Software Design and Testing

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License, citation, and acknowledgments

License and Citation

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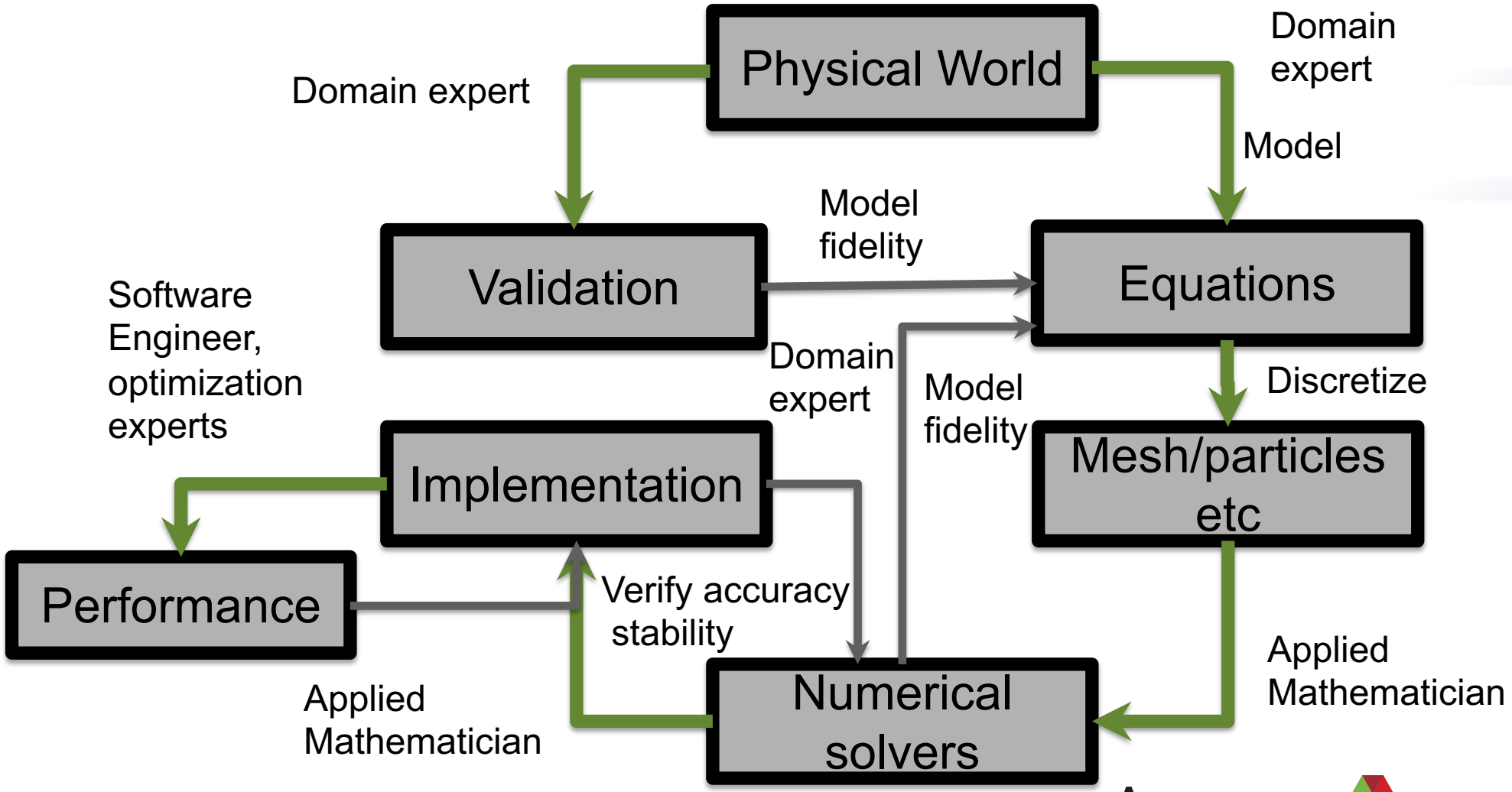
Argonne NATIONAL LABORATORY

ECP EXASCALE COMPUTING PROJECT

DESIGN

Science with Simulations Partial Workflow



Motivation for Software Design

The default mode of growth by accretion leads to unmanageable software

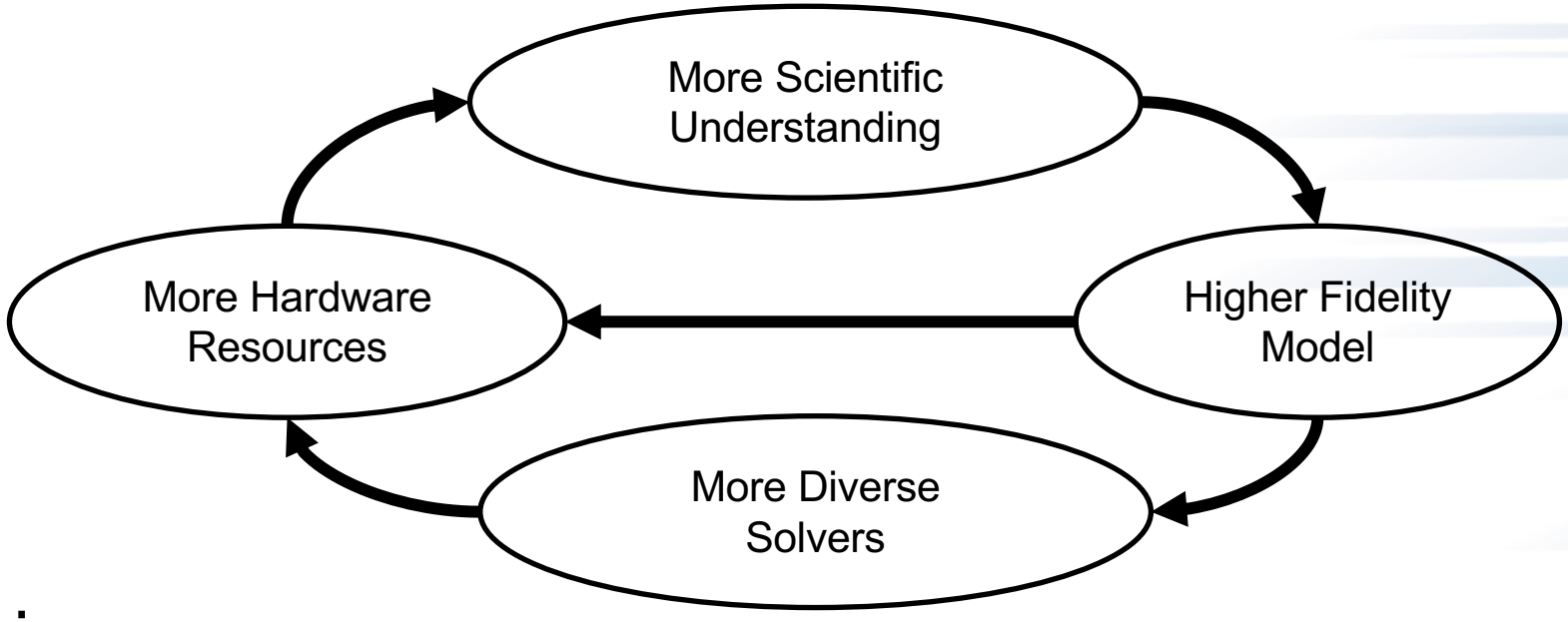
- Increases cost of maintenance
- Parts of software may become unusable over time
- Inadequately verified software produces questionable results
- Increases ramp-on time for new developers
- Reduces software and science productivity due to technical debt

Technical debt --> Consequence of Choices

Quick and dirty collects interest which means more effort required to add features.

It is extremely important to recognize that science through computing is only as credible as the software that produces it

SCIENCE WITH HIGH PERFORMANCE COMPUTING



- Compute on expensive, rare resources
- Software continuously evolving
- Many components of the software under research

Taking stock

- Software architecture and process design is an overhead
  - Value lies in avoiding technical debt (future saving)
  - Worthwhile to understand the trade-off

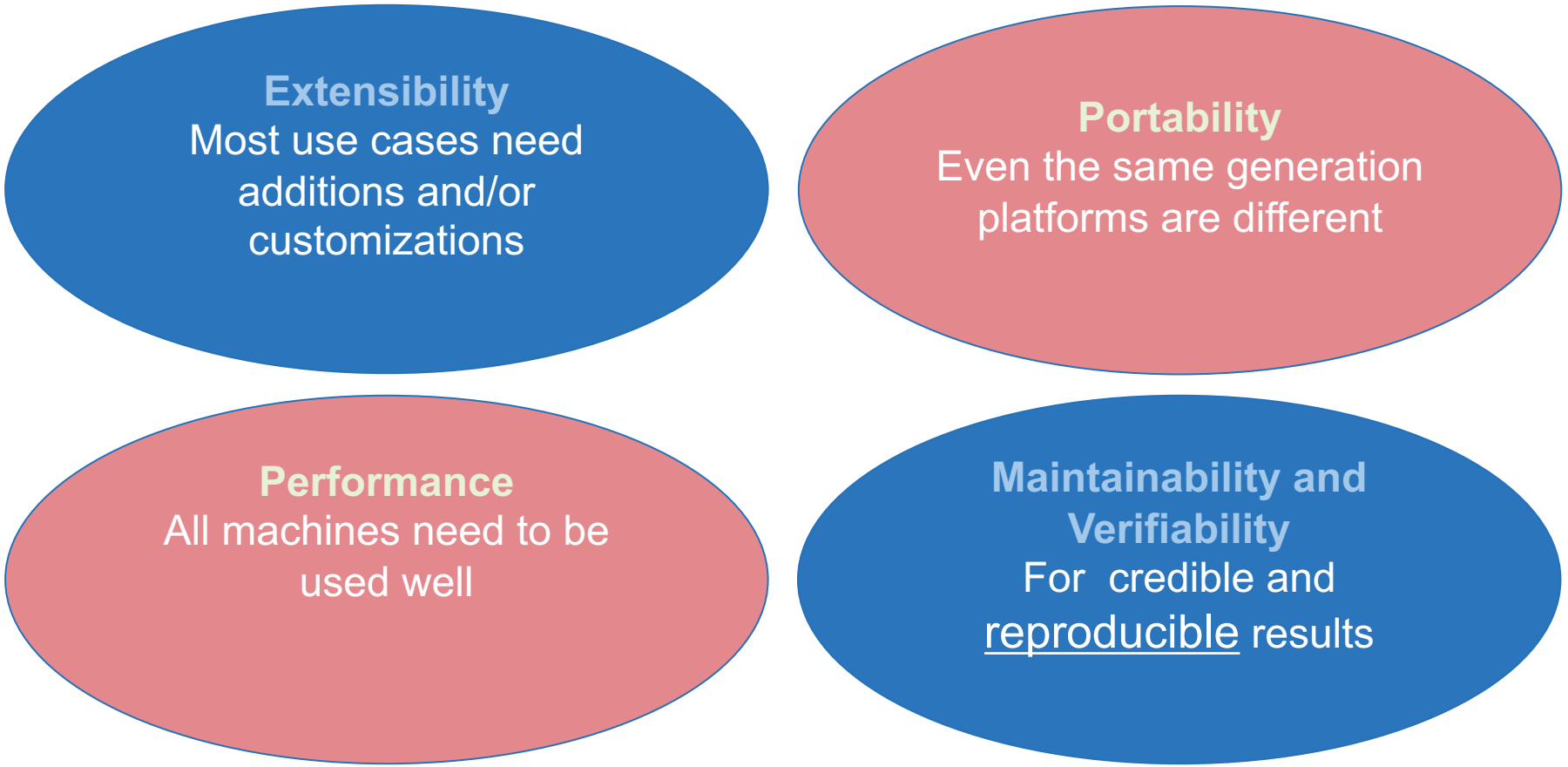
- The target of the software
  - Proof-of-concept
  - Verification
  - Exploration of some phenomenon
  - Experiment design
  - Analysis
  - Other …

Cognizant of resource constraints

Dictate the rigor of the design and software process

Architecting scientific codes

Desirable Characteristics



Architecting scientific codes

Desirable Characteristics

Extensibility
Well defined structure and modules
Encapsulation of functionalities

Portability
Even the same generation platforms are different

Performance
All machines need to be used well

Maintainability and Verifiability
For credible and reproducible results

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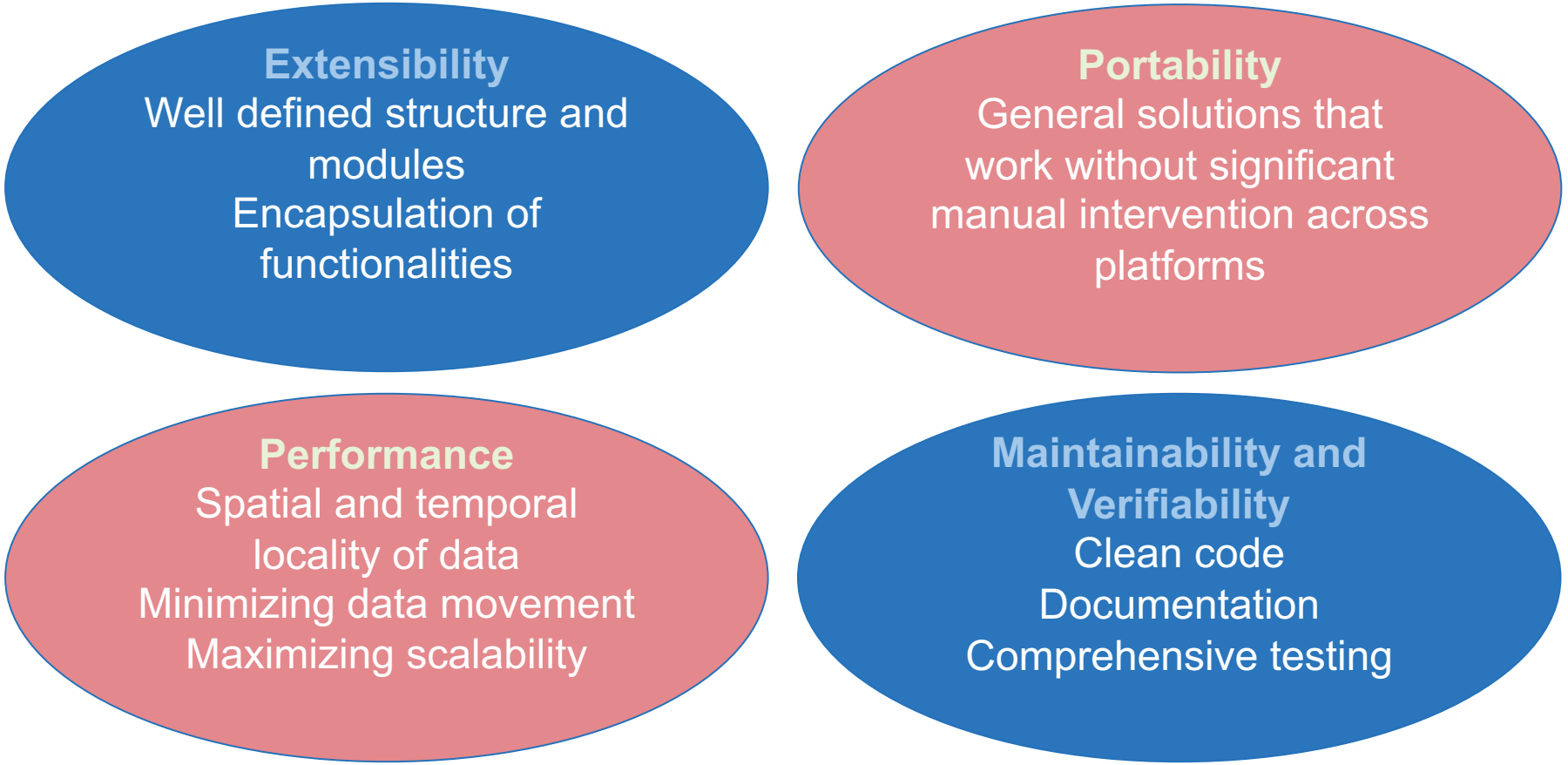
Clean code
Documentation
Comprehensive testing

Architecting scientific codes

Why it is challenging



Architecting scientific codes

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Extensibility
Same data layout not good for all solvers. Many corner cases. Necessary lateral interactions

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A version for each class of device => combinatorial explosion

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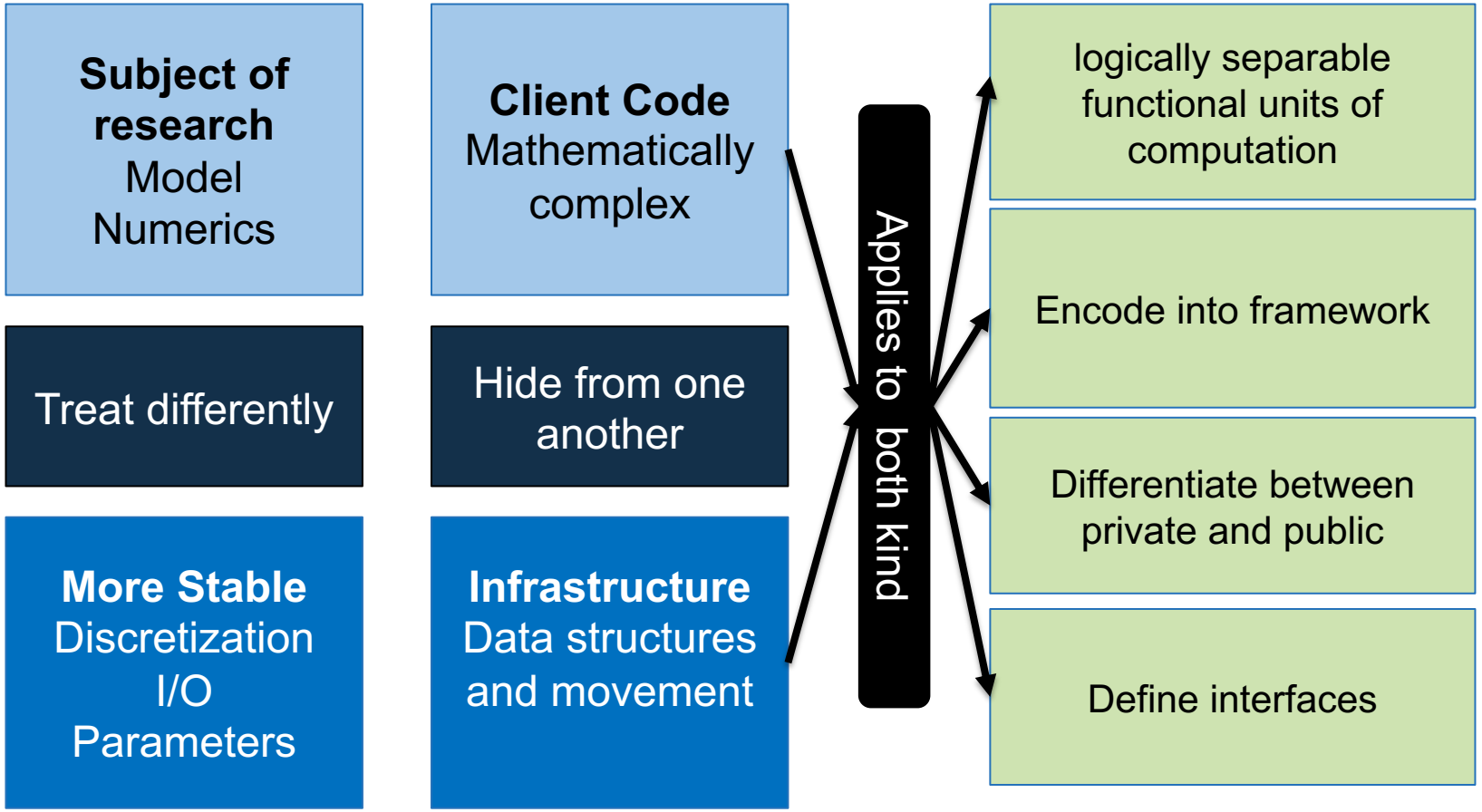
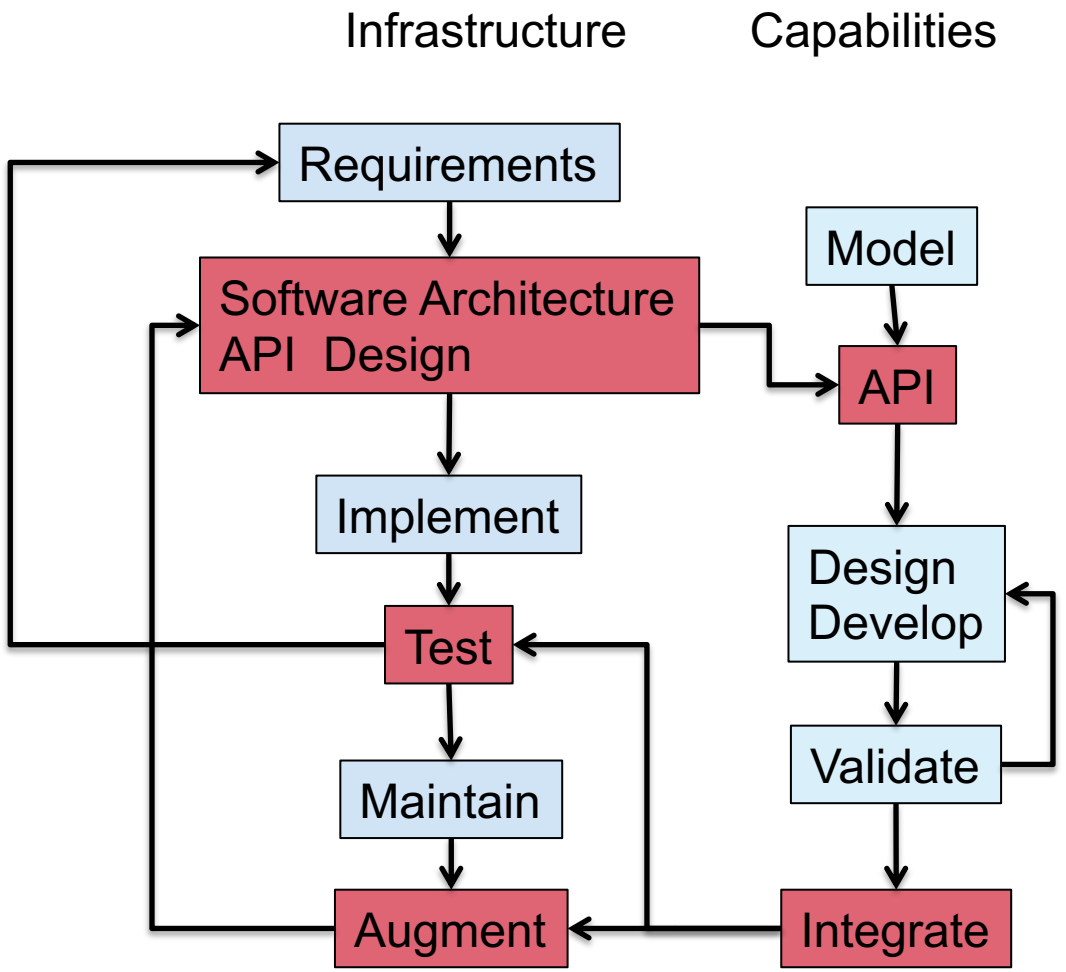
Maintainability and Verifiability
Wrong incentives
Designing good tests is hard

Architecting scientific codes

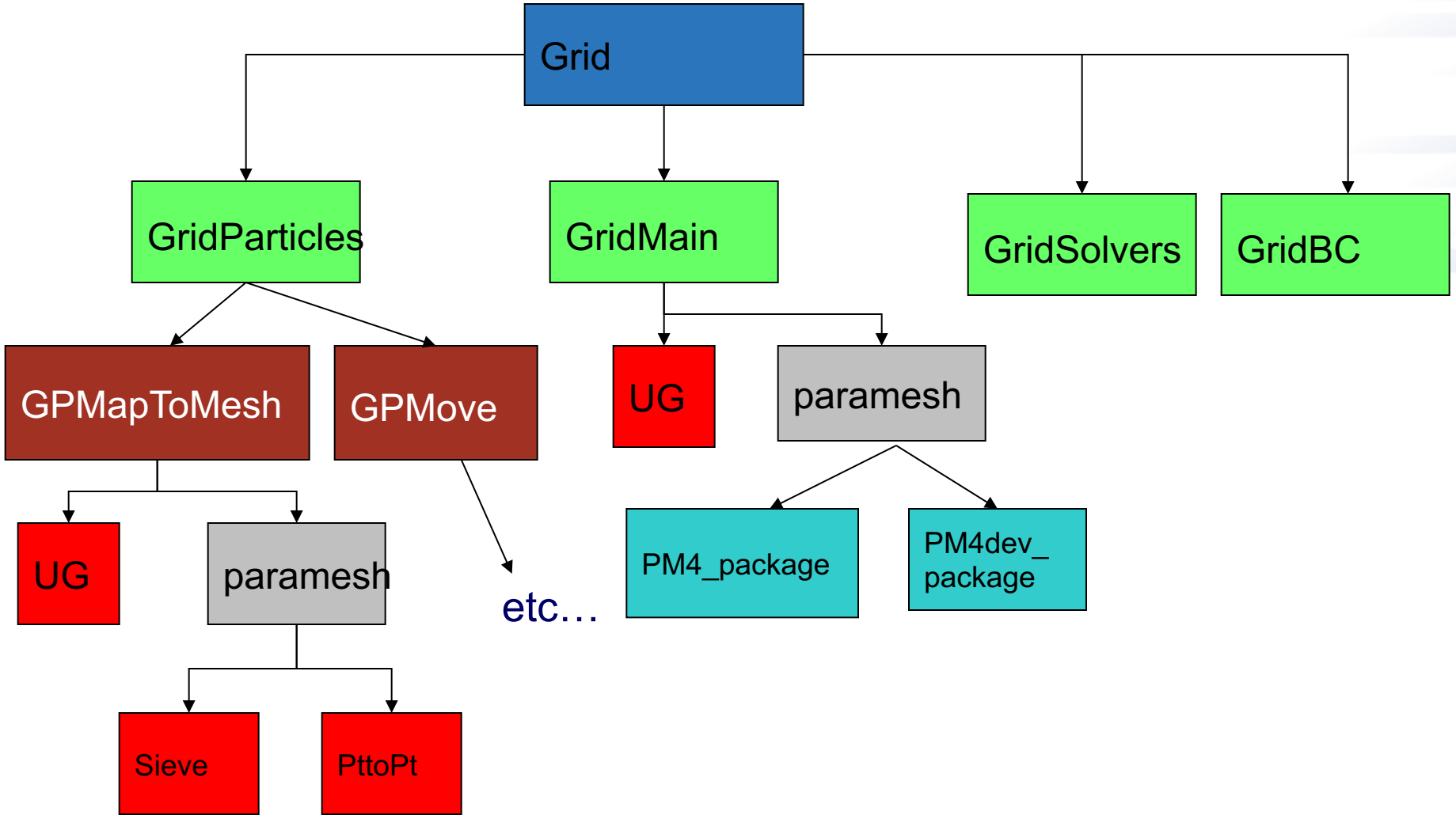
Taming the Complexity: Separation of Concerns



A successful model



Example From FLASH – Grid Unit



Example From FLASH: EOS interface Design

- Hierarchy in complexity of interfaces
  - For collection of points
  - For sections of a block
- Different levels in the hierarchy give different degrees of control to the client routines
  - Most of the complexity is completely hidden from casual users
  - More sophisticated users can bypass the wrappers for greater control
- Done with elaborate machinery of masks and defined constants

```
physics/Eos/Eos
physics/Eos/Eos_finalize
physics/Eos/Eos_getAbarZbar
physics/Eos/Eos_getData
physics/Eos/Eos_getParameters
physics/Eos/Eos_getTempData
physics/Eos/Eos_guardCells
physics/Eos/Eos_init
physics/Eos/Eos_logDiagnostics
physics/Eos/Eos_nucDetectBounce
physics/Eos/Eos_nucOneZone
physics/Eos/Eos_putData
physics/Eos/Eos_unitTest
physics/Eos/Eos_wrapped
```

Preparing for future

- Much larger codes
  - Transition time much longer than before
  - Platform life <<< code lifecycle
  - Platform life ~= transition time
  - Same generation has different platforms
- No single machine model to program to
- Need to deepen parallel hierarchy and lift abstraction
  - Let abstraction and middle layers do the heavy lifting for portability
  - Many ideas, little convergence.

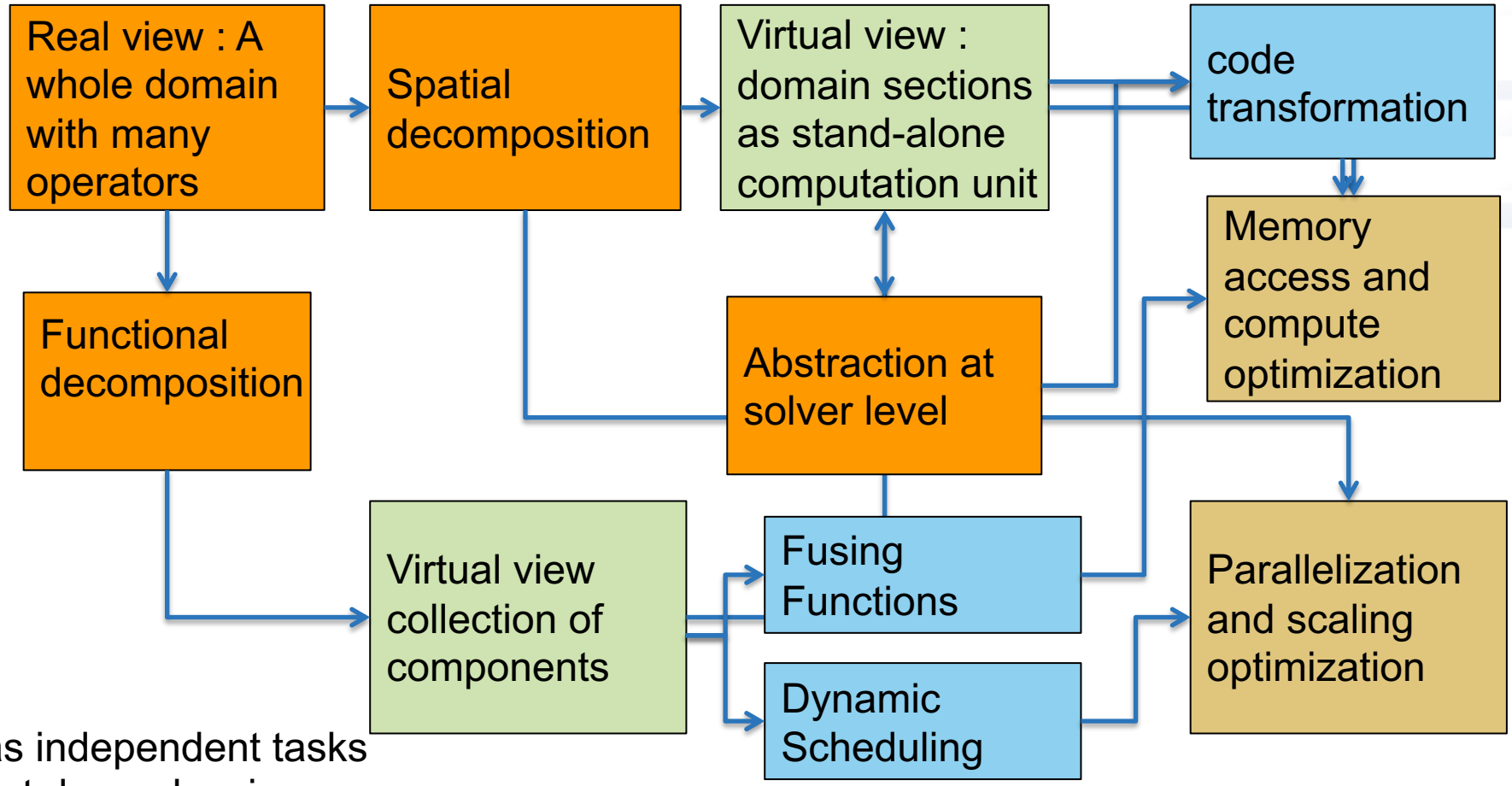
Overarching Theme

- Differentiate between physical view and virtual view
- Simpler world view at either end enables separation of concerns
- Hard-nosed trade-offs

Design considerations - new

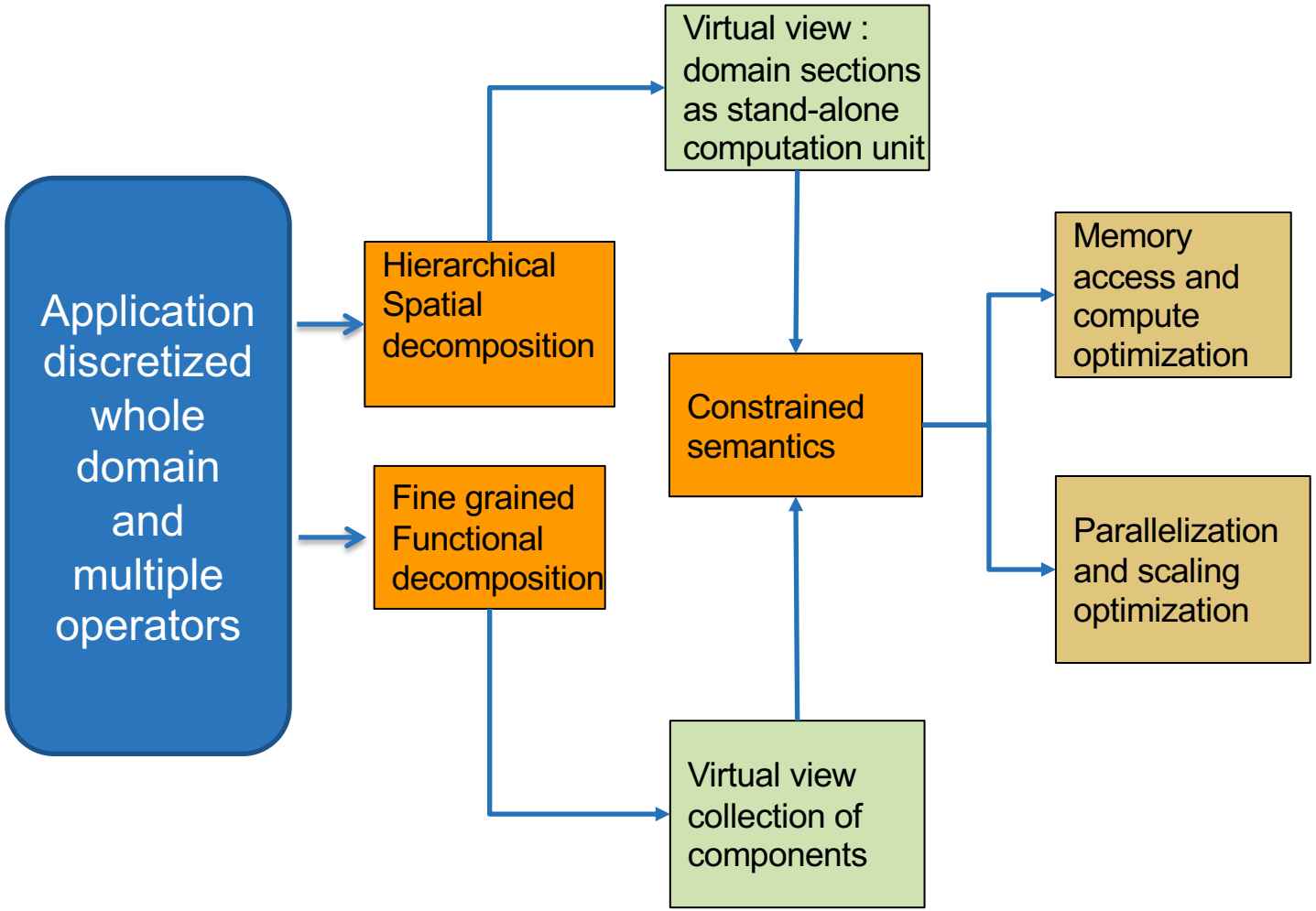
- Composing tasks
  - Components or kernels
- Task orchestration
  - Mapping tasks to devices
    - CPU, accelerators, specialized devices
  - Managing data movement between devices

Example: PDE's

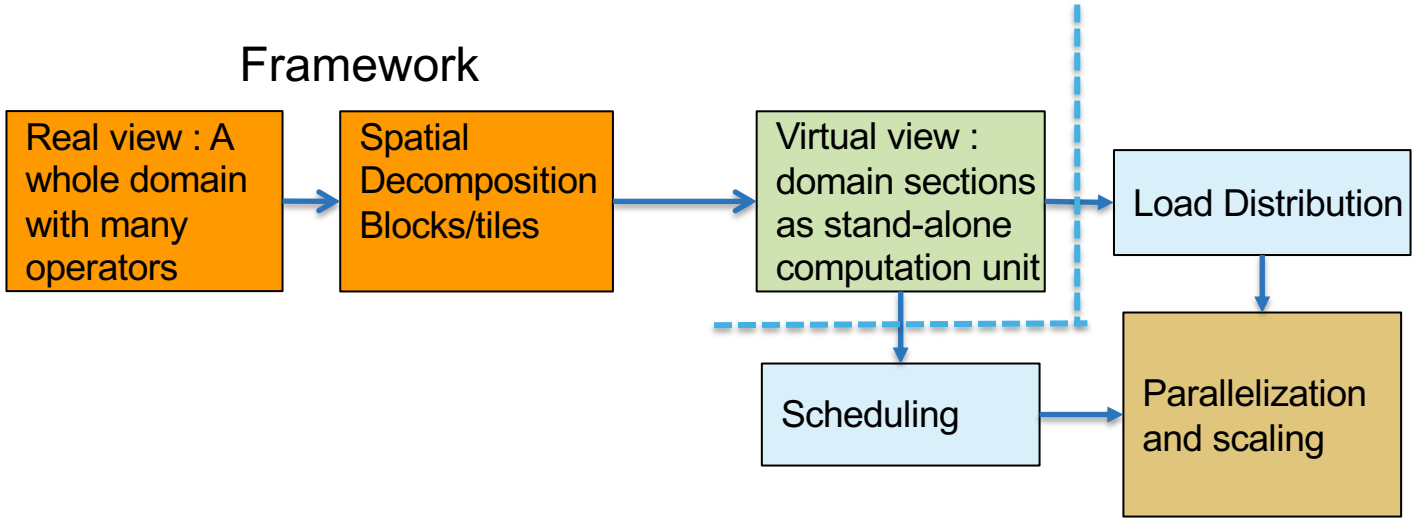


Write solvers as independent tasks
Explicitly call out dependencies
Expose fusion possibilities

The flash approach

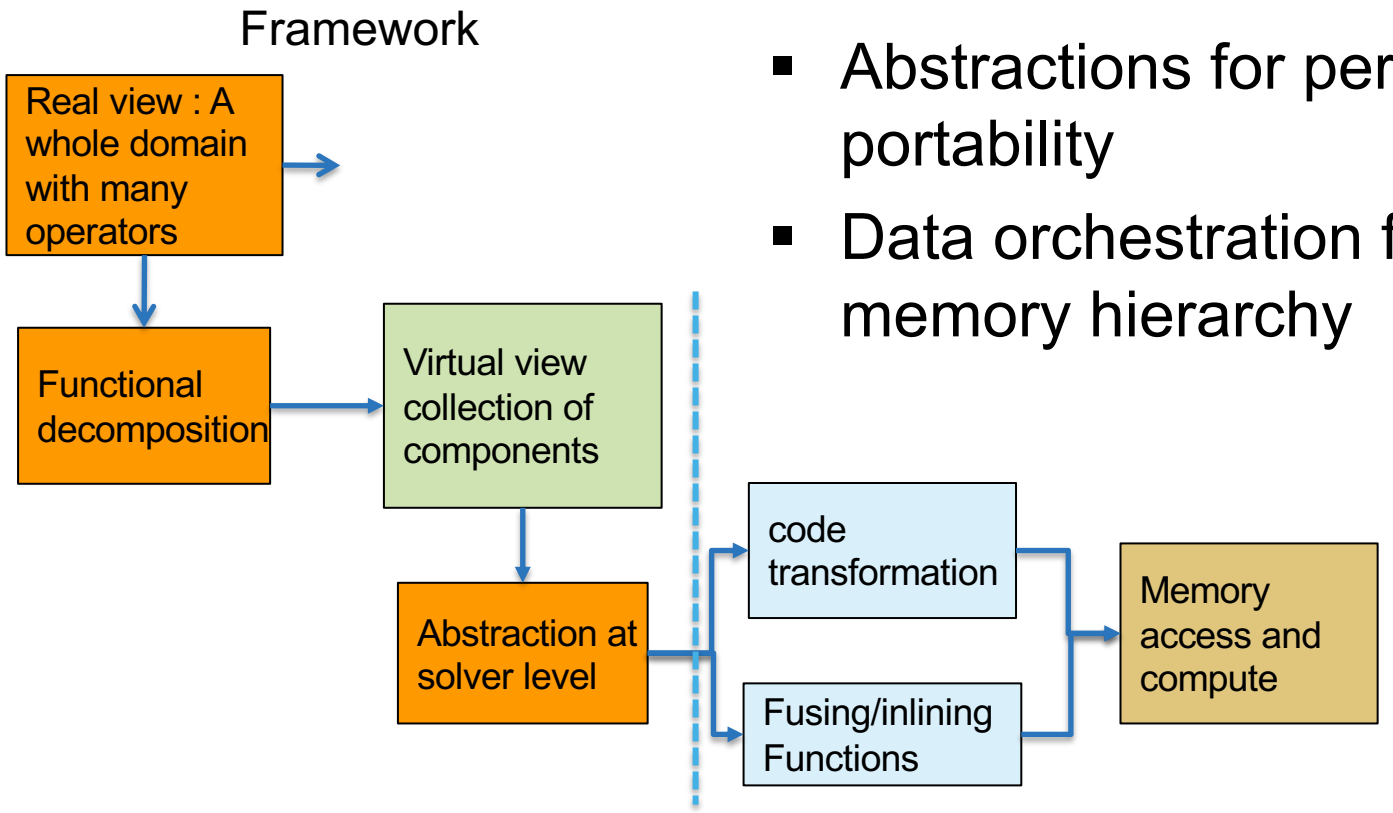


Components in play: infrastructure



- AMR infrastructure: refinement, load balancing, work redistribution
- Scheduling and data movement at block and operator level

Components in Play: operators



- Abstractions for performance portability
- Data orchestration for memory hierarchy

Putting it all Together

- The construction of operators
  - Express computation in the form of stencil operators or other appropriate abstraction
  - Specify the part of the domain, and the conditions under which the operators apply
    - Use masks to take care of branching
- Mix-mode parallelism
  - Parameters to control the degree of tiling or other forms of mix-mode parallelism
    - Could be handed to the compiler when technology arrives
  - Framework forms the data containers
- Dynamic tasking
  - Smarter iterators that are aware of mix-mode parallelism and dependencies
  - The iterating loops give up control and do while loops

Some available Options

- Many efforts to provide tools to application developers
  - KoKKOs : Integrated Option with polymorphic arrays
  - Raja :
  - TiDA, HTA : managing tiling abstractions
  - GridTools : comprehensive solution from CSCS-ETH
  - Dash : managing multilevel locality
  - Task based processing – OCR, charm++, HPX, Quark etc
  - Language based solutions – Julia, Chapel, UPC++ etc
  - Domain specific languages

Other Things to Consider

- Leverage existing software
  - Libraries may have better solvers
    - Off-load expertise and maintenance
  - Examine the interoperability constraints
    - Many times the cost is justified even if there is more data movement
- More available packages are attempting to achieve interoperability
  - See if a combination meets your requirements
- May be worthwhile to let the library dictate data layout if the corresponding operations dominate

Institute an extremely rigorous verification regime at the outset

TESTING AND VERIFICATION

Verification

- Code verification uses tests
  - It is much more than a collection of tests
- It is the holistic process through which you ensure that
  - Your implementation shows expected behavior,
  - Your implementation is consistent with your model,
  - Science you are trying to do with the code can be done.

Stages and types of verification

- During initial code development
  - Accuracy and stability
  - Matching the algorithm to the model
  - Interoperability of algorithms
- In later stages
  - While adding new major capabilities or modifying existing capabilities
  - Ongoing maintenance
  - Preparing for production

Challenge with Exploratory Software

- Verification implies one knows the outcome
  - The outcome is achieved or not achieved
- What if one doesn't exactly know the outcome?
  - Software is meant to understand the expected outcome

Other specific verification challenges

- Functionality coverage
- Particularly true of codes that allow composability in their configuration
- Codes may incorporate some legacy components
  - Its own set of challenges
    - No existing tests at any granularity
- Examples – multiphysics application codes that support multiple domains

Challenges with legacy codes

Checking for coverage

- Legacy codes can have many gotchas
  - Dead code
  - Redundant branches
- Interactions between sections of the code may be unknown
- Can be difficult to differentiate between just bad code, or bad code for a good reason
  - Nested conditionals

Code coverage tools are of limited help

Components of Verification

- Testing at various granularity
  - Individual components
  - Interoperability of components
  - Convergence, stability and accuracy
- Validation of individual components
- Testing practices
- Error bars
  - Necessary for differentiating between drift and round-off
- Selection of tests for coverage

Regular Testing

- Part of ongoing verification
- Automating is helpful
- Can be just a script
- Or a testing harness

Jenkins
C-dash
Custom
(FlashTest)

- Essential for large code
  - Set up and run tests
  - Evaluate test results
- Easy to execute a logical subset of tests
  - Pre-push
  - Nightly
- Automation of test harness is critical for
  - Long-running test suites
  - Projects that support many platforms

Good Testing Practices

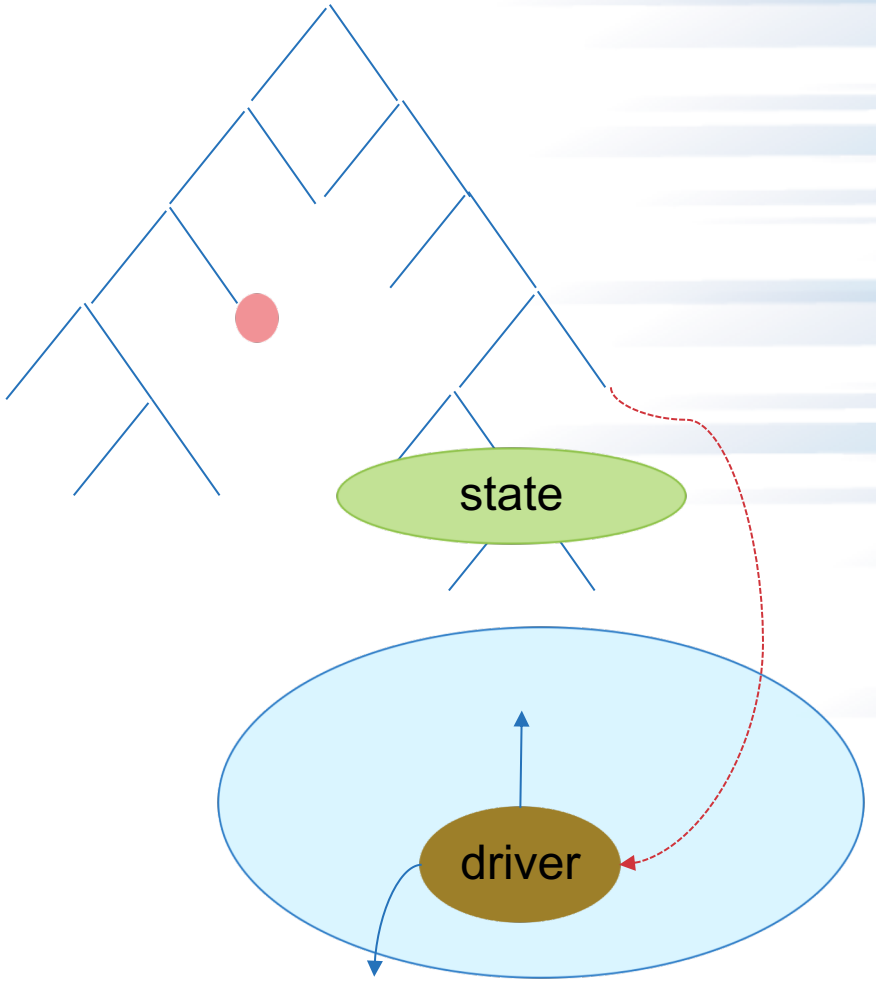
- Must have consistent policy on dealing with failed tests
  - Issue tracking
    - How quickly does it need to be fixed?
    - Who is responsible for fixing it?
- Someone should be watching the test suite
- When refactoring or adding new features, run a regression suite before check in
  - Add new regression tests or modify existing ones for the new features
- Code review before releasing test suite is useful
  - Another person may spot issues you didn't
  - Incredibly cost-effective

Test Development

- Development of tests and diagnostics goes hand-in-hand with code development
  - Non-trivial to devise good tests, but extremely important
  - Compare against simpler analytical or semi-analytical solutions
- When faced with legacy codes with no existing tests
  - Isolate a small area of the code
  - Dump a useful state snapshot
  - Build a test driver
    - Start with only the files in the area
    - Link in dependencies
      - Copy if any customizations needed
  - Read in the state snapshot
  - Verify correctness
    - Always inject errors to verify that the test is working

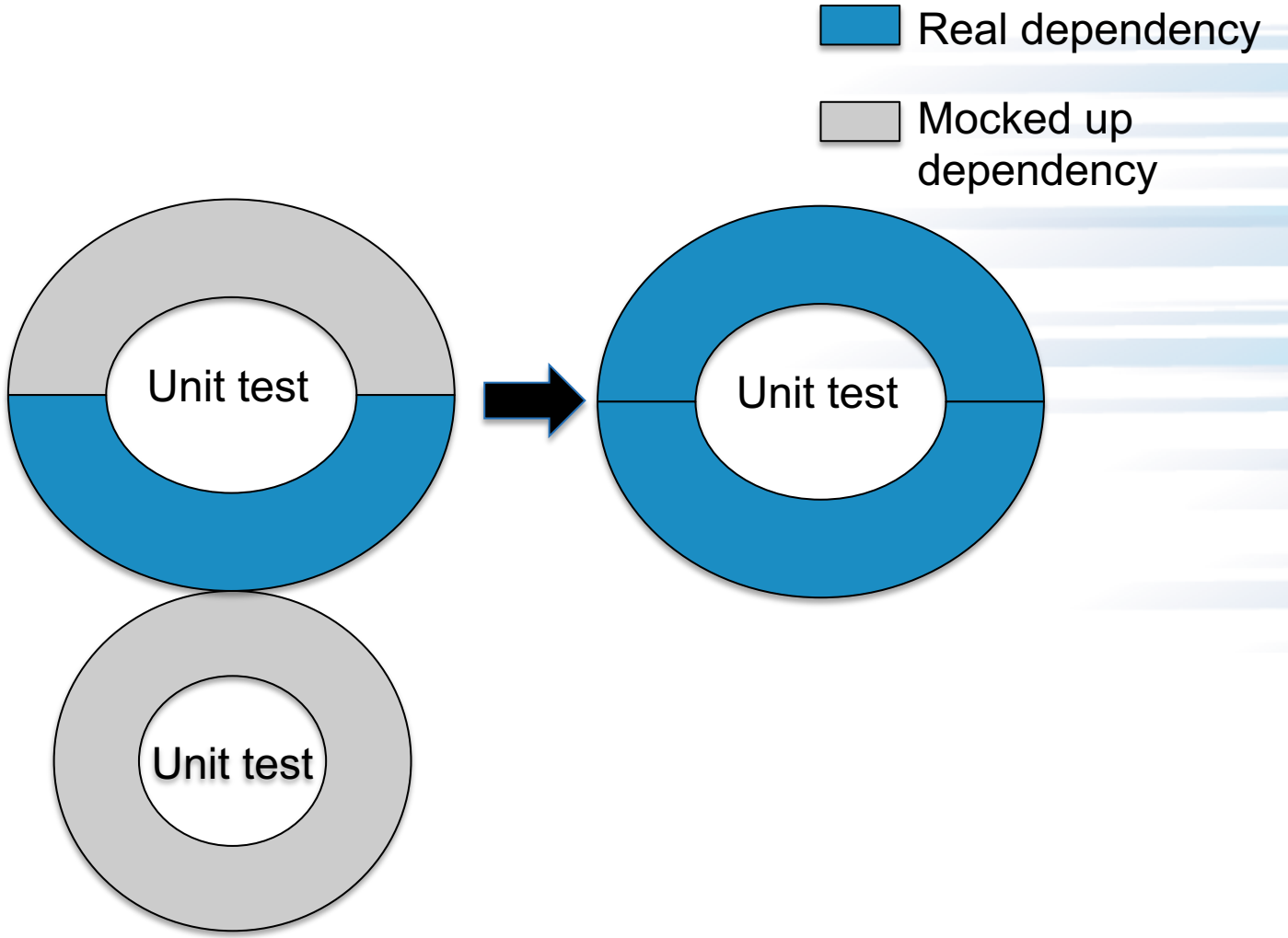
Example from E3SM

- Isolate a small area of the code
- Dump a useful state snapshot
- Build a test driver
  - Start with only the files in the area
  - Link in dependencies
    - Copy if any customizations needed
- Read in the state snapshot
- Restart from the saved state



Workarounds for Granularity

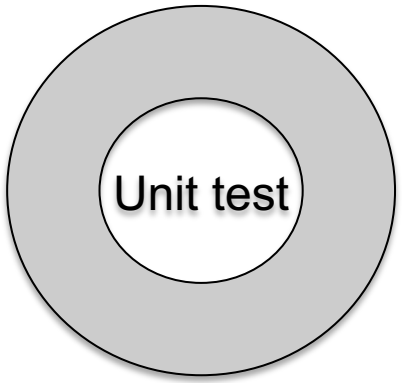
- Approach the problem sideways
  - Components can be exercised against known simpler applications
  - Same applies to combination of components
- Build a scaffolding of verification tests to gain confidence

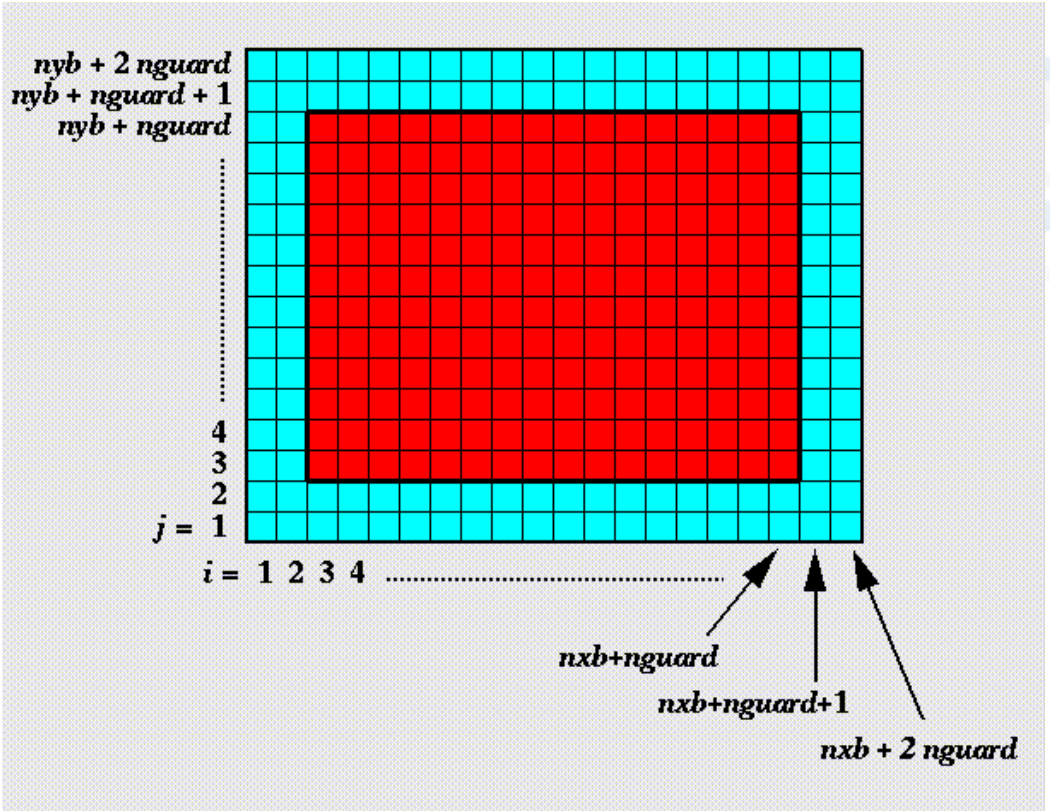


Example from FLASH

Unit test for Grid

- Verification of guard cell fill
- Use two variables A & B
- Initialize A in all cells and B only in the interior cells (red)
- Apply guard cell fill to B





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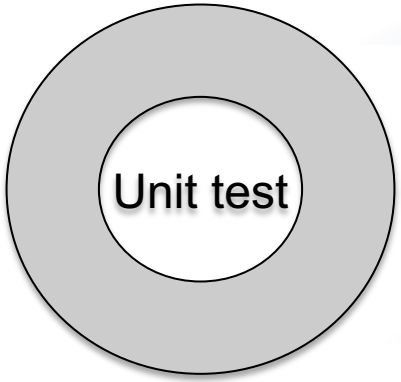


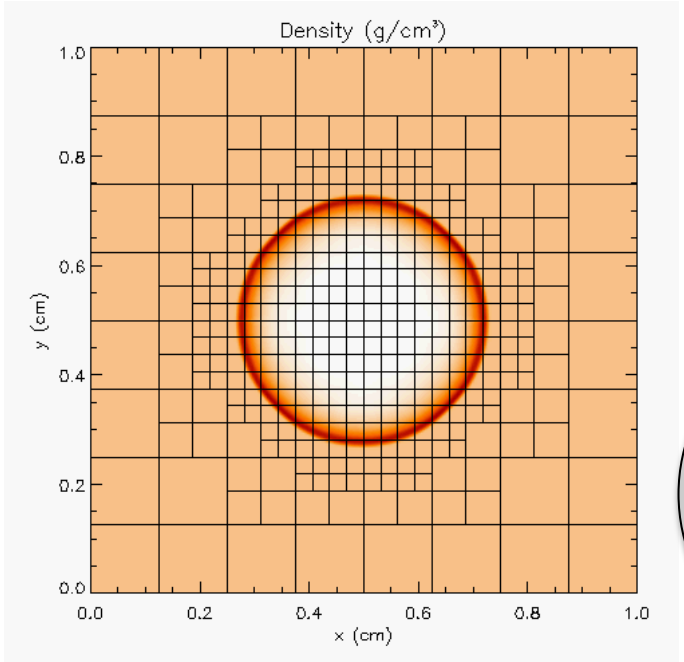
Unit test for Equation of State (EOS)

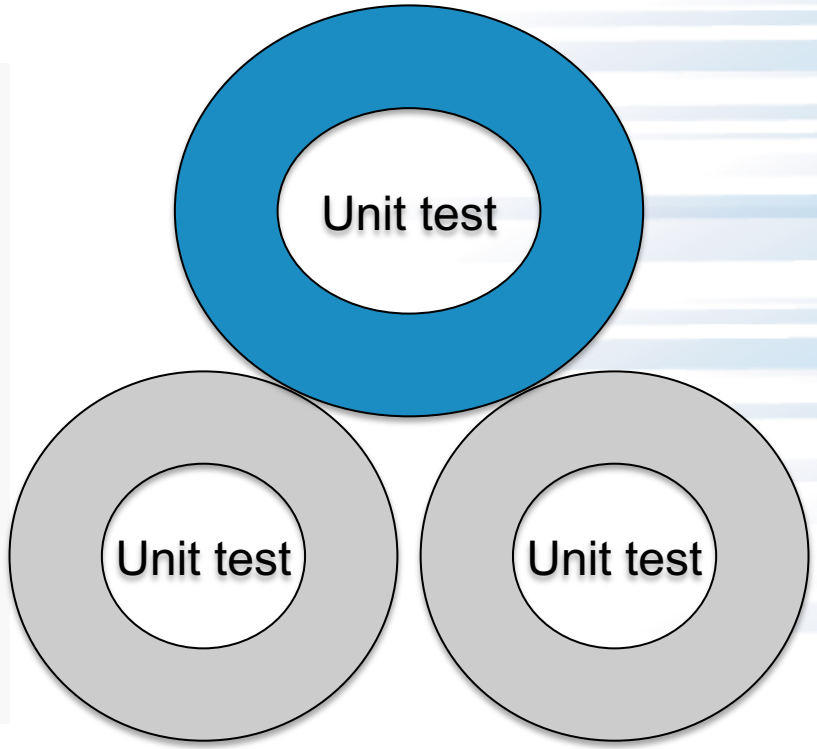
- Three modes for invoking EOS
  - MODE1: Pressure and density as input, internal energy and temperature as output
  - MODE2: Internal energy and density as input temperature and pressure as output
  - MODE3: Temperature and density as input pressure and internal energy as output
- Use initial conditions from a known problem, initialize pressure and density
- Apply EOS in MODE1
- Using internal energy generated in the previous step apply EOS in MODE2
- Using temperature generated in the previous step apply EOS in MODE3
- At the end all variables should be consistent within tolerance

Example from FLASH

Unit test for Hydrodynamics

- Sedov blast wave
- High pressure at the center
- Shock moves out spherically
- FLASH with AMR and hydro
- Known analytical solution





Though it exercises mesh, hydro and eos, if mesh and eos are verified first, then this test verifies hydro

More testing needed for Grid using AMR
Flux correction and regridding

Example from FLASH

Reason about correctness for testing Flux correction and regridding

IF Guardcell fill and EOS unit tests passed

- Run Hydro without AMR
  - If failed fault is in Hydro
- Run Hydro with AMR, but no dynamic refinement
  - If failed fault is in flux correction
- Run Hydro with AMR and dynamic refinement
  - If failed fault is in regridding

Selection of tests

- Two purposes
  - Regression testing
    - May be long running
    - Provide comprehensive coverage
  - Continuous integration
    - Quick diagnosis of error
- A mix of different granularities works well
  - Unit tests for isolating component or sub-component level faults
  - Integration tests with simple to complex configuration and system level
  - Restart tests
- Rules of thumb
  - Simple
  - Enable quick pin-pointing

Why not always use the most stringent testing?

- Effort spent in devising tests and testing regime are a tax on team resources
- When the tax is too high…
  - Team cannot meet code-use objectives
- When is the tax is too low…
  - Necessary oversight not provided
  - Defects in code sneak through
- Evaluate project needs
  - Objectives: expected use of the code
  - Team: size and degree of heterogeneity
  - Lifecycle stage: new or production or refactoring
  - Lifetime: one off or ongoing production
  - Complexity: modules and their interactions

Commonalities

- Unit testing is always good
  - It is never sufficient
- Verification of expected behavior
- Understanding the range of validity and applicability is always important
  - Especially for individual solvers

Test Selection

- First line of defense – code coverage tools (demo later)
- Necessary but not sufficient – don't give any information about interoperability

- Build a matrix
  - Physics along rows
  - Infrastructure along columns
  - Alternative implementations, dimensions, geometry
- Mark <i,j> if test covers corresponding features
- Follow the order
  - All unit tests – including full module tests
  - Tests representing ongoing productions
  - Tests sensitive to perturbations
  - Most stringent tests for solvers
  - Least complex test to cover remaining spots

Example

	Hydro	EOS	Gravity	Burn	Particles
AMR	CL	CL		CL	CL
UG	SV	SV			SV
Multigrid	WD	WD	WD	WD	
FFT			PT		

- A test on the same row indicates interoperability between corresponding physics
- Similar logic would apply to tests on the same column for infrastructure
- More goes on, but this is the primary methodology

Tests	Symbol
Sedov	SV
Cellular	CL
Poisson	PT
White Dwarf	WD

TAKEAWAYS

- UNDERSTAND YOUR NEEDS
- DO THE COST-BENEFIT ANALYSIS
- ADOPT WHAT WORKS FOR YOU WITHOUT INCURRING TECHNICAL DEBT
- DESIGN WITH PORTABILITY, EXTENSIBILITY, REPRODUCIBILITY AND MAINTAINABILITY IN MIND
- VERIFY … VERIFY … VERIFY

…….QUESTIONS ?