Benesh: a Programming Model for Coupled Scientific Workflows

Philip E. Davis*, Pradeep Subedi*, Shaohua Duan*, Lee Ricketson◊, Jeffrey A.F. Hittinger◊, Manish Parashar*

* Rutgers Discovery Informatics Institute, Rutgers University, Piscataway, NJ

◊ Lawrence Livermore National Laboratories, Livermore, CA

Introduction

- What I am talking about today is Benesh
  - a programming model for scientific workflows
  - makes it easier to combine existing codes into complex workflows
  - allows interactions be specified separately from the codes themselves
- What I am NOT talking about today
  - An architecture or performance model for Benesh
- Apologies on terminology (coupling, composition, workflow, …)

Programming In-situ Workflows

- What do I mean by in-situ workflows?
  - A single scientific computing experiment (simulation, analysis, viz, etc.)
  - Different programs (components) of the workflow run together, actively exchanging data
- Multiphysics workflow
  - Multiple simulations working together to solve some larger/more complex problem
  - E.g. split in space (WDMApp), split on physics (plasma + laser), split in medium (ice+sea)
  - *Solutions* are coupled in some mathematical regime
  - *Codes* must exchange data to accomplish this regime
- Common programming methods for workflows
  - *ad hoc* – directly code interactions into software packages; difficult to change and maintain
  - *Orchestration* – decompose workflow into many discrete tasks, orchestrator satisfies dependencies and launches new tasks; difficult to refactor legacy codes, loss of autonomy

Outline

1. Benesh Overview
2. Model Elements
3. Example
4. Future Work

Benesh

- A programming model for developing in-situ workflows
  - Take existing codes and make them work together
  - Abstractions aimed at supporting multiphysics use cases
- Programming-language hooks for a preparing an existing code for use in a Benesh workflow
- Workflow description language for specifying the interactions of workflow components
  - Provide enough information about the workflow to make interactions flexible
- (**In progress**) Middleware for instantiating Benesh workflows efficiently

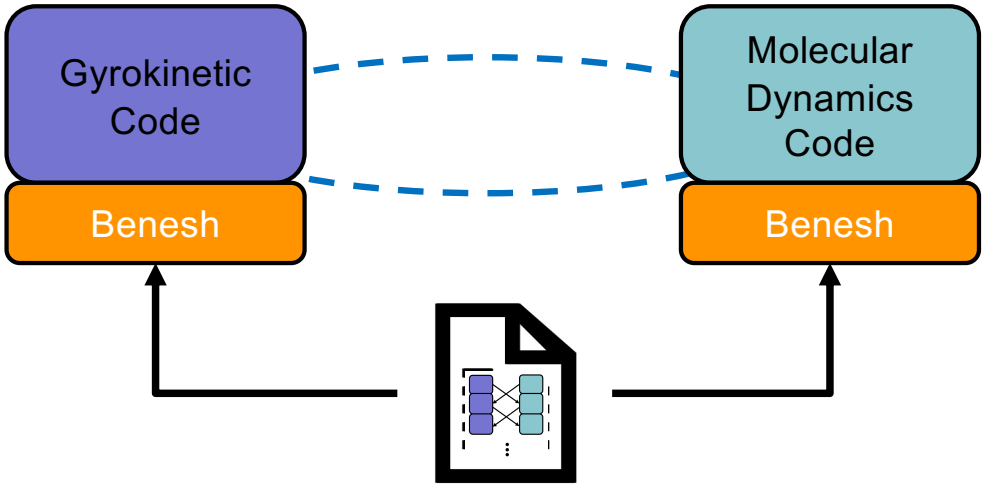
Goals

1. Reuse existing code

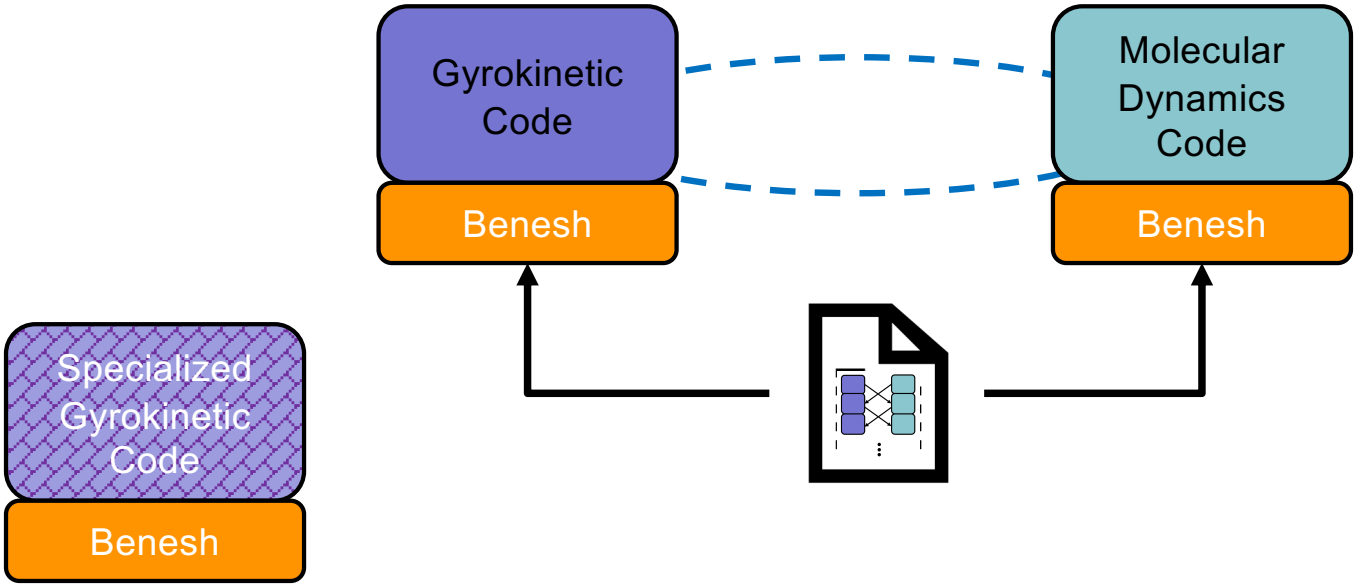
2. Rapid experimentation
   - Adding and removing components
   - Swapping components
   - Changing schemes

3. Consolidation of workflow language
   - Make interactions explicit

Benesh



Benesh


Gyrokinetic Code
Benesh
Molecular Dynamics Code
Benesh
Specialized Gyrokinetic Code
Benesh

Benesh – Language Concepts

- Interface – What can be done by a component?
  - Each component implements an abstract interface that is declared as part of the workflow description. This encapsulation of components allows component functionality to be modularized
- Data Target Rules – How should interactions occur?
  - Makefile-like rules define dependencies and ‘recipes’ for creating data objects
  - Invocation of target rules automatically invokes dependent rules
- Touchpoints – When should interactions occur?
  - Points in the code where workflow interactions occur / dependencies to advance are satisfied
  - Touchpoints are where workflow and component-level tasks are synchronized.
  - Touchpoints signal when to invoke data target rules

Benesh – Model Features

- Workflow is composed with a service-oriented architecture
  - Well-defined interface is implemented by each component
  - Borrow interface concepts from OO programming
- Workflow components are autonomous
  - Parallel (conceptual) execution tracks for workflow and component-level operations
- Workflow interactions are *choreographic*
  - Components have a shared understanding of the workflow
  - Components coordinate their activities when necessary

Language Elements

- Abstract Component Interface model
  - Declare the interface that codes must provide in order to fill the role of a component in a workflow
  - Define the data objects that are visible at the workflow level
- Workflow data model
  - Define the global data domain and how this domain maps into workflow components
- Workflow choreology
  - Recipes for realizing component interactions
  - What kind of component state changes or data events trigger these interactions
- Code Binding API

Abstract Component Interface

- Interface in the OO sense
- Any component that can act in a particular role of a workflow provides this interface
  - Can simulate a plasma over the required domain in the required way
  - Can perform the required analysis
  - Can visualize the simulation in the desired way
- This is the abstraction of the codes in terms of how they interact, and the developer must instantiate this interface
- Function signatures and local data structures
- State transition markers from code (touchpoints)

```
interface <name>:
    <type><dim> <var_name>
    <type>{}    <set_name>

    <method_name>():
        in: <var_list>
        out: <var_list>

    <method_name>(<arg>):
        in: <var_list>
        out: <var_list>

touchpoints:
    <pamaterized names>
```

Workflow Data Model

- Defines the parameters of a data domain
  - Will later be bound to interface data structures
  - Can be changed on a run-by-run basis in order to resize or redistribute the data domain between components
- Contains information to map data to components
  - Boundaries, overlaps, etc can be derived
- Does NOT contain information on mapping ranks to data
  - May be determined or changed after the workflow starts

```
domain <domain_name>:
    range: [<start>,<end>]
    periodic: (<val>,…<val>)
    domain <subdomain_name>:
        range: [<start>,<end>]
        periodic: (<val>,…<val>)
```

Workflow choreology

- Component declaration
  - Components instantiate an interface using a particular program

- Data rules
  - A makeflow-type syntax that takes the form of

```
target: dependencies
  procedure
```

- State transition/synchronization
  - Operations that take place when a component (or the workflow as a whole) reaches some defined location (this ties the user code state to the workflow state.) See examples.

Workflow choreology – component declaration

- Bind workflow components to a particular role (interface) that component interfaces provide.
- Interface refers to the abstract interfaces that already declared.
- Credential is provided by the component as part of the client bindings.
- Different credentials refer to different implementations of the same role.

```
component <comp_name>(<interface>)[<credential>]
```

```
component Generator1(ArrayBuilder1D)[random]
component Generator2(ArrayBuilder1D)[exponent]
component Analyzer(ArrayCompare1d)[maxdiff]
```

Workflow choreology – target generation rules

- 'makeflow'-style target definition
  - Target name and dependencies, followed by a "recipe"
- Rules call interface methods
- Parameterize rules with %{} syntax (allow some manipulation of variables, e.g. %[[t-1]])
  - e.g. Generator2.x.1 depends on Generator2.x.0

```
<comp_name>.<var_name>.<version>: <dependencies>
    <procedure>
```

```
Generator1.x.0:
Generator1.x.%{t}: Generator1.x.%[[t-1]]
    Generator1.build_array(seed) in=x.%[[t-1]] ; out= x.%{t}

Generator2.x.0:
Generator2.x.%{t}: Generator2.x.%[[t-1]]
    Generator2.build_array(seed) in=x.%[[t-1]] ; out= x.%{t}

Analyzer.diff.%{t}: Generator1.x.%{t} Generator2.x.%{t}
    Analyzer.x.%{t} < Generator1.x.%{t}
    Analyzer.y.%{t} < Generator2.y.%{t}
    Analyzer.compare_array()
```

Workflow choreology – touchpoint rules

- Rules for synchronizing component activity and state with workflow activity and state
- Touchpoints (identified by what's to the right of '@') are reached at certain points in the component code

```
<comp_name>@<touchpoint_name>:
    <target>
```

```
Generator1@ts.%{t}:
    Generator1.x.%{t}

Generator2@ts.%{t}:
    Generator2.x.%{t}

Analyzer@ts.%{t}:
    Analyzer.diff.%{t}
```

Code Binding API

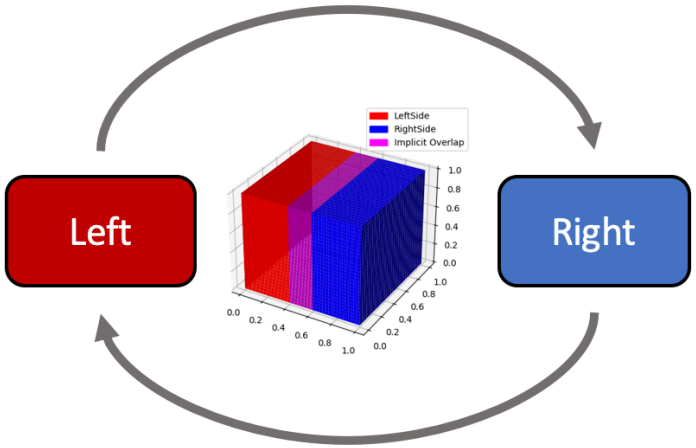
- API calls to bind component code
- Binding syntax depends heavily on language capabilities (e.g. function pointers in C)
- Future work to create preprocessor
- Benesh will need to manage variable buffer(s), so a data accessor API is required in some languages.

```
bind_method(function_pointer, ”method_name”)
touchpoint(“touchpoint_name”)
bind_domain(“domain_name”, “variable_name”, range)

bind_data(data_pointer, “data_name”)
 ---or---
var_access_scalar(buffer_pointer, “variable_name”, TYPE)
var_access_buffer(buffer_pointer, “variable_name”, TYPE)
var_access_iter(iter_pointer, “variable_name”, …)
…
```

Example Workflow

- Solve a physical quantity (u) on a 3D domain
  - Unit cube
  - Split into left and right subdomains
- Suppose two different u-solvers
  - `speedy`
  - `special`
- Solve each subdomain with a separate simulation component, exchanging boundary data for consistency



ad hoc method - lockstep

```
do_timestep():
    du = sxxx_calc_du(u)
    u = sxxx_advance(u, du)
...
while(ts++):
    ...
    do_timestep()
    ...
```

```
do_timestep():
    wait_for_other()
    read_boundaries(u)
    du = sxxx_calc_du(u)
    u = sxxx_advance(u, du)
    write_boundaries(u)
    signal_other()
...
while(ts++):
    ...
    do_timestep()
    ...
```

ad hoc method - lockstep

- Boundary exchanges hides complexity
  - Both codes must agree on boundary domain and data organization
- Swapping out codes requires maintaining this order of operations
- Changes in domain need to be coordinated
- Further splitting the domain would require more complex coordination operations

```
do_timestep():
    wait_for_other()
    read_boundaries(u)
    du = sxxx_calc_du(u)
    u = sxxx_advance(u, du)
    write_boundaries(u)
    signal_other()
...
while(ts++):
    ...
    do_timestep()
    ...
```

ad hoc Changing scheme

```
do_timestep():
    wait_for_other()
    read_boundaries(u)
    du = sxxx_calc_du(u)
    u = sxxx_advance(u, du)
    write_boundaries(u)
    signal_other()
...
while(ts++):
    ...
    do_timestep()
    ...
```

```
do_timestep():
    write_boundaries(u)
    read_boundaries(u)
    du = sxxx_calc_du(u)
    u = sxxx_advance(u, du)
    signal_other()
    wait_for_other()
...
while(ts++):
    ...
    do_timestep()
    ...
```

Ad hoc changing scheme

- Do we understand the data consistency requirements for the remainder code?

```
do_timestep():
    write_boundaries(u)
    read_boundaries(u)
    du = sxxx_calc_du(u)
    u = sxxx_advance(u, du)
    signal_other()
    wait_for_other()
...
while(ts++):
    ...
    do_timestep()
    ...
```

Preparing the code for Benesh

```
do_timestep():
    du = sxxx_calc_du(u)
    u = sxxx_advance(u, du)
...
while(ts++):
    ...
    do_timestep()
    ...
```

```
benesh_bind_method("calc_du", sxxx_calc_du)
benesh_bind_method("advance", sxxx_advance)
benesh_bind_data("u", u)
benesh_bind_data("du", du)

...
while(ts++):
    ...
    benesh_touchpoint("ts.%d" % ts)
    ...
```

Benesh Workflow Definition

```
interface explicit3d:
    real<3> u
    real<3> du
    calc_du(real):
        in: u
        out: du
    advance(real):
        in: u, du
        out: u
    touchpoints:
        ts.%n
```

```
domain Global:
    periodic(a, a, a)
    range: [0,1] x [0,1] x [0,1]
    domain Left:
        range: [0,.6] x [0,1] x [0,1]
    domain Right:
        range: [.4,1] x [0,1] x [0,1]
```

Benesh Target Generation Rules - lockstep

```
real dt = .01
real t

Left.u.0:
    t = 0
Left.u.%{ts}: Left.u.%[[ts-1]] Right.u.%[[ts-1]]
    boundary(Left.u.%[[ts-1]] < Right.u.%[[ts-1]]
    Left.calc_du(t) : in=u.%[[ts-1]] ; out=du.%[[ts-1]]
    Left.advance(dt) : in=u.%[[ts-1]], du.%[[ts-1]] ; out=u.%{ts}

Right.u.0:
Right.u.%{ts}: Left.u.%{ts} Right.u.%[[ts-1]]
    boundary(Right.u.%[[ts-1]] < Left.u.%{ts}
    Right.calc_du(t)  in=u.%[[ts-1]] ; out=du.%[[ts-1]]
    Right.advance(dt) in=u.%[[ts-1]], du.%[[ts-1]] ; out=u.%{ts}
    t = t + dt
```

Benesh Target Generation Rules – scheme change

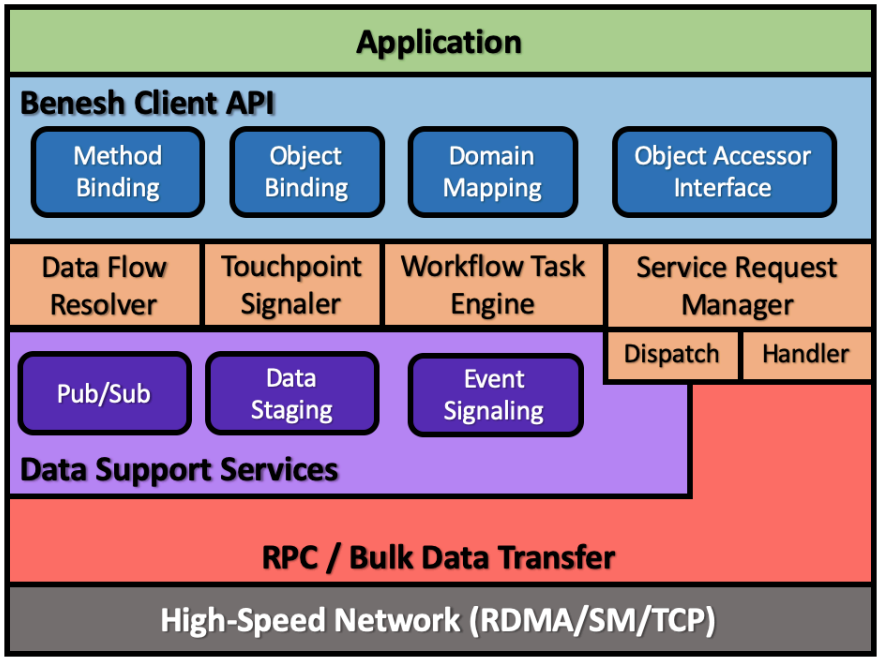
```
real dt = .01
real t

Left.u.0:
    t = 0
Left.u.%{ts}: Left.u.%[[ts-1]] Right.u.%[[ts-1]]
    boundary(Left.u.%[[ts-1]] < Right.u.%[[ts-1]]
    Left.calc_du(t) : in=u.%[[ts-1]] ; out=du.%[[ts-1]]
    Left.advance(dt) : in=u.%[[ts-1]], du.%[[ts-1]] ; out=u.%{ts}

Right.u.0:
Right.u.%{ts}: Left.u.%[[ts-1]] Right.u.%[[ts-1]]
    boundary(Right.u.%[[ts-1]] < Left.u.%[[ts-1]]
    Right.calc_du(t)  in=u.%[[ts-1]] ; out=du.%[[ts-1]]
    Right.advance(dt) in=u.%[[ts-1]], du.%[[ts-1]] ; out=u.%{ts}
    t = t + dt
```

Future Work – Development of Supporting Middleware

- Develop middleware to actualize Benesh workflows
  - Leverage and extend composable* data services
- Create performance model for workflow-level operations
  - Portable between execution spaces



Future Work – Binding Interface

- Interface binding is based on high-level features of the code
- It is desirable to minimize the work of preparing a code for Benesh
- Code annotation/pragma and introspection tools may be a better solution than runtime API hooks

Acknowledgements

- The research at Rutgers was conducted as part of the Rutgers Discovery Informatics Institute.

- This research was supported 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 also supported by the U.S. Department of Energy, Office of Science, Advanced Scientific Computing Research, under Contract DE-AC02-06CH11357.