Efficient Scientific Computing School – 13th Edition

Exploiting Heterogeneous Architectures: Applications and Lessons Learned

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```
mirror object to mirror
irror_mod.mirror_object
peration == "MIRROR_X":
irror_mod.use_x = True
irror_mod.use_y = False
irror_mod.use_z = False
 operation == "MIRROR_Y"
irror_mod.use_x = False
irror_mod.use_y = True
irror_mod.use_z = False
 operation == "MIRROR_Z"
irror_mod.use_x
```

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CBG Max Planck Institute of Molecular Cell Biology and Genetics

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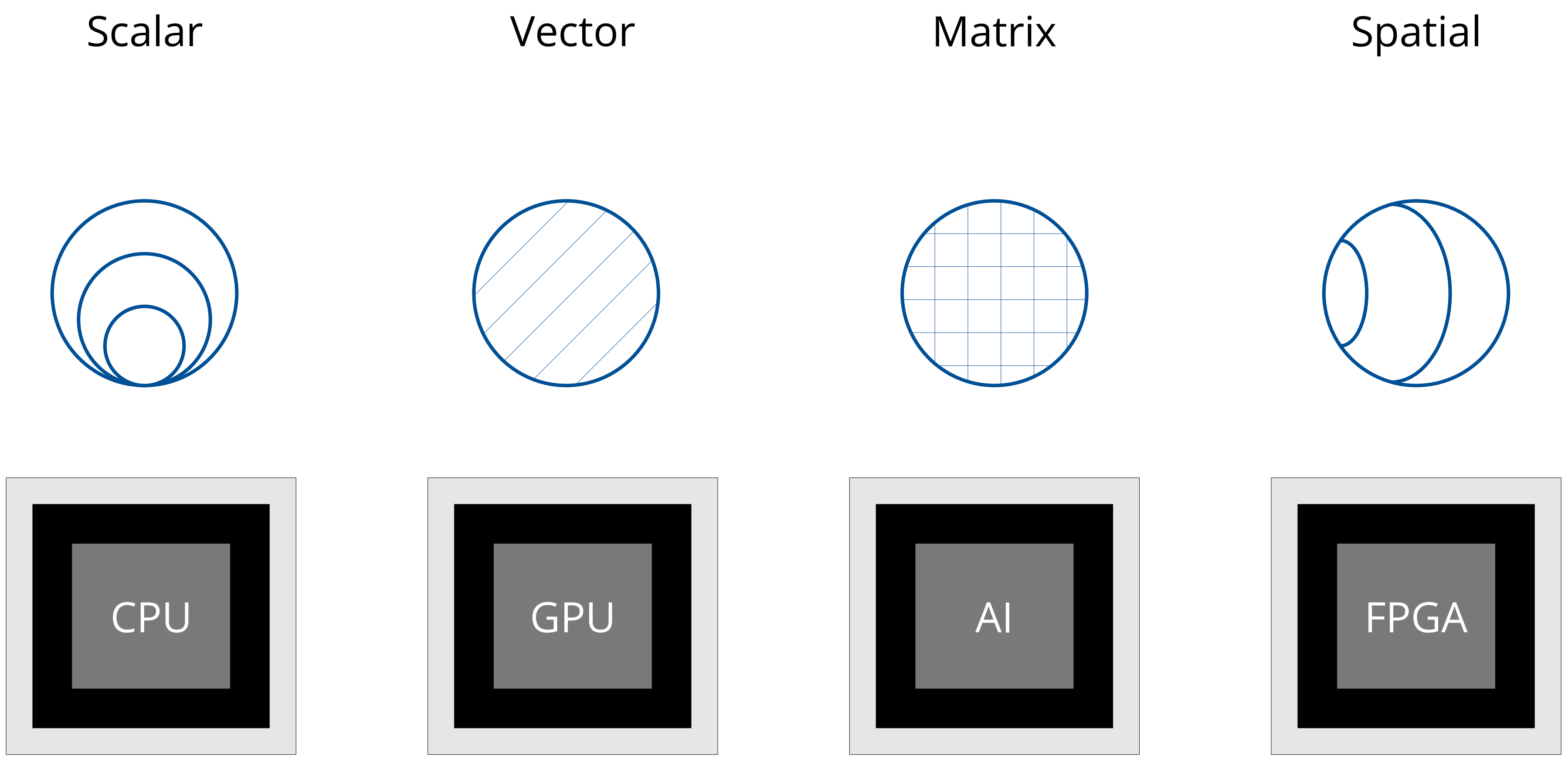
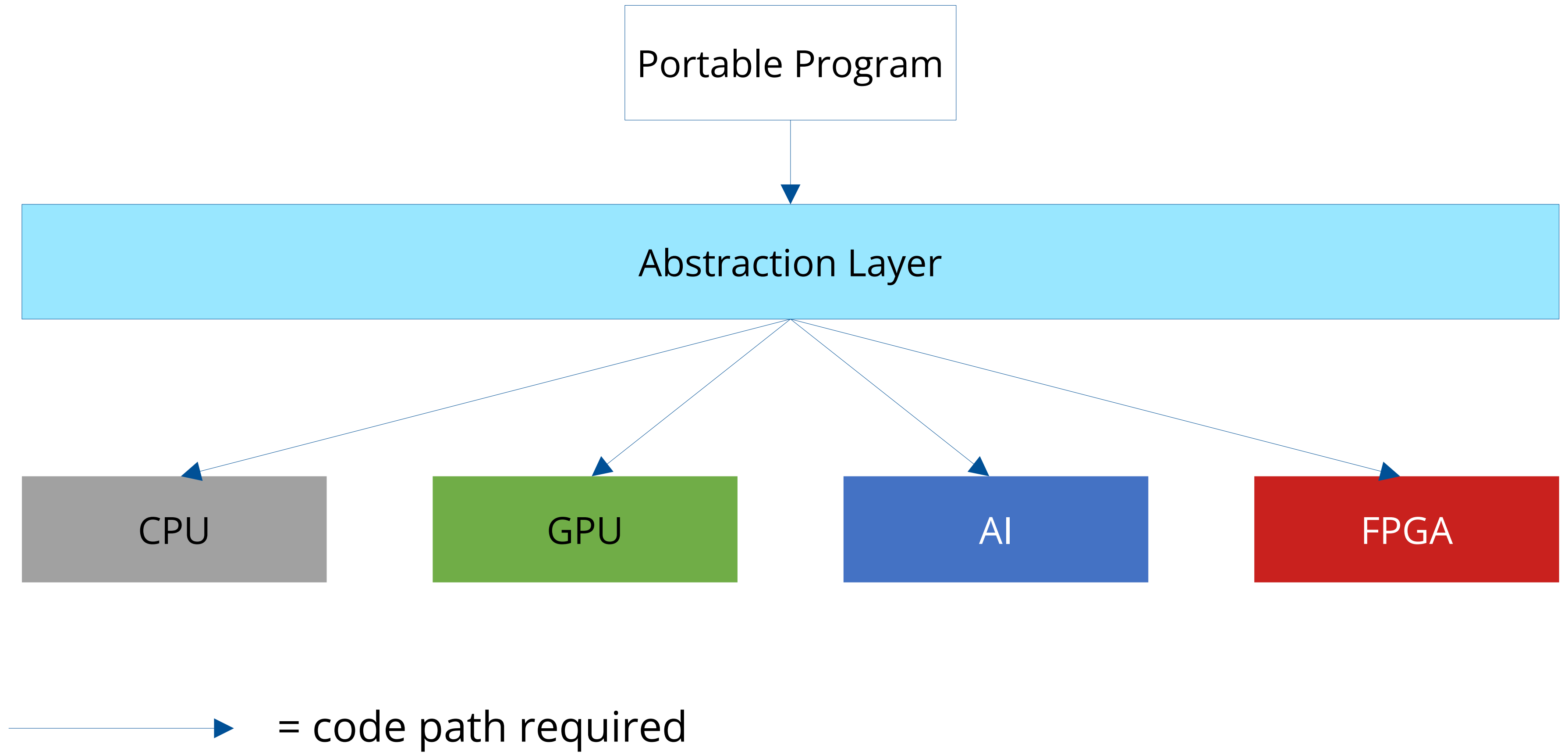
Recap

Workload Patterns



General Idea



Available Libraries

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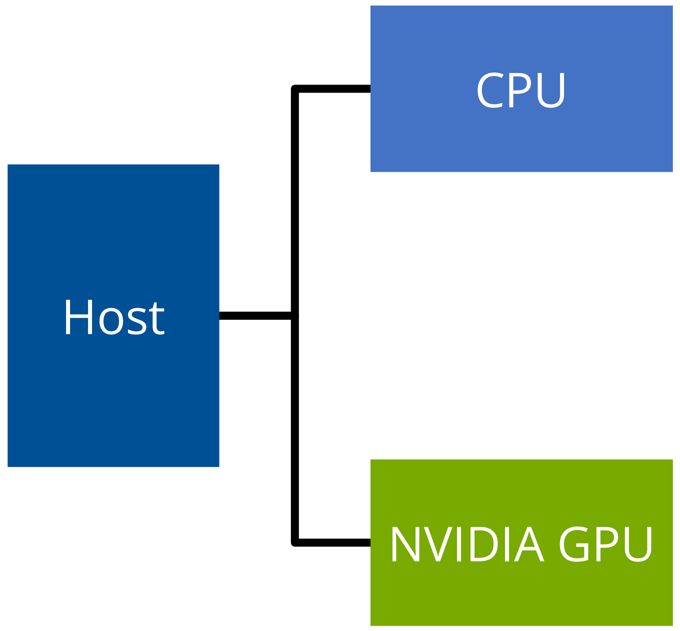
Programming Heterogeneous Systems

Heterogeneous Systems

- Real-world scenario: Use all available compute power
- Also real-world scenario: Multiple different hardware types available
- Requirement: Usage of one back-end per hardware platform
- Requirement: Back-ends need to be interoperable



Mastering Heterogeneous Systems

Why Do We Need This?

Can’t we just decide on one accelerator?

- In one word: Yes.

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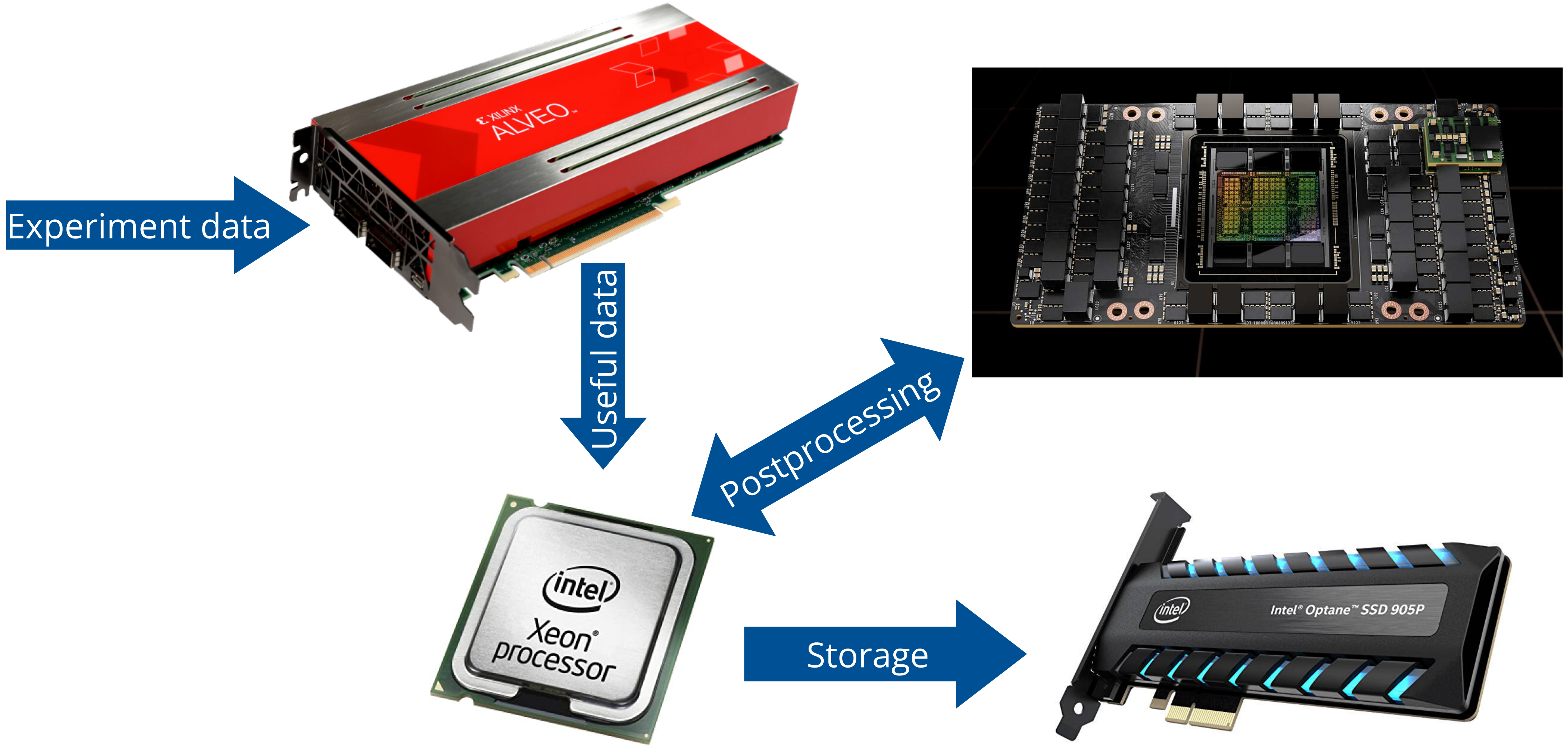
- Questions to ask yourself:
  - What is the expected lifetime of the application?
  - Is the accelerator suitable for all required algorithms?
  - If not, what is the penalty for using a non-ideal accelerator?
  - Do you have enough money to buy another accelerator?

Example Setup



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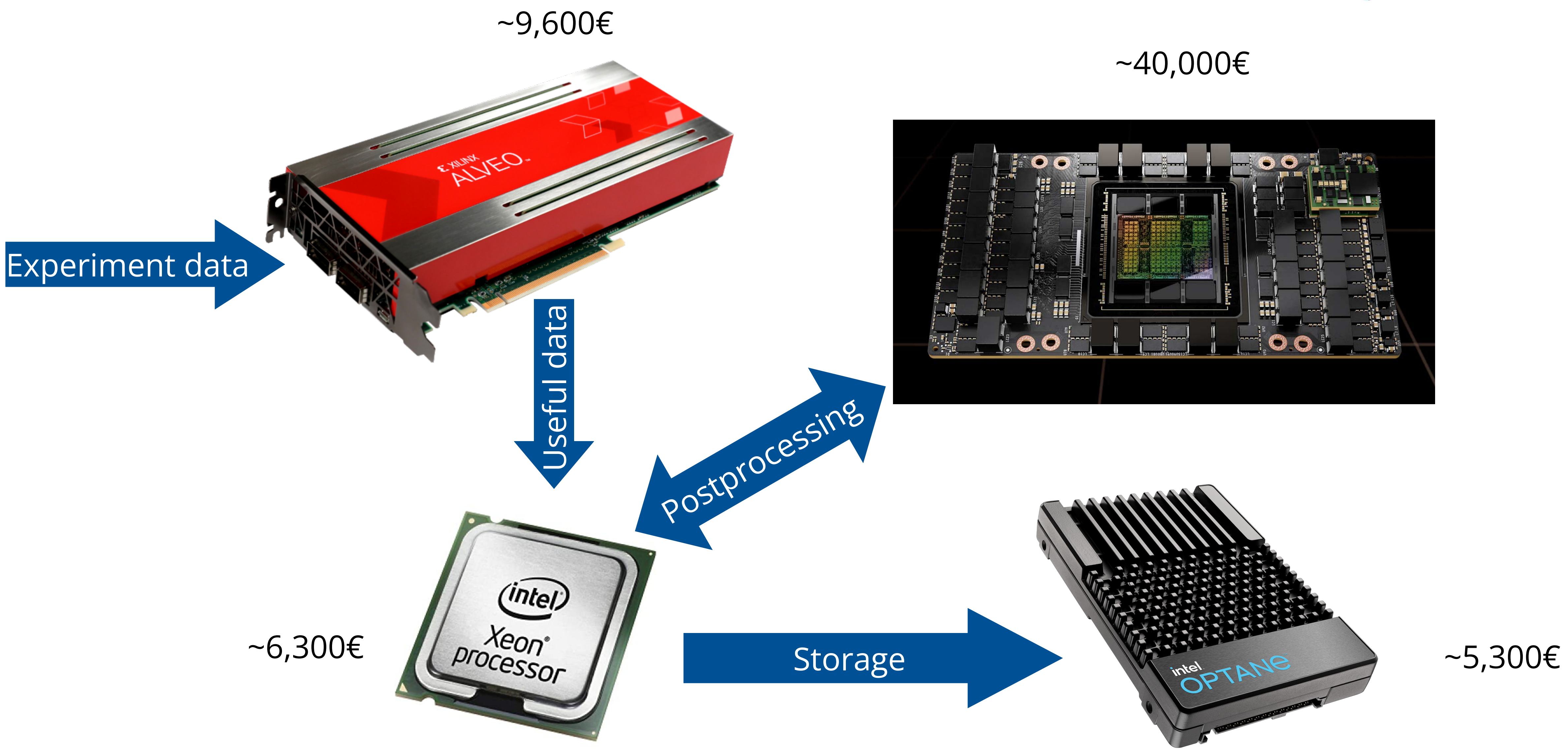

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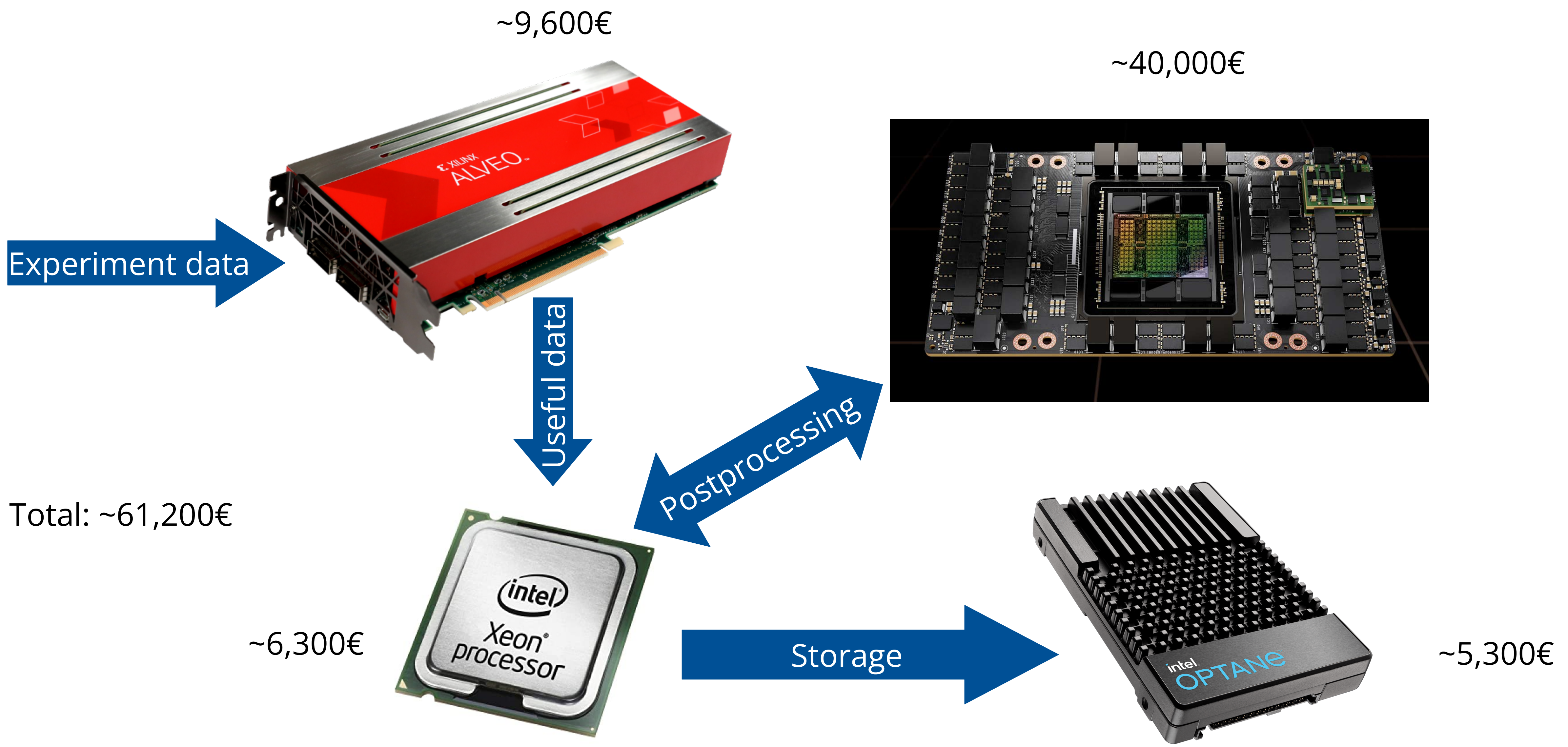

How Do We Control the Setup?

Bad solution

We can program each component individually using its native API!

- Requires detailed API knowledge for each platform
- Vendor lock-in for each component

How Do We Control the Setup?

Good solution

We use an abstraction layer for the entire application.

- Single API available for all underlying platforms
- Individual components can be easily exchanged

Real World Example: Porting Efforts

My Boss Walked Into My Office…

“Are you interested in testing alpaka on an experimental cluster?”

- New ARM-based CPU hardware available on cluster
- Node type #1: Fujitsu A64FX
  - Featured in Fugaku supercomputer (Fastest supercomputer from June 2020 – November 2021, currently #2)

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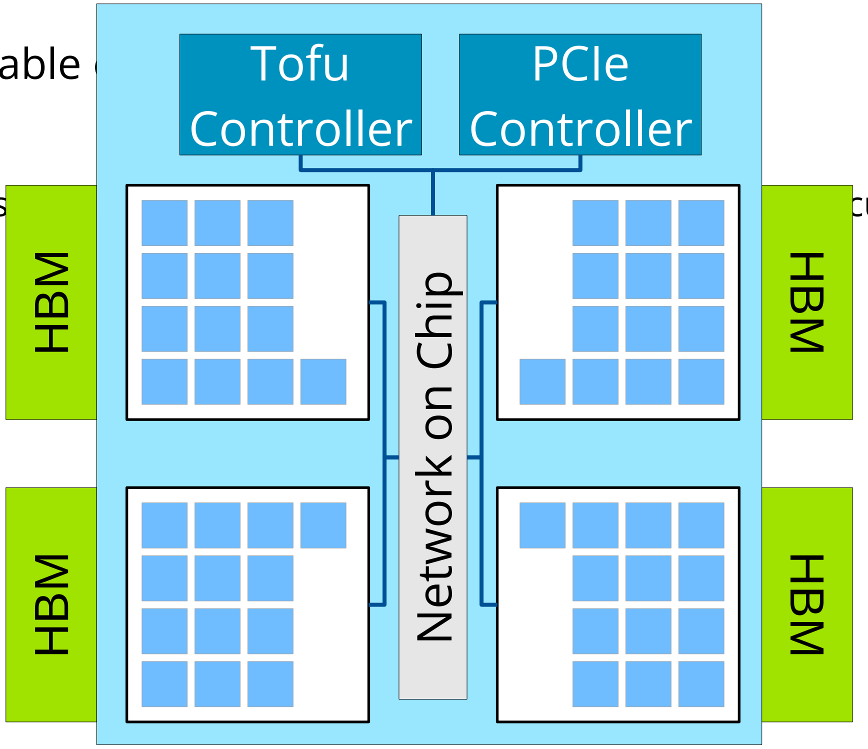

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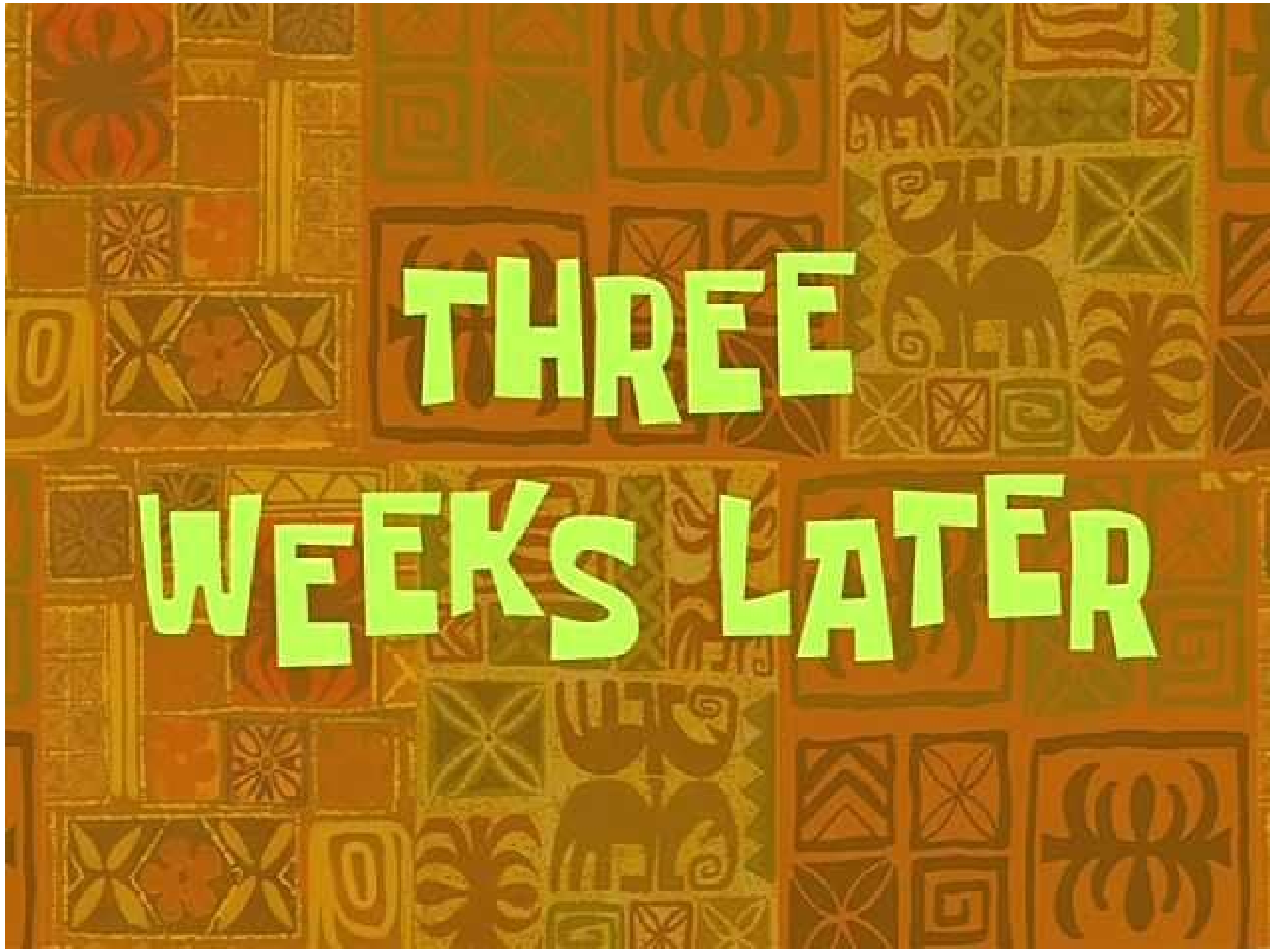
- Node type #1: Fujitsu A64FX
  - Featured in Fugaku supercomputer (Fastest supercomputer from June 2020 – November 2021, currently #2)
- Node type #2: Ampere Altra CPUs + NVIDIA A100 GPUs
  - Envisioned for enterprise-grade server applications
  - 80 cores @ 3.30 GHz (max)
  - No SIMD registers


THREE
WEEKS LATER

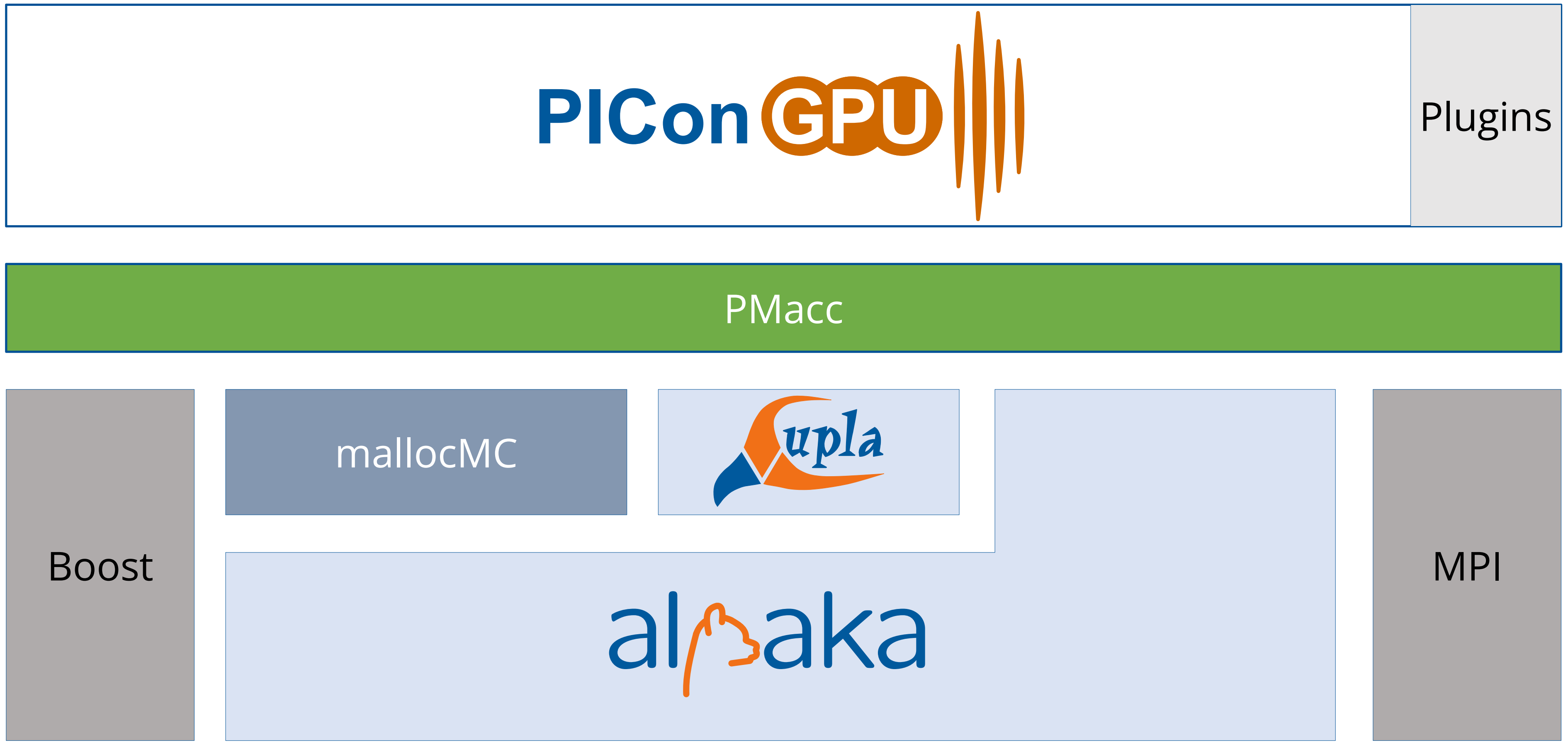
Three Weeks Later…

“We want you to port PIConGPU to the experimental hardware.”

- Fully relativistic, 3D3V particle-in-cell code
- Implements various numerical schemes to solve the PIC cycle
- Full restart and output capabilities
- 2D and 3D live view and diagnostic tools
- Many plugins available
- Utilization of several thousand GPUs possible
- 2013: Finalist of Gordon Bell prize (for scalability to > 18,000 GPUs)

https://www.github.com/ComputationalRadiationPhysics/picongpu

PIConGPU Software Stack



Porting Effort

Required efforts

- Some dependencies were not available on the cluster → self-compiled
  - Boost 1.78.0
  - libpng /pngwriter
  - openPMD
- PIConGPU's build system required support for `armclang++` compiler

Worked out-of-the-box

- Could compile for CPU architecture and utilize all CPU cores
- Could immediately utilize NVIDIA GPUs

→ **no C++ code changes required!**

Benefits of Using alpaka

Using alpaka saved several hours of porting efforts!

- alpaka's core is written in **standard** C++17
- x86-specific parts were made optional in 2021

  → Improvements in alpaka directly improve existing user code
- Utilization of ARM CPUs through alpaka's OpenMP back-end
- Utilization of NVIDIA GPUs through alpaka's CUDA back-end

Example: Maintenance & Future-Proofing

Example: CERN CMS Patatrack

- CMSSW reconstruction software currently (Run-3) runs on ~30,000 x86 CPUs
- Run-4 planned for 2027+ will see several hardware / detector upgrades for experiment
- CPUs will not be performant enough to process (much) larger data sizes
- Accelerators are required

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- **How to plan for the future?**

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Benefits of Abstraction Layers

- Unified API for users

  → Vendor and hardware type (almost) do not matter
- Support for future hardware is not the user’s problem

  → Implementers of abstraction layers will deal with this
- Easy comparison of hardware types
- **Less technical debt**

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