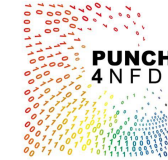


From HPC to the Edge

Alpaka, LLAMA and other animals

Michael Bussmann

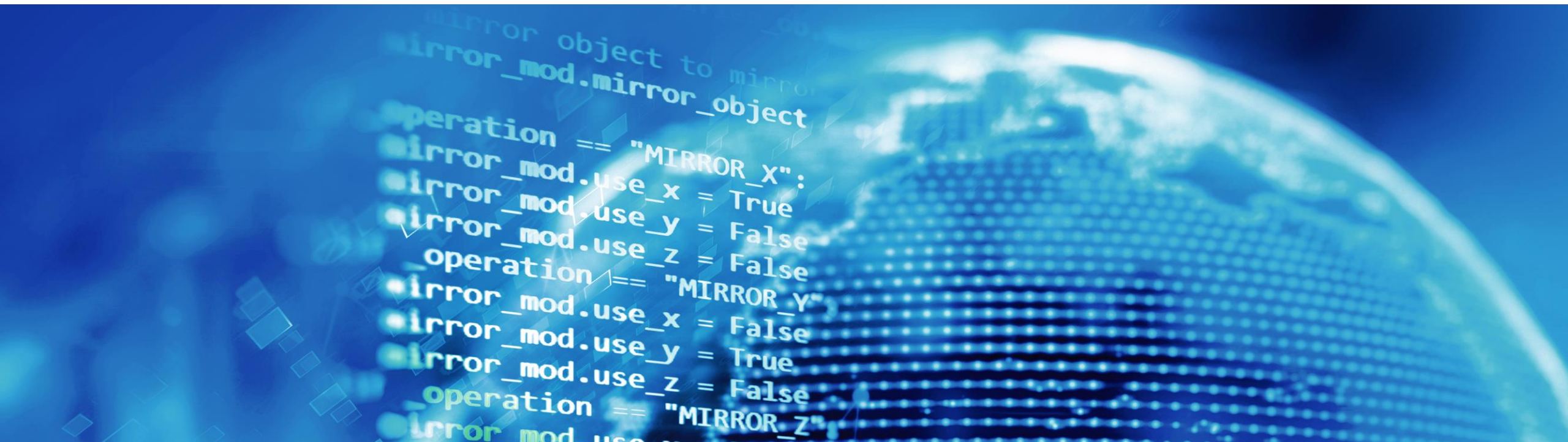
DFG - NFDI



CASUS

CENTER FOR ADVANCED
SYSTEMS UNDERSTANDING

www.casus.science

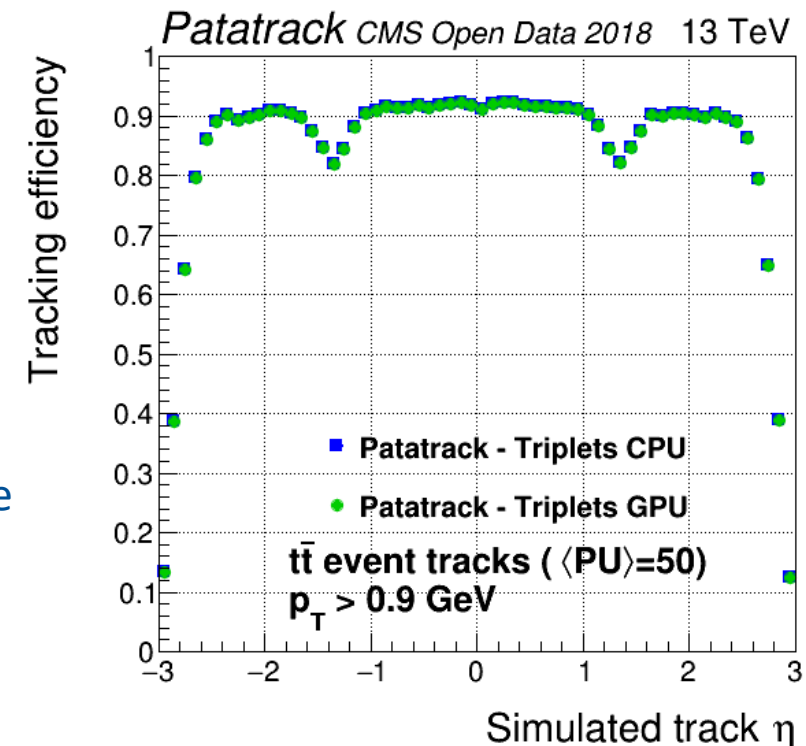


Challenges in parallel programming today

High data rates, complex algorithms, Sustainability

Throughput & Sustainability

- **Memory bound:** Throughput is decisive to use your hardware efficiently
- **Development cycles:** Hardware is changing every two years
- **A zoo without a keeper:** CPUs, GPUs, FPGAs, ARM, RISC-V
- **Reproducibility & trust:** Algorithms have to do the same regardless of Hardware

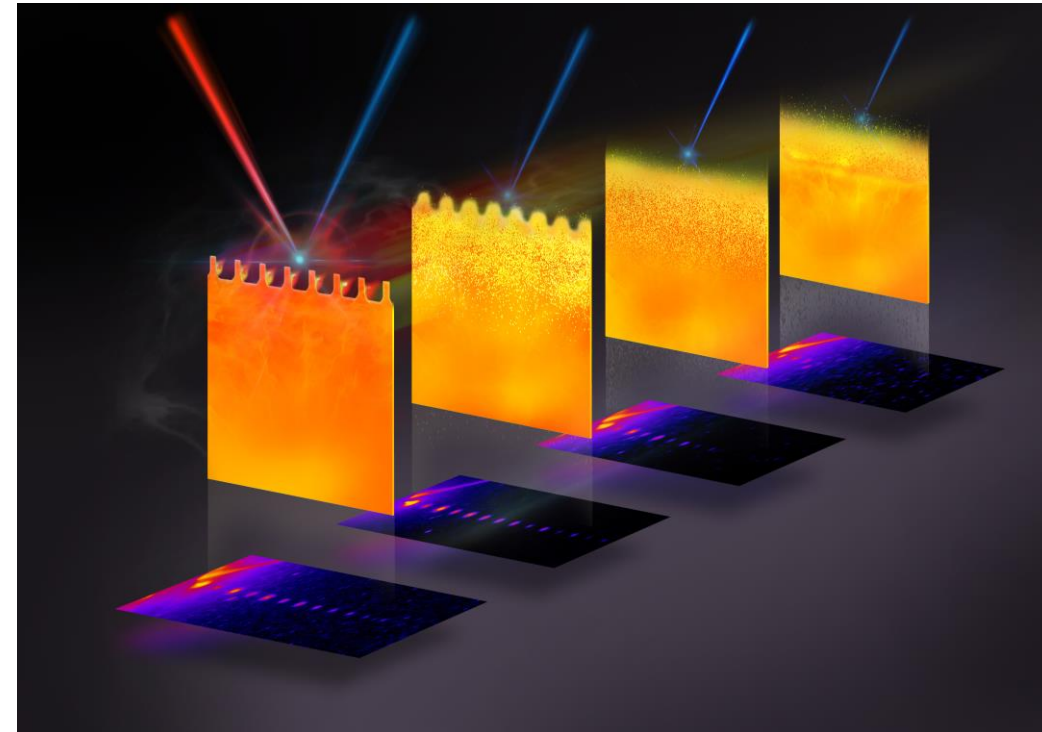


Challenges in parallel programming today

What it takes to use your hardware

How to use your hardware the best you can

- **Data locality** is key, so you need to express your data dependencies
- **Data layout** is (still) important, so you need to be able to change it
- **Parallel efficiency** = Express both data + task parallelism
- Do not write to disk if you can, **stream your data**



Data Locality: Know and express your data dependencies

REDGRAPES: Express your task parallelism by data dependencies

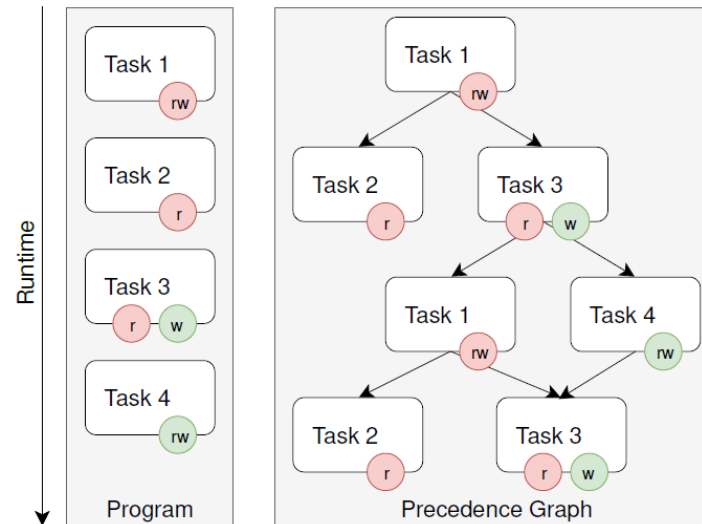
Data Dependencies

Example Code

```
rg::IOResource< int > a, b;  
  
for( ... ) {  
    task([]( auto a ) { *a = 2; },  
        a.write());  
    task([]( auto a ) { printf("%d", *a); },  
        a.read());  
    task([]( auto a, auto b ) { *b = *a; },  
        a.read(),  
        b.write());  
    task([]( auto b ) { *b += 1; },  
        b.write());  
}
```

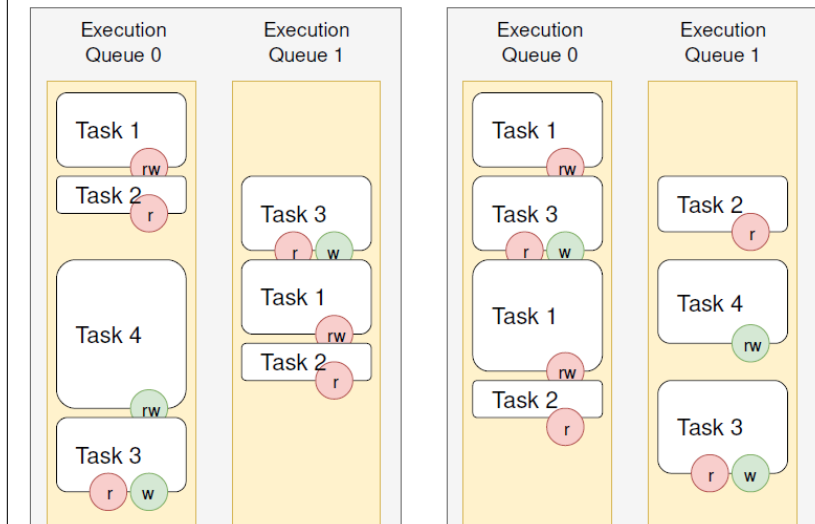
Task Tree

Declarative Task Dependencies



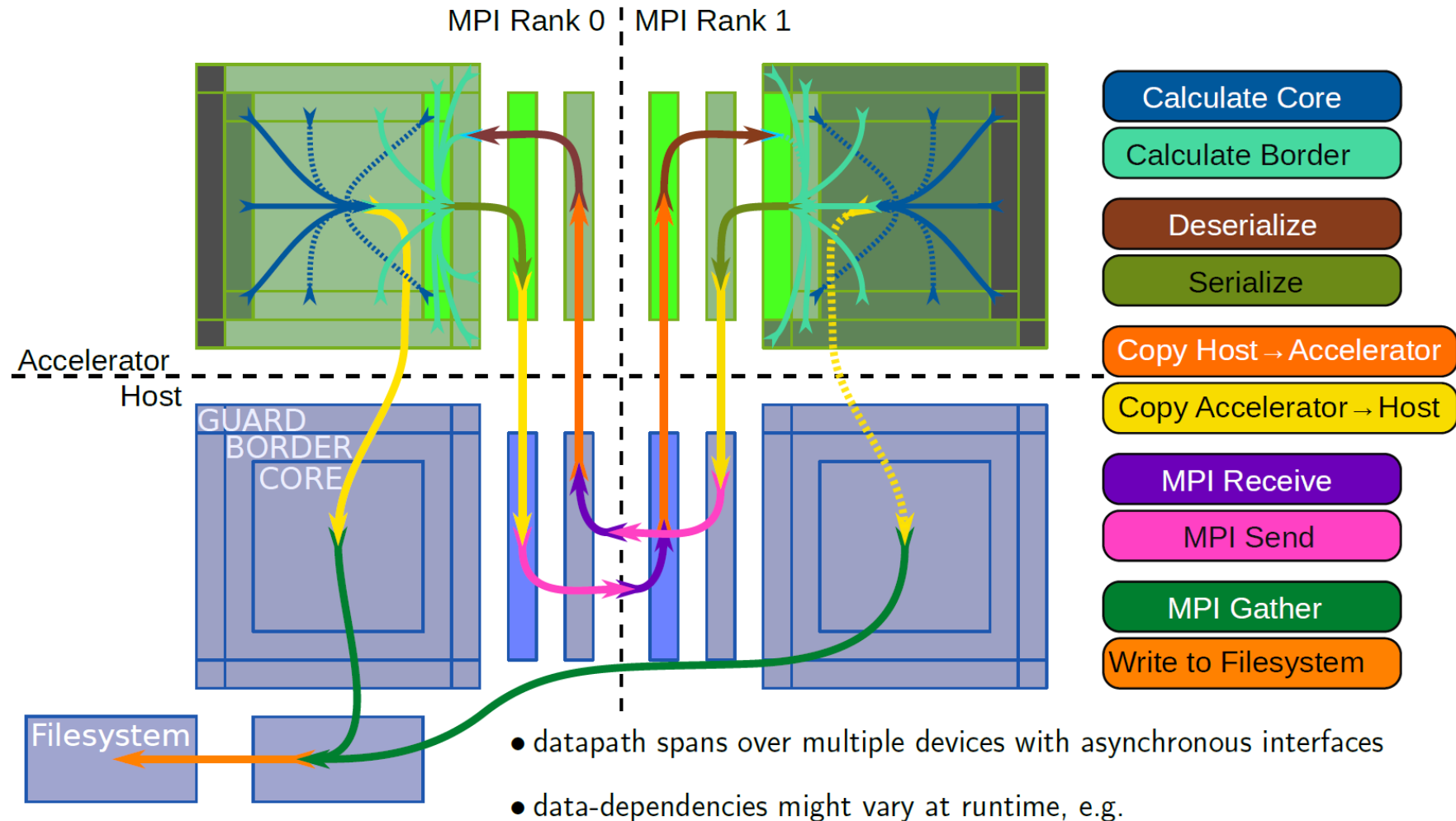
Scheduling Strategy

Possible Schedules



Data Locality: Know and express your data dependencies

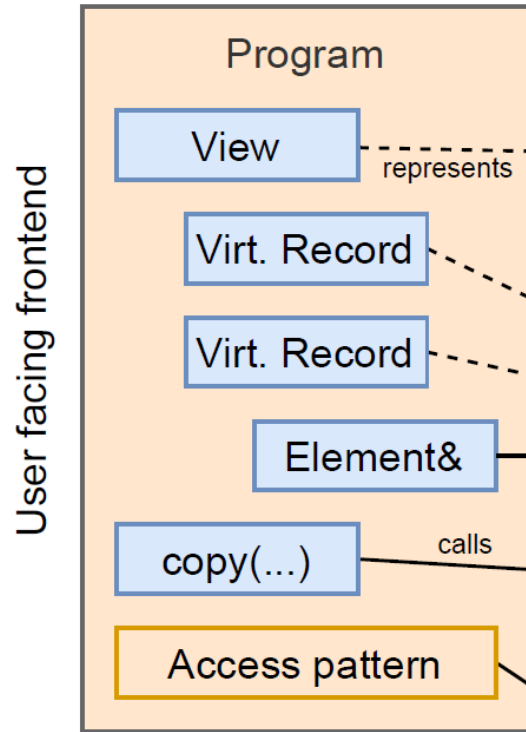
REDGRAPES: Express your task parallelism by data dependencies



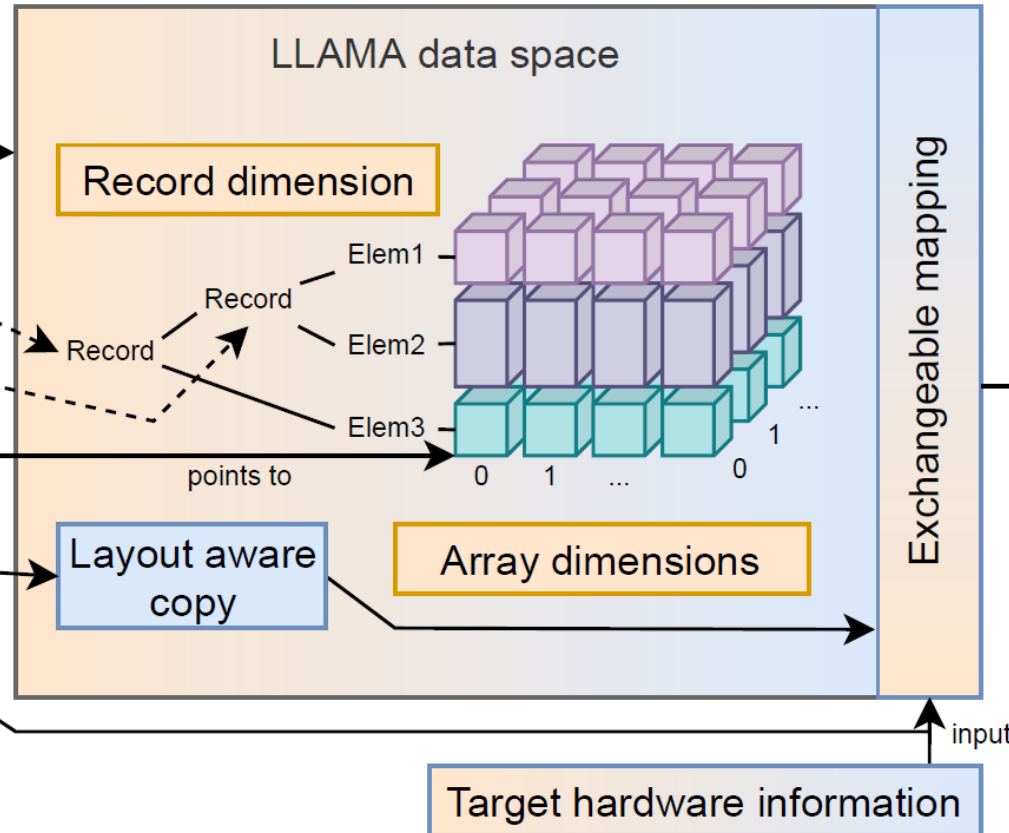
Data Layout: Layouts change, but code should not

LLAMA: Efficient data layouts without changing your code

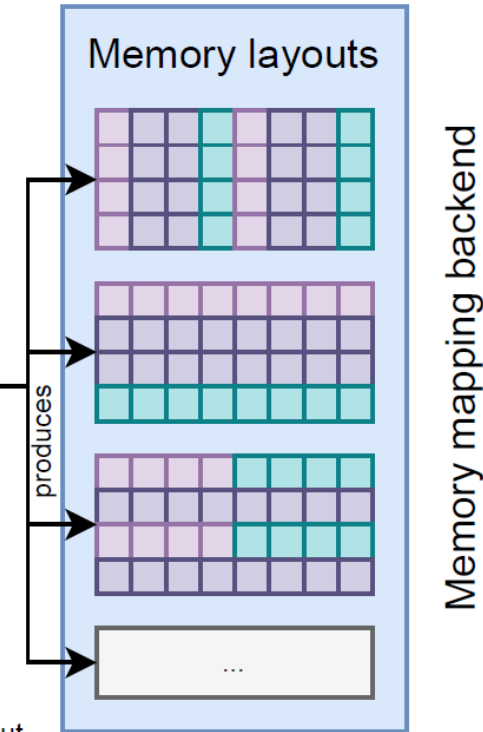
User side Data Types



Mapping

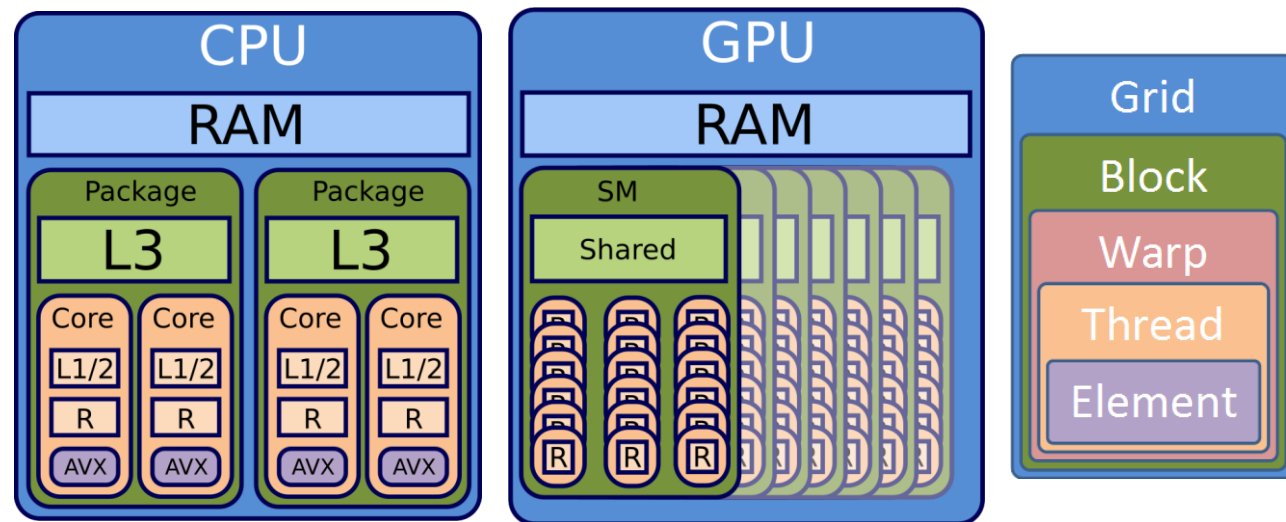


Efficient Layout



Parallel Efficiency: Express parallelism across platforms

ALPAKA: Single-source programming for CPUs, GPUs & FPGAs



```

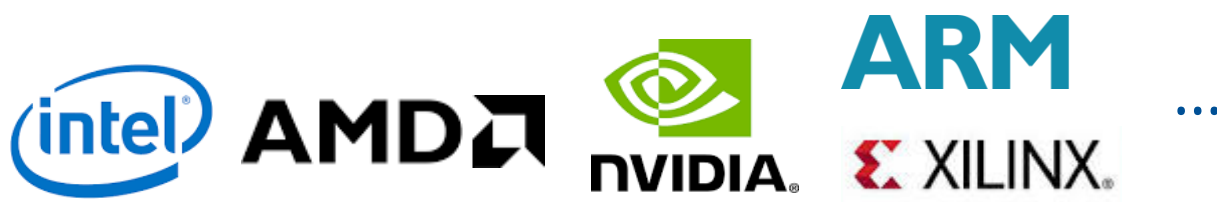
#ifdef CUDA_ENABLE
    // CUDA Kernel implementation
    // ...

#elif OPENMP_ENABLE
    // OpenMP implementation
    // ...

#else
    // Sequential CPU implementation
    // ...

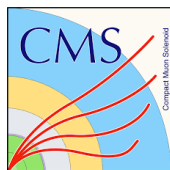
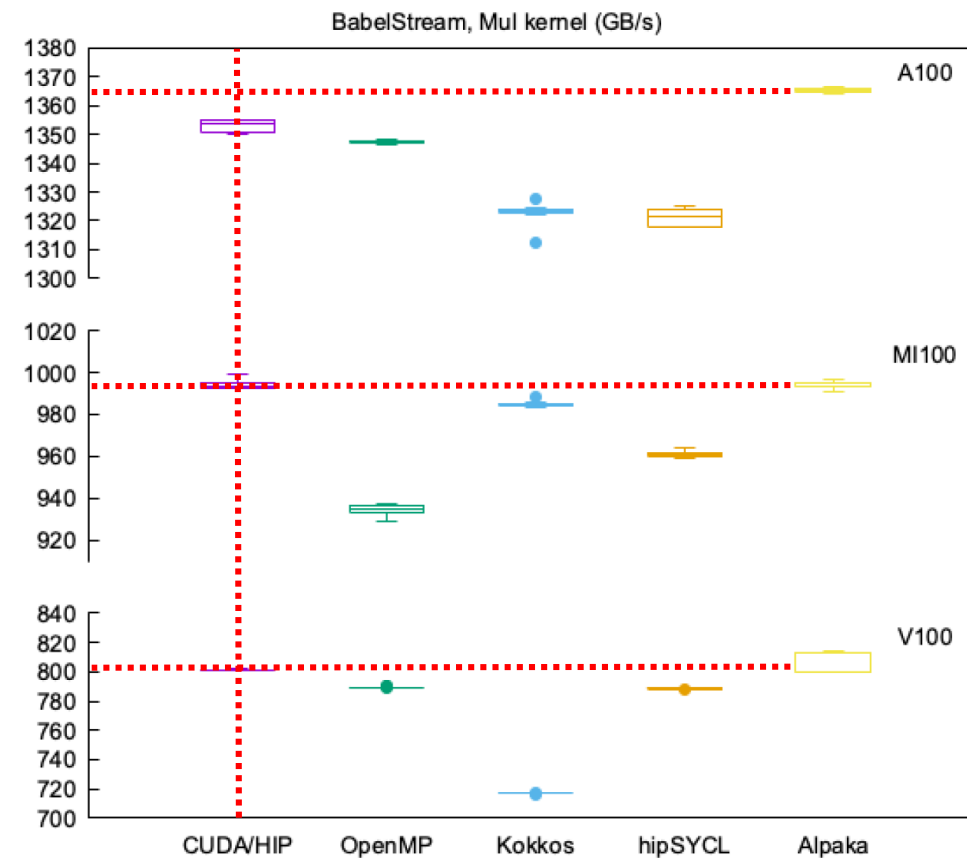
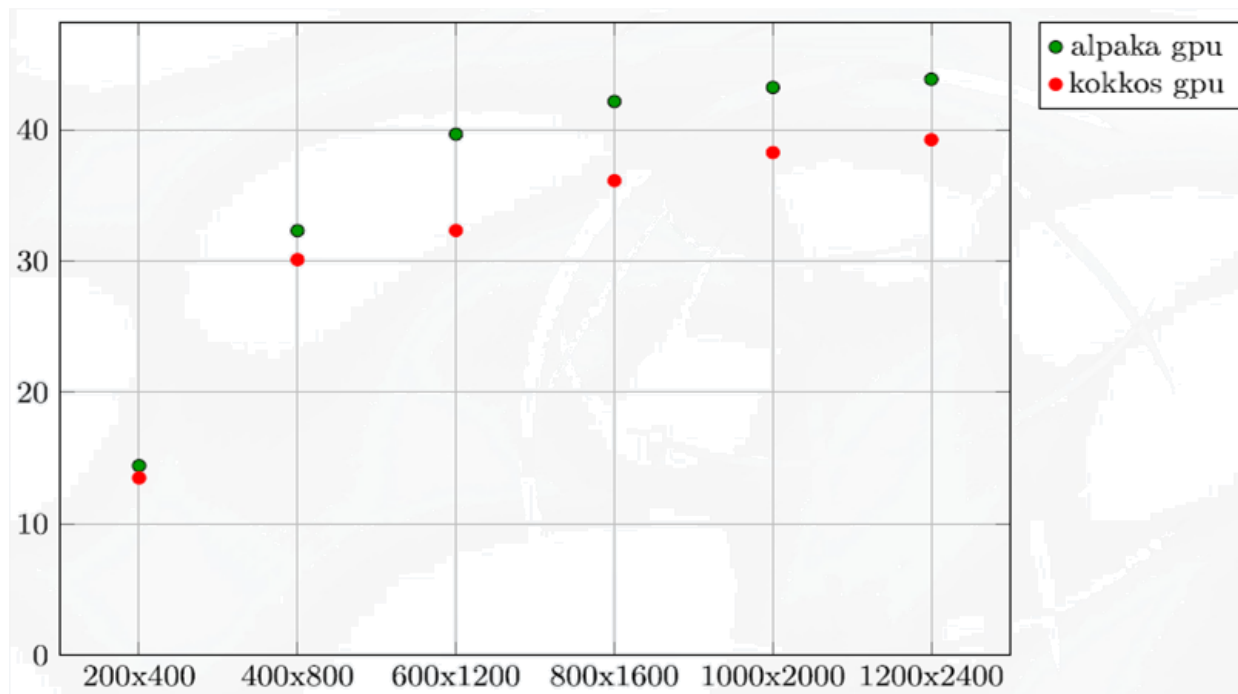
#endif

```



ALPAKA: Single-source programming for CPUs, GPUs & FPGAs

ALPAKA: Close to native performance



ALPAKA: Single-source programming for CPUs, GPUs & FPGAs

Close to native performance

Alpaka CUDA PTX

```
mov.u32    %r3, %ctaid.x;
mov.u32    %r4, %ntid.x;
mov.u32    %r5, %tid.x;
mad.lo.s32 %r1, %r4, %r3, %r5;
setp.ge.s32 %p1, %r1, %r2;
@%p1 bra  BB6_2;

cvta.to.global.u64 %rd3, %rd2;
cvta.to.global.u64 %rd4, %rd1;
mul.wide.s32    %rd5, %r1, 8;
add.s64        %rd6, %rd4, %rd5;
ld.global.f64  %fd2, [%rd6];
add.s64        %rd7, %rd3, %rd5;
ld.global.f64  %fd3, [%rd7];
fma.rn.f64     %fd4, %fd2, %fd1, %fd3;
st.global.f64  [%rd7], %fd4;
```

Native CUDA PTX

```
mov.u32    %r3, %ctaid.x;
mov.u32    %r4, %ntid.x;
mov.u32    %r5, %tid.x;
mad.lo.s32 %r1, %r4, %r3, %r5;
setp.ge.s32 %p1, %r1, %r2;
@%p1 bra  BB6_2;

cvta.to.global.u64 %rd3, %rd2;
cvta.to.global.u64 %rd4, %rd1;
mul.wide.s32    %rd5, %r1, 8;
add.s64        %rd6, %rd4, %rd5;
ld.global.nc.f64 %fd2, [%rd6];
add.s64        %rd7, %rd3, %rd5;
ld.global.f64  %fd3, [%rd7];
fma.rn.f64     %fd4, %fd2, %fd1, %fd3;
st.global.f64  [%rd7], %fd4;
```



alpaka

I have a C++ CUDA code and am too lazy to port it

CUPLA: Making portable ALPAKA code without effort

Native CUDA Code

```
// CUDA kernel
__global__ void kernel(/* Args */)
{
    /* CUDA code */
}

// Kernel launch
dim3 gridSize(42, 1, 1);
dim3 blockSize(256, 1, 1);
kernel<<<gridSize, blockSize>>>(/* Args */);
```

Portable CUPLA Code

```
// include CUPLA-to-CUDA header
#include <cuda_to_cupla.hpp>

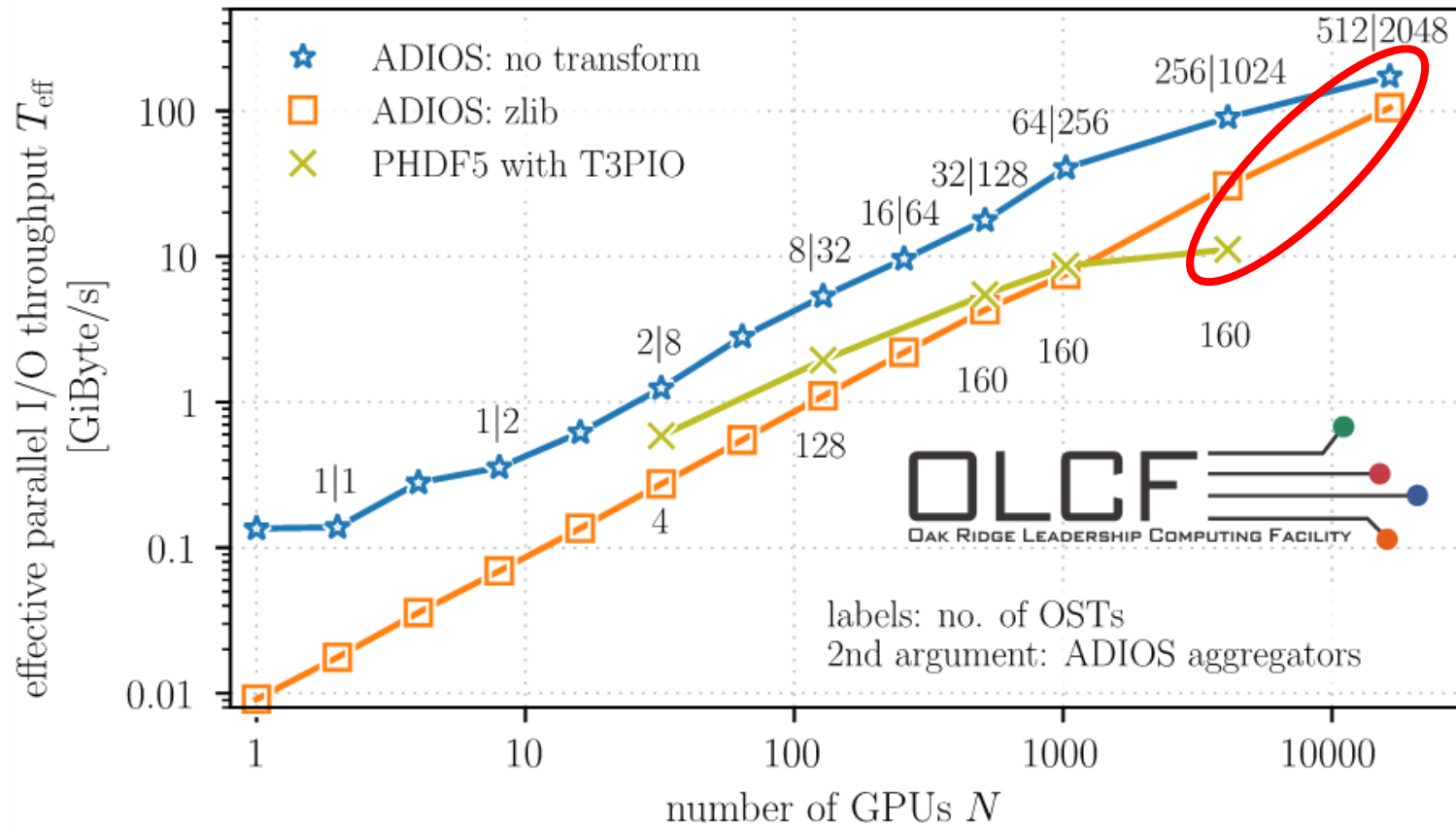
// replace kernel definition with functor definition
struct Kernel {
    template<typename TAcc>
    ALPAKA_FN_ACC
    void operator()(TAcc const& acc,
                   /* Args */) const
    {
        /* CUDA code */
    }
};

// Kernel launch
dim3 gridSize(42, 1, 1);
dim3 blockSize(256, 1, 1);
CUPLA_KERNEL(Kernel)(gridSize, blockSize)(/* Args */);
```



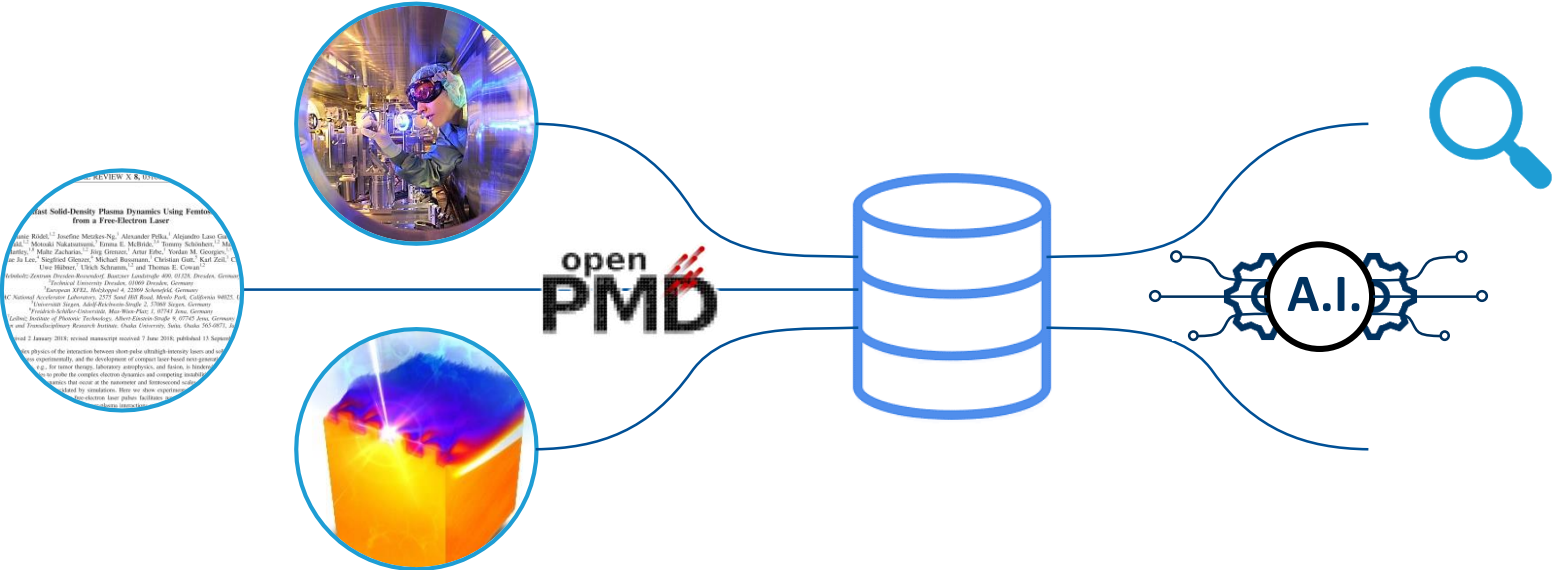
I/O is seriously limited

OPENPMD: F.A.I.R. I/O and streaming for the Exascale era



OPENPMD: F.A.I.R. I/O and streaming for the Exascale era

OPENPMD: Streaming workflows for Analysis, Simulation & AI



REVIEW A. & U. ...
Fast Solid-Density Plasma Dynamics Using Femto-
Pulses from a Free-Electron Laser
Janis Ködder,^{1,2} Ines-Marie Morlock-Ng,³ Alexander Pylka,⁴ Alejandro-Luis Garcia,⁵
Mitsuru Nakatsunagi,⁶ Emma E. McBride,⁷ Timothy Schifano,⁸ M.
S. Jentsch,⁹ Maja Zarkovic,¹⁰ Eug. Gerasim,¹¹ Andrei Ephe,¹² Yoonan M. Gougeon,¹³
Jun-Ju Lee,¹⁴ Siegfried Glenz,¹⁵ Michael Beumann,¹⁶ Christian Goh,¹⁷ Karl Zosel,¹⁸ C.
Ulrich Hübner,¹⁹ Ulrich Schramm,²⁰ and Thomas E. Cowan²¹
¹Maxwell Institute for Quantum and Laser Photonics, Lancaster University, LA1 4YW, Lancaster, UK
²Department of Physics, Lancaster University, LA1 4YW, Lancaster, UK
³Department of Physics, Lancaster University, LA1 4YW, Lancaster, UK
⁴Department of Physics, Lancaster University, LA1 4YW, Lancaster, UK
⁵Department of Physics, Lancaster University, LA1 4YW, Lancaster, UK
⁶Department of Physics, Lancaster University, LA1 4YW, Lancaster, UK
⁷Department of Physics, Lancaster University, LA1 4YW, Lancaster, UK
⁸Department of Physics, Lancaster University, LA1 4YW, Lancaster, UK
⁹Department of Physics, Lancaster University, LA1 4YW, Lancaster, UK
¹⁰Department of Physics, Lancaster University, LA1 4YW, Lancaster, UK
¹¹Department of Physics, Lancaster University, LA1 4YW, Lancaster, UK
¹²Department of Physics, Lancaster University, LA1 4YW, Lancaster, UK
¹³Department of Physics, Lancaster University, LA1 4YW, Lancaster, UK
¹⁴Department of Physics, Lancaster University, LA1 4YW, Lancaster, UK
¹⁵Department of Physics, Lancaster University, LA1 4YW, Lancaster, UK
¹⁶Department of Physics, Lancaster University, LA1 4YW, Lancaster, UK
¹⁷Department of Physics, Lancaster University, LA1 4YW, Lancaster, UK
¹⁸Department of Physics, Lancaster University, LA1 4YW, Lancaster, UK
¹⁹Department of Physics, Lancaster University, LA1 4YW, Lancaster, UK
²⁰Department of Physics, Lancaster University, LA1 4YW, Lancaster, UK
²¹Department of Physics, Lancaster University, LA1 4YW, Lancaster, UK



Tools for the NFDI Data Challenge from HPC to Edge

Open, F.A.I.R. & fast



alaka



upla



AMA



open
PMD



DAPHNE
4NFDI



PUNCH
4NFDI