A Community Roadmap to Robust Science in High-throughput Applications

robustscience.org

Workflows Interoperability

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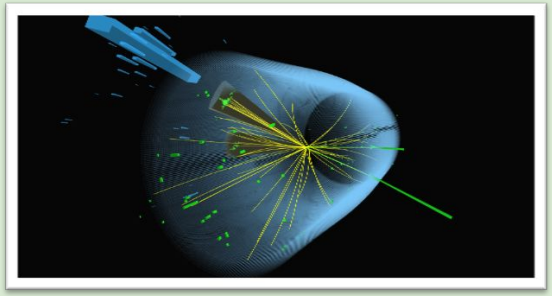
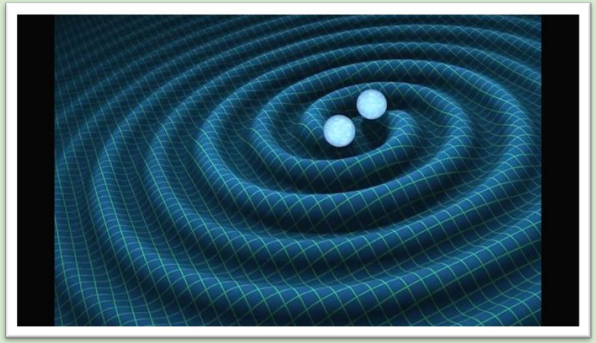
Scientific Workflows

As workflows continue to be adopted by scientific projects and user communities, they are becoming **more complex**



Catering to these workflow features and demands requires **workflow systems research** and **development at several levels**, from algorithms and systems all the way to user interfaces



Workflows are being designed that can analyze **terabyte-scale datasets**, be composed of **millions of individual tasks** that execute for milliseconds up to several hours, process data streams, and process static data in object stores

Workflows Interoperability

To a varying degree, workflow systems implement separately:

- **Language** for wiring workflow inputs/outputs
- Plugin system for connecting possible (often cmd line) **tools**
- **Control** mechanisms (e.g. fault tolerance, loops, choices)
- **Data management** facilities
- Possible **execution backends**
- Ways to connect **multiple workflows** (e.g. nesting)
- **Reproducibility** aspect for sharing workflows
- **Provenance** recording/logging

Workflows Interoperability

There has been an explosion of workflow (orchestration) technologies in the last ten years. Each one serves a different user community or underlying compute engine, albeit with substantial technical and conceptual overlap.

Underlying reasons for divergence:

- Use cases with completely different workflow structures.
- Resources with very different optimization goals.
- Execution systems with fundamentally different capabilities.

There are some missed opportunities for **interoperability**:

- Can user workflows be ported between systems?
- Can provenance be captured in similar ways?
- Can workflow systems be plugged into different engines?

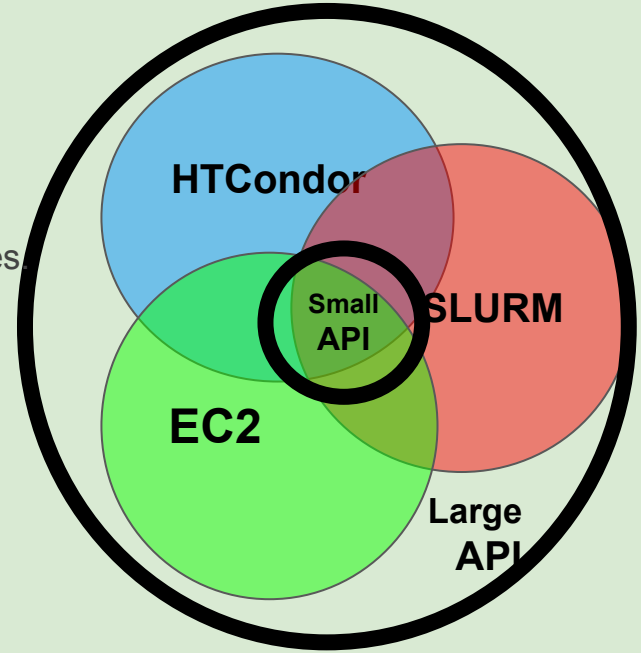
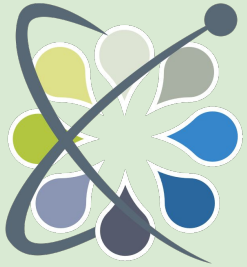


Image courtesy from Douglas Thain (University of Notre Dame) Workflows Community Summit

Workflows Interoperability Efforts



Task execution: DRMAA, GA4GH APIs *(TRS, WES)*, OGF *(JSDL, OGSA)*

Data access: S3**,** DRS, GridFTP, …

Syntactic: Common Workflow Language, Workflow Description Language

Semantic: Bioschemas, EDAM, wfdesc, Biocompute Object, IWIR Metaworkflows, CWFR

Packaging: RO-Crate, BioConda, BioContainers *(Docker/Singularity)*, Debian-Med

Data: HDF5, VOTable, CSV On the Web, SBML (COMBINE), HL7 FHIR, DFDL

Metadata: DCAT2, Codemeta, Datacite, schema.org, W3C PROV

Repository: WorkflowHub.eu, Dockstore, nf-core, PegasusHub, Galaxy Toolshed, bio.tools

Platforms and Hardware: HTC, HPC, OpenCL, Rosetta 2

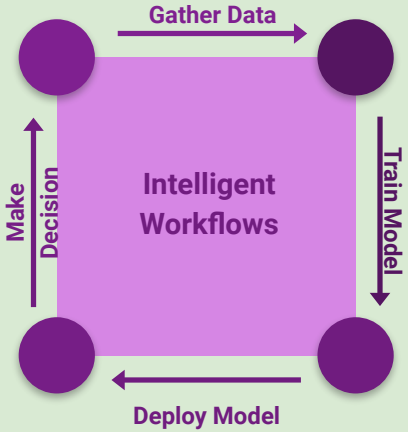
Slide courtesy of Stian SoilandReys (University of Manchester)
Workflows Community Summit

AI Workflows

AI Workflows have artificial intelligence / machine learning systems as workflow components, sub-components and/or orchestrators.

Interoperability is even harder due to the following **challenges:**

- **Data driven** computing
- **Heterogeneity** in software *and* hardware
- Distributed, edge and high-frequency computing
- Simulation results are not necessarily the product
- Leveraging fast-paced developments, driven by industry, not science



Slide courtesy of Luc Peterson (LLNL)
Workflows Community Summit

FEEDBACK OPPORTUNITIES

This project needs your feedback and there are 3 ways that you can contribute:

- **No. 1 Before the Cafe:** On the website there is a form available, per cafe, where you can provide use cases for the session in relation to the topic question.

- **No. 2 At the Cafe:** Contribute to the MURAL design-thinking application tool during and after the session.

- **No. 3 After the Cafe:** Complete the post-workshop survey designed by the Assessment Team.

Visit the project website at: **robustscience.org**