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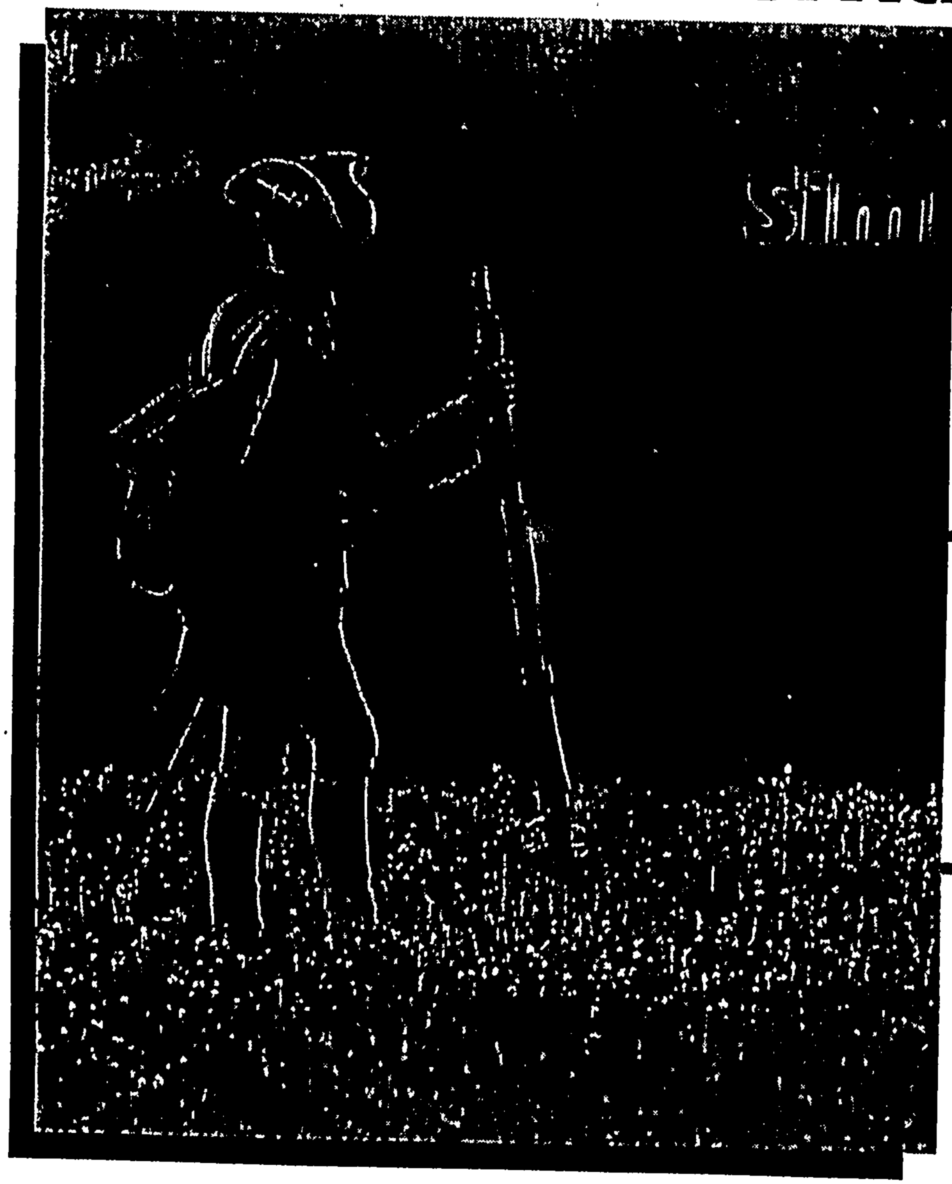

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Recent Progress in 3D EM/EM-PIC Simulation with ARGUS and Parallel ARGUS

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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.

ARGUS uses a domain decomposition algorithm [2], coupled with memory management and data handling techniques, to optimize the use of physical memory for each problem and to efficiently move data between physical memory and disk 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. 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 only by available disk storage and by the overhead of disk I/O, rather than by the size of physical memory and/or paging space.

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,

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

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

where $B=\mu H$, $D=\varepsilon E$, and λ is the eigenvalue we seek. The presence of the 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 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 Paramid 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.

References

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