Scientific Software Design

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Better Scientific Software tutorial @ SC21

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License and Citation

- **The requested citation the overall tutorial is: David E. Bernholdt, Anshu Dubey, Patricia A. Grubel, Rinku K. Gupta, and Gregory R. Watson, Better Scientific Software tutorial, in the International Conference for High-Performance Computing, Networking, Storage, and Analysis (SC21), St. Louis, MO, USA and online, 2021. DOI: 10.6084/m9.figshare.16556628**
- Individual modules may be cited as *Speaker, Module Title*, in Better Scientific Software tutorial…

Acknowledgements

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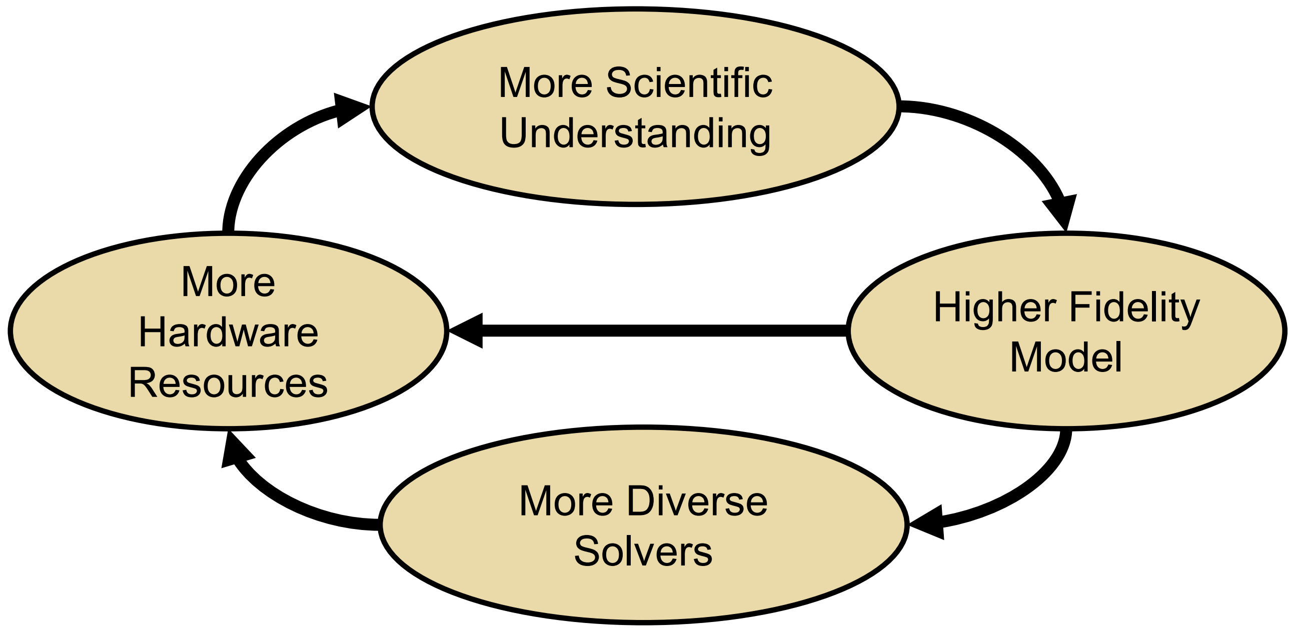
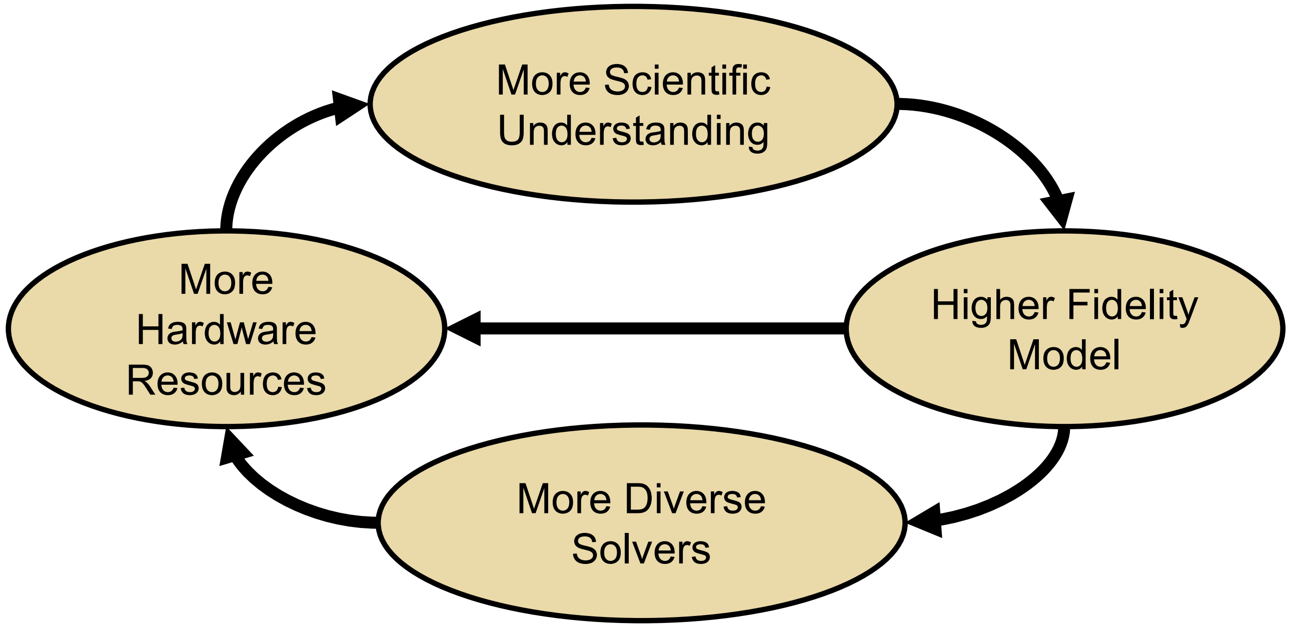
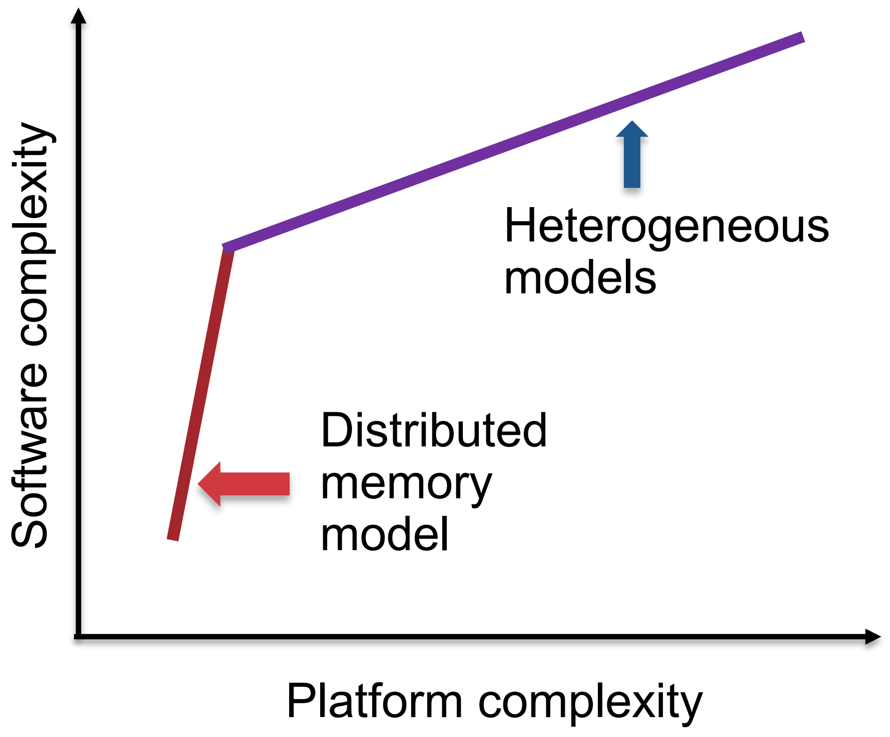
HPC Computational Science Use-case



HPC Computational Science Use-case





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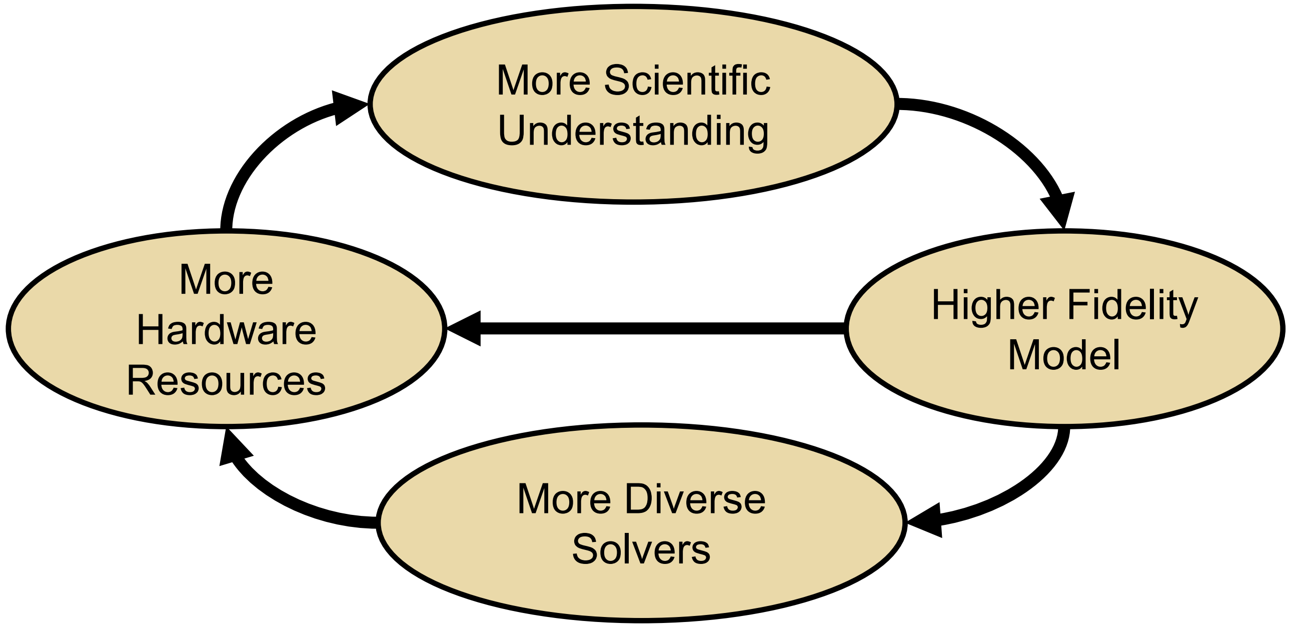
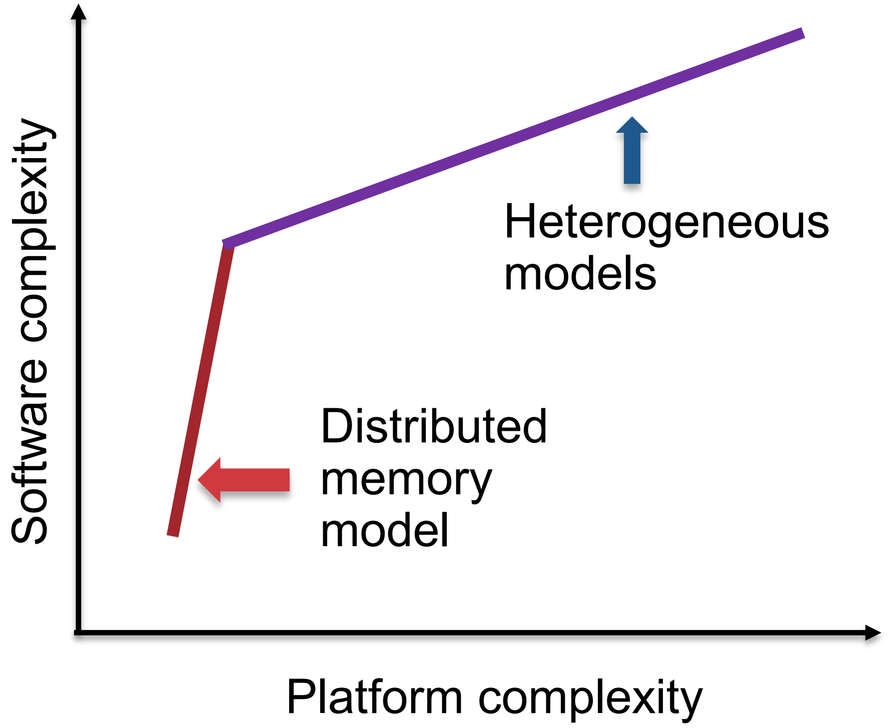




- ❑ Many components may be under research
- ❑ Software continuously evolves
- ❑ All use cases are different and unique

General Design Principles for HPC Scientific Software

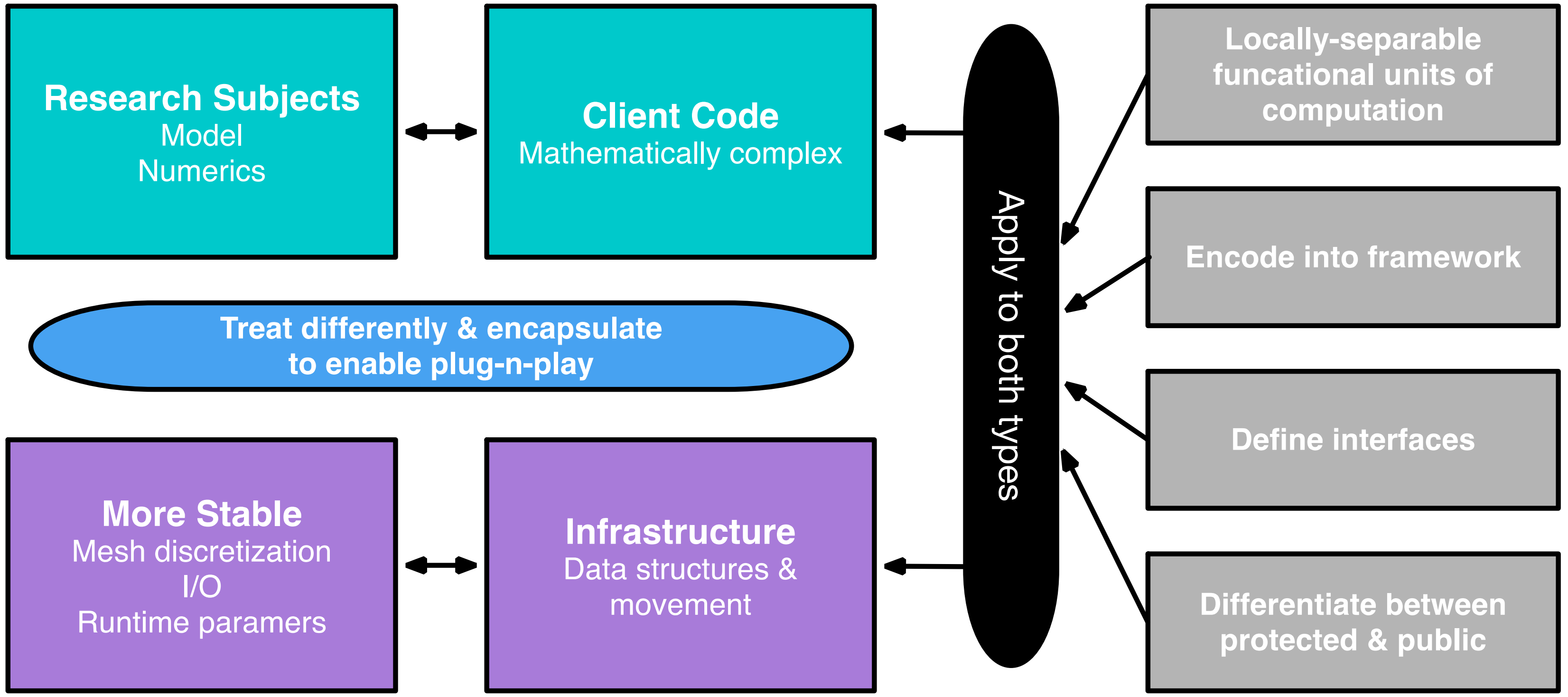
Considerations

- ❑ 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

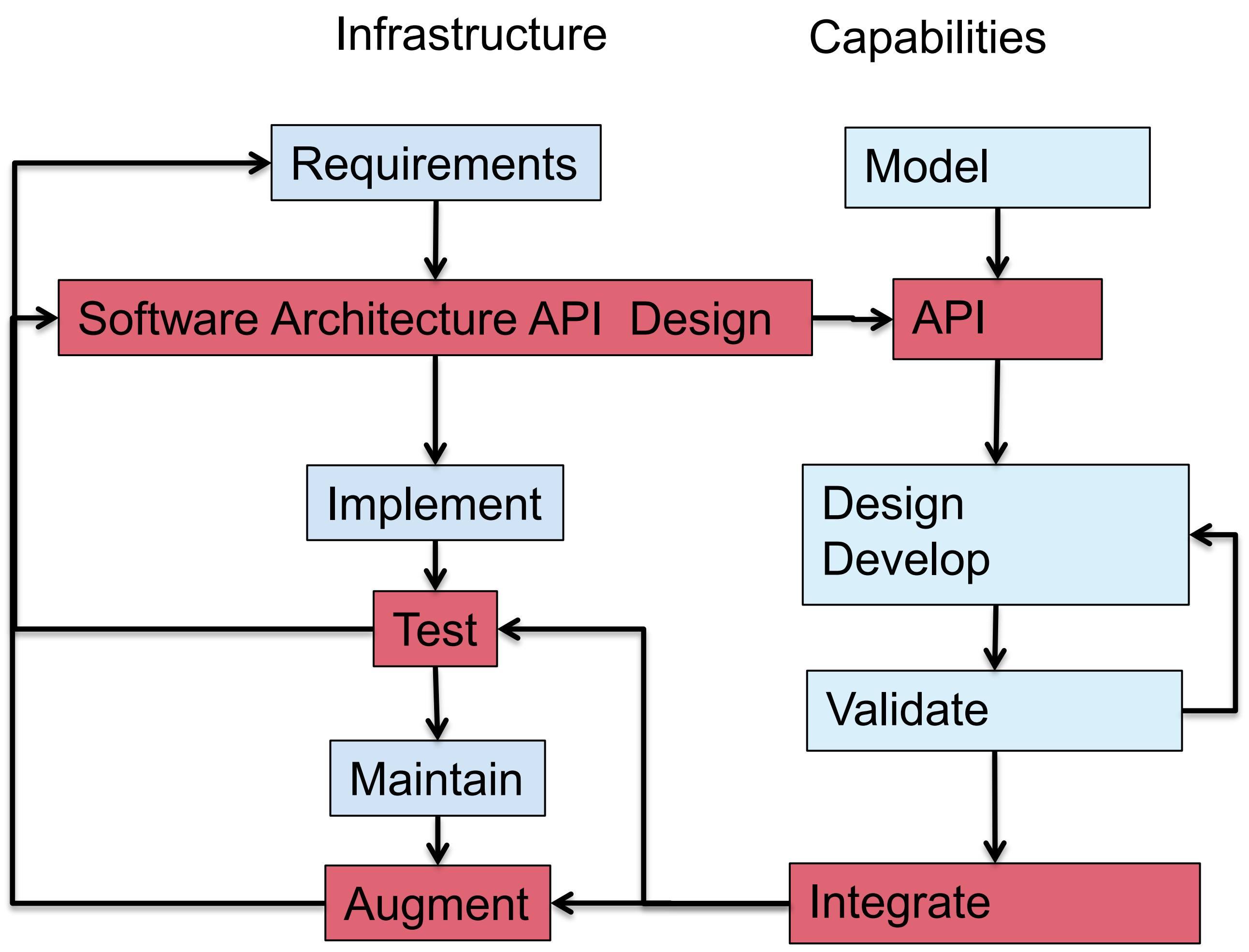
General Design Principles for HPC Scientific Software



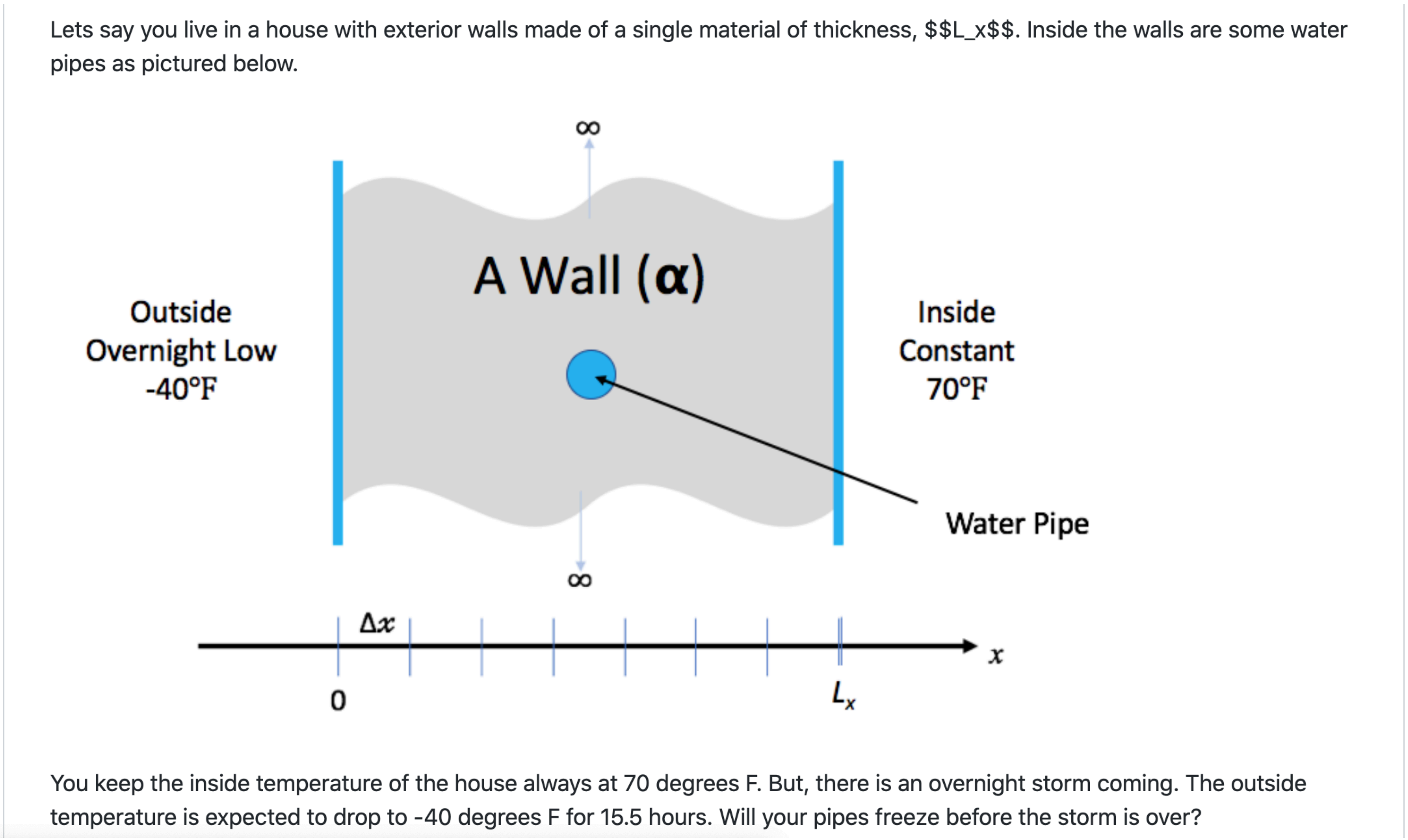
Research Subjects
Model
Numerics
Client Code
Mathematically complex
Treat differently & encapsulate to enable plug-n-play
More Stable
Mesh discretization
I/O
Runtime paramers
Infrastructure
Data structures & movement
Apply to both types
Locally-separable funcational units of computation
Encode into framework
Define interfaces
Differentiate between protected & public

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

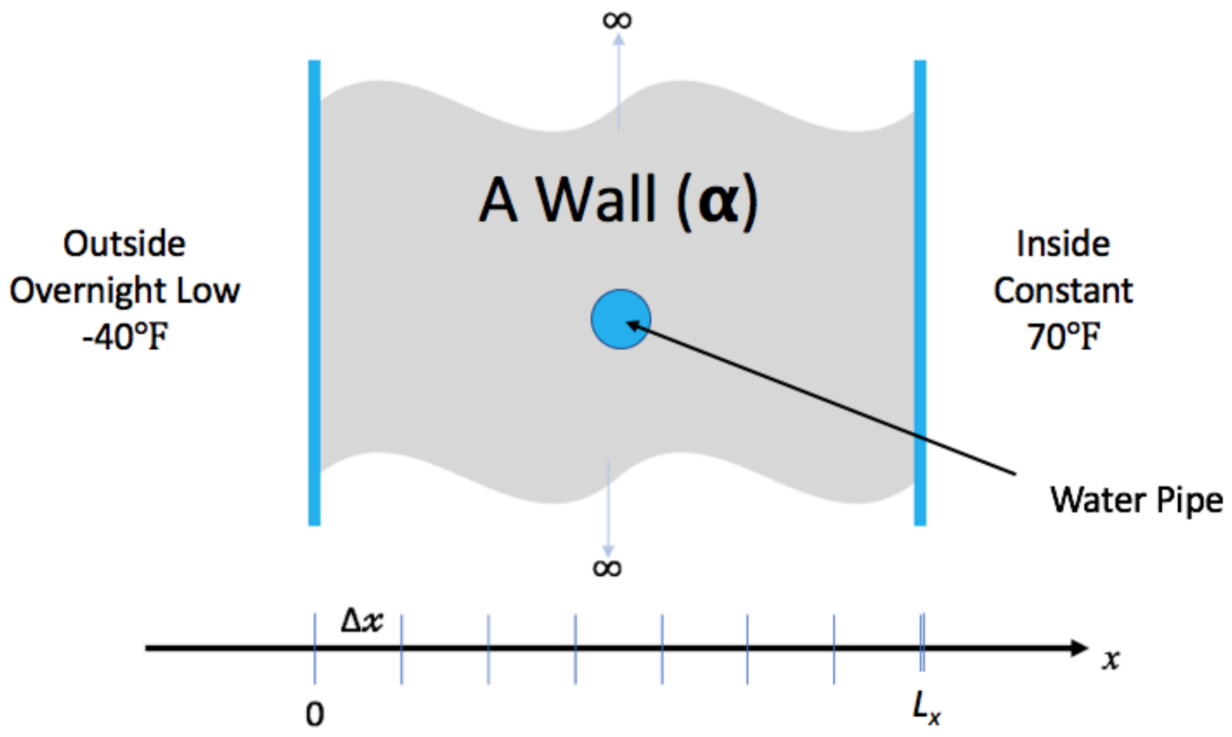
A Design Model for Separation of Concerns



The Running Example



Lets say you live in a house with exterior walls made of a single material of thickness, $$L_x$$. Inside the walls are some water pipes as pictured below.



You keep the inside temperature of the house always at 70 degrees F. But, there is an overnight storm coming. The outside temperature is expected to drop to -40 degrees F for 15.5 hours. Will your pipes freeze before the storm is over?

Problem Specification - Design Considerations

- Specification
  - Solve heat equation with some initial and boundary conditions
  - Apply different integration methods

- What is infrastructure here?
  - Discretization/ State
  - Verification
  - I/O
  - Application of initial conditions
  - Runtime parameters
  - Comparison

- What is model here?
  - Initial conditions
  - Boundary conditions
  - Integration

Infrastructure API

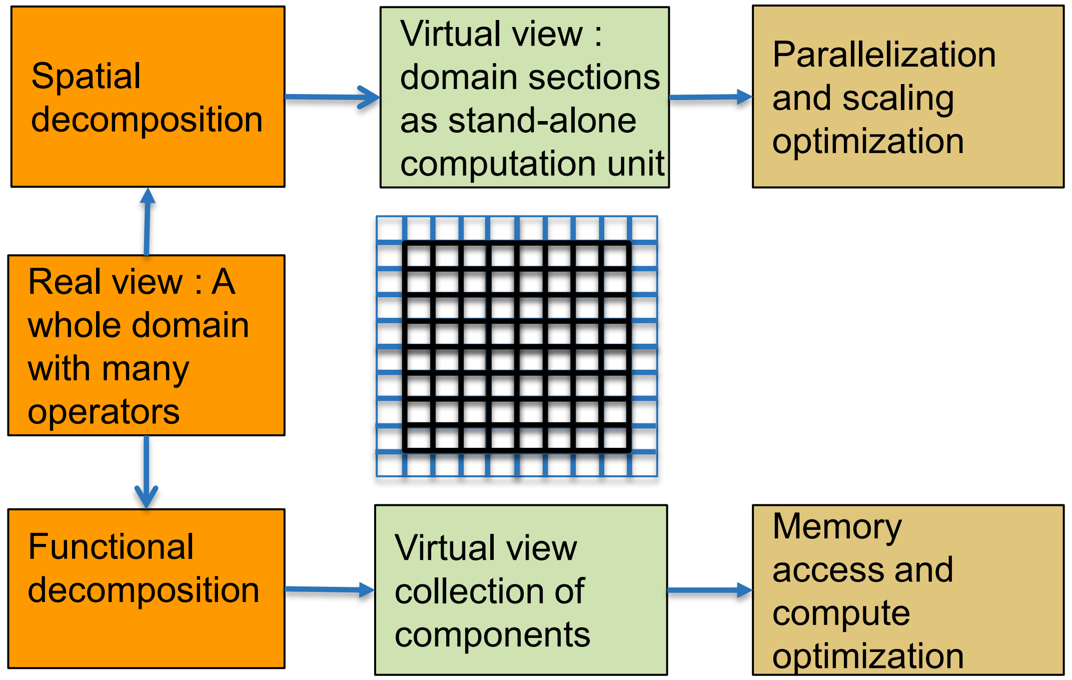
- **process_args**(int argc, char **argv)
- static void **initialize**(void)
- void **copy**(int n, double *dst, double const *src)
- void **write_array**(int t, int n, double dx, double const *a)
- void **set_initial_condition**(int n, double *a, double dx, char const *ic)

Numerics API

- double **l2_norm**(int n, double const *a, double const *b)
- bool **update_solution_crankn**(int n, double *curr, double const *last, double const *cn_Amat, double bc_0, double bc_1)
- bool **update_solution_upwind15**(int n, double *curr, double const *last, double alpha, double dx, double dt, double bc_0, double bc_1)
- bool **update_solution_ftcs**(int n, double *uk1, double const *uk0, double alpha, double dx, double dt, double bc0, double bc1)
- void **compute_exact_solution**(int n, double *a, double dx, char const *ic, double alpha, double t, double bc0, double bc1)

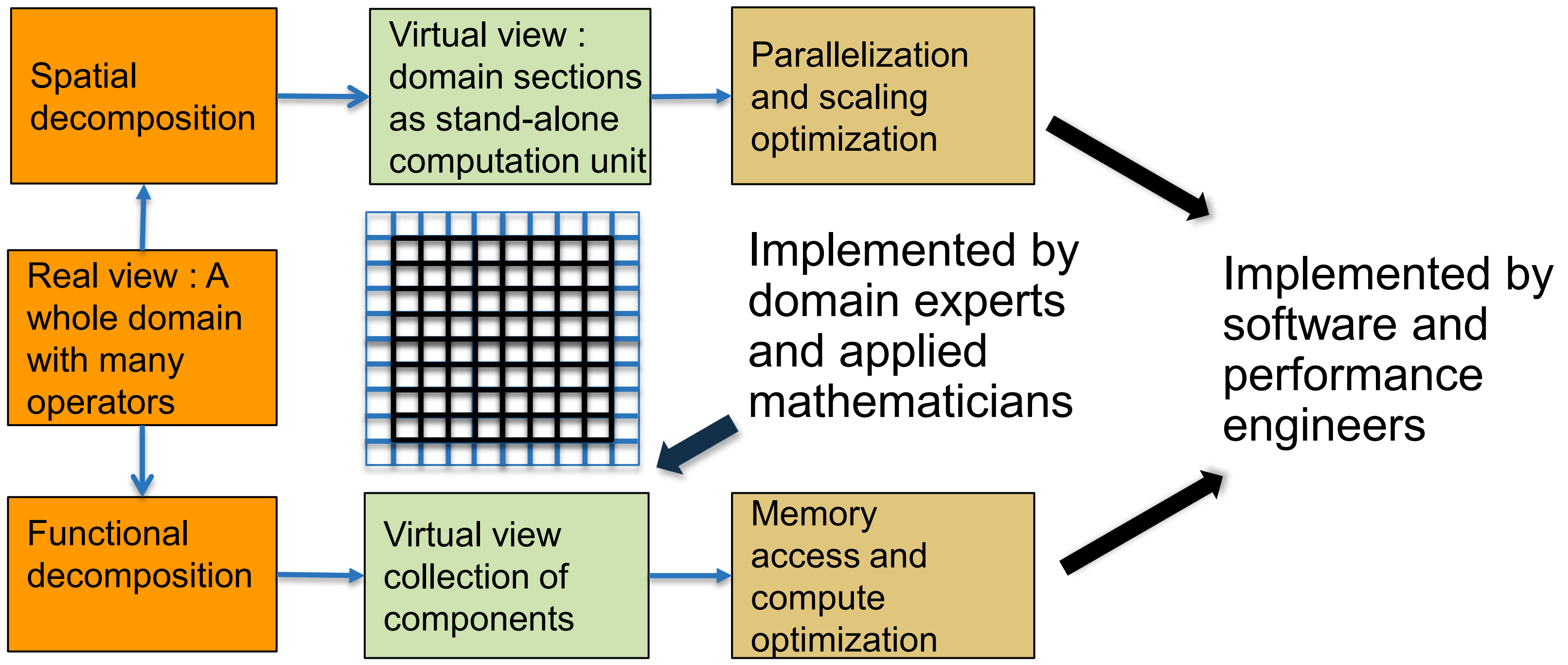
Example: Architecting Multiphysics PDEs

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


Spatial decomposition
Virtual view : domain sections as stand-alone computation unit
Parallelization and scaling optimization
Real view : A whole domain with many operators
Functional decomposition
Virtual view collection of components
Memory access and compute optimization

Example: Multiphysics PDEs for Distributed Memory Parallelism

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

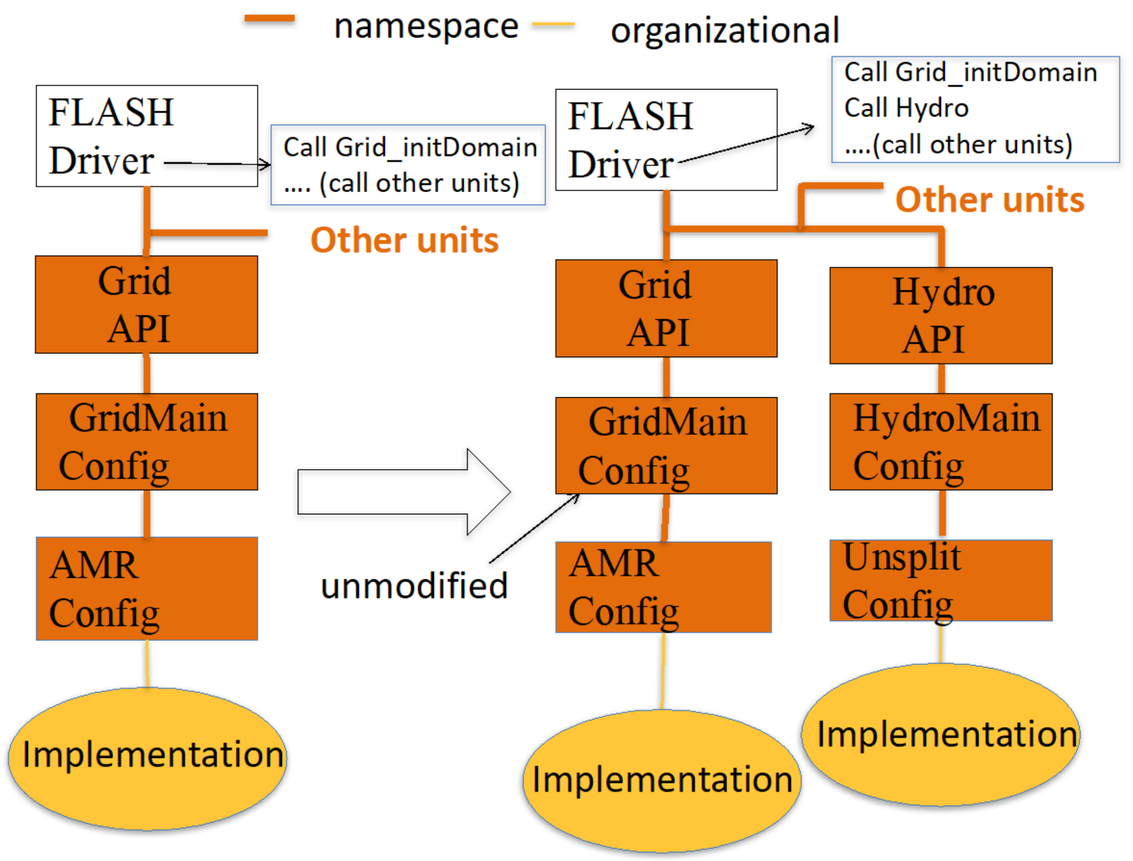

Spatial decomposition
Virtual view : domain sections as stand-alone computation unit
Parallelization and scaling optimization
Real view : A whole domain with many operators
Implemented by domain experts and applied mathematicians
Implemented by software and performance engineers
Functional decomposition
Virtual view collection of components
Memory access and compute optimization

Example: Design for Extensibility from FLASH, Now Flash-X

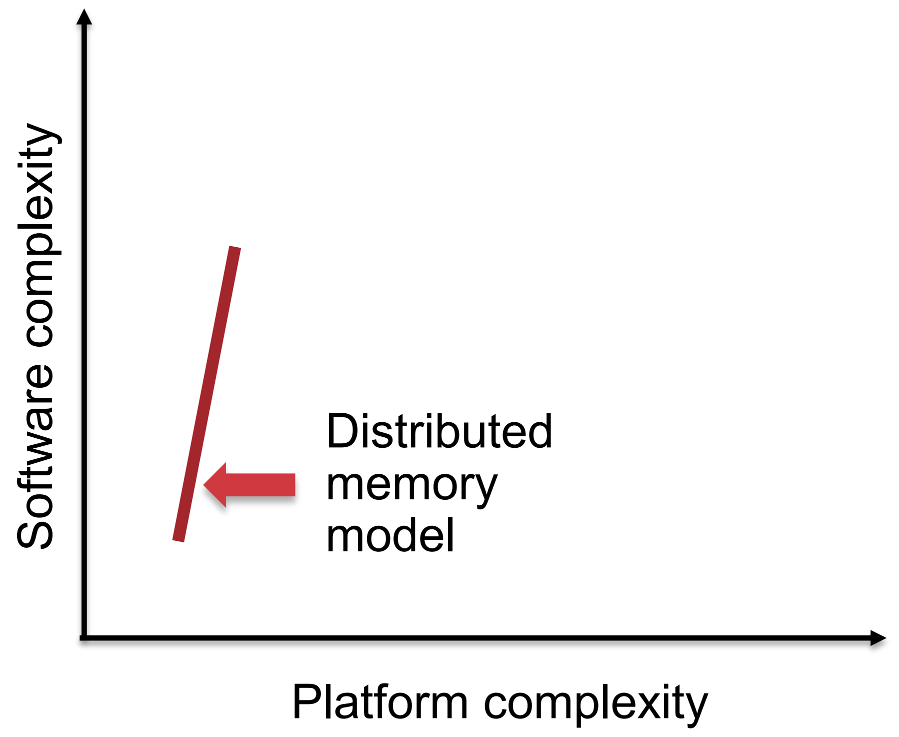
Assumed that capabilities will be added for better models

- Assembly from components
- Decentralized maintenance of metadata
- Python tool to parse and configure
- OOP implemented through Unix directory structure and configuration tool

Key idea is distributed intelligence

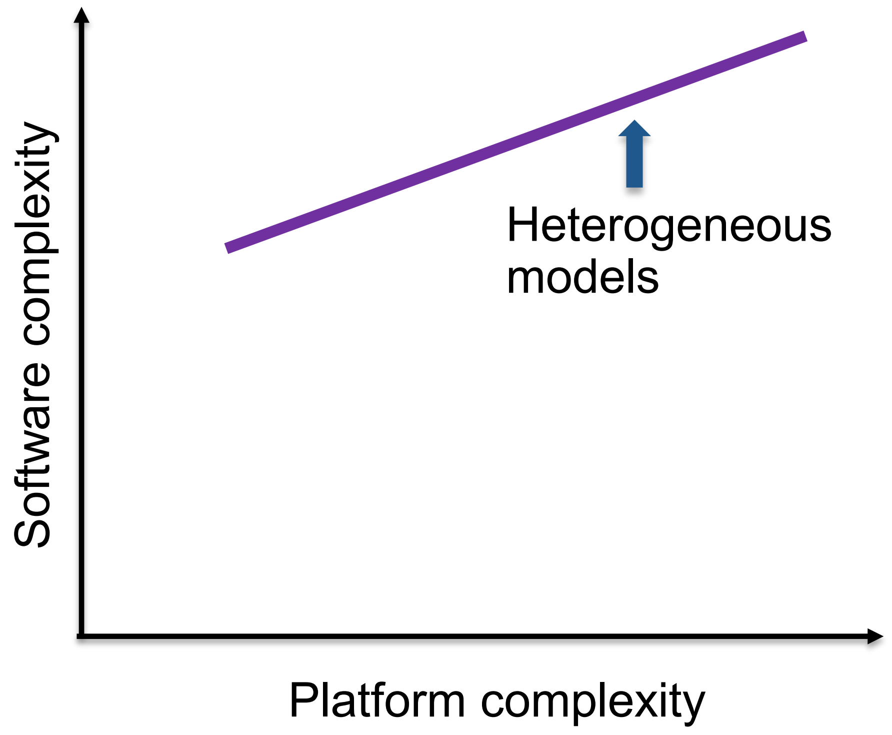


Takeaways Until Now



- 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?

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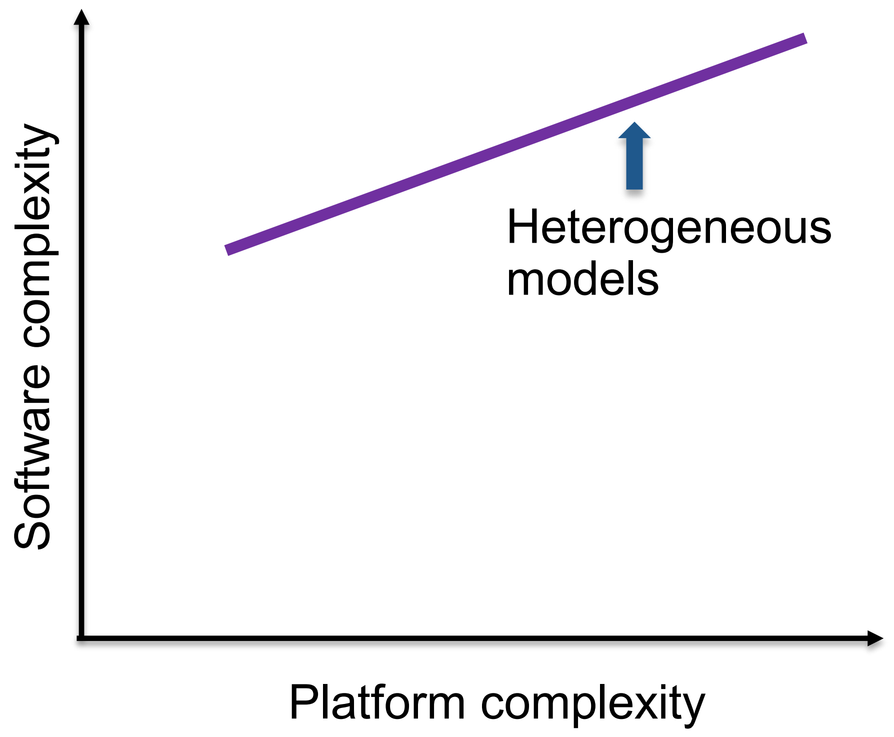

- Question - do the design principles change?
- The answer is – not really
- The details get more involved

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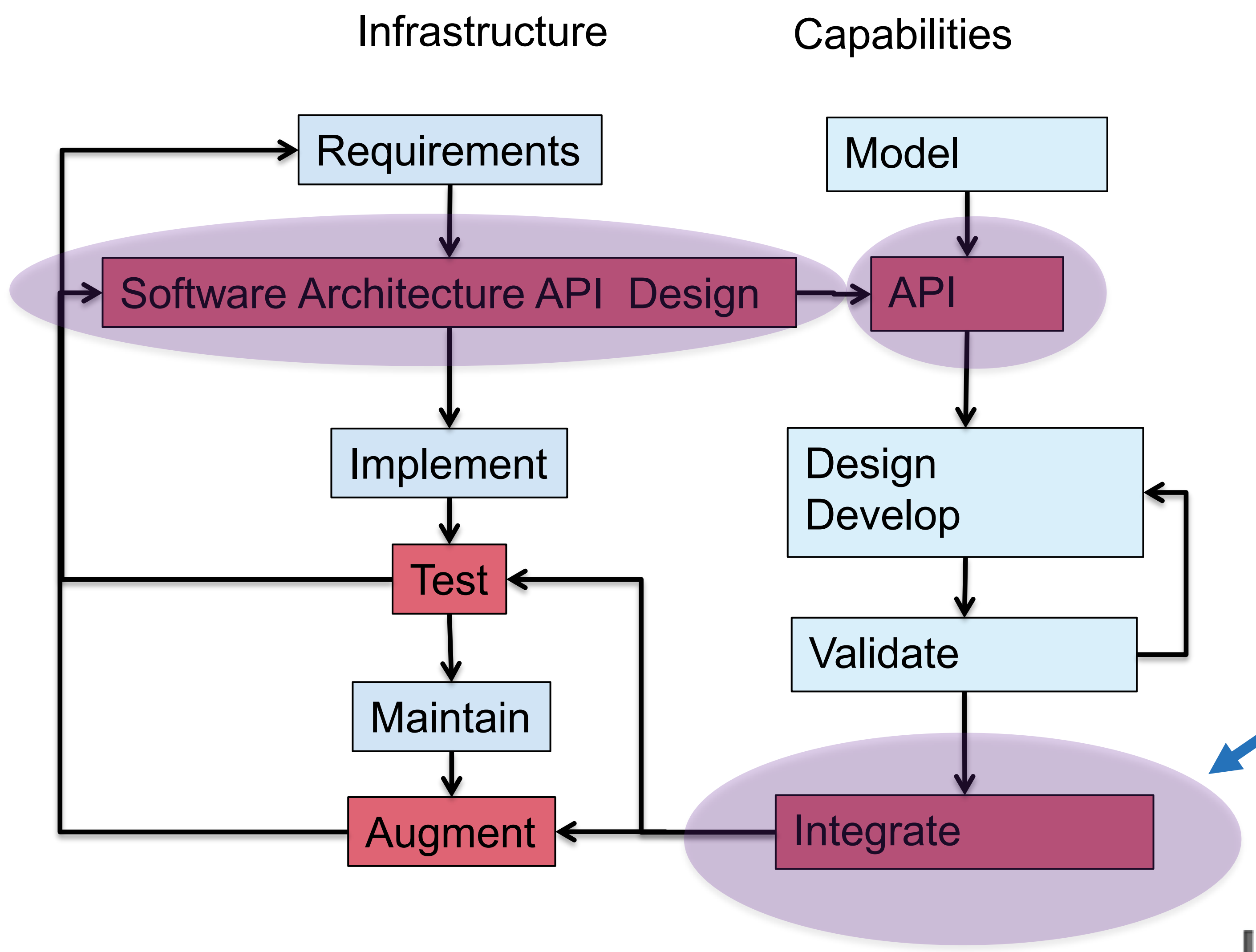
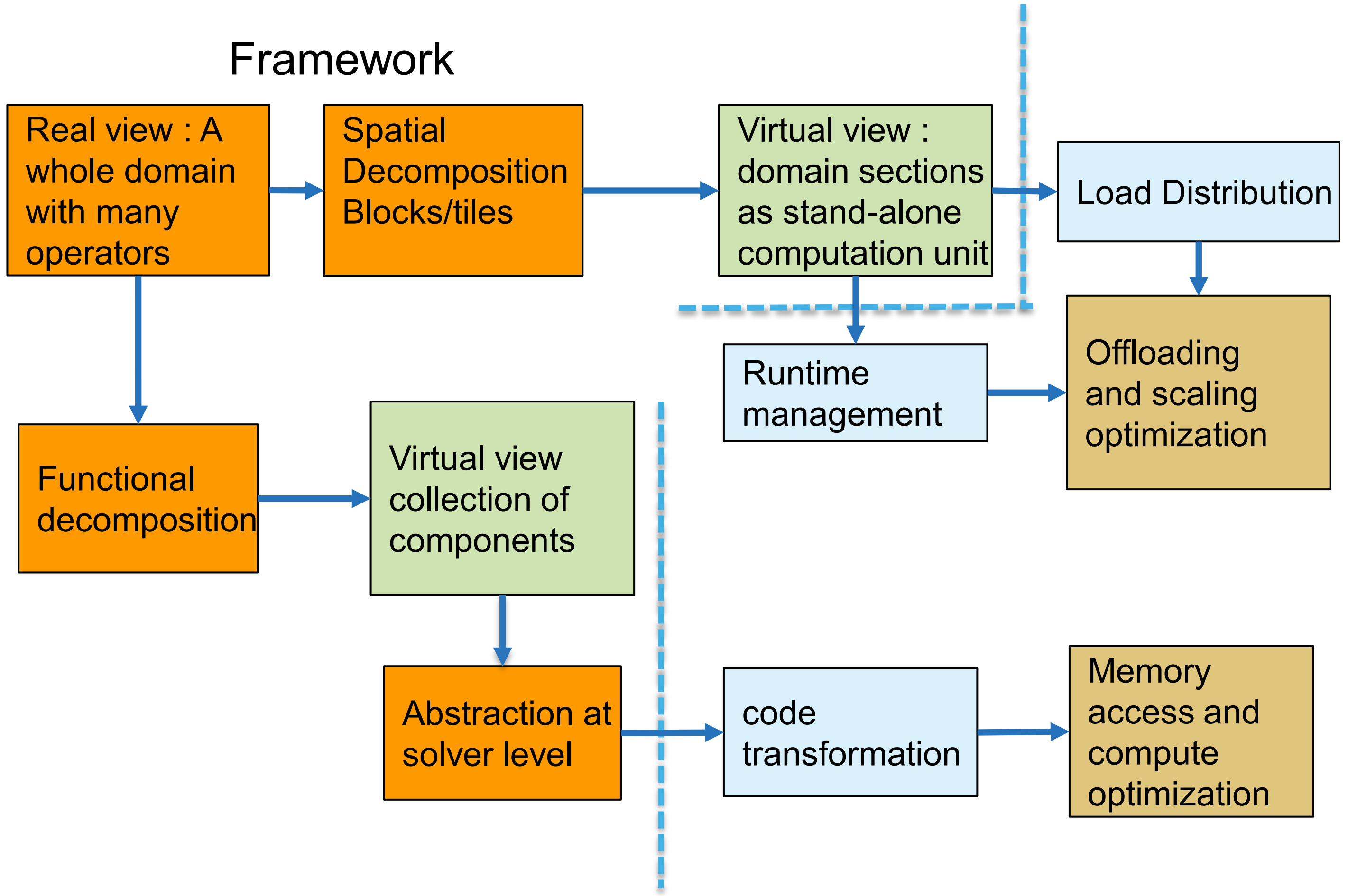


This is where maximum change is likely

Design Guidance For Performance Portability

- Design for Hierarchical parallelism
- Design towards several thousand threads
- Design for a hierarchical memory space
- Design patterns that count, allocate, and reuse memory
- Avoid exposing/using non-portable vendor-specific options

Features and Abstractions that must Come in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Real view : A whole domain with many operators
Spatial Decomposition Blocks/tiles
Virtual view : domain sections as stand-alone computation unit
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code transformation
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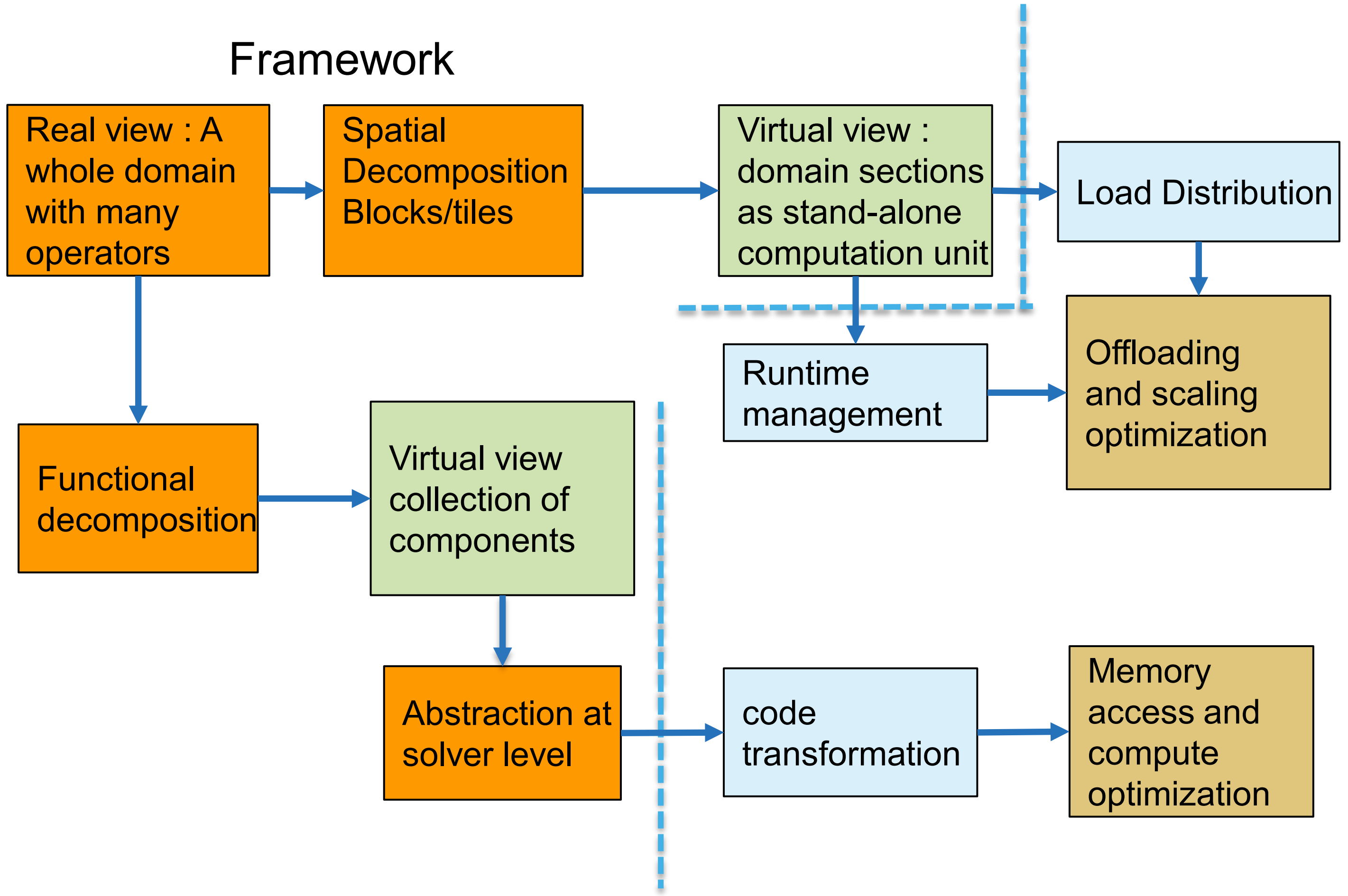
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How do abstraction layers work

- ❑ 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.

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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Even when using third party abstraction tools understanding the code’s structure and needs is critical for performance portability
… that translates to investing in design

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More complex data orchestration system for asynchronous computation

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://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