Status of the Los Alamos Accelerator Code Group

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Abstract. Since 1986, the Los Alamos Accelerator Code Group (LAACG) has received funding from the U.S. Department of Energy. The LAACG is a national resource for members of the accelerator community who use and/or develop software for the design and analysis of particle accelerators, and beam transport systems. We distribute accelerator design and simulation codes such as the POISSON/SUPERFISH group of codes, PARMELA, PARMILA, TRACE 3-D, and others via the world-wide web, and maintain an online compendium of accelerator codes at http://laacg1.lanl.gov/laacg/componl.html. We presently have over 1300 registered users world-wide using our codes and accessing our website. An update of recent LAACG activities and projects for the upcoming year will be discussed. This work is supported by the U. S. Department of Energy Office of Science, Division of High Energy Physics.

1. Brief History of the Los Alamos Accelerator Code Group

Since 1986, the Los Alamos Accelerator Code Group (LAACG) has received funding from the U.S. Department of Energy. The LAACG is a national resource for members of the accelerator community who use and/or develop software for the design and analysis of particle accelerators, and beam transport systems. We distribute accelerator design and simulation codes via the world-wide web and maintain an online compendium of accelerator codes at http://laacg1.lanl.gov/laacg/componl.html. Figure 1 shows the website layout for the code compendium. We presently have over 1300 registered users world-wide using our codes and accessing our website. The code group resides in the Accelerator Physics and Engineering Group, LANSCE-1, at Los Alamos National Laboratory. Initially, funding was received to maintain and document a standard version of POISSON/SUPERFISH, a collection of programs for calculating static magnetic and electric fields, and radio-frequency electromagnetic fields in either 2-D Cartesian coordinates or axially symmetric cylindrical coordinates. Designers of modern high-energy physics machines use POISSON/SUPERFISH to design magnets, accelerator cavities, and other beam-line components. Significant improvements in the accuracy and ease of use of the POISSON/SUPERFISH group of codes have resulted due to the past efforts of members of the LAACG. In the early 1990s the LAACG added support of other workhorse accelerator design codes: PARMELA, PARMILA and TRACE 3-D. At about the same time, due to rapidly increasing desktop computing capabilities, the code group began migration of these programs from older mainframe computers to PC desktop machines. Now all the supported codes run on PC desktop machines.

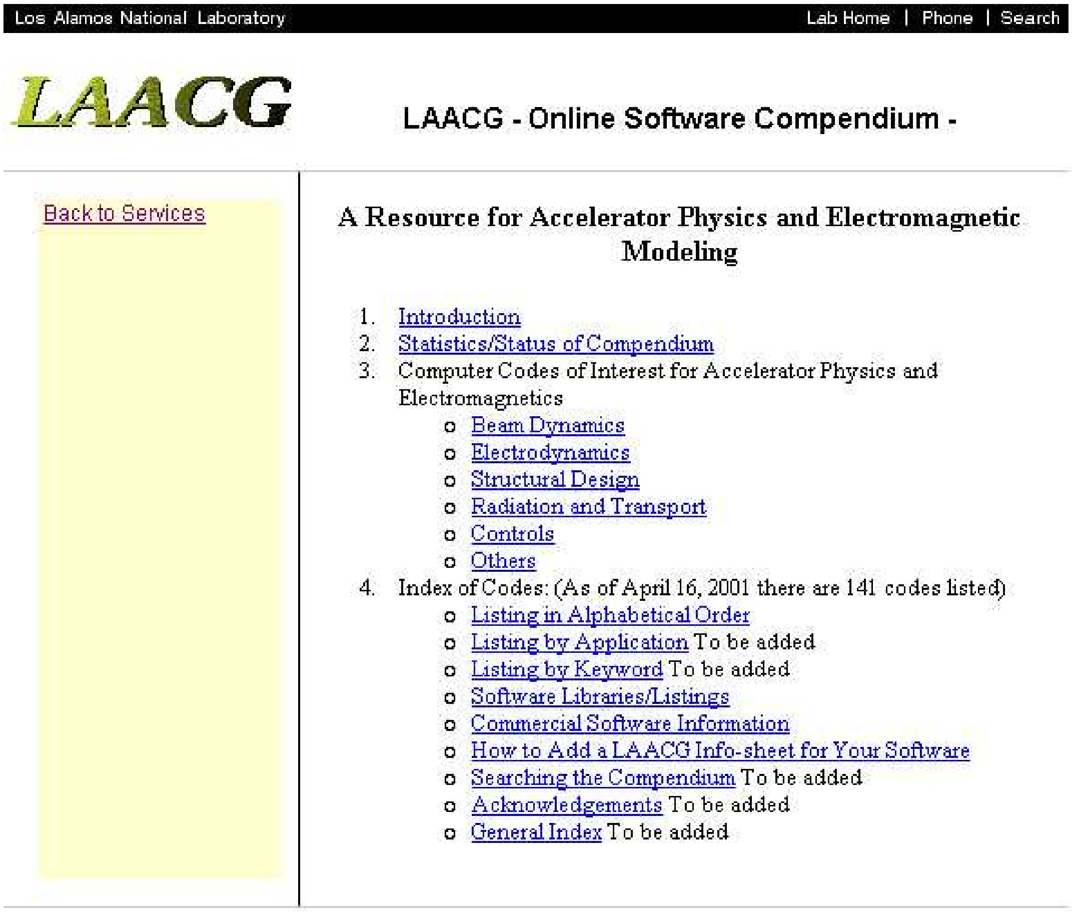

Figure 1. Code compendium website layout.

2. Impact of the LAACG

The codes maintained by the LAACG are currently being used in the design and simulation of accelerators and beam delivery systems presently funded through several divisions of the DOE Office of Science and other funding sources. Many of these projects are of national importance such as the Spallation Neutron Source (SNS) now being constructed at Oak Ridge National laboratory, at SLAC for LCLS and NLC, at BNL for RHIC, at universities such as UCLA, the University of Maryland, the University of Indiana, and Michigan State University, and several companies in industry including Advanced Energy Systems and AccSys Technology, Inc.

A review of major conference and workshop proceedings (e.g. the International Linac Conference, the Particle Accelerator Conference, the European Particle Accelerator Conference, the International Conference on the Application of Accelerators in Research and Industry, and others) shows that, in any given year, several hundred papers are published for which the research presented involved codes developed and maintained by the LAACG. Several of these publications also include comparisons between codes, indicating that similar alternate software is being developed at other institutions. However, these codes are always benchmarked against the LAACG codes. Another trend that is visible is the development of software at other institutions that basically provides graphics interfaces and uses the LAACG codes as the calculation tools (or uses output from the LAACG codes as input for secondary calculations).

3. Present LAACG Activities

Present LAACG activities include: (1) maintenance and enhancement of certain widely used software packages, including POISSON/SUPERFISH, PARMILA, PARMELA, PARMTEQ, and TRACE 3-D; (2) consultation, education, and gathering/dissemination of information related to computational accelerator physics; (3) the distribution of software and documentation via the Internet; and (4) maintenance of the official LAACG website. The continued high-level use of the above-mentioned codes, which have over 1300 registered users world-wide, demonstrates the great value of the LAACG to the national and international accelerator communities. Additionally, every year, the code group is pleased to grant the requests of instructors at universities and at special accelerator schools (USPAS, CERN) to use LAACG codes (POISSON/SUPERFISH, PARMELA, and TRACE 3-D) in the classroom as part of their graduate-level instruction in accelerator physics and engineering.

Many improvements to the codes have resulted through national and international collaborations with our users and through regular feedback regarding how the codes are serving the needs of the community. Future code enhancements such as including the capability to model low-energy superconducting accelerator structures could impact the design of facilities such as the Rare Isotope Accelerator (RIA) now being planned by collaboration between Argonne National Laboratory and Michigan State University, and the Accelerator Demonstration Test Facility (ADTF) being planned as part of the Advanced Accelerator Applications Program (AAA). Codes like PARMELA have already been used to enhance the performance of existing machines such as the Stanford Linear Collider. Additionally, these codes may be required to help design the next- generation light source.

Recently, in order to reach some of our future goals, we have begun to collaborate with members of the Accelerator Controls and Automation Group (LANSCE-8) in our division and have added a member of that group to the LAACG. Members of this group will help us to eventually modernize our workhorse codes by allowing modularization of beam-physics calculations through object-oriented programming methods. Modularization will increase the application flexibility of these codes. Additionally, we are working towards standardizing the input format for our distributed codes. This will also increase the application flexibility of the codes.

4. The LAACG Design Codes

POISSON/SUPERFISH – *is a 2-D code package of more than 30 programs for the design of RF cavities, magnet components, electrostatic elements, and waveguide devices*. An over-relaxation method is used to solve the generalized Poisson's equation in two dimensions. Eigenfrequencies and fields for arbitrarily shaped two-dimensional waveguides in Cartesian coordinates and three-dimensional axially symmetric RF cavities in cylindrical coordinates can be determined. The package contains codes to generate a very accurate triangular mesh adjusted to conform to the problem geometry, to plot the fields and to evaluate auxiliary quantities of interest in the design of drift-tube linac (DTL) cavities, coupled-cavity linac (CCL) cells, radio-frequency quadrupole (RFQ) cavities and other devices. For example, the code calculates transit-time factors, power losses, and the effect of perturbations. Several codes are included for automatically tuning DTL, CCL, and RFQ cavities by iterating on a selected portion of the geometry.

PARMILA – *is a multi-particle design and transport code for ions historically used to design drift-tube linacs (DTLs).* The name comes from the phrase, "***P****hase* ***a****nd*

***R**adial **M**otion in **I**on **L**inear **A**ccelerators*". The code has been extended to also design coupled-cavity linacs, and elliptical-cavity superconducting linac structures. A "drift-kick" method is used to transform the beam, represented by a collection of particles, through the linac to study the beam dynamics performance of the design.

PARMELA – *is a multi-particle beam dynamics code used primarily for electron-linac beam simulations.* The name comes from the phrase, "***P**hase **a**nd **R**adial **M**otion in **E**lectron **L**inear **A**ccelerators.*" It is a versatile code that transforms the beam, represented by a collection of particles, through a user-specified linac and/or transport system. It includes several space-charge calculation methods. Particle trajectories are determined by numerical integration through the fields. This approach is particularly important for electrons where some of the approximations used by other codes (e.g. the "drift-kick" method commonly used for low-energy protons) would not hold. PARMELA works equally well for either electrons or ions although is computationally slower due to the numerical integrations. PARMELA can read field distributions generated by the POISSON/SUPERFISH group of codes. Members of the code group won a LANL 2000 Distinguished Copyright Award for this code.

PARMTEQ – *and several other RFQ design codes comprise this group of codes and are used to design high-performance radio-frequency quadrupole (RFQ) linacs.* PARMTEQ is an acronym for "***P**hase **a**nd **R**adial **M**otion in a **T**ransverse **E**lectric **Q**uadrupole*". The codes have been experimentally verified in some detail by working hardware at Los Alamos and at other laboratories around the world. As we learn more about linac performance, both experimentally and theoretically, we continue to update these codes. Partial and complete RFQ design-code distributions are available. A partial distribution contains the codes necessary to design the RFQ vane profile and analyze the beam performance including the effects of higher order multipole field components and image charges. A complete distribution also includes the code VANES and several related programs, which generate and analyze machine instructions for numerically controlled machining of the vanes. Multi-particle simulations of the RFQ design are also possible with these codes.

TRACE 3-D – *is an interactive first-order beam-dynamics program that calculates the envelopes of a bunched beam, including linear space-charge forces, through a user-defined transport system.* It provides an immediate graphics display of the envelopes and the phase-space ellipses in three dimensions. This code is extremely useful for laying out beam transport lines and for determining beam matching parameters.

5. FY 2002 Highlights

The LAACG suite of PC codes (PARMELA, PARMILA, RFQ Codes, POISSON/SUPERFISH, and TRACE 3-D) continued to be supported and enhanced in FY 2002. A description of some of these activities follows. More detailed accounts can be found in the "Changes" files distributed with the codes, available on the LAACG fileservers. Additionally, some updating of information and links in the online code compendium was completed.

POISSON/SUPERFISH – (highlights from more than 40 code modifications)

At user request, the POISSON/SUPERFISH codes now support an unlimited number of materials. Program VGAPLOT was retired and replaced by the Windows plotting program WSFPLOT, which includes several hard copy choices, arrow and circle plots to show field amplitude and direction, numbered axes, and other features. New utility programs update user preferences in an "INI file," and convert experimental measurements of cavity frequencies between ambient conditions and vacuum at operating temperature. Modifications to point selection and harmonic polynomial functions improved the accuracy of the field interpolator. Several new features were added to the suite of RF-tuning programs. At the suggestion of a user at LBNL, we added new problem variables to the POISSON and PANDIRA harmonic analysis that allow off-axis placement of the analysis circle. We fixed some reported problems in the postprocessors SF7 and Force. All codes now use the robust programming practice that declares "IMPLICIT NONE" in every program unit, an extensive overhaul that allowed us to discover and work around a serious bug inherent to the Windows 98 and Windows ME operating systems.

PARMELA – (highlights from more than 20 code modifications)
Version 3, which was released last year, has proven robust enough so that we have discontinued support of version 2. The 3-D space-charge routine has new limits on the mesh aspect ratio while still allowing high-energy electrons to be treated correctly. Several beam-line elements have additional options, some at user request. Drifting particles whose velocity falls to zero are now treated properly in the presence of a static electric field. The code now writes multiple plot files for large problems (> 2 GB), eliminating a code crash. The plotting code, PARGRAF, includes new options, including color-coded particle densities, output of time-step emittance, and beam-size data. Input of Twiss parameters now uses the same convention as the programs PARMILA and TRACE 3-D.

PARMILA – A new 3-D space-charge algorithm has been added to more accurately simulate the performance of beams with high-aspect ratios. The code group benchmarked performance of PARMILA against four other codes as a part of an international collaboration on linac-design techniques. New features and plotting routines have also been added to help evaluate linac designs, and aid in the development and understanding of machine-commissioning techniques. PARMILA was used to design the SNS linac that is presently under construction and is being modified for use during its commissioning. PARMILA has become a large code. An effort to separate the accelerator design and beam dynamics functions of the code is presently underway with the goal of improving the ease of use of the code.

TRACE 3-D – A more robust data entry routine was added. This routine parses the namelist-like entries for syntax errors and reports the specific error, saving users considerable time debugging an input file.

IMPACT – Many enhancements were made to the Impact code (an object-oriented three-dimensional parallel particle-in-cell code for studying high intensity beam dynamics) to increase its applicability to a wider range of problems and to improve performance. The code treats mean-field Coulomb interactions along with the dynamics of charged particles accelerator electromagnetic fields. The code includes two types of integrators, one based on a Hamiltonian approach and another based on the direct integration of the Lorentz-force equations. The code's 3-D parallel Poisson solvers treat six types of boundary conditions. The Lorentz-force based solver has been modified to have a time-step sub-cycle for the space-charge force calculation. This allows several steps, using different external fields, to use the same space-charge forces, which speeds up the Lorentz integrator. External field transformation functions needed for error studies using the Lorentz integrator with all six boundary conditions were added. The restart capability (portable to all high performance computers) was modified so that each processor in a multi-processor run will read from a file. The random sampling of an initial distribution was improved. A new beam-line element, EMfld, provides users the flexibility of using complex external-focusing and -accelerating structures in the simulation. We used the code to study a “cross-plane resonance” phenomena discovered by Ingo Hofmann [1], which may lead to halo amplitudes significantly larger than previously expected.

POSTER – This graphics postprocessor is currently under development by C. Thomas Mottershead and is a new addition to the LAACG suite of codes. We anticipate making a version of this code available on the web soon. POSTER converts data files into Postscript form for plotting. It also includes several high-performance data processing/analysis capabilities. Its primary utility is to layout linacs, circular accelerators and beam lines that have been designed by the popular accelerator design codes. However, it has also been used to visualize results from multiparticle simulations and actual measured beam data. Figure 2 shows two examples of the sophisticated data processing and plotting capabilities of POSTER. Figure 2A shows a layout of the LANSCE Proton Storage Ring that is produced directly by reading a MARYLIE output file. All dimensions of the ring layout including the specific locations of each of the beam line elements are accurately portrayed to scale by the program. Figure 2B is a plot of the real-space transverse cross-section of a beam containing a halo. In this example the graded logarithmic color scale indicates halo beam fraction decades. This postprocessor will be extended to provide a seamless interface to PARMILA, PARMELA, TRACE 3-D, MARYLIE, DIMAD, TRANSPORT, and TEAPOT. POSTER will read the input files for these codes and generate accurate physical layouts of beam lines and accelerator lattices. An online version of a users manual will also be available. POSTER has been used rather extensively for beam-line layouts completed as part of the Advanced Hydrotest Facility Project, as well as others.

CODE COMPARISONS – In an attempt to validate our linac-design codes we undertook a program to benchmark the performance of 5 codes: PARMELA, PARMILA, IMPACT, and two codes developed by K. Crandall at TechSource, LINAC and PARTRAN, against each other by simulation of the beam dynamics in the high-intensity SNS linac design as the basis of comparison. The comparison showed all 5 codes to be in close agreement. This exercise, involving an international collaboration, laid the initial groundwork for standardization of the I/O of all the codes to facilitate further collaborations and comparisons in the future.

6. Future Plans

Present funding levels for the code group do not allow any new initiatives to be undertaken. However, it is anticipated that the future level of DOE support may increase. As a result, we are considering several new initiatives for the future. These are discussed below along with our ongoing activities.

6.1 Ongoing Activities

Code Development and Distribution – The LAACG will continue to develop, maintain, and distribute the following codes: POISSON/SUPERFISH, PARMILA, PARMELA, PARMTEQ, and TRACE 3-D. A major area of emphasis will be to upgrade all source codes to the Fortran 90 standard. The POISSON/SUPERFISH suite of codes has already been upgraded to the Fortran 90 standard. A near-term goal will be to complete conversion of the PARMILA code, with conversion of all the codes in the next few years. Conversion of all the codes to this standard is a long-term goal of the LAACG

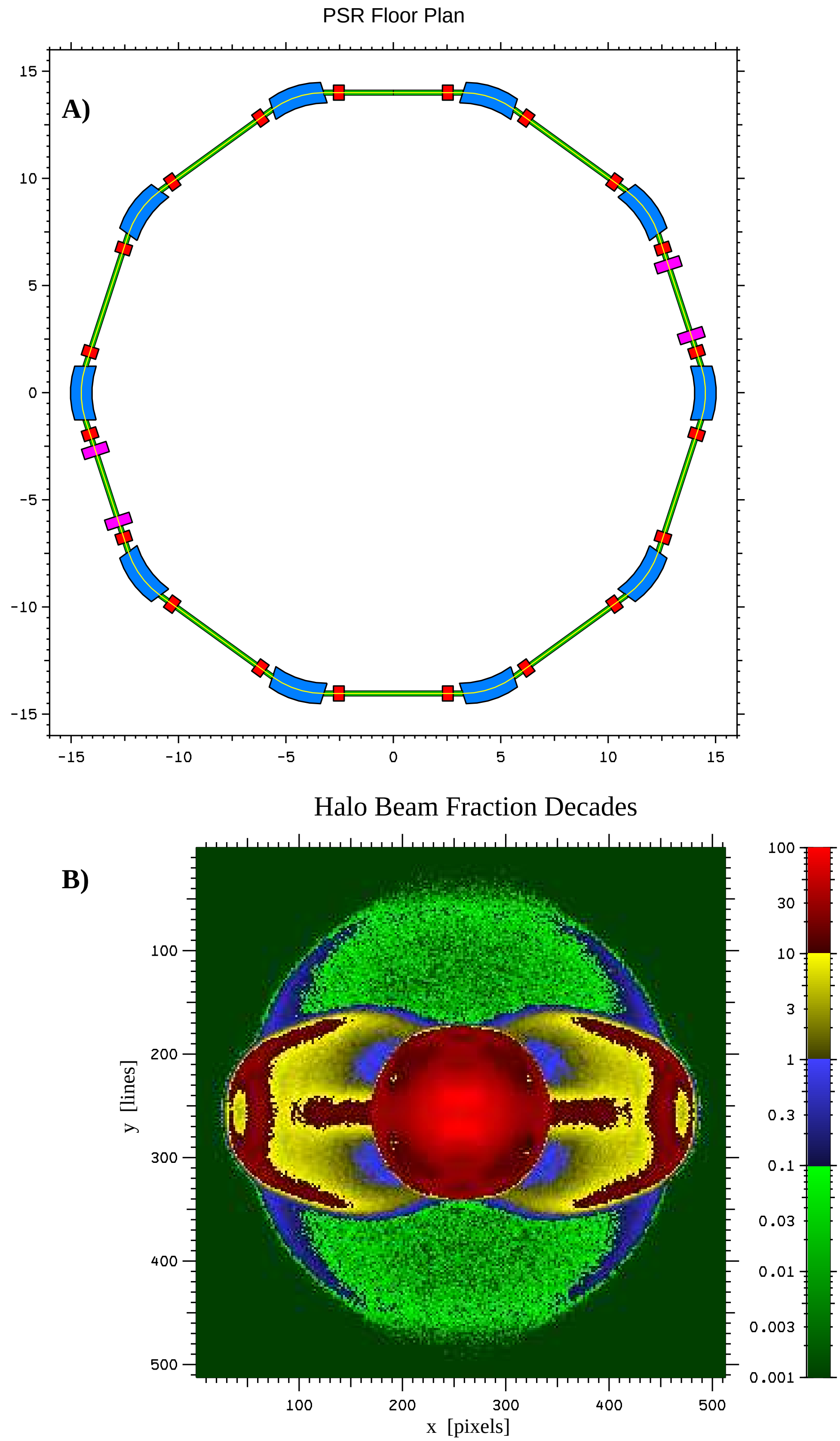

Figure 2. POSTER plotting examples: A) LANSCE Proton Storage Ring layout, B) Plot of the real-space transverse cross-section of a beam containing a halo where the graded logarithmic color scale indicates halo beam fraction decades.

and will facilitate the eventual release of Linux versions of all these codes, thereby increasing our user base significantly. Another major area of emphasis will be to improve the user interfaces of these codes. Other code development activities will include:

> POISSON/SUPERFISH – Windows versions of the general-purpose plotting codes will be released (A beta-test version has been very well received in the community.), the ability to use file editors while in a major application will be implemented, several obsolete features no longer needed on fast, modern computers will be eliminated, and the 600-page online users manual will be revised.
>
> PARMELA – The next major release will include 3-D field maps for RF and static fields, and coherent synchrotron radiation effects for electron beams in bends. PARMELA will likely be the first of the beam dynamics codes released as either a Linux or Windows version.
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> TRACE 3-D – The next release will include new Windows dialog boxes with tabular entry of variables, replacing old-style cryptic text commands.
>
> RFQ CODES – Work is underway to bring the source codes for these programs up to modern standards. The next versions will use robust coding in Fortran 90 similar to that already implanted in POISSON/SUPERFISH. In addition, two important features will be added to the beam-dynamics simulation code PARMTEQ: a 3-D space charge routine, and implementation of the dynamic aperture effect.

Web Site Maintenance / Compendium of Accelerator Codes – The LAACG will continue to maintain the official web site and online compendium of accelerator codes. At present, the online compendium is incomplete with many pages not yet containing the required descriptive text or appropriate links. We expect to be able to correct all major compendium deficiencies during FY 2003, although improvement of the web site and updating the compendium is expected to be an ongoing activity of the LAACG. Acquisition of a new server running the Linux operating system is also a goal for FY 2003. Switching to a Linux-based server will allow improved capabilities such as online searching along with implementation of software not presently available under the MS-Windows environment to track our web site traffic.

6.2 New Initiatives

External Advisory Panel – As a means of better setting priorities for the LAACG and to better serve our user community, we will establish an external advisory panel. A volunteer panel comprised of users from several other national laboratories and universities will be formed. One to two meetings per year via e-mail or phone conference will be used to address issues and set priorities to best utilize the LAACG funding.

Universal Input Format – Through recent interactions with many of the international users of our distributed codes, some consensus has been reached as to what a universal input file format might look like. The impetus for standardizing an input file format would be to allow ease of simulation of the same problem using various codes throughout the world. In particular, this would be extremely useful in expediting code benchmarking. We expect to specifically define this format with the help of our users. Our final goal is to, as much as is possible, implement this input format with all of our distributed codes.

Superconducting (SC) Accelerating Structure Modeling – At present, modeling of SC elliptical accelerating cavities is included in the PARMILA code. These cavities have historically been used in electron accelerators (β=1) and will soon be used in the high-energy section of the Spallation Neutron Source (SNS) proton linac. However, there is increasing national and international interest in the use of low-β accelerating structures such as spoke resonators that could be used to eliminate the majority of normal-conducting accelerating structures in a proton or ion linac, for example, for systems like accelerator transmutation of waste, etc. LANSCE-1 presently has codes used for modeling the beam dynamics of these low-β accelerating structures. We plan to either incorporate the modeling of these cavities into the PARMILA code or to develop our present codes to a state that would eventually allow distribution through the LAACG. This work would be carried out as part of our present code-development activities. An additional future project will be the modeling of other types of quarter-wave and half-wave resonators that are now also becoming of interest for low-β SC applications. Interest in these cavities exists since they will be used for the proposed RIA Project.

Code Modernization – A long-term goal of the LAACG is to eventually move away from codes having a monolithic, procedural architecture. This is typical of most legacy codes, making them difficult to maintain, upgrade, and distribute. We believe that porting the simulation algorithms and numerical techniques to a modern, modular, and object-oriented architecture has the potential to significantly reduce the overhead associated with code maintenance. Additionally, we believe this approach will increase the range of applications and ease of use of the codes. A major new area of application for this modern modular programming approach is the implementation of sophisticated beam modeling algorithms as part of an accelerator control system. Major advances in control system sophistication related to beam tailoring and fault recovery/management will be required for operation of complex accelerator systems. Example applications for such a system include an energy-producing waste transmutation plant where tolerances to accelerator faults is very low and beam down-time must be reduced significantly below what is presently tolerated in research facilities, significant improvements in beam control required to reach luminosity goals in future colliders, and the very tight tolerances required for successful operation of the next 4^{th}-5^{th} generation light sources. As a first step, we plan to modernize/modularize the beam dynamics calculations for a drift-tube linac as an initial test case. Simulation results will be benchmarked against the PARMILA code. A specific part of the modularization process is documentation of the physics approximations and numerical methods used in the codes. This is particularly urgent since many of the key individuals having developed these codes over the last 10-15 years will retire within the next 2-5 years. We will begin this documentation process in FY 2003.

IMPACT Code Development – Past LAACG funds were used to support the development of advanced computing applications. We would like to continue to develop the IMPACT code in collaboration with R. Ryne and J. Qiang, the developers of this code and both now at Lawrence Berkeley National Laboratory, into another work-horse user-friendly code that can eventually be distributed through the LAACG.

Specifically, we would work on making the code portable for use on both large multi-processor clusters and smaller desktop systems. Improvement of user interfaces and documentation would also be a goal.

MARYLIE Collaboration – MARYLIE is a Lie-algebraic particle beam transport and tracking program particularly useful for doing higher-order optics in transport lines and circular storage rings. Dr. C. Thomas Mottershead has been a long-time collaborator with Professor Alex Dragt at the University of Maryland (UM) in the development of this code. Other members of LANSCE-1 have also made contributions to this code. Continued code development and possibly the eventual distribution of MARYLIE through the LAACG is being discussed. The LAACG would also attempt to build up a larger user base for the code and to maintain the code while continuing to participate in future code development activities.

7. LAACG Members

A new leader has recently been appointed and additional members have been added to the LAACG in order to meet future goals including succession planning. The present members of the LAACG are listed below:

Dr. Robert Garnett, *Code Group Leader* - parallel computing, consulting.
Dr. Christopher Allen - Code modernization, accelerator controls.
Dr. James Billen - POISSON/SUPERFISH, PARMELA, PARMTEQ code development, consulting and distribution.
Dr. Frank Krawczyk - Website maintenance, code compendium, consulting.
Dr. C. Thomas Mottershead - MARYLIE and POSTER code development.
Dr. Harunori Takeda - PARMILA code development and consulting.
Dr. Lloyd Young - POISSON/SUPERFISH, PARMELA, PARMTEQ code development, consulting, and distribution.

With the exceptions of Drs. Allen and Mottershead, all other present members of the LAACG (including the new Code Group Leader) have been members in excess of 5 years.

8. Contact Us

For any questions, comments, or suggestions regarding the codes we distribute, their use, or our policies, please feel free to contact us at:

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References

[1] Qiang J, Hoffman I, Ryne R 2001 Proc. Particle Accelerator Conference