Software

Numerical Modeling of Nanoelectronic Devices

Nanoelectronic Modeling 3-D (NEMO 3-D) is a computer program for numerical modeling of the electronic structure properties of a semiconductor device that is embodied in a crystal containing as many as 16 million atoms in an arbitrary configuration and that has overall dimensions of the order of tens of nanometers. The underlying mathematical model represents the quantum-mechanical behavior of the device resolved to the atomistic level of granularity. The system of electrons in the device is represented by a sparse Hamiltonian matrix that contains hundreds of millions of terms. NEMO 3-D solves the matrix equation on a Beowulf-class cluster computer, by use of a parallel-processing matrix·vector multiplication algorithm coupled to a Lanczos and/or Rayleigh-Ritz algorithm that solves for eigenvalues. In a recent update of NEMO 3-D, a new strain treatment, parameterized for bulk material properties of GaAs and InAs, was developed for two tight-binding submodels. The utility of the NEMO 3-D was demonstrated in an atomistic analysis of the effects of disorder in alloys and, in particular, in bulk $In_xGa_{1-x}As$ and in $In_{0.6}Ga_{0.4}As$ quantum dots.

This program was written by Gerhard Klimeck, Fabiano Oyafuso, R. Chris Bowen, and Timothy Boykin of Caltech for **NASA's Jet Propulsion Laboratory**. *Further information is contained in a TSP (see page 1).*

This software is available for commercial licensing. Please contact Don Hart of the California Institute of Technology at (818) 393-3425. Refer to NPO-30520.

Organizing Diverse, Distributed Project Information

SemanticOrganizer is a software application designed to organize and integrate information generated within a distributed organization or as part of a project that involves multiple, geographically dispersed collaborators. SemanticOrganizer incorporates the capabilities of database storage, document sharing, hypermedia navigation, and semantic-interlinking into a system that can be customized to satisfy the specific information-management needs of different user communities. The program provides a centralized repository of information that is both secure and accessible to project collaborators via the World Wide Web. SemanticOrganizer's repository can be used to collect diverse information (including forms, documents, notes, data, spreadsheets, images, and sounds) from computers at collaborators' work sites. The program organizes the information using a unique network-structured conceptual framework, wherein each node represents a data record that contains not only the original information but also metadata (in effect, standardized data that characterize the information). Links among nodes express semantic relationships among the data records. The program features a Web interface through which users enter, interlink, and/or search for information in the repository. By use of this repository, the collaborators have immediate access to the most recent project information, as well as to archived information. A key advantage to SemanticOrganizer is its ability to interlink information together in a natural fashion using customized terminology and concepts that are familiar to a user community.

Software development activities were directed by Richard M. Keller of **Ames Research Center**. *For further information, access http://sciencedesk.arc.nasa.gov and http://io.arc.nasa.gov.*

Inquiries concerning rights for the commercial use of this invention should be addressed to the Patent Counsel, Ames Research Center, (650) 604-5104. Refer to ARC-15070-1.

Eigensolver for a Sparse, Large Hermitian Matrix

A parallel-processing computer program finds a few eigenvalues in a sparse Hermitian matrix that contains as many as 100 million diagonal elements. This program finds the eigenvalues faster, using less memory, than do other, comparable eigensolver programs. This program implements a Lanczos algorithm in the American National Standards Institute/International Organization for Standardization (ANSI/ISO) C computing language, using the Message Passing Interface (MPI) standard to complement an eigensolver in PARPACK. [PARPACK (Parallel Arnoldi Package) is an extension, to parallel-processing computer architectures, of ARPACK (Arnoldi Package), which is a collection of Fortran 77 subroutines that solve large-scale eigenvalue problems.] The eigensolver runs on Beowulf clusters of computers at the Jet Propulsion Laboratory (JPL). The package is open-source software and is distributed under the terms of the GNU Lesser General Public License (LGPL) on the Internet through the Open Channel Foundation at http://www.openchannelsoftware.com/.

This program was written by E. Robert Tisdale, Fabiano Oyafuso, Gerhard Klimeck, and R. Chris Brown of Caltech for **NASA's Jet Propulsion Laboratory**. *Further information is contained in a TSP (see page 1).*

This software is available for commercial licensing. Please contact Don Hart of the California Institute of Technology at (818) 393-3425. Refer to NPO-30834.

Modified Polar-Format Software for Processing SAR Data

HMPF is a computer program that implements a modified polar-format algorithm for processing data from spaceborne synthetic-aperture radar (SAR) systems. Unlike prior polar-format processing algorithms, this algorithm is based on the assumption that the radar signal wavefronts are spherical rather than planar. The algorithm provides for resampling of SAR pulse data from slant range to radial distance from the center of a reference sphere that is nominally the local Earth surface. Then, invoking the projection-slice theorem, the resampled pulse data are Fourier-transformed over radial distance, arranged in the wavenumber domain according to the acquisition geometry, resampled to a Cartesian grid, and inverse-Fourier-transformed. The result of this process is the focused SAR image. HMPF, and perhaps other programs that implement variants of the algorithm, may give better accuracy than do prior algorithms for processing strip-map SAR data from high altitudes and may give better phase preservation relative to prior polar-format algorithms for processing spotlight-mode SAR data.

This program was written by Curtis Chen of Caltech for **NASA's Jet Propulsion Laboratory**. *Further information is contained in a TSP (see page 1). This software is available for commercial licensing. Please contact Don Hart of the California Institute of Technology at (818) 393-3425. Refer to NPO-30906.*

∑ e-Stars Template Builder

e-Stars Template Builder is a computer program that implements a concept of enabling users to rapidly gain access to information on projects of NASA's Jet Propulsion Laboratory. The information about a given project is not stored in a data base, but rather, in a network that follows the project as it develops. e-Stars Template Builder resides on a server computer, using Practical Extraction and Reporting Language (PERL) scripts to create what are called "e-STARS node templates," which are software constructs that allow for project-specific configurations. The software resides on the server and does not require specific software on the user machine except for an Internet browser. A user's computer need not be equipped with special software (other than an Internet-browser program). e-Stars Template Builder is compatible with Windows, Macintosh, and UNIX operating systems. A user invokes e-Stars Template Builder from a browser window. Operations that can be performed by the user include the creation of child processes and the addition of links and descriptions of documentation to existing pages or nodes. By means of this addition of "child processes" of nodes, a network that reflects the development of a project is generated.

This program was written by Brian Cox of Caltech for **NASA's Jet Propulsion Laboratory**. *Further information is contained in a TSP (see page 1).*

This software is available for commercial licensing. Please contact Don Hart of the California Institute of Technology at (818) 393-3425. Refer to NPO-40089.

⊚ Software for Acoustic Rendering

SLAB is a software system that can be run on a personal computer to simulate an acoustic environment in real time. SLAB was developed to enable computational experimentation in which one can exert low-level control over a variety of signal-processing parameters, related to spatialization, for conducting psychoacoustic studies. Among the parameters that can be manipulated are the number and position of reflections, the fidelity (that is, the number of taps in finite-impulse-response filters), the system latency, and the update rate of the filters. Another goal in the development of SLAB was to provide an inexpensive means of dynamic synthesis of virtual audio over headphones, without need for special-purpose signal-processing hardware. SLAB has a modular, object-oriented design that affords the flexibility and extensibility needed to accommodate a variety of computational experiments and signal-flow structures. SLAB's spatial renderer has a fixed signal-flow architecture corresponding to a set of parallel signal paths from each source to a listener. This fixed architecture can be regarded as a compromise that optimizes efficiency at the expense of complete flexibility. Such a compromise is necessary, given the design goal of enabling computational psychoacoustic experimentation on inexpensive personal computers.

This program was written by Joel D. Miller of QSS Group, Inc., for **Ames Research Center**. *For further information, access http://human-factors.arc.nasa.gov/SLAB/. Refer to ARC-14991-1.*