Simulations Explain High-Energy-Density Experiments

MAXIMIZING energy density—the amount of energy stored in a given volume—is a common research theme at Lawrence Livermore. Energy density can take many forms. Aeronautical engineers want a fuel with maximum energy density for rocket liftoff. High-energy-density foods are vital to endurance athletes, such as cyclists in the Tour de France. The object with the highest energy density ever created by humankind is an exploding thermonuclear weapon.

Recently, a Computing Grand Challenge project on Livermore’s Atlas supercomputer simulated the results from two sets of laser-driven high-energy-density (HED) experiments. These simulations have helped explain the physics behind what was seen and measured in the experiments.

In one set of experiments, researchers zapped very small reduced-mass targets with ultrahigh-intensity lasers to get the dense targets as hot as possible. (See the box on p. 14.) Such targets, which produce high-energy electrons, protons, and x rays, are being considered as backlighters for radiography diagnostics on the 192-beam laser system at the National Ignition Facility (NIF).

In a second set of experiments, researchers used intense laser light to create a laser wakefield accelerator to speed up electrons in a low-density plasma. Such accelerators are anticipated to reach energies of 10 gigaelectronvolts (GeV,
1 billion electronvolts) over a meter, which is much shorter than the multikilometer length of most particle accelerators.

“In the laboratory, tightly focused, intense laser light in ultrashort pulses is one of the most efficient ways to quickly transfer large amounts of energy into a small volume of material,” says physicist Scott Wilks, who led the Grand Challenge project. “In fact, it is the basis for the fast-ignitor fusion concept.” In 2007, the Laboratory’s annual Computing Grand Challenge Program allocated 83.7 million hours of machine time on the Atlas and Thunder supercomputers to just 17 research projects, one of which was Wilks’s.

“Intense” laser light means more than a quintillion watts of energy per square centimeter ($10^{18} \text{ W cm}^2$). During HED experiments, laser light slams into a tiny target and then interacts with the plasma that is created. This interaction generates electrons that move in targeted materials at almost the speed of light. Diagnostic devices abound, but understanding the results can be difficult because laser energy and plasma interact in complex, highly nonlinear ways.

Simulating the physics of the experiments on powerful supercomputers is often the only way to both understand the results in detail and develop physical insight into these complex processes. Simulations can parse the physical constituents that affect the whole and examine microscopic details not easily detected during an experiment. In addition, computer simulations can explore regimes of temperature, density, and pressure that experiments cannot yet achieve, serving as a guide for future experiments. Ultimately, scientists must depend on both experiments and simulations working in tandem to advance HED physics research.

Explaining the Unexpected

In one set of HED experiments, researchers used ultrahigh-intensity lasers with ultrashort pulses to zap one side of a reduced-mass target. “These very small, square targets [100 micrometers across and 7 micrometers thick] were initially designed for studying certain aspects of neutron stars,” says physicist Hui Chen. “Our goal was to get a dense target as hot as possible in the presence of a large magnetic field.”

The 2007 experiments performed on the Callisto laser in Livermore’s Jupiter...
Laser Facility showed that the target did get hot, but an unexpectedly large number of protons were ejected from the entire surface of the target. In contrast, when a laser zaps a larger (millimeter size) target, a beamlike pattern of protons blows off the back of the target.

To simulate Chen’s experimental results, physicist Andreas Kemp used the Particle Simulation Code (PSC), a particle-in-cell code specifically designed for studying electrons in a high-energy plasma. The computational capabilities of Atlas allowed Kemp to simulate laser–plasma interactions in reduced-mass targets at full scale from first principles.

In a two-dimensional (2D) simulation of a large target, electrons accelerated by the laser generated an electric field on both the top and bottom of the target. In a simulation of a smaller, “finite” reduced-mass target, large electric fields developed on the sides of the target as well, which explained the signal detected all around the target in experiments. This simulation showed that shrinking a target to a smaller size does not increase target temperature but instead increases the total number of ions accelerated from all of its surfaces. In fact, it was precisely the pattern seen in Chen’s puzzling data. A 3D simulation also predicted maximum proton energies out the back of the target to be about 5 megaelectronvolts, which agreed with experimental results. Results from the Atlas simulations indicate that smaller targets may be more efficient ion accelerators than larger targets, which could make fast ignition using proton beams competitive with hot electron–based fast ignition.

Kemp notes that a full-physics code such as PSC is expensive to run. As a consequence, he performed just a few 3D simulations. In addition, Kemp developed a number of 1D simulations that were derived from 2D results. He found that the interface where the laser interacts with the plasma recedes significantly. A series of in-depth, 1D simulations helped researchers understand the hydrodynamics at the interface.

Kemp was delighted to have so much dedicated computer time. Laser–plasma interaction simulations are highly complex and computationally intensive. “Although the events we simulate occur on a subpicosecond timescale [less than a trillionth of a second], hundreds of CPUs [central processing units] running in parallel for a long time are needed to examine the many interactions in that brief moment of activity,” says Kemp.

In the past, PSC has been run for limited periods on machines at the National Energy Research Scientific Computing Center in Berkeley, California, and on the Earth Simulator in Japan. “The access we had to Atlas made quite a difference,” says Kemp. “We could do a run, make some changes, and do another run. The time on Atlas allowed us to make a lot of progress.”
Simulations Ride the Wave

In the second set of HED experiments simulated on Atlas, a short-pulse, high-intensity laser system accelerated electrons within a plasma. The 2004–2006 experiments were run by the Laser Optics and Accelerator Systems Integrated Studies (LOASIS) Program on the LOASIS laser at Lawrence Berkeley National Laboratory under the leadership of Wim Leemans and in collaboration with Simon Hooker’s group from Oxford University. They demonstrated that gigaelectronvolt beams can be produced by a channel-guided laser plasma accelerator.

In these experiments, a laser pulse propagates through a low-density plasma channel, leaving behind a plasma density oscillation, or wakefield. The electric field of this wakefield pulls electrons forward, accelerating them thousands of times faster, and hence requiring much shorter distances, than a conventional particle accelerator. (See the box on p. 15.)

Experiments and simulations to date have demonstrated production of 1-GeV energies over a distance of 3 centimeters and indicate that a laser wakefield accelerator (LWFA) could reach energies of 10 GeV in a mere meter. The availability of an accelerator this small could put experiments with high-energy electron beams in many laboratories.

Simulations on Atlas probed the dynamics of how electrons are trapped by the wake to better understand the LOASIS experiments and to plan future experiments. The LWFA simulations were conducted by physicists Cameron Geddes and Estelle Cormier-Michel of LOASIS and by David Bruhwiler and John Cary of Tech-X Corporation in Boulder, Colorado. The team performed the simulations using the particle-in-cell capabilities of VORPAL, a parallel computational framework. Tech-X scientists, who have collaborated for several years with the LOASIS group, developed VORPAL.

Although simulations in the past have shown how the particles are trapped and concentrated as they outrun the wake, a crucial challenge has been to accurately model the particle beam’s divergence and energy spread. Particle-in-cell simulations of plasma incorporate particles moving in space with an electromagnetic field on a grid. “The particles are discrete objects,” says Bruhwiler, “while the electromagnetic field is continuous.” The discrete particles and interpolation from the grid create noise in the simulations.

The time on Atlas gave the team the opportunity to improve VORPAL’s algorithms and reduce this noise by weighting both forces and particle currents more smoothly across the grid. “The particles are discrete objects,” says Bruhwiler, “while the electromagnetic field is continuous.” The discrete particles and interpolation from the grid create noise in the simulations.

The first experiments with a high-energy, ultrashort-pulse laser were performed at Lawrence Livermore in 1996 on the Petawatt laser, which delivered a record-setting 1.25 petawatts (quadrillion watts) of power. The Petawatt laser was developed to test the fast-ignition concept for inertial confinement fusion. Achieving the fast-ignition route to nuclear fusion requires a detailed understanding of electron generation and transport, some of which has come from experiments using reduced-mass targets (RMTs).

Physicist Hui Chen performed the most recent RMT experiments in 2007 on the ultrashort-pulse Callisto laser in Livermore’s Jupiter Laser Facility. She was also at Rutherford Appleton Laboratory in the United Kingdom when the first-ever RMT experiments were performed in 2003. Earlier experiments examined x-ray production from RMTs and confirmed important characteristics such as high temperatures and heating uniformity. Tiny RMT targets may be useful as highly efficient ion accelerators, with accelerated protons providing the energy required to ignite a larger target.
In 2006, during the highest-energy laser wakefield acceleration experiments to date, scientists at Lawrence Berkeley National Laboratory accelerated electrons to energies exceeding 1 gigaelectronvolt (GeV) over a distance of just 3.3 centimeters. The high electron energies achieved with moderate input laser energy demonstrated just how effective a laser wakefield can be for accelerating electrons.

Two parameters must work together precisely to achieve efficient electron acceleration. One parameter is the plasma’s density profile. A plasma density channel—a structure with lower plasma density along the axis of the laser beam—is essential to extend and control the laser’s focus over longer distances than would otherwise be possible. This focusing must be done at low plasma densities to allow for the acceleration of electrons to high energies before outrunning the wake. The second parameter is the shape of the laser pulse, including its power and length, which drives the wake’s oscillations. If the amplitude of the oscillations is too low, no particles are trapped. Too high of an amplitude results in uncontrolled trapping, which degrades beam quality.

Just as a surfer can ride the wake of a powerboat, so can electrons ride a “wakefield” behind a laser beam channeling through plasma.

Atlas simulations have been used to design experiments planned for 2012 at LOASIS. These experiments are expected to generate 10-GeV energies in a channel half a millimeter wide and a meter long. The plasma’s density will need to be lower than in past experiments to maintain the necessary conditions over the longer distance. Because a 3D simulation of a single centimeter of beam propagation requires a million CPU hours, modeling a meter-long stage with traditional particle-in-cell codes is prohibitive. However, Bruhwiler successfully used 1D simulations to verify 10-GeV energy gain and evaluate the evolution of the laser beam over a 1-meter length. By comparing these results with those from much faster, reduced-physics algorithms, he was able to simulate 10-GeV LWFAs in 2D and 3D.

**The Power of Atlas**

All of these HED experiments and simulations help bring the Laboratory closer to its goal of achieving inertial confinement fusion on NIF and to applying HED science to new particle accelerators. “This grand challenge project not only gave us the computer time needed to quickly make a lot of progress toward understanding the underlying physics by doing many smaller runs,” says Wilks, “but also allowed us to simulate full-scale laser–target experiments in 3D for the first time. We learned a great deal about the complex ways that intense, short-pulse lasers transfer their energy to electrons.”

—Katie Walter

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