Scientific Software Design

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• The requested citation the overall tutorial is: David E. Bernholdt, Anshu Dubey, Mark C. Miller, Katherine M. Riley, and James M. Willenbring, Software Productivity Track, in Argonne Training Program for Extreme Scale Computing (ATPESC), August 2020, online. DOI: 10.6084/m9.figshare.12719834

• Individual modules may be cited as Speaker, Module Title, in Software Productivity Track...

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Architecting scientific codes

Desirable Characteristics and Why They are Challenging

Extensibility

Well defined structure and modules
Encapsulation of functionalities
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Well defined structure and modules
Encapsulation of functionalities

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

Spatial and temporal locality of data
Minimizing data movement
Maximizing scalability

Same data layout not good for all solvers. Many corner cases. Necessary lateral interactions
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Desirable Characteristics and Why They are Challenging

### Extensibility
- Well defined structure and modules
- Encapsulation of functionalities
- Same data layout not good for all solvers. Many corner cases. Necessary lateral interactions

### Performance
- Spatial and temporal locality of data
- Minimizing data movement
- Maximizing scalability
- Low arithmetic intensity solvers with hard dependencies. Proximity and work distribution at cross purposes
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Desirable Characteristics and Why They are Challenging

Portability

General solutions that work without significant manual intervention across platforms
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Desirable Characteristics and Why They are Challenging

Portability

General solutions that work without significant manual intervention across platforms

Tremendous platform heterogeneity
A version for each class of device => combinatorial explosion
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Desirable Characteristics and Why They are Challenging

Portability

General solutions that work without significant manual intervention across platforms

Verifiability and Maintainability

Clean code
Documentation
Comprehensive testing

Tremendous platform heterogeneity
A version for each class of device => combinatorial explosion
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Desirable Characteristics and Why They are Challenging

Portability

General solutions that work without significant manual intervention across platforms

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

Verifiability and Maintainability

Clean code
Documentation
Comprehensive testing

Wrong incentives
Designing good tests is hard
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Taming the Complexity: Separation of Concerns

Subject of research
Model
Numerics

More Stable
Discretization
I/O
Parameters
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Treat differently

More Stable
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Taming the Complexity: Separation of Concerns

Subject of research
Model
Numerics

Client Code
Mathematically complex

Treat differently

More Stable
Discretization
I/O
Parameters

Infrastructure
Data structures and movement
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Taming the Complexity: Separation of Concerns

- **Subject of research**
  - Model
  - Numerics

- **Client Code**
  - Mathematically complex

- **More Stable**
  - Discretization
  - I/O
  - Parameters

- **Infrastructure**
  - Data structures and movement

- Treat differently
- Hide from one another
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Taming the Complexity: Separation of Concerns

Subject of research
Model
Numerics

Client Code
Mathematically complex

Treat differently

More Stable Discretization
I/O Parameters

Infrastructure
Data structures and movement

Hide from one another

logically separable functional units of computation

Encode into framework

Differentiate between private and public

Define interfaces

Applies to both kind
A Design Model for Separation of Concerns

Requirements
- Implement
- Test
- Maintain
- Augment

Software Architecture API Design

Capabilities
- Model
- API
- Design
- Develop
- Validate
- Integrate
Design Considerations

• 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
Design Considerations

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

- **Model/numerics design**
  - Abstract away the infrastructure knowledge as much as possible
  - Encapsulate
  - Let model needs guide API
  - Design flexible API to accommodate quick upgrades to methods
- **Simple is better**
  - Flexibility Vs transparent to the user
    - Flexibility wins
The Running Example

Let's 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)
- static void r83_np_fa(int n, double *a)
- static void r83_np_sl ( int n, double const *a_lu, double const *b, double *x)
- 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)
- void compute_exact_solution(int n, double *a, double dx, char const *ic, double alpha, double t, double bc0, double bc1)
- bool update_solution_ftcs( int n, double *uk1, double const *uk0, double alpha, double dx, double dt, 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
- Virtual view: collection of components
- Memory access and compute optimization

Example: Architecting Multiphysics PDEs
A Design Model for Separation of Concerns

Requirements → Software Architecture API Design → Implement → Test → Maintain → Augment

Capabilities

API Design → API → Design Develop → Validate → Integrate → Model

This worked with distributed memory parallelization model
No longer sufficient needs refinement
Additional Considerations for Infrastructure

- **Configurability**
  - Components or kernels
  - Levels of access (hierarchical)
  - Layered API

- **Task orchestration**
  - Mapping tasks to devices
  - CPU, accelerators, specialized devices
  - Managing data movement between devices
Example: Architecting Multiphysics PDEs

Separation of Concerns, Tasks

Framework

- Real view: A whole domain with many operators
- Spatial Decomposition Blocks/tiles
- Virtual view: domain sections as stand-alone computation unit
- Load Distribution
- Parallelization and scaling optimization
- Dynamic Scheduling

- load balancing, work redistribution
- Meta-information about domain sections
- Possible asynchronization at block and operator level
- No compute optimization here
Example: Architecting Multiphysics PDEs

- Abstractions for performance portability
- Ability to express operations at a higher level

- Toolchain to configure
- Compilers to optimize

Framework

Real view: A whole domain with many operators

Functional decomposition

Virtual view collection of components

Abstraction at solver level

- Code transformation
- Fusing/inlining Functions
- Memory access and compute optimization
Other Considerations

• 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 a rigorous verification regime at the outset
TAKEAWAYS

• DIFFERENTIATE BETWEEN SLOW CHANGING AND FAST CHANGING COMPONENTS OF YOUR CODE
• TAKE YOUR TIME TO UNDERSTAND THE REQUIREMENTS OF YOUR INFRASTRUCTURE
• IMPLEMENT SEPARATION OF CONCERNS
• DESIGN WITH PORTABILITY, EXTENSIBILITY, REPRODUCIBILITY AND MAINTAINABILITY IN MIND
• LEVERAGE EXISTING CAPABILITIES WHERE POSSIBLE

……..QUESTIONS ?