SCIENTIFIC AND ENGINEERING SEMICONDUCTOR DEVICE SIMULATION TOOLS AS A WINDOWS APPLICATION

FINAL REPORT

H. L. GRUBIN

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SCIENTIFIC RESEARCH ASSOCIATES, INC.
50 NYE RD., PO BOX 1058
GLASTONBURY, CT 06033

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H. L. Grubin

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Scientific Research Associates, Inc.
50 Nye Rd., P.O. Box 1058
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13. ABSTRACT *(Maximum 200 words)*

A bottleneck associated with numerical simulations of quantum feature size semiconductor devices, has been the absence of a menu driven program that does not require user knowledge of the solution algorithm for the device equations. Under this SBIR study SRA transferred quantum transport algorithms, originally developed for supercomputer simulations to a PC environment. This resulted in (1) program execution via menu based *Microsoft Windows*-type interface, (2) user-defined parameters (dimension, doping, material property, voltage, etc.), (3) an intuitive user interface, and (4) acceptable execution and throughput times when compared to workstations and supercomputers. Under the Phase II study SRA configured three numerically robust software programs (plus operating manuals) for *PC-Windows* operation. These codes are ready for sale. The Fortran based simulation algorithms are: (1) SRA's algorithm for solving the quantum Liouville equation in the coordinate representation; (2) SRA's one-dimensional quantum hydrodynamic algorithm; (3) SRA's two dimensional quantum hydrodynamic algorithm configured for HEMT simulations. The first two algorithms include time dependence. The algorithms can provide device parameters for coupling to standard commercially available circuit packages.

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Quantum transport, semiconductor devices, PC windows based simulations, quantum hydrodynamics, quantum Liouville equation

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Scientific and Engineering Semiconductor Device Simulation Tools as a Windows Application

Introduction

This document summarizes Scientific Research Associates, Inc. (SRA) SBIR work on the development of PC Windows based semiconductor device design software. The two primary goals of the program were (1) transitioning super-computer based numerical algorithms to desktop PCs, and (2) demonstrating a viable commercialization plan. Both goals were achieved.

The Software

Three algorithms were configured for PC operation. The algorithms were *DenMat*, a program designed for solving the quantum Liouville equation in the coordinate representation; *QHD-CAD*, a program designed for solving the one dimensional time dependent quantum hydrodynamic equations; and *2D- QHD*, a program for solving the steady state time independent two dimensional quantum hydrodynamic equations. Manuals for each of these programs were prepared. A brief summary of each of these programs is contained in this report. Detailed discussions of the programs are contained in the *User Manuals*, which are also included in this report.

The software and manuals were delivered to Dr. Dwight Woolard at the beginning of the summer of 1997.

Commercialization

A key goal of the program is the commercialization of the software. The procedures for commercialization were established and are currently operational. At present all of the software is accessible via the Internet. SRA has created a site specifically for the sale and distribution of its software. Presently, *QHD-CAD* is available for distribution. To obtain the software an individual must access the SRA homepage: *http://www.srassoc.com.* The homepage contains a description of the company as well as instructions for accessing the software. There is also a link to the physics behind the equations solved in the *QHD-CAD* software.

If the registration is accepted by SRA the *USER* is invited to download the software from the SRA website. The primary software is contained in a self-extracting file. The software consists of an *executable* with an online help menu, sample files, a *USER* manual, and a *read me* file with instructions for setting up the software. By design, the executable is 'missing' several lines of code. The additional lines of code are contained in another file, called the *service* file. The *service file* has a lifetime of twenty-four hours. All computations are performed locally on the user PC. Presently, the software can be accessed with *Windows 95* and *Windows NT.* The software can be used with *Windows 3.1.* The latter will require Win32s files, which are available free of charge from the *Microsoft* website. The online help menu is not accessible to *Windows 3.1* users.

Presently, **users are not charged for downloading the self-extracting files. User charges are based upon the number of times the service file is downloaded.** A schedule of fees is described at SRA's website. Army Research Office reviewers are invited to access this software at no cost. Interested reviewers should skip the registration site and go to the download page at the SRA website with the *USER NAME: ARMYRES,* and *PASSWORD: ARMYRESR.*

The sequence of accessing the software is different for first-time and subsequent users, and is summarized in the figures 1 and 2.

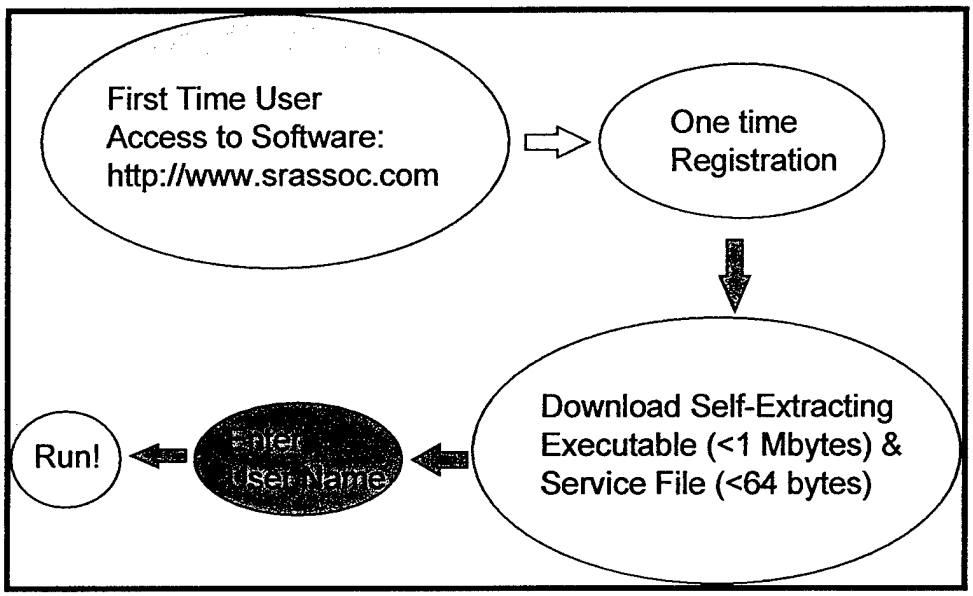


Figure 1. Downloading sequence for registration and first time access to the QHD-CAD files.

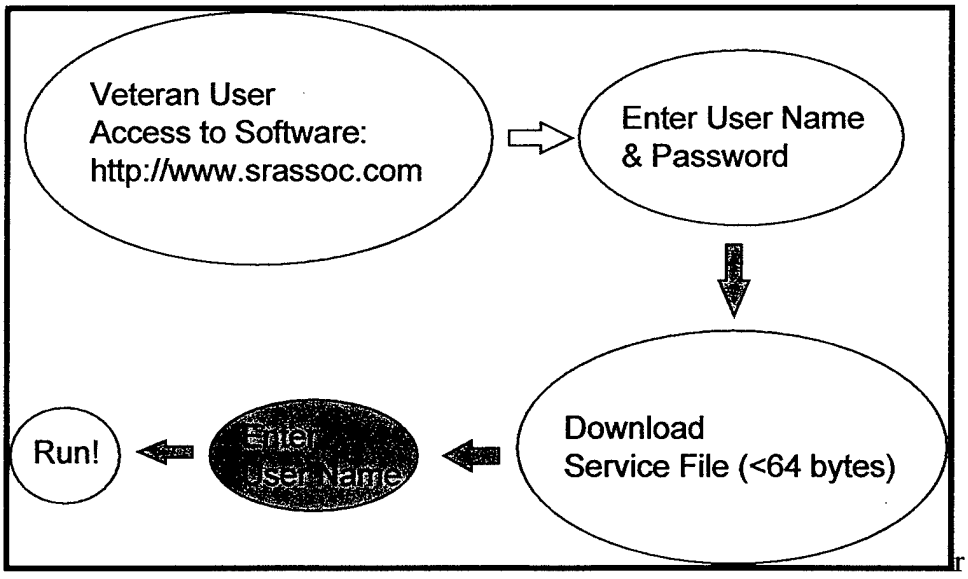
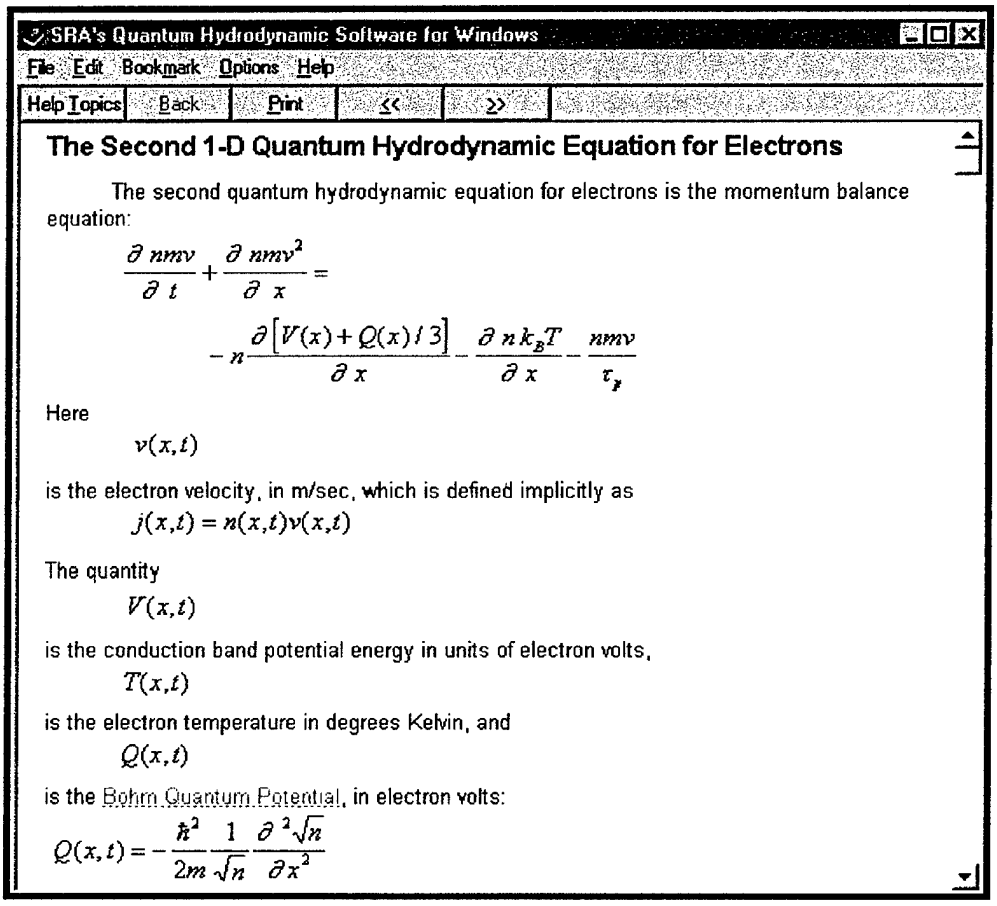


Figure 2. Downloading sequence for veteran users.

The One-and Two Dimensional Quantum Hydrodynamics Software: QHD-CAD

The quantum hydrodynamics equations have been described in a number of publications, and a variant of the SRA work is presently being offered by SILVACO. The equations are described both at the SRA website and in the online manual, which accompanies this final report. An illustration of this is shown below, which is taken from the online help menu distributed with the one dimensional QHD software.



The quantum hydrodynamic equations algorithms in one dimension permit detailed transient studies to be undertaken and have been used to provide a discussion of gain at 500 GHz in resonant tunneling devices. One of the important features of the quantum hydrodynamics code is its ability to deal with long devices.

The Quantum Liouville Equation in the Coordinate Representation

There is considerably more physics associated with this representation. We have been able to provide validation of the software for the equilibrium case. This was done by performing fairly long analytical calculations of the charge density for specified heterostructure configurations. In addition, while this has not been incorporated into the interface we have included a dissipation model that allows us to retrieve the

semiconductor drift and diffusion equation results. This is a major step in making a transition from quantum transport to classical models.

The Manuals

The bulk of this final report is made up of manuals for each of the programs configured for the PC. In anticipation that each of the manuals will be used separately, they have been separately paginated.

Publications

In 1995 a book chapter was published that included detailed results of calculations using the quantum Liouville equation in the coordinate representation.

D. K. Ferry and H. L. Grubin, **Modeling of Quantum Transport in Semiconductor Devices,** Solid State Physics, **49**, 283-448, Academic Press, 1955.

Participating Personnel

Dr. Harold L. Grubin

Dr. T. R. Govindan

Mr. J. R. Kreskovsky

Mr. Oleg Kirshon