Computer Science Department

Potential of I/O-Aware Workflows in Climate and Weather

Limitless Storage
Limitless Possibilities

https://hps.vi4io.org

Julian M. Kunkel, Luciana Pedro, Bryan Lawrence, Glenn Greed, David Matthews, Hua Huang

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LIMITLESS **POTENTIAL** | LIMITLESS **OPPORTUNITIES** | LIMITLESS **IMPACT**

Climate/Weather Workflows

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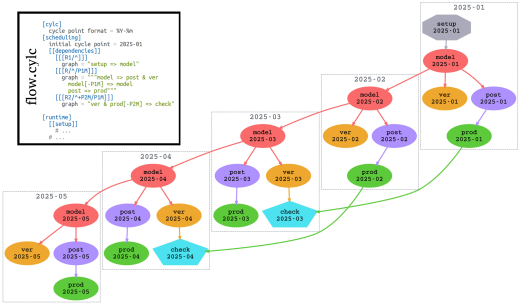
- A workflow consists of many steps
  - Repeated for simulation time
  - E.g., weather for 14 days
- Scientists use **Cylc** to handle such **cycling** workflows
- Cylc workflow specifies
  - Tasks with commands
  - Environment variables
  - Dependencies



Workflow Execution

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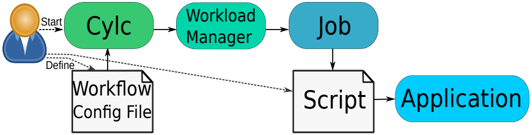
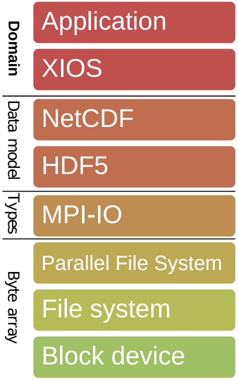
1. Cylc analyzes workflow
   - Creates a job script for each task
   - Submits to workload manager
2. Wflow manager allocates resources
   - Starts a job with env. vars
3. Job script runs applications
   - File names set by
     - env. var
     - command
   - May depend on cycle

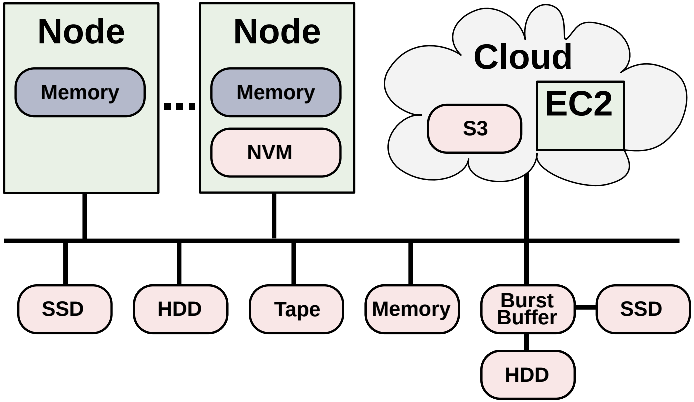


- The data dependency between tasks is currently stored implicitly

Execution Environment



I/O path for an MPI-parallel application. HDF5 can be replaced with ESDM.



Example of an heterogeneous HPC landscape

Earth-System Data Middleware

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- Part of the ESiWACE Center of Excellence in H2020
  - Centre of Excellence in Simulation of Weather and Climate in Europe

  https://www.esiwace.eu
- Integrated as NetCDF backend

ESDM provides a transitional approach towards a vision for I/O addressing

- Scalable data management practice
- The inhomogeneous storage stack
- Suboptimal performance and performance portability
- Data conversion/merging

EU funded Project: ESiWACE

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The Centre of Excellence in Simulation of Weather and Climate in Europe

- Representing the European community for
  - Climate modelling and numerical weather simulation
- Goals in respect to HPC environments:
  - Improve efficiency and productivity
  - Supporting the end-to-end workflow of global Earth system modelling
  - Establish demonstrator simulations that run at highest affordable resolution
- Funding via the European Union’s Horizon 2020 program (grant #823988)

http://esiwace.eu

esiwace
CENTRE OF EXCELLENCE IN SIMULATION OF WEATHER AND CLIMATE IN EUROPE

Data Center Perspective: Utilization of HPC Resources

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Projects run in Data Centers

- Proposals may include: Time needed, CPU (GPU) hours, storage space
- After resources are granted scientists basically do what they want
  - Some limitations, e.g., quota, compute limit
  - But actual usage and access patterns?
  - The system is not aware what possibly could happen
  - The data center does not know suffiently what users do
- Additionally: Execution uses often tools with 40year old concepts

Projects executed in Cern/LHC and other big experiments

- A detailed planning of activities is performed
- Experiments are proposed with detailed plans (time, resource utilization)

Outline

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Planning HPC Resources: An Alternative Universe

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- Scientists deliver
  - detailed but abstract workflow orchestration
  - containers with all software
  - data management plan with data lifecycle
  - time constraints and budget
- Data centers and vendors
  - Simulate the execution before workflow is executed
  - Estimate costs, energy consumption
  - Determine if it is the best option to run
- Systems
  - Utilize the information to orchestrate I/O
  - Make decisions about data location and placement:
    - Trade compute vs. storage and energy/costs vs. runtime
  - Ensure proper execution
- Provoking: Big data technology is ahead of HPC in such an agenda

Vision: Exploit Workflow Knowledge

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- Enhance workflow description with IO characteristics
  - Needed input
  - Generated output and its characteristics
  - Information Lifecycle (data life)
    - How long to keep data, type of data...
  - ⇒ Explicit input/output definition (dependencies) instead of implicit
- Smarter IO scheduling
  - Considering the hardware/software environment
  - Data placement: Transfer, migration, staging, replication, allocation
  - Data reduction: data compression and data recomputation
- ⇒ Providing a separation of concern
  - Scientist declares workflow including IO
  - System maps workflow to hardware using expert knowledge and ML

Extended Workflow Description

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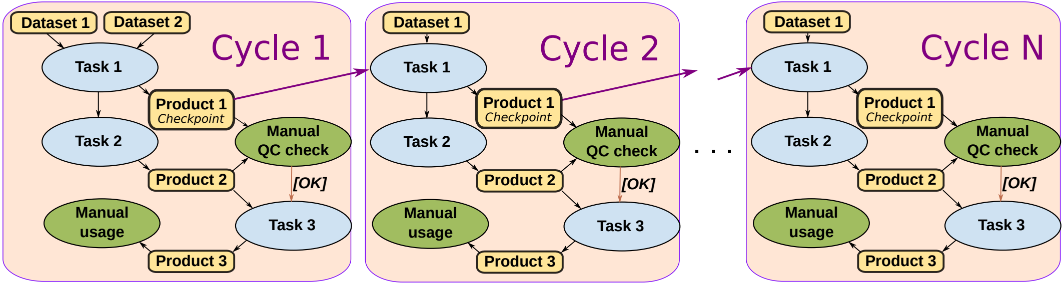

- Enhance workflow description with IO characteristics
  - Input required
  - Output generated and its characteristics

Smarter IO Scheduling: Advantage for Data Placement

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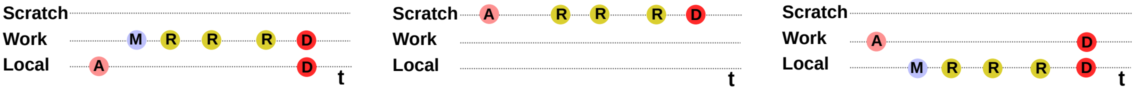
Scenario

- Consider three file systems: local, scratch, and work
  - Local is a compute-node local storage system
- Data can be stored on any of these storage systems
- Scheduler to optimize data placement throughout life cycle to hardware

Alternative life cycles for mapping a dataset (Selection)



Local and work file systems | Scratch file system only | Local and work file systems

Allocation, **M**igration, **R**eading, and **D**eleting

Outline

Design Overview

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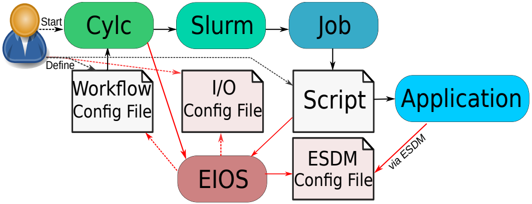
Relevant components

- Configuring system information
- Extending the workflow description
- Providing a smart I/O scheduler (EIOS)

Modified workflow execution

1. Cylc analyzes workflow
   - EIOS provides Slurm variables
2. Wflow manager allocates resources
   - May schedule on nodes of prev. jobs
3. Job script runs applications
   - EIOS generates pseudo filenames encoding scheduling information



Configuring System Information

- Reuse the Earth-System Data Middleware (ESDM) configuration file
  - Contains available storage targets, performance model, further information

```
"backends": [
    {"type": "POSIX", "id": "work1", "target": "/work/lustre01/projectX/",
        "performance-model" : {"latency" : 0.00001, "throughput" : 500000.0},
        "max-threads-per-node" : 8,
        "max-fragment-size" : 104857600,
        "max-global-threads" : 200,
        "accessibility" : "global"
    },
    {"type": "POSIX", "id": "work2", "target": "/work/lustre02/projectX/",
        "performance-model" : {"latency" : 0.00001, "throughput" : 200000.0},
        "max-threads-per-node" : 8,
        "max-fragment-size" : 104857600,
        "max-global-threads" : 200,
        "accessibility" : "global"
    },
    {"type": "POSIX", "id": "tmp", "target": "/tmp/esdm/",
        "performance-model" : {"latency" : 0.00001, "throughput" : 200.0},
        "max-threads-per-node" : 0,
        "max-fragment-size" : 10485760,
        "max-global-threads" : 0,
        "accessibility" : "local"
    }
] ...
```

Extending Workflow Description

- Additional IO workflow file (later to be integrated)
- EIOS knows workflow from Cylc and reads this file

```
[Task 1]
  [[inputs]]
    topography = "/pool/input/app/config/topography.dat"
    checkpoint = "[Task 1].checkpoint$(CYCLE - 1)"
    init       = "/pool/input/app/config/init.dat"

  [[outputs]]
    [[[varA]]] # This is the name of the variable
      pattern = 1 day
      lifetime = 5 years
      type = product
      datatype = float
      size = 100 GB
      precision.absolute_tolerance = 0.1

    [[[checkpoint]]]
      pattern = $(CYCLE)
      lifetime = 7 days
      type = checkpoint
      datatype = float
      dimension = (100,100,100,50)
```

Smarter I/O Scheduler

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- Provides hints for colocating tasks with data
  - Create dummy file name to include schedule (e.g., prefer local storage)
  - ESDM parses the schedule information and enacts it (if possible)
- Optimizing data placement strategy in ESDM/workflow scheduler
  - Utilizing hints for IME to pin data to cache
  - Storing data locally between depending tasks (using modified Slurm)
  - Optimizing initial data allocation (e.g., alternating storage between cycles)

These changes are planned as part of the ESiWACE project

- Relevant for climate/weather applications and achievable now
- Considered to be intermediate and leading towards the vision

Summary and Conclusions

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Goals of our vision and design

- Separation of concerns between developer/user and system optimization
- Scientists enhances workflow descriptions with IO characteristics
- System exploits workflow specification considering system characteristics

Outlook: Opportunities Knowing Workflows

- Performance modelling (simulation or via. recorded behavior)
  - Imagine to include compute model, too
  - Analyse: How long will the workflow run, costs to run it on a given platform?
  - What if analysis: How to change the system / storage to improve performance?
- Data centers may require submission of workflow descriptions for proposals
  - Data center could predict benefit, costs, explore how to run it optimally
  - May hand over to vendors, explore signposting to alternative systems