Software Design Insights for Longevity of Scientific software

EXASCALE COMPUTING PROJECT

IDEAS productivity

better scientific software

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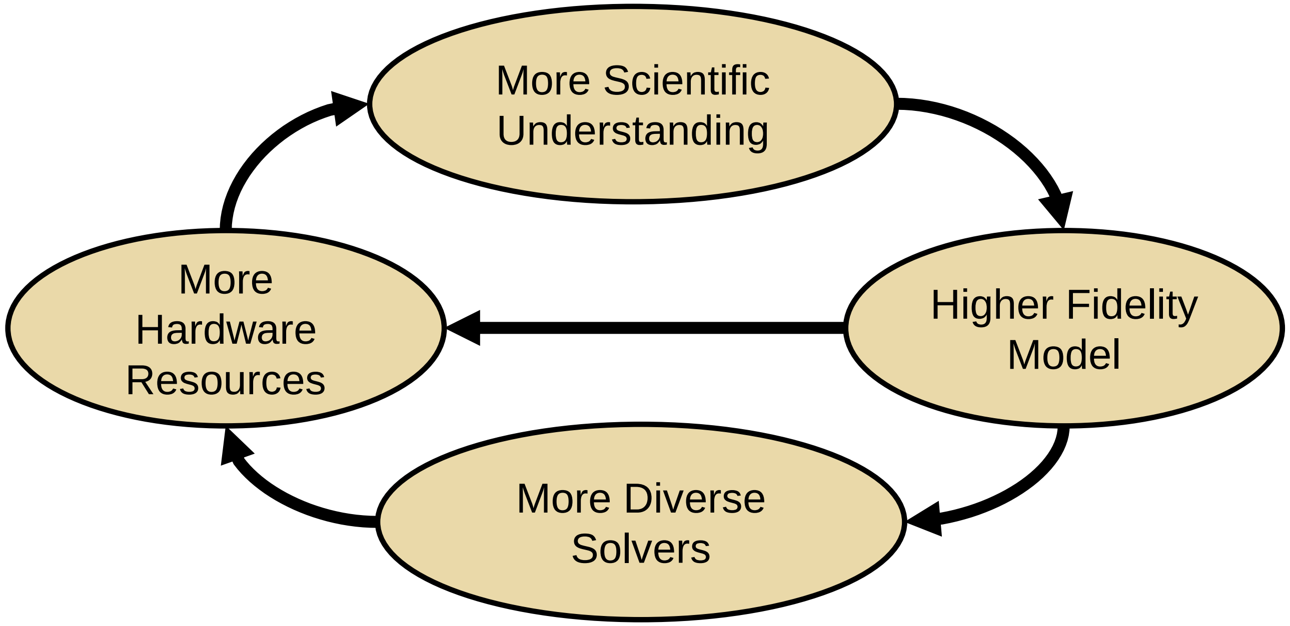
HPC Computational Science Use-case



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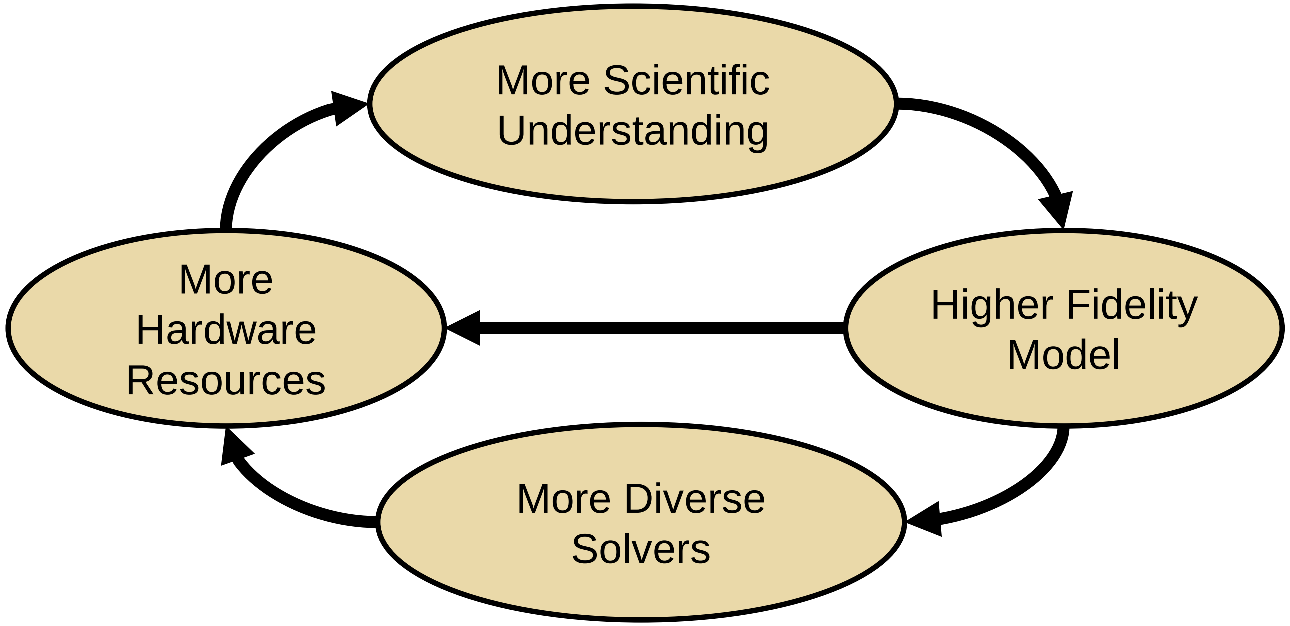
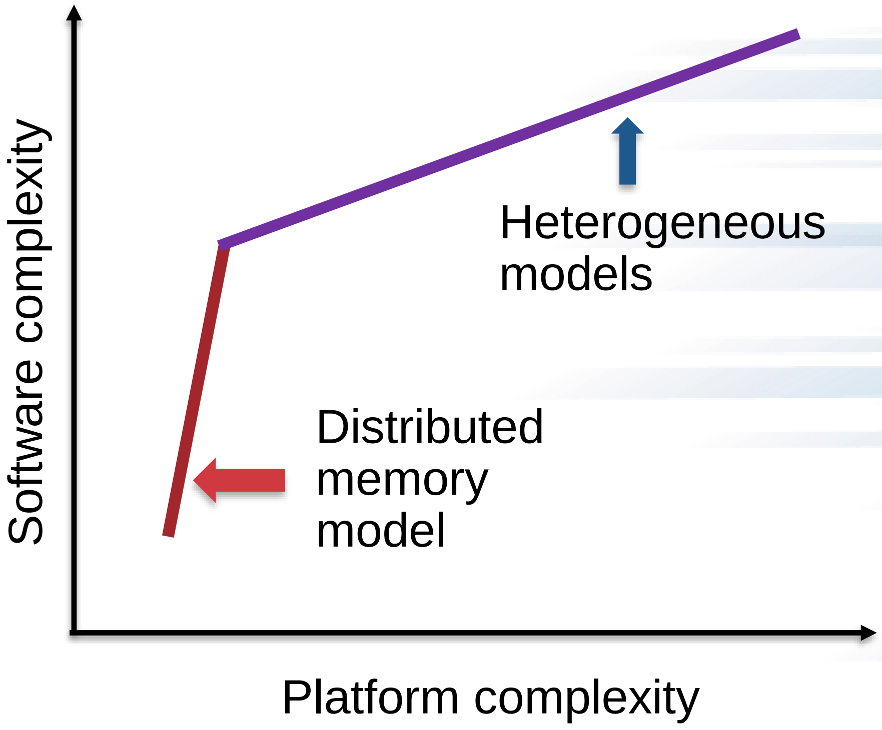




- ❑ Many components may be under research
- ❑ Software continuously evolves
- ❑ All use cases are different and unique

General Design Principles for HPC Scientific Software

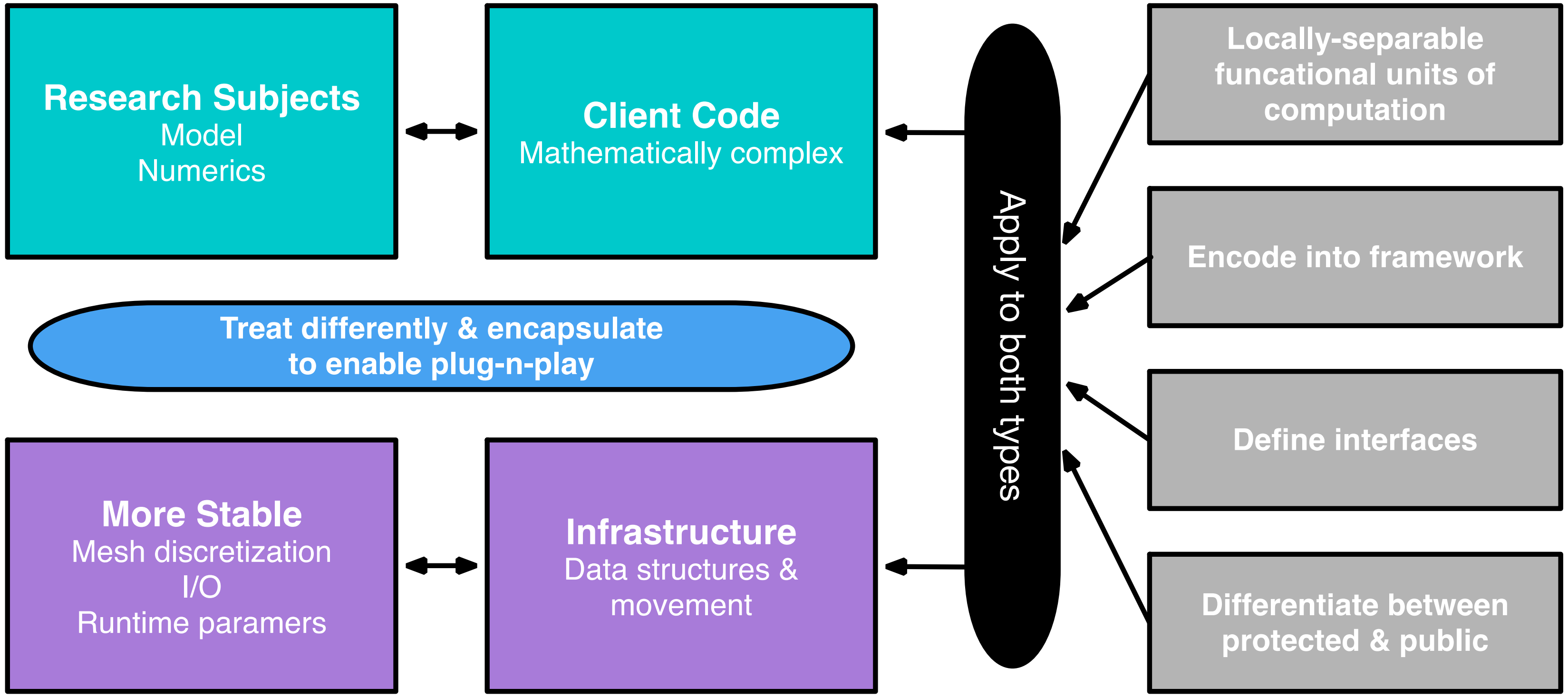
Considerations

- ❑ 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

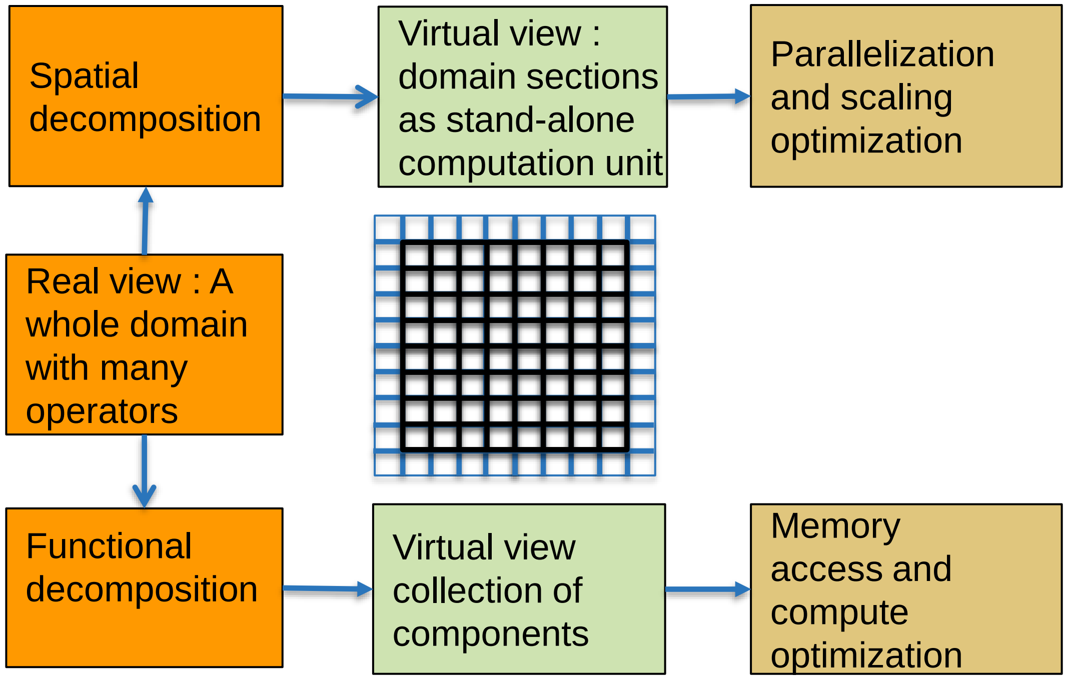
General Design Principles for HPC Scientific Software



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

Example: Multiphysics PDEs for Distributed Memory Parallelism

- Virtual view of domain and functionalities
- Decomposition into components and definition of interfaces



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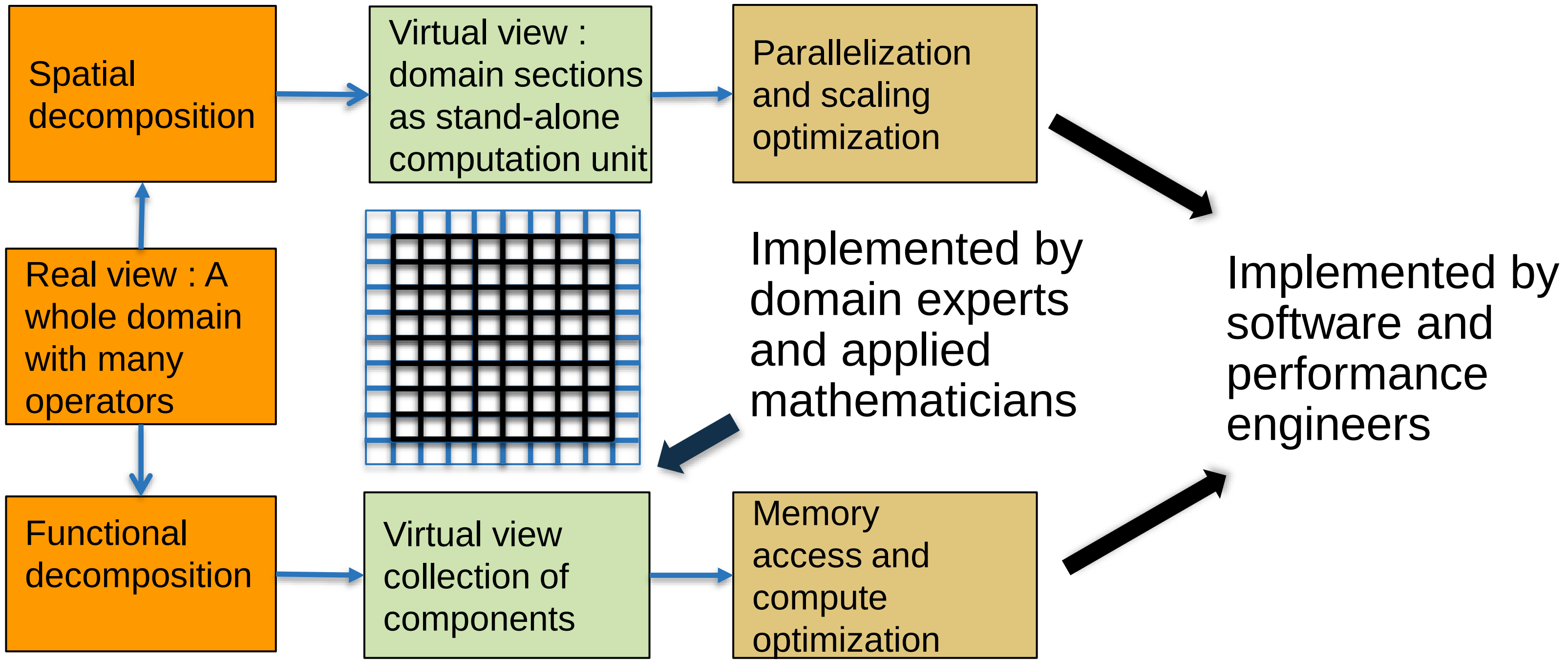
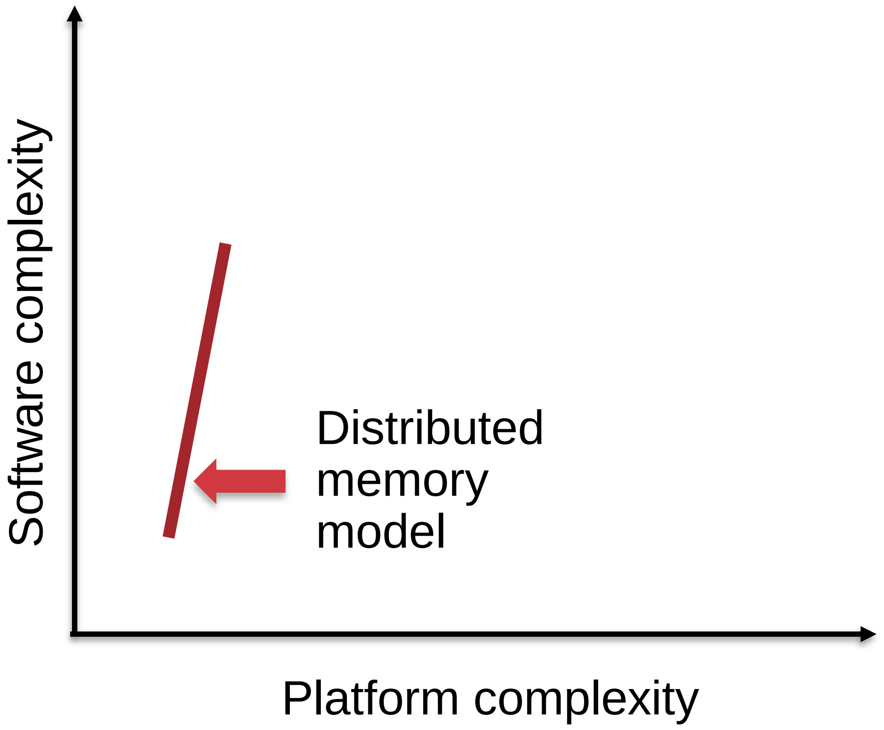
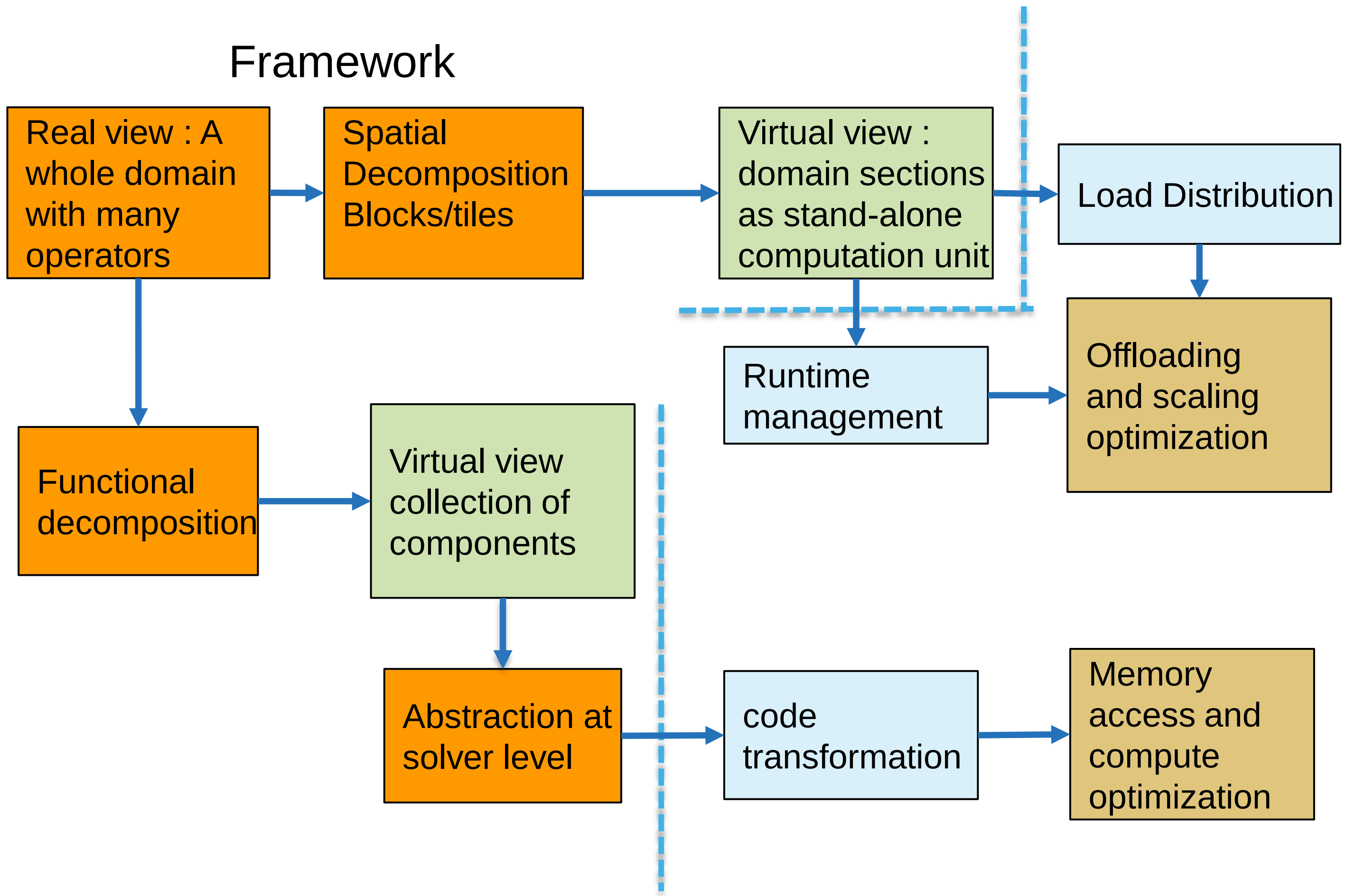


Takeaways Until Now



- 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

Features and Abstractions that must Come in



Underlying Ideas

Make the same code work on different devices

- A way to let compiler know that ”this” expression can be specialized in many ways
- Definition of specializations

Template meta-programming in abstraction layers

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Template meta-programming in abstraction layers

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

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… that translates to investing in design

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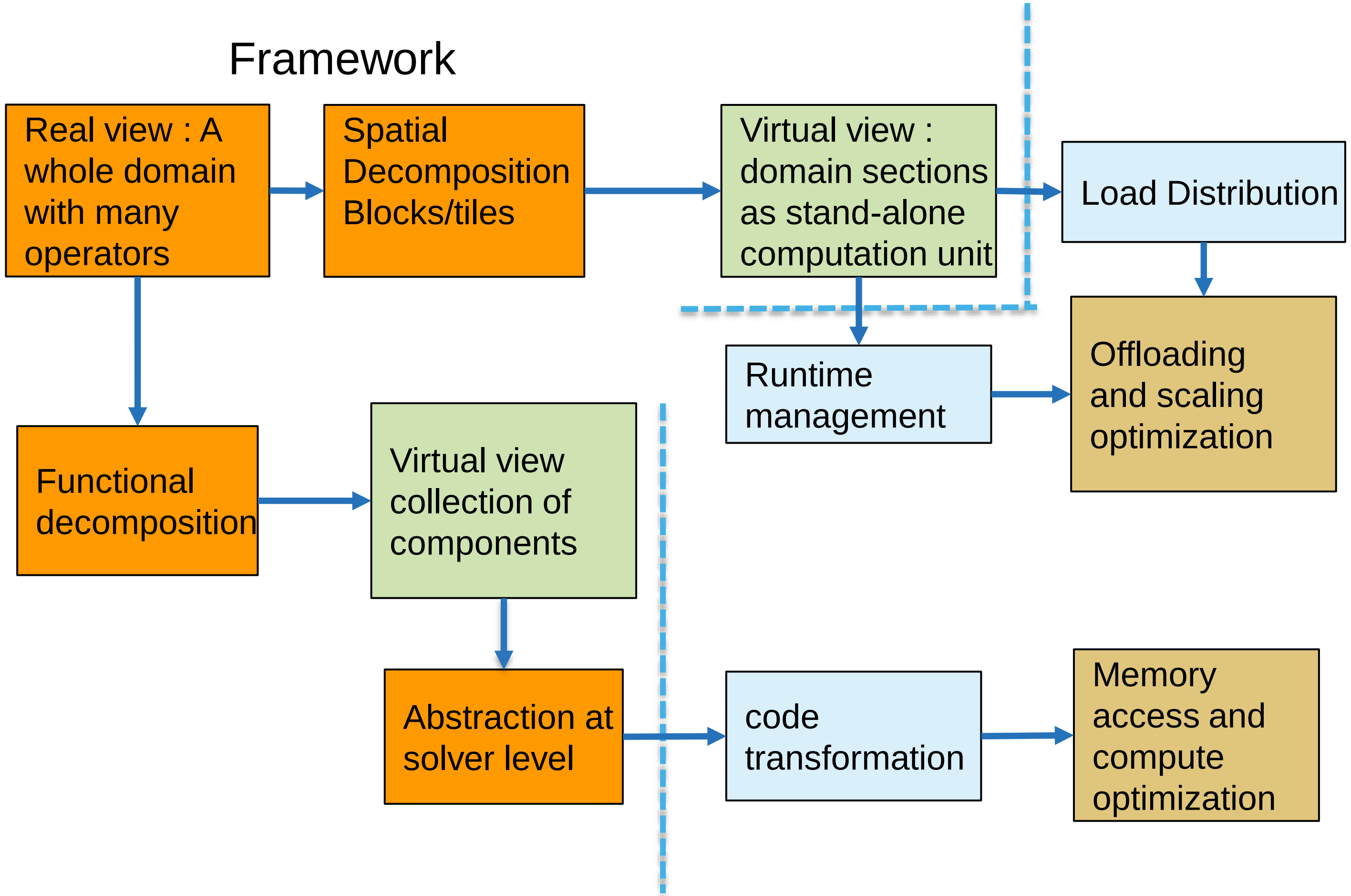

How do abstraction layers work

- 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

Performance depends upon how well the mapping is done.

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://figshare.com/articles/presentation/SC20_Tutorial_Better_Scientific_Software/12994376?file=25219346

https://bssw.io/blog_posts/performance-portability-and-the-exascale-computing-project

https://www.exascaleproject.org/event/kokkos-class-series

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