DYFLOW: A flexible framework for orchestrating scientific workflows on supercomputers

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Outline

• Motivation
• DYFLOW Approach
• DYFLOW capabilities: demonstration with example
• Future Work
Modern scientific workflows are complex:
Support for adaptive workflows is important now more than ever

Traditional workflows – loosely coupled

- Involves complex tasks (e.g., graph and machine learning based approaches)
- Large-scale coupling involving petabytes of data
  - I/O becomes the performance bottleneck

Paradigm shift towards in situ workflows
- Memory to memory transfers replace disk writes
  - On-node memory buffers, e.g. ADIOS
  - Off-node dedicated servers, e.g. Dataspaces

In situ workflows – tightly coupled

Dynamic challenges
- Dealing with interference since tasks share compute nodes
- Dealing with changes in data-flow rate
- Automating handling of data-driven events
- Handling failures...

...
Modern scientific workflows are complex:
Static nature of resource assignment on supercomputers

- No dynamic resource assignment
- No or limited support for handling data-driven events or failures
- No flexibility

Resource overprovisioning => Underutilized resources

No orchestration to adapt resources based on changing requirements of workflow tasks at runtime
DYFLOW

A workflow orchestration service that reuses existing support from widely used workflow management services.

Specification of workflow tasks with one-time resource requirement.

Specification of workflow orchestration needs.

Compute nodes

Cluster Batch Scheduler

Static scheduling

Workflow Management Service

DYFLOW
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DYFLOW: Dynamic model

Features:

Flexibility:
Provides comprehensive constructs at different stages that enable end-users to configure and automate workflow orchestration as a user desires

Ease of expression and reusability across workflows tasks and parallel architectures
DYFLOW: Dynamic model (Monitor)

User defined sensors

What data to gather?
Method to use for data gathering?
How to **group** and **reduce** data to form a metric?

Framework:

Manages sensors - set and reset sensors as task run and stop
Manage collection and reduction of distributed data at scale
Support different types of data **gathering**, grouping and reduction methods

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![Diagram](image-url)

- **Running workflow**
- **Real-time data**
- **Control signals**
- **Reduced metrics**
- **User-defined workflow orchestration settings**
- **Action plan** (feasible set of low-level actions)
- **Arbitration**
- **Decision**
- **User defined sensors**
- **Monitor**
- **Actuation**
- **Workflow Management Service**
DYFLOW: Dynamic model (Decision)

User defined policies

- What evaluation condition determines an event of interest?
- Suggested high-level actions?
- Frequency of evaluation?

Framework:

- Manages policies
- Trigger evaluation conditions at the desired frequency
- Support different types of evaluation conditions and high-level actions

Diagram:

- Decision
  - Real-time data
  - User-defined workflow orchestration settings
  - Reduced metrics
- Monitor
- Actuation
  - Control signals
- Workflow Management Service
  - Action plan (feasible set of low-level actions)
- Arbitration
- Action plan (feasible set of low-level actions)
DYFLOW: Dynamic model (Arbitration)

User defined rules

End-users can assist in
• Conflict resolution by setting task priorities
• Identification of dependent actions by declaring task dependencies

Framework:
• Resolves conflicting high-level actions
• Identifies dependent actions
• Maps high-level to low-level actions
• Determine resource assignments
• Suspend processing incoming suggestions to avoid repeatedly applying the same actions

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DYFLOW: Dynamic model (Actuation)

Workflow developers:
- Extend DYFLOW via plugin interface to enable Actuation to invoke the workflow management services

Framework:
- Provide wrappers for plugin interfaces with the services (low-level actions) requested by the Actuation. E.g. stopping the tasks

**User-defined workflow orchestration settings**

- Reduced metrics
- Action plan (feasible set of low-level actions)
- Decision
- Arbitration

**Monitor**
- Real-time data
- Control signals

**Actuation**
- Action plan (feasible set of low-level actions)
- Workflow Management Service

**Workflow developers**
- Stop/Start or relaunch tasks with a new resource assignment
- Inquire about current resources assignment
- Inquire about resource status
- ....
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DYFLOW: IMPLEMENTATION

Capabilities

- Improve Throughput
- Improve Performance
- Handle Node Failure
- Handle data-driven Events

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DYFLOW: Handling Node Failure

LAMMPS

Tightly coupled Workflow

Summit
A high-end supercomputer at
Oak Ridge National Lab

<sensor id="STATUS" type="ERRORSTATUS">  
  <group-by>  
    <group granularity="task" reduction-operation="FIRST"/>  
  </group-by>  
</sensor>

<policy id="RESTART_ON_FAILURE">  
  <eval operation="GT" threshold="128"/>  
  <sensors-to-use>  
    <use-sensor id="STATUS" granularity="task"/>  
  </sensors-to-use>  
  <action>RESTART</action>  
  <frequency seconds="30"/>  
</policy>
DYFLOW: Handling Node Failure

Failure recovery (Summit): Event timestamps (min:sec) and duration

- Workflow restart after node failure using additional node in the allocation from the job scheduler
- Simulation restarts from the last checkpoint
- Time to restart reflects the decision frequency of 30 sec
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Future work

• Improving Arbitration stage
  • To manage the heterogeneous resources assignments at runtime
  • Use machine learning to make better arbitration decisions, based on history, to improve conflict resolution, policy priorities, etc.

• Improving Actuation stage
  • Exploring controllable actions that allows users to dynamically alter running workflow, for instance, controlling what and how data flows between tasks.
**DYFLOW:** A flexible framework for orchestrating scientific workflows on supercomputers

To summarize ...

- **DYFLOW** is a generic framework that automates the orchestration of scientific workflows on supercomputers based on user-defined criteria
- Provides end-users with comprehensive and easy-to-use constructs to express and customize the orchestration of their workflow at different stages of runtime management
- Supports adaptive workflows with various capabilities to improve throughput and performance, handle failures and data-driven events
- Integrates with existing workflow management services and utilizes their workflow management support

Questions?

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