Accelerated Scientific Discovery with AI-driven Experiments in support of IFE

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Executive Summary

Recent advances in data science including breakthroughs in deep learning algorithms and advanced computational hardware will make it possible to accelerate scientific discovery by several orders of magnitude by conducting experiments at high repetition rates (HRR) (>10 shots/hour) with current and future generation high power lasers. Machine learning (ML) has shown utility in many areas of everyday life from reading hand-written text to self-driving cars and more recently in scientific applications relevant to IFE research (Spears, 2018) (Hatfield P. W., 2021). As safely operating self-driving cars at high speed requires synchronizing the inputs from a variety of sensors in real time, so to does safely operating a HRR laser facility designed to maximized a particular application, such as IFE. The example of self-driving cars provides a template for creating self-driving laser experiments where heterogeneous data is combined to operate the many components a single laser experiment (or "shot"). For this to be realized the laser (energy, pulse duration, focal spot, etc.) and target characteristics (foil thickness, shape, etc.) must be controlled and characterized prior to the shot while HRR-capable diagnostics must be rapidly and accurately analyzed after the laser has been delivered to the target. Prior to the experiment, 100's-1k's of simulations (ensemble simulations) can be used to scan a large set of input parameters such as laser energy and pulse shape. Deep learning can then be used to create fast "surrogate models" (Djordjević, 2021) that can be used to guide experimental exploration, and retrained with experimental data (Gaffney, 2019) (Humbird, 2019) to provide a basis for improving the fidelity of HED modeling capability. Coupled with artificial intelligence (AI), it will be possible to make decisions that will "drive" experiments to explore vast regions of high-dimensional parameter space for optimizing experimental quantities and ultimately improving the physics models used to simulate them. Along with the more obvious aspects of HRR experiments, IFE research will also need massive increases in speed for target development, production, characterization, and alignment. AI is already making an impact on the NIF as it is being used to identify optical defects on the main beam line with success rates that exceed that of trained experts

(Trummer, 2018). Lastly, ML will be necessary to handle (filter, analyze, store) the incredible amounts of data generated by experiments at HRR and ensemble simulations. Further developing these technologies and more importantly integrating them into autonomous experimental facilities will provide a path forward for rapid and efficient scientific progress for exploring the highly non-linear science inherent to inertial fusion energy (IFE).

Introduction

Until recently, much of laser-driven high energy density (HED) physics research has focused on large, energetic drivers (lasers, pulsed power machines) that are mostly single shot (about 1 shot / hour). Multiple high-repetition-rate (HRR), high-intensity short- pulse lasers have recently come online around the world (>1 shot/minute), with many more poised to be built in the next few years including kJ-class nanosecond pulse-duration drivers (Dyer, 2021). These lasers introduce a radical paradigm shift in the way HED experiments could be operated (Ma, 2021), however, the technology to utilize them to their full potential (i.e. at >1 Hz) lags behind. Typically, the process for scientific discovery has been a slow process compared to the possibilities offered by integrating AI technologies with HRR experimental platforms. First, theory and simulations developed over months/years provide a scientific hypothesis as the basis for a proposal for experimental time on a given laser facility; once accepted, experimentalists work to design targets and diagnostics (months); the experiments are executed, providing 10-100 datapoints; finally, time-consuming data analysis is performed and compared to new simulations to understand the experimental data and provide a new scientific hypothesis or proposed changes to experiments. In order to accelerate the rate of scientific discovery, target production/characterization, laser configuration/diagnostics, and experimental diagnostic analysis must all be able operate at commensurate rates. There are three main thrusts where ML can be useful for HRR experiments: (i) For fast laser/experimental data analysis; (ii) For autonomous real-time laser/target/diagnostic control; and (iii) Developing surrogate models for physics exploration/optimization. To enable this, advanced computational methods such as ML must be leveraged to analyze multi-modal data while AI can combine heterogeneous data and interpret it to guide experimental exploration without human intervention. Figure 1 shows the eventual vision for a fully integrated laser-driven experimental system that capitalizes on HRR and a series of feedback loops to simultaneously accelerate both empirical discovery and computer model development. First, the laser must be able to operate safely and with high stability while making changes proposed by a controlling algorithm. Next targets must be delivered on demand, ideally with some flexibility in construction, adequately characterized, and aligned prior to shot time. Diagnostics must also be able to operate in the hostile experimental environment without using traditional recording media such as image plate or film (M. J.-E. Manuel, 2020), and importantly be analyzed both rapidly and accurately (Mariscal, 2021) (Simpson, 2021). In order to compare experimentally acquired data to simulations, both sets of data will need to be combined in a "latent" space where important features have been distilled through ML. All pieces of this loop will benefit from the application of ML to increase speed while maintaining high accuracy. It is important to note that when fusion becomes robust and reliable, the machine repetition rate will necessarily increase by many orders of magnitude from what the current-generation ICF research facilities operate at. Thus, the integration of these technologies will be a key underpinning of a safe and stable power plant.

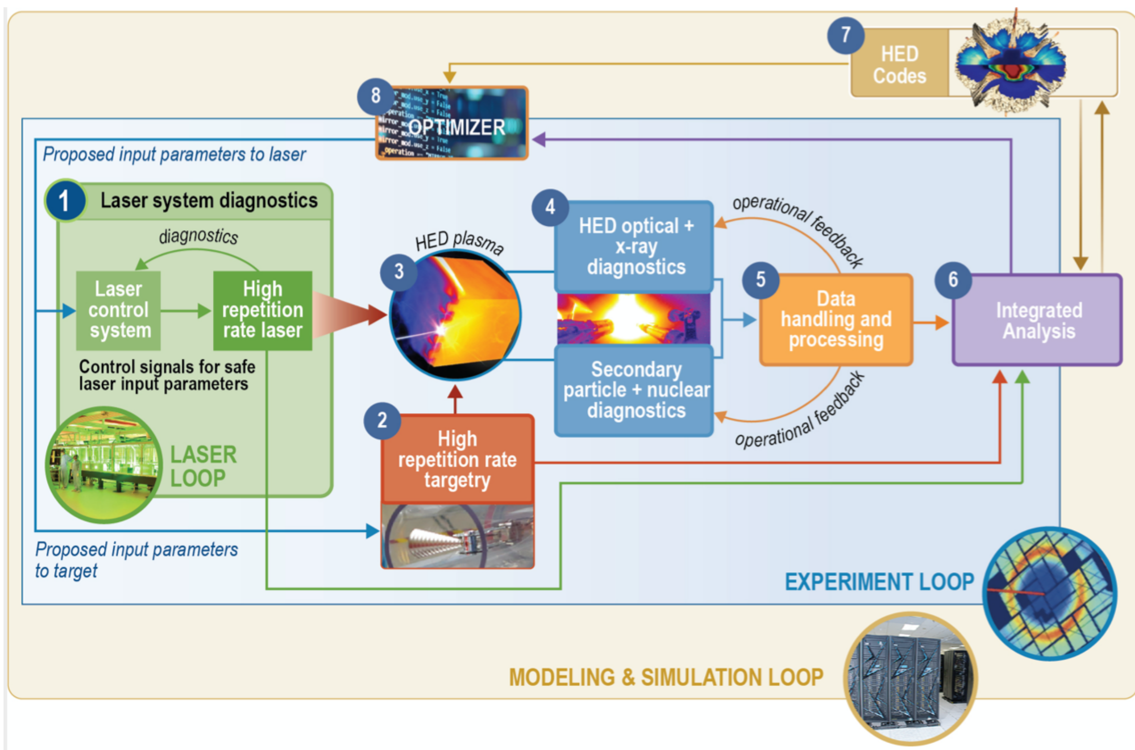

Figure 1: Outline of integrated HRR loops for rapid scientific advancement. The green, blue, and tan loops all rely on extremely fast & accurate analysis through ML in order to safely and intelligently operate the integrated system for self-driving science exploration. (from T. Ma, et al., (Ma, 2021))

Machine learning has made large strides over the last decade and has shown great utility in science, especially in regions where large datasets ("big data") can be generated. Some examples include classification of astrophysical objects (Jacobs, 2020), predictions of tokamak disruption (Rea, 2018), or identification of damage defects in optics used on the National Ignition Facility (Trummer, 2018), and prediction or optimization of ICF designs (Hatfield P. W., 2019) (Anirudh, 2020)and HED experiments (Martin, 2018). Demonstrations of the use of neural networks for analysis of diagnostic data from laser-driven experiments are increasing and showing the ability to exceed human-tended analysis in accuracy while decreasing the time to complete analysis by many orders of magnitude (from hours to milliseconds) (Mariscal, 2021) (Simpson, 2021). Further, by connecting simulations to diagnostic models it will be possible to perform "enhanced" multi-modal analysis where parameters that are impossible (or extremely difficult) to measure can be deduced. As a simple example, it is possible to deduce the pressure of an ideal gas by measuring the temperature, density, and volume without directly measuring it. In the context of IFE, advanced simulations codes would replace the ideal gas law to, for example, deduce the pressure achieved during an ICF implosion. At multi-Hz experimental rates, it is likely that several GB/s of data will be produced, or about a TB every 15 minutes. At such rates, ML will likely be needed to enable on-the-fly data reduction, filtration, and storage where decreased latency in these processes can be enhanced by ML-enabled "edge" computing near diagnostics (Bhardwaj, (2021).). Additionally, ML is being incorporated into laser control systems to ensure stable and safe operation (Galvin, 2018). Finally, AI has demonstrated utility in understanding highly non-linear systems such as inertial confinement fusion (Gaffney, 2019) (Hatfield P. W., 2019) (Humbird, 2019). To develop quick surrogate models, hundreds or thousands of low-dimensional or reduced-fidelity radiation-hydrodynamics or particle-in-cell (PIC) simulations are generated and using deep learning is used to develop surrogate models that can interpolate across wide swaths of parameter space (laser intensity, target thickness, etc.) to inform predictions of experimental outcomes. By enabling HRR experiments, it will be possible to generate the many thousands of data samples that are necessary to create a data-driven model.

Integrating all of the aforementioned pieces through AI will be necessary to realize the full potential of IFE research at high repetition rates. For example, a surrogate model generated from many simulations can provide a base model to which the experimental data can be compared. By utilizing transfer learning, these models can in principle be retrained on-the-fly with streaming NN-analyzed experimental data to combine multi-modal data and create real-world-informed models. In turn, these empirically informed models can be used to improve the physics models contained in HED codes. In this way, it will be possible to drastically accelerate the rate of learning from HRR experimental systems in support of key components of IFE.

Key Metrics

- Laser technology has enabled high-energy (10's J-kJ) multi-Hz operation. Compared to shot/hr facilities, this represents an opportunity to increase data throughput by ~36,000X.
- While lasers can operate at multi-Hz, control systems often still require "hands on" operation. ML must be leveraged to provide the fine control and exquisite stability that would be necessary for a IFE power plant.
- A typical NIF shot produces ~150 GB of data (laser and experimental data). If data is comparable, a rep-rated IFE facility could in principle generate 1.5 TB/second which quickly becomes "big data" and intractable via conventional "brute force" analysis. Data pipeline handling through AI will be necessary to filter, analyze, and retain important data.
- Human-operated analysis could take several hours to analyze a single piece of data while an optimized analysis algorithm may take several seconds to generate the reduced quantities of interest. An optimized NN for analysis can in principle analyze large (several MP) data on the millisecond time-scale, representing a 1,000X speed increase.
- It is now possible to utilize 1,000's of reduced fidelity simulations to scan multi-dimensional parameter space. While this is still computationally expensive, machine learning can be used to create surrogate models that interpolate between sparsely sampled parameter space. These models are thousands of times faster to evaluate (Kluth, 2020) for comparison/retraining during HRR experimental operations and have proven to be predictive of "future" experiments with relatively sparse datasets (Humbird, 2019).

Program Outline

To increase the rate of learning from HRR facilities in support of IFE, we propose a program that would seek to *integrate experiments and simulations , through machine learning and AI*.

Simulation groups should work to develop a robust methodology to rapidly scan input parameters and develop neural networks that can point to areas of interest and optimization.

Computational advances utilizing AI to guide ensemble simulation exploration (as in ICF) should be leveraged as the framework for experimental exploration.
Experimental efforts should focus on integrating the machine learning models to monitor and control the laser, targets, and analyze diagnostics. Significant research in HRR-capable target delivery systems and diagnostics should be made along with emphasis on the need to be able to actively control them.

Each of these pieces will rely on advanced computational algorithm development and utilization of the best available hardware to eventually integrate experiments and simulations to fully realize autonomous discovery. Further enhancements in experimental operation speed (analysis, targeting, data handling) may be realized through the use of low power computing located near data sources (i.e. “edge computing”), which should also be explored. Researchers should partner with DOE advanced computational groups and the beamline accelerator to community to incorporate large-scale data handling strategies and the incorporation of edge computing, such as at LLNL’s high performance computing facilities and LCLS-II for 1 MHz experiments. Advanced computational methods investments focused on integrating experimental and simulations systems will both broaden the study of IFE parameter space and increase the rate of learning by more than three orders of magnitude.

Collaborations with institutions in the US and facilities and abroad that have already had early successes with real-time experimental optimization (Shalloo, 2020) (Dann, 2019) should be strengthened. Investments in current HRR-capable facilities, such as those found in LaserNetUS, should be made in order demonstrate these technologies in preparation for future HRR HED facilities such as SLAC’s MEC-U (short pulse (150J, 150fs 10Hz); a 100J-class long pulse (10Hz); and a kJ long pulse).

Data standardization for both experiments and simulations should be emphasized to further increase the ability to share and collaborate between groups. The ability to quickly share data will be vital to progress in IFE research. By standardizing data and communication protocols, it may be possible to enable multi-facility, multi-scale experiments where lower power drivers can develop models that can be validated at larger scale facilities. This could then lead to further speed increases in learning for IFE.

While many of the component advanced computational techniques are in everyday use for scientific applications, it will be necessary to emphasize the integration of these systems with HRR facilities to utilize DOE investments to their full scientific potential. Ultimately, investments in this area stand to increase scientific payoffs in support of IFE by several orders of magnitude. Demonstrations of AI-driven laser facilities will serve as roadmaps for safely operating IFE facilities with stable output.

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