Scientific Knowledge Discovery
Cross Cutting Science –Coevolution of Experiments and simulations
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Amber Boehnlein

Preface:

The interplay between simulation and experiments at DOE facilities is increasingly important to advance the state of scientific discovery. As simulations of physical phenomena become increasingly precise and accurate, there will be wider applicability in the design of facilities, detectors and experiments and subsequent improvement of the simulations. In some cases, the experiment may be conceptually designed using one domain simulation, and the scientific results of the experiment used to improve the simulation of an entirely different domain. Such cases can drive requirements for scientific knowledge discovery.

Introduction:

In many domains, simulations drive experiments and experiments drive simulations. Improving the process and technologies that enable interplay and feedback will advance scientific discovery potential.

The state of the simulations and models and their connection to appropriate scientific communities varies dramatically from domain to domain; a few selected domains are outlined below.

High Energy Physics:

One domain science that fully integrates simulation and modeling into accelerator and experimental design and results is High Energy Physics. Codes for theoretical calculations and predictions are foundational to scientific understanding—such codes range from Lattice QCD calculations to generators to predict cross sections and topologies for proposed extensions of the Standard Model such as Supersymmetric Models. General purpose toolkits that encapsulate the effects of the passage of particles through matter are used to understand physical signatures that will be observed in the detectors and to model background radiation to appropriately design shielding. The approval process for any accelerator or detector

construction project includes the validation of benchmark physics channels and the demonstration of the instrument efficiency against those benchmarks.

There usually are several implementations or parameters that cover different regions of phase space. For that reason, experiments are sometimes designed for the specific purpose of benchmarking or tuning simulations so that those simulations can be used to predict physical phenomena. One such experiment is The Large Hadron Collider forward (LHCf) experiment that uses forward collisions in the Large Hadron Collider to simulate cosmic rays in laboratory conditions. Studying how collisions inside the LHC cause similar cascades of particles will help physicists to interpret and calibrate large-scale cosmic-ray experiments that can cover thousands of kilometres. (http://home.web.cern.ch/about/experiments/lhcf).

Even in this case, in which the community is aware of the tools, there are issues that limit scientific discovery.

A Multi-Domain Example:

There are existing cross disciplinary examples which draw on experimental and computational results from multiple fields.

A recent example demonstrates the connection between plasma physics and astrophysics to understand the origin and energy spectrum of high energy cosmic rays. Results from the Fermi Glast Space telescope confirms that expanding shock waves from ancient supernovas are the origin of cosmic rays observed on earth [2]. The physical mechanism for generating these collision shock waves remains an open question. Recent simulations have demonstrated that filamentary structures in high-energy density plasmas can be driven in laser-plasma interactions and lead to the formation of collisionless shocks with properties similar to the ones that are believed to occur in astrophysics. Realizing this experimental program will be an iterative process using progressively more powerful lasers, comparing the results to the plasma simulation which may require advances in computational science for plasma physics by requiring increased precision or finer granularity, ability to visualize the results, the possible addition of

physical effects at second or third order. At the same time, the MDH codes for type II supernovae collapse may need to be benchmarked against the Fermi results and perhaps modified as a result of the high energy density experiments. Realizing this science will require the sharing of data, information and knowledge across multiple different domains

Issues:

- Intellectual property—not all simulations are openly available
- Identifying knowledge gaps between simulation and experiment
- Frameworks, tools and analytics that enable comparable analysis of simulated and experimental/observational data including appropriate uncertainty quantification/error analysis.
- Enabling discovery of appropriate tools and results
    - Registry of codes and capabilities
    - Digital Object Identifiers for codes
    - Common/comparable Metadata and data formats
    - Community based analysis of the strengths and weaknesses of simulations that cover the similar domain space
    - Development of common benchmarks and references
    - Literature searches

Conclusion:

[1] R. A. Fonseca et al., OSIRIS: A Three-Dimensional, Fully Relativistic Particle in Cell Code for Modeling Plasma Based Accelerators, 2331 (2002)
[2] M. Ackermann, et al., Detection of the Characteristic Pion-Decay Signature in Supernova Remnants, *Science* 339 6121 (2013)
[3] G. Gregori et al. Generation of scaled protogalactic seed magnetic fields in laser-produced shock waves, Nature 481, 480 (2012).
[4] S.H. Glenzer, R. Redmer, X-ray Thomson Scattering in High Energy Density Plasmas, Rev. Mod. Phys. 81(4), 1625 (2009).
[5] F. Fiuza, R. A. Fonseca, J. Tonge, W. B. Mori, and L. O. Silva, Weibel-instability-mediated collisionless shocks in the laboratory with ultraintense

lasers, Physical Review Letters 108, 235004 (2012)