The Workflow Project at LLNL

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Exascale systems are required to increase predictive capability but by themselves will not greatly enhance end-to-end analyst productivity. The workflow project aims to improve user efficiency in setting up, managing, and analyzing exascale simulations via three efforts: Siboka, C2C, and ROVER.

1. NNSA Workflow Challenges

- Problem setup can take many weeks
- Large multi-disciplinary teams
- Multi-year campaigns
- Uncertainty Quantification / ensembles
- Certified by director, reported to congress
- Security and access control requirements

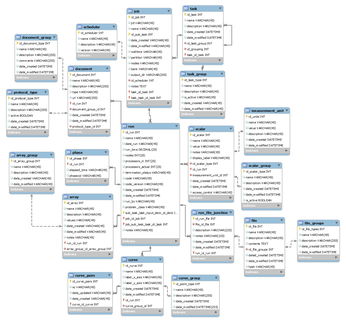
2. The workflow project seeks to:

- Adapt infrastructure to meet exascale challenges
- Enable integration of modern analytics tools by our users
- Create an ecosystem of components for users
- Create infrastructure to enable pedigree & provenance
- Work to federate/virtualize disparate servers and portals

3. Siboka: building blocks for exascale workflows and analytics

Sina: simulation insight & analysis

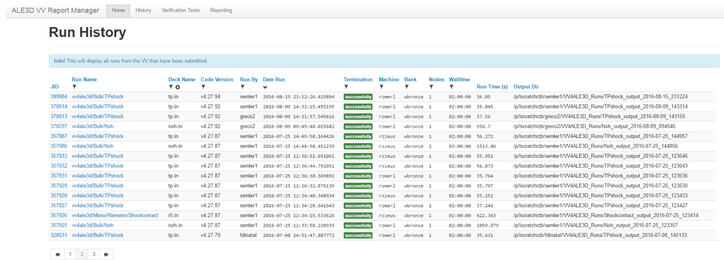
- Data collection for *meta-data* and *non-bulk inputs and outputs*
- SQL & NoSQL representations
- Python API & CLI for queries
- Designing JSON schema and tools for simulation information
- Imported 50,000K inertial confinement fusion simulations
- Plan open-source release in 2018



SQL Schema for simulation information

Simulation management

- **VV4ALE3D** web app for running validation suite integrated in Livermore Computing
- **MaestroWF:** serverless lightweight workflow execution, on github.com



4. C2C: 'contours to codes', enabling a common contour format for applications

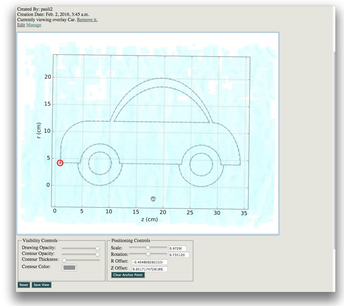
Contours are *a common fundamental geometric* input to the modeling process, and must be accurate, pedigreed, and sharable

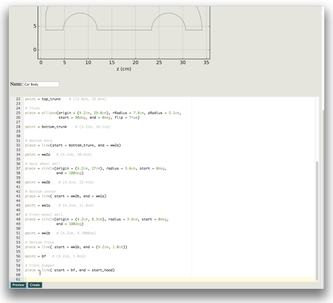
Goal: Drastically reduce time required for problem setup and peer-review and reduce duplication of user efforts in setting up new problems

We are leveraging a code-agnostic file format developed by LANL and building tooling around this format to enable problem setup & interchange

C2C tools are integrated with PMESH to generate meshes for the **MARBL** Exascale Computing Project application code

We created a prototype repository structure for contour information and supporting documents



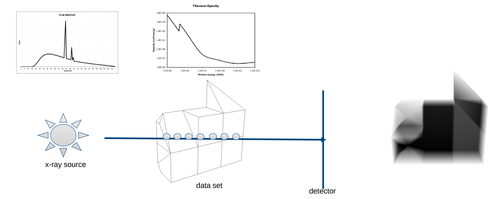


5. ROVER: volume rendering and multi-group radiography

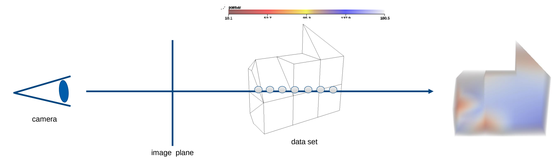
Quantitative diagnostic images are crucial in many NNSA application areas

- Can require 100's of photon energy groups
- Sampling of many time steps

ROVER provides a distributed, high performance, hardware accelerated ray tracing and compositing package for radiography and volume rendering



Radiography mode uses multi-group sources and opacities

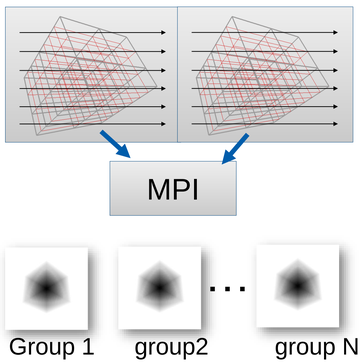


Volume rendering mode uses standard RGB color channels

ROVER ray-tracing has been incorporated into VTK-m and deployed in VisIt

ROVER includes scalable multi-group compositing (right)

Open source release coming soon!



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