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Dissemination and Support of ARGUS for Accelerator Applications

Contract Number DE-AC05-91ER40625

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Introduction

This document is a status report for DOE Contract Number DE-AC05-91ER40625, entitled *Dissemination and Support of ARGUS for Accelerator Applications*, and covers the period from April 24, 1991 to April 14, 1995.

The effort has two broad goals, which have been prioritized by DOE, as follows:

- To enhance the ARGUS code for use in practical accelerator design simulations.
- To release ARGUS to the accelerator community through the Los Alamos Accelerator Code Group (LAACG.)

During the contract period, ARGUS versions 24 and 25 have been released. An upgraded version 25 (ARGUS v.25c) will be released in July, 1995, and will include all of the features that are tested and working at the conclusion of the DOE-funded effort. Version 26 will be released in December, 1995, and will include ARGUS enhancements that were made under DOE funding, but were not fully tested and ready for release at the conclusion of the program.

The effort that consolidated version 24 established a set of core capabilities that all ARGUS modules could access. A Unicos version of the code was established to accommodate the transition from CTSS to Unicos at NERSC (the National Energy Research Supercomputer Center at Lawrence Livermore National Laboratory.) This version was released at NERSC in August 1992.

Version 25 incorporated several major improvements:

- A new frequency-domain module was incorporated into ARGUS that can handle degenerate modes, lossy materials, and periodic boundary conditions with sub-phase specification, and that can utilize the ARGUS data handling machinery for multi-block operation.
- HDF output was implemented to allow ARGUS to send data to visualization tools.
- A plasma chemistry capability was included in the steady-state PIC module to allow ionization, stripping, electron attachment, charge exchange, and other ion rate processes to occur within the PIC calculation.
- New structure input options for figures of translation (extrusion) and figures of revolution were implemented.

This ARGUS release is supported on all Cray platforms and on the IBM RS6000 Unix workstation platform. Version 25 was released in February 1994.

The ARGUS v.26 release includes a new S-parameter module, a graphical user interface, and a post-processor. It operates on SUN workstation platforms in addition to the Cray and IBM platforms that were already supported.

The ARGUS dissemination and support activities have proceeded in parallel with code enhancement. Training courses have been held at UCLA (March 1993) and at U. of Maryland (March 1994.) ARGUS has been represented at the US Accelerator Schools at Harvard University (June 1993) and at U. of Indiana at Bloomington (June 1994.) ARGUS will be featured again this year at the Accelerator School at the University of Washington in Seattle (June 1995.)

On-line ARGUS support is available at NERSC through ARGUS man pages, at the SAIC ftp node at mclapo.saic.com, through the SAIC MOSAIC home page, and through ARGUS bulletin boards maintained at SAIC and at NERSC.

Current ARGUS documentation, available over the Internet, includes the ARGUS User's Guide and the ARGUS Primer, a tutorial for new users, and the ARGUS Technical Reference Manual and Programmer's Guide.

To date more than 70 users have been trained in the use of ARGUS. The source code, code libraries and documentation are freely available on SAIC's anonymous ftp server (which can also be accessed over Internet via GOPHER and MOSAIC.) Approximately one download per week is logged on the ftp server, out of several logins that occur each week. There is a similar level of activity at NERSC, where the ARGUS executable is maintained in the PUBLIC directory.

ARGUS execution requires a license from SAIC. These licenses have been issued freely to all DOE users. Sixty-three (63) licenses were E-mailed to ARGUS users between October 1993 and October 1994.

The following table summarizes the status of ARGUS v. 26 vs. the statement of work:

Code Development Task	Status	Release Version
User interface in a workstation environment	TAE-based MOTIF interface exists for ARGUS grid, structure and field block set up.	ARGUS v.26.
Open boundary conditions	Open BC's, based on the Lindman algorithm, are supported in the time-domain electromagnetic modules. The frequency-domain module supports sub-phase periodic BC's.	ARGUS v.25.
Lossy elements in the frequency domain module	New FD module treats lossy materials up to a maximum loss tangent.	ARGUS v.25.
Post-processor for electromagnetic simulations	Field energy and impedance integrals, as well as wall loss calculations based on a perturbative technique (for walls that are good conductors), are available.	ARGUS v.26.
Conformal gridding	Conformal gridding is needed mainly for wall loss computations. Triangular gridding was planned for this task, but is inadequate for good wall-loss results. Research on interpolated-wall boundary conditions is in progress. This type of BC will allow stairstep grids to be used, as in ARGUS, but will interpolate fields to the true wall position in each cell when applying boundary conditions.	Not yet available for release.
S parameters	A time-domain driven-frequency module with generalized external ports is available.	ARGUS v.26.

ARGUS Overview

Figure 1. The ARGUS simulation model. ARGUS provides a simulation framework linking field solvers and particle-in-cell modules together in a shared data environment with common system utilities for structure input, memory management, data handling, and visualization.

ARGUS is an integrated, three-dimensional, volumetric simulation model for systems involving electric and magnetic fields and charged particles, including the capability to embed materials in the simulation region^{1,2,3}. The code offers the capability to carry out

- ¹ A. Mankofsky, *Three-Dimensional Electromagnetic Particle Codes and Applications to Accelerators, Linear Accelerators and Beam Optics Codes*, (E.R. Eminheizer, ed., A.I.P. Conf. Proc. No. 177, American Institute of Physics, New York, 1988), p. 137.
- ² C.L. Chang, D. Chernin, A. Drobot, K. Ko, M. Kress, A. Mankofsky, A. Mondelli, and J. Petillo, *Three-Dimensional Modeling of Accelerators*, Proc. Conf. on Computer Codes and the Linear Accelerator Community (R.K. Cooper, ed., Los Alamos National Lab., January 22-25, 1990, Los Alamos Report LA-11857-C, 1990), p. 27.
- ³ J.J. Petillo, A. Mankofsky, W.A. Krueger, C. Kostas, A.A. Mondelli, and A.T. Drobot, *Applications of the ARGUS Code in Accelerator Physics*, **Computational Accelerator Physics** (R. Ryne, ed., A.I.P. Conf. Proc. No. 297, American Institute of Physics, New York, 1994), p.303.

time-domain and frequency-domain electromagnetic simulations of complex physical systems. ARGUS uses a Boolean solid-model structure input capability that can include essentially arbitrary structures on the computational domain. It has a modular architecture that allows multiple physics packages to access the same data structure and to share common code utilities. Physics modules are in place to compute electrostatic and electromagnetic fields, the normal modes of rf structures, driven-frequency rf solutions, and self-consistent particle-in-cell (PIC) simulation in either a time-dependent mode or a steady-state mode. The PIC modules include multiple particle species, the Lorentz equations of motion, and algorithms for the creation of particles by emission from material surfaces, injection onto the grid, and ionization.

Domain Decomposition in ARGUS

ARGUS uses a domain-decomposition algorithm⁴, coupled with memory management and data handling techniques, to optimize the use of core memory for each problem and to efficiently move data between core and disk memory during the calculation. A large problem is divided into blocks which are independently processed in core. The data-handling module uses overlapped I/O to move the data blocks between disk and core as they are needed by various code modules. The ARGUS modules are designed for compatibility with this data structure. The disk I/O is table driven, so that the I/O sequence for each algorithm is independently optimized. With these techniques the maximum problem size in ARGUS is limited by the available disk storage and by the overhead of disk I/O, rather than by the size of core memory. This architecture is also compatible with parallel processing within ARGUS; each block can be processed by a separate cpu.

Structure Specification

The structure input in ARGUS is carried out using combinatorial geometry. The code stores a library of basic three-dimensional objects (e.g. a rectangular solid, an elliptical cylinder, an ellipsoid, etc.). These objects are combined by the user with logical operations (to either *add* or *delete* the library object) to produce structures of arbitrary shape. The structures so specified are represented on the computational grid by a *structure mask* array, which stores the material and electrical properties of each cell on the grid.

Material properties can be associated with structures. The code allows perfectly-conducting materials, as well as materials with complex values of both permittivity and permeability; hence lossy materials are allowed. Furthermore, the permittivity and permeability may be specified as diagonal tensors to treat certain classes of non-isotropic materials.

Field Solver Module

The three-dimensional fields required in ARGUS can be computed in the electrostatic approximation or as solutions to Maxwell's equations in either the time domain or the frequency domain. These solvers can be used to compute fields for the PIC module, or as stand-alone field solvers for calculating field profiles, S parameters, capacitance, or the normal-mode frequencies and impedances of rf structures, for example.

⁴ A. Mankofsky, J.L. Seftor, C.L. Chang, K. Ko, A.A. Mondelli, A.T. Drobot, J. Moura, W. Aimonetti, S.T. Brandon, D.E. Nielson, Jr., and K.M. Dyer, *Domain Decomposition and Particle Pushing for Multiprocessing Computers*, Comp. Phys. Commun. **48**, 155 (1988).

Electrostatic Solvers. ARGUS offers two types of three-dimensional electrostatic solver. The first is a general, iterative solver for Poisson's equation, using Chebyshev-accelerated SOR⁵. The second uses a direct Fast-Fourier-Transform (FFT) method with a capacitance-matrix technique to match the potential across field blocks and to satisfy the boundary conditions on internal structures embedded on the grid. The FFT method is faster, but applies to a more limited set of problems.

Electromagnetic Solvers. ARGUS solves the complete set of Maxwell's equations in either the time domain or the frequency domain. The solutions for the electric and magnetic fields can be analyzed in a postprocessor to provide integrated field quantities, such as impedances, field energy, etc. These solvers handle non-isotropic, lossy materials.

The frequency-domain algorithm solves for the resonant modes of an rf structure with an algorithm based on a polynomial iteration method developed by Tückmantel⁶.

The initialization of the fields in the time domain can be carried out by introducing waves at ports, by driving specified currents on the grid, or by initializing specific fields on the grid. The electric and magnetic fields can be recorded as functions of time at specified witness points and Fourier analyzed to obtain the frequency content of the solution. The time-domain solver is not limited to the steady-state regime, but can provide the full time evolution of the fields.

The port boundary conditions allow arbitrarily shaped apertures at the edges of the simulation domain to represent waveguides that can carry rf power into or out of the simulation. ARGUS solves for the waveguide modes for the specified port shape, at a known frequency, and uses these modes to either drive rf fields into the simulation or to allow rf power to escape from the simulation. Outgoing power at the port aperture is decomposed into waveguide modes, and each modal component is matched out at the mode's phase velocity. With this port capability, the user can set up and execute S-parameter calculations in the ARGUS time-domain EM module. To analyze a multi-port structure, the user would drive one port, in succession, at specified frequencies, and compute the power flowing into and out of each port. The S parameters are then calculated from the ratios of the power flowing in the various ports to the power injected at the driven port.

ARGUS also supports periodic and open, radiating boundary conditions in the time domain, using the Lindman algorithm⁷, and periodic boundary conditions with user-specified phase advance across the period length in the frequency domain.

⁵ L.A. Hageman and D.M. Young, *Applied Iterative Methods* (Academic Press, New York, 1981).

⁶ J. Tückmantel, *An Improved Version of the Eigenvalue Processor SAP Applied in URMEL*, CERN/RF 85-4 (1985).

⁷ E.L. Lindman, "Free-Space" Boundary Conditions for the Time-Dependent Wave Equation, *J. Comp. Phys.* 18, 66 (1975).

Particle-in-Cell (PIC) Module

PIC simulation offers a means of solving for charged-particle flows and fields in a self-consistent manner⁸⁻¹¹. As charged particles move in the local electric and magnetic fields, they alter the local space charge and current density fields. These altered source fields then act in Maxwell's equations to modify the electric and magnetic fields. The PIC algorithm couples these two phenomena at each cycle of the simulation.

Particles can be injected at specified surfaces on the grid or emitted from material surfaces. The emission algorithm can be either space-charge limited or the emission of a prescribed current. Particles can be removed by rate processes (e.g., stripping) in the grid volume, or by absorption on material surfaces or at the edges of the grid.

ARGUS supports two major types of PIC module, dynamic PIC and steady-state PIC. The dynamic PIC module is an implementation of the full, time dependent PIC algorithm, where the fields are updated after each particle time step. This module can run with either electrostatic or electromagnetic self-fields, in addition to applied fields. It includes a "moving window" option for a moving bunch in a smooth pipe. The steady-state PIC algorithm iteratively launches successive generations of particles in fixed fields and tracks their flow across the entire grid, allocating space charge as the particles pass through each cell. The resulting space-charge density is used in Poisson's equation to update the electrostatic field for the next generation of particles. The algorithm converges when successive particle generation reproduce the same fields and flows.

⁸ O. Buneman, Phys. Rev. **115**, 503 (1959).

⁹ J.M. Dawson, Phys Fluids **5**, 445 (1962).

¹⁰ R.W. Hockney and J.W. Eastwood, **Computer Simulation Using Particles** (McGraw-Hill, New York, 1981).

¹¹ C.K. Birdsall and A.M. Langdon, **Plasma Physics via Computer Simulation** (McGraw-Hill, New York, 1985).

ARGUS Capabilities Compared With Commercial EM Software

The ARGUS code offers capabilities that are generally comparable with those available in other commercial electromagnetic software packages. Most commercial software systems do not offer the integrated electromagnetic capability that is available in ARGUS, although some offer features lacking in ARGUS. The following table summarizes the differences between ARGUS v.26 and several other well-known simulation tools.

Software	Grid	Geometry	Solvers	Post Processors	Materials	Boundary Conditions	Interfaces
ARGUS (SAIC)	SRN	D	✓	✓	✓	✓	✓
MAFIA (MAFIA)	STN	D	✓	✓	✓	✓	✓
HFSS (Hewlett-Packard)	UTN	C	✓	✓	✓	✓	✓
EMAS (MacNeil-Schwendler)	UTN	C	✓	✓	✓	✓	✓
OPERA (Vector Fields)	UTN	C	✓	✓	✓	✓	✓
MICROWAVE EXPLORER (Compact)	UTN	C	✓	✓	✓	✓	✓
SOS (Mission Research)	SRN	D	✓	✓	✓	✓	✓

S=structured grid
 U=unstructured grid
 R=rectangular cells
 T=triangular cells
 N=non-uniform cells

D=discretized structure
 C=conformal structure

L=lossy material allowed
 H=hysteresis included

P=sub-phase periodic BC

ARGUS Applications in Accelerator Simulation

ARGUS has been applied to the design and analysis of accelerator components, such as rf cavities¹² and low-energy beam transports¹³. The code has also found broader applications in the design of rf power tubes and the modeling of solid-state rf circuits (e.g., MIMIC's.)

Helix TWT Cold Test

The frequency-domain module in ARGUS can treat complex fields, where the imaginary part allows the model to treat lossy materials and to handle periodic boundary conditions with sub-phase specification. This latter feature is particularly useful when attempting to compute the dispersion curves for long, periodic structures. The usual periodic boundary condition imposes a phase shift of 2π across the computational grid. If the user needs to impose a different phase shift across the symmetry period of the structure, he does so by modeling several structure periods to build up a phase shift of 2π (or π with an electric-wall symmetry plane.) The ARGUS algorithm allows the user to specify the phase shift to be imposed across the computational grid, thereby enabling him to map out a dispersion curve while modeling only a single structure period.

This module has been used to calculate the cold test properties of a helix traveling-wave tube (TWT). Figure 2 shows the ARGUS representation of the helix TWT, including the metallic vanes that are used to reduce dispersion. (ARGUS uses sub-grid metallic structures to include these vanes. Most helix TWT codes are unable to model this essential feature in the tube's design.) The dielectric rods that support the helix were also included in the simulation, but are not shown on the figure. The ARGUS simulation used an $80 \times 80 \times 20$ grid, and computed six eigenvectors for each phase shift selected.

The dispersion curve for the helix TWT is displayed on the figure. The two lowest modes are plotted on the figure. The various curves for each mode show the effects of the dielectric supports and the metallic vanes on each mode. These results compare favorably with experimental cold-test measurements of this tube at Northrop Corporation.

¹² K. Ko, T.G. Lee, N. Kroll, and S. Tonewaga, *A Three-Gap Klystron Output Cavity at X-Band*, SLAC-PUB-5760 (1992).

¹³ J.J. Petillo and A.A. Mondelli, *LEBT Modeling with ARGUS*, Proc. 1991 Part. Accel. Conf. (San Francisco, CA, May 6-9, 1991, IEEE Cat. No. 91CH3038-7, 1991), Vol. 1, p. 315.

Figure 2. Cold-test analysis of a helix TWT with ARGUS. The metallic structures, as represented in ARGUS, are shown in (a). The helix is an ARGUS "primitive" shape, which can be simply specified by the user. The vane structures in the figure are ideal planar perfectly conducting elements to model very thin metal sheets used for dispersion reduction in the fundamental mode. Dielectric support rods are included in the simulation, but are not shown in (a). The dispersion curves for the lowest two modes are shown in (b). The various curves show the results for the helix alone, with the dielectric support rods included, and with the metallic vanes included.

Cavity-Waveguide Coupling Calculation

An important problem in the design of rf linacs is the coupling between the waveguide that feeds rf power to the linac and the cavity through which the beam is accelerated. The designer needs to know the coupling coefficient, the frequency shift, and the external Q due to the waveguide, as well as the fields in the aperture of the coupling iris. This problem is difficult for time-domain simulation because accelerator cavities are often very high- Q structures, and therefore require many rf periods to fill.

ARGUS has been employed in a collaboration between SAIC and AccSys Technology, Inc. to calculate the external Q of the drift-tube linac (DTL) cavities in the injector for the Superconducting Super Collider (SSC)¹⁴. The intrinsic Q of the DTL cavities is approximately 40,000. Figure 3 shows the DTL waveguide-cavity structure, as represented in ARGUS. The internal drift-tube structures were represented as an equivalent load, represented by a dielectric rod.

The simulations utilized published methods^{15,16,17} for inferring the external Q with a three-dimensional electromagnetic eigenvalue solver. The method requires the eigenvalue solver to be exercised several times, with the waveguide shorted at different distances from the iris, thereby allowing a resonance curve of frequency vs. phase shift to be calculated. The design is a trade-off between external Q , the field strength in the iris aperture, and the cavity mode distortion due to the aperture.

A comparison of the ARGUS results with measured data at AccSys is shown in the figure as a plot of external Q and frequency shift as functions of the iris aperture. The experimental data is plotted on the figure and agrees with the simulations within the experimental uncertainty.

Merging Beamlet Pre-Accelerator for an Electrostatic Quadrupole Accelerator

ARGUS has been employed at Lawrence Berkeley Laboratory to support planned experiments to merge 200 mA of multi-beamlet H^- at 100 keV into a single-channel electrostatic quadrupole accelerator (ESQ), which will boost the beam to 200 keV¹⁸. ARGUS was used to explore the merging of 19 beamlets in a configuration shown in Figure 4.

The ARGUS simulations modeled a pre-accelerator which accelerates particles from 6.5 keV to 100 keV in a three-electrode configuration, as shown in the figure. The evolution

¹⁴ J. Petillo, W. Krueger, A. Mondelli, and J. Potter, *Frequency Domain Determination of the Waveguide Loaded Q for the SSCL Drift Tube Linac*, Proc. 1993 Part. Accel. Conf. (Washington, DC, May 17-20, 1993, IEEE Cat. No. 93CH3279-7), Vol. 2, p.1004.

¹⁵ N. Kroll and D. Yu, *Computer Determination of the External Q and Resonant Frequency of Waveguide-Loaded Cavities*, Part. Accel **34**, 231 (1990).

¹⁶ Y. Goren and D. Yu, *Computer-Aided Design of Three-Dimensional Waveguide-Loaded Cavities*, SLAC/AP-73 (1989).

¹⁷ R. Gluckstern and R. Li, *Calculation of Cavity/Waveguide Coupling*, Proc. 1988 Linear Accel. Conf. (Newport News, VA, Oct. 3-7, 1988, CEBAF Report No. 89-001), p. 356.

¹⁸ C.F. Chan and M.C. Vella, *Design of a Merging Beamlet Pre-Accelerator for an Electrostatic Quadrupole Accelerator (ESQ)*, Proc. 1993 Part. Accel. Conf. (Washington, DC, May 17-20, 1993, IEEE Cat. No. 93CH3279-7, 1993), Vol. 4, p. 3157.

of the particle trajectories and the particle phase space are modeled by the code to establish a matched injection of the merged beamlets into the ESQ.

Figure 3. Waveguide-cavity coupling analysis for the SSC drift-tube linac. The ARGUS representation of the DTL cavity-waveguide system for the SSC injector is shown in (a). The computed and measured results for the external Q and frequency shift as functions of the iris aperture height (at 12 cm width) are shown in (b). The experimental measurements were made at AccSys Technology, Inc.

3D Calculation of a Merging Beamlet Pre-accelerator

Chen-Pai Chen

$I = 200\text{mA}$, total H^+ current from 19 apertures
 $E_0 = 6.5\text{keV}$, initial beamlet energy
 $E = 100\text{keV}$, final beam energy
 $V = 0, 80, 93.5\text{kV}$, electrode voltages

Initial Phase Space

Final Phase Space

Figure 4. Modeling of a Merging-Beamlet Pre-Accelerator for an ESQ. The ARGUS code was used at LBL to model the merging 19 beamlets in a pre-accelerator that accelerates 200 mA from 6.5 keV to 100 keV prior to acceleration into a single-channel ESQ. The equipotentials and electrode configuration are shown in (a), together with particle trajectories. The initial phase space is shown in (b), displaying the 19 independent beamlets. The final phase space, in (c), shows the beamlets merged and ready for injection into the ESQ channel.

ARGUS Code Releases

The schedule for ARGUS development and distribution can be described in terms of the schedule for ARGUS base version releases. During this contract, SAIC has prepared three ARGUS base versions (ARGUS v24 - ARGUS v26) for release.

Each new base version release has been distributed to the entire ARGUS user community, and has been accompanied by user training initiatives, such as user support workshops and courses at the US Particle Accelerator School. Recent releases have included support for Unix workstation platforms, which has helped to increase interest in ARGUS from users who have limited access to Cray supercomputers.

The code is released freely over the Internet, but users are required to obtain licenses from SAIC.

The following table summarizes the major capabilities associated with each of the ARGUS base versions:

ARGUS v24

Official Release:
November 1991

Upgrade Release (NERSC):
August 1992

ARGUS ported from Cray/CTSS to Cray/Unicos.

Uniform capabilities from module to module:

- Compatible diagnostics in steady-state and dynamic PIC modules.
- Space-charge-limited emission in both PIC modules.
- FFT electrostatic solver (CYCLOP) in dynamic PIC.
- Driven electrostatic field boundary conditions allowed so that dynamic PIC can be run with driven electrostatic fields.

ARGUS User's Guide

ARGUS v25

Beta Release:
March 1993

Official Release:
February 1994

Upgrade Release:
July 1995 (planned)

ARGUS ported to IBM RS6000 Unix workstation.

New electromagnetic (EM) frequency-domain module:

- Faster and more accurate.
- Uses ARGUS multi-block structure.
- Improved treatment of degenerate modes.

- Lossy materials included (for small loss tangent).
- Periodic BC with sub-phase specification.
- More intuitive user input.
- Performance diagnostics provided.

Plasma chemistry model in steady-state PIC.

New input structures:

- Figure of revolution.
- Extruded figure.

HDF output for data transfer to visualization tools.

Macro processor for ARGUS input.

ARGUS Primer Manual.

ARGUS v26

**Planned Official Release:
December 1995 (planned)**

ARGUS ported to SUN Sparc10 workstation.

Generalized external ports for EM time domain:

- Arbitrary port aperture cross-section allowed at the edges of the computational domain.
- Driven mode(s) as field drivers.
- Outgoing radiation matched to normal port modes.

EM Post-processor:

- Field energy and impedances.
- S parameters between generalized external ports from driven EM time-domain solution.
- Wall losses (for discretized wall) using perturbative approach.

Graphical user interface (GUI).

Technical Reference Manual.

ARGUS Code Development Activities

ARGUS v.24

ARGUS v.24 is a consolidation of the capabilities of the various ARGUS modules that had evolved in disparate directions, under diverse user-supported applications, over several years before the start of this contract effort. The primary function of this release has been to provide a stable code base on which to layer new code capabilities.

This version is the first to include UNICOS as a supported operating system on the Cray computer. ARGUS v.24 was released to the public through the National Energy Supercomputer Center (NERSC) in August 1992; this was the first broad-scale code release under this contract.

Major technical features in ARGUS v.24 are as follows:

- **Space-charge-limited emission of particles in the steady-state PIC module** was implemented for emission from flat surfaces, thus bringing the time-dependent and steady-state PIC modules into alignment.
- **Voltage-driven electrostatic PIC simulations** were enabled by linking the electrostatic field-solver modules, including time-dependent voltage boundary conditions, to the time-domain PIC module.

ARGUS v.25

ARGUS v.25 was released as a beta version at the UCLA ARGUS Workshop in March 1993. Upgrades were released through the summer and fall of 1993, and the official base version was released in February 1994. An upgraded release is planned for July 1995.

This version is a major upgrade of ARGUS over the previous base version. ARGUS v.25 includes many new features that greatly expand the code's capability to treat accelerator physics and design problems. The major new features are described below.

New frequency-domain solver

The frequency-domain solver in ARGUS v.24 has been replaced in v.25 with a new module that supports the use of complex fields and that has incorporated the following improvements that make the algorithm faster, more accurate, and friendlier to use:

- **Faster and more accurate than the previous version.** The new module uses information from the previous basis vector solution to reduce the number of iterations needed for subsequent basis vectors.
- **Improved treatment of degenerate modes.** ARGUS v.25 includes a "reseeding" algorithm that assists the frequency-domain algorithm in finding all the eigenvectors associated with a degenerate eigenvalue.
- **Periodic boundary condition with sub-phase specification.** The complex field implementation supports the use of a user-specified phase factor in the periodic boundary condition. This feature allows the user to obtain the complete dispersion relation from a single, well-resolved period of the structure.
- **Compatible with lossy materials.** Lossy materials (complex material properties) are allowed by the complex-field representation used in ARGUS v.25. This feature is available in v.25 for small loss tangent.

- **Multi-block capability.** The implementation of the frequency-domain algorithm in ARGUS v.25 uses the domain decomposition machinery in ARGUS to allow the user to split a large problem into multiple blocks. The ARGUS v.24 module was only a single-block implementation.
- **More intuitive input structure.** The user input for the frequency-domain module in ARGUS v.25 allows the user to specify the number of modes he wants to compute and the frequency band in which he expects those modes to occur. The user no longer needs to be concerned with algorithm-dependent input quantities, such as shift factors and iteration counts, that were required in the v.24 input.
- **Performance diagnostics.** The frequency-domain module in ARGUS v.25 provides performance diagnostics that allow the user to determine whether the modes presented are physical or spurious. The diagnostics are designed to measure $\text{div } \mathbf{D}$ (to test for electrostatic modes) and to compute the tolerance to which the solution satisfies the original eigenvalue equation.

Chemistry module in steady-state PIC

The steady-state PIC module has been augmented in ARGUS v.25 to include rate equations that change the species populations, in effect allowing plasma chemistry problems to be addressed in ARGUS.

The chemistry model in ARGUS allows rate equations of the following form,

$$\frac{dN_i}{dt} = \sum_{j=1}^n \gamma_{ij} N_j^{\alpha_{ij}}$$

where n is the total number of species, N_i is the density of the i -th specie in a particular spatial cell, and γ_{ij} is the rate at which specie i is created or destroyed in collisions involving specie j . The exponent α_{ij} allows additional flexibility in the model so that, for example, certain types of multi-body collisions can be included. The rates γ_{ij} are allowed to depend on the spatial cell number through the use of spatial form factors.

The chemistry module runs only under the steady-state PIC module in ARGUS. It therefore iterates to the steady-state solution of the rate equations consistent with the particle trajectories in the applied and self fields.

New structure input options

Two new classes of input structures are now allowed in ARGUS. These are figures of revolution (generalized torus) and figures of translation or extruded figures (generalized cylinder). In each case the user describes the cross-section of the structure, which can be an arbitrary closed planar curve, and rotational or translational symmetry is used to sweep out a three-dimensional volume.

HDF output files

ARGUS uses a version of GRAFLIB that runs over NCAR to produce its own graphics output as GKS metafiles. These files can be viewed with standard utilities, like GPLOT.

In addition, ARGUS v.25 includes the capability to generate HDF output files. These files can be read by many visualization packages (e.g., NCSA Image Tools). HDF files are easily transported over computer networks so that, for example, ARGUS results from a run on a Cray can be brought to a workstation for visualization. The availability of HDF output allows the user to examine his results using advanced, interactive visualization tools in a local workstation environment.

In addition, since HDF is a protocol for data representation, it offers a vehicle for users to transfer data from ARGUS to other codes.

Input macro processor

A macro-processing capability for ARGUS input files has been introduced with the ARGUS v.25 release. The processor allows the user to define macros that simplify the specification of ARGUS input variables for his application by letting him associate intuitive symbols with specific ARGUS variables.

Workstation platform support

ARGUS v.25 is the first ARGUS version to run on other than Cray platforms. The code was ported to the Unix operating system, as implemented on the IBM RS6000 platform. This activity was a natural extension of the translation from CTSS to Unicos two years ago. Ports to other Unix platforms are planned for future ARGUS releases.

Documentation

ARGUS v.25 has been released with an on-line Users' Guide and a Primer Manual that teach users how to prepare an ARGUS input file, and provide examples of problems typically encountered in accelerator physics applications.

The ARGUS Users' Guide was developed by SAIC in 1991, and has been upgraded for each new ARGUS release since then.

The ARGUS Primer was developed in collaboration with the LAACG, and was first released at the ARGUS v.25 release workshop at UCLA in March, 1993.

A first version of the ARGUS Technical Reference Manual and Programmer's Guide will be available with the upgrade release (ARGUS v.25c) in July 1995.

ARGUS v.26

ARGUS v.26, scheduled for release in December 1995, will include all of the features developed under this contract. (These features are already available to users through alpha versions at SAIC.)

Time-harmonic electromagnetic solutions

ARGUS v.26 includes a new module to compute driven single-frequency solutions of Maxwell's equations. Such solutions can be used to post-process S parameters, the coefficients that describe the RF coupling between apertures (ports) in a simulation. In an N-port network, the S parameters will form a matrix, S_{ij} , where each element represents the power flow in the j -th port for unit power drive in the i -th port. These quantities are frequency-dependent, and are related to the port impedance and admittance.

A time-domain, driven-field solver for ARGUS has been written as an engine for the S-parameter calculation. This solver computes the electromagnetic fields in the structure at a specified frequency. The implementation of the module has required the development of a generalized port algorithm that allows ports of arbitrary shape to be specified. (The present ARGUS code only allows rectangular external ports.) The electromagnetic eigenvalue solver (frequency-domain module) in ARGUS has been adapted to compute the waveguide mode spectrum in the port so that specified modes can be driven and outgoing waves can be decomposed and properly matched into outgoing waveguide modes.

User interface

A MOTIF-compliant user interface for ARGUS set-up is available with the ARGUS v.26 release. The interface is being built using the TAE GUI builder developed by NASA. It can be run from an X-terminal, or under X-windows on a workstation. The ARGUS v.26 version of the interface will support grid, multi-block and structure setup. It will allow reuse of previous input files.

Figure 5. ARGUS Graphical User Interface. The ARGUS GUI is designed to help the novice user quickly become proficient with the code, while providing a valuable time saver for experienced users of ARGUS.

Post-processor for field diagnostics

ARGUS v.26 includes a post-processing capability for computing field energy, impedances, S parameters, and wall losses.

Workstation platforms

ARGUS v.26 supports the SUN platform, in addition to Cray and IBM RS6000.

Documentation

The ARGUS Technical Reference Manual and Programmer's Guide will be available as part of the ARGUS v.26. This document provides information on the algorithms and program structure used in ARGUS. A first version of this document will be available starting in July 1995 (for ARGUS v.25c.)

ARGUS Dissemination Activities

ARGUS Release Schedule

The ARGUS code has been released through the SAIC-LAACG collaboration. Each release version typically appears in a pre-release (beta) version, followed by an official release. Often, an upgraded release is created after the official release to correct major bugs and to release new features.

During the execution of this contract two major ARGUS releases have occurred:

- (1) ARGUS v.24 was released in November, 1991. An upgraded version was released through NERSC in August, 1992.
- (2) ARGUS v.25 was released as a beta version in March, 1993. The official release was in February, 1994. (An upgrade version, ARGUS v.25c, will be released in July 1995.)

ARGUS v.25 was originally scheduled for release in July, 1993. Since the beta release in March was very stable, additional time was devoted to generating a polished version for the IBM RS6000 workstation.

ARGUS Release Mechanism

Beginning with the ARGUS v.25 release, the source code, code libraries, and documentation have been freely available through Internet using

- Anonymous ftp at SAIC (mclapo.saic.com)
- Gopher server
- MOSAIC

In addition, the ARGUS Cray executables and documentation are available in the NERSC public directory.

All of the physics code in ARGUS is available as source code. System routines and graphics routines are maintained as an executable library for each supported platform.

ARGUS execution requires the user to have an ARGUS license from SAIC. Licenses are encrypted files that identify the user and authorize specific ARGUS versions to run on specific platforms for a specified time period. SAIC makes licenses available for free to any DOE or NERSC users who request them. SAIC has issued 63 licenses over the year from October 1993 to October 1994. Typically one new user downloads ARGUS from the SAIC server each week.

ARGUS releases are well advertised through the following channels:

- ARGUS Bulletin Board (maintained by SAIC)
- NERSC Bulletin Board
- Posting on the *sci.physics.accelerators* Internet news group
- E-mail to all current ARGUS users
- ARGUS workshops
- US Accelerator School

User Training Sessions

Several ARGUS training sessions have been held. Initially, sessions were held to acquire beta testers and to train the LAACG staff in the use of ARGUS. ARGUS workshops are now held to train new users.

- (1) A training session was held at the SSC Laboratory in June, 1991.
- (2) The LAACG staff was trained in the use of ARGUS through a user training seminar at LANL in September, 1991.
- (3) An ARGUS workshop for the LAACG staff was held at SAIC in November, 1992.
- (4) An ARGUS Release workshops was held at UCLA in March, 1993.
- (5) An ARGUS Release workshops was held at U. of Maryland in March, 1994.
- (6) SAIC taught the ARGUS portion of courses on "Computations in Accelerator Physics" at the US Accelerator Schools held at Harvard University in June 1993.
- (7) SAIC taught the ARGUS portion of courses on "Computations in Accelerator Physics" at the US Accelerator Schools held at U. of Indiana at Bloomington in June 1994.
- (8) SAIC will offer the course again this year at the University of Washington in Seattle in June 1995.

ARGUS Release for Unix Workstations

The emergence of workstation platforms with performance approaching that of the Cray has led to user interest in the creation of ARGUS release versions that will run on Unix workstation platforms. As a result, SAIC has included a version of ARGUS for the IBM RS6000 workstation as a part of the ARGUS v.25 release. SAIC has also ported ARGUS to a SUN Sparc10 platform for release in v.26.

Interaction with the LAACG

Training sessions. The LAACG became ARGUS users at a training session at LANL in September, 1991. An additional training workshop was held at SAIC in November, 1992 to prepare the LAACG to support the upcoming ARGUS v.25 release. That workshop included lectures on the ARGUS code architecture and algorithms, and a review of ARGUS input procedures.

ARGUS Primer. The LAACG staff worked through several simple test problems in accelerator physics during the November, 1992 training course. These problems have formed the starting point for the ARGUS Primer, which was released at the UCLA workshop in March, 1993, and is currently the major ARGUS training tool.

Release workshop. Dick Cooper and Jean Browman from LAACG were co-instructors with SAIC at the UCLA release workshop in March, 1993. Dick Cooper worked on the U. of Maryland workshop as an SAIC consultant.

The reduction in force for the LAACG took a severe toll on the level of staff availability in that group at the critical time when they were becoming significant ARGUS supporters. After the staff cut-backs, the LAACG's ability to take on the ARGUS support and dissemination role, as planned, never materialized. Except for brief periods, SAIC has filled this role throughout this contract.

Appendix 1

**A. Mondelli,
EM Simulation Using 3-D Modeling,
Wireless Design and Development (February 1994)**

EM Simulation Using 3-D Modeling

by Alfred A. Mondelli, Science Applications International Corp. (SAIC)

ARGUS is an integrated, three-dimensional, volumetric simulation model for systems involving electric and magnetic fields and charged particles, including the capability to embed materials in the simulation region. The code offers the capability to carry out time-domain and frequency-domain electromagnetic simulations of complex physical systems.

Previous RF design codes have tended to be single-function tools with limited geometrical capability. In contrast, ARGUS offers a Boolean solid model structure input capability that can include essentially arbitrary structures on the computational domain, and a modular architecture that allows multiple physics packages to access the same data structure and to share common code utilities. Physics modules are in place to compute electrostatic and electromagnetic fields, the normal modes of RF structures, and self-consistent particle-in-cell (PIC) simulation in either a time-dependent mode or a steady-state mode. The PIC modules include multiple particle species, the Lorentz equations of motion, and algorithms for the creation of particles by emission from material surfaces, injection onto the grid and ionization.

Domain Decomposition in ARGUS

ARGUS uses a domain-decomposition algorithm, coupled with memory management and data handling techniques, to optimize the use of core memory for each problem and to efficiently move data between core and disk memory during the calculation. A large problem is divided into blocks that are independently processed in core. The data-handling module uses overlapped I/O to move the data blocks between disk and core as they are needed by various code modules. The ARGUS modules are designed for compatibility with this data structure. The disk I/O is table driven so that the I/O sequence for each algorithm is independently optimized. With these techniques the maximum problem size in ARGUS is limited by the available disk storage and by the overhead of disk I/O rather than by the size of core memory. This architecture is also compatible with parallel processing within ARGUS. Each block can be processed by a separate CPU.

Structure Specification

The structure input in ARGUS is carried out using combinational geometry. The code stores a library of basic three-dimensional objects (e.g. a rectangular solid, an elliptical cylinder, an ellipsoid, etc.). These objects are combined by the user with logical operations (to either add or delete the library object) to produce structures of arbitrary shape. The structures so specified are represented on the computational grid by a structure mask array, which stores the mate-

ARGUS integrated simulation model.

Cold-test simulation of a helix TWT. This simulation includes the helix structure (shown in black), as well as dielectric support rods and metallic dispersion-control vanes (not shown). Colored field isosurfaces show the field pattern for a normal mode. Several modes can be computed, with multiple phase shifts, to generate the complete cold dispersion curve for this device.

Electrical stability analysis for a MMIC packaging. Colored field isosurfaces show the electrical field distribution for a normal mode of a C-band T/R module for a phased-array radar.

rial and electrical properties of each cell on the grid.

Material properties can be associated with structures. The code allows perfectly conducting materials as well as materials with complex values of both permittivity and permeability; hence lossy materials are allowed. Furthermore, the permittivity and permeability may be specified as diagonal tensors to treat certain classes of non-isotropic materials.

across field blocks and to satisfy the boundary conditions on the internal structure embedded on the grid. The FFT method is faster, but applies to a more limited set of problems.

Electromagnetic Solvers. ARGUS solves the complete set of Maxwell's equations in either the time domain or the frequency domain. The solutions for the electric and magnetic fields can be analyzed by the code to provide integrated field quantities, such as impedances, field energy, etc. These solvers can handle nonlinear, nonisotropic, lossy materials.

The initialization of the fields in the time domain can be carried out by introducing waves at ports, by driving specified currents on the grid, or by initializing specific fields of the grid. The electric and magnetic fields can be recorded as functions of time at specified witness points and Fourier analyzed to obtain the frequency content of the solution. The time-domain solver is not limited to the steady-state regime, but can provide the full time evolution of the fields.

Particle-in-Cell (PIC) Module

PIC simulation offers a means of solving for charged-particle flows and fields in a self-consistent manner. It can be used to calculate the hot-test performance for diverse RF devices. As charged particles move in the local electric and magnetic fields, they alter the local space charge and current density fields. These new source fields then act in Maxwell's equations to modify the electric and magnetic fields. The PIC algorithm couples these two phenomena at each cycle of the simulation.

Particles can be injected at specified surfaces on the grid or emitted from material surfaces. The emission algorithm can be space-charge limited or the emission of a prescribed current. Particles can be removed by rate processes (e.g. stripping) in the grid volume or by absorption on material surfaces at the edge of the grid.

Field Solver Module

The three-dimensional fields required in ARGUS can be computed either in the electrostatic approximation or as solutions to the full time-dependent Maxwell's equations. Two types of electrostatic solvers (using direct or iterative methods) and two types of electromagnetic solvers (frequency domain or time domain) are available within ARGUS. For example, these solvers can be used to compute fields in the PIC module, or as stand-alone field solvers for calculating field profiles, capacitance, or the cold-test properties of RF structures.

Electrostatic Solvers. ARGUS offers two types of three-dimensional electrostatic solvers. The first is a general, iterative solver for Poisson's equation, using Chebyshev-accelerated SOR (Successive OverRelaxation). The second uses a direct Fast-Fourier-Transform (FFT) method with a capacitance-matrix technique to match the potential

ARGUS Applications in RF Simulations

ARGUS has been applied to the design and analysis of many devices and components used in RF systems, including cold-test calculations for microwave coupled-cavity tubes and helix TWTs, and the analysis of the RF modes in MMIC circuits and MMIC packaging structures. Calculations with lossy materials have been carried out to model severs in a microwave amplifier and high-order-mod dampers in a gyrokystron amplifier circuit. The ARGUS code also has found many applications in the RF design of accelerator structures and in the study of particle sources.

Appendix 2

J. Petillo, A. Mankofsky, W. Krueger, C. Kostas, A. Mondelli, and A. Drobot,
Applications of the ARGUS Code in Accelerator Physics,
Proc. 1993 Computational Accelerator Physics Conference
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COMPUTATIONAL ACCELERATOR PHYSICS

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ABSTRACT

ARGUS is a three-dimensional, electromagnetic, particle-in-cell (PIC) simulation code that is being distributed to U.S. accelerator laboratories in collaboration between Science Applications International Corporation (SAICTM) and the Los Alamos Accelerator Code Group (LAACG). It uses a modular architecture that allows multiple physics modules to share common utilities for grid and structure input, memory management, disk I/O, and diagnostics. Physics modules are in place for electrostatic and electromagnetic field solutions, frequency-domain (eigenvalue) solutions, time-dependent PIC, and steady-state PIC simulations. All of the modules are implemented with a domain-decomposition architecture that allows large problems to be broken up into pieces that fit in core and that facilitates the adaptation of ARGUS for parallel processing. ARGUS operates on either Cray or workstation platforms, and a MOTIF-based user interface is available for X-windows terminals. Applications of ARGUS in accelerator physics and design are described in this paper.

DESCRIPTION OF ARGUS

The ARGUS code^{1,2} has been under development at SAIC since 1983. It is a general-purpose three-dimensional simulation code. The code architecture is specifically designed to handle the problems associated with three-dimensional simulations. It uses sophisticated memory management and data handling techniques³ to deal with the large volume of data that is generated in three-dimensional simulations. Recent work by Leabrook Computing, Ltd. shows that the domain decomposition technique used in ARGUS provides a suitable framework for coarse-grained parallelization of the code.

A modular architecture is employed so that ARGUS is in fact a system of three-dimensional codes (numerical modules) that utilize a common data structure and share utilities for structure input, grid generation, memory management, data handling, and diagnostics. The codes allow complicated geometrical structures to be represented on the computational grid. The grid can be nonuniform in all three dimensions. Cartesian and cylindrical coordinate systems have been implemented throughout ARGUS; some of the modules also support toroidal and mixed coordinates. Physics modules are in place to compute electrostatic and electromagnetic fields, the eigenmodes of rf structures, and PIC simulation in either a time-dependent mode or a steady-state mode. The PIC modules include multiple particle species, relativistic particle dynamics, and algorithms for the creation of particles by emission from material surfaces and by injection onto the grid. A plasma chemistry module allows species to be created or destroyed based on specified rate processes.

The structure input in ARGUS is carried out through combinatorial geometry. The code stores a library of basic three-dimensional objects (e.g., a rectangular solid, an elliptical cylinder, an ellipsoid, etc.). These objects are combined by the user with logical operations (to either *add* or *delete* the library object) to produce structures of arbitrary shape. The structures so specified are represented on the computational grid

by a *structure mask* array, which stores the material and electrical properties of each cell on the grid.

Figure 1. ARGUS modular code architecture.

Material properties can be associated with structures. The code allows perfectly-conducting materials, as well as materials with complex values of both permittivity and permeability; hence lossy materials are allowed. Furthermore, the permittivity and permeability may be specified as diagonal tensors to treat certain classes of non-isotropic materials.

ARGUS has a wide variety of diagnostic plots that are selected by user input and are available at run time. These include set-up graphics, contour and arrow plots

of field quantities, and plots of particle trajectories and phase space. The code also will allow the user to create HDF files for exporting data to other visualization tools.

SOME EXAMPLES FROM THE ARGUS PRIMER

The current code release (ARGUS v.25) includes an ARGUS Primer, which provides a tutorial for new ARGUS users. It presents a set of simple example problems that illustrate how to use the features in ARGUS. The Primer will also be used in testing future ARGUS releases and ARGUS installations on new computing platforms. A subset of the examples featured in the Primer are presented here.

The "Tombstone" Cavity

An example in the MAFIA User's Guide consists of analyzing the normal modes of the structure shown in Figure 2. The structure is a cylindrical drift tube attached to a cavity made of a rectangular box topped with a half cylinder. MAFIA and ARGUS represent this structure in different ways. ARGUS uses a "stairstep" representation on the grid, while MAFIA allows triangular "half cells". (Half-cell masking will be included in a future ARGUS release.)

Figure 2. The "Tombstone" cavity.

Cold Test of the "Tombstone" Cavity

A comparison of ARGUS and MAFIA cold-test results for the "Tombstone" cavity are given in Figure 3. The ten lowest modes of the structure were computed. The discrepancy is generally in the 1-2% range, and is due to the differences in the structure representation by the two codes. This result is consistent with other comparisons of these codes on comparable meshes. With finer meshing, the codes agree more closely.

Figure 3. Comparison of ARGUS and MAFIA results for "Tombstone" cavity cold test.

Wake Fields in the "Tombstone" Cavity

Figure 4. Wake fields due to a Gaussian bunch passing through the "Tombstone" cavity.

By initializing a Gaussian bunch of heavy particles in the time-dependent PIC module, and allowing them to drift through a structure, the user can cause ARGUS to create wake fields in the structure. This method was employed to display the wake

fields in the "Tombstone" cavity. Figure 4 shows three snapshots of the particles and axial electric field as the bunch traverses the structure. The Gaussian bunch was placed on the axis of the cylindrical drift tube and launched into the tombstone cavity. The particles are visible in the figure as a line charge on axis. In the first frame, time step 25, the particles are just entering the tombstone cavity from the lower drift tube. In the second frame, time step 75, they are just leaving the tombstone cavity and entering the upper drift tube. In the third frame, time step 125, they are leaving the upper drift tube (by being absorbed on the upper boundary of the simulation).

Radiating Open Waveguide in the Time Domain

The ability of the ARGUS code to handle open, radiating boundary conditions in the time domain sets it apart from several other codes. Two separate utilities exist for carrying out this capability. The first is a "port" boundary condition, which treats a specified opening in the simulation boundary as though it were connected to a waveguide extending to infinity. The second is an implementation of the Lindman⁴ algorithm for radiating boundaries. While the port condition only matches the boundary for radiation at a specified frequency, the Lindman condition is a general outgoing wave boundary condition.

This simulation provides a demonstration of the Lindman algorithm for the simple example of a rectangular waveguide that is driven at the lower end, and open at the upper end. Figure 5 shows the radiation fields at two time steps, selected to show the phase slippage at the top (open) boundary.

Figure 5. A radiating waveguide in the time domain.

WAVEGUIDE-CAVITY COUPLING

An important problem in the design of rf linacs is the coupling between the waveguide that feeds rf power to the accelerator and the cavity through which the beam is accelerated. The designer needs to know the coupling coefficient, the frequency shift, and the external Q due to the waveguide, as well as the fields in the

aperture of the coupling iris. This problem is difficult for time-domain simulation codes because accelerator cavities often are very high-Q structures, and therefore require very many rf cycles to fill.

ARGUS has been employed in a collaboration between SAIC and AccSys Technology, Inc. to model the external Q of the drift-tube linac (DTL) cavities in the injector for the Superconducting Super-Collider (SSC). The intrinsic Q of the DTL cavities is approximately 40,000. Figure 6 shows the aperture in the waveguide cavity system, as represented in the ARGUS model. The drift-tube structures are represented by an "equivalent load," consisting of a dielectric rod.

Figure 6. ARGUS representation of the DTL cavity/waveguide structure for the SSC injector.

The methods used for the solution are based on published techniques^{5,6,7} for using electromagnetic frequency-domain algorithms to compute the external Q in high-Q cavity-waveguide systems. They require the eigenvalue solver to be exercised several times, with the waveguide shorted at different distances from the iris, thereby allowing a resonance curve of frequency vs. phase shift, like that shown in Figure 7, to be mapped out. The figure shows the resonance curve for a round iris, 12 cm in diameter. This analysis is repeated for different choices of the iris dimensions until a suitable design point is realized. The design is a trade-off between the external Q, the field strength in the iris aperture, and the cavity mode distortion due to the aperture.

AccSys has built an experimental test-stand which allowed the ARGUS results to be compared with measured data. The results of that test are shown in Figure 8, which presents the external Q and frequency shift as functions of the iris aperture length, for a fixed aperture width of 12 cm. The experimental data are plotted on the figure and agree with the simulations to within the experimental uncertainty.

AccSys Technology, Inc. is under contract to build the DTL cavities for the SSC Laboratory, and has used these simulations to verify the accuracy of their experimental test data prior to constructing full-scale cavities (which are approximately 10 m in length). Dr. Jim Potter of AccSys has collaborated with SAIC in this effort,

and provided the experimental data which was compared with the ARGUS simulations in Figure 8.

Figure 7. Phase shift vs. frequency for a 12 cm diameter iris aperture.

Figure 8. External Q and frequency shift vs. iris length for the DTL cavity/waveguide system. ARGUS simulation results are compared with experimental measurements (courtesy of J. Potter, AccSys Technology, Inc.)

HELIX TRAVELING-WAVE TUBE

The frequency-domain solver in ARGUS v.25 can treat complex fields, where the imaginary part allows the model to treat lossy materials and to handle periodic boundary conditions with sub-phase specification. This latter feature is particularly

useful when attempting to compute the dispersion curves for long, periodic structures. The usual periodic boundary condition imposes a phase shift of 2π across the computational grid. If the user needs to impose a different phase shift across a symmetry period of the structure, he does so by modeling several structure periods to build up a phase shift of 2π (or π with an electric wall symmetry plane). The ARGUS v.25 algorithm allows the user to specify the phase shift to be imposed across the computational grid, thereby enabling him to map out a dispersion curve while modeling only a single structure period.

This module has been used to cold test a helix traveling-wave tube (TWT), developed by Northrup Corporation. Figure 9 shows the ARGUS representation of the helix TWT, including the metallic vanes that are used to short the fields between the helix supports. The supports (not shown in the figure) are dielectric rods that are attached to the helix and to the outer cylindrical wall. The ARGUS simulation model employed a $80 \times 80 \times 20$ grid, and requested six eigenvectors for each phase shift selected.

Figure 9. ARGUS structure plot for the metallic regions in the Northrup helix TWT.

The dispersion curve for the helix TWT is displayed in Figure 10. The figure shows the effect of the supports and the metallic vanes on the dispersion curve. The vanes are needed to flatten the dispersion curve (i.e., to reduce the dependence of the phase velocity on frequency). They are modeled in ARGUS as two-dimensional metallic sheets. Most three-dimensional electromagnetic codes are unable to include sub-cell features of this type, and therefore do not succeed in cold test analyses of devices like the helix TWT. Comparison with experimental data at Northrup indicate that the phase velocity corresponding to Figure 10 differs from the measured phase velocity by approximately 10%, but this difference can be largely accounted for by

adjusting the contact area between the support rods and the helix. (The phase velocity of a helix TWT is known to be very sensitive to the area of contact.)

Dr. Gunther Doehler of Northrup Corporation has graciously provided a description of the helix TWT geometry, and has compared the ARGUS simulation results with his experimental data.

Figure 10. Dispersion curve for the Northrup helix TWT.

ACKNOWLEDGMENT

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Appendix 3

A. Mankofsky, J. Petillo, W. Krueger, and A. Mondelli,

***Recent Progress in 3D EM/EM-PIC Simulation
with ARGUS and Parallel ARGUS,***

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Recent Progress in 3D EM/EM-PIC Simulation with ARGUS and Parallel ARGUS

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ARGUS is an integrated, three-dimensional, volumetric simulation model for systems involving electric and magnetic fields and charged particles, including materials embedded in the simulation region [1]. The code offers the capability to carry out time domain and frequency domain electromagnetic simulations of complex physical systems. Previous codes have tended to be single-function tools, with limited geometrical capability. In contrast, ARGUS offers a Boolean solid model structure input capability that can include essentially arbitrary structures on the computational domain, and a modular architecture that allows multiple physics packages to access the same data structure and to share common code utilities. Physics modules are in place to compute electrostatic and electromagnetic fields, the normal modes of RF structures, and self-consistent particle-in-cell (PIC) simulation in either a time-dependent mode or a steady-state mode. The PIC modules include multiple particle species, the Lorentz equations of motion, and algorithms for the creation of particles by emission from material surfaces, injection onto the grid, and ionization.

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In this paper, we present an updated overview of ARGUS, with particular emphasis given to recent algorithmic and computational advances. These include a completely rewritten frequency domain solver which efficiently treats lossy materials and periodic structures, a parallel version of ARGUS with support for both shared memory parallel vector (i.e., Cray) machines and distributed memory massively parallel MIMD systems, and numerous new applications of the code.

Frequency Domain Calculations

The ARGUS frequency domain solver calculates the eigenvalues and eigenvectors of 3D structures. It is useful for finding the complex resonances of enclosed cavities such as are commonly found in accelerators and microwave devices.

Previously, the ARGUS algorithm was restricted to finding purely real eigenmodes, i.e., lossy materials were not properly accounted for in the calculation. In addition, a device's dispersion relation could be found only by modeling many periods of the structure; this required an inordinately large number of cells, with correspondingly long running times. Both restrictions have been eliminated in the latest release of ARGUS.

Physical model

The equations of interest in the frequency domain are the Fourier-transformed Maxwell equations,

$$\lambda \mathbf{B} = -\nabla \times \mathbf{E},$$

$$\lambda \mathbf{D} = \nabla \times \mathbf{H} + \sigma \mathbf{E},$$

where $\mathbf{B} = \mu \mathbf{H}$, $\mathbf{D} = \epsilon \mathbf{E}$, and λ is the eigenvalue we seek. The presence of the $\mathbf{E}$ term in the second equation leads to dissipation. Physically, this term represents resistive elements in the system, which give rise to eigenvalues with a negative real part and therefore lead to damping of a set of modes. This damping could also be due to a lossy dielectric, in which case ϵ is complex, representing the loss tangent of the dielectric.

The simple inclusion of a resistive term in the model subtly changes the properties of the system, necessitating a complete revision of the numerical procedure used to solve for the eigenmodes.

Numerical algorithm

The new ARGUS frequency domain algorithm is based on techniques developed by Tückmantel [3]. The underlying premise of the method is that a sequential application of the shifted Maxwell operator to a trial solution will project out a subspace which contains only a few lowest eigenvectors. An equivalent matrix problem on this subspace will have the same eigenvalues as the overall problem. In the presence of complex materials, the eigenvalues of the Maxwell operator occur either in complex pairs (λ, λ^*), or else are purely real and negative ($-\lambda_1, -\lambda_2$).

To reduce a trial solution to a subspace requires a proper set of shift factors, which come in complex pairs. We have used shifts of the form $s_n = \alpha_n + i\beta_n$, where α_n and β_n are sequential iteration parameters, used as follows:

$$\mathbf{B}^{n+1} = -\nabla \times \mathbf{E}^n + s_n \mathbf{B}^n,$$

$$\mathbf{D}^{n+1} = \nabla \times \mathbf{H}^n - \sigma \mathbf{E}^n + s_n \mathbf{D}^n,$$

followed by

$$\mathbf{B}^{n+2} = -\nabla \times \mathbf{E}^{n+1} + s_n^* \mathbf{B}^{n+1},$$

$$\mathbf{D}^{n+2} = \nabla \times \mathbf{H}^{n+1} - \sigma \mathbf{E}^{n+1} + s_n^* \mathbf{D}^{n+1}.$$

A proper choice for α_n and β_n can be used to project out eigenvectors that have eigenvalues in a specific region of the complex plane. In our formulation, the trial vectors consist of the meshwide E , which is complex.

This generalization of the ARGUS frequency domain algorithm to the complex plane also allows the trivial imposition of an arbitrary phase shift at a periodic boundary. By modeling a single period of a structure (an immediate savings in terms of problem size and running time relative to a multi-period structure) and making a number of small runs each with a different phase shift, dispersion curves can be now be calculated with far less computational cost than previously possible.

Parallel ARGUS

The domain decomposition methods used in ARGUS are naturally suited to parallel processing. Each field block, or group of field blocks, can be assigned to a separate CPU; data shared across block interfaces [2] is then simply sent from one CPU to another, with appropriate synchronization. Particles can be treated in a similar fashion.

This approach maps particularly well onto message passing schemes for parallelization. Using PAXX (a portable data transport library with underlying support for the PVM, PARMACS, and Intel NX protocols), major portions of ARGUS have been parallelized and run on both the Transtech Pyramid MPP and the Cray C90. The entire effort required the addition of approximately 400 lines of code, predominantly in the areas of setup, diagnostics, and memory management. The key pieces of new code - those implementing the message passing and synchronization at block interfaces - were confined to only a few routines. No changes were required to any of the fundamental ARGUS algorithms.

Preliminary timings on a 16-node parallel system indicate overlaps approaching 98% for a 32 block EM solve with 124,000 mesh points. Even higher efficiencies can be obtained by assigning three or more blocks per node and processing the outer blocks on each node first, so that the data transport between nodes can be completely overlapped with the calculation. On the other hand, the efficiency is reduced slightly when complex internal structures are included in the simulation, but this is simply an artifact of the masking algorithm presently used in ARGUS, and does not have any fundamentally negative implications for the more general application of the parallel code.

Recent ARGUS applications

ARGUS has been applied to the design and analysis of a wide variety of electromagnetic devices and components. Recent areas include cavity design for a drift tube linac, ICRH antenna design for heating of Tokamak plasmas, diamond reactor design for plasma processing, and RF calculations for microwave coupled-cavity tubes, helix TWTs, and MMIC circuits and packaging structures. ARGUS has also found many applications in the RF design of accelerator structures, and in the study of particle sources, charged particle beams, and antennas. We present several representative examples.

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- [3] J. Tückmantel, "An Improved Version of the Eigenvalue Processor SAP Applied in URMEI," CERN/EF/RF 85-4 (1985).

Appendix 4

Alfred Mondelli

ARGUS Now Available at NERSC

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diagonal tensors to treat certain classes of non-isotropic materials.

ARGUS has a wide variety of diagnostic plots that are selected by user input and are available at run time.

The structure setup can be viewed in two diagnostics, either as slices through the grid or as a two-point perspective plot, to display the structure mask on the grid. Users can select which type of structure (e.g., material) to plot, or can request that all structures be plotted together.

Any field quantity on the grid can be displayed as a contour plot. Vector field quantities may be displayed either as arrow plots or as contour plots for any component of the vector. These plots may be generated at user specified time intervals in a time-domain electromagnetic solve or a time-dependent PIC simulation, for each eigenmode solution from the frequency-domain electromagnetic solver, or at each iteration of a steady-state PIC simulation. In addition the time-dependent modules (PIC and time-domain electromagnetic) have the capability of saving and plotting time histories of any field component at a set of specified sample points. These time histories can be Fourier analyzed by the code to display the frequency spectrum associated with the time dependence. Integrals over field quantities, to compute field energy and impedance, are also available.

The particle diagnostics consist of phase space projections on any two-dimensional or three-dimensional subsurface of the six-dimensional phase space. Diagnostics to process beam emittance are also available.

New ARGUS Features Under Development

ARGUS is undergoing a substantial enhancement in preparation for the code release next year. That release will include a new frequency domain algorithm capable of treating complex eigenvalues (i.e., lossy materials). A new periodic boundary condition, with arbitrary phase advance per period, will be included. Finally, a MOTIF-based user interface that runs on UNIX workstations under X-windows will be available. Extensive code documentation improvements are also in progress.

ARGUS Applications

ARGUS has been applied to a broad spectrum of problems. The electrostatic solvers have been used as stand-alone codes to analyze the dc component of the fields in a cross-field amplifier tube. They have also been used with the PIC module to carry out steady-state simulations of electron guns, depressed electron collectors, ion guns, and low-energy electrostatic ion accelerators.

The electromagnetic modules in ARGUS have been used to carry out cold-test calculations for microwave coupled-cavity tubes and accelerator structures. Calculations with lossy materials have been carried out to model severs in a microwave amplifier and high-order-mode dampers in a gyrokystron amplifier circuit. ARGUS has modeled the double output cavity for the SLAC klystron. It has also been applied to the analysis of the rf modes in MMIC circuits and MMIC packaging structures.

Knowing the cold-test fields in an rf structure from ARGUS, it is possible to inject single test particles and to determine the transfer of energy between the electromagnetic fields and the particles. This type of calculation can be used, for example, to compute start-oscillation criteria and linear gain in an rf amplifier.

Full PIC simulations have been carried out to study instabilities in the particle flow in a magnetically-insulated transmission line (using electromagnetic fields) and to model heavy-ion beam transport (with electrostatic fields) in a periodic magnetic quadrupole lattice for the heavy-ion fusion program.

¹ A. Mankofsky, "Three-Dimensional Electromagnetic Particle Codes and Applications to Accelerators," *Linear Accelerator and Beam Optics Codes*, C.R. Eminheizer, ed., A.I.P. Conf. Proc. No. 177 (American Institute of Physics, New York, 1988), p. 137ff.

² C.L. Chang, D. Chernin, A. Drobot, K. Ko, M. Kress, A. Mankofsky, A. Mondelli, and J. Petillo, "Three-Dimensional Modeling of Accelerators," *Proc. of the Conf. on Computer Codes and the Linear Accelerator Community*, R.K. Cooper, ed. (Los Alamos National Laboratory, January 22-25, 1990, LA-11857-C), p. 27.

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ARGUS Now Available at NERSC

Alfred Mondelli, Science Applications International Corporation

The ARGUS code system, a set of three-dimensional simulation modules for plasma physics, beam research, and electromagnetics, is now available to NERSC users. ARGUS was developed by Science Applications International Corporation (SAIC).

The Department of Energy is sponsoring a collaboration between SAIC and Los Alamos National Laboratory to release ARGUS to all DOE users through the Los Alamos Accelerator Code Group (LAACG). The code will become available through LAACG, with user support and documentation, in the first quarter of 1993. The current release at NERSC is a beta version that is being made available to NERSC users in anticipation of the release next year. Until then, while NERSC consultants will provide a first line of user support, SAIC will provide basic support by phone and E-mail. If there is sufficient demand, user training sessions will be scheduled at SAIC in McLean, Virginia. There will be a fee to cover staff and materials expenses for training sessions at SAIC.

The beta version of the code is available in the /usr/local/pub directory on the CRAY/C, F, and Y. Type:

```
man argus
```

for instructions on how to access ARGUS and the ARGUS User's Guide, and to retrieve a file containing sample input files.

Description of ARGUS

The ARGUS code^{1,2} has been under development at SAIC since 1983. It is a

general-purpose three-dimensional simulation code. The code architecture is specifically designed to handle the problems associated with three-dimensional simulations. It uses sophisticated memory management and data handling techniques to deal with the large volume of data that is generated in three-dimensional simulations.

A modular architecture is employed so that ARGUS is in fact a system of three-dimensional codes (numerical modules) that use a common data structure and share utilities for structure input, grid generation, memory management, data handling, and diagnostics (see Figure 1).

The codes allow complicated geometrical structures to be represented on the computational grid, which can be nonuniform in all three dimensions. Cartesian coordinates are implemented throughout ARGUS, although some of the modules also support cylindrical and toroidal coordinates. Physics modules are in place to compute electrostatic and electromagnetic fields, the eigenmodes of rf structures, and PIC (Particle-in-Cell) simulation in either a time-dependent mode or a steady-state mode. The PIC modules include multiple particle species, relativistic particle dynamics, and algorithms for the creation of particles by emission from material surfaces and injection onto the grid. A plasma chemistry module allows species to be created or destroyed based on specified rate processes.

The structure input in ARGUS is carried out through combinatorial geometry. The code stores a library of

ARGUS is a set of three-dimensional simulation modules for plasma physics, beam research, and electromagnetics.

Figure 1. ARGUS modular code architecture.

basic three-dimensional objects (e.g., a rectangular solid, an elliptical cylinder, an ellipsoid, etc.). These objects are combined by the user with logical operations (to either *add* or *delete* the library object) to produce structures of arbitrary shape. The structures so specified are represented on the computational grid by a *structure mask* array, which stores the material and

electrical properties of each cell on the grid.

Various material properties can be associated with structures. The code allows perfectly conducting materials, as well as materials with complex values of both permittivity and permeability; hence lossy materials are allowed. Furthermore, the permittivity and permeability may be specified as

diagonal tensors to treat certain classes of non-isotropic materials.

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