

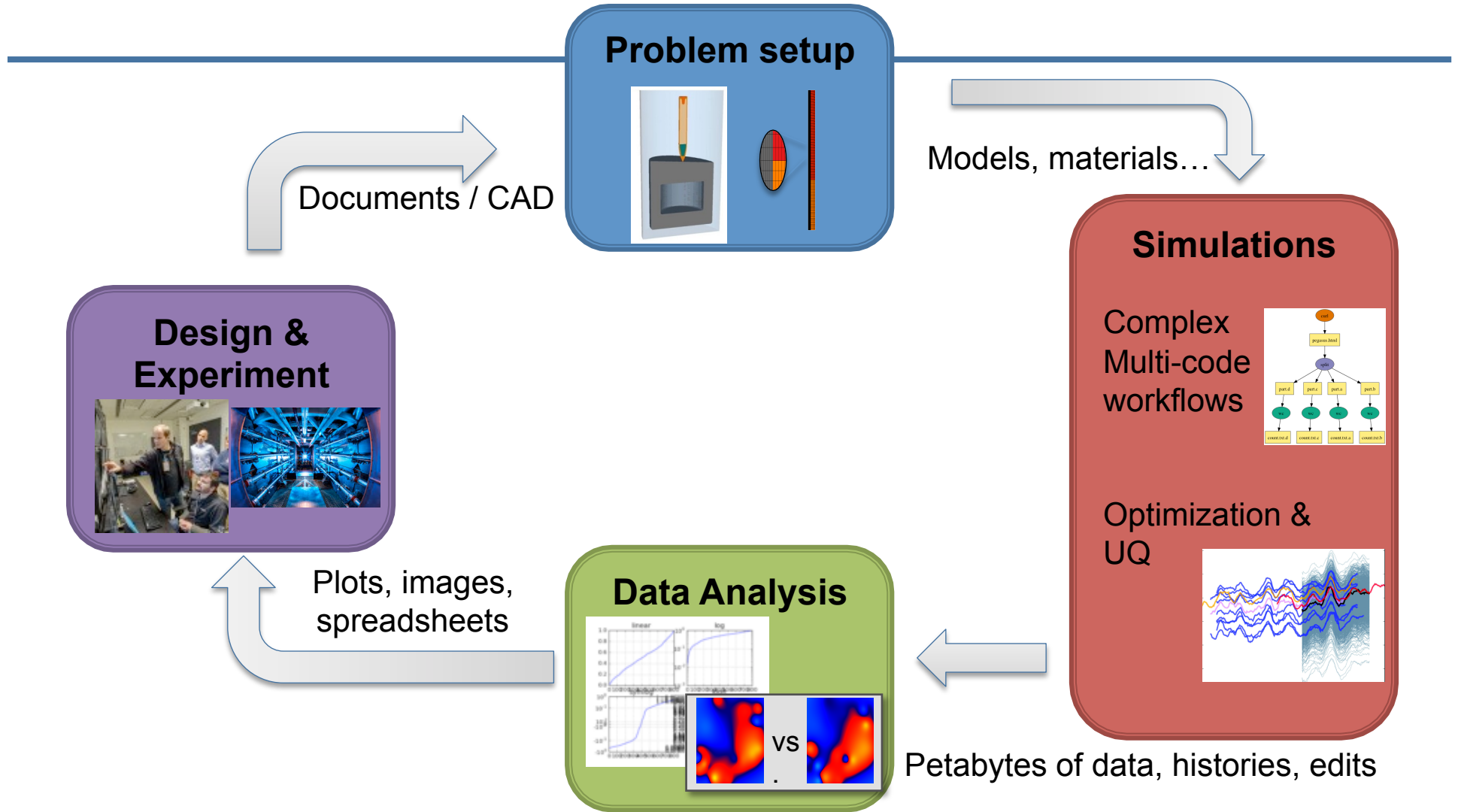
Workflow Project Overview

Daniel Laney
Workflow Project Lead

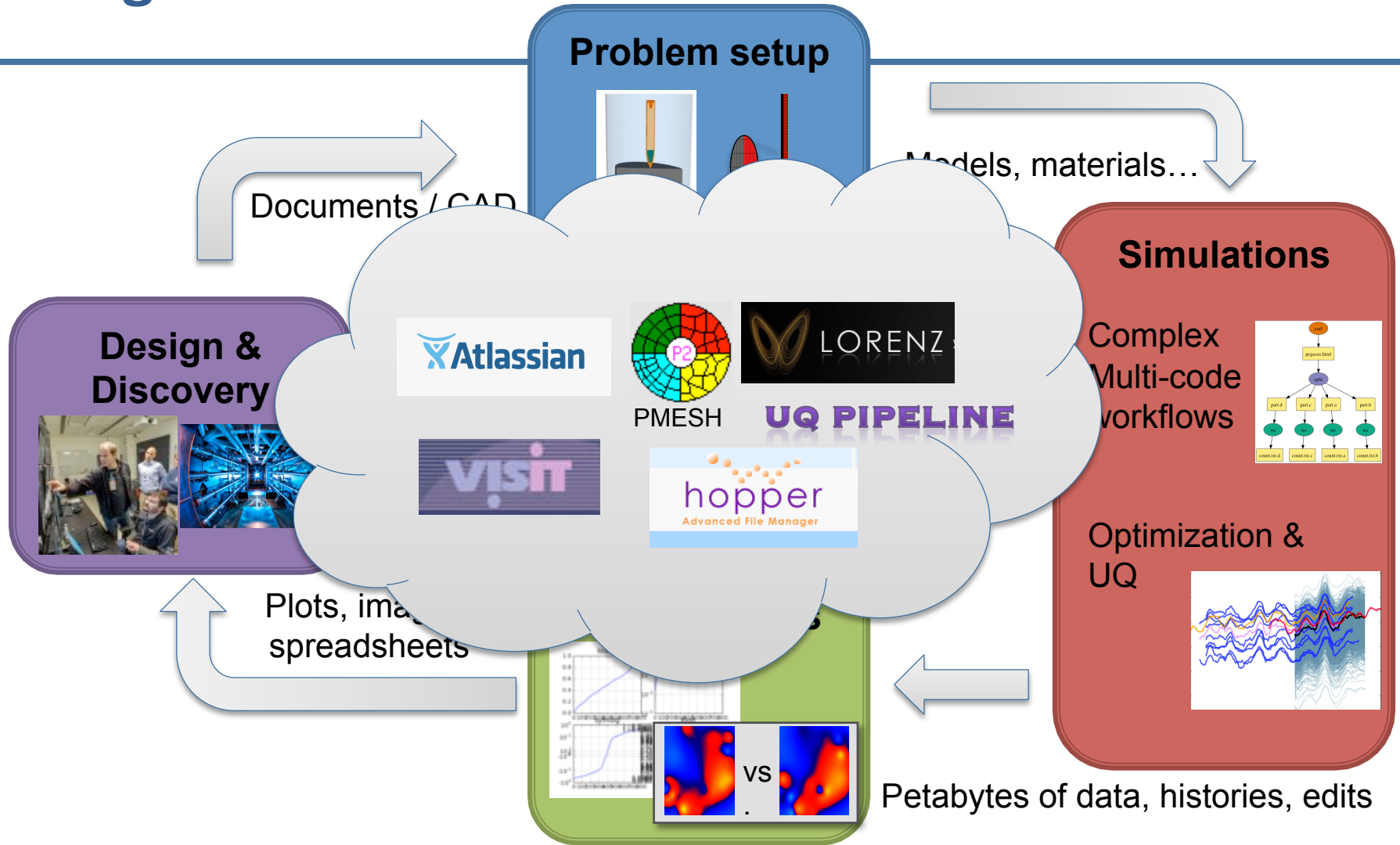
February 25, 2016



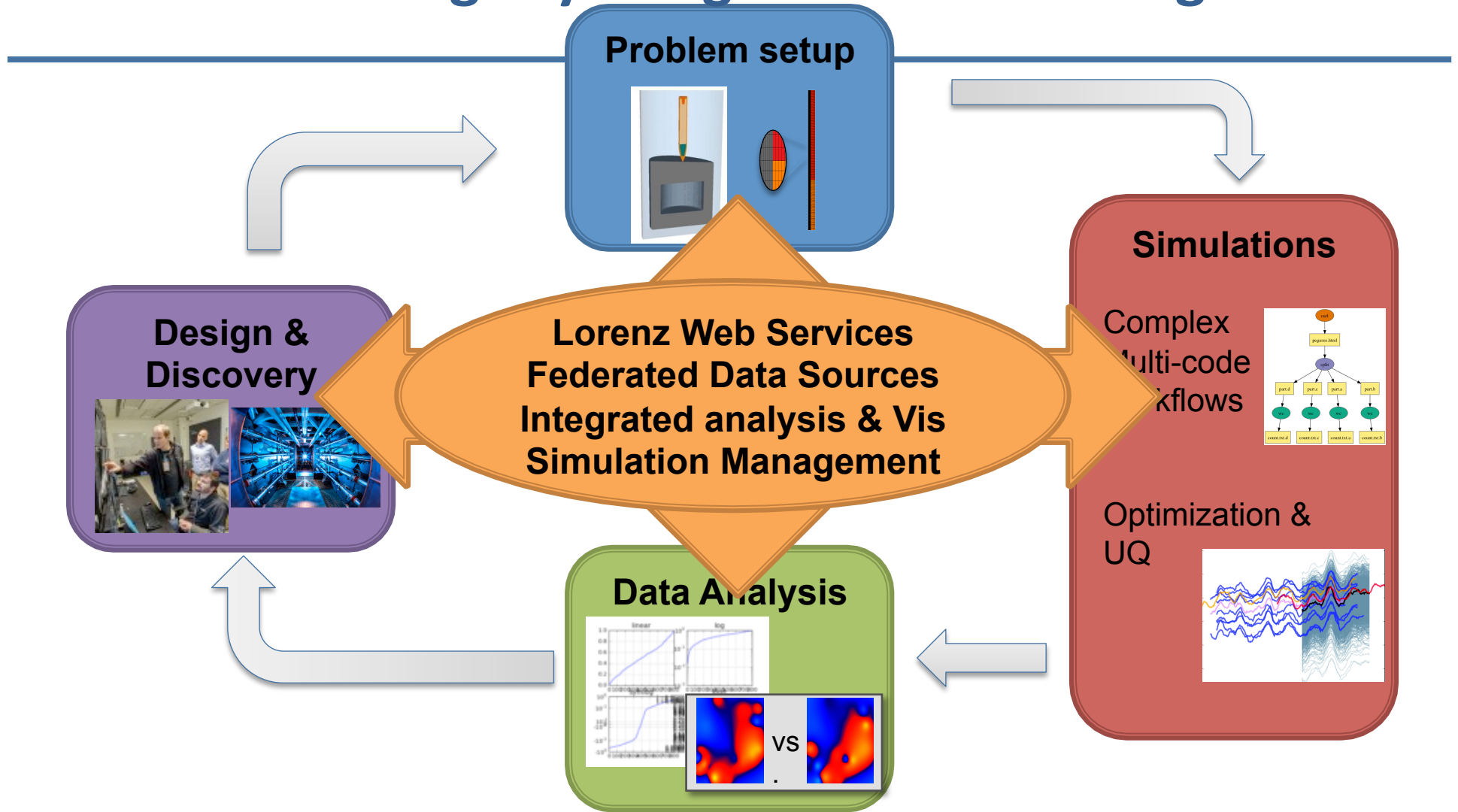
Our users have a diverse set of complex, iterative workflows



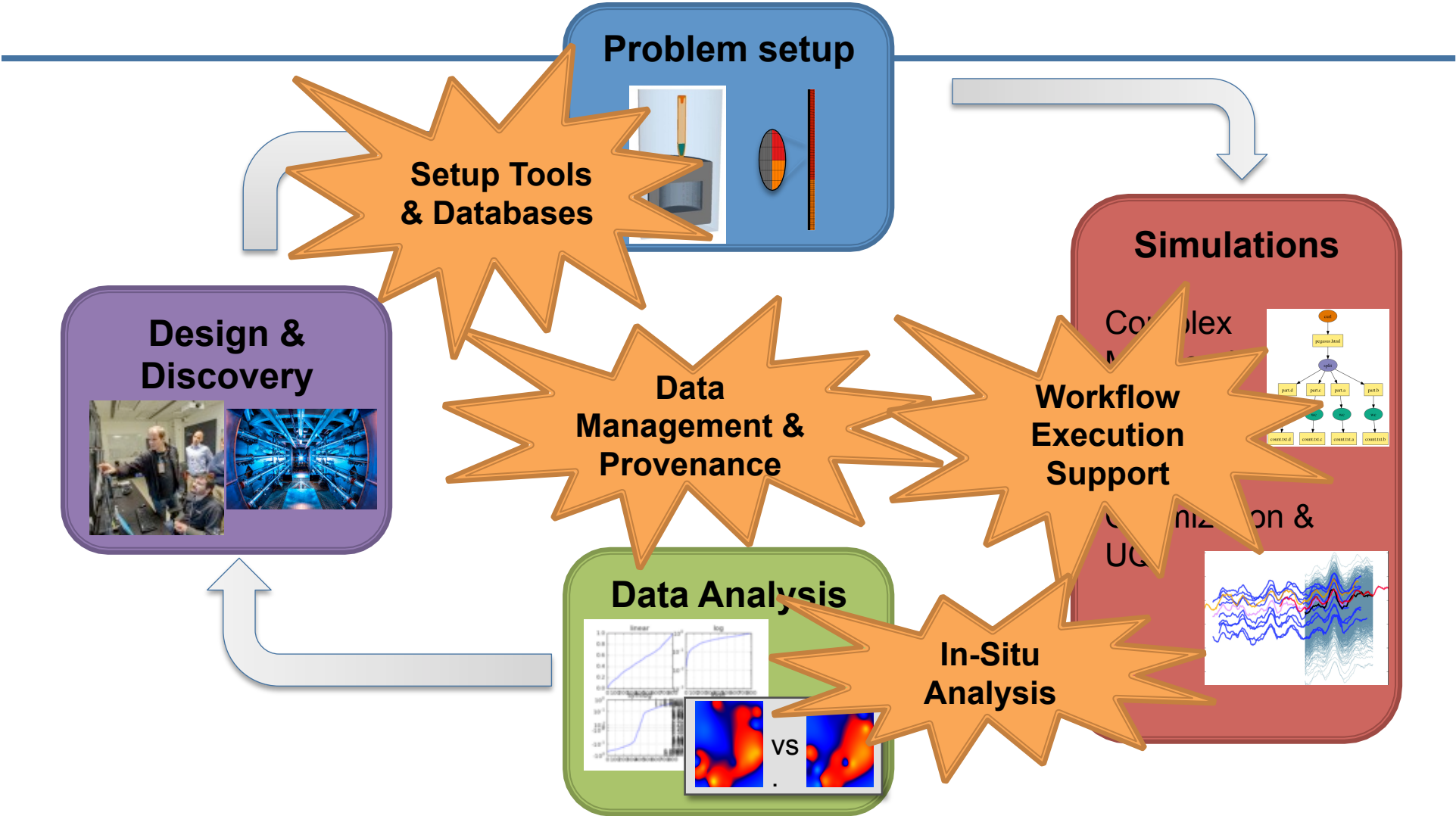
We provide a rich set of tools, but lack an integrated workflow environment for our users



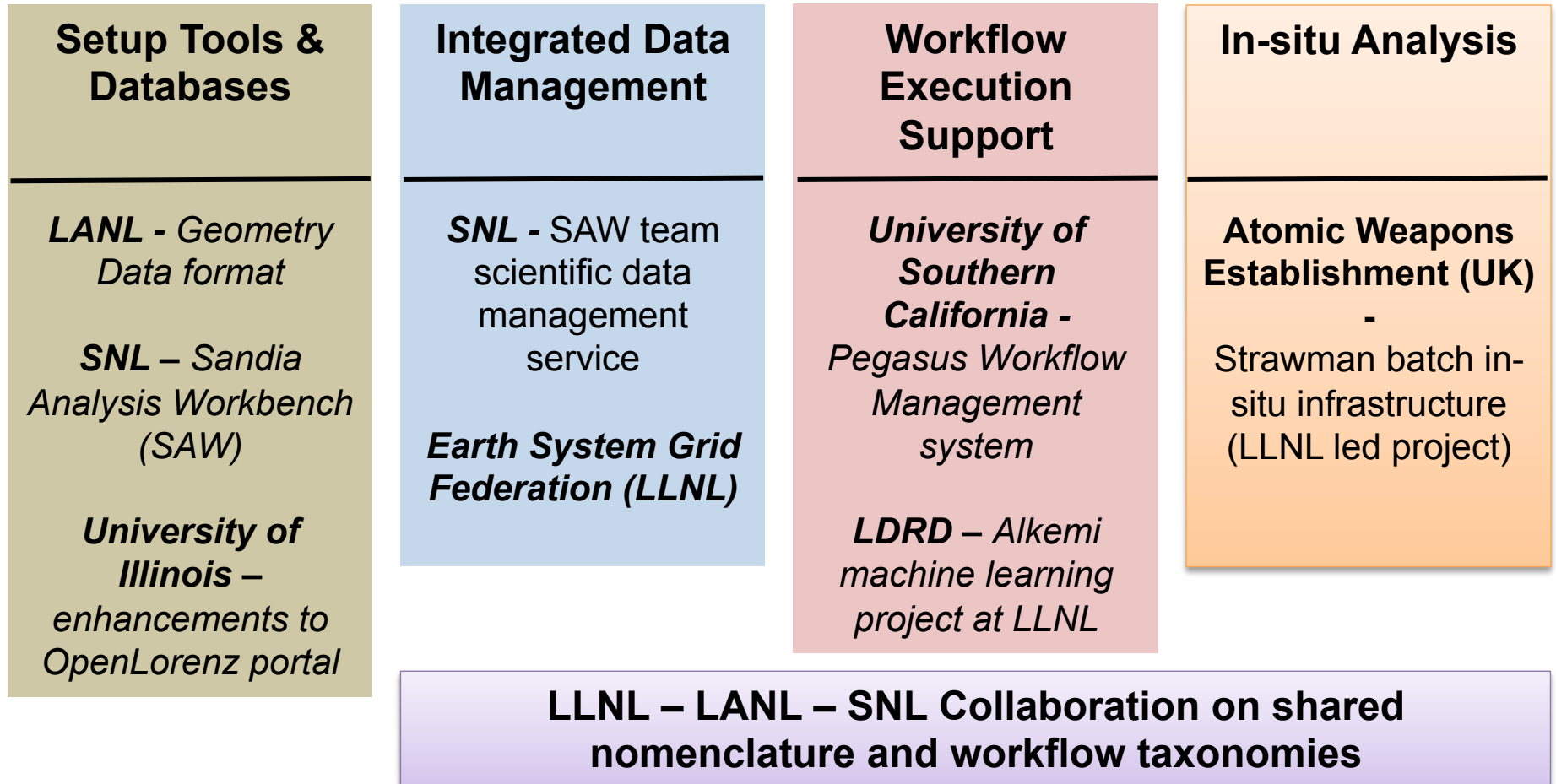
Our vision is to unify our tools around Lorenz services and tightly integrated data management



ATDM must close several gaps to realize this vision



ATDM efforts in these areas are leveraging new collaborations and partnerships



Geometry database and Contour Central demonstrator

- **Goal:** Common input geometry specification across multiple validated codes and labs
- Simple versioning and powerful editing of files
- Associating hierarchies of documents and geometry components

Created By: paul12
Creation Date: Feb. 2, 2016, 3:45 a.m.
Currently Viewing Overlay Car: Remonte Jr.
Edit Message

Visibility Controls: Drawing Opacity: Contour Thickness: Contour Color: Positioning Controls: Scale: 0.9736, Rotation: 0.4548062821551, R Offset: 0.4548062821551, Z Offset: 0.551272721302

Name	Type	Creation Date	Z Offset	R Offset
Wheel 1	Contour	Feb. 2, 2016, 3:40 a.m.	0	0
Wheel 2	Contour	Feb. 2, 2016, 3:40 a.m.	0	0
Windows	Contour	Feb. 2, 2016, 3:40 a.m.	0	0

Name	Type	Creation Date
Car Body	Contour	Feb. 2, 2016, 3:44 a.m.
Hub 1	Contour	Feb. 2, 2016, 3:39 a.m.
Hub 2	Contour	Feb. 2, 2016, 3:40 a.m.
Wheel 1	Contour	Feb. 2, 2016, 3:40 a.m.
Wheel 2	Contour	Feb. 2, 2016, 3:40 a.m.
Windows	Contour	Feb. 2, 2016, 3:40 a.m.

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```

ATDM

PMESH

LANL

We are planning to co-develop a scientific data management infrastructure with Sandia

- **Goal:** to develop light weight components that can be utilized by both labs
- Share costs of surveying prior-art and new software development
- Status:
 - We have combined the initial set of requirements of both labs
 - Now working on logistics

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handles multi-gigabyte files, it is not designed to store large numbers of such files, nor can it handle larger files in the terascale or larger regimes that cannot be easily moved. Ideally, in the next generation server, such files could be handled by first-class references to external data, so files residing on other systems could be easily referenced *in situ*. Besides improving scalability, this would allow the new SDM server to federate with other data management systems.

Requirements

The existing SAW SDM system sees daily use by a large user base at Sandia. The team has many ideas for improvements, but the number of user-requested improvements to the server itself is small. Therefore for the purposes of this proposal, we'll take the technical requirements for a new SDM server to be first and foremost to preserve the capabilities of the existing system, and supplement that main requirement with a short list of new business and technical requirements.

New business requirements are:

- Low- or no-cost at runtime
- Explicit support for external data references
- Easy adoption outside of Sandia (i.e., highly portable and extensible)

Existing capabilities and characteristics that must be preserved are:

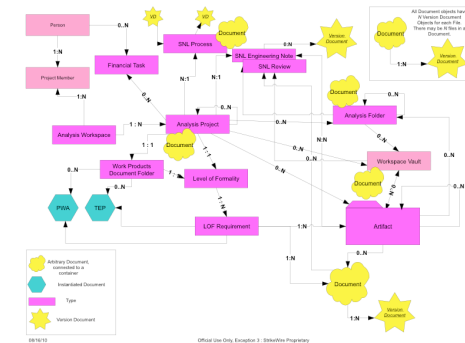
- Organizing documents into hierarchical folders and projects
- Storing arbitrary metadata about documents
- Versioning of documents
- Storing dependencies and relationships between documents and projects
- Storing documents on a filestore, and metadata in a database
- An NTK-compatible security model, with Kerberos and ACL (e.g., Sandia's metagroups) integration
- Java-based or Java-compatible
- Runs on Linux Server
- Full data migration must be possible
- Production (24/7/365) quality capability
- Complete backup/restore capability, including all

New user-requested capabilities:

- Performance improvements (specially???)
- Improved search capabilities (full-text search)

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VV4ALE3D: a validation suite for ALE3D based on a new framework for managing simulations

- **Goal:** to build extensible and plug-in oriented tools for managing and running suites of applications across WCI
- Integrating Web Technologies
 - Lorenz
 - Visualization and Analytics
- Helping to define data management requirements (SNL)
- Early target for Pegasus workflow engine evaluation (USC)

ATDM

Lorenz
(LC)

University
of Illinois

Pegasus
(USC)

ALE3D VV Report Manager [Home](#) [Configure Groups](#) [Run Tests](#) [History](#) [Verification Tests](#)

Run History

Info! This will display all runs from the VV that have been submitted.

Info! This is an experimental feature that will display a general overview of the success or failure of a run. This will include things to how accurately actual results compared to expected results, if the run terminated successfully, or by comparing other variables of interest.

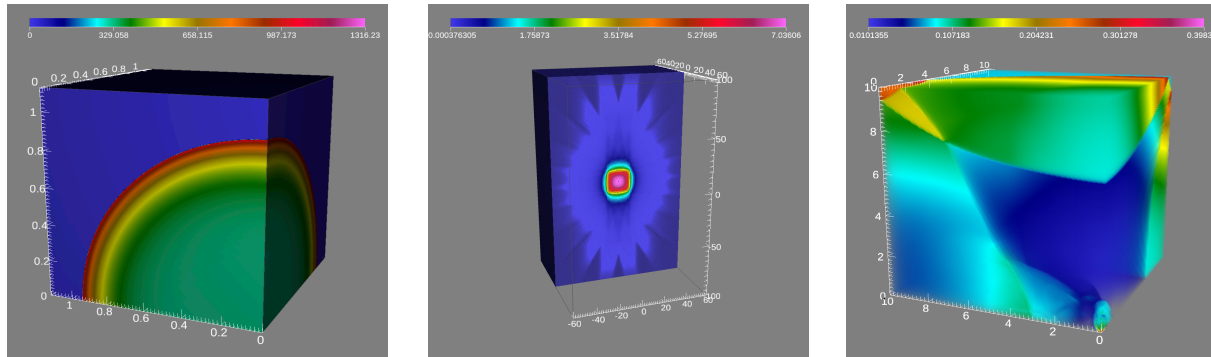
Potential Color Meaning

- Green - Actual matched expected
- Red - Actual did not match expected (completely off)
- Yellow - Actual was closeior results could not be determined

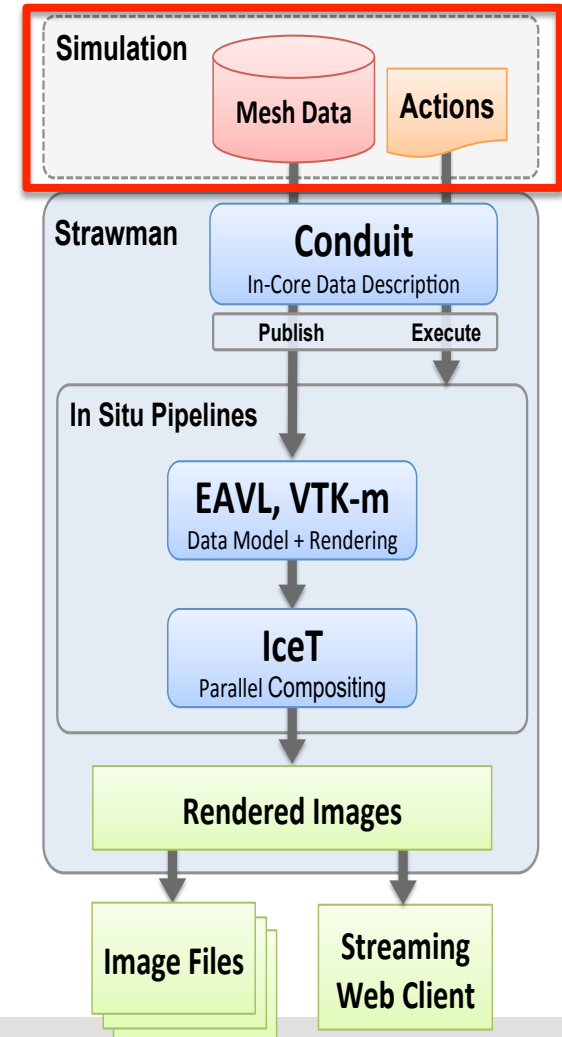
Run ID	Run Name	Sims Run	Date Run	Machine	Code Version	Processors	Wall Clock Time	Results	Rerun Tests
09152	Regression Run		11-01-2015	RZAlastor	4.6.2	256	2h		Rerun
09151	Regression Run		11-01-2015	RZAlastor	4.6.2	256	2h		Rerun
09150	Regression Run		11-01-2015	RZAlastor	4.6.2	256	2h		Rerun
09149	Version Update		10-30-2015	RZAlastor	4.6.2	256	1h		Rerun
09148	Regression Run		10-26-2015	RZAlastor	4.6.1	256	3h		Rerun

In-situ Analysis

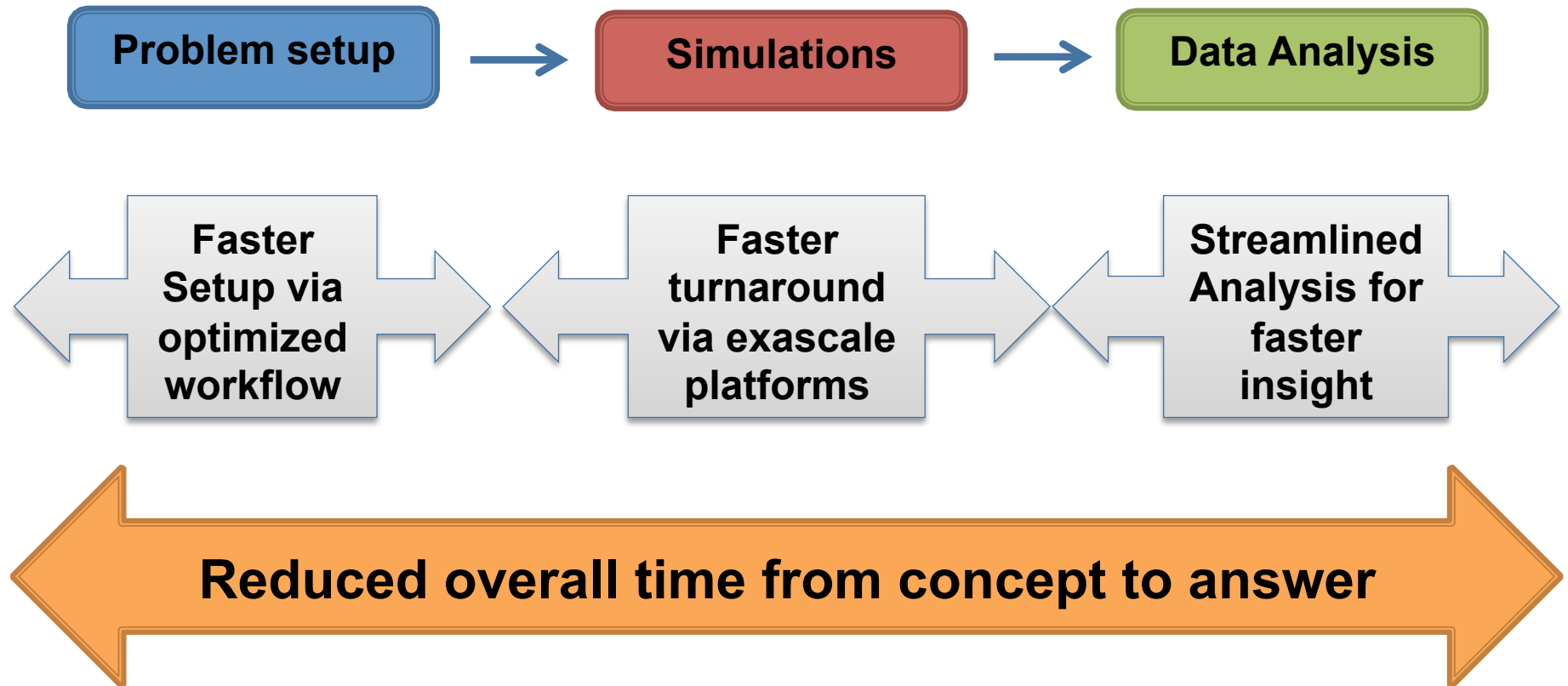
Strawman: a batch in-situ infrastructure for GPU-enabled analysis and visualization (with AWE in UK)



LULESH	Kripke	CloverLeaf3D
Hydrodynamics	Neutron Transport	Hydrodynamics
Unstructured	Uniform	Rectilinear
C++	C++	FORTTRAN



Our goal is a cohesive workflow environment that enables our users to harness exascale computing





**Lawrence Livermore
National Laboratory**