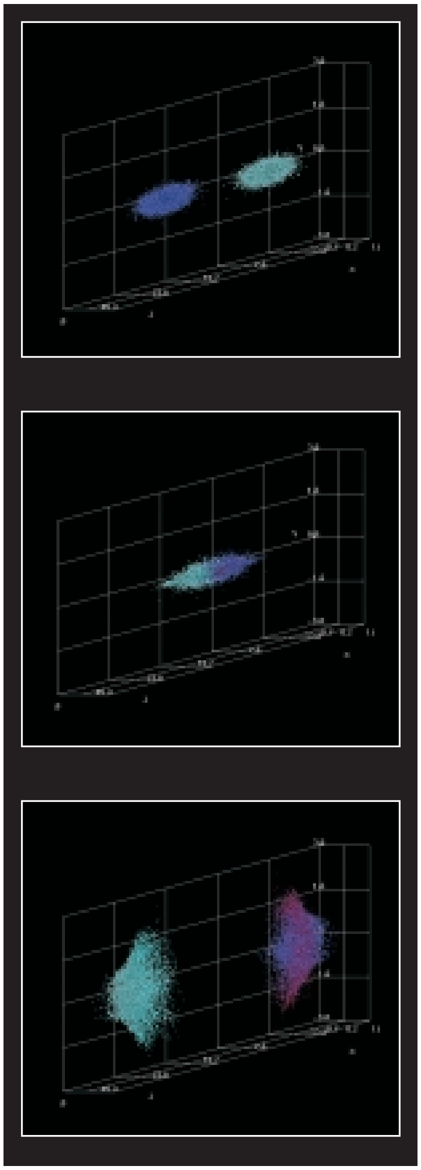
THE SYNTHESIS OF ACCELERATOR SCIENCE AND ADVANCED COMPUTING

Developing Extraordinary Tools for Extraordinary Science

ERNEST ORLANDO LAWRENCE invented the cyclotron seven decades ago, and though much has changed since then, his namesake laboratory in Berkeley, Lawrence Berkeley National Laboratory (LBNL), remains committed to leadership in accelerator science and technology. While operating and enhancing state-of-the-art facilities like the Advanced Light Source (ALS), LBNL researchers are designing future accelerators, including a “fourth generation” light source and “drivers” for heavy ion fusion. They are also developing novel laser- and plasma-based accelerator concepts that will extend the frontiers of accelerator science. Advanced computing is playing a key role in these important accelerator programs at LBNL.

LBNL operates several U.S. Department of Energy, Office of Science facilities including the Advanced Light Source (left) and the National Energy Research Scientific Computing Center (above).



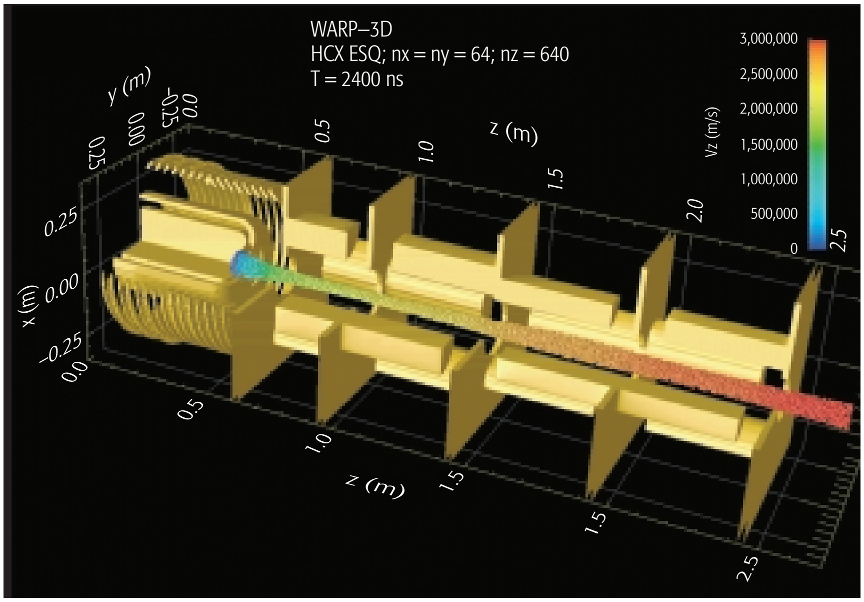
These figures show a collision between two bunches of particles modeled using a new, parallel simulation code developed at LBNL. Such large-scale simulations, like this one performed on NERSC's IBM/SP supercomputer, help accelerator physicists understand the electromagnetic interaction between beams in a collider. This ability is used both to improve the performance of existing machines and to facilitate design decisions for next-generation accelerators.

JI QIANG (AFRD) AND CRISTINA SIEGERIST (NERSC).

PARTICLE ACCELERATORS are critical to research in many fields—in fact, they are relevant to all four strategic elements in the science portfolio of the Department of Energy's Office of Science. The DOE Office of Science has been largely responsible for the development of the nation's major accelerator facilities. This is particularly true of its programs in High Energy and Nuclear Physics, Basic Energy Sciences, and Fusion Energy Sciences. These accelerator facilities include high-energy colliders, synchrotron light sources, and spallation neutron sources, and they are critical to research in many fields, including high energy physics, nuclear physics, materials science, chemistry, and the biosciences.

Accelerators have also been proposed that address national needs related to energy, the environment, and national security. Examples include accelerator-driven fusion and fission energy systems, accelerators for nuclear waste transmutation, and accelerators for radiography of hydrodynamic systems. On a smaller scale, particle accelerators and the technologies associated with them have many other applications that are highly beneficial to society. Examples include medical isotope production, irradiation and sterilization of biological hazards, particle beams for medical irradiation therapy, superconducting magnets for medical MRI, ion implantation, and beam lithography. As these examples show, particle accelerators are extremely important to scientific and technological progress and to improving the quality of people's lives.

ADVANCED COMPUTING is essential for studying and enhancing existing accelerators and for designing future accelerators. Today's major accelerator facilities are among the largest and most complex of all scientific instruments. Designing upgrades to expand the operational envelopes of these facilities requires large-scale simulations run on parallel computers. The next generation of accelerators will present even greater challenges as designs expand the frontiers of beam intensity, beam energy, and system complexity. The three-dimensional, nonlinear, multi-scale, many-body, and time-dependent characteristics of future accelerator design problems, and the complexity and immensity of the associated computations, add up to extreme technical difficulty.



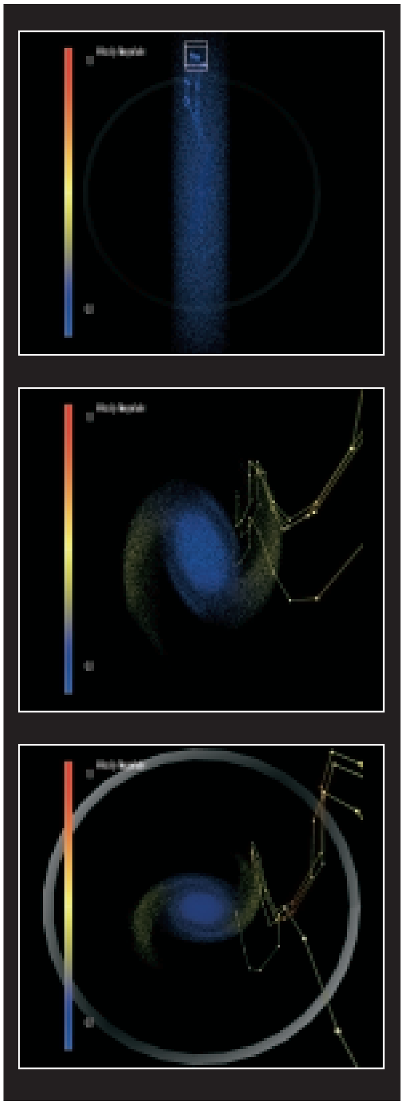
The applications of accelerators extend far beyond their origins in high-energy and nuclear physics. This is a frame from a WARP3D simulation of an intense, high-current, space-charge-dominated heavy-ion beam's progress through the High-Current Experiment (HCX). The HCX is the present step in a program, performed jointly with Lawrence Livermore National Laboratory and Princeton Plasma Physics Laboratory, to develop heavy-ion accelerators as efficient and cost-effective "drivers" for inertial fusion energy. This 3D time-dependent simulation followed the space-charge dominated beam from the ion source through a series of electrostatic quadrupole focusing elements, as in the current configuration of the actual experiment at LBNL. On an ultrascale computer at a sustained performance of 100 Tflop/s, end-to-end simulation of a full scale driver is expected to require approximately 20 hours of computing time.

JEAN-LUC VAY (LBNL), AND DAVE GROTE AND
ALEX FRIEDMAN (LLNL).

LBNL is playing a major role in developing a new generation of accelerator modeling codes for the terascale era and the upcoming ultrascale era of high performance computing. (Ultrascale supercomputers—expected by 2005—will achieve a performance of more than 100 trillion operations per second, or Tflop/s.) Within LBNL, several organizations are collaborating to develop these new capabilities. The organizations include the Accelerator Modeling and Advanced Computing Program, the Center for Beam Physics, and the Heavy Ion Fusion Virtual National Laboratory in the Accelerator and Fusion Research Division (AFRD); the Advanced Light Source Division; the Computational Research Division; and the National Energy Research Scientific Computing Center (NERSC). LBNL is also a co-lead laboratory on a SciDAC accelerator modeling project. Through these and other projects, LBNL is developing a new generation of accelerator modeling codes in collaboration with several national laboratories and universities. LBNL's work has two main areas of emphasis: development of beam dynamics codes, and development of codes for simulating advanced accelerator concepts.

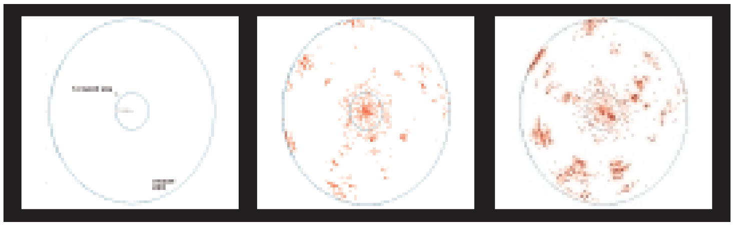
SIMULATION STUDIES OF BEAM DYNAMICS

As particle beams are accelerated and focused, they undergo tremendously complicated interactions with their environment. This environment includes the electromagnetic fields of the accelerator (including wakefields), the beam itself (e.g., space-charge effects and intrabeam scattering), fields from other beams (as in a collider or a multi-beam fusion driver), interactions with secondary particles (for example, the electron-cloud effect), and interactions with radiation fields. These phenomena can produce beam halos, degrade the beam quality, and result in beam instabilities that limit accelerator performance. Working with institutions such as LANL, FNAL, BNL, UCLA, and U. Maryland, LBNL is developing a new generation of beam dynamics codes to model these and other effects on parallel computers. The codes include IMPACT (a high-intensity linac simulation code), MaryLie/IMPACT (which will extend IMPACT's capabilities to circular machines), BeamBeam3D (a code for modeling colliding beams), and Langevin3D (for the self-consistent simulation of intrabeam scattering and electron cooling systems).



In these frames showing the time-dependent density evolution of an intense beam, the high density region is the beam core. Selected particles of interest, depending on the physical problem under study, are shown as streamlines. In this case, the streamlines correspond to halo particles in a very low density region far from the core. The spiral arms show the result of the beam's being injected improperly into the accelerator, which in this case is a separated sector cyclotron.

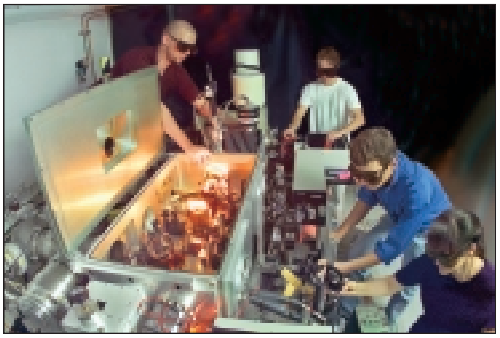
ANDREAS ADELMANN AND CRISTINA SIEGERIST, NERSC.



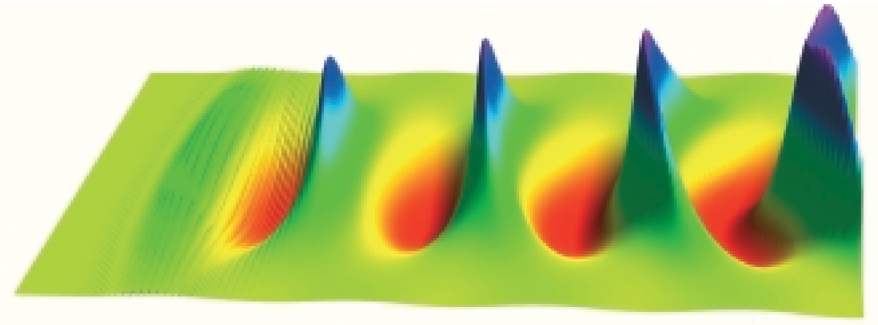
The "electron-cloud effect" is one of many phenomena that were only recently discovered, or hitherto could be neglected, that are significant in some of today's accelerators and will take on even greater importance in future accelerators. Electron-cloud instabilities are important in today's high intensity proton rings (like the LANL PSR) and B-factories (PEP-II and KEK-B). The effects will be even greater in future machines like the SNS accumulator ring and the LHC. This simulation shows, from left to right, a sequence of frames from a simulation showing the buildup of the electron cloud, a buildup so great that it can disrupt the main beam being accelerated.

MIGUEL FURMAN AND MAURO PIVI, AFRD.

SIMULATION OF ADVANCED ACCELERATOR CONCEPTS

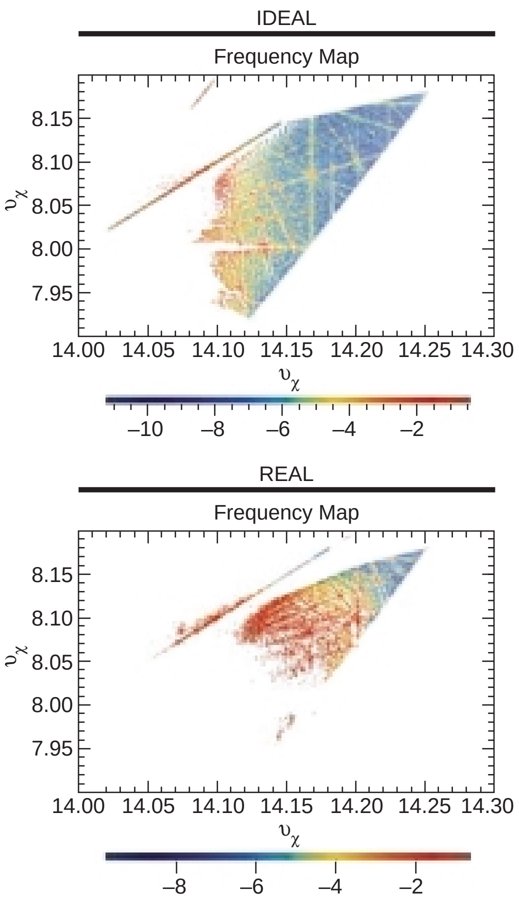


Since high energy accelerators cannot grow in size indefinitely, it will be necessary to develop new technologies capable of higher acceleration gradients. One possible approach is to use the extremely high fields that can be generated in lasers and plasmas. If these benchtop experiments could be developed into useable accelerators of much smaller size than today's, the payoff would be immense, not only in high-energy physics but in wide-ranging applications of compact accelerators to scientific research, industry, and medicine. Thanks to the confluence of successful small-scale experiments, terascale computing resources, and parallel 3D codes for modeling laser/plasma accelerators, it is now possible for full-scale simulations to play a pivotal role in guiding experiments. In addition, the fundamental physics inherent in ultra-intense laser and beam-plasma interactions is rich in nonlinear, ultrafast, and relativistic physics. The insight gained from large-scale particle-in-cell codes is essential for unraveling this new physics.



Berkeley Lab excels in the areas of theoretical, computational and experimental research on advanced laser-driven plasma-based accelerators. These devices are capable of sustaining ultrahigh accelerating gradients (10-100 GV/m, some three orders of magnitude beyond conventional technology) at their present laboratory scale, and are promising candidates as future compact high-energy accelerators and as drivers for novel short-pulse radiation sources. The accelerating field comes from an electron density wave generated by the radiation pressure of a high-intensity laser pulse moving through a plasma. The centerpiece of the experimental program at l'OASIS Laboratory (Laser Optics and Accelerator Systems Integrated Studies) is a 10 TW, 50 fs, 10 Hz Ti:sapphire laser system. The laser is now being upgraded to 100 TW. The highly nonlinear laser-plasma interaction is modeled numerically with relativistic fluid-Maxwell codes and with particle-in-cell codes. Here we see a simulation of the plasma density wave (propagating from left to right after being excited in the wake of a high-intensity laser pulse), obtained from a fluid code.

BRADLEY SHADWICK, ERIC ESAREY, AND WIM LEEMANS, AFRD.



These simulated frequency maps are based on the ideal ALS lattice (top) and on the actual machine with its measured magnetic-field imperfections (bottom). Blue areas represent electron trajectories with no diffusion (no change in frequency over time), and red areas represent particles with high rates of diffusion. The differences in the two figures illustrate how machine imperfections significantly increase the size of the region where electron trajectories have high diffusion rates and are unstable. Frequency map techniques are now seen as extremely valuable tools for determining the optimal operating points (machine settings) of light sources. The techniques are so powerful that, in the future, it is likely that they will be integrated into on-line control systems.

CHRISTOPH STEIER AND DAVID ROBIN,
ADVANCED LIGHT SOURCE.

DEVELOPING AND APPLYING NEW MODELING TECHNIQUES

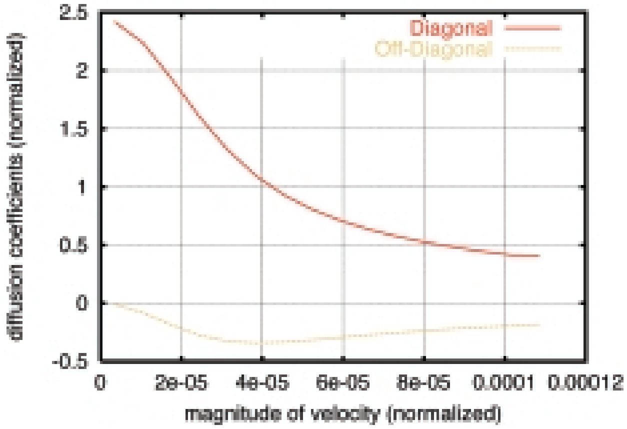
Developments in Computational Accelerator Science involve not only software but also the development of new algorithms and modeling techniques. One area where LBNL researchers have made a key contribution is in regard to the understanding of the beam dynamics in particle storage rings through frequency map analysis. In particle storage rings, resonance excitation can cause irregular or chaotic particle motion and eventual loss of particles. Obtaining a detailed global view of the beam dynamics is crucial for optimizing the performance of the storage rings. Accelerator physicists at LBNLs Advanced Light Source (ALS) have collaborated with Jacques Laskar, an astronomer at France's Bureau des Longitudes, on storage-ring applications of his technique of studying the global dynamics of multidimensional systems through frequency-map analysis. Frequency maps can be generated from knowledge of the beam positions on each revolution around the ring. The beam positions can either be calculated from an optics model or measured in the storage ring. Using the beam position data, a fast-converging modified Fourier technique then generates a quasi-periodic approximation to the trajectories from which the fundamental frequencies are extracted. Evaluation of the variation of these frequencies over time allows one to determine if the motion is regular or diffusive. The researchers have demonstrated that the generation of frequency maps, using measured beam positions, sensitively reveals the strength of harmful resonances. They have also shown that these measured frequency maps agree extremely well with frequency maps obtained using an optics model which includes measured magnetic-field imperfections. Frequency map analysis has proven to have excellent predictive capability in regard to finding operating points in parameter space that optimize storage ring performance.

SCIDAC ACCELERATOR MODELING PROJECT

LBNL has a leading role in a DOE Office of Science project, Advanced Computing for 21st Century Accelerator Science and Technology, which is part of the Scientific Discovery through Advanced Computing (SciDAC) program. The SciDAC accelerator modeling project is run by the Office of High Energy and Nuclear Physics (HENP) in partnership with the Office of Advanced Scientific Computing Research. Under this project, accelerator scientists are collaborating with computer scientists, applied mathematicians, and other Information Technology experts to develop a new generation of accelerator modeling codes. These codes, targeted toward parallel computing platforms, will enable large-scale three-dimensional simulations of accelerators to solve the most challenging and important problems in accelerator design and analysis.

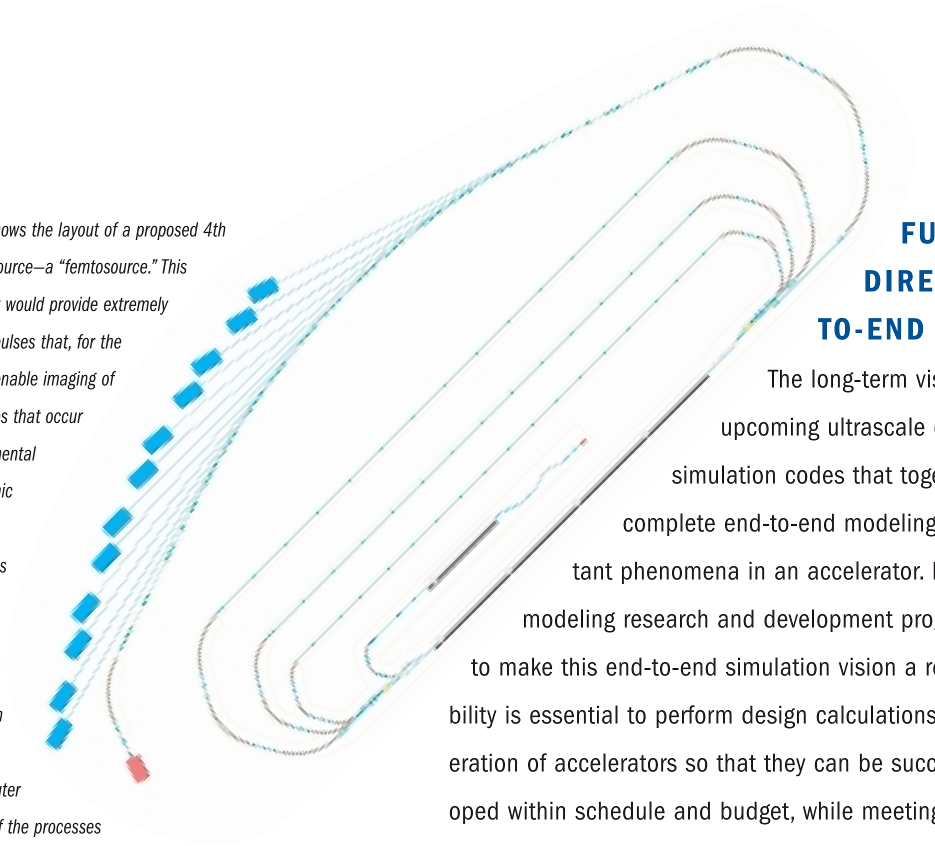
Under this project LBNL has developed new algorithms and software that are benefiting several HENP projects. The activities include:

- modeling beam-beam interactions in the Large Hadron Collider
- modeling beam-beam interactions in the Tevatron
- collaboration on simulation of the Fermilab booster and the BNL booster
- Next Linear Collider damping ring design involving use of the MaryLie code to simulate beam dynamics in wiggler magnets
- modeling laser/plasma accelerators, including recent experiments at SLAC and experiments at LBNL's l'OASIS laboratory



This figure shows the diffusion coefficients as a function of velocity from a simulation that includes the effects of multiple small-angle scattering. The data were computed using the parallel code LANGEVIN3D. This code, developed by SciDAC project members at LANL and LBNL, is the first code to model the Fokker-Planck equation in three dimensions using a first-principles treatment of the damping and diffusion coefficients. Previous idealized calculations based on the Spitzer approximation assumed that the diagonal coefficient (top curve) was a constant, and the off-diagonal term (bottom curve) was zero. As is evident from the figure, the self-consistent calculation shows qualitative differences compared with the idealized approximation. An accurate calculation of these coefficients is essential for determining the long-term behavior and relaxation rate of collisional beams and plasmas. Such self-consistent simulations would be impossible without terascale computers.

SALMAN HABIB (LANL), AND JI QIANG AND ROBERT RYNE (LBNL).



This schematic shows the layout of a proposed 4th generation light source—a "femtosource." This future accelerator would provide extremely short hard-x-ray pulses that, for the first time, would enable imaging of dynamic processes that occur within the fundamental timescale of atomic motion. The many complex processes involved in the production and manipulation of the electron beam require intensive end-to-end computer simulation. One of the processes requiring significant computer modeling is the effect of space-charge forces in the low-energy electron bunch from the source through the early stages of acceleration in the injector linac. In addition, tracking of the bunch through the lattice (oval paths) and beamlines leading to the experimental areas (blue boxes), accounting for realistic errors in components, is essential for understanding emittance growth and mitigating undesired effects. Simulations on high performance computers are critical for important design decisions in order to reduce cost and risk and optimize performance.

FUTURE DIRECTION: END-TO-END MODELING

The long-term vision for the upcoming ultrascale era is an array of simulation codes that together provide complete end-to-end modeling of all the important phenomena in an accelerator. LBNL's accelerator modeling research and development programs are helping to make this end-to-end simulation vision a reality. This capability is essential to perform design calculations for the next generation of accelerators so that they can be successfully developed within schedule and budget, while meeting demanding performance requirements dictated by the science.

For more information on how advances in computer techniques are being put to use in the particle-accelerator field by Berkeley Lab and its collaborators, including links to technical papers and movies of many of these simulations, please visit the Accelerator Modeling and Advanced Computing (AMAC) program website at **http://amac.lbl.gov,** or contact Robert D. Ryne, AMAC Program Leader, at RDRyne@lbl.gov