Refactoring Scientific Software

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License and Citation

- **The requested citation the overall tutorial is:** Anshu Dubey, David E. Bernholdt, Greg Becker, and Jared O'Neal, Software Productivity and Sustainability track, in Argonne Training Program on Extreme-Scale Computing, St. Charles, Illinois, 2023. DOI: 10.6084/m9.figshare.23823822.
- Individual modules may be cited as *Speaker, Module Title*, in *Tutorial Title*, …

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What is Refactoring

Definition: Refactoring is a disciplined technique for restructuring an existing body of code, altering its internal structure without changing its external behavior.

- Different from development
  - You have a working code
  - You know and understand the behavior
  - You have a baseline that you can use for comparison

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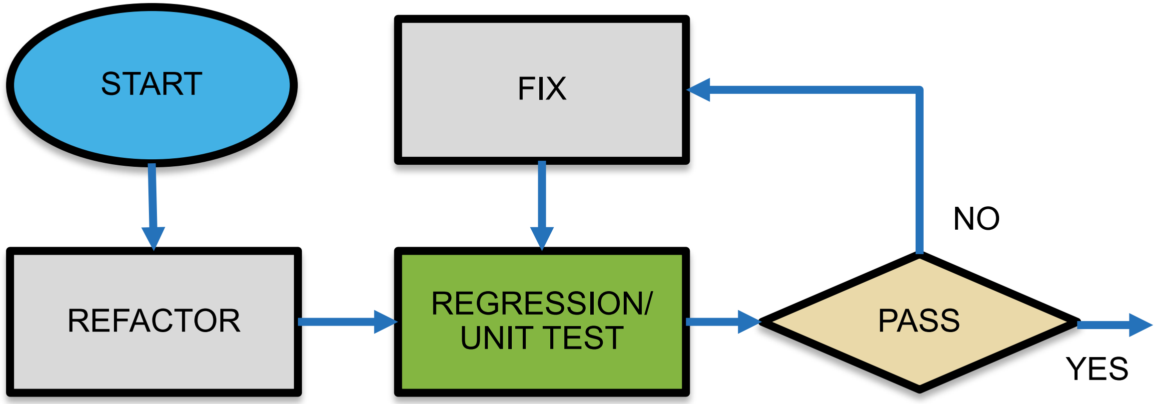
- General motivations
  - Modularity enhancement
    - Improve sustainability
  - Release to outside users
    - Easier to use and understand
  - Port to new platforms
    - Performance portability
  - Expand capabilities
    - Structural flexibility

An Example Workflow



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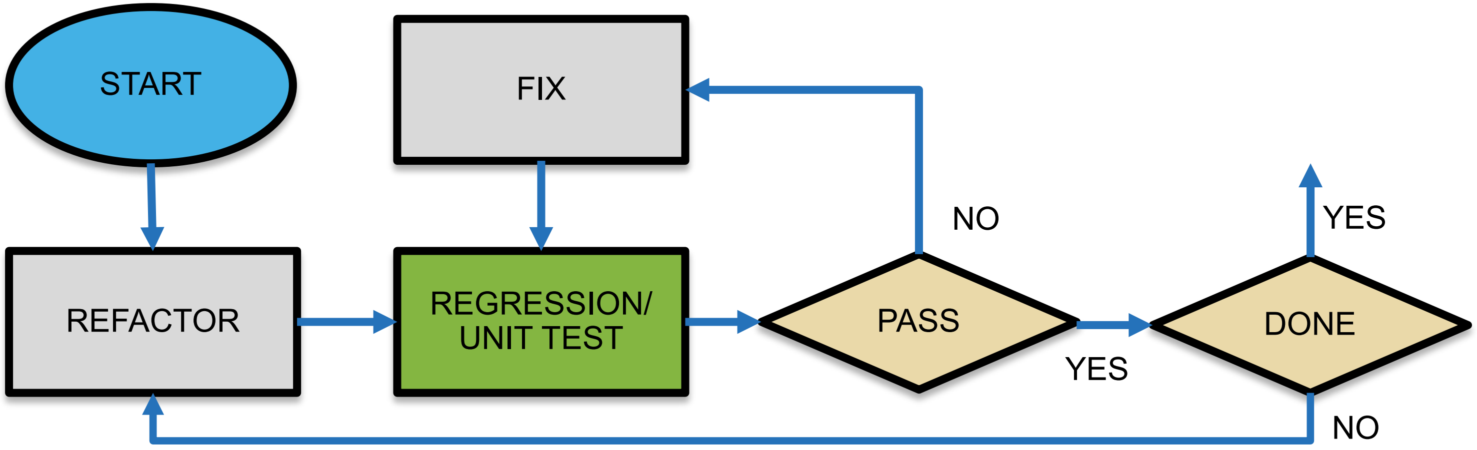

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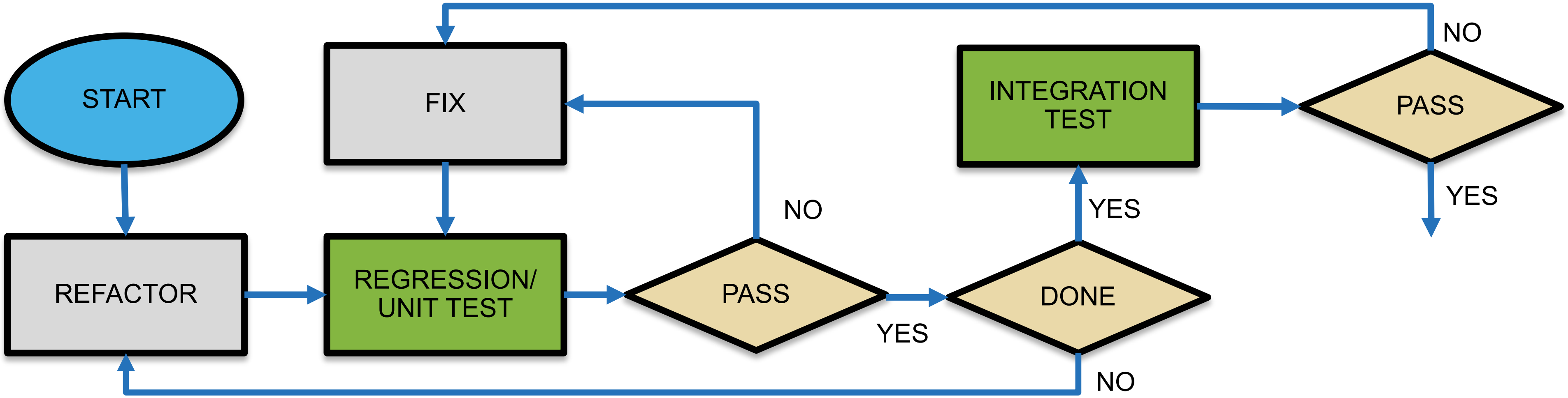

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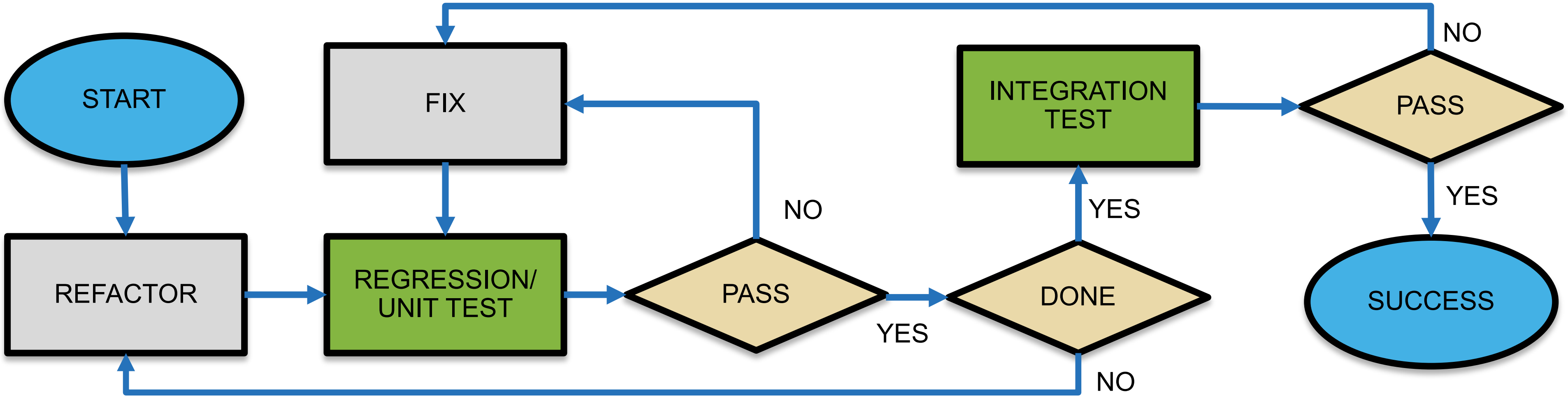
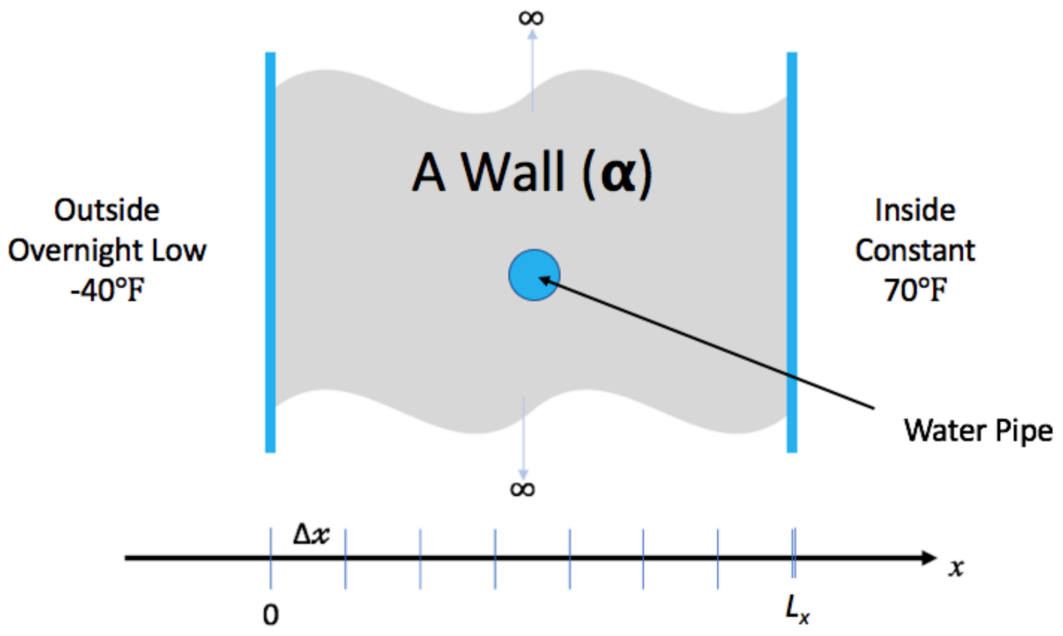


Look at the Running Example

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?

Consider two versions of this code…

- One is a single file with monolithic code
- The other is modularized reusable maintainable code
- If we had only the first version, we would be refactoring to get to the second

Considerations for Refactoring

- Know why you are refactoring
  - Is it necessary
  - Where should the code be after refactoring
- In heat example version 1
  - It is necessary because
    - It is a monolithic code
    - No reusability of any part of the code
    - Devising tests is hard
    - Limited extensibility
  - Where do we want to be after refactoring
    - Closer to the second version
    - More modular, maintainable and extensible

Considerations for Refactoring

- Know the scope of refactoring
  - How deep a change
  - How much code will be affected
- In heat example
  - No capability extension
  - No performance consideration
  - Cleaner, more maintainable code

To modularize the monolithic code…

- Separate out utilities, generalize interfaces
- Put global definitions in a header file
- Create a general build function
- No new code or intrusive changes

Before Starting

- Know your cost estimates
- Verification
  - Check for coverage provided by existing tests
  - Develop new tests where there are gaps
  - Make sure tests exist at different granularities
    - There should be demanding integration and system level tests

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  - on acceptable behavior change
  - error bounds
    - bitwise reproduction of results unlikely after transition
- Map from here to there

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Incorporate testing overheads into refactoring cost estimates

Exercise: Refactoring `bssw-tutorial/hello-numerical-world`

- I am taking the clean solution and generalizing the update_solution interface
  - Motivation: Do not want to change heat.C for adding another method
  - For this exercise we will use “ftcs” and “upwind15” as alternative options

Preparing for Refactoring – check coverage

- Run ./heat runame="ftcs_results"
- Run gcov heat.C
- Examine heat.C.gcov

- A dash indicates non-executable line
- A number indicated the times the line was called
- ###### indicates line wasn't exercised

```
HDR = Double.H
SRC = heat.C utils.C args.C exact.C ftcs.C upwind15.C crankn.C
OBJ = $(SRC:.C=.o)
GCOV = $(SRC:.C=.C.gcov) $(SRC:.C=.gcda) $(SRC:.C=.gcno) $(HDR:.
H=.H.gcov)
EXE = heat

# Implicit rule for object files
%.o : %.C
        $(CXX) -c -coverage $(CXXFLAGS) $(CPPFLAGS) $< -o $@

# Linking the final heat app
heat: $(OBJ)
        $(CXX) -coverage -o heat $(OBJ) $(LDFLAGS) -lm
```

```
    -:  143:static bool
  500:  144:update_solution()
    -:  145:{
  500:  146:    if (!strcmp(alg, "ftcs"))
  500:  147:        return update_solution_ftcs(Nx, curr, last, alpha, dx, dt, bc0, bc1);
#####:  148:    else if (!strcmp(alg, "upwind15"))
#####:  149:        return update_solution_upwind15(Nx, curr, last, alpha, dx, dt, bc0, bc1);
#####:  150:    else if (!strcmp(alg, "crankn"))
#####:  151:        return update_solution_crankn(Nx, curr, last, cn_Amat, bc0, bc1);
#####:  152:    return false;
  500:  153:}
    -:  154:
    -:  155:static Double
  500:  156:update_output_files(int ti)
    -:  157:{
  500:  158:    Double change;
    -:  159:
  500:  160:    if (ti>0 && save)
    -:  161:    {
#####:  162:        compute_exact_solution(Nx, exact, dx, ic, alpha, ti*dt, bc0, bc1);
#####:  163:        if (savi && ti%savi==0)
#####:  164:            write_array(ti, Nx, dx, exact);
#####:  165:    }
```

Preparing for Refactoring – get baselines

- Call to upwind15 not exercised
- Run ./heat alg="upwind15" runame="upwind_results

```
      -:  143:static bool
    500:  144:update_solution()
      -:  145:{
    500:  146:    if (!strcmp(alg, "ftcs"))
  #####:  147:        return update_solution_ftcs(Nx, curr, last, alpha, dx, dt, bc0, bc1);
    500:  148:    else if (!strcmp(alg, "upwind15"))
    500:  149:        return update_solution_upwind15(Nx, curr, last, alpha, dx, dt, bc0, bc1);
  #####:  150:    else if (!strcmp(alg, "crankn"))
  #####:  151:        return update_solution_crankn(Nx, curr, last, cn_Amat, bc0, bc1);
  #####:  152:    return false;
    500:  153:}
      -:  154:
```

- We have baselines for ftcs and upwind

```
ahilya:clean dubey$ ls ftcs_results/
clargs.out                    ftcs_results_soln_00000.curve   ftcs_results_soln_final.curve
ahilya:clean dubey$ ls upwind_results/
clargs.out                    upwind_results_soln_00000.curve upwind_results_soln_final.curve
ahilya:clean dubey$
```

Refactoring – The starting code

```
extern bool
update_solution_ftcs(int n,
    Double *curr, Double const *last,
    Double alpha, Double dx, Double dt,
    Double bc_0, Double bc_1);

extern bool
update_solution_upwind15(int n,
    Double *curr, Double const *last,
    Double alpha, Double dx, Double dt,
    Double bc_0, Double bc_1);

extern bool
update_solution_crankn(int n,
    Double *curr, Double const *last,
    Double const *cn_Amat,
    Double bc_0, Double bc_1);
```

```
if (!strncmp(alg, "crankn", 6))
    initialize_crankn(Nx, alpha, dx, dt, &cn_Amat);
```

- Interfaces are not identical
- crankn has an extra argument
- It also has an extra step in initialization

Refactoring

- Generalize the interface

```
extern bool
update_solution(int n,
    Double *curr, Double const *last,
    Double alpha, Double dx, Double dt,
    Double const *cn_Amat,
    Double bc_0, Double bc_1);
```

- Modify the makefile

Refactoring

- Generalize the interface

```
extern bool
update_solution(int n,
    Double *curr, Double const *last,
    Double alpha, Double dx, Double dt,
    Double const *cn_Amat,
    Double bc_0, Double bc_1);
```

- Modify the makefile

```
HDR = Double.H
SRC1 = heat.C utils.C args.C exact.C ftcs.C
SRC2 = heat.C utils.C args.C exact.C upwind15.C
SRC3 = heat.C utils.C args.C exact.C crankn.C
OBJ1 = $(SRC1:.C=.o)
OBJ2 = $(SRC2:.C=.o)
OBJ3 = $(SRC3:.C=.o)

EXE1 = heat1
EXE2 = heat2
EXE3 = heat3
```

IDEAS productivity
ECP EXASCALE COMPUTING PROJECT

Refactoring

- Generalize the interface

```
extern bool
update_solution(int n,
    Double *curr, Double const *last,
    Double alpha, Double dx, Double dt,
    Double const *cn_Amat,
    Double bc_0, Double bc_1);
```

```
HDR = Double.H
SRC1 = heat.C utils.C args.C exact.C ftcs.C
SRC2 = heat.C utils.C args.C exact.C upwind15.C
SRC3 = heat.C utils.C args.C exact.C crankn.C
OBJ1 = $(SRC1:.C=.o)
OBJ2 = $(SRC2:.C=.o)
OBJ3 = $(SRC3:.C=.o)

EXE1 = heat1
EXE2 = heat2
EXE3 = heat3
```

- Modify the makefile
- Add null implementations of initialize_crank in ftcs and upwind15

Refactoring

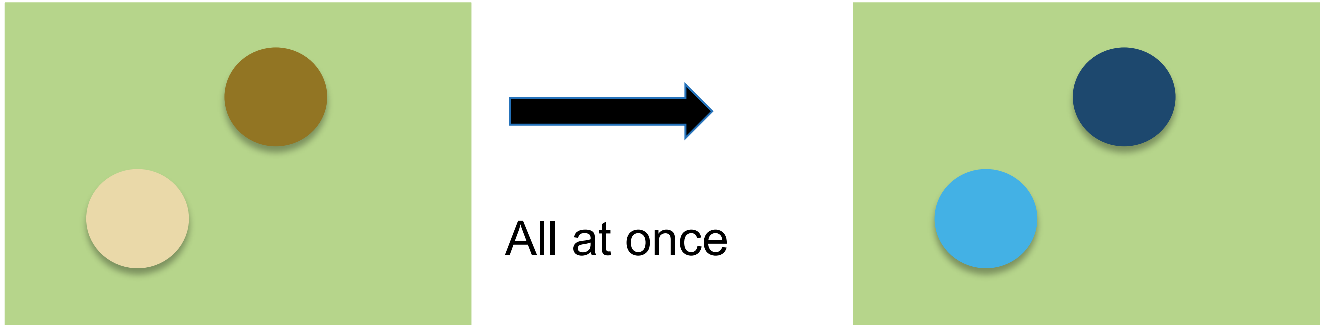
```
void
initialize_crankn(int n,
    Double alpha, Double dx, Double dt,
    Double **_cn_Amat)
{
}

bool
update_solution(int n, Double *curr, Double const *last,
    Double alpha, Double dx, Double dt,
    Double const *cn_Amat,
    Double bc_0, Double bc_1)
{
    Double const f2 = 1.0/24;
    Double const f1 = 1.0/6;
    Double const f0 = 1.0/4;
    Double const k = alpha * alpha * dt / (dx * dx);
    Double const k2 = k*k;
```

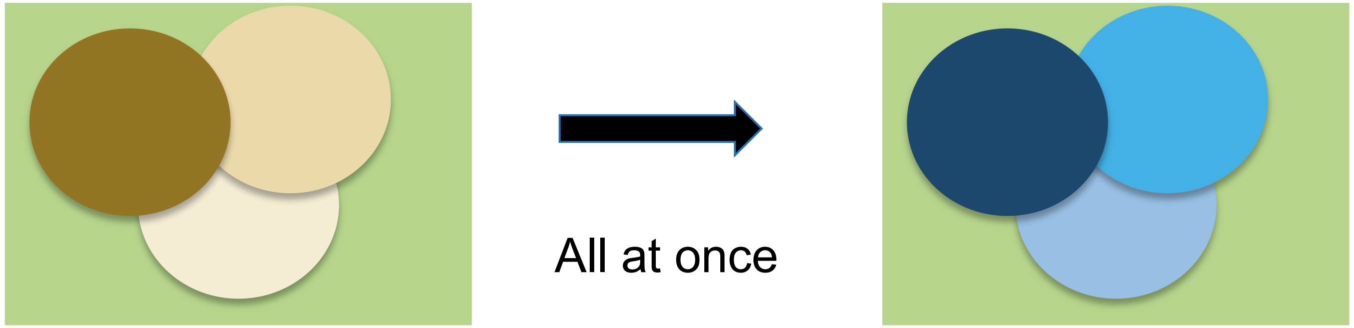
- make heat1
- Run ./heat runame="ftcs_results"
- Make heat2
- Run ./heat runame="upwind_results"
- Verify against baselines

Map from Here to There: On ramp plan

Proportionate to the scope

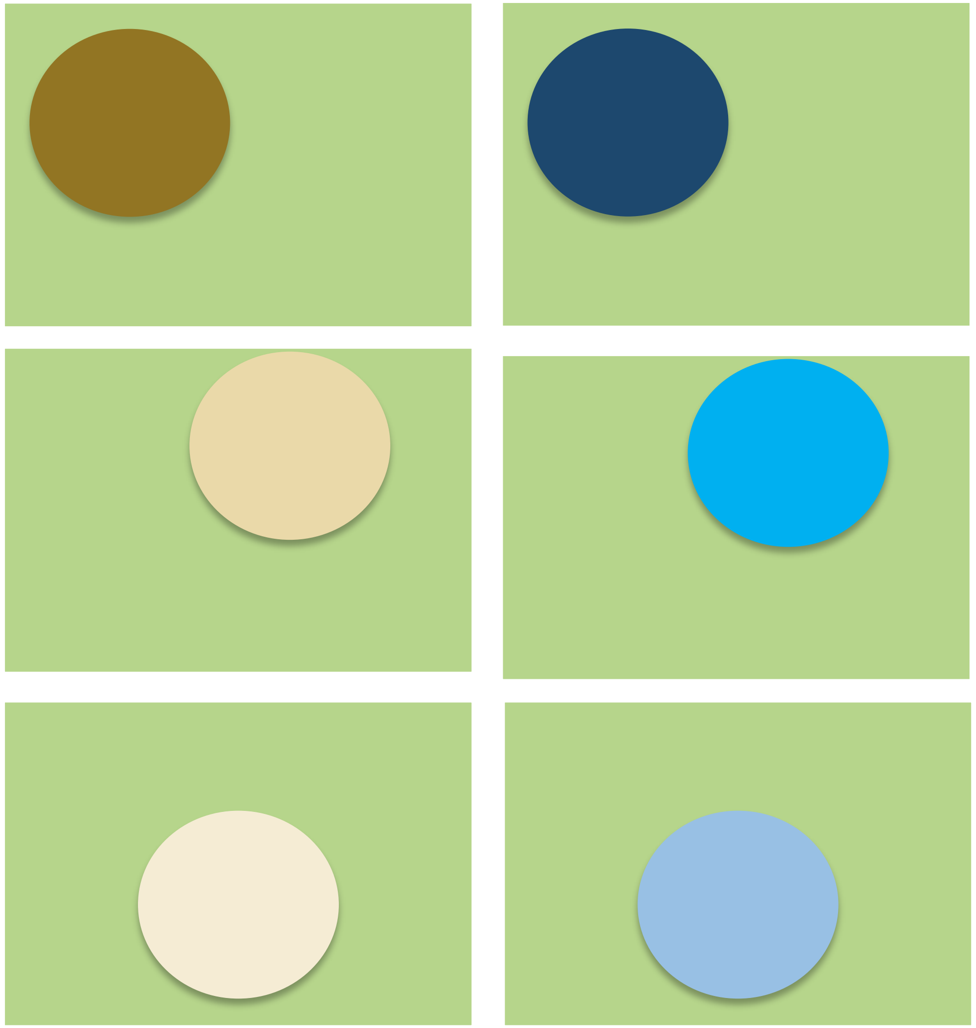


Scattered independent changes - May be OK



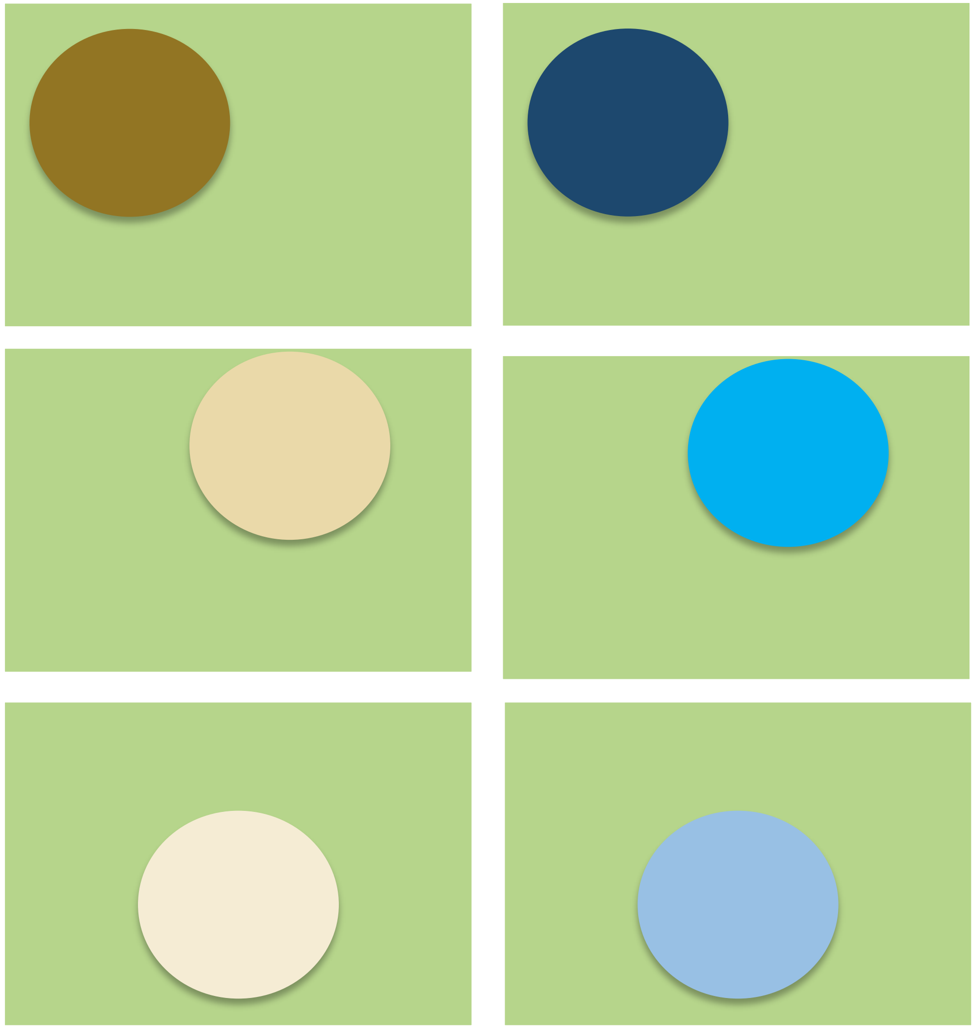
Invasive large-scale change in the code - Bad idea

Map from Here to There: On ramp plan1



- Turn off all modules except for the one being refactored.
- Have a way of testing in intermediate stages
- Do this for all modules that need refactoring independently

Map from Here to There: On ramp plan1



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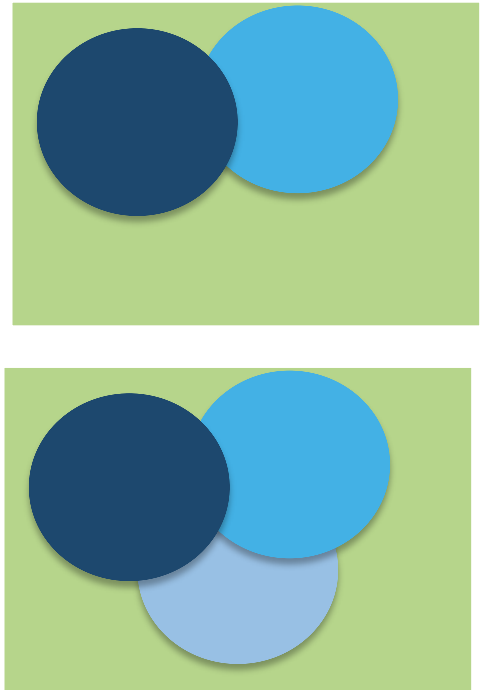
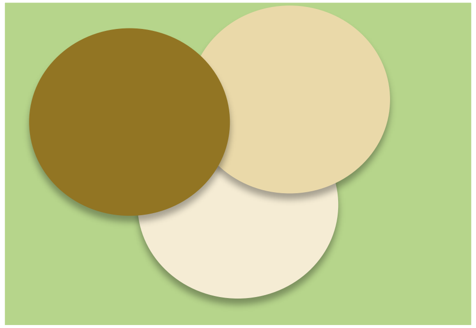
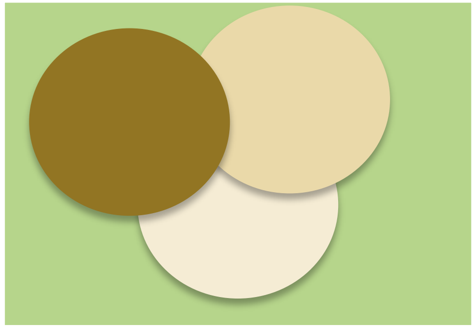


- One by one turn on more than one refactored module

Map from Here to There: On ramp plan2

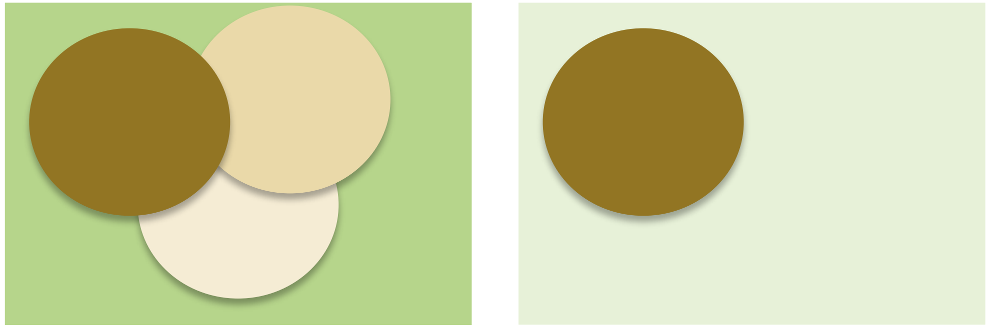


Map from Here to There: On ramp plan2



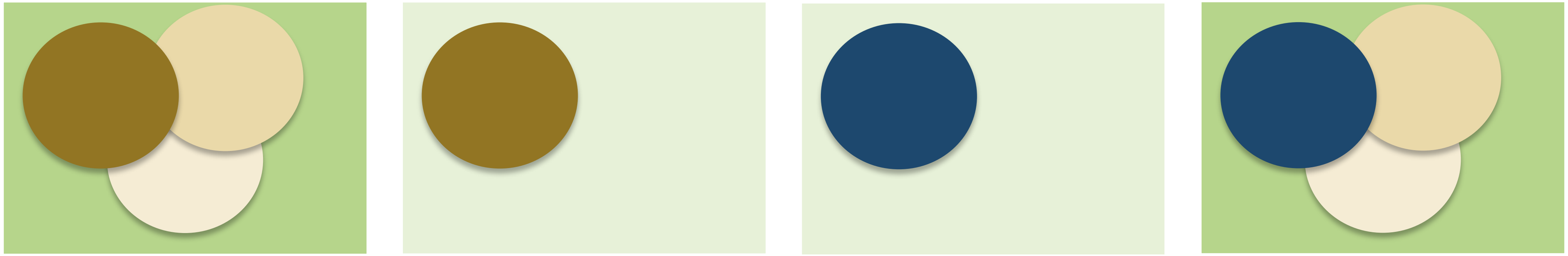
- Build a separate environment for testing refactored module

Map from Here to There: On ramp plan2



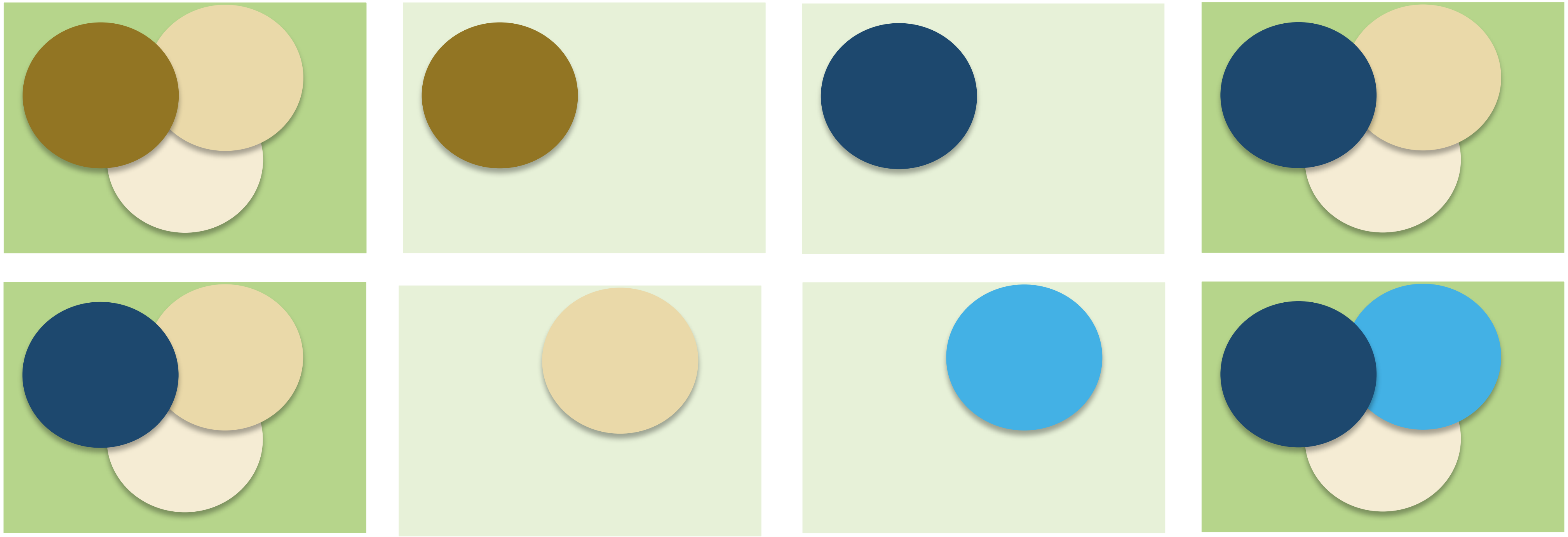
- Build a separate environment for testing refactored module
- Copy over the module in this isolated environment

Map from Here to There: On ramp plan2



- Build a separate environment for testing refactored module
- Copy over the module in this isolated environment
- Put back refactored module

Map from Here to There: On ramp plan2



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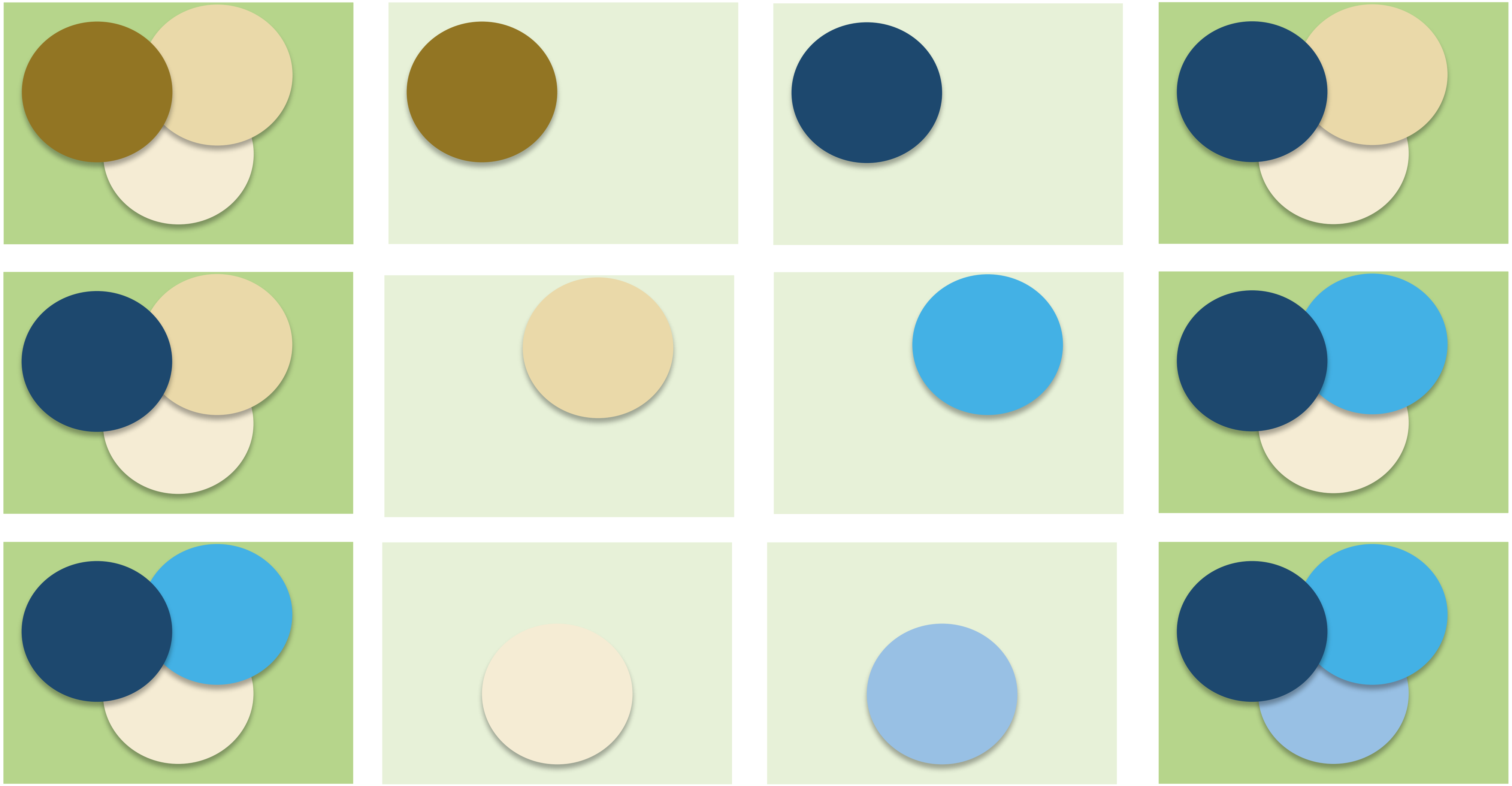

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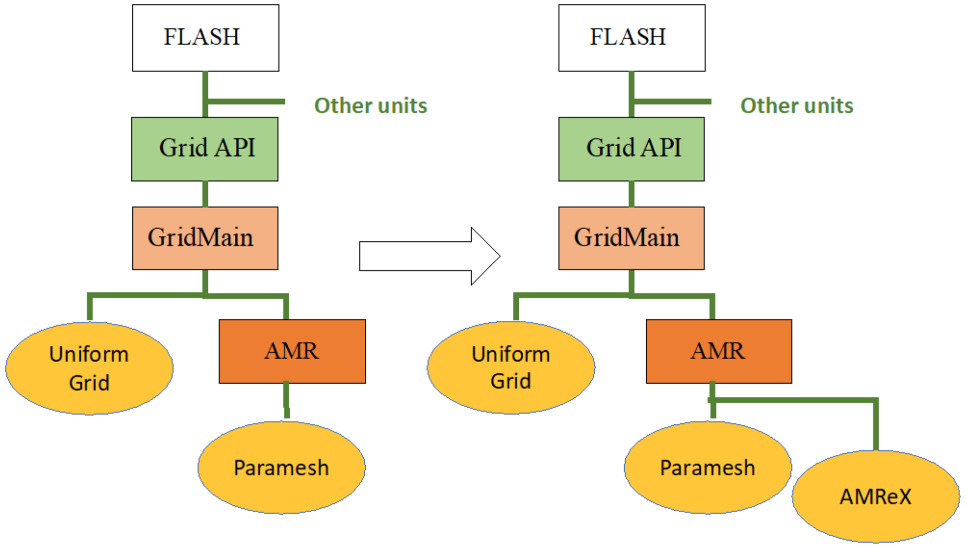
A Real-World Example: FLASH to Flash-X

Refactoring to supporting a different AMR library

Goal: Replace Paramesh with AMReX

Plan: Getting there from here
- On ramping
- Design
- Intermediate steps
- Realizing the goal



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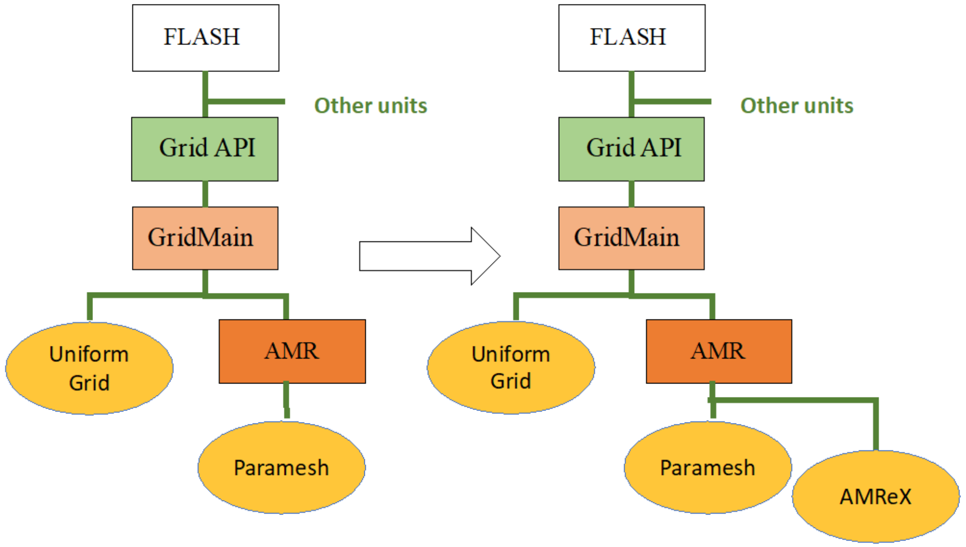
Refactoring to supporting a different AMR library

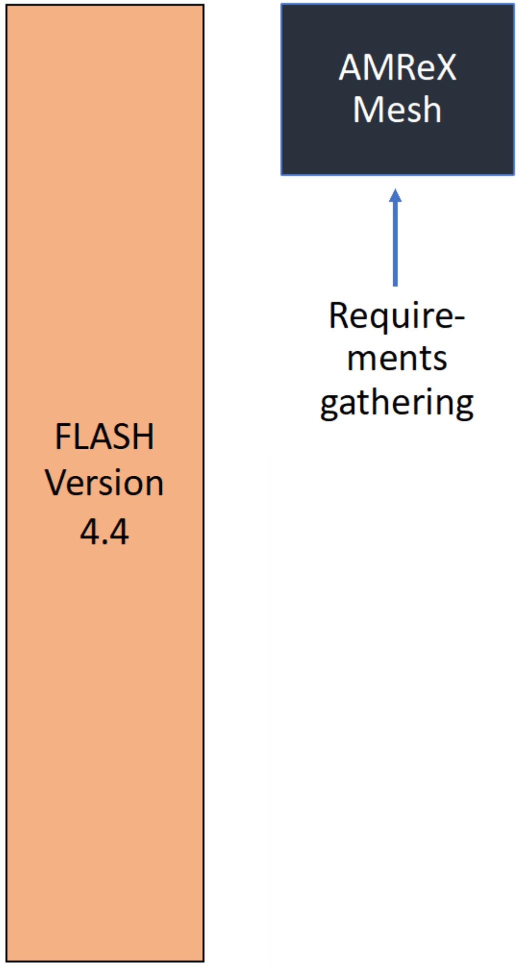
Goal: Replace Paramesh with AMReX

Plan: Getting there from here
- On ramping
- Design
- Intermediate steps
- Realizing the goal

- Cost estimation
  - 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



Steps in the Flash-X Refactoring : a mix of strategies



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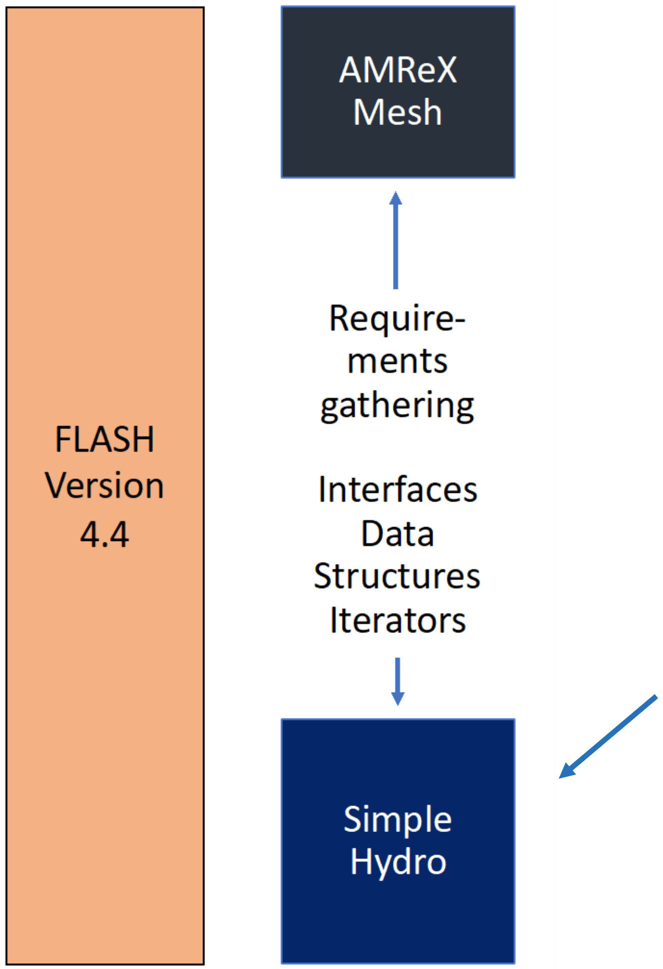
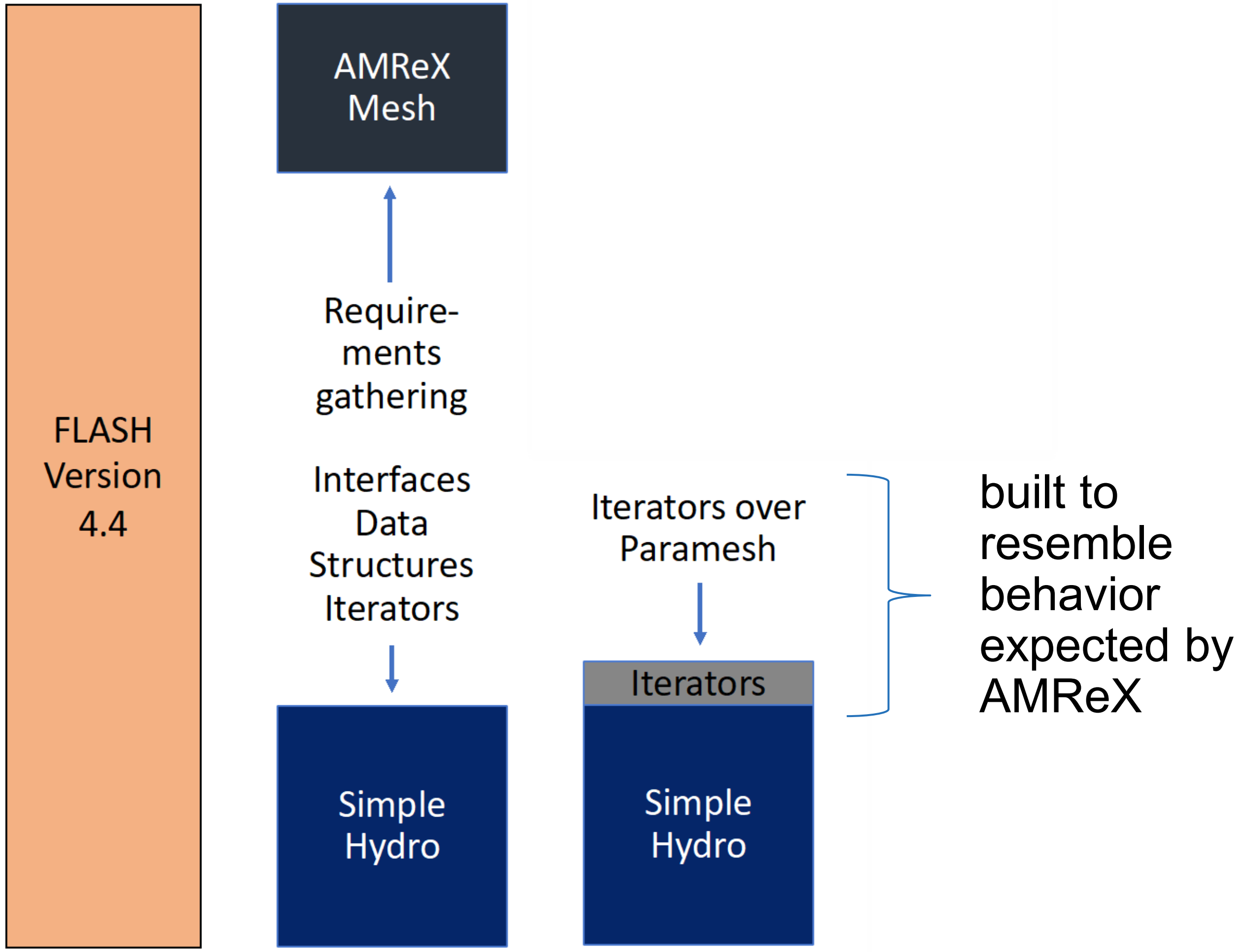
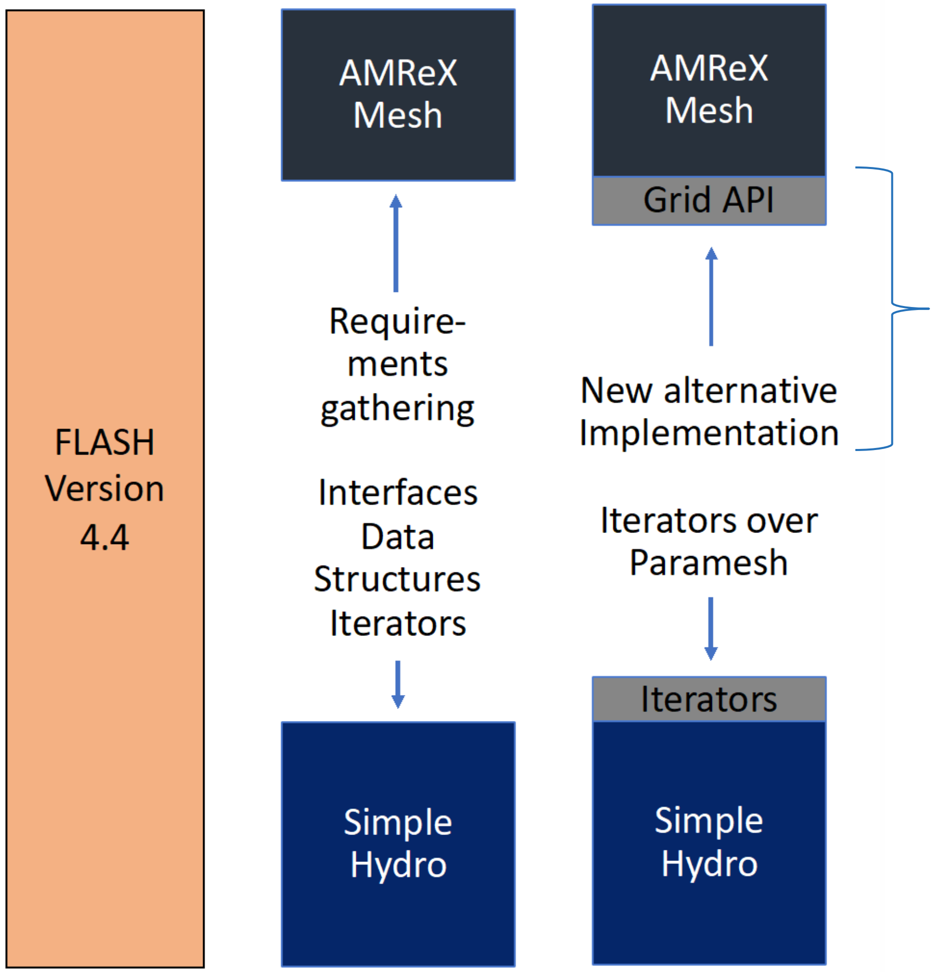


Part of a simpler environment for refactoring and testing

Steps in the Process

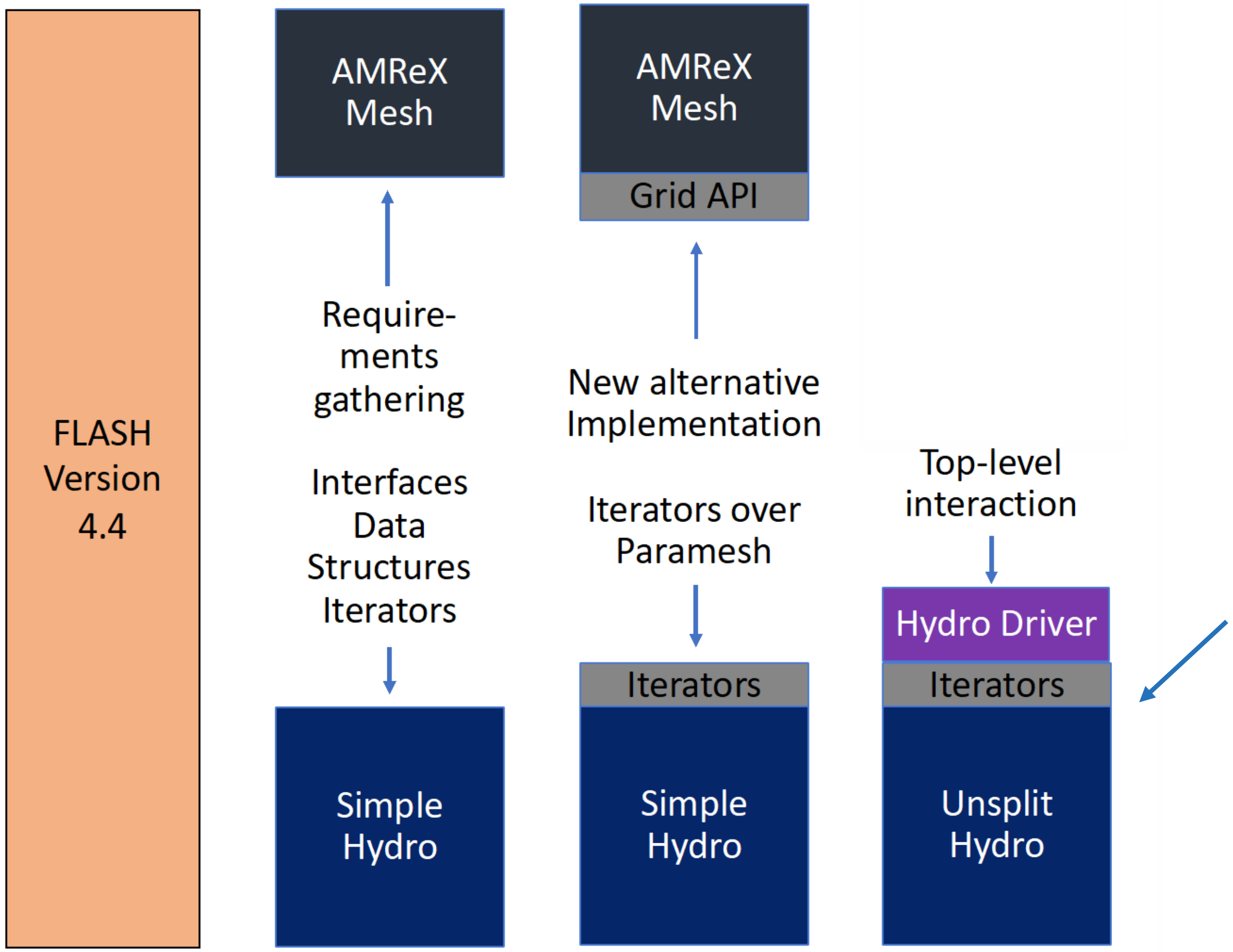


Steps in the Process



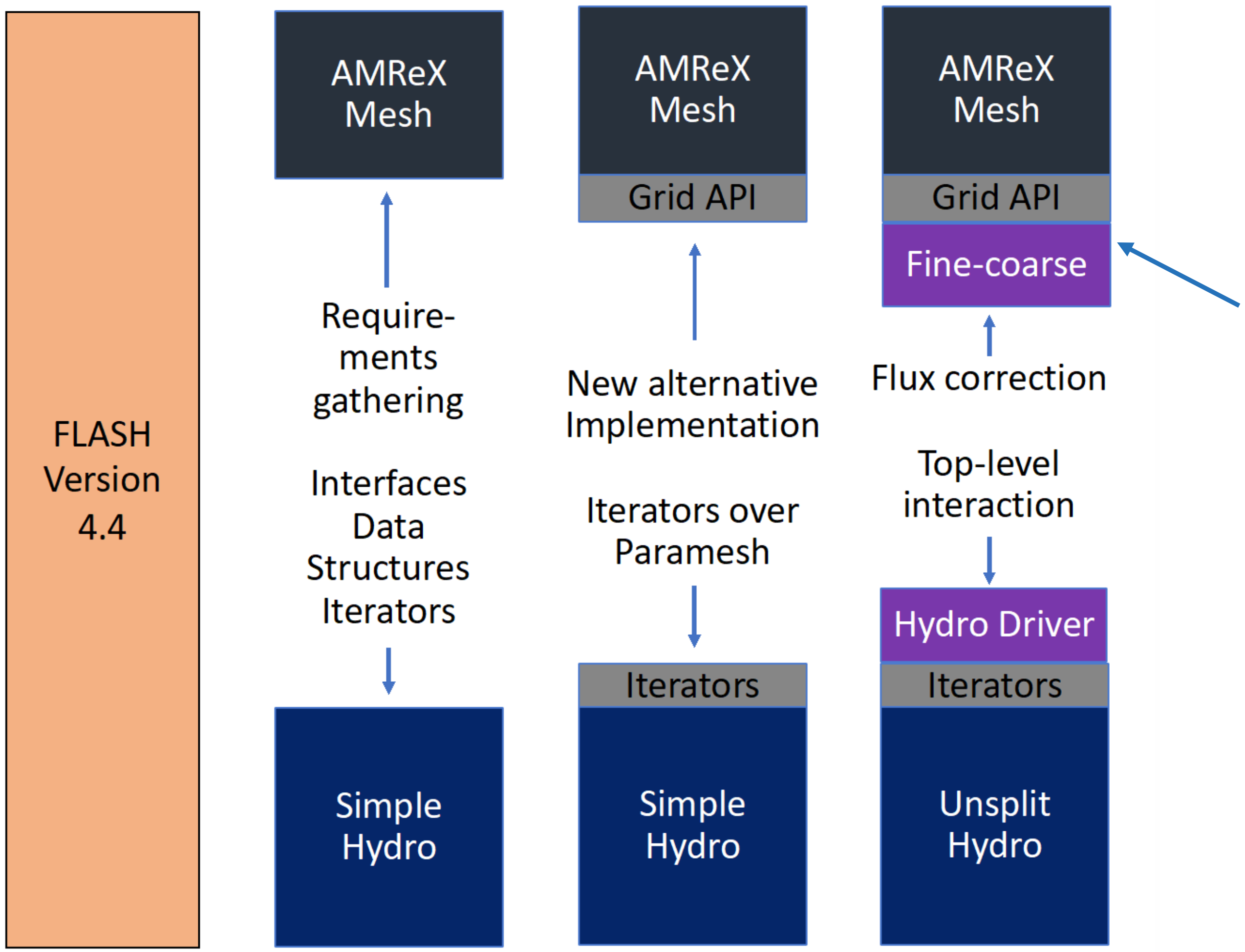
Refactored Grid interface made compatible with AMReX

Steps in the Process



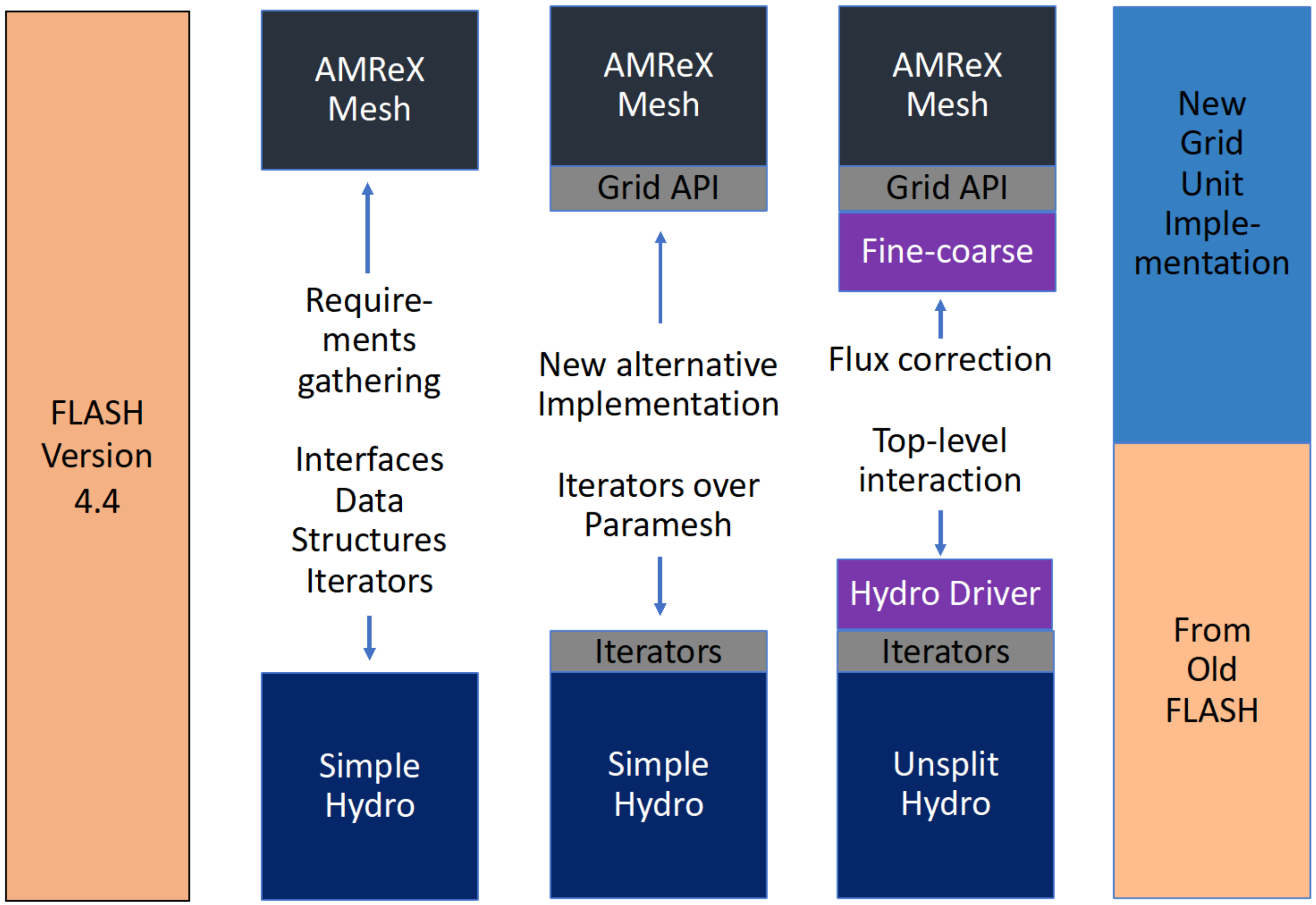
Bring back the real environment but turn off some features related to AMR

Steps in the Process



Turn on all AMR features needed in the final stage

Steps in the Process



To Have a Good Outcome from Refactoring

1. Know why
2. Know how much
3. Know the cost
4. Plan
5. Have strong testing and verification
6. Get buy-in from stakeholders