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ComPASS Final Report

Tech-X Corporation

"Community Petascale Project for Accelerator Science and Simulations"
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Activity description

Tech-X is participating across the full range of ComPASS activities.

Our efforts in the *Advanced Accelerators* area primarily involve modeling of laser plasma accelerator (LPA) concepts and experiments. Our work directly supports the LOASIS Program and the BELLA Project at Lawrence Berkeley Lab (LBL). We are collaborating with scientists at LBL and also at the University of California Los Angeles (UCLA).

Our efforts in the *Beam Dynamics* area primarily involve electron cooling and electron cloud simulations. For electron cooling, we collaborate primarily with Brookhaven National Lab (BNL) scientists, and our work is relevant to the coherent electron cooling (CeC) proof-of-principle experiment at BNL, as well as more general concepts for the electron-ion collider (EIC) concept. For electron cloud work, we collaborate primarily with Fermi National Accelerator Lab (Fermilab) scientists, including support of experiments.

Our efforts to date in the *Electromagnetics* area primarily involve superconducting RF (SRF) cavity modeling, including computations of frequencies, modes and quality factors. We have worked directly with cavity designers at Fermilab, Thomas Jefferson National Accelerator Facility (JLab) and the Cockcroft Institute in the UK, with an emphasis on crab cavity modeling for the Large Hadron Collider (LHC).

Advanced Accelerators

In this section, we summarize our contributions to laser plasma accelerator (LPA) simulations and associated software development/testing, in support of present and planned experiments at the LOASIS Program of LBL, including the BELLA Project. Our work has been collaborative with LOASIS Program staff members, who are also part of the ComPASS project team, and also with UCLA scientists.

During the first year of the project, emphasis was made on software verification of 3D laser plasma accelerator (LPA) simulations via benchmarking of the time-explicit codes Vorpal and OSIRIS, as well as the quasi-static code QuickPIC, results published in [1]. This work was a collaborative effort between Tech-X, the SciDAC personnel at UCLA and members of the ComPASS team at LBNL. We considered a Ti-Sapphire laser pulse entering a constant density electron plasma and propagating for a short distance. We compared 2D color contour plots and 1D lineouts of the laser electric field, the longitudinal plasma wakefield, and the electron density. Agreement between Vorpal and OSIRIS was found to be quite good, lending confidence in the validity of both codes. Although QuickPIC does not capture the short-scale space/time oscillations driven by the laser pulse, it accurately models physical features on the scale of the plasma wavelength/frequency. Subsequently, we performed benchmarking of the laser envelope model and the cold relativistic fluid algorithm in Vorpal using the same parameters, both showing good agreement with the previously obtained results.

During the period of the project Vorpal was successfully ported to various high performance computing centers. Vorpal was run on the ATLAS machine at LLNL and on all super-computer systems at NERSC. Although parallel I/O performance with hdf5 was limited initially on the Lustre file system, extensive discussions with NERSC consultants allowed us to greatly improve performance, enabling production runs on 10^4 processors with excellent efficiency. Production simulations routinely use > 4,000 processors on NERSC machines (Franklin initially and now Hopper). Weak scaling studies of Vorpal electromagnetic PIC simulations showed excellent efficiency up to 16,384 Franklin cores. Recently we also obtained > 90% efficiency in scaling up to 24,576 cores on Hopper. Weak scaling is the key metric for LWFA simulations, because our need for higher resolution is only limited by the availability of processors to make the wall clock run times acceptable.

We successfully demonstrated efficient modeling of meter-scale 10 GeV LPA stages, in support of the BELLA project at LBNL [2]. Numerical noise issues were mitigated using higher order particle shapes, in particular, we showed that the use of 3^{rd} order splines is critical for noise reduction and correct simulation of beam energy spread and emittance [3,4]. Concurrently, a uniquely powerful 3D parallel charged fluid algorithm has been implemented in Vorpal and works well for weakly non-linear laser pulses ($a_0 < 2$), with no particle driven noise, and can also be used in hybrid with an externally injected beam that is represented by particles. The hybrid technique can dramatically reduce the numerical noise associated with conventional PIC, so that ultra-low beam emittances in LPA can be correctly modeled. This algorithm is 2^{nd} order accurate intracell density variation and is robust in the presence of strong gradient and plasma/vacuum interface. It has been successfully benchmarked against PIC, as noted above.

Two practical approaches for simulating meter-scale, 10 GeV, LPA stages have been demonstrated [5]. The first approach is to scale all physical quantities with the plasma density, such that the simulation is conducted with an artificially high density [6]. In the quasilinear regime (a_0 <2), this approach correctly captures all relevant physics, including beam loading, with two major exceptions: 1) the number of laser pulse Rayleigh ranges is reduced and so any betatron oscillations of the pulse width (and corresponding oscillations of the plasma wake) are not correct; and 2) the number of oscillations within the laser pulse envelope is reduced, which could exaggerate non-ponderomotive effects. This method was used to study how shaping of the laser pulse transversely can help optimize the properties of the accelerated electron beam in a 10 GeV quasi-linear LPA stage [7,8,9]. It was shown that, as shaping the transverse pulse shape can control the transverse forces in the wakefield, one can control the emittance and radius of the accelerated beam. This can be used to increase the matched beam radius, and effectively increase the accelerated charge.

The second approach is to use reduced models with which full scale 10 GeV stages can be simulated. The laser envelope, or ponderomotive guiding center (PGC) model reduce disparities of length by averaging the laser wavelength, allowing for larger grid spacing and hence larger time step [10,11]. This approach nicely complements the first approach, because the number of Rayleigh ranges and corresponding betatron oscillations of the laser pulse width are correctly captured, and because non-ponderomotive effects are neglected (rather than being exaggerated). In any case, non-ponderomotive effects are weak in the quasi-linear regime. The envelope model implementation in Vorpal has shown speedup of ~10,000 over time-explicit PIC. The primary limitation of this method is that spectral broadening due to pump depletion cannot be accurately captured in the final 20% to 30% of the interaction length. Improvements have been made to the algorithm in Vorpal to allow propagating the laser further into depletion, using the envelope phase tracking feature. The envelope model has been successfully benchmarked against fully time explicit PIC as noted above. (This work was partially funded by SBIR/DOE phase I grants).

Significant speedup can also be achieved by performing simulation in a boosted frame [12,13,14]. This technique uses the same size grid as lab-frame PIC simulations, and hence can efficiently use ~ 10,000 cores or more, but requires orders of magnitude fewer time steps. We collaborated with the group at LBNL to successfully implement in Vorpal the techniques initially introduced by J.-L. Vay et al. in WARP [13]. We obtained good agreement between boosted frame and lab frame simulations, with speedup up to 35,000 compare to conventional PIC [15]. We also performed successful benchmarking with the code WARP, which results were published in [12].

The fluid algorithm, mentioned above, has been shown to work well in the Lorentz boosted frame. Fluid updates for the PGC algorithm have been implemented, and initial testing has shown reasonable results when compared with PIC.

Vorpal simulations were used to design and interpret electron beam injection in LPA, in collaboration and in support of the experimental program at LBNL.

The envelope model was used to model the down-ramp injection technique [16,17,18].

We performed thorough parameter scan to guide experimental set-up for colliding pulse induced injection [19,20,21]. The simulations predicted density and timing windows for charge in the experiments and were used to improve experimental parameters. Effects of realistic laser modes fit to the experiment and of laser guiding were also simulated to optimize performance. In this context, we made use of the SciDAC visualization software VisIT to visualize large 3D data set, with the goal of building a high quality movie, showing the interaction and injection process. (This work was partially funded by DOE/NNSA-NA22 grant).

Motivated by the increase interest in using ionization of a high-Z gas to inject an electron beam in a LPA, we implemented a general formula for the tunneling ionization rate [22,23,24] in Vorpal, which was previously limited to a few gases, which ionization rate and ionization potentials were recorded in the TxPhysics library. The general formula calculates the ionization rate for any atom, provided the ionization potential. Simulations results obtained with Vorpal were successfully benchmarked against VLPL [25,26] simulations at LBNL. This effort supports ongoing experiments from the LOASIS program at LBNL.

A new scheme was introduced, in which injection through colliding pulses propagating transversely help reduce the transverse emittance of the injected beam. This model is used in conjunction with the ionization of nitrogen atoms to increase the beam charge [27]. Simulations were done using the codes VLPL and Vorpal and the results successfully benchmarked.

In order to better interpret the simulations, we collaborated with researchers from the VACET project and LOASIS program at LBNL to produce VisIT parallel three-dimensional rendering, allowing rapid visualization of large simulations outputs, and automate detection, characterization and fast parallel tracking of trapped particle bunches in the simulation [28,29,30,31,32].

The ComPASS project partly funded efforts to improve the Vorpal code usability. We developed in-line documentation for Vorpal and input file validation. Thanks to the new implementation the input file syntax can now be validated before a Vorpal job is run. This was integrated in VorpalComposer, which is a powerful new graphical interface that facilitates the use of Vorpal by managing both workflow and 3D visualization via VisIt. We also developed physics examples that are distributed to the user to facilitate introduction to Vorpal usage.

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Beam Dynamics — Electron Cooling

In this section, we summarize the status of work on simulating the physics of electron cooling, in collaboration with the electron cooling group of BNL.

In the first year of the project, a semi-analytic binary collision model was used with electrostatic particle-in-cell (ES-PIC) Vorpal simulations, via operator splitting, to capture the self-fields of the electron distribution around an ion. The ES-PIC solvers in Vorpal use the Trilinos library from SNL to solve Poisson’s equation. To test this approach, in collaboration with the COMPASS team at BNL and with Y. Derbenev at Jefferson Lab, Vorpal was used to conduct initial simulations of the modulator section of the coherent electron cooling (CEC) proof-of-principal experiment, using electrostatic PIC and advanced noise reduction techniques.

During the project, we installed Vorpal on the BNL linux cluster, along with the IDL-based visualization utility VorpalView. We also conducted a VORPAL training session at BNL for V. Litvinenko, A. Fedotov, E. Pozdeyev and others. Additionally, we made Vorpal available at NERSC for use by BNL and JLab scientists. Tech-X now manages a NERSC repository for use by all ComPASS collaborators doing work funded by the NP office.

In the second year of the project, much of the focus of the electron cooling effort was redirected toward modeling the coherent electron cooling concept, which requires completely different algorithmic approaches. In this case, it is not necessary to model the close binary collisions of the ions, making it unnecessary to use the binary collision algorithm used in Year 1. Instead, it is only necessary that the electron density and velocity fluctuations be modeled accurately.

To this purpose, great success was found with the δf PIC algorithm rather than electrostatic PIC. Instead of requiring extremely large numbers of simulation particles like electrostatic PIC, the δf PIC algorithm uses perturbation theory to minimize particle noise, thus enabling simulation of very subtle density and velocity wakes in a thermal electron distribution, and which scales well on many processors.

We performed 3D electrostatic δf PIC simulations of the electron response to a single ion in the CeC modulator. These simulations were conducted with Vorpal using ~500 cores on Franklin at NERSC. We compared our simulation results with the analytical predictions of Wang and Blaskiewicz [33].

In the third year of the project, Vorpal simulations were conducted to model electron cooling using three algorithms: electrostatic PIC, the semi-analytical binary collision model, and δf PIC.

Conventional electron cooling simulations were performed with Vorpal using the semi-analytic binary-collision algorithm and electrostatic PIC, but scaling these approaches to more than 1000 cores was found to be difficult and unnecessary, due to the success of the δf PIC approach and the shift in emphasis to modeling the CeC system. Therefore, the δf PIC algorithm was used instead. Vorpal simulations of a single Au^{+79} ion in the modulator section of the CeC system were shown to scale well up to 4096 processors on Franklin. These modulator simulations were validated by comparison with theory in an appropriate limit and used to address regimes not accessible by theory [34]. Work on relativistic unmagnetized electron cooling was included in a manuscript that was submitted to the New Journal of Physics [35]. The results of this effort were presented in an invited talk at the HB2010 workshop [36].

In the fourth year of the project, significant improvements were made to the particle I/O in Vorpal by taking advantage of the "striping" capabilities of the Lustre filesystem at NERSC. With changes made to the particle I/O, using appropriate striping, a 13x reduction in dump time was achieved on Franklin with 1.8B particles distributed (not completely evenly) across 2048 cores. Striping on Hopper II reduced the write time from long enough to hit the debug limit (> 20 min) to just 2-3 minutes.

Also to support the coherent electron cooling (CeC) proof-of-principle experiment at Brookhaven National Lab, we used Vorpal to model both JLAB's DC electron gun [37] and a new superconducting 112 MHz 1.5 MV SRF gun [38]. We have set up the geometry for both guns in Vorpal and propagated relevant particle distributions to the respective gun exits. Detailed parameter scans are not complete but are planned for the near future.

We have also contributed to the use of Vlasov/Poisson capabilities in Vorpal for modeling Debye shielding of ions in an electron beam with density gradients [39]. Additionally, we made effective use of the SciDAC visualization software VisIt [40]. We developed a VisIt-compatible Python script to visualize and create animation frames showing ion shielding in the modulator section. In the process we came across a bug in the (then) current VisIt release on Windows, which we communicated to a forum moderator at VisItUsers.org.

In the final year of the project, Vorpal simulations of the CeC modulator were performed with more than ~12,000 processors on Franklin at NERSC. In the process, a bug in parallel HDF5 was found preventing the use of more than 8000 processors. This bug has been observed by the HDF Group, and they are working on a fix. In the mean time, a temporary fix has been added to Vorpal to allow scaling to 16000 processors. A more complete fix is being implemented now.

Improvements have also been made to the accuracy of the model used in Vorpal δf PIC simulations of the modulator. Prior simulations assumed a uniform electron density in the modulator, and included no external focusing or space charge, so it was also constant in time. For accurate simulation, it is important to model how the shielding cloud around an ion changes when the uniform, constant density assumption is no longer true.

Assuming constant and linear radial-focusing fields, we compared a 1D Vlasov model to 1D δf PIC simulations. The agreement between these two models was excellent and described in our PAC 2011 proceedings paper [41]. Adding space-charge effects to these simulations, we applied a 2D model of the transverse structure of the beam as the focusing was increased. The solution for the ion shielding was obtained using Delta-f PIC. These results are in our IPAC 2012 proceedings paper [42].

In both cases we obtained results for stationary as well as moving ions in regions where the background density is not constant, as well as in the center of the beam where the density is more uniform. We can compare the results of our numerical simulations with the predictions of Wang and Blaskiewicz [33]. In the numerical simulations, when the ion is in the center of the beam, the numerical results compare well to the theory of Wang and Blaskiewicz. When the ion is near the edge of the beam, the results match qualitatively to the theory towards the interior of the beam where the density is increasing. Towards the edge of the beam where the density is decreasing, the simulations show a reduced response. This makes sense because the plasma frequency is lower where the density is lower, so the shielding response in this region is slower.

In addition to improved modulator simulations, efforts were made to expand simulation of the CeC system beyond the modulator. To that end, Python scripts were developed to extract the necessary bunching and energy modulation data from Vorpal simulations of the modulator and converting these quantities to Genesis particle distributions. Genesis is then used to model the FEL section of the CeC system. After the FEL, the evolution of the charge density modulation in the kicker was simulated with Vorpal and compared with 1D theory. We presented these results at the 2012 International Particle Accelerator Conference [43]. Lastly, we developed algorithms to track an ion's motion in the kicker and compute the net cooling force it experiences during this time.

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Beam Dynamics — Electron Cloud

In this section, we summarize the status of work on modeling the physics of electron clouds in high-intensity accelerators, in collaboration with researchers at Fermilab. Electron cloud modeling was not in the original research plan, but was added in order to support researchers at Fermilab who are trying to understand the best way to mitigate the performance-limiting effects of electron plasma formation for Project X. Electron cloud work did not start until the second year of the project.

During this performance period we reallocated some funding from electromagnetics to beam dynamics in order to support the simulation of electron cloud buildup in the Main Injector and modeling of traveling wave RF diagnostics of electron cloud density. We combined electromagnetics and beam dynamics to help understand rf diagnostics for electron cloud measurement, in support of experiments at the Fermilab Main Injector. The image below shows transmission through an electron cloud of an rf wave used as a diagnostic for cloud density. The cloud is shown as red particles. The amplitude of the rf wave is shown as the color contours. The beam pipe is elliptical with dimensions of the pipe in the Fermilab Main Injector. VORPAL provides unique capability to combine electromagnetics and beam dynamics.

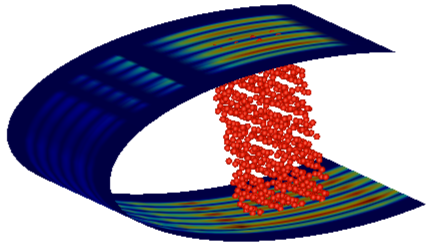

Figure 1: VORPAL result showing transmission through an electron cloud of an rf wave used as a diagnostic for cloud density. The cloud is shown as red particles. The amplitude of the rf wave is shown as the color contours. The beam pipe is elliptical with dimensions of the pipe in the Fermilab Main Injector. VORPAL provides unique capability to combine electromagnetics and beam dynamics.

This work provided the basis for supporting modeling efforts at Fermilab on the build up of electron clouds during this and subsequent performance periods. Using Vorpal, Tech-X researchers collaborated closely with Fermilab researchers to develop accurate models of electron plasma build up over many bunch crossings, and in varying magnetic field configurations, such as drift, dipole, and quadrupole sections of the Main Injector.

During this performance period we continued to make progress in the simulation of rf diagnostics of electron clouds in the Main Injector. This work gives important insights into the dynamics of particle accelerators such as Project X and the potential for mitigation of destabilizing effects of electron clouds on particle beams. Typical Particle-In-Cell (PIC) simulations may accurately model cloud dynamics; however, due to the large range of temporal scales needed to model side band production due to electron cloud modulation, typical PIC models may not be the best choice. We advanced numerical modeling of rf electron cloud diagnostics by replacing kinetic particles with an equivalent plasma dielectric model, for a simplified system with no boundaries. This demonstrated the potential of using advanced models to simulate rf diagnostics in electron clouds, in order to better understand rf transmission diagnostic experimental data at Fermilab.

The plasma dielectric model provides significant speedup and increased numerical stability, while still providing accurate models of rf phase shifts induced by electron cloud plasmas over long time scales. Figure (2) below shows typical spectra produced by modulating the plasma dielectric for a plane wave traveling through a uniform density electron plasma with no external magnetic fields. Modulating the dielectric constant produces side bands in the rf spectra, with a height that is linearly related to the plasma density. For the plane wave case in a uniform density cloud, the linear theory is known, and these simulations provided the basis for modeling electron cloud rf diagnostics in realistic configurations with non-uniform densities and magnetic field configurations with beam pipe effects in subsequent performance periods.

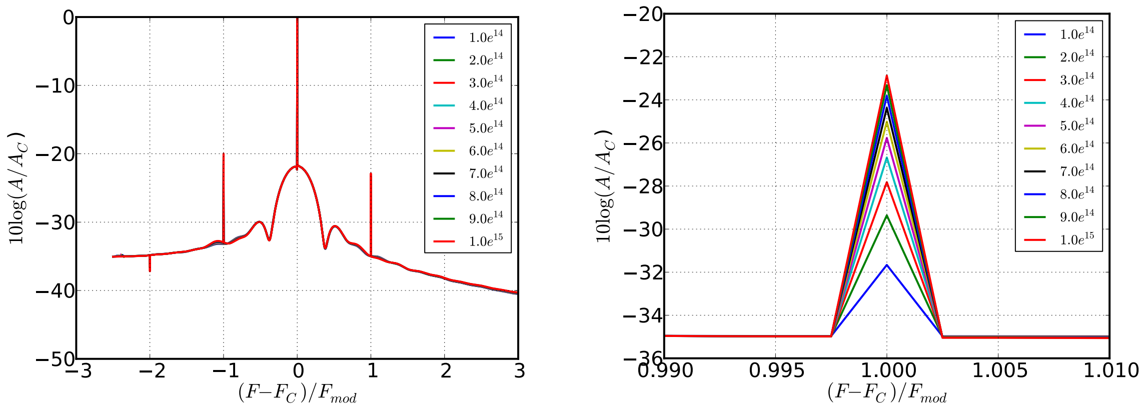

Figure **Error! Main Document Only.**. Simulated side band spectra for plane waves in uniform density electron plasmas obtained in numerical experiments by modulating a plasma dielectric representation of electron clouds. The height of the first side band is a measure of the electron cloud density, and is linear in density, as expected from theory.

In this performance period we also helped Fermilab researchers perform detailed benchmarks between Vorpal and POSINST codes for electron cloud simulations, in order to understand the effects of different parameterizations, such as Secondary Electron Yield (SEY) models on the dynamics of electron cloud build up. For these benchmarks, a large number of 2D electrostatic Vorpal simulations were performed and compared to similar POSINST simulations. While initial results showed significant discrepancies, model agreement was found to be good when model parameterizations were sufficiently equivalent. Of primary importance were the details of the SEY model in the case of high peak emission value.

In the last year of the project, we focused on developing new algorithms for modeling travelling wave rf diagnostics of electron clouds based on a plasma dielectric model as opposed to kinetic modeling of plasma particles. We improved our plasma dielectric model to incorporate port boundary conditions, which allowed us to simultaneously absorb rf power at one frequency at the open boundaries of our simulations, and to inject traveling wave rf at the source end of the simulation. This improved our simulation efficiency by eliminating the need for long unphysical regions at the boundaries to absorb rf power and reduce numerical reflection off of the boundaries. We also improved our model so that it accurately describes the dielectric properties of the electron plasma with metallic boundaries (beam pipe), non-uniform density plasmas, and external magnetic field configurations (dielectric tensor formulation). These new simulation capabilities were demonstrated by simulations of electron cloud rf diagnostics in realistic beam pipe configurations. Since one needs to resolve both the rf signal (~2 GHz) and the modulation frequency (~10 MHz), it was important to develop models that are numerically stable over many time steps. Our simulations exhibited remarkable stability over more than 50 million FDTD iterations, and accurately reproduced side band structure observed in experiments at Fermilab.

Figure (3) below shows a snapshot of rf propagating in a square cross section beam pipe in these simulations. Note the damping of the wave due to the slightly lossy plasma dielectric in this simulation. Figure (4) below shows a comparison between plasma-induced phase shifts in a non-uniform magnetic field configuration (wiggler field) for uniform and non-uniform cloud densities. These results indicate that the effects of cloud density evolution and magnetic field configuration will have significant effects on the interpretation of experimental data in terms of deducing the actual plasma density based on rf measurements in high-intensity accelerators.

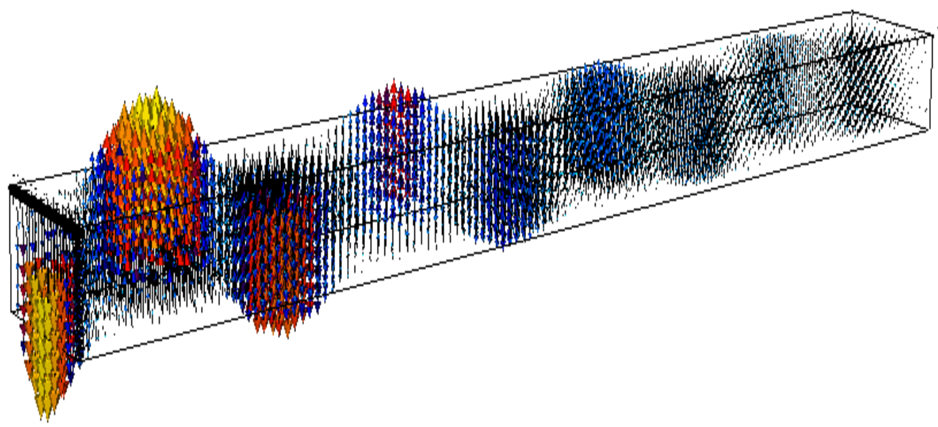

Figure 3: Simulated rf propagation in a square cross section beam pipe through a modulated plasma dielectric representing an electron cloud. Modulation of the dielectric tensor produces side bands similar to those observed in experiments at the Main Injector.

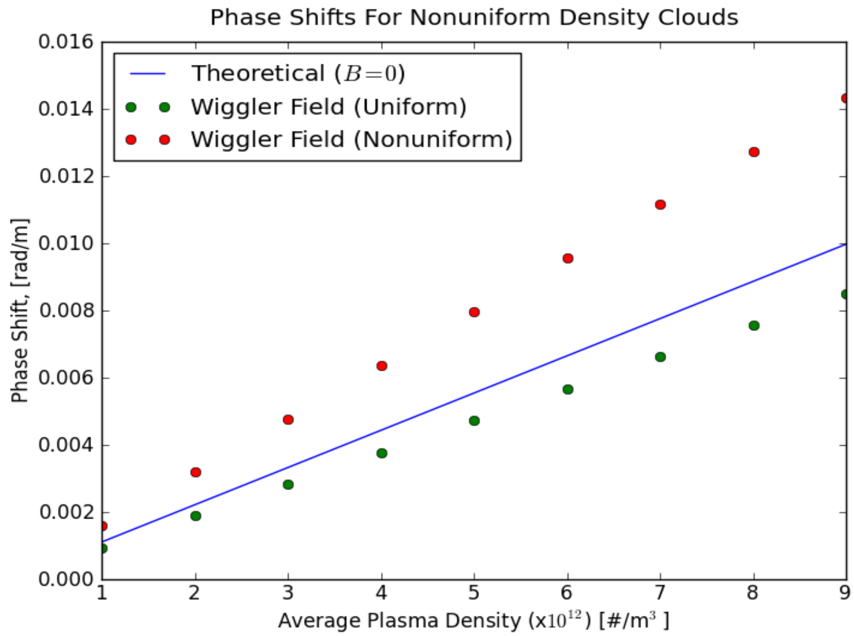

Figure 4: Comparison of plasma-induced phase shifts in simulations with a complicated non-uniform magnetic field configuration (wiggler field), with two different plasma density distributions. For uniform plasmas, which fill the entire beam pipe, the phase shifts, as derived from the side band height, are lower than the nominal case with no magnetic field. However, the case in which the electron cloud has higher density near the center of the beam pipe, and lower density near the edges, while retaining the same overall density, the phase shifts are larger. This indicates that plasma density variations and magnetic field configurations will play an important role in determining actual plasma density based on rf experimental data.

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Electromagnetics

A major aspect of the Tech-X electromagnetics work for ComPASS-2 was the accurate, efficient computation of eigenmodes and frequencies in RF accelerating cavities with complex geometries. These computations were enabled by the development, early in the project, of post-processing software for VORPAL for mode and frequency extraction from time-domain simulations. The description of the algorithm has been published in [44]. One unique aspect of this algorithm is that it can accurately extract frequencies even when modes are nearly degenerate.

This algorithm was applied highly successfully to the modeling of crab cavities for the LHC. Frequency computations, accurate to parts in 10^5, were performed for the cavities as a function of indentation. Initial computations showed disagreement with both MAFIA calculations and experimental results. To resolve these discrepancies, simulations were performed of the A15 cavity, which were fabricated by a more precise machining process than the previous prototype, and thus provided better dimensional accuracy to the simulations. The VORPAL frequency computations then deviated from experimental measurements by 2 MHz (out of 3.9 GHz). To investigate this issue further, we performed a set of calculations for a cavity with a 25 mm difference in the equator radius; this change yielded a 2 MHz shift in frequency values that brought them to within hundreds of kHz of the experimental measurements. This prompted our experimental collaborators to perform more precise measurements of the A15 cavity. These measurements found manufacturing errors that resulted in differences in the cavity geometry from the preliminary results, and repeating the VORPAL simulations with the more precise geometry resulted in the simulations agreeing with the measurements to within experimental error. This served as a rigorous benchmarking of the VORPAL frequency computation capability; ultimately our calculations were shown to be accurate to 2 parts in 10^5 [45–47]. Thus, new simulation capability was able to help experimentalists diagnose and correct manufacturing issues with crab cavities.

We also completed an analysis of the frequencies and Q values of the crabbing modes and the same-order modes (SOMs) for an 800 MHz JLAB/UK/Tech-X elliptical crab cavity design for the LHC. The analysis was also performed using VORPAL and the Werner-Cary frequency extraction method described in [44]. The goal of this work was to benchmark mode frequencies and Q values from Microwave Studio (MWS) simulations carried out by Graeme Burt and co-workers, where they were limited in the resolution they could use because they could only run in serial.

Calculating Q values depends sensitively on the boundary conditions, since small amounts of reflection from the numerical boundaries can have a large effect on the rate at which energy leaves the simulation and therefore on Q. Therefore a first goal of our work was to understand where to place the boundaries. Initial simulations, with the end pipes and on-cell couplers shortened, resulted in a mode analysis that was far from expected values. Consequently, we moved the numerical boundaries further out. This required large-scale, parallel runs (running at NERSC with ~2000 processors). For the runs with the far away boundaries, we were still able to use 5 mm resolution, while the serial MWS simulations used 10-20 times fewer cells. The results of the computations compared favorably with the MWS results and thus VORPAL provided a benchmark for the lower-resolution MWS simulations.

More recently, we applied the capabilities developed in this project to investigate the effects of dispersion in multi-cell RF cavities. Specifically, we investigated the origin of modes trapped in the beam pipe between two 9-cell ILC cavities [48], observed in [49], and which could degrade beam quality. We first simulated a single cell of the cavity, varying the phase shift across the cell to compute the longitudinal band structure. We found that the pipe cutoff frequency lay within a longitudinal photonic band gap (PBG), providing the confinement necessary for a trapped mode. Computations of the mode with simulations of an entire pair of 9-cell cavities verified that the PBG mechanism was responsible for the longitudinal confinement. Further, we found that reducing the beam pipe radius so that the cutoff frequency is increased above the PBG eliminates the trapped mode, presenting a possible strategy for mitigating these modes. These results have been submitted for peer review [50]. This work used both the Dey-Mittra cut-cell boundaries and the VORPAL frequency extraction tool [44] to perform the computations. We also took advantage of another capability developed as part of this project, namely the implementation of the electromagnetic update on graphics processing units (GPUs). This enabled us to perform the computations rapidly on the Dirac GPU testbed cluster at NERSC. The GPU development is described further below.

Another major development in this project was the implementation of a "controlled dispersion" electromagnetic update in VORPAL. The algorithm provides for numerical dispersion-free propagation of plane waves along a grid axis in vacuum. It does so by performing a particular smoothing of a field during one of the Maxwell updates. This eliminates numerical Čerenkov radiation from a relativistic particle bunch propagating through a structure, providing much greater accuracy in wakefield simulations. The algorithm was applied to a wakefield simulation of the Cornell B-cell cavity. The procedure used in the algorithm also gives rise to an implicit method for consistently initializing the self-fields of a beam propagating through a pipe, thus avoiding unphysical transition radiation without simulating over a long formation length. The controlled dispersion also provides for much greater accuracy in the group velocity of a laser pulse propagating along an axis in an LPA simulation. Details and applications of the algorithm, with an emphasis on the benefit for simulations of LPA stages, were submitted for peer review [51]. Benefits were also shown for LPA self-injection simulations [52].

Related to this development was the implement of the moving window with boundaries. With this feature, the simulation domain can be shifted at the speed of light to follow a relativistic electron bunch. We extended this feature to enable the boundaries associated with perfectly conducting structures, represented either as a stairstepped boundary or with the more accurate cut-cell treatment, to be shifted as well. We also enabled testing on large numbers of processors, and we conducted studies into how the controlled dispersion algorithm could be used together with the moving window and complicated SRF cavities for complete wakefield simulations.

Other activities included performing initial evaluation of multipacting in Project X cavity designs [53–55]. The present design for the 3 GeV linac driver for Project X involves 650 MHz cavities of both $b = 0.6$ and $b = 0.9$. In collaboration with Jefferson Lab, Tech-X researchers conducted a preliminary analysis of multipacting in a proposed design of a 650 MHz cavity for the Project X linac. We also published a new fully implicit charge-conserving algorithm for electromagnetic particle-in-cell (EMPIC) simulations [56].

We conducted synergistic work in developing software for visualizing cavities and the associated large datasets, as part of VizSchema [57]. This is an application-independent specification of the attributes needed for data visualization. This allows data for, e.g., cavities to be visualized using the VisIt tool, being developed under the SciDAC program, through development of a data reader plugin that can interpret VizSchema. We have made this plugin available to the community. Use of this plugin led to the receipt of an OASCR Award for Scientific Visualization at the 2008 Scientific Discovery through Advanced Computation Conference for the video, "Visual Inspection of a VORPAL Modeled Crab Cavity" [58], based on the cavity simulations described above.

Finally, we investigated the possibility of improving frequency-domain electromagnetic solver performance using state-of-the-art linear algebra techniques. Specifically, recent advances in multigrid techniques point the way towards efficient iterative solvers. These would enable tackling the largest electromagnetic problems, since they scale linearly in both computation time and memory. We prototyped a code that combines several of these advances, including complex preconditioner shift and smoothed aggregation. We demonstrated efficient solves of two-dimensional photonic crystal systems. We discovered the remarkable property that solver performance improves for parameters of physical interest, namely with frequencies in the bandgap.

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