Verification and Refactoring

Better Scientific Software Tutorial

Anshu Dubey

Argonne National Laboratory

ISC High Performance Conference

June 16, 2019

License, citation, and acknowledgements

License and Citation

Acknowledgements

- This work was supported by the U.S. Department of Energy Office of Science, Office of Advanced Scientific Computing Research (ASCR), and by the Exascale Computing Project (17-SC-20-SC), a collaborative effort of the U.S. Department of Energy Office of Science and the National Nuclear Security Administration.
- This work was performed in part at the Argonne National Laboratory, which is managed by UChicago Argonne, LLC for the U.S. Department of Energy under Contract No. DE-AC02-06CH11357

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

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

Test Definitions

- Unit tests
  - Test individual functions or classes
- Integration tests
  - Test interaction, build complex hierarchy
- System level tests
  - At the user interaction level

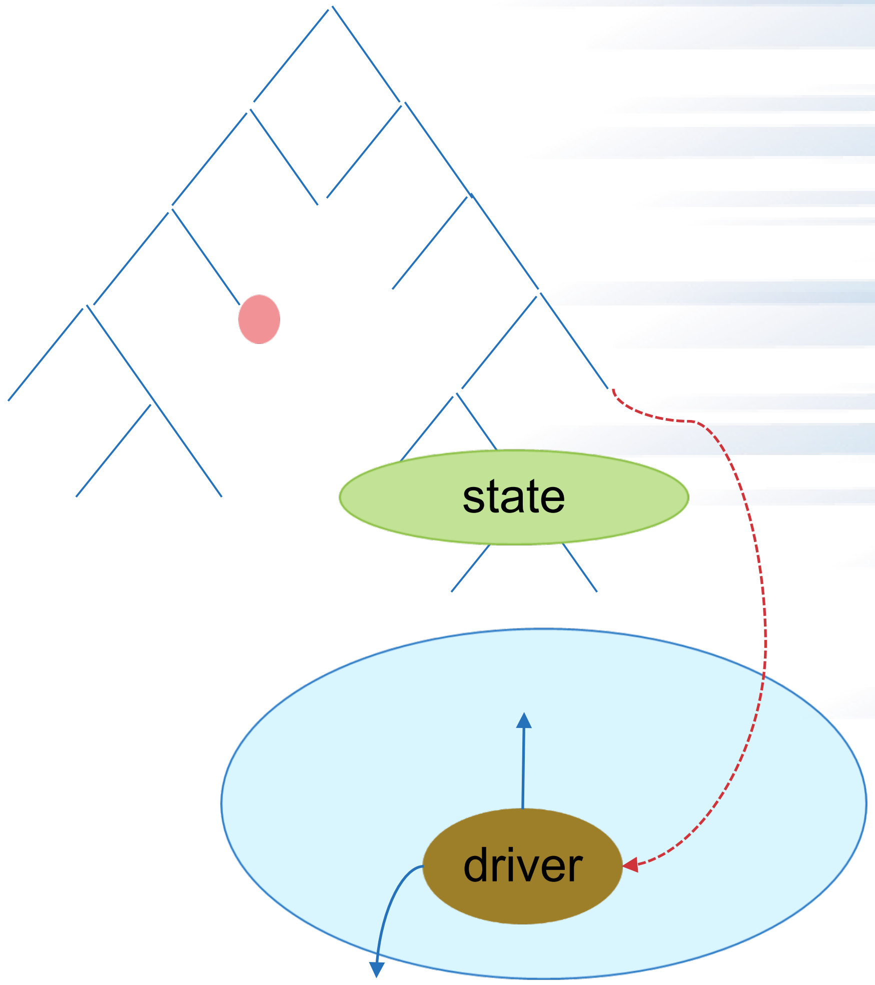
- Restart tests
  - Code starts transparently from a checkpoint
- Regression (no-change) tests
  - Compare current observable output to a gold standard
- Performance tests
  - Focus on the runtime and resource utilization

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
  - More creative approach becomes necessary
- Verify correctness
  - Always inject errors to verify that the test is working

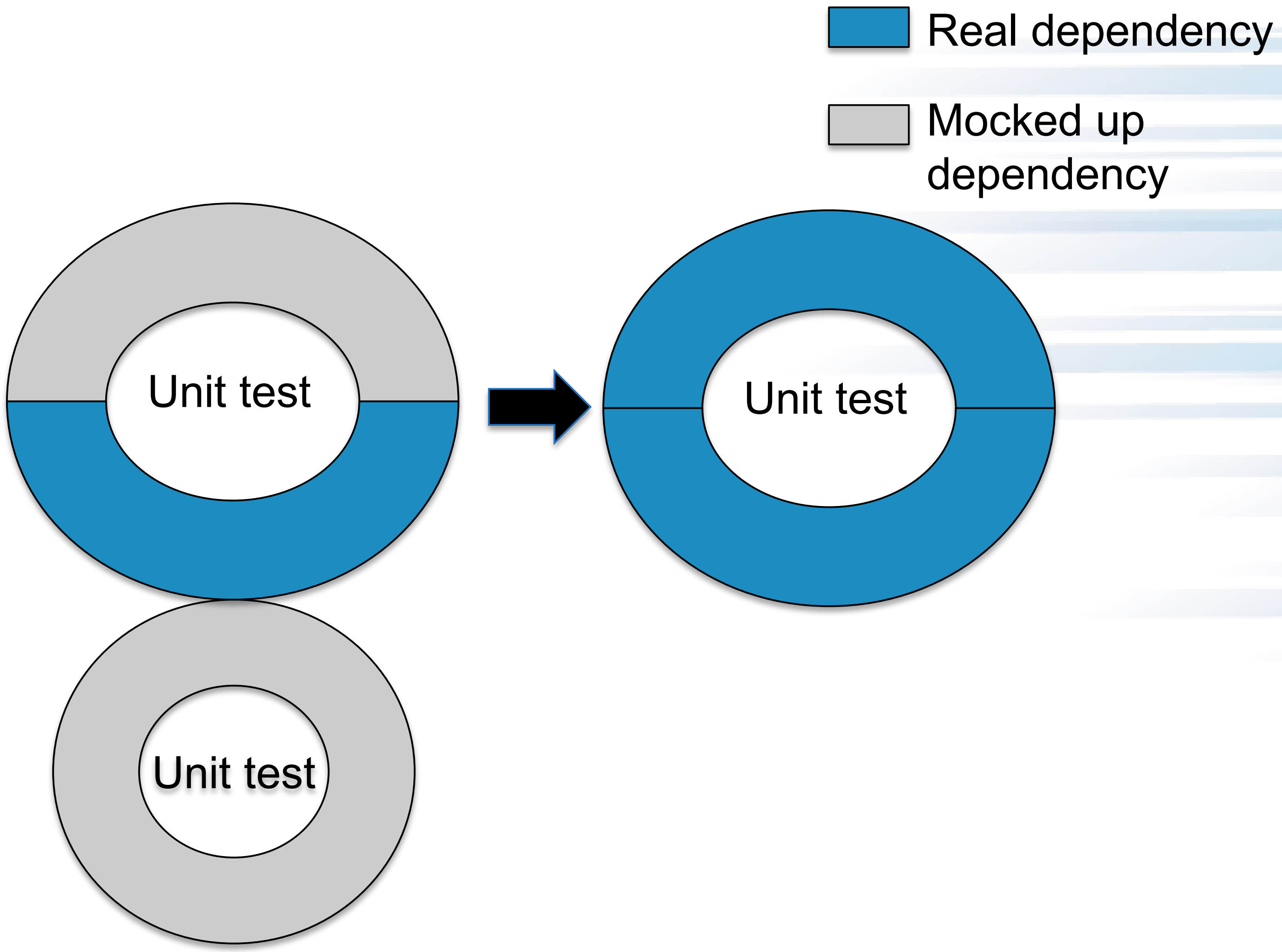
Example from E3SM

- 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

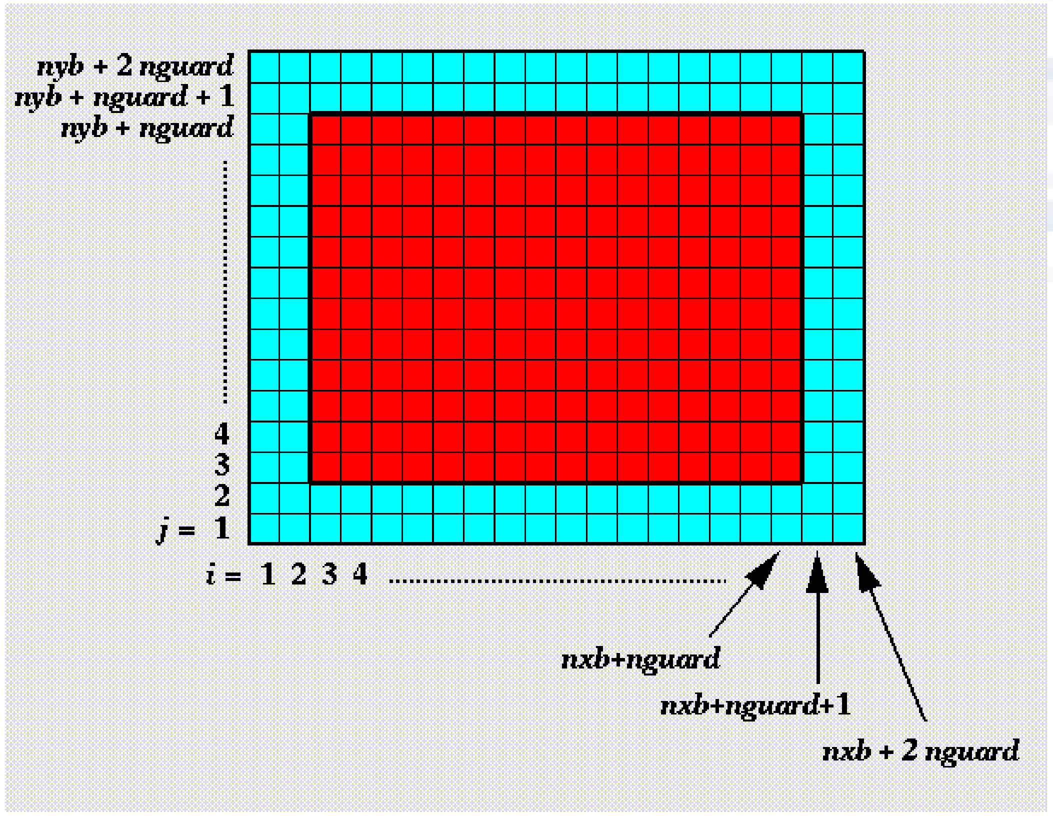
- Approach the problem sideways
  - Components can be exercised against known simpler applications
  - Same applies to combination of components
- Build a scaffolding of verification tests to gain confidence

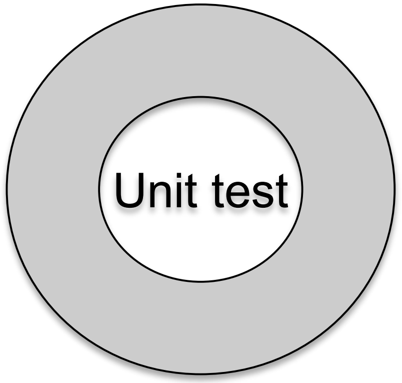


Example from FLASH

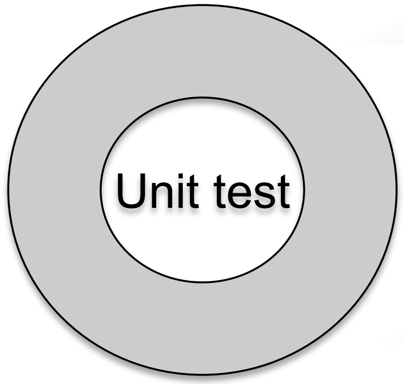
Unit test for Grid

- 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





Example from Flash



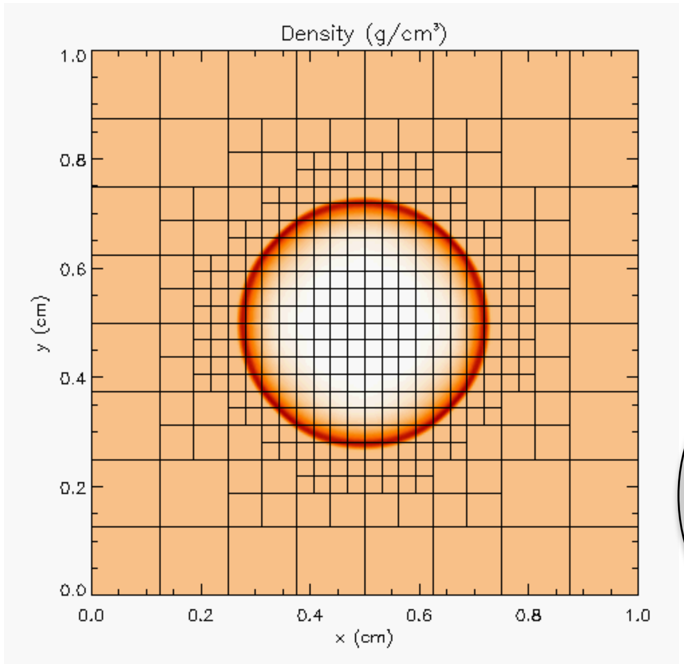
Unit test for Equation of State (EOS)

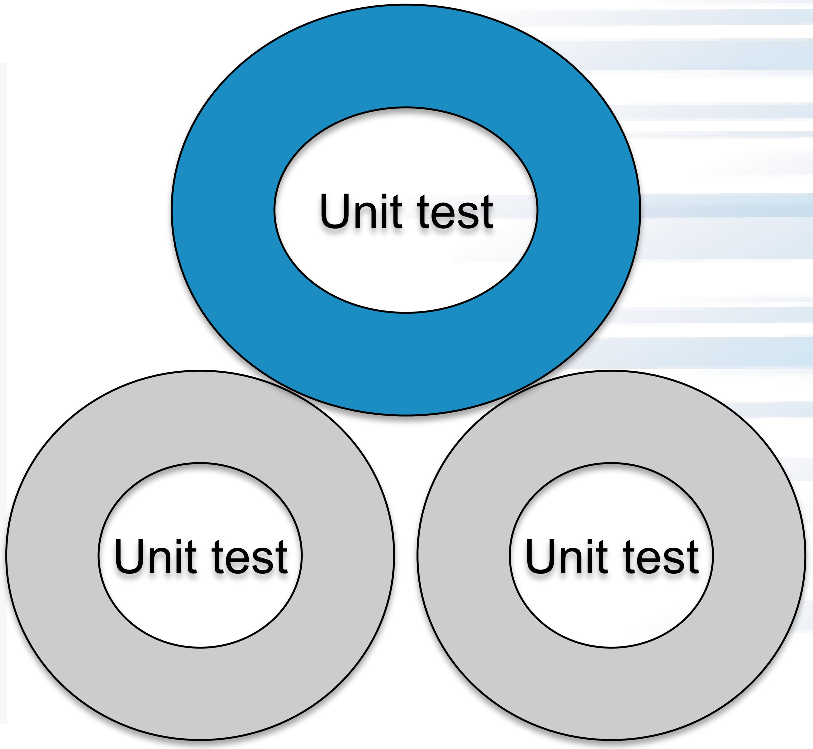
- Three modes for invoking EOS
  - MODE1: Pressure and density as input, internal energy and temperature as output
  - MODE2: Internal energy and density as input temperature and pressure as output
  - MODE3: Temperature and density as input pressure and internal energy as output
- Use initial conditions 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

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		

Tests	Symbol
Sedov	SV
Cellular	CL
Poisson	PT
White Dwarf	WD

- 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

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

Refactoring

Considerations

- Know why you are refactoring
  - Is it necessary
  - Where should the code be after refactoring
- Know the scope of refactoring
  - How deep a change
  - How much code will be affected
- Estimate the cost
  - Expected developer time
  - Extent of disruption in production schedules
- Get a buy-in from the stakeholders
  - That includes the users
  - For both development time and disruption

Cost estimation

When development and production co-exist

- Potential for branch divergence
- Policies for code modification
  - Estimate the cost of synchronization
  - Plan synchronization schedule and account for overheads
- Anticipate production disruption
  - From code freeze due to merges
  - Account for resources for quick resolution of merge issues

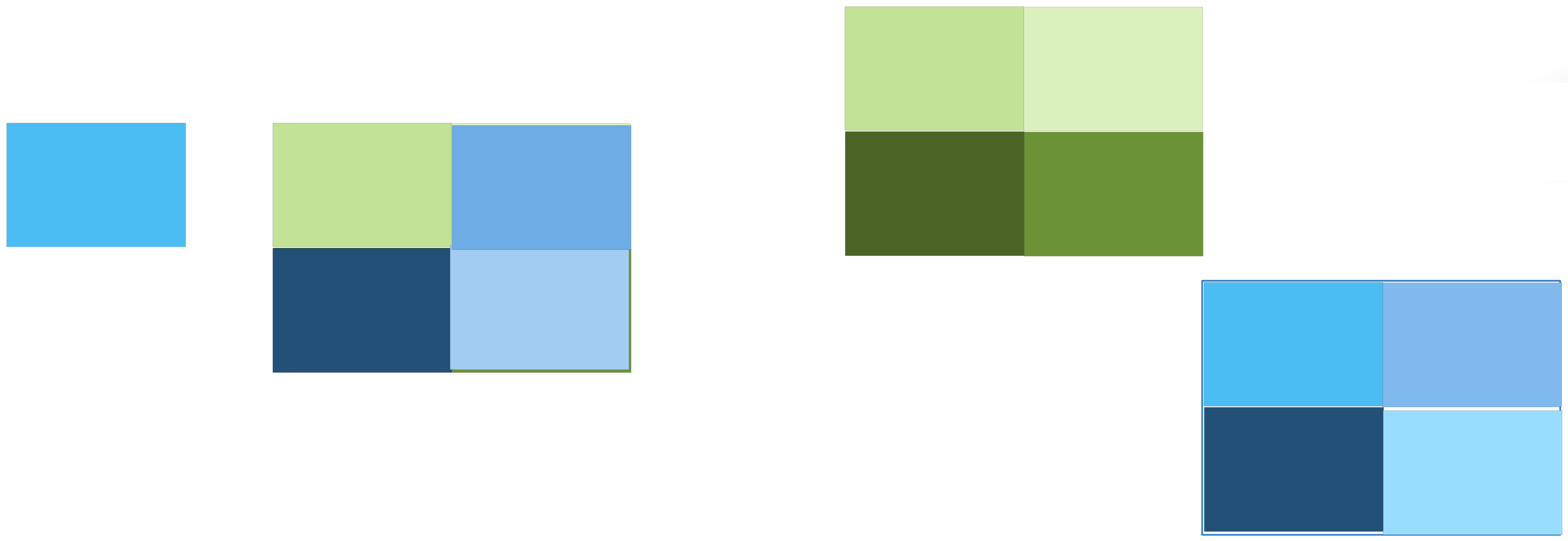
This is where buy-in from the stake-holders is critical

Before Starting

- Know bounds on acceptable behavior change
- Know your error bounds
  - Bitwise reproduction of results unlikely after transition
- Map from here to there
- Check for coverage provided by existing tests
- Develop new tests where there are gaps

Incorporate testing overheads into refactor cost estimates

On ramp plan

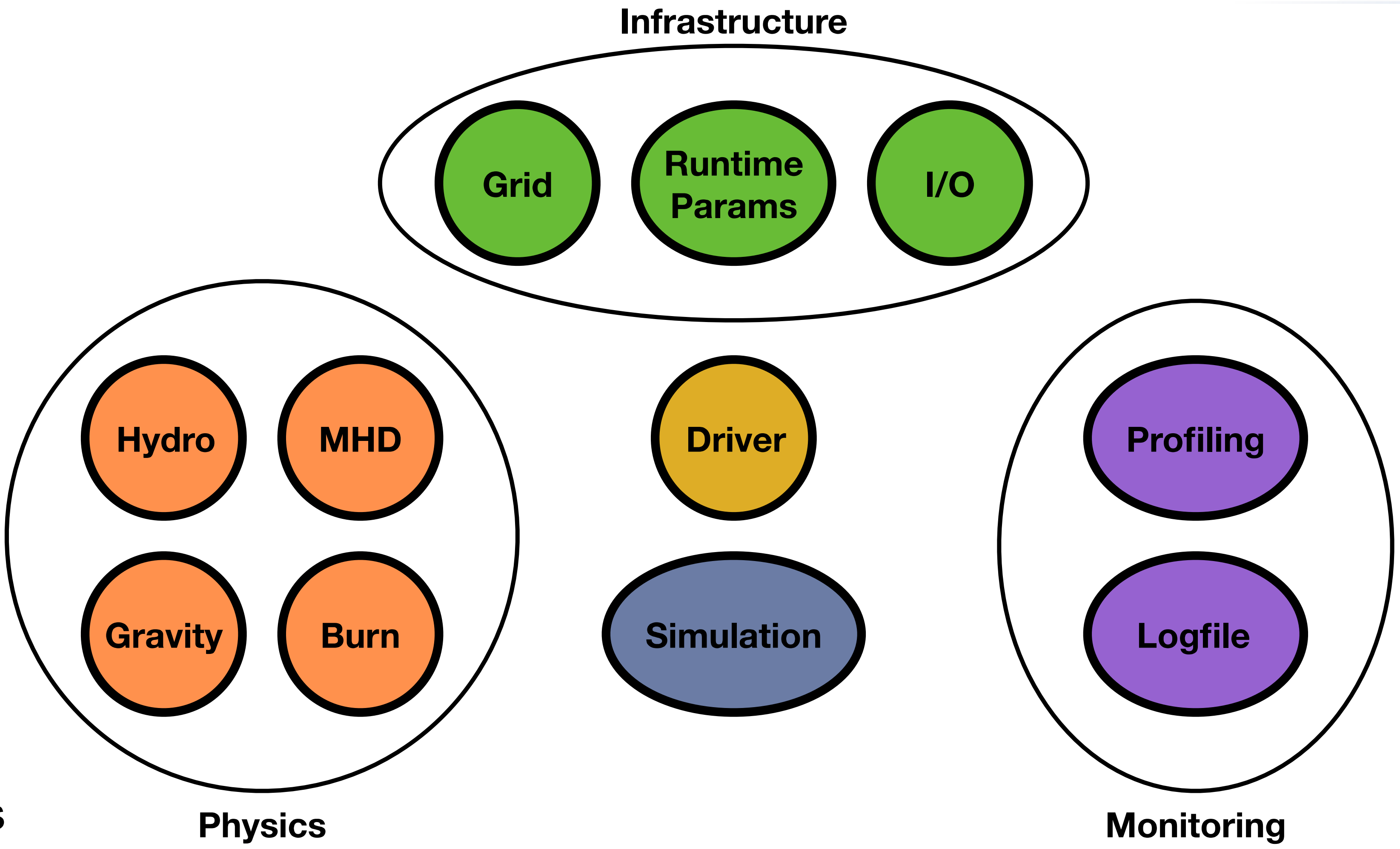


- Incrementally if at all possible
- Small components, verified individually
- Migrated back

- Alternatively migrate them into new infrastructure

Example FLASH

- Grid
  - Manages data
  - Domain discretization
- Hydro
  - `simpleUnsplit`
  - `Unsplit`
- Driver
  - Time-stepping
  - Orchestrates interactions



FLASH5

Refactoring for Next Generation Hardware

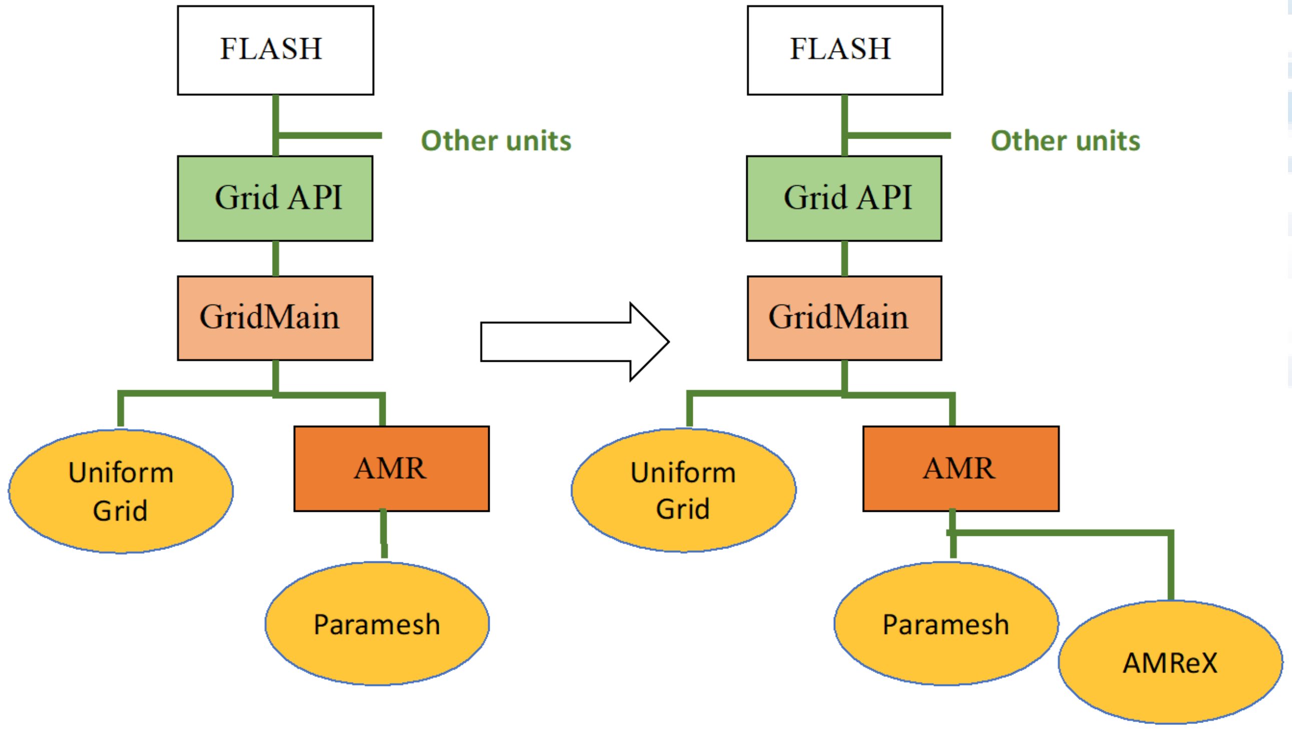
AMReX - Lawrence Berkeley National Lab

- Designed for exascale
- Node-level heterogeneity
- Smart iterators hide parallelization

Goal: Replace Paramesh with AMReX

Plan:

- Paramesh & AMReX coexist
- Adapt interfaces to suit AMReX
- Refactor Paramesh implementation
- Compare AMReX implementation against Paramesh implementation



Refactoring plan

Design

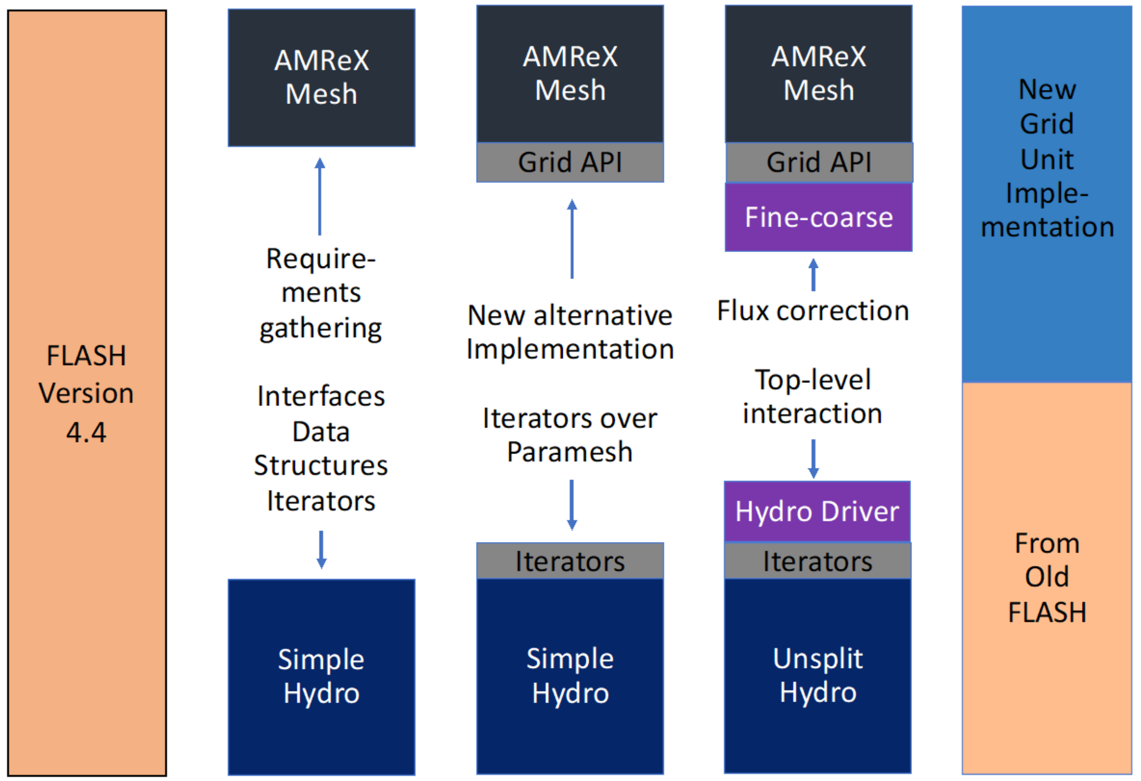
- Degree & scope of change
- Formulate initial requirements

Prototyping

- Explore & test design decisions
- Update requirements

Implementation

- Recover from prototyping
- Expand & implement design decisions



Phase 1 - design

Sit, think, hypothesize, & argue

- Derive and understand principal definitions & abstractions
- Collect & understand Paramesh/AMReX constraints
  - Generally useful design due to two sets of constraints?
- Collect & understand physics unit requirements on Grid unit
- Design fundamental data structures & update interface
  - AMReX introduces iterators over blocks/tiles of mesh
  - Package up block/tile index with associated mesh metadata
- Minimal prototyping with no verification

Phase 2 - prototyping

Quick, dirty, & light

- Implement new data structures
  - Evolve design/implementation by iterating between Paramesh & AMReX
- Explore Grid/physics unit interface
  - `simpleUnsplit` Hydro unit
- Discover use patterns of data structures and Grid unit interface
- Adjust requirements & interfaces

Verification

- Single `simpleUnsplit` simulation
- Quantitative regression test with Paramesh
- Proof of concept with AMReX *via* qualitative comparison with Paramesh

Phase 3 - implementation

Toward quantifiable success & Continuous Integration

- Derive & implement lessons learned
  - Clean code & inline documentation
- Update `Unsplit` Hydro
- Hybrid FLASH
  - AMReX manages data
  - Paramesh drives AMR
- Fully-functioning simulation with AMReX
- Prune old code

Verification

- Git workflow
- Grow test suite / CI with Jenkins
- Add new feature/test
  - Create Paramesh baseline with FLASH4.4
  - Refactor Paramesh implementation
  - Implement with AMReX & compare against Paramesh baseline

Other resources

Software testing levels and definitions:
http://www.tutorialspoint.com/software_testing/software_testing_levels.htm

Working Effectively with Legacy Code, Michael Feathers. The legacy software change algorithm described in this book is very straight-forward and powerful for anyone working on a code that has insufficient testing.

Code Complete, Steve McConnell. Includes testing advice.

Organization dedicated to software testing: https://www.associationforsoftwaretesting.org/

Software Carpentry: http://katyhuff.github.io/python-testing/

Tutorial from Udacity: https://www.udacity.com/course/software-testing--cs258

Papers on testing:
http://www.sciencedirect.com/science/article/pii/S0950584914001232
https://www.researchgate.net/publication/264697060_Ongoing_verification_of_a_multiphysic
s_community_code_FLASH

Resources for Trilinos testing:
Trilinos testing policy: https://github.com/trilinos/Trilinos/wiki/Trilinos-Testing-Policy
Trilinos test harness: https://github.com/trilinos/Trilinos/wiki/Policies--%7C-Testing

Agenda

Time	Module	Topic	Speaker
2:00pm-2:40pm	01	Overview of Best Practices in HPC Software Development	Anshu Dubey, ANL
2:40pm-3:20pm	02	Better (Small) Scientific Software Teams	David E. Bernholdt, ORNL
3:20pm-4:00pm	03	Improving Reproducibility through Better Software Practices	David E. Bernholdt, ORNL
4:00pm-4:30pm		*Break*	
4:30pm-5:15pm	04	Verification & Refactoring	Anshu Dubey, ANL
5:15pm-6:00pm	05	Git Workflow & Continuous Integration	Jared O'Neal, ANL

https://r.isc-hpc.com/tut130

(Please note the R before our domain)

FEEDBACK

IDEAS productivity

ECP EXASCALE COMPUTING PROJECT