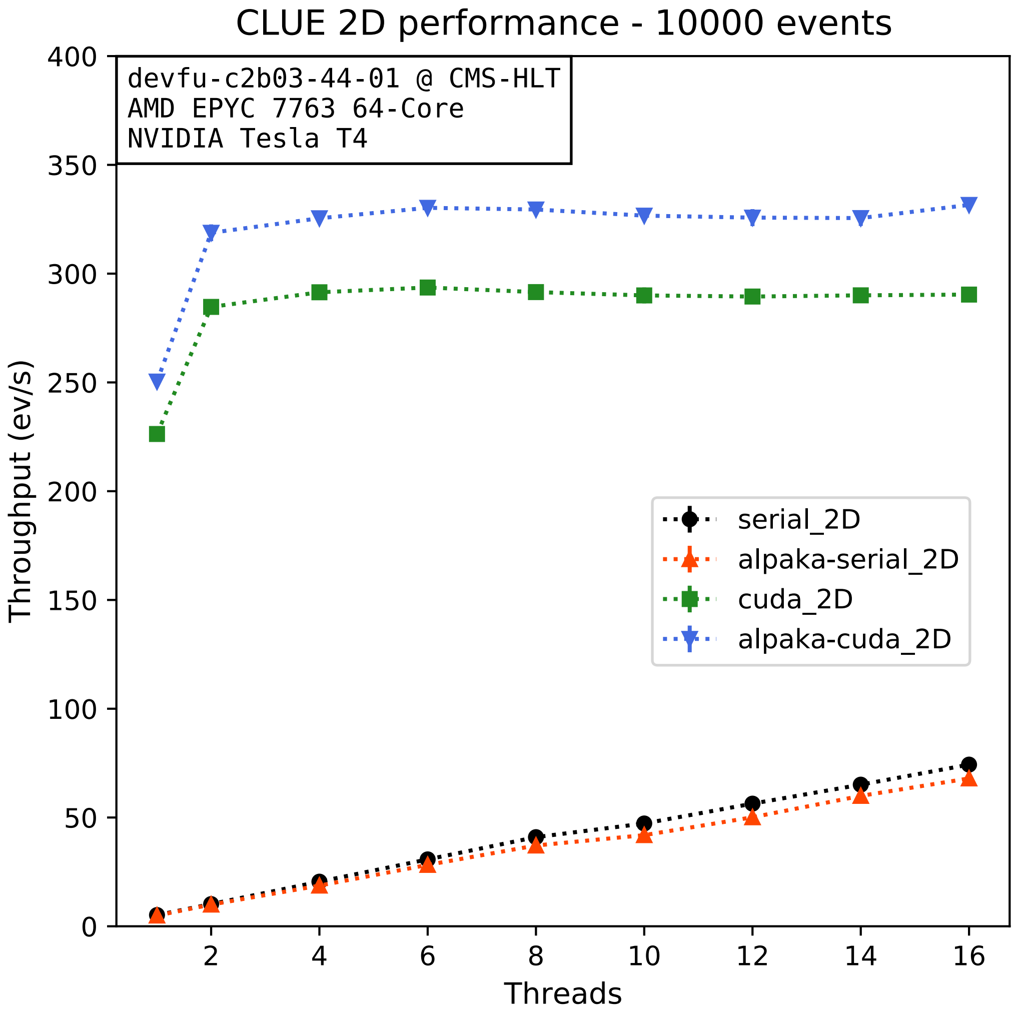
Called when launching the kernel

Equivalent to CUDA __global__

CPU/GPU alpaka: same as CUDA, with a user-defined helper function that accounts for an additional "***elements***" abstraction layer

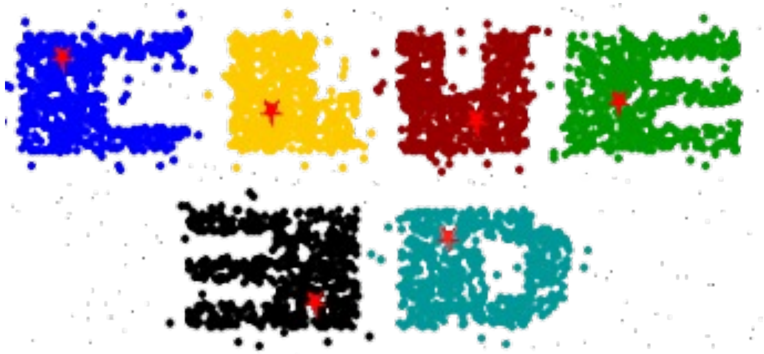
- Work division organized in Grids-Blocks-Threads-Elements

CLUE - Performance plot

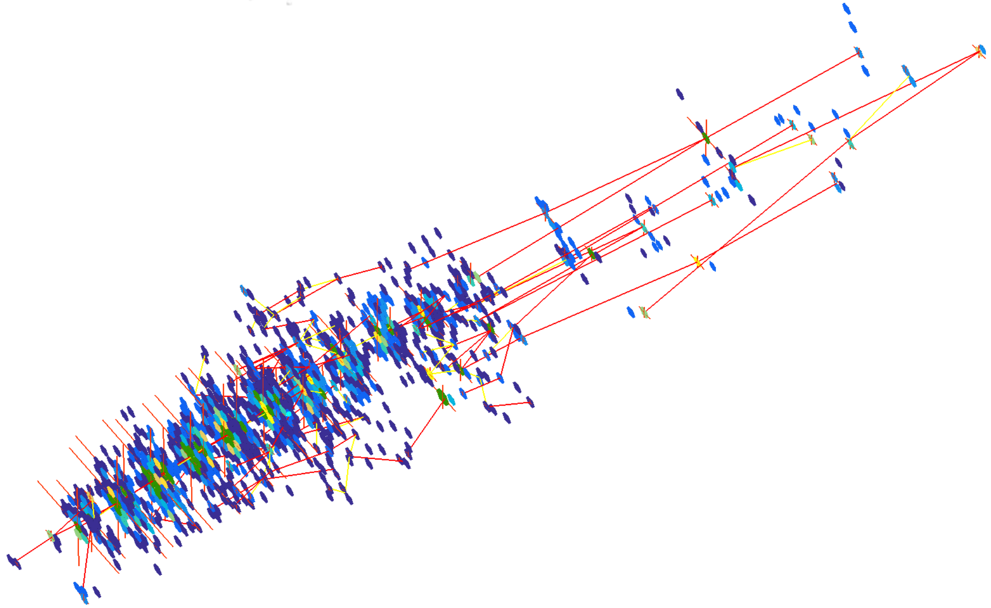


- **Alpaka** with the **serial** backend ***scales linearly*** with the number of threads (concurrent events), ***the same way*** as the **native serial** implementation
- **Alpaka** with the **cuda** backend has the ***same scaling*** of the **native cuda** implementation. Two points are under investigation:
  - Other applications **do not show** that alpaka is faster than cuda
  - It seems that I/O operations and the computing capability of the GPU are limiting the scaling for threads > 4

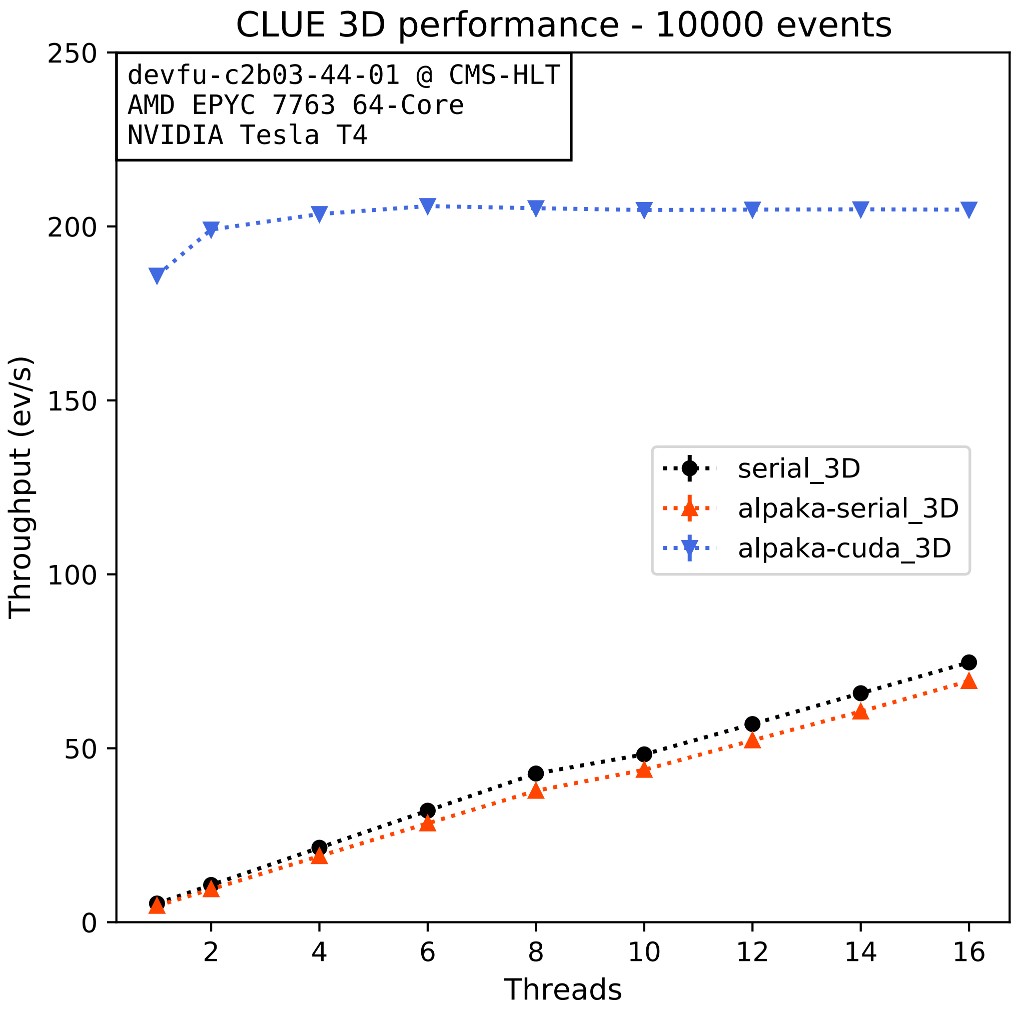
CLUE 3D (WIP)



- **3D version of the CLUE algorithm** to reconstruct particle showers in multi-layer high granularity calorimeters
- Builds 3D objects ***starting from clusters*** built with CLUE 2D
- Serial implementation currently used by the HGCAL reconstruction framework (TICL) in CMSSW
- **Ported to alpaka and can run on GPU now!**
- For more information, check **Wahid Redjeb's poster "The TICL reconstruction at the CMS Phase-2 High Granularity Calorimeter Endcap"** on Thursday



CLUE 3D – Performance plot



- **Alpaka** with the **serial** backend ***scales linearly*** with the number of threads (concurrent events) ***the same way*** as the **native serial** implementation
- **Alpaka** with the **cuda** backend provides a a high throughput of **~200 events/second**
  - Compared with serial and the same number of threads (i.e. 2), throughput is more than 20 times higher
  - Also for CLUE 3D, throughput on GPU seems limited by I/O operations

Work in progress and future plans

- CLUE has been ported to another performance portability library: **SYCL/oneAPI** (credits to ***Luca Ferragina*** and ***Juan Jose Olivera Loyola***)
  - Performance under study
  - CLUE 3D expected to be ported as well
  - For more information, check **Aurora Perego's poster** "**Experience in SYCL/oneAPI for event reconstruction at the CMS experiment**" on Tuesday
- A python library named **CLUEstering** (credits to ***Simone Balducci*** and ***Alessandro Mancini***) has been developed
  - Generalization of CLUE to N dimensions
  - Python binding to C++ serial implementation
  - Expected binding to C++ alpaka implementation in future

Conclusions

- The alpaka performance portability library is **an interesting solution** in the era of heterogeneous computing
  - ***Write the code once, compile it, and run it on different backends!***
  - Performance **close to native implementations**
  - New backends are planned and/or in development (i.e. SYCL)
- CLUE represents a **useful testbed** for performance portability solutions
  - Simple application
  - Tests have been made with both alpaka and SYCL/oneAPI
- CLUE 3D is the **first algorithm**, within the HGCAL-TICL reconstruction framework, that has been **ported directly from serial C++ to alpaka**
  - Optimizations still ongoing

Thanks for your attention

CLUE repository: heterogeneous-clue

CLUE original paper: CLUE

email: cms-patatrack@cern.ch

Backup

Porting to Alpaka: what to know

- Programming strategy *inspired by* CUDA
  - Easy porting CUDA-to-alpaka
  - Same way of organizing the work division – ***Grids-Blocks-Threads*** + additional abstraction layer ***Elements*** that can be exploited for vectorization
- Performance is close to the native backend
  - No overhead with respect to native CUDA or HIP/ROCm
- Alpaka objects behave like shared_ptrs → must be passed by value or const reference
- native buffers (vectors, arrays, …) must be ported to alpaka buffers, which **don't have a default constructor**

Kernel launch comparison

```
kernel_compute_histogram<<<gridSize, blockSize, 0, stream_>>>(d_hist.get(), d_points.view(), host_pc.x.size());
```

CUDA baseline

```
auto WorkDiv1D = cms::alpakatools::make_workdiv<Acc1D>(gridSize, blockSize);
alpaka::enqueue(
    queue_,
    alpaka::createTaskKernel<Acc1D>(WorkDiv1D, KernelComputeHistogram(), hist_, d_points.view(), d_points.n));
```

alpaka: kernels are enqueued in task objects