



Scientific Software Design



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Better Scientific Software tutorial @ SC22

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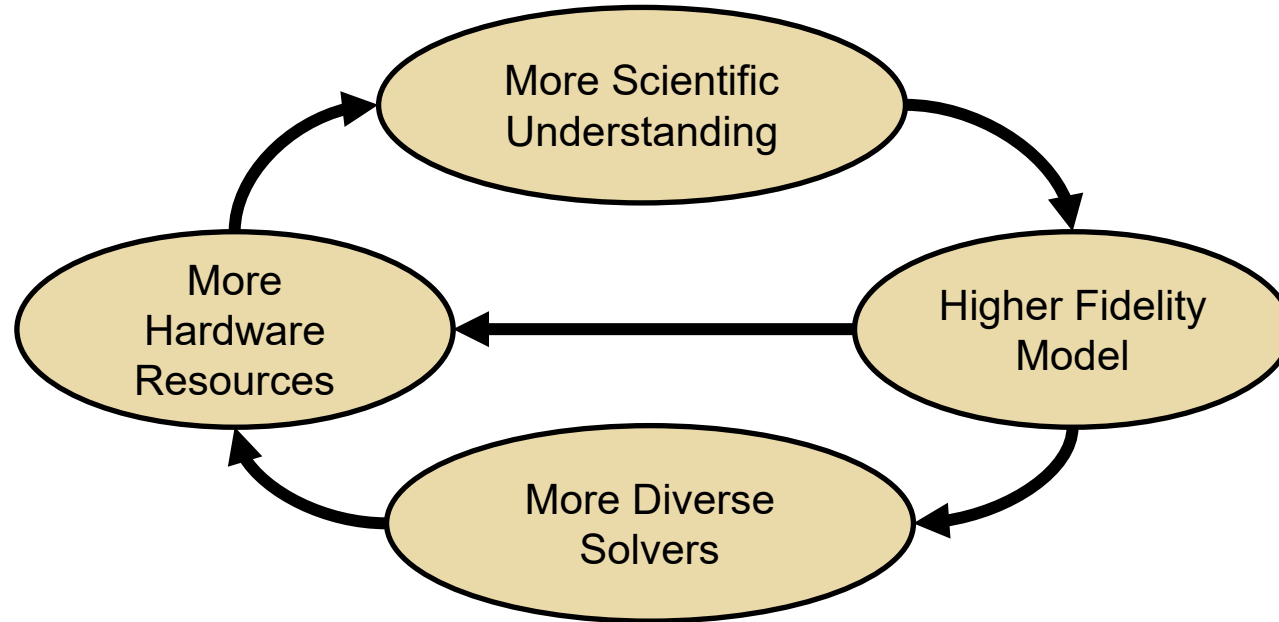
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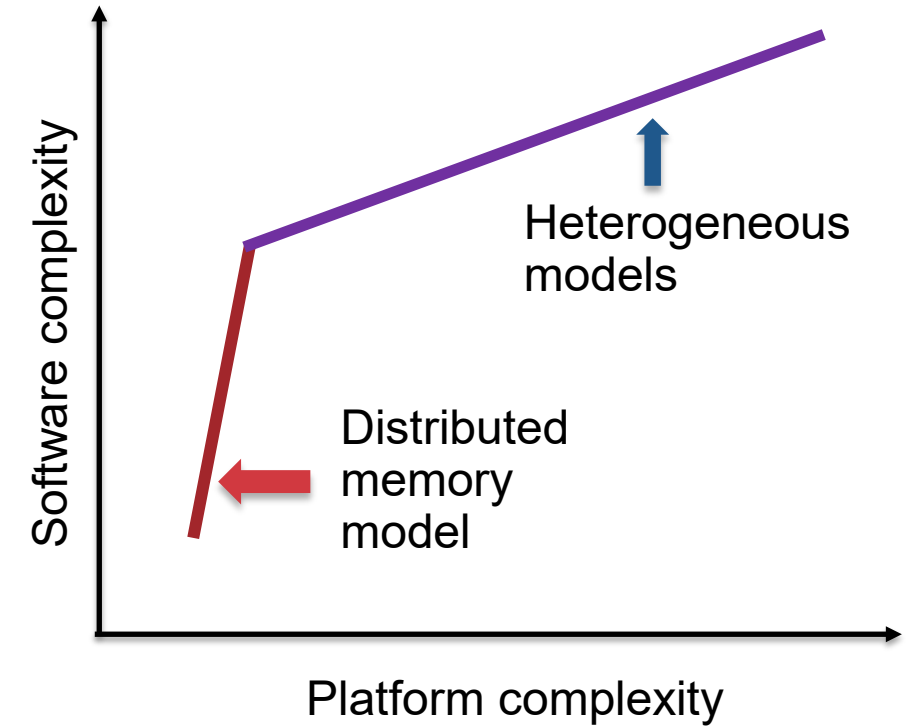
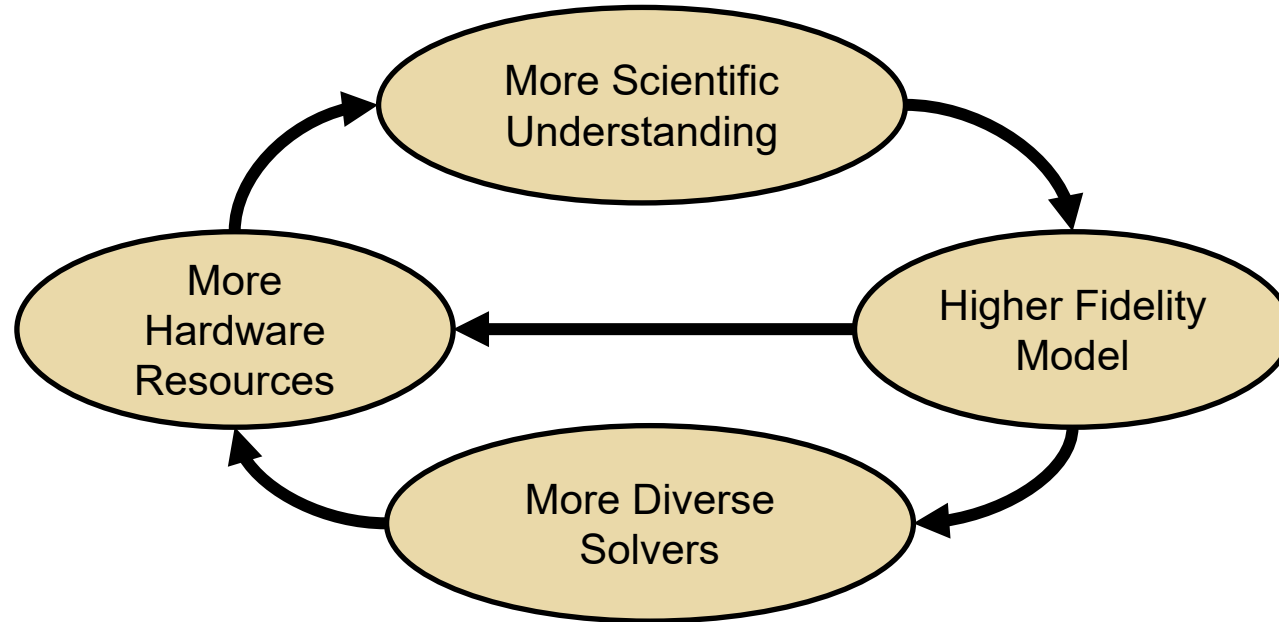
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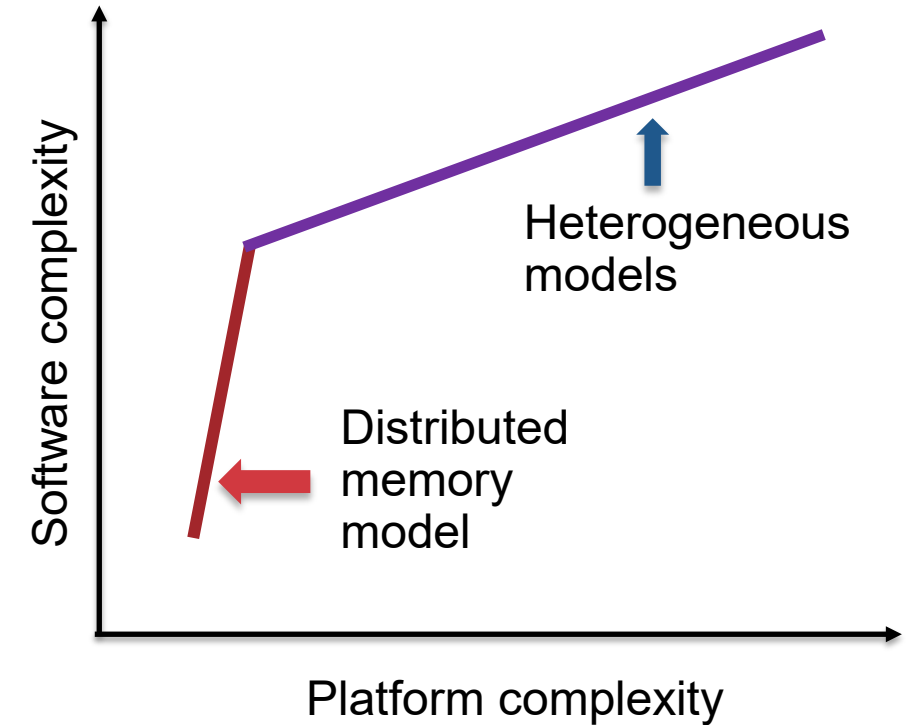
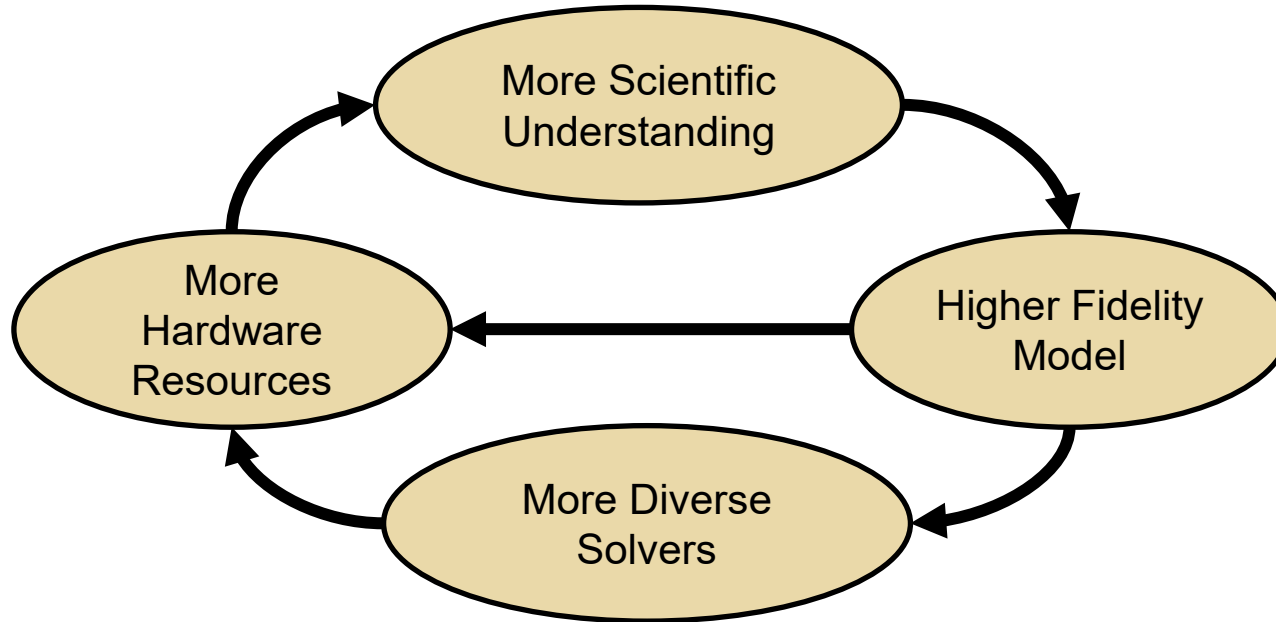
HPC Computational Science Use-case



HPC Computational Science Use-case



HPC Computational Science Use-case



- ❑ Many components may be under research
- ❑ Software continuously evolves
- ❑ All use cases are different and unique

General Design Principles for HPC Scientific Software

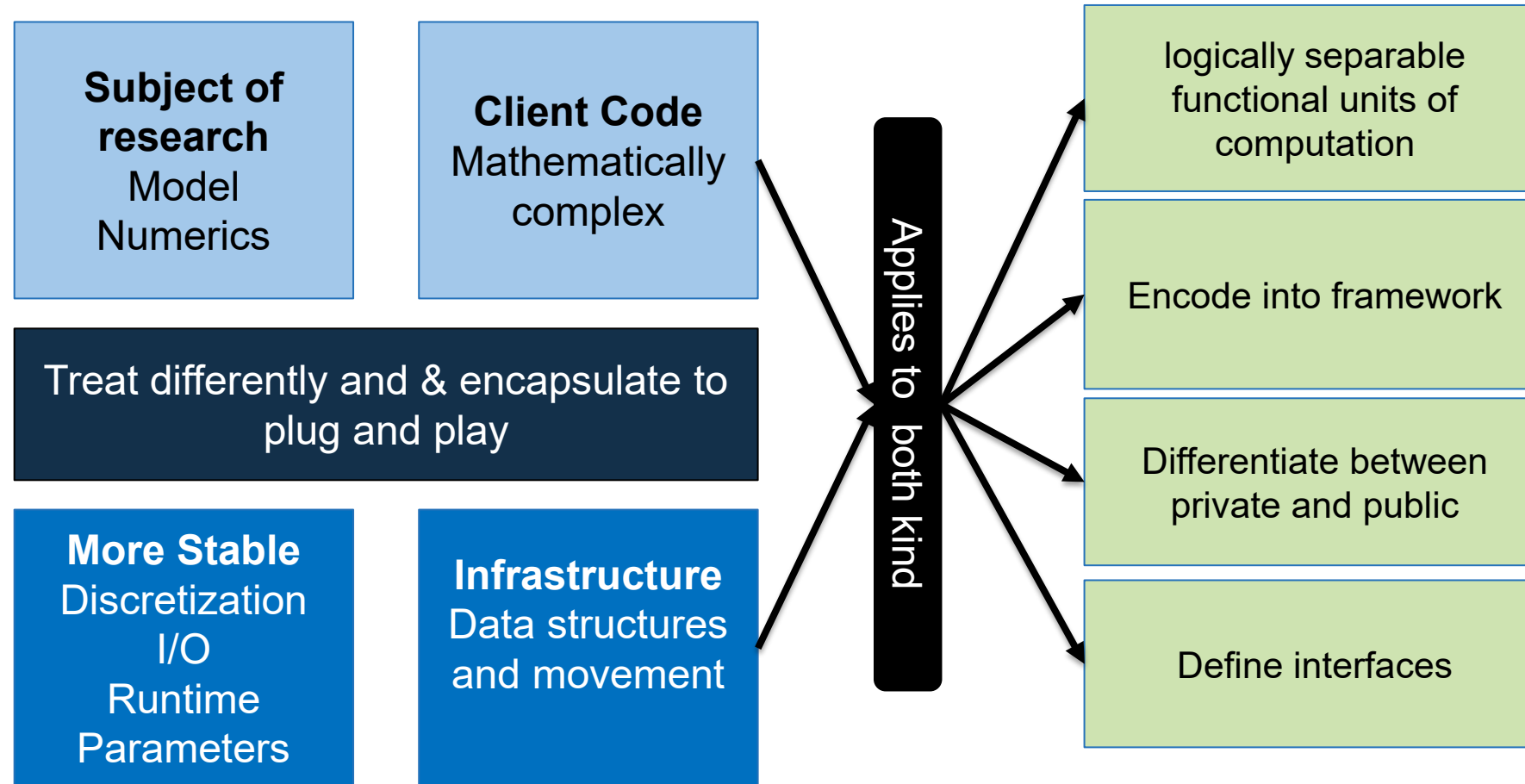
Considerations

- ❑ Multidisciplinary teams
 - ❑ Many facets of knowledge
 - ❑ To know everything is not feasible
- ❑ Two types of code components
 - ❑ Infrastructure (mesh/IO/runtime ...)
 - ❑ Science models (numerical methods)
- ❑ Codes grow
 - ❑ New ideas => new features
 - ❑ Code reuse by others

Design Implications

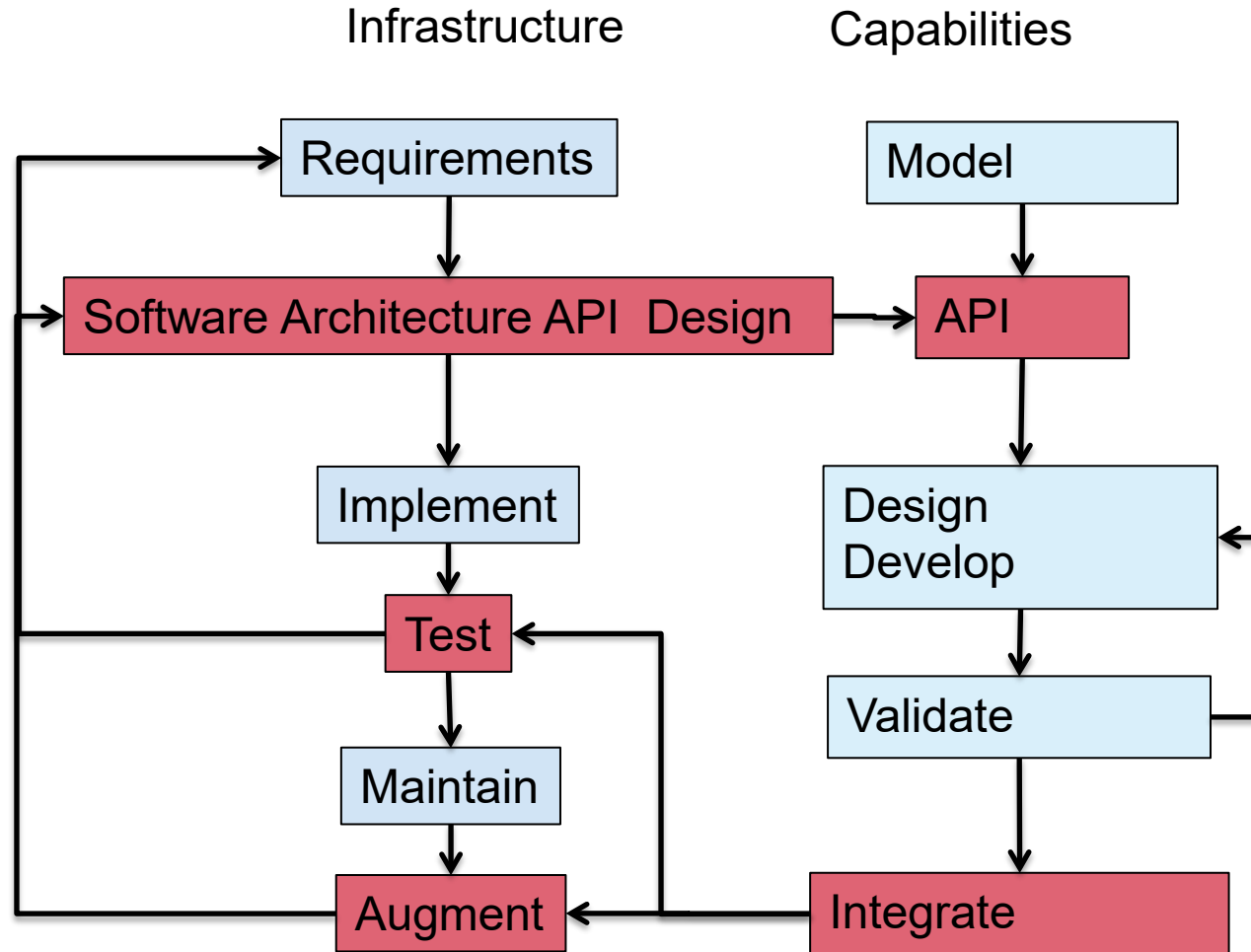
- ❑ Separation of Concerns
 - ❑ Shield developers from unnecessary complexities
- ❑ Work with different lifecycles
 - ❑ Long-lasting vs quick changing
 - ❑ Logically vs mathematically complex
- ❑ Extensibility built in
 - ❑ Ease of adding new capabilities
 - ❑ Customizing existing capabilities

General Design Principles for HPC Scientific Software



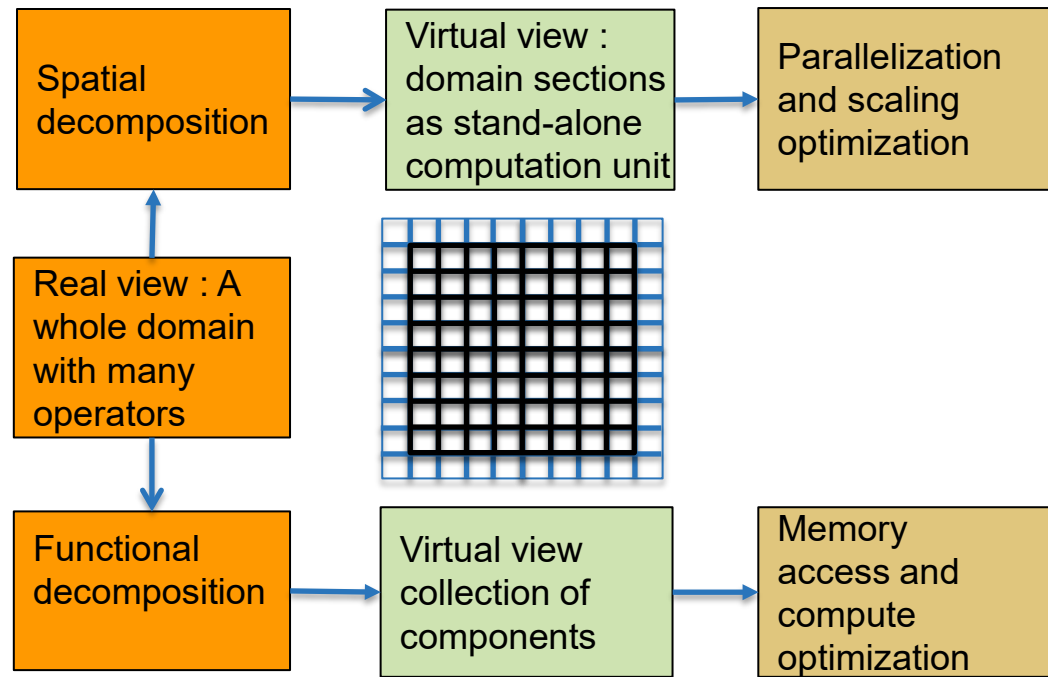
Design first, then apply programming model to the design instead of taking a programming model and fitting your design to it.

A Design Model for Separation of Concerns



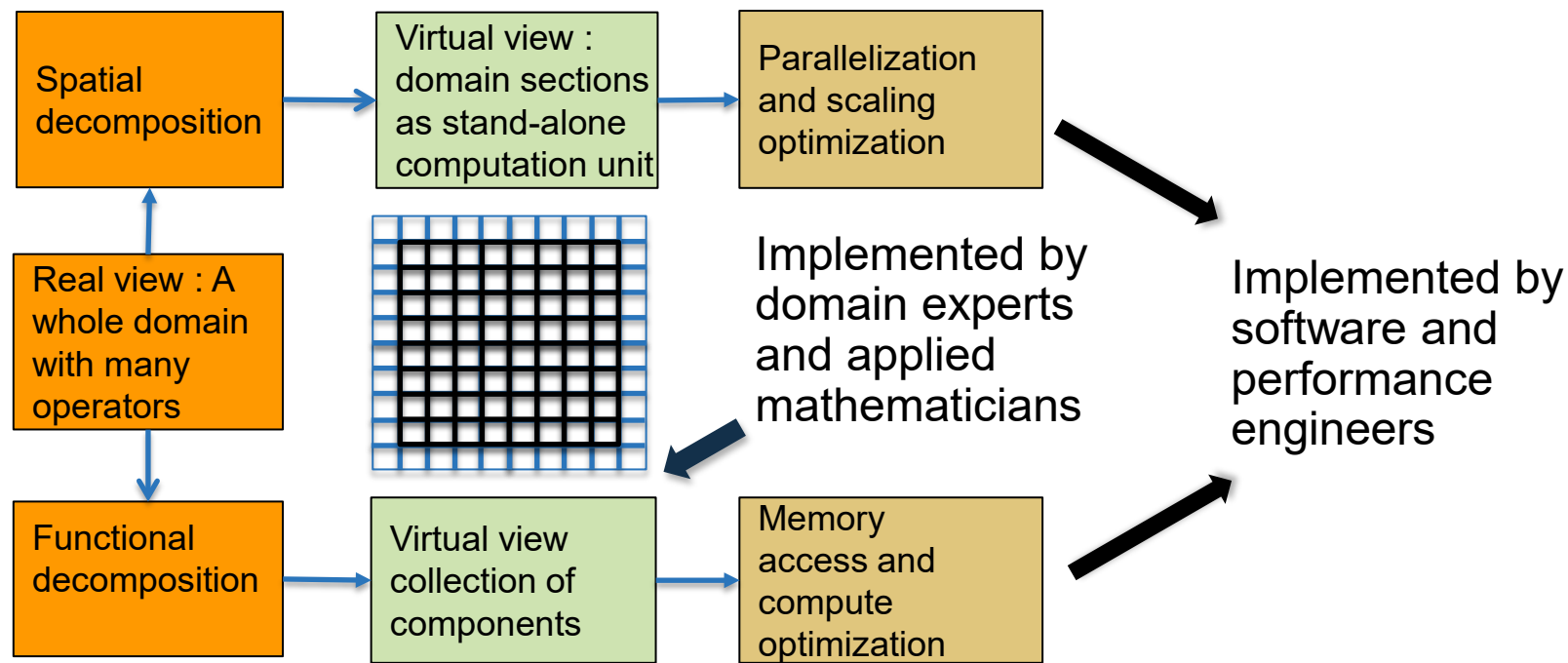
Example: Architecting Multiphysics PDEs

- Virtual view of functionalities
- Decomposition into units and definition of interfaces

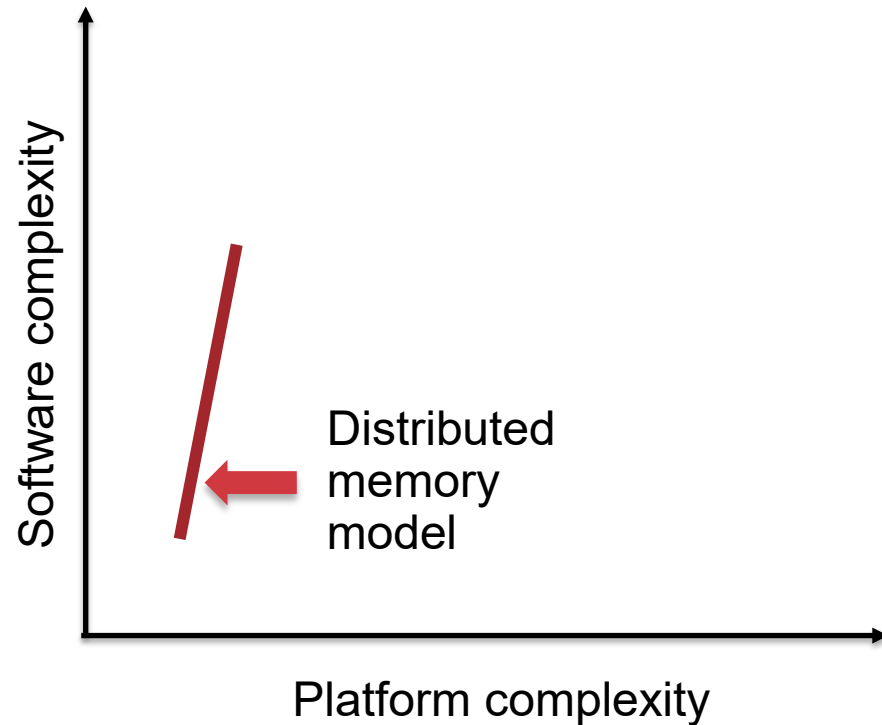


Example: Multiphysics PDEs for Distributed Memory Parallelism

- Virtual view of functionalities
- Decomposition into units and definition of interfaces

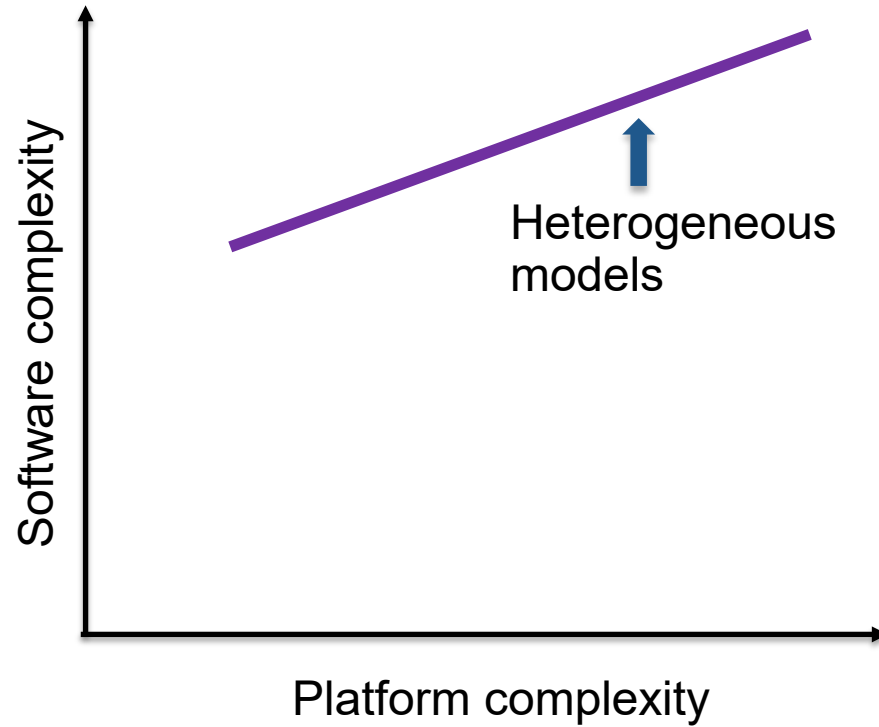


Takeaways Until Now



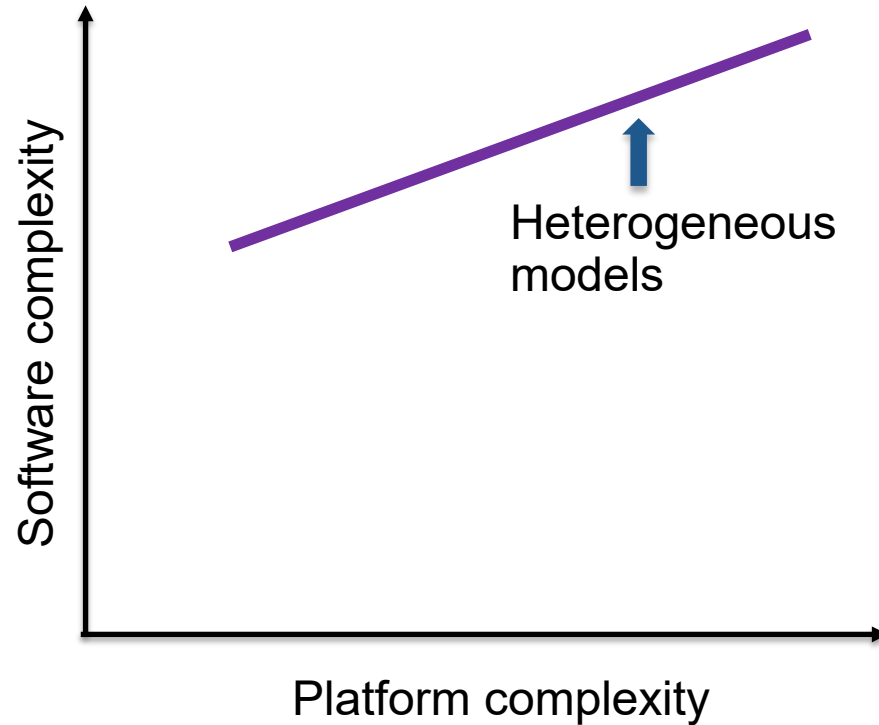
- Differentiate between slow changing and fast changing components of your code
- Understand the requirements of your infrastructure
- Implement separation of concerns
- Design with portability, extensibility, reproducibility and maintainability in mind
- Do not design with a specific programming model in mind

A New Paradigm Because of Platform Heterogeneity



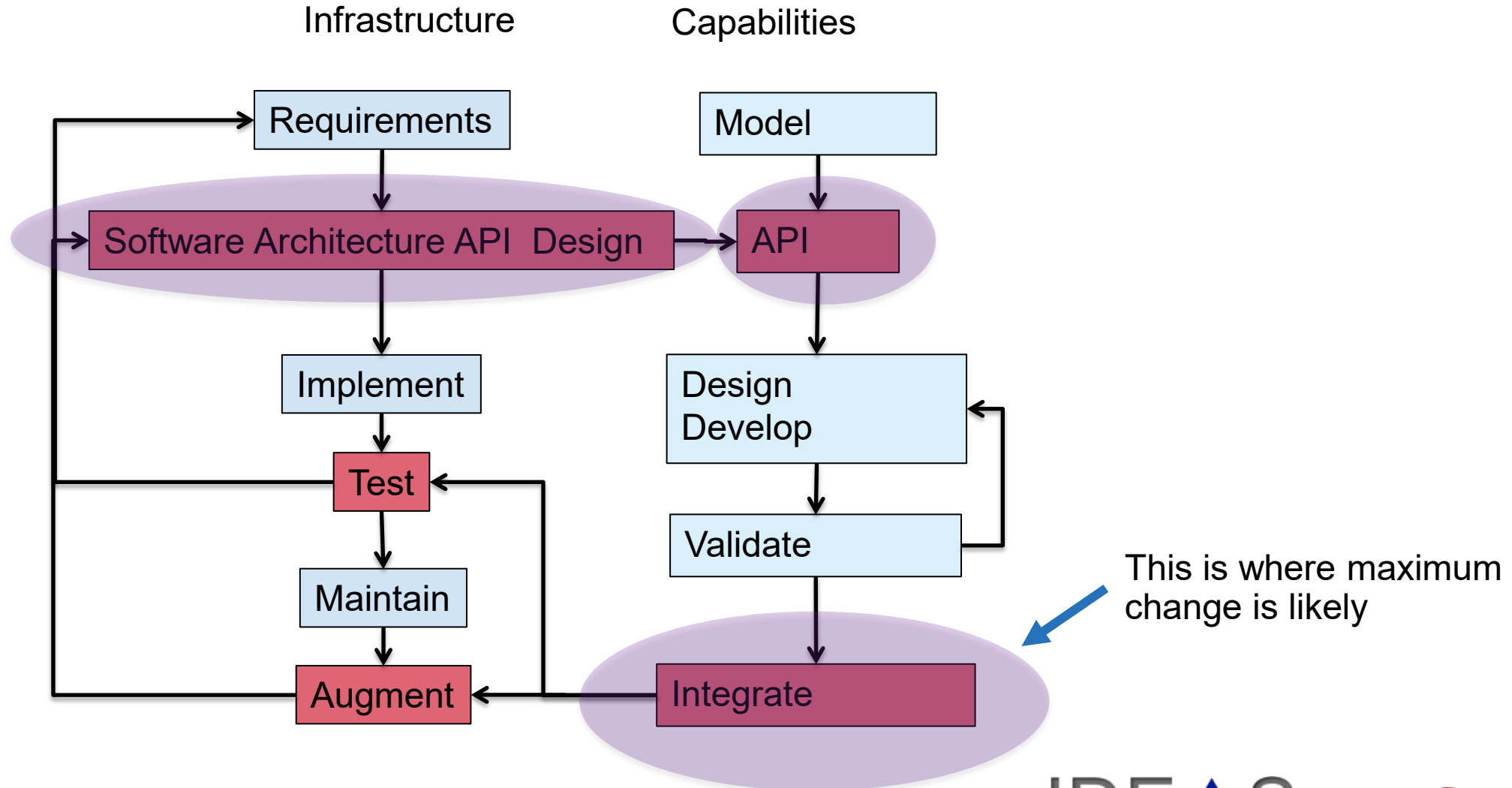
- Question - do the design principles change?

A New Paradigm Because of Platform Heterogeneity



- Question - do the design principles change?
- The answer is – not really
- The details get more involved

Handling Heterogeneity – Hardware and Software



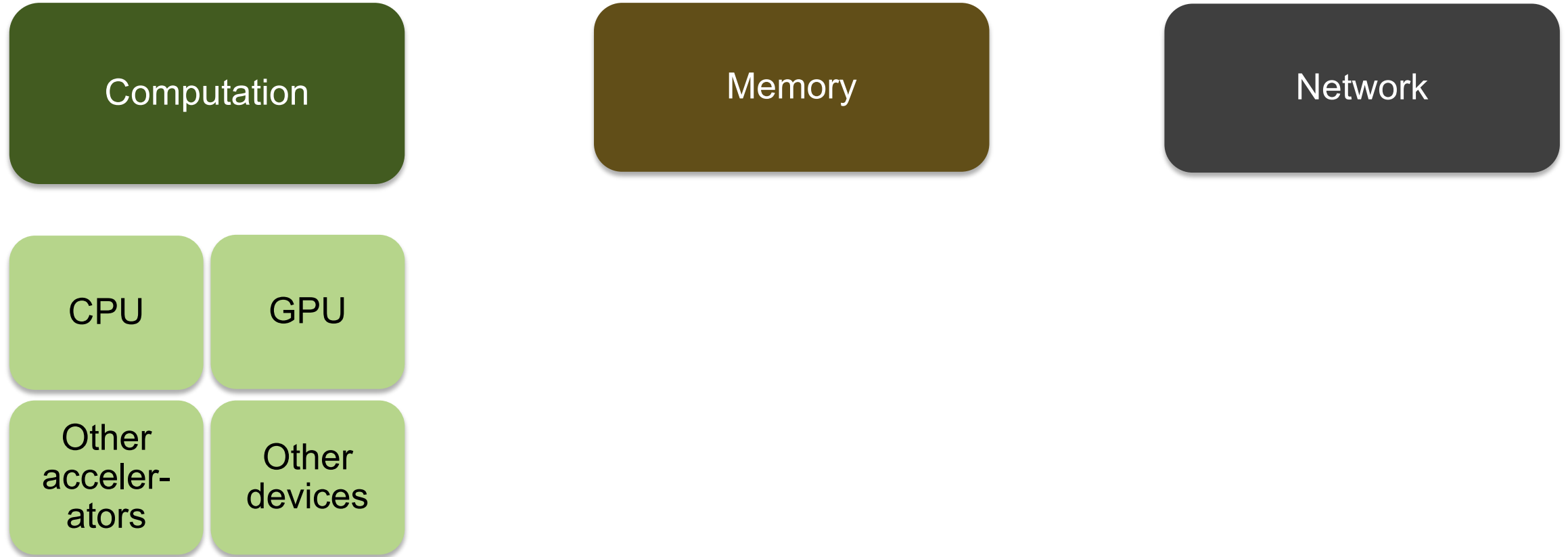
Platform Heterogeneity

Computation

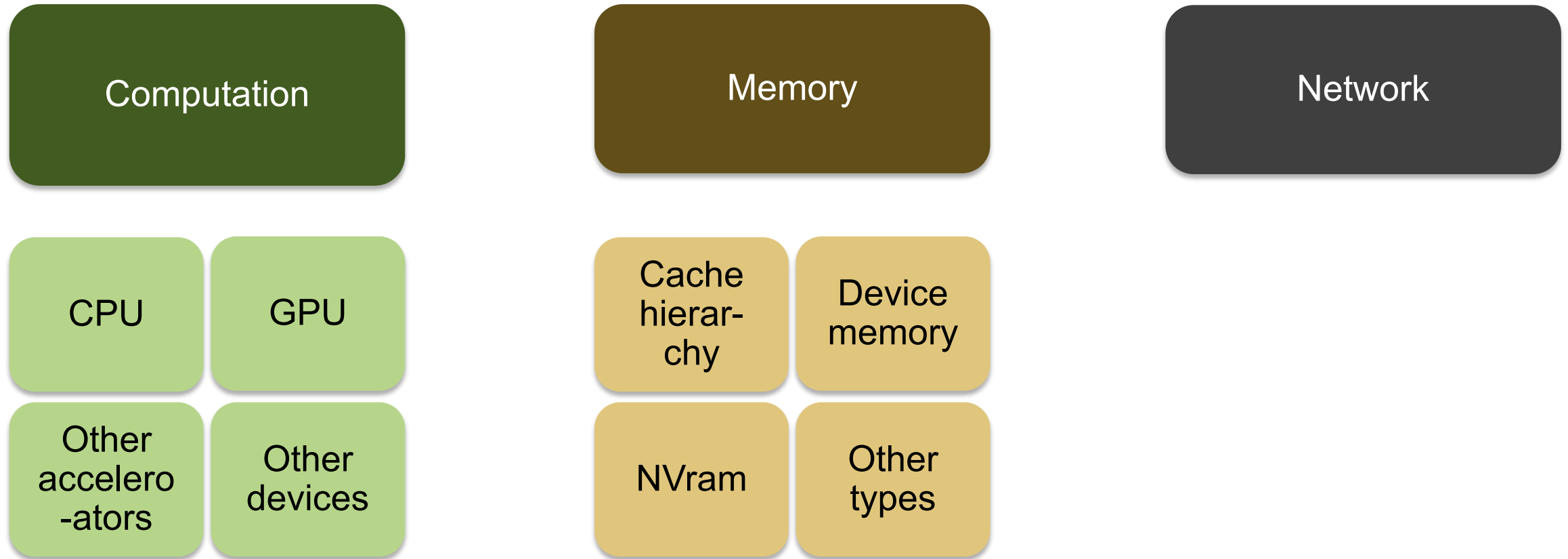
Memory

Network

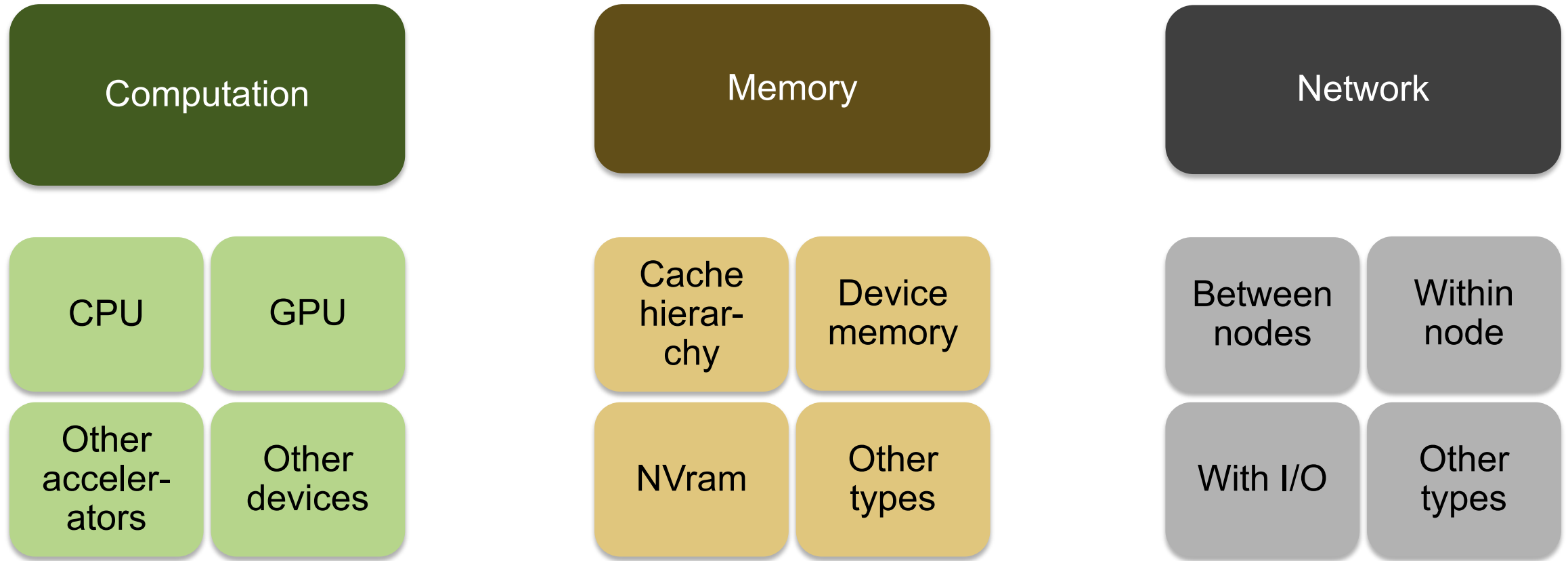
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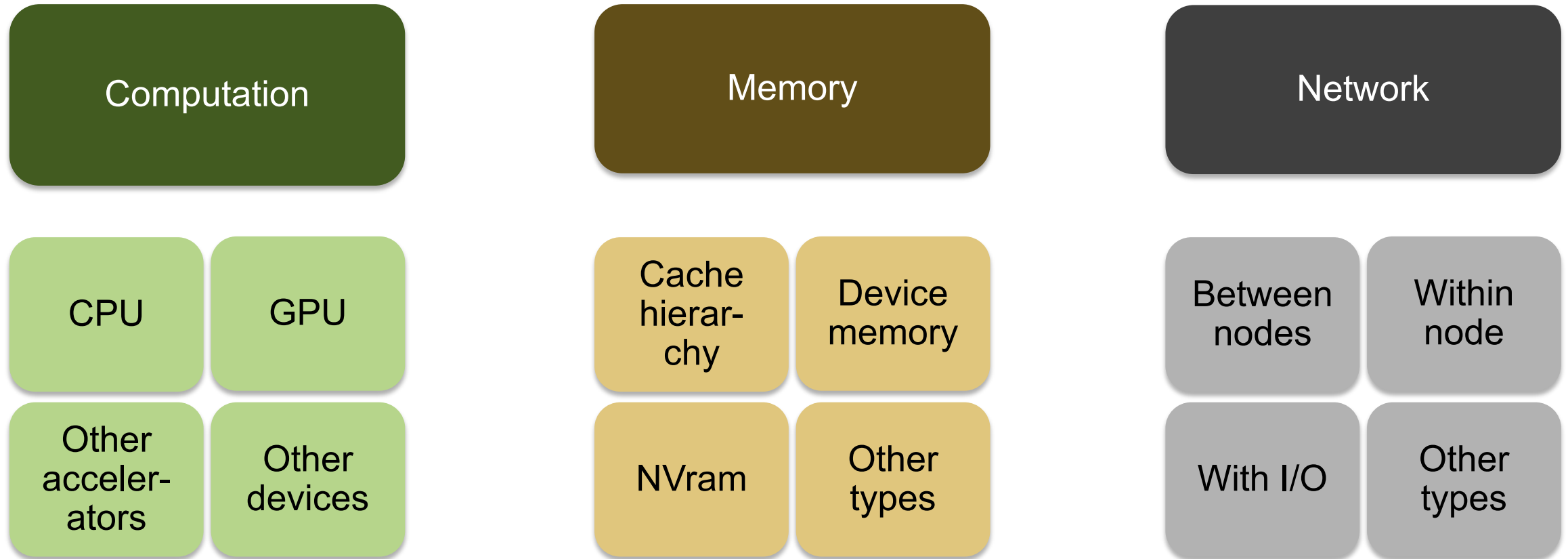
Platform Heterogeneity



Platform Heterogeneity



Platform Heterogeneity



And memory access models: unified memory / gpu-direct / explicit transfer

Mechanisms Needed by the Code

Mechanisms to unify expression of computation

- Minimize maintained variants of source suitable for all computational devices
- Reconcile differences in data structures

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Mechanisms to move work and data to computational targets

- Moving between devices
 - Launching work at the destination
 - Hiding latency of movement
- Moving data off node

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- Figuring out the map
 - Expression of dependencies
 - Cost models
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So, what do we need?

- Abstractions layers
- Code transformation tools
- Data movement orchestrators

Underlying Ideas: Unification of Computational Expressions

Make the same code work on different devices

Same algorithm different data layouts or operation sequence:

- A way to let compiler know that "this" expression can be specialized in many ways
- Definition of specializations
- Often done with template meta-programming

More challenging if algorithms need to be fundamentally different

- Support for alternatives

Underlying Ideas: Moving Work and Data to the Target

Parallelization Models

Hierarchy in domain decomposition

- Distributed memory model at node level – still very prevalent, likely to remain so for a while
- Also done with PGAS models – shared with locality being important

Assigning work within the node

- “Parallel For” or directives with unified memory
- Directives or specific programming model for explicit data movement

More complex data orchestration system for asynchronous computation

- Task based work distribution

Underlying Ideas: Mapping Work to Targets

This is how many abstraction layers work

- Infer the structure of the code
- Infer the map between algorithms and devices
- Infer the data movements
- Map computations to devices
- These are specified either through constructs or pragmas

**It can also be the end user who figures out the mapping
In either case performance depends upon how well the mapping is done**

Mechanisms Needed by the Code : Example Flash-X

Mechanisms to unify expression of computation

Macros with inheritance

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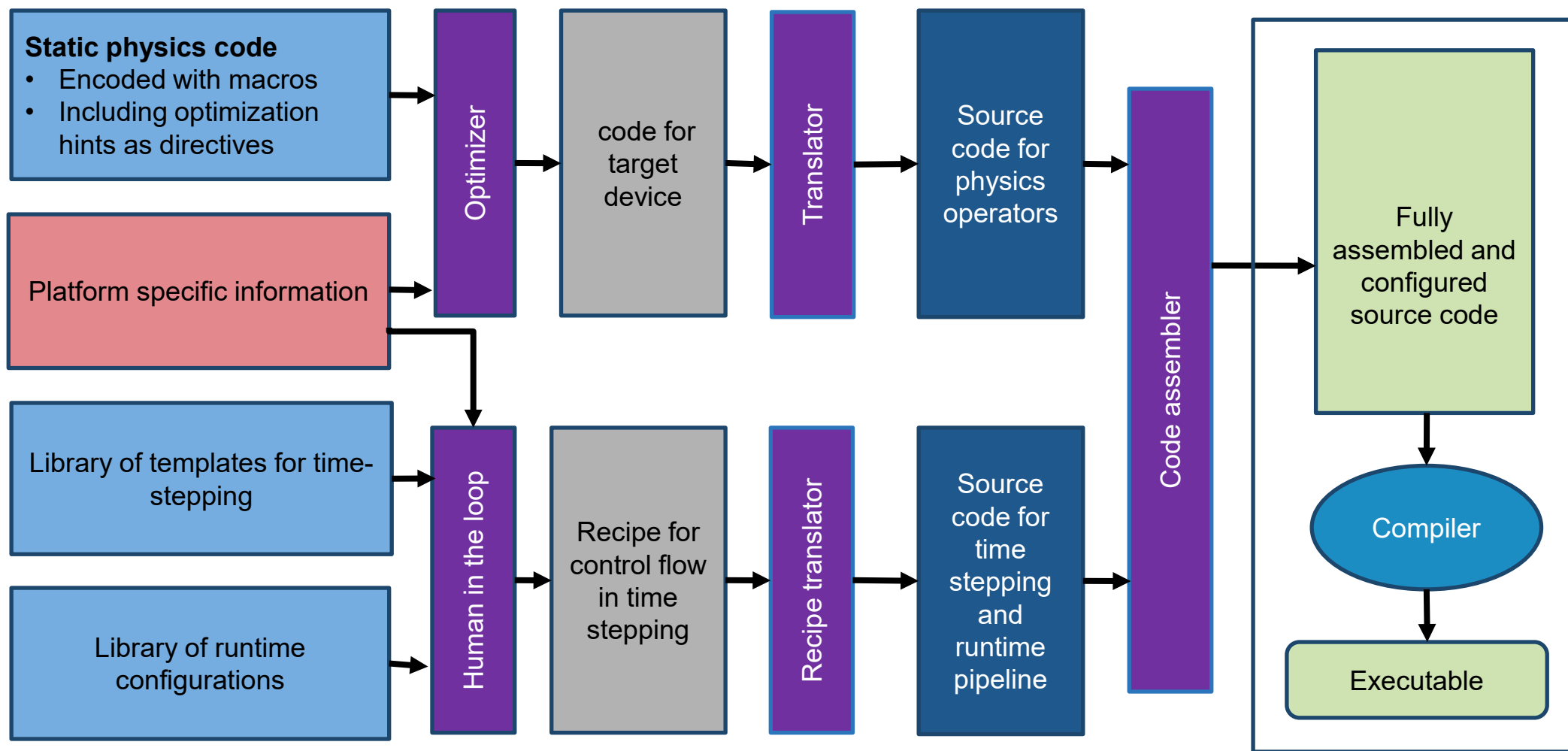
Domain specific runtime

Mechanisms to map work to computational targets

DSL for recipes with code generator

Composability in the source
A toolset of each mechanism
Independent tool sets

Overview of Flash-X Design Approach with Separation of Concerns in tools



Final takeaways

- The key to both performance portability and longevity is careful software design
- Extensibility should be built into the design
- Design should be independent of any specific programming model
- Composability and flexibility help with performance portability
- Resources:
 - <https://www.exascaleproject.org/>
 - <https://doi.org/10.6084/m9.figshare.13283714.v1>
 - https://bssw.io/blog_posts/performance-portability-and-the-exascale-computing-project
 - <https://www.exascaleproject.org/event/kokkos-class-series>
 - [A Design Proposal for a Next Generation Scientific Software Framework](#)
 - [Software Design for Longevity with Performance Portability](#)