PROGRAMMING ABSTRACTIONS FOR ORCHESTRATION OF HPC SCIENTIFIC COMPUTING

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SETTING THE STAGE

What should my ideal computational tool do?

Everything really.

- Scan my brain
- Figure out what I want
- Scan the literature
- Figure out the equations
- Auto-generate the code
- Run it
- Analyze the data

I am happy to present the results.

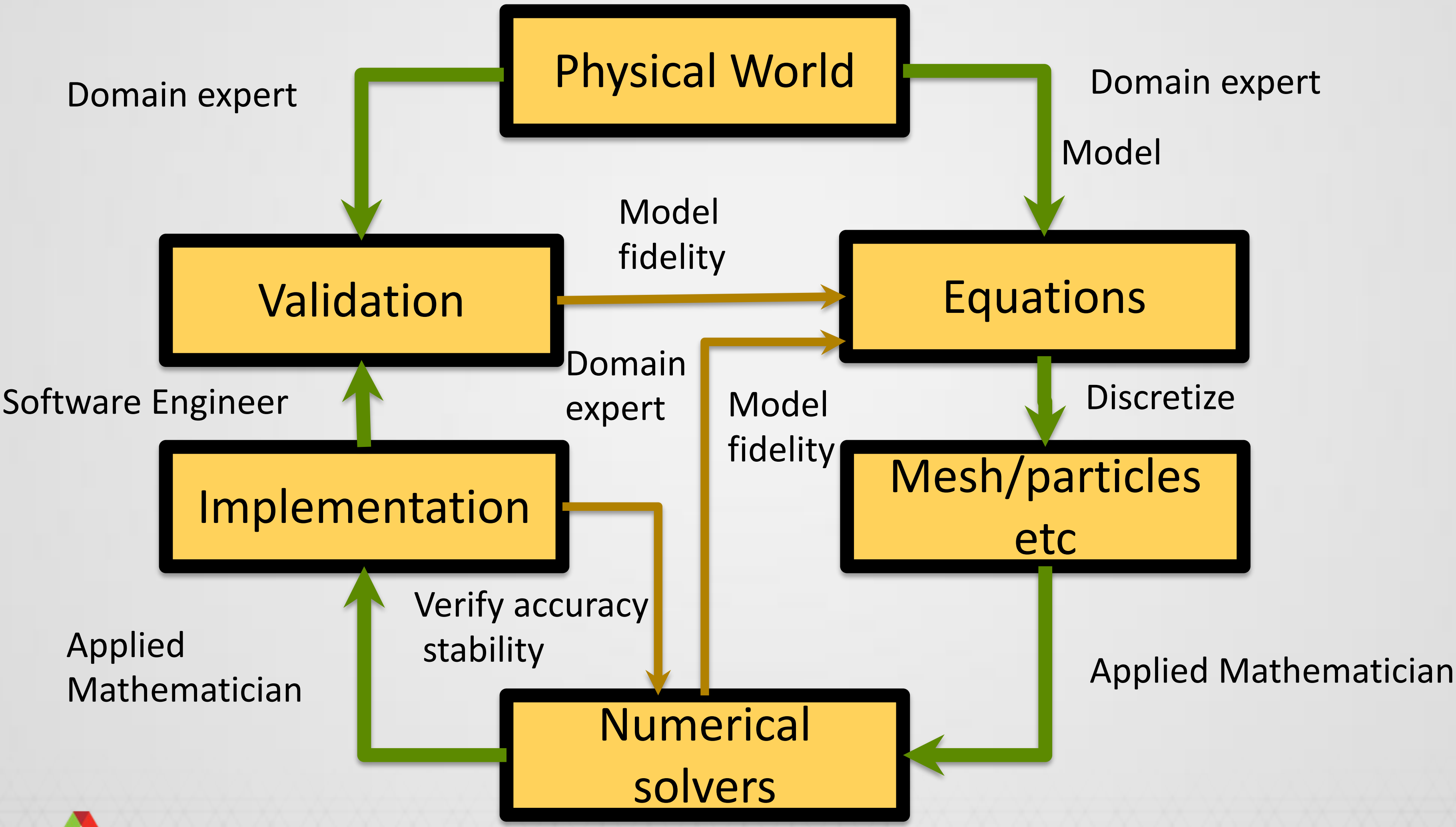
SETTING THE STAGE

Since programming models and other tools are not so obliging, let me reduce the complexity by several orders of magnitude.

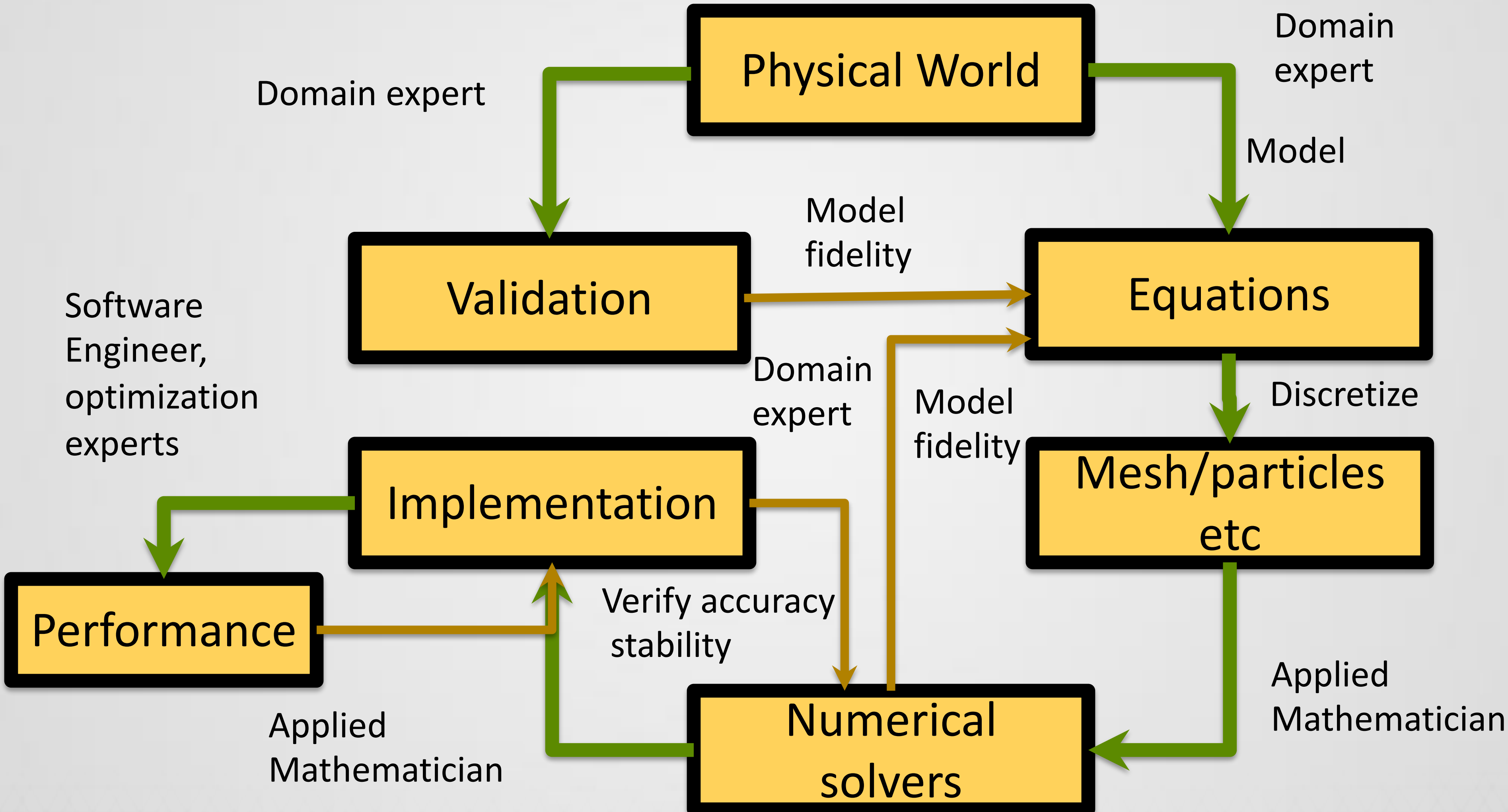
If we were starting a new multiphysics exascale software project today, that expects to have long term use for scientific discovery, how should we design the software?

Chapel designers seem to think the way I do. I like the abstractions and the design, let me explain why.

SCIENCE CODE DEVELOPMENT



THERE IS MORE



ARCHITECTING SCIENTIFIC CODES

Desirable Characteristics

Extensibility
Most use cases need additions and/or customizations

Portability
Even the same generation platforms are different

Performance
All machines need to be used well

Maintainability and Verifiability
For credible and reproducible results

ARCHITECTING SCIENTIFIC CODES

Desirable Characteristics

Extensibility
Well defined structure and modules
Encapsulation of functionalities

Portability
General solutions that work without significant manual intervention across platforms

Performance
Spatial and temporal locality of data
Minimizing data movement
Maximizing scalability

Maintainability and Verifiability
Clean code
Documentation
Comprehensive testing

ARCHITECTING SCIENTIFIC CODES

Why it is challenging

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

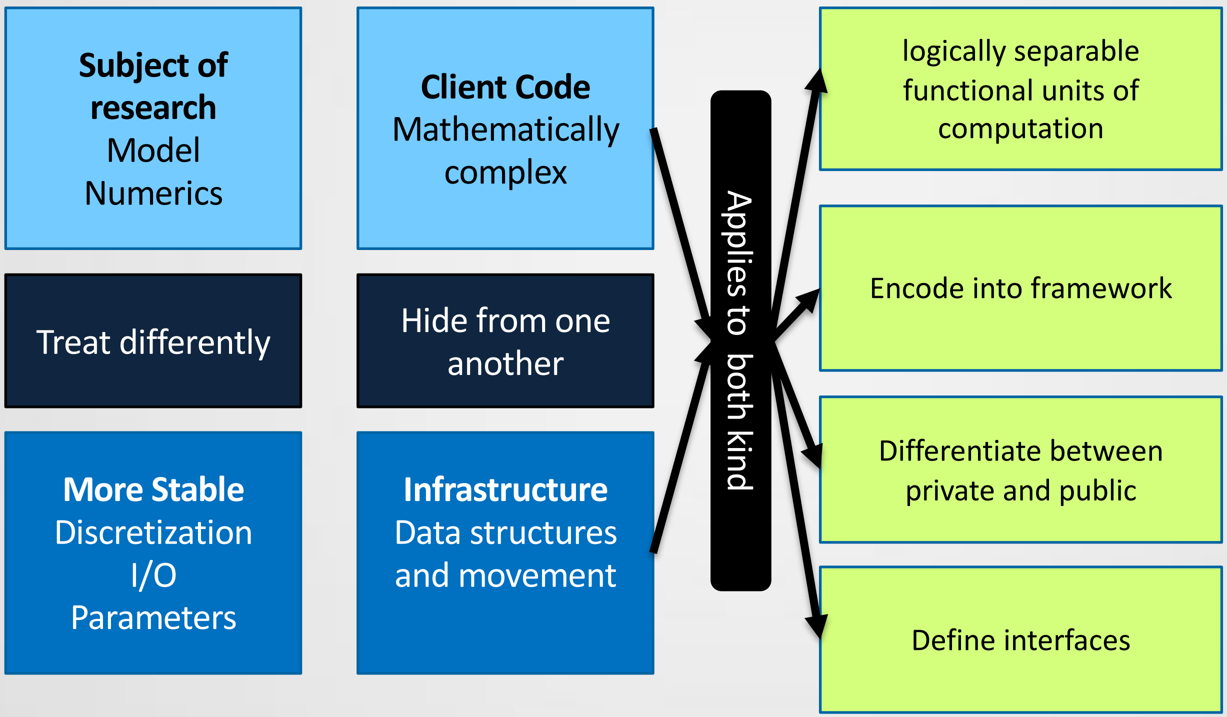
Portability
Tremendous platform heterogeneity
A version for each class of device => combinatorial explosion

Performance
Solvers with low arithmetic intensity but hard sequential dependencies
Proximity and work distribution at cross purposes

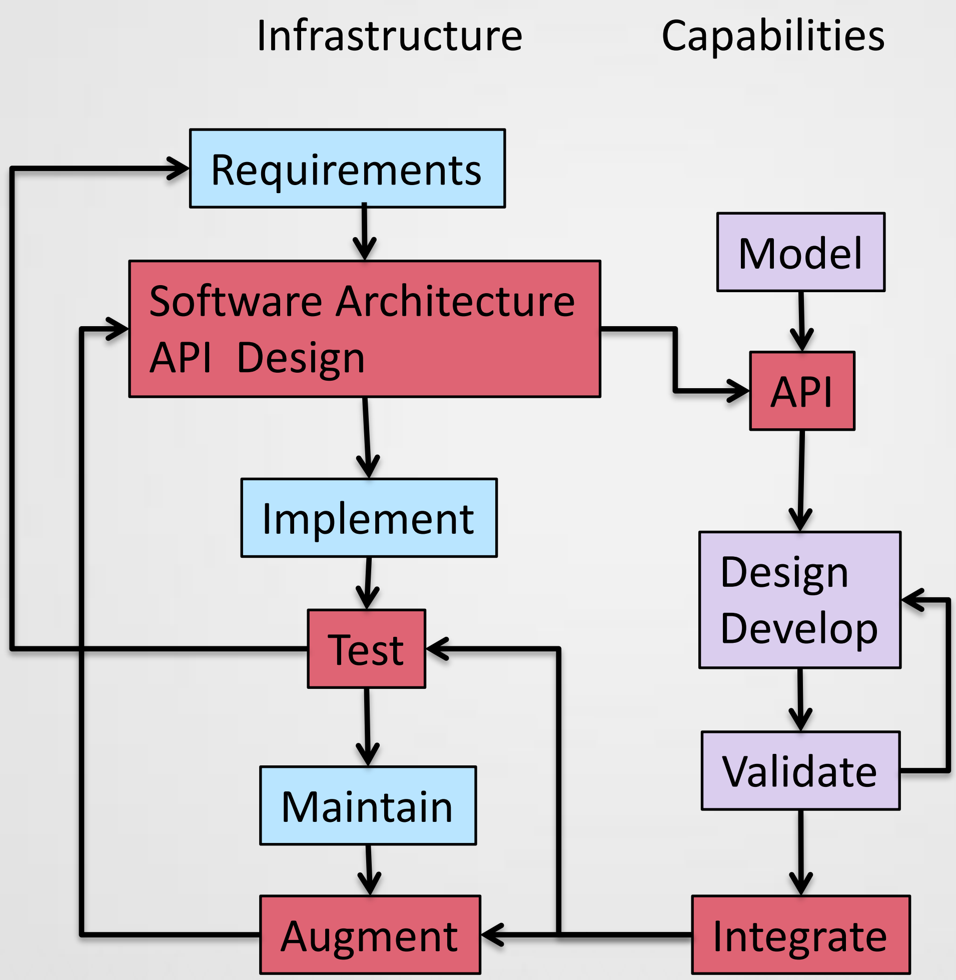
Maintainability and Verifiability
Wrong incentives
Designing good tests is hard

DESIGN APPROACH

Taming the Complexity: Separation of Concerns



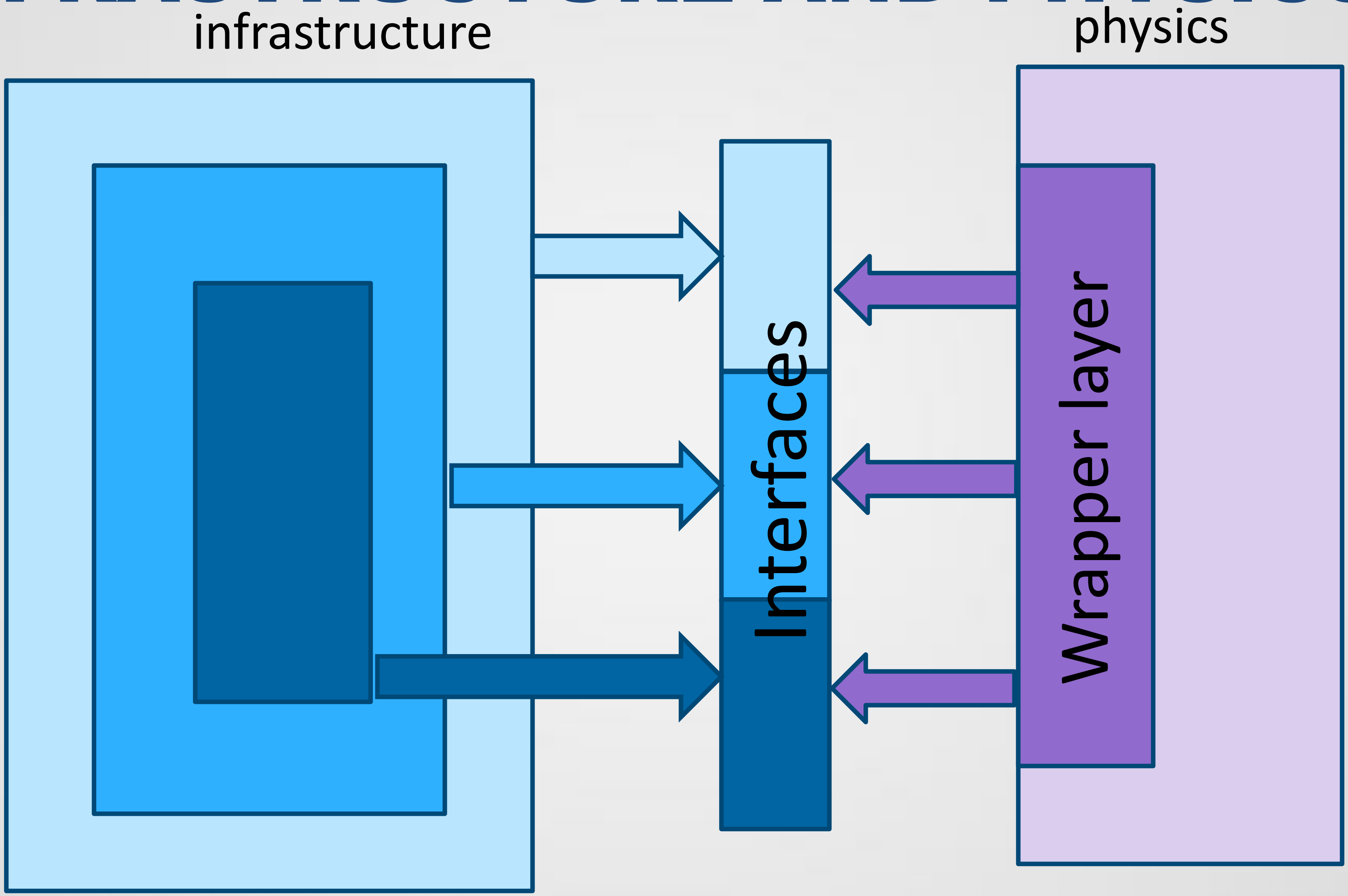
SEPARATION OF CONCERNS



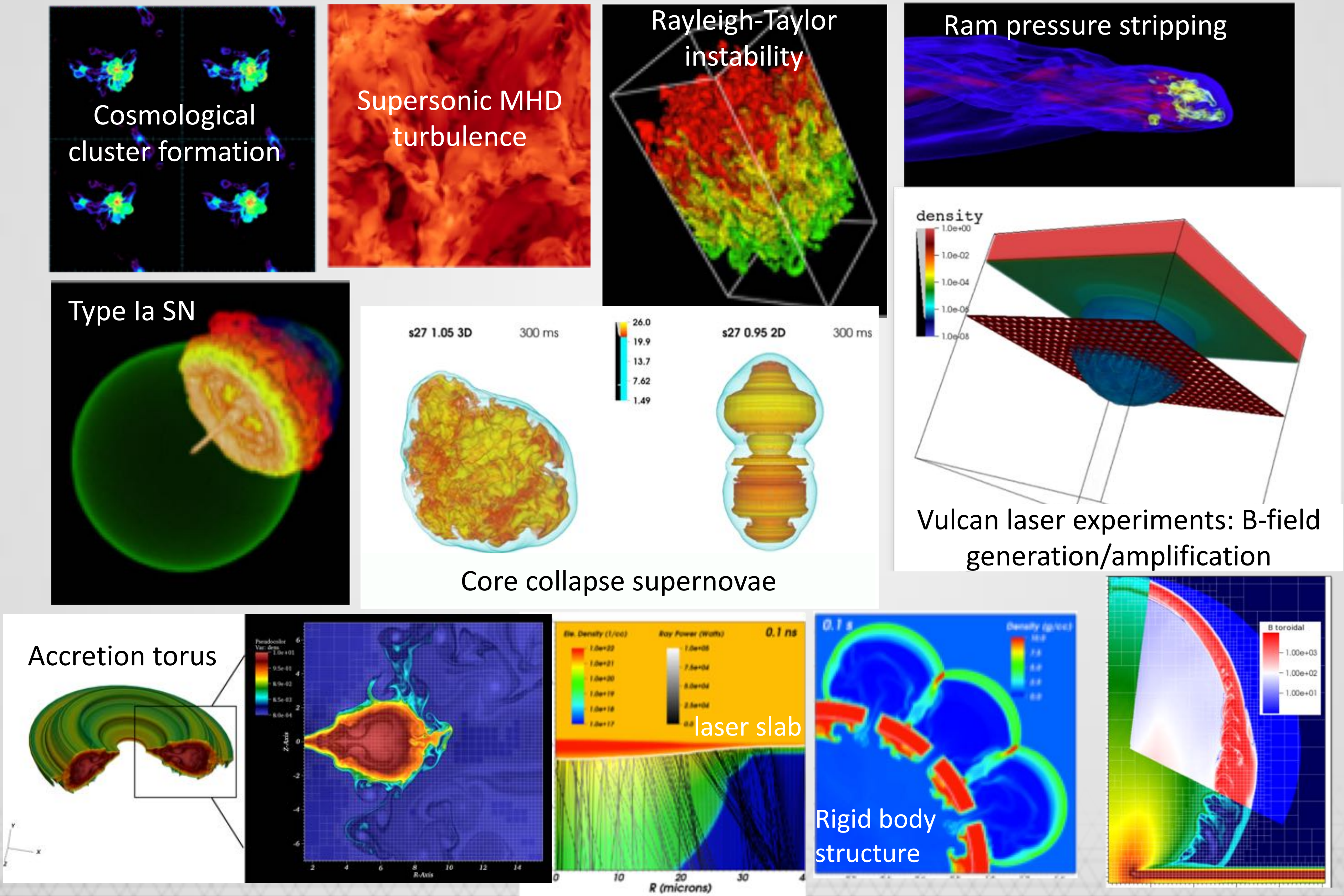
DESIGN PHILOSOPHY

- Infrastructure design
  - Take time to discuss, iterate over requirements and specification
  - Keep end users involved
    - Not doing so leaves possible options on the table
- Simple is better
  - Flexibility Vs transparent to the user
    - Flexibility wins
- Hierarchical access to features

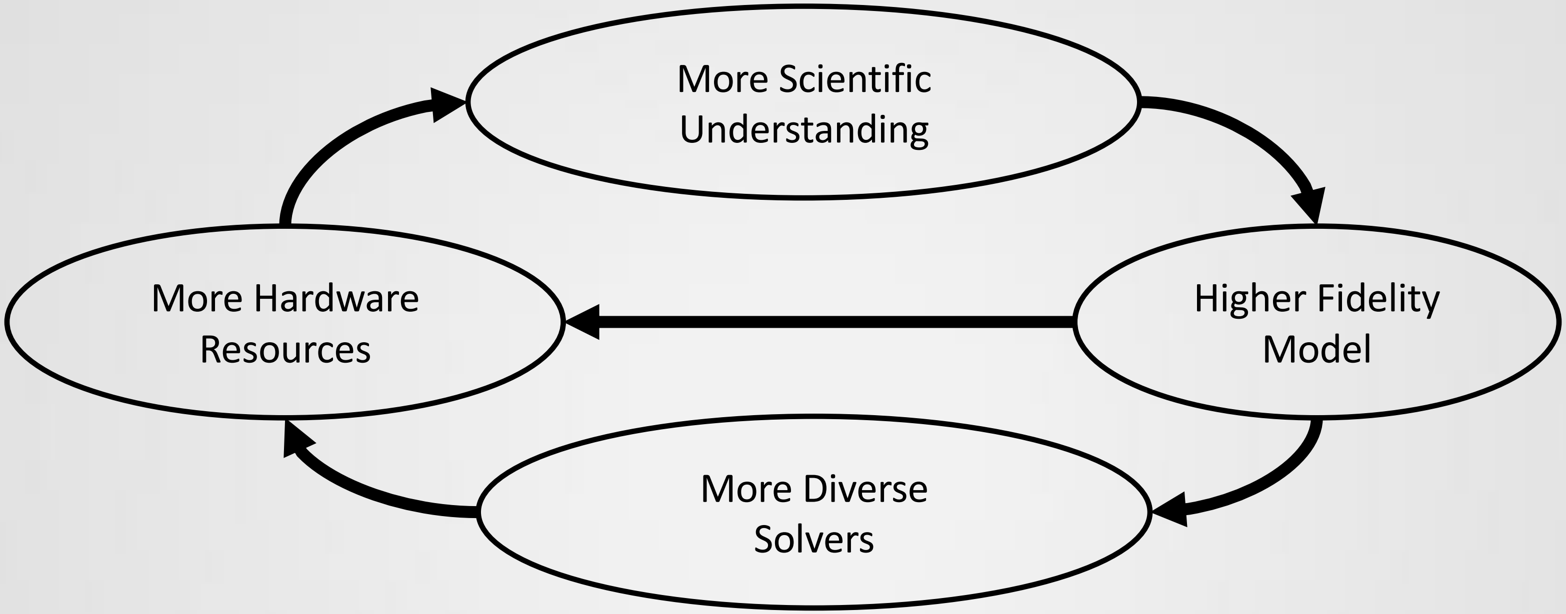
INTERACTION BETWEEN INFRASTRUCTURE AND PHYSICS



Example Software: FLASH



SCIENCE USING FLASH



- ❑ Many components under research
- ❑ Software continuously evolving
- ❑ Compute on expensive, rare resources
- ❑ All use cases are different and unique

FLASH CODE BASICS

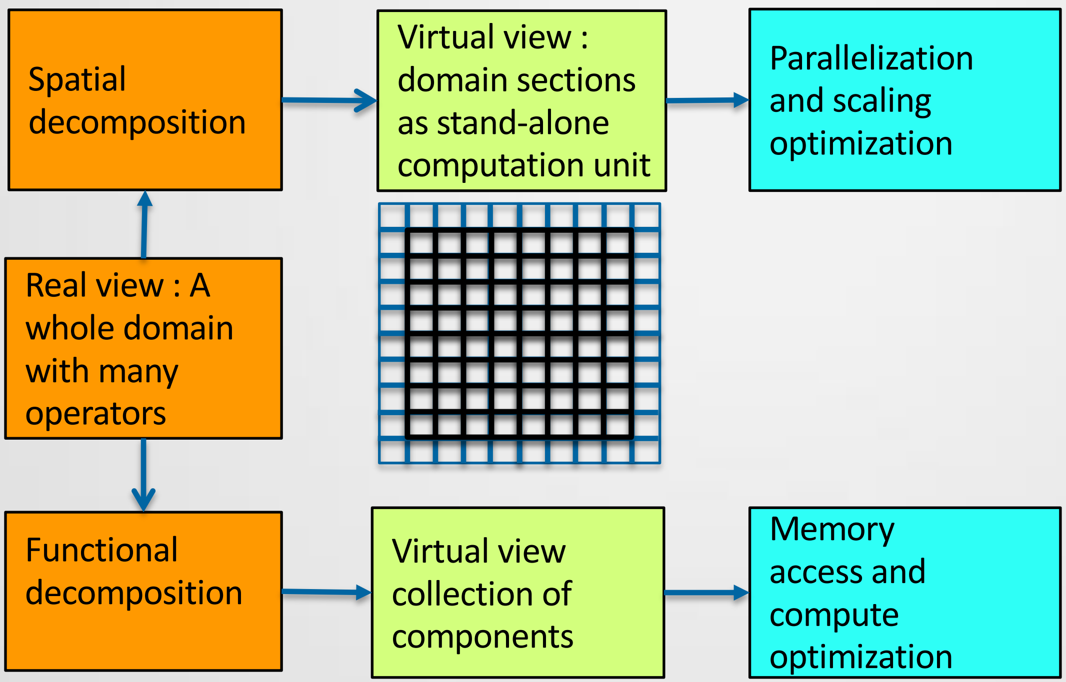
- An application code, composed of encapsulated functional *units*.
  - Units are combined and composed to form applications
  - Not one monolithic binary, each problem has its own distinct binary
- Setup tool (python) parses Config files, picks specific implementations of units and composes full application
  - Units can have alternative implementations
    - Three implementations of mesh are supported
  - Composability implies any of the implementations can be picked
- Mostly Fortran, some C, about 1.5 million lines of code
- Portable, and until recently performance portable

DESIGN CONSIDERATIONS

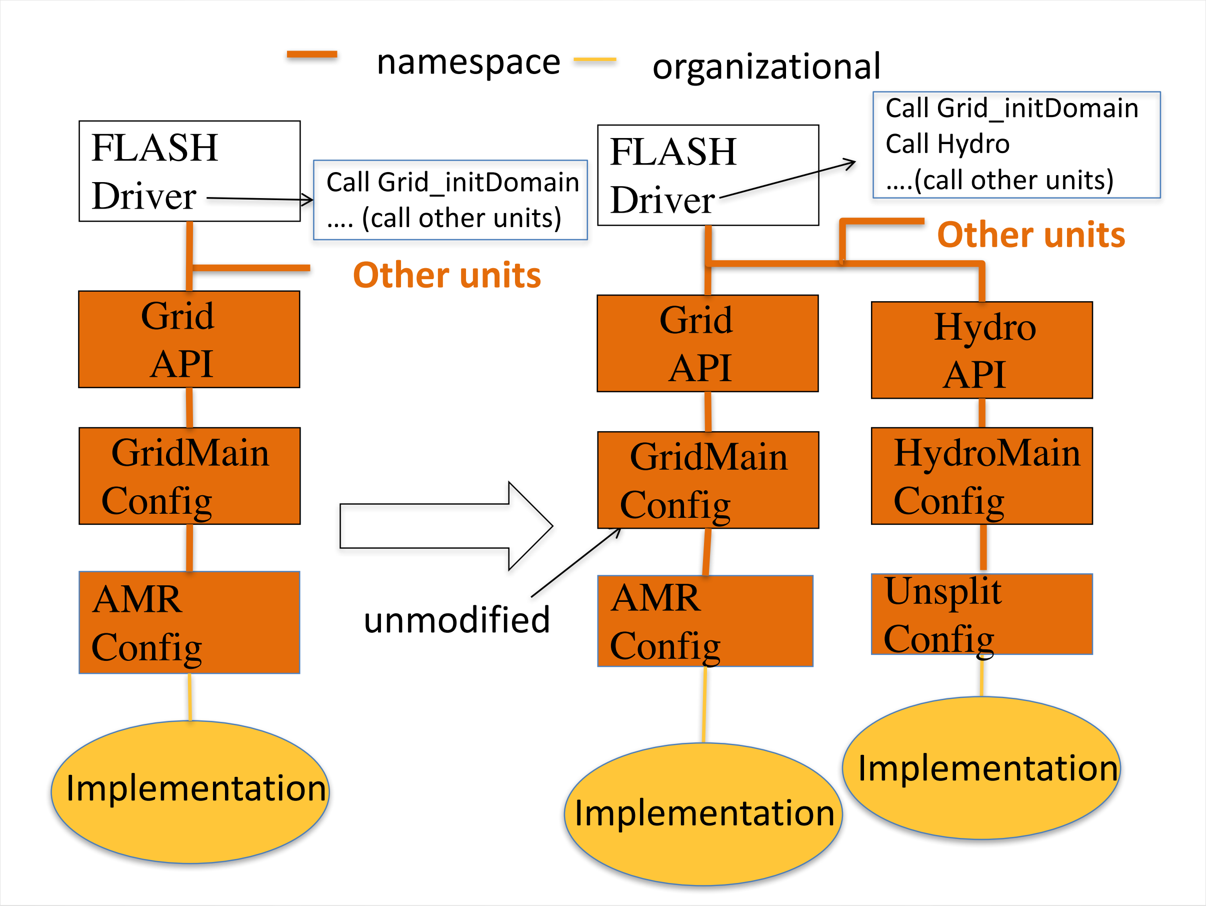
- Encapsulation and interfaces
- Separation of concerns
- Extensibility
- Locality
- Composability
- Orchestration
- Cost accounting

ENCAPSULATION

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

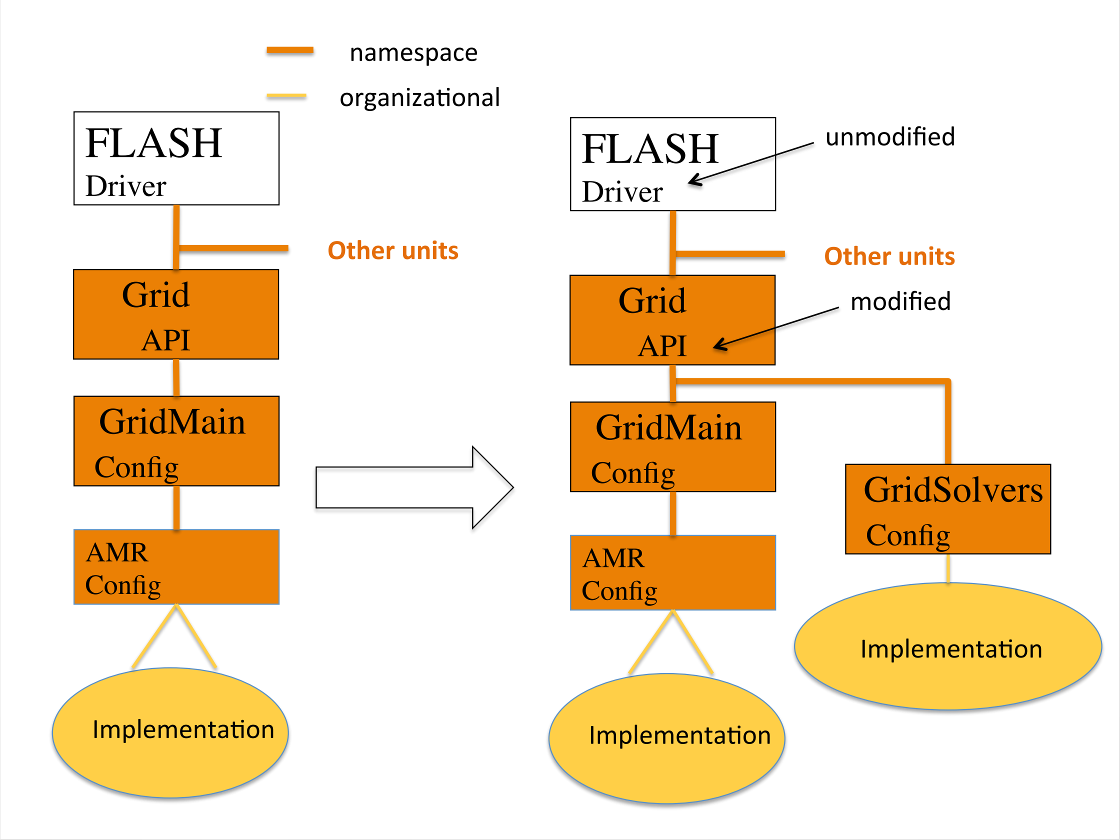


EXTENSIBILITY
ADD A UNIT

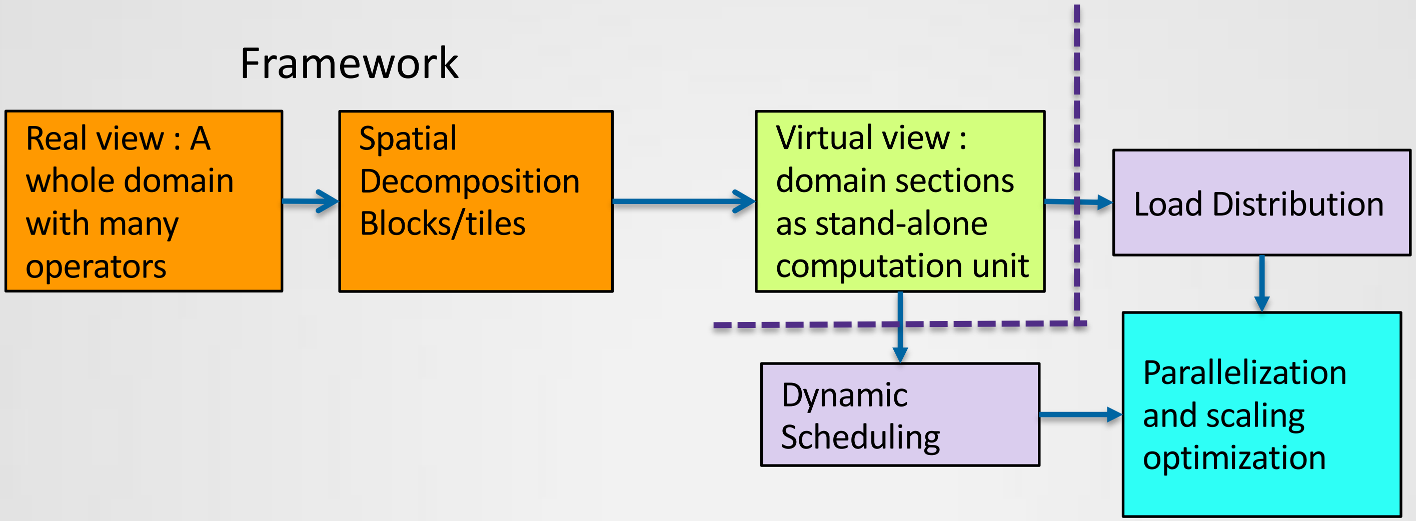


EXTENSIBILITY AND LOCALITY

ADD A SUBUNIT



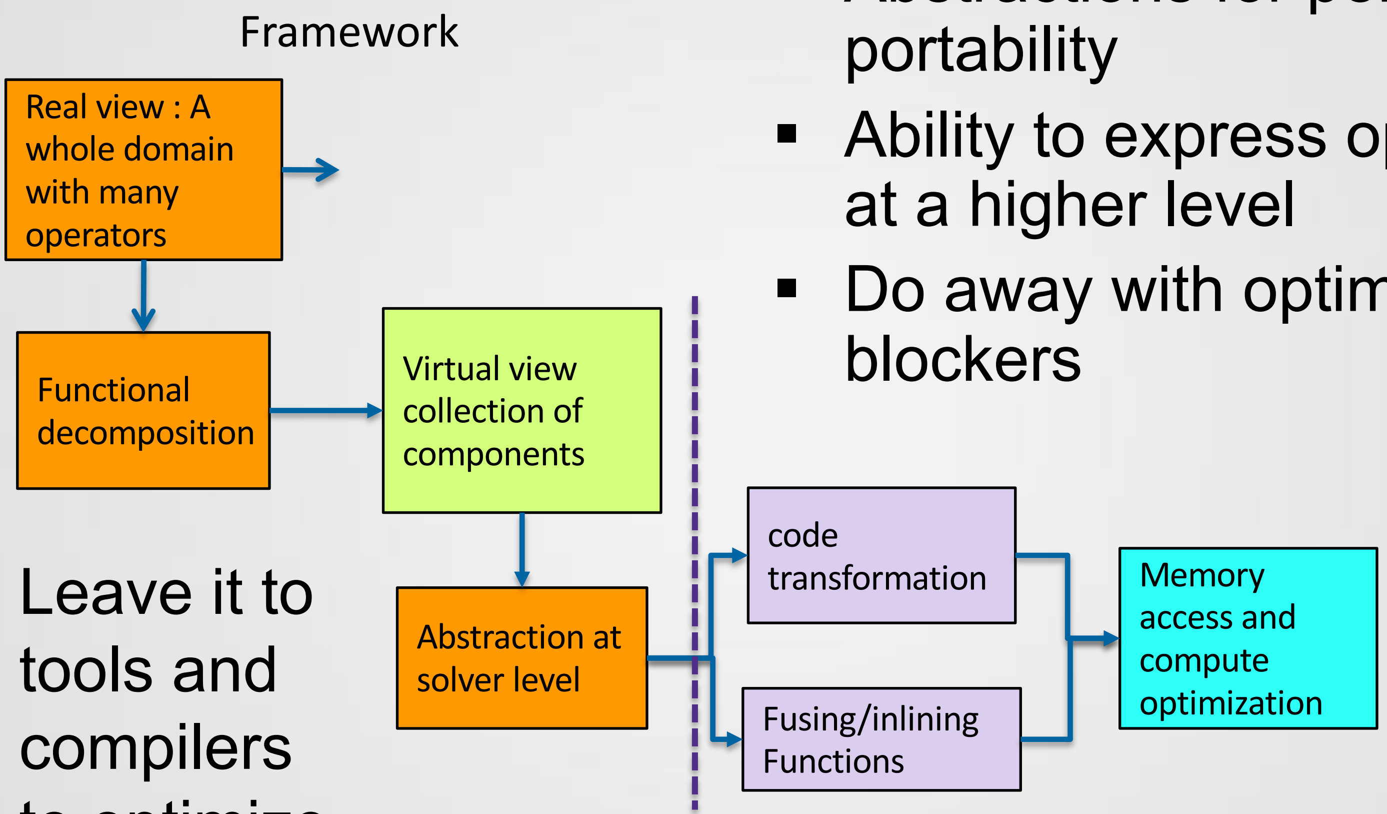
COMPOSABILITY



- AMR infrastructure: refinement, load balancing, work redistribution
- Meta-information about domain sections
- Asynchronization at block and operator level
- No kernel optimization in this part

COMPOSITION

- Abstractions for performance portability
- Ability to express operations at a higher level
- Do away with optimization blockers



- Leave it to tools and compilers to optimize

CODE TRANSFORMATION

- Two different scopes
  - The usual one
    - Write code once, generate ”optimized” code for the target
    - Down at the level of loop nests or kernels
      - Best done for limited scope computations
    - We intend to use transpiler being developed by collaborators
    - Turns IR into constrained python, optimized code generated from there.
  - The not so usual one
    - High level orchestration of operators
    - Determined during application configuration
    - Communicated to the runtime in part

ORCHESTRATION SYSTEM

- Task composer – used for configuration
  - Extension of the original FLASH “Config” files
  - A configuration DSL
  - Encode meta-information for application construction in FLASH-specific syntax as needed

A primer on how FLASH framework configures application.

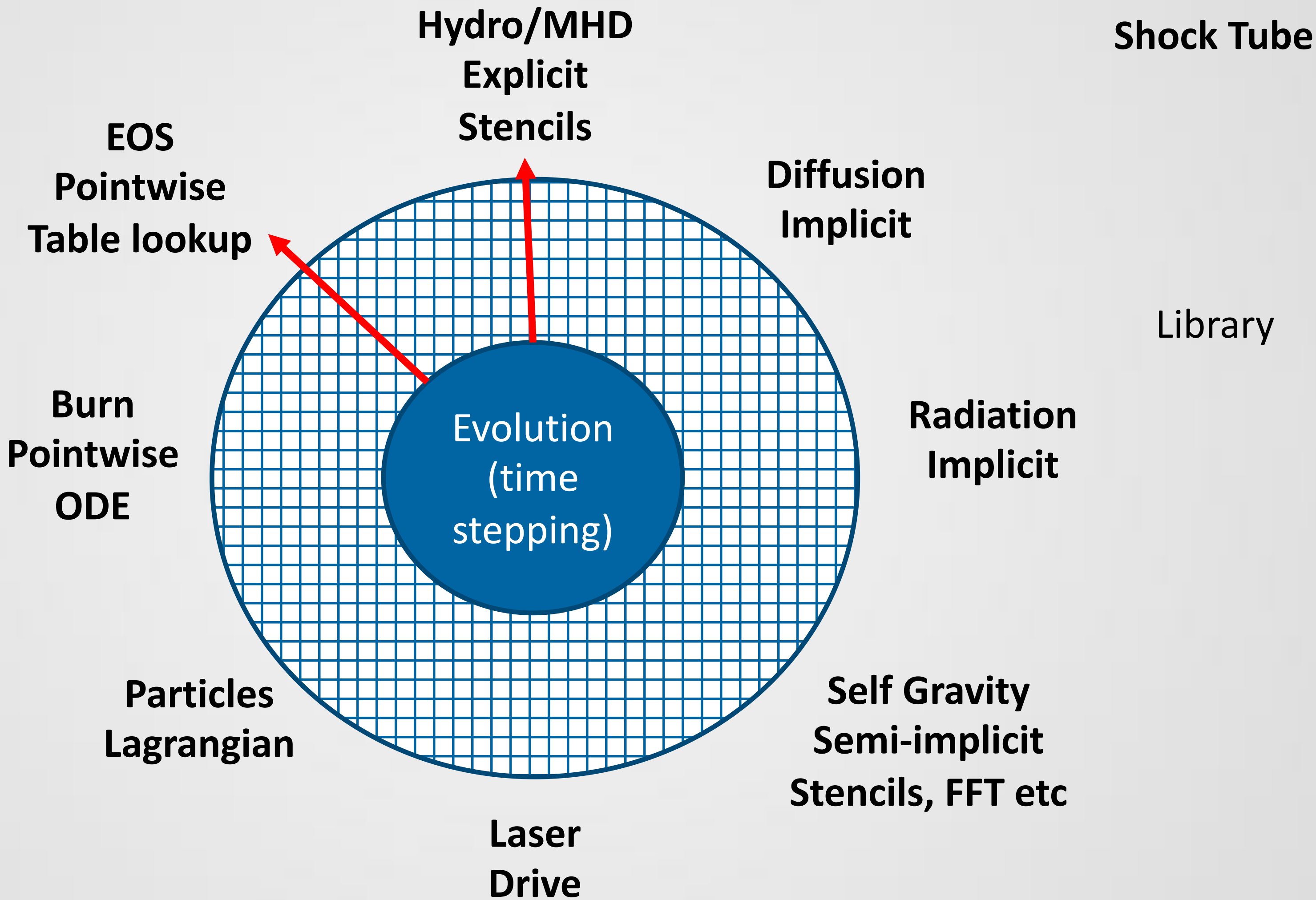
CONFIG FILES

```
REQUIRES Driver
REQUIRES physics/Hydro
REQUIRES physics/Eos/EosMain/Helmholtz
REQUIRES physics/sourceTerms/Burn/BurnMain/nuclearBurn
REQUIRES Simulation/SimulationComposition

PARAMETER xhe4       REAL   0.0 [0.0 to 1.0]
PARAMETER xc12       REAL   1.0 [0.0 to 1.0]
PARAMETER xo16       REAL   0.0 [0.0 to 1.0]
```

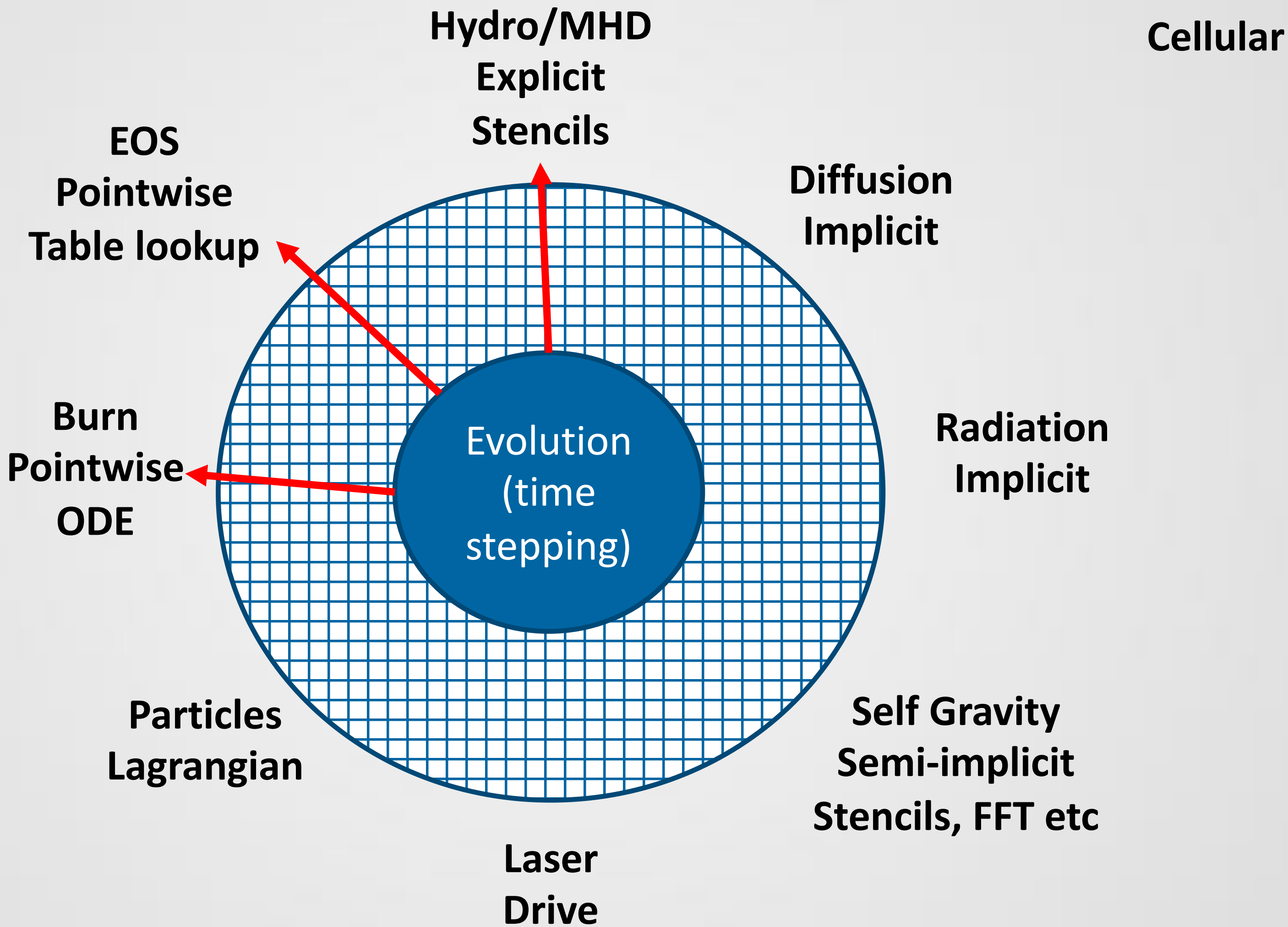
- Can exist anywhere in the directory structure
- Encode all meta-information for that level
  - Unit dependencies
  - State variables needed
  - State variables that need reconciliation at fine-coarse boundaries
  - Runtime environment

CONFIGURATION



Dubey et al, Parallel Computing 2009

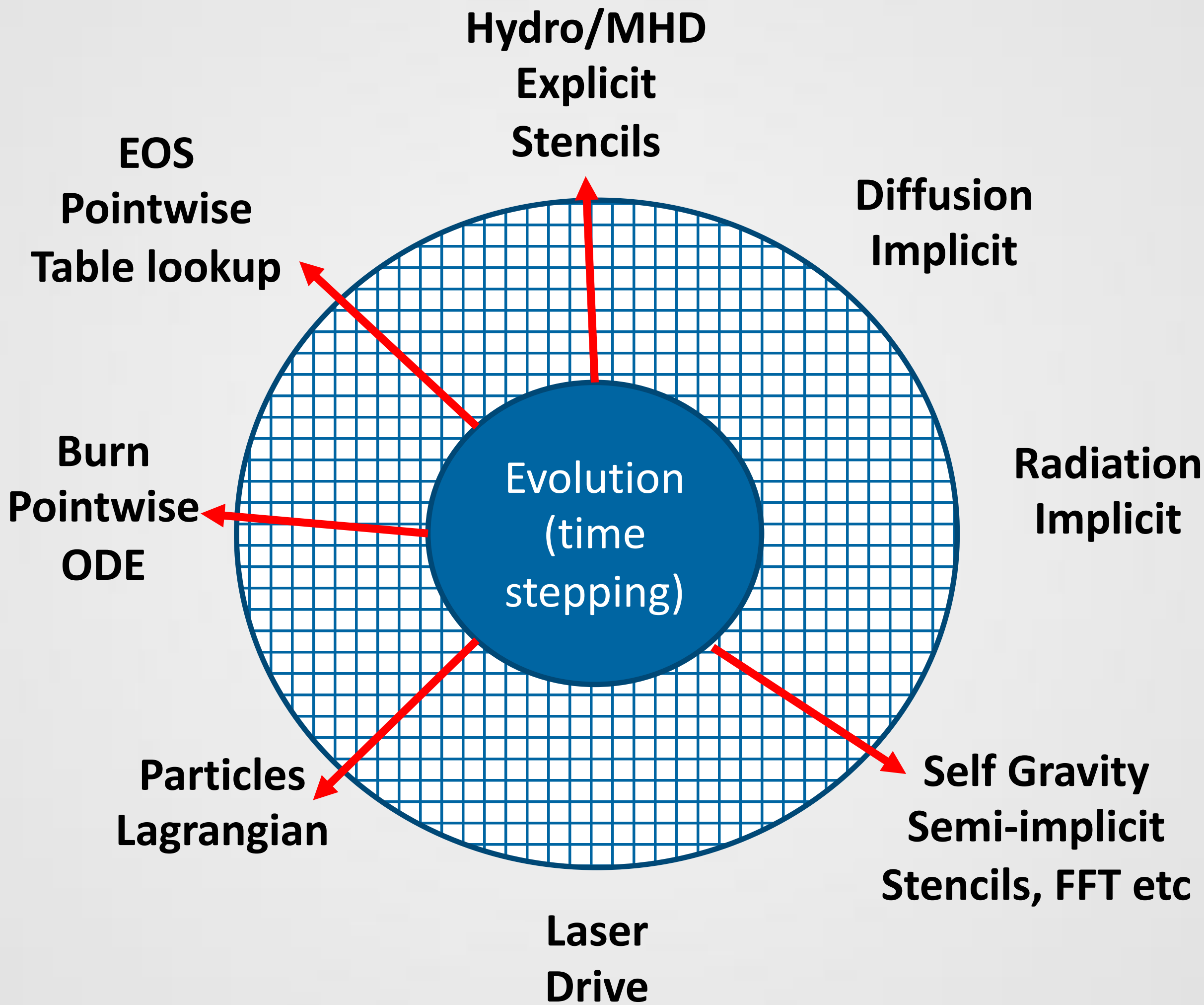
CONFIGURATION



Dubey et al, Parallel Computing 2009

CONFIGURATION

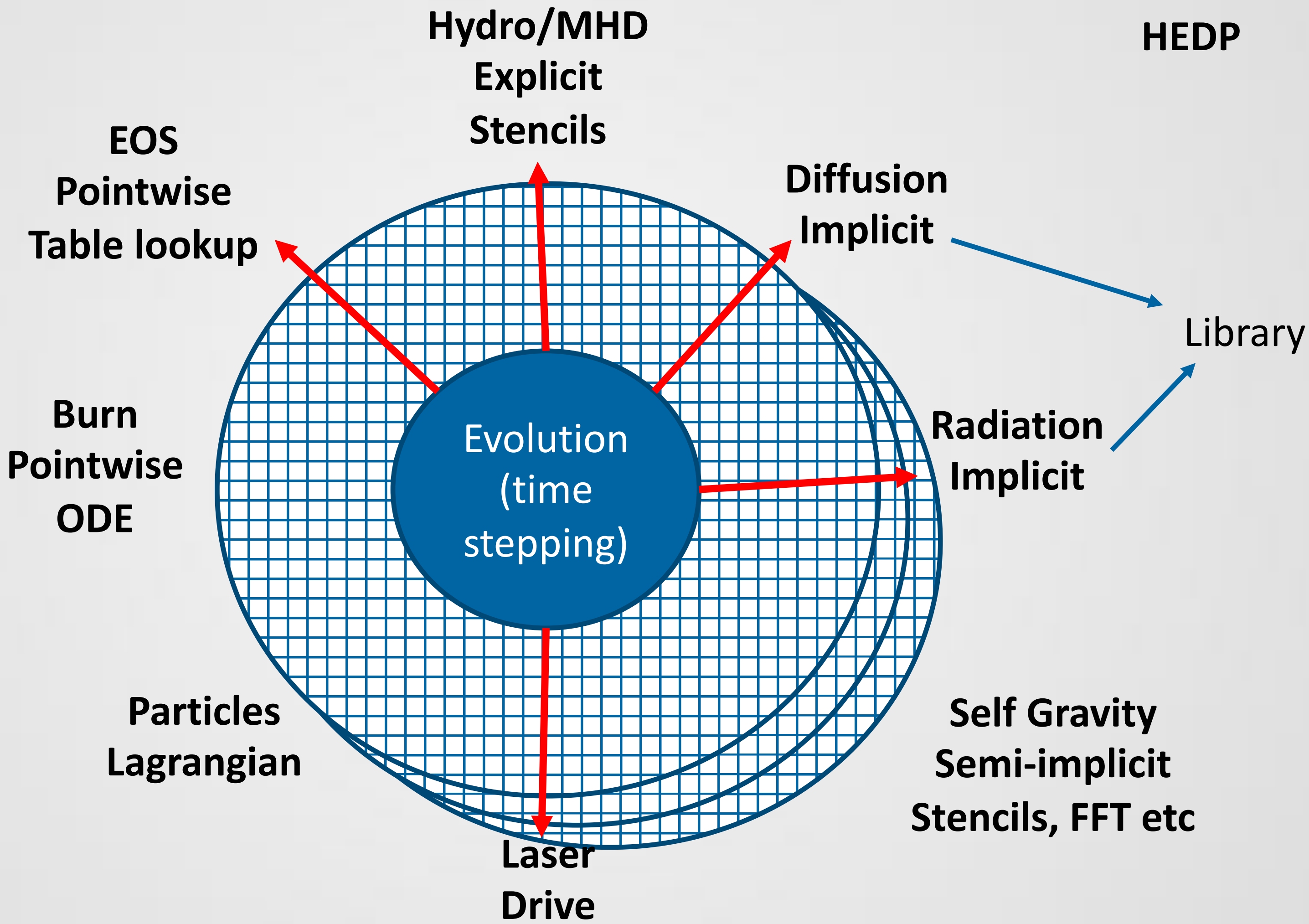
GCD



Dubey et al, Parallel Computing 2009

CONFIGURATION

HEDP

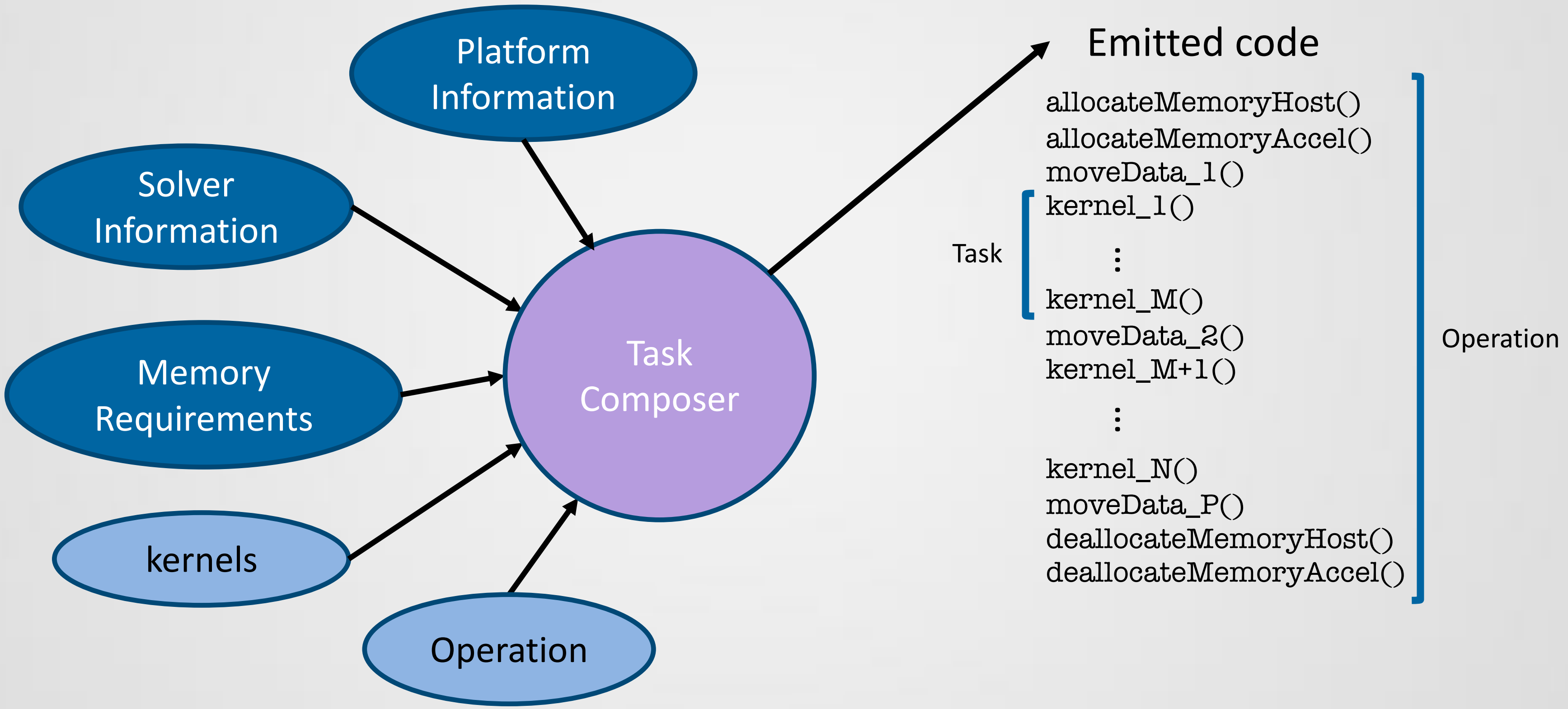


Dubey et al, Parallel Computing 2009

COMPOSER FILES

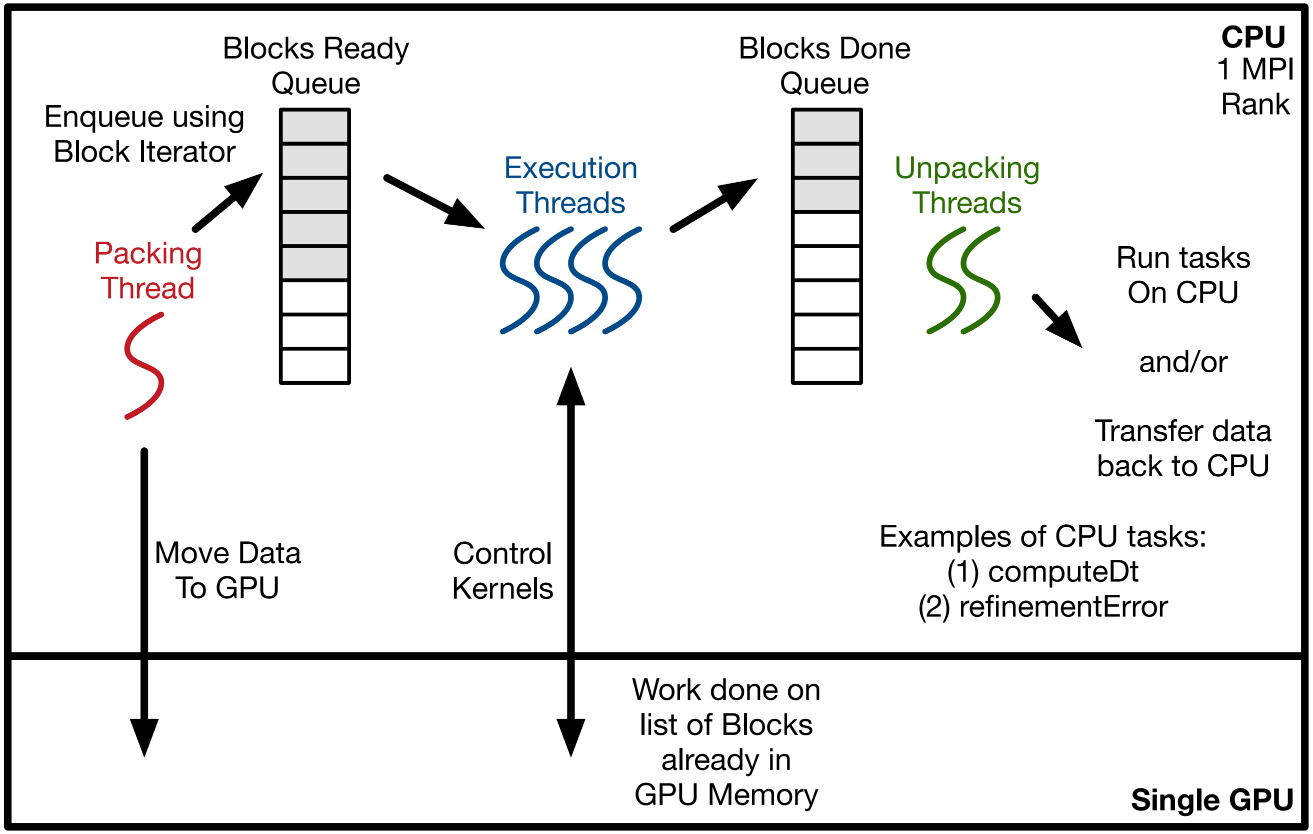
- Same philosophy
- Keep them separate from Config files
  - More complex
  - Functionally different
  - Operate at individual unit level
- Build a separate tool
  - Could be a DSL compiler
    - We prefer to keep it simple
    - Time will tell if we can
- Parse the meta-information and produce executable code

OUR VISION



Platform Information
Solver Information
Memory Requirements
kernels
Operation
Task Composer
Emitted code
allocateMemoryHost()
allocateMemoryAccel()
moveData_1()
kernel_1()
⋮
kernel_M()
moveData_2()
kernel_M+1()
⋮
kernel_N()
moveData_P()
deallocateMemoryHost()
deallocateMemoryAccel()
Task
Operation

RUNTIME ORCHESTRATION



Task Composition: scheduleComputations(gpu={gcFill, computeFluxes, updateSoln, Eos}, cpu={computeDt}, moveDataBack=True)

BUILDING THE CODE

- Configuration in three stages
  - Stage 1 – the usual running of setup script
  - Stage 2 – run the task composer
  - Stage 3 – run the transpiler
- Run make as usual
- The orchestrator generated in the process
  - Launches various threads that control run time
  - May or may not interact with AMReX asynchronization

Lot of open questions still, but we believe that this is the right approach

WHY THIS WAY - PARALLELISM

- MPI is not difficult, decomposition is
- In parallelization neither all nor none is good
  - All – leave everything to the compiler
    - Domain specific knowledge lost – wasted opportunity
    - Compilers get impossible job, cannot optimize
  - None – orchestrate everything explicitly
    - Not feasible for even moderately complex application
    - Impossible from productivity perspective
- Whichever model is used, understanding the parallelizable structure of application is critical
- Constructs to encode the understanding needed

WHY THIS WAY - KERNELS

- C++ => Pushing a needlessly complex language that lacks basic structures
  - If there is a mesh there are 3D arrays
    - meta-data built and carried around
    - Explicit order of access and order of operations
  - No graceful way to encode lack of dependence
- Maintainable code in clean constructs, perhaps in python eventually
- We can also exploit alternative implementations at arbitrary granularity

ADVANTAGES

- All code can be compiled with standard compilers
- Constructs for expressing parallelism at different granularities
- Limit intelligence needed in any one tool
- Domain knowledge encoded in composer file, helps with optimizations

This is why I think Chapel designers think the way I do.

Questions ?