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High-Quality Electron Beams From a Laser Wakefield Accelerator

C.G.R. Geddes[1,2], Cs. Toth[1], J. van Tilborg[1,3], E. Esarey[1], C.B. Schroeder[1], D. Bruhwiler[4], C. Nieter[4], J. Cary[4,5], & W.P. Leemans[1]
[1]Lawrence Berkeley National Laboratory; [2]University of California, Berkeley; [3]Technische Universiteit Eindhoven; [4]Tech-X Corporation; [5]University of Colorado, Boulder

In work that brings the promise of laser driven particle accelerators dramatically closer to reality, with the potential to shrink accelerators from miles in length to meters and open new applications from medicine to high energy physics, researchers at Lawrence Berkeley National Laboratory have produced high quality electron beams in an accelerating structure only a few millimeters long.

The experimental results were then analyzed by running the VORPAL plasma simulation code on supercomputers at DOE's National Energy Research Scientific Computing Center (NERSC) at Berkeley Lab. The results were published in the Sept. 30 issue of Nature magazine, which chose an image from the NERSC simulations for the magazine's cover.

The work was done by the L'OASIS group (L'OASIS stands for Laser Optics and Accelerator Systems Integrated Studies), led by Wim Leemans of the Center for Beam Physics in Berkeley Lab's Accelerator and Fusion Research Division. To analyze the experiment, Cameron Geddes used the VORPAL code developed by David Bruhwiler, John R. Cary and Chet Nieter of the Tech-X Corporation of Boulder, Colorado, to model the results on supercomputers at NERSC. This modeling, which is partially supported by DOE's Scientific Discovery through Advanced Computing (SciDAC) Accelerator Modeling project, allowed the scientists to see the details of the evolution of the experiment.

"With VORPAL, one can see the laser pulse breakup and the injection of particles into the laser-plasma accelerator," said Cary, CEO of Tech-X Corp. and a professor of physics at the University of Colorado. "This allows one to understand how the injection and acceleration occur in detail so that the experiment's designers can figure out how to optimize the process."

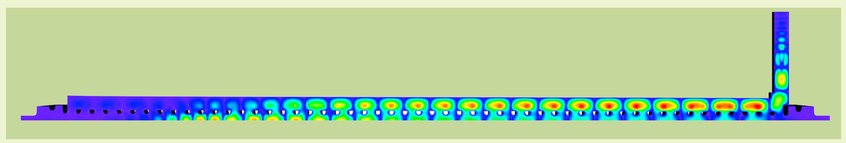
Plasma density variation driven by the radiation pressure of an intense laser pulse that is guided by a preformed plasma channel. The laser pulse travels upwards and different colors indicate different densities. Associated with the density variation is an electric field that travels like a wake behind a motor boat. The field is thousands of times stronger than in a conventional accelerator, allowing compact devices. The channel acts like an optical fiber for extremely intense laser pulses and extends the focused propagation distance. This results in trapping and acceleration of electrons to 100 million volts in a distance on the order of a millimeter and the generation of high quality beams.

X-Band Linear Collider R&D in Accelerating Structures Through Advanced Computing

Zenghai Li, Nathan T. Folwell, Lixin Ge, Adam Guetz, Valentin Ivanov, Marc Kowalski, Lie-Quan Lee, Cho-Kuen Ng, Greg Schussman, Ravindra Uplenchwar, Michael Wolf[1], and Kwok Ko, SLAC, [1]University of Illinois, Urbana-Champaign, USA
Proceedings of the 9th European Particle Accelerator Conference, July 5-9, 2004, Lucerne, Switzerland

The parallel electromagnetic, finite element eigensolver Omega3P developed at SLAC has been used to find the normal modes in the Damped Detuned Structure (DDS), considered to be the baseline design for the Next Linear Collider (NLC). The accelerating structure comprises 55 cells with variations from cell-to-cell of order microns to detune the dipole modes, while the mode damping is provided by cell-coupling to four vacuum manifolds that run the length of the structure to terminate in matched loads. The DDS design aims to suppress the long-range dipole wakefields that are harmful to the long bunch train operation of the proposed NLC while providing maximum accelerating gradient.

Previous theoretical studies on the DDS dipole wakefields have been limited to simplified lumped circuit models that can calculate only the two lowest bands in the dipole mode spectrum. Using Omega3P, a SciDAC AST team led by SLAC has succeeded in finding the dipole wakefields in a DDS prototype H6OVG4 with realistic geometries and higher bands included. This is the first-ever end-to-end simulation of an entire accelerating structure only made possible by the advent of parallel computing and unstructured grids, and also by achievements in meshing and solvers resulting from the collaboration with the Math ISICs (TSTT and TOPS).



Eigenmode with high kick factor/low Q from Omega3P in 1st band of the H60VG4.

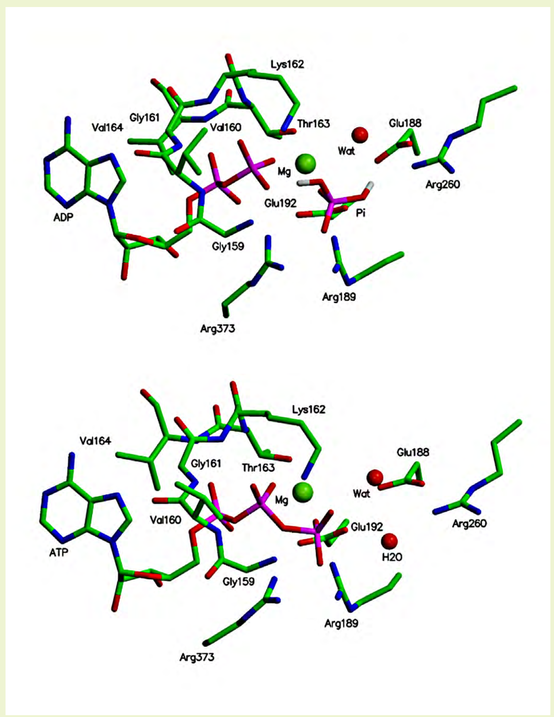
The Omega3P computations were performed on 512 processors of the IBM/SP machine at NERSC, requiring more than 400 GB of memory for a problem size of 2.3 million degrees of freedom or 94.5 million non-zeros. It took Omega3P 3179 sec to solve for 120 complex eigenpairs in the DDS when modeled with quadratic elements. The figure shows a dipole mode that couples to the damping manifold and is absorbed in matched loads at the HOM coupler downstream. A total of 400 complex eigenmodes covering the spectrum up to 30 GHz have been obtained to form the sum for the wakefield which is found to be in good agreement with time-domain simulation results from the parallel solver Tau3P.

The Missing Link Between Thermodynamics and Structure in F_1-ATPase

W. Yang[1], Y. Q. Gao[2], Q. Cui[3], J. Ma[4], and M. Karplus[1,5]
[1]Harvard University; [2]California Institute of Technology, [3]University of Wisconsin, [4]Baylor College of Medicine, [5]Universite´ Louis Pasteur
Proceedings of the National Academy of Sciences, vol. 100, no. 3, February 4, 2003

F_1F_o-ATP synthase is the enzyme responsible for most of the ATP synthesis in living systems. The catalytic domain F_1 of the F_1F_o complex, F_1-ATPase, has the ability to hydrolyze ATP. A fundamental problem in the development of a detailed mechanism for this enzyme is that it has not been possible to determine experimentally the relation between the ligand binding affinities measured in solution and the different conformations of the catalytic β subunits (β_{TP}, β_{DP}, β_E) observed in the crystal structures of the mitochondrial enzyme, MF_1.

Using free energy difference simulations for the hydrolysis reaction $ATP+H_2O \longrightarrow ADP+P_i$ in the β_{TP} and β_{DP} sites and unisite hydrolysis data, we are able to identify β_{TP} as the "tight" ($K_D = 10^{-12}$ M, MF_1) binding site for ATP and β_{DP} as the "loose" site. An energy decomposition analysis demonstrates how certain residues, some of which have been shown to be important in catalysis, modulate the free energy of the hydrolysis reaction in the β_{TP} and β_{DP} sites, even though their structures are very similar. Combined with the recently published simulations of the rotation cycle of F_1-ATPase, the present results make possible a consistent description of the binding change mechanism of F_1-ATPase at an atomic level of detail.



The calculated structures of β_{TP} site with ATP/H_2O (lower) and ADP/P_i (upper) as ligands. In the binding sites, substrates interact directly with several charged protein residues, which play essential role in controlling the relative chemical potential between ATP/H_2O and ADP/P_i.

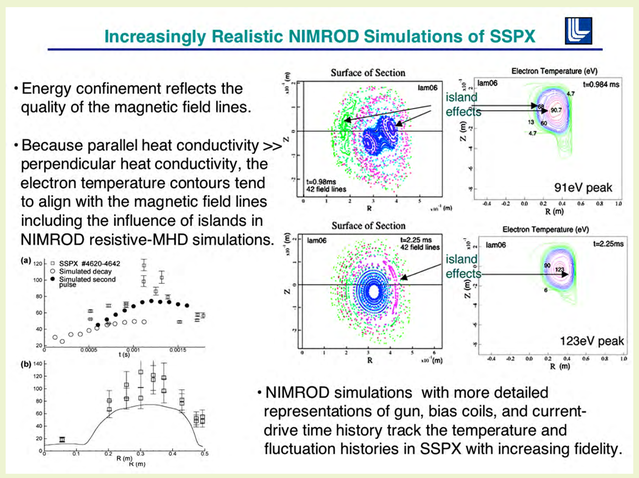
Massively Parallel Simulation of the SSPX Magnetic Fusion Experiment

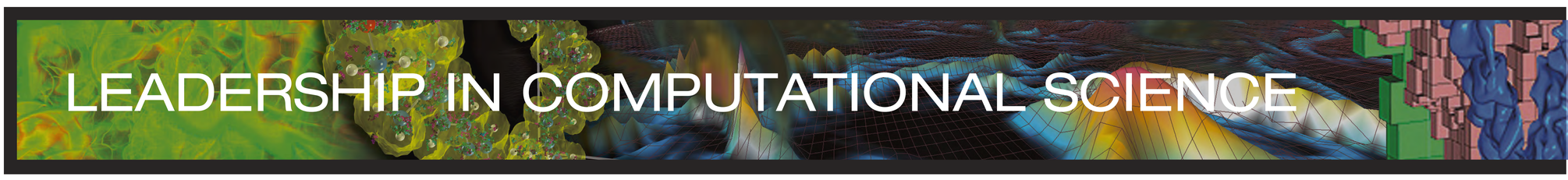
C. R. Sovinec and G.A. Cone, University of Wisconsin, Madison; B.I. Cohen, E.B. Hooper, and H. S. McLean, University of California Lawrence Livermore National Laboratory
"Numerical Investigation of Transients in the SSPX Spheromak," submitted to *Physical Review Letters,* 2004; for NIMROD see *Journal of Computational Physics,* 195, 355, March 2004

The spheromak is a compact, self-organized, toroidal plasma configuration in which confining magnetic fields are produced by poloidal and toroidal currents flowing in the plasma; there are no toroidal magnetic field coils linking the plasma. A spheromak can be formed and sustained by injecting magnetic helicity and energy from a magnetized coaxial plasma gun (powered by a capacitor bank) into a conducting shell, or flux conserver. The spheromak is an interesting fusion concept because the ratio of the plasma pressure to the magnetic energy density is relatively high in a spheromak, and the fusion cross-section depends on the square of the pressure, while the capital cost increases with the magnetic field strength.
The goal of theoretical studies in support of the SSPX spheromak experiment at the Lawrence Livermore National Laboratory is to understand the important physics issues affecting the experiment.

The modeling attempts to match and predict the experiment, and successful theory and simulation efforts can lead to improvements in the performance of the experiment. A recurrent theme in the modeling is magnetic field-line quality in a driven spheromak. Direct numerical simulations of formation, sustainment and magnetic reconnection using the nonlinear, resistive MHD code NIMROD with more detailed representations of the gun geometry, magnetic bias coils, and current-drive time history track the temperature and magnetic fluctuation histories and reconstructions of the magnetic structure in SSPX with increasing fidelity.

One of the graphics shows temperature time histories from a series of NIMROD simulations that compare favorably to SSPX Thomson scattering data. The other set of graphics shows the corresponding electron temperature contours at two different times in one of the NIMROD simulations, which align with the magnetic topology including the effects of magnetic islands arising from magnetic fluctuations. The plasma has continued to heat at the expense of magnetic energy during a partially driven resistive decay as the system becomes more axisymmetric and energy confinement improves.





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