Final Report

NAQEDA: a software tool for nanoelectronics modeling and design

(NRC-IRAP Project #700796)

Nanoacademic Technologies Inc.
March 31, 2012

Abstract

In this IRAP supported R&D project entitled "NAQEDA: a software tool for nanoelectronics modeling and design", the key innovative objective is to develop modeling methods based on atomistic quantum principles for accurately predicting nonequilibrium and nonlinear charge/spin quantum transport in nanoelectronics and nanotechnology. NAQEDA – stands for NanoAcademic Quantum Electronic Design Automation, is to have unprecedented capability to handle device structures involving a few hundred atoms all the way to one million atoms or more, without relying on phenomenological parameters. In the past three years, a seven-phase R&D plan was carried out and NAQEDA has reached essentially all the original goals set out in our project proposal. This final report will summarize the entire work in sever sections according to the NRC-IRAP Final Report Guidelines.

1. Project Title, NRC-IRAP Project Number

Project Title: NAQEDA: a software tool for nanoelectronics modeling and design

NRC-IRAP Project Number: 700796.

2. Identify project results in concrete terms measured against the project's objectives

The project's objectives as set out in the original proposal are quoted here: "The overall objective of the proposed NAQEDA project is to develop a modeling method and implement it into a software tool to accurately predict nonlinear and non-equilibrium quantum transport properties of nanoelectronic devices from atomic and quantum principles, for nanostructures having much larger number of atoms than what can be analyzed today. The goal is to reach one million atoms which is the size needed to simulate realistic switching devices". This overall objective is subdivided into six sub-objectives which we summarize our accomplishments for each of them, as below.

2.1. Develop a linear scaling methodology and implement it into our NEGF DFT first principles modeling tool, such that the total computation time needed for modeling device property

will scale nearly linearly in N. At present, all NEGF-DFT methods have at least N-square scaling.

We have completely achieved this sub-objective. This is the main and most important sub-objective of the entire NAQEDA project. For this sub-objective, we developed a proprietary technique that achieved linear scaling within NEGF-DFT self-consistent method for systems up to N ~ 20,000 atoms (Si MOSFET transistor structure) using a modest computation cluster with modest memory requirement for the computing nodes of the cluster. For N ~ 1 million (1M) atoms, we developed a tight binding (TB) potential method with quantum transport emphasis, that also scales linearly with N. Importantly, our TB parameters are obtained from NAQEDA first principles calculations on quantum transport systems. Fig.1 plots the linear-scaling and memory behavior of NAQEDA test run by the NEGF-DFT self-consistent method; Fig.2 plots the same characteristics for the tight-binding run – reaching beyond 1M atoms.

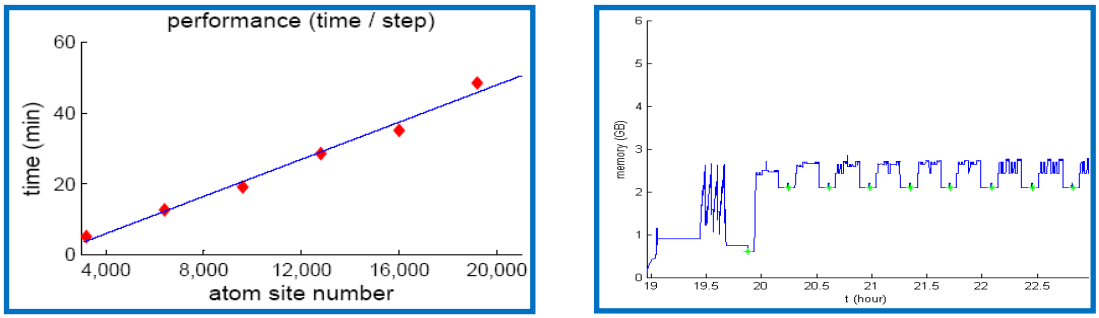

Fig.1 NAQEDA run using the NEGF-DFT self-consistent method for a Si MOSFET structure having upto N=19,200 atomic sites. The atomic structure is periodic in x-direction and 10nm thick in the y-direction. Left: computing time per NEGF-DFT self-consistent step versus the channel length of the transistor, showing a clear linear scaling behavior all the way to N=19,200 atomic sites. Right: memory usage during the N=12,800 atom run, versus the computation time. The highest memory usage is less than 3GB per computing core. The calculations were done on a modest cluster of 160 cores.

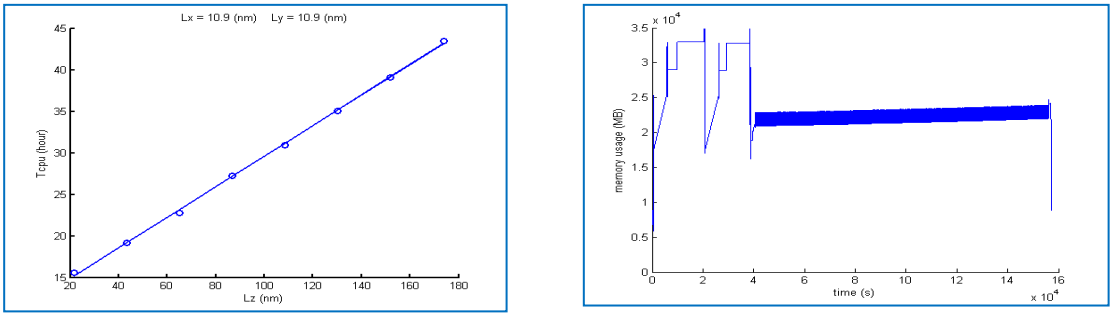

Fig.2 NAQEDA run using the tight-binding potential with transport emphasis method, for Si MOSFET structures up to 1,024,000 Si atoms (over 1 million). The atomic structure has a cross section of $(10.9nm)^2$. Left: computation time versus length of the transistor, showing a clear linear scaling behavior. The last point is at L_z=173.8nm (1,024,000 atoms), and it took about two days running on a 12-core computing node. Right: the memory usage of the 1M-atom run versus computing time. The highest memory usage is not more than 36 GB – namely 3GB/core is adequate for the 1M atom transport calculation.

2.2. Develop fast numerical methods for iterative convergence. At present, all NEGF-DFT methods take at least ten times more iteration steps to converge atomic potential for open systems (devices) at non-equilibrium, than that is needed for closed systems of equal size. Reduce this convergence factor to within five by using more advanced convergence criterion.

Our R&D allowed us to identify the issues related to this troublesome problem. When at non-equilibrium, the electrochemical potentials of the left electrodes (μ_L) and right electrodes (μ_R) are different (they are setup by the external bias voltages). For NEGF-DFT self-consistent modeling, the electronic density matrix in the device channel region must be self-consistently solved iteratively until the electrons "know" that the left and right chemical potentials are different – at μ_L and μ_R, respectively. Since each iteration step only changes the atomic potential slightly, it requires many iteration steps to converge a non-equilibrium density matrix. This situation is dictated by the physics that could not be overcome. On the other hand, we have developed various techniques into NAQEDA to "guess" a good initial atomic potential: this is possible because we know the values of μ_L and μ_R. This way, if a good initial condition is setup before the self-consistent iteration run, it helps to significantly reduce the total number of iterative steps. In end, modest number of iteration steps is needed to run the device simulation. Table 1 below shows that to converge (with high accuracy) a two-probe Si transistor structure with 19,200 atomic sites, 267 iteration steps were sufficient. We however also found that the number of iteration steps is not universal, for different problems this number is different. Our R&D clearly points to the importance for setting up a good initial condition at non-equilibrium situations.

Structure	Size	# of atoms	NEGF-DFT run	Convergence
Leads :	1 X 20 X 1	320 atomic spheres (2880 Orbitals)		
Two probe 1	1 X 20 X 20	6400 atomic spheres (57600 Orbitals)	107 DFT steps, 5.5 min/step, total 9.8 hours	Potential 1.0 x 10^{-5} Charge 1.23 x 10^{-5} per atom
Two probe 2	1 X 20 X 40	12800 atomic spheres (115200 Orbitals)	195 DFT steps, 14 min/step, total 46 hours	Potential 1.0 x 10^{-5} Charge 6.2 x 10^{-6} per atom
Two probe 3	1 x 20 x 60	19200 atomic spheres (172800 Orbitals)	267 DFT steps, 30 min/step, total 134 hours	Same as above

Table 1. NAQEDA run using the NEGF-DFT self-consistent method on Si MOSFET atomic structures. The last row gives the characteristic of the largest NEGF-DFT run: N = 19,200 atomic sites. It took 267 self-consistent iteration steps which are not that much more in comparison to typical DFT simulations at much smaller values of N (e.g. even for N =200, it typically will require about 100 steps to converge).

2.3. Develop automatic error control, fast scattering states computation, distributed memory management, and efficient mathematical algorithms so that nanoelectronic device structures having N~10,000 atoms can be analyzed on a moderate PC cluster (~16 Quad-core).

We have accomplished all of this sub-objective. The Fig.1,2 and Table 1 above show the simulation characteristics. As far as the fast scattering states computation, we have developed two methods: the first is based on Green's functions and the second is based on scattering matrices. Both methods gave identical results and their computation times are also similar. For distributed memory, the k-sampling, E-sampling, real-space potential computation, principal layer calculation, tri-diagonal matrix inversion for Green's function computations etc., are all done by distributed memory approach. These account for over 80% of the numerically intensive part of the NAQEDA software. The only relevant part that has not been distributed in memory is the Poisson equation solver which we wish to get done in the very near future. Finally, we have discovered proprietary mathematical algorithms that allow us to more efficiently calculate large systems.

2.4. Develop methodology and implement it for generating tight binding (TB) potential with transport emphasis. These TB potentials should produce quantitative results accurately comparable to those obtained from NEGF-DFT first principles approach for quantum transport modeling. Generate TB potential with transport emphasis for about 20 different atoms commonly used in nanoelectronics such as Si, Ge, Ga, As, P, O, H, N, B, Cu, Al, C, Au, Fe, Ni, Co, Mg etc.. Judiciously select open device structures involving combinations of these atoms in the process of TB generation.

This sub-objective has been completely reached. In particular, a special software module called "nanoskif" – stands for Nanoacademic Slater-Koster Integrals Fitting package, is integrated into NAQEDA that fits the TB potential parameters. Our R&D showed that the relevant target of the fitting procedure is the electronic bands near the Fermi level. Using nanoskif, we have derived all the necessary TB parameters for all the semiconductor materials that are relevant to the IT technology (including and beyond the materials of atoms listed above). Nanoskif is an extremely powerful module of NAQEDA. Fig. 3 is a verification of the TB parameters for Si transistor structure. For a *perfect* Si structure, the transmission coefficient must equal to the number transmission channels. The latter can be calculated by just counting the number of electronic bands that cross the Fermi level – thus known. As shown in Fig.3, the calculated transmission coefficient versus energy using the TB parameters, are in excellent agreement with the known values for the entire energy range. The largest error is less than 1.4%.

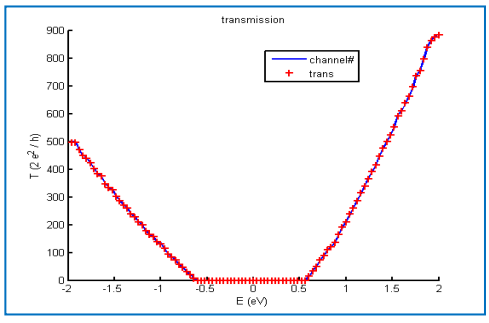

Fig.3.Transmission coefficient T vs. energy E, obtained by the TB model in NAQEDA (red). The system is a perfect Si transistor structure having 1,024,000 atoms. Blue: number of the transmission channels that can be counted for. The agreement is essentially perfect.

As another demonstration of the well behavior of our TB parameters obtained by the nanoskif module of NAQEDA, in Fig.4 we plot the calculated density of states (DOS) of Si bulk crystal (black curve, shifted upward for better showing the comparison), and Si films of thickness N_y which is the unit-cell number. For large N_y, the TB curves must converge to the bulk curve – and they do. This is a very strong check of our TB parameters: even for films with surfaces and dangling bonds, they work very well.

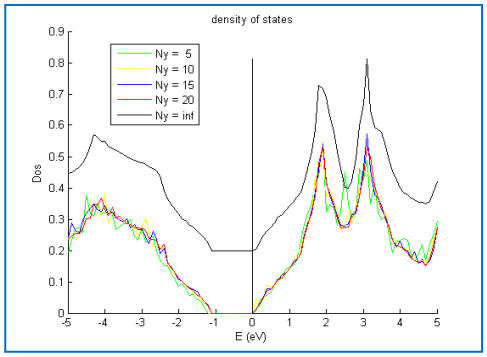

Fig.4. Density of states of Si versus electron energy. Black curve is for bulk crystal (shifted upward to show better the comparison). Other curves are for Si films with thickness N_y as shown in the legend. For large N_y, the curves approach that for the bulk. Note, N_y=15 is equivalent to 8nm. This is a strong verification of the well behavior of the TB parameters.

Finally, Fig. 5 is a periodic table showing available TB-parameters (for atoms in red) we have generated which are included into a database of NAQEDA. When using the software, by clicking the atomic symbol, the details of the potentials are shown.

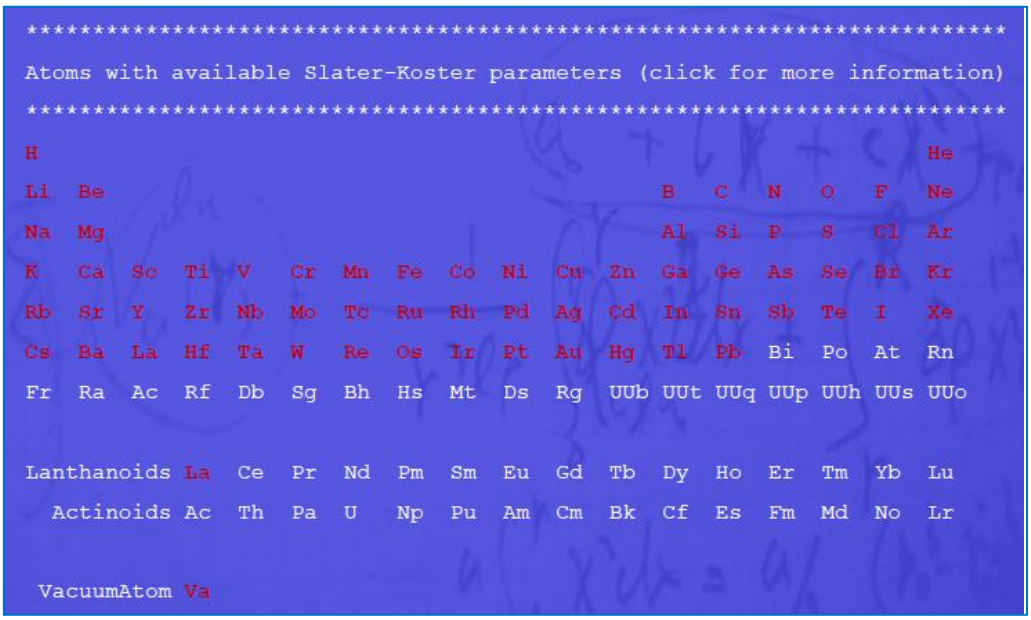

Fig.5. Using nanoskif, we have generated TB parameters with transport emphasis for the atoms in red. In the atomic sphere approximation, the vacuum sphere has also a potential, which is generated as well.

Suite 256
7005 Blvd. Taschereau
Brossard QC J4Z 1A7 Canada
www.nanoacademic.com
Tel: (450)904-1626
Fax: (450)904-1555
email: guo@nanoacademic.ca

2.5. Develop methodology and implement it for efficiently computing transmission coefficients for atomic structures having million-atom level size. Together with sub-objective #4, demonstrate capability of modeling nanoelectronic device structures at million-atom level.

This sub-objective has been completely reached. The Fig.1,2 and Table 1 above already showed the simulation characteristics, all the way to the million-atom level. Fig.6-left plots the I-V characteristics of a double-gate MOSFET calculated parameter-free by NAQEDA from atomistic first principles. As a comparison, Fig.6-right plots the same I-V characteristics obtained by an effective mass model based on many phenomenological parameters. The agreement is excellent.

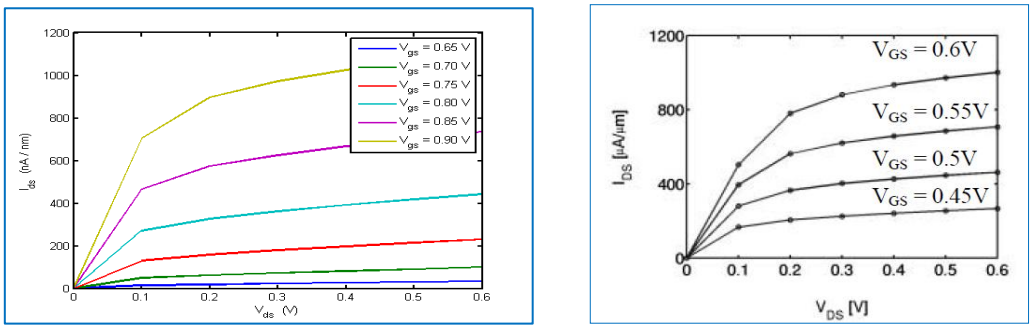

Fig.6. I-V characteristics of a Si double-gate transistor. Left: by NAQEDA. Right: by effective mass model (figure from PhD thesis, Zhibin Ren, Purdue Univ.) that is based on many phenomenological parameters. The agreement is very good. Note that in NAQEDA, the potential zero is set by the vacuum level. But in the effective mass result, it is unknown (hence the gate voltage scale is different).

2.6. Develop a friendly GUI to package NAQEDA into an easy to use modeling tool. Apply proper IP protection for NAQEDA

This sub-objective is partially achieved: we have developed a GUI but it requires further refinement. At the moment, this GUI is based on the plotting library java3D. However, since java3D so far has not supported 64-bit computer nodes, we plan to re-develop it using a different plotting library. If java3D will come out with a 64-bit version, then such re-development will not be needed. Fig.7 below shows a screen shot of our GUI during the process of building a two-probe transistor structure.

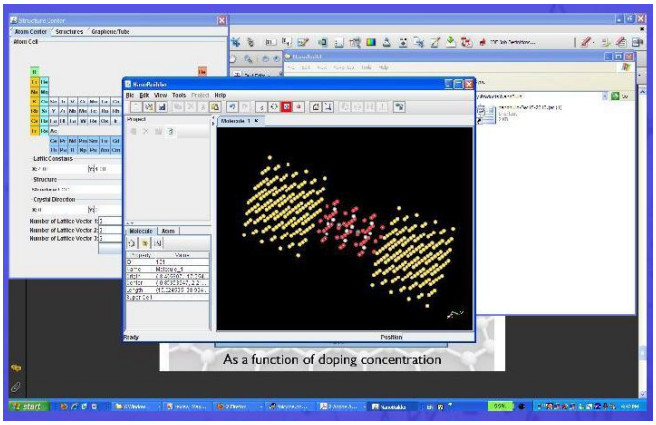

Fig.7. Screen-shot of the GUI that is being used to build two-probe transistor structure.

In summary, we have satisfactorily reached essentially all the objectives of this project. Most importantly, we have developed proprietary IP that allows us to reach device modeling goals of unprecedented sizes and accuracy. The NAQEDA has been very thoroughly verified against exactly solvable models, against parameter based methods, and against a lot of experimental data. NAQEDA is now standalone software that is being beta-tested by us and by our potential customers.

3. Describe the technical achievements and difficulties encountered

The main technical achievements in NAQEDA can be summarized in the following list:

(1) In order to model nanoelectronic devices that is relevant to the emerging technology, one must be able to: (a) accurately model atomic nanostructures from N~10,000 up to 1M atoms; (b) accurately predicting band gaps of semiconductors from density functional theory for systems having N~10,000 or more atoms; (c) accurately handle the doping of atomic impurities into semiconductor materials and carry out configuration average very efficiently for large N cases; (d) efficiently handle complicated device boundary conditions and nonequilibrium quantum transport conditions. We have achieved all these very important technical advances.

(2) Associated with the accurate band gap predictions, discovery of a practical approach for using the modified Becke-Johnson potential (MBJ) in device structures having materials interfaces.

(3) Associated with (2), investigating about 25 semiconductor materials and determining the c-parameter in the MBJ potential for all of them.

(4) The development of efficient linear scaling methods in both NEGF-DFT self-consistent method and the TB-potential method.

(5) Associated with (4), discovery and implementation of new mathematical theorems and algorithms that allow the calculation of both equilibrium and non-equilibrium density matrix of very large systems.

(6) The development of the nanoskif module that allows the generation of TB parameters with transport emphases.

(7) The discovery and implementation of a method to automatically add empty atomic spheres at appropriate positions in the atomic structure of semiconductor and insulator materials, such that the atomic sphere approximation can be easily applied by users. The discovery and implementation of a method to automatically optimize the size (radius) and positions of the empty atomic spheres.

(8) Associated with the above, discovery of new methods for parallel computation of quantum transport properties (such as conductance); discovery of new methods for monitor and control of computer memory during large scale device simulation.

(9) Associated with all the above, the development of error control for the approximations that allow device modeling at the 1M atom level.

(10) Development of methods to predict the influence of external magnetic fields to quantum transport properties of nanostructures self-consistently at nonequilibrium from atomic first principles.

(11) Discovery and implementation on how to carry out first principles self-consistent modeling of nonequilibrium quantum transport in nanostructures having more than two electrodes.

(12) The development of a general method for transforming any types of Matlab data into XML for subsequent data exchanges.

(13) Discovering a new concept of *density of the scattering states* (DOSS) that wash out unwanted background states, predicting much clearer physical pictures of device operation.

(14) Implementing three-dimensional non-collinear and non-planar spin structure for open systems such that emerging spintronic devices can now be modeled.

(15) Discovery of the use of several new numerical convergence criteria, leading to better computation convergence for NEGF-DFT calculations under non-equilibrium.

(16) Discovery how to handle disorder sites with more than two atomic components at non-equilibrium.

(17) Discovery and implementation of a new iterative algorithm for solving the nonequilibrium vertex correction (NVC) equations efficiently.

(18) Discovery and implementation of a new technique for solving coherent potential approximation (CPA) and NVC at very small impurity concentrations without solving them iteratively.

(19) Discovery of how to calculate Madelung potential for half-infinite electrodes.

(20) Implementation of all 2-dimensional symmetry groups and time-reversal symmetry, as well as many other methods to drastically reduce computation time.

(21) Implementation of multi-contour in complex contour integral which improved numerical convergence.

The main technical difficulties encountered are listed below:

[1] Our R&D discovered that there is no iterative technique for computing the non-equilibrium density matrix by the NEGF, thus a direct calculation of the density matrix by matrix inversion must be used. For large systems, this is extremely inefficient. We devoted tremendous effort to solve this problem.

[2] Our R&D discovered that all existing linear scaling methods in DFT were based on the locality principle that exists in equilibrium. But for nonequilibrium quantum transport modeling, the locality principle breaks down, rendering all existing linear scaling methods non-applicable. We devoted tremendous effort to solve this problem.

[3] For very large systems N > 10,000 atoms, self-consistency at nonequilibrium is very hard to reach; this is especially true at large external voltages (bias and gate voltages). The

only way to rectify this problem is to increase the computational speed for each computation step – by good parallel computing algorithms; and by choosing better initial conditions of the modeling. We devoted tremendous effort to this direction.

[4] The linear scaling is achieved in NAQEDA along the quantum transport direction – this is the most relevant length scale in device modeling. Nevertheless, the computation scales as $O(M^2)$ along the transverse direction of the atomic structure, where M is the matrix size of the cross section of the atomic structure. No efficient solution to further rectify the computation issue in the transverse direction was found so far.

4. Is there a possibility of an intellectual property (patent or other) arising from the project?

The answer is yes. While some of the ultimate technical details will be protected as trade secrets, we are aiming to initial file two patents applications. The first is associated with the nanoskif module: its methods and the generated TB potentials with transport emphasis. The second is associated with the NEGF-DFT methods of solving nonequilibrium quantum transport in nanostructures having N~20,000 atoms. Other proprietary IPs may also be patented in the near future.

5. Identify the project's impact as of project completion date and forecast for the next twelve months based on the benefits to Canada outcomes you identified in your proposal

This project has extremely significant impact to the competitiveness of our company because NAQEDA is extraordinarily innovative and no software in the world has capabilities coming close to it. NAQEDA has brought our modeling technology to the level of a design tool that can be used by circuit design engineers or act as a plug-in to circuit design tools in the large EDA market. It is the only design tool based on atomistic first principles in the world. It will position our firm as the leader in a potentially large but currently empty market space. This is extremely significant. Nanoelectronics is at the heart of present and near future IT technology, it is a field of intensive international R&D as well as competition due to its profound economic and scientific implications. The NAQEDA project provided us a unique opportunity which we seized to produce the most powerful software solution for quantum electronic design automation; as such a major challenge in EDA has been solved here by our firm. In addition, the IPs generated within this project have large potential applications to many other fields, including certain sectors in energy, defense, security, biotech and environmental.

Our R&D project benefits Quebec and Canada through jobs in high tech, training of highly qualified personnel and, in the near future, revenue generation. Even though not directly paid by the IRAP funds, seven students (both graduate and undergraduate) and postdoctoral fellows from two universities were trained in our firm by doing development work under the supervision of our employees. Dr. Tao Ji was hired by the firm to be part of the project team (he chose to leave the firm at the end of February 2012 to pursue his other interests). As summarized above, this

project has generated important IPs in a strategic sector of high-tech industry. It allowed our firm to develop its most powerful product which we project will generate considerable revenue.

6. What are your plans for commercialization of the results from this project?

During the R&D phase of this project, we have already made many contacts, visits, and discussions with interested parties from industry and academia, including people at the most important and largest firms in the world such as Intel, IBM, Synopsys, Cadens, other important players such as Altera, ProPlus, Magwel etc.. Exchanges with people in these companies allowed us to aim at what is urgently needed by electronics industry.

With the R&D phase completed, commercialization starts in four different ways simultaneously:

1. We will continue discussing and pursuing partnership with large TCAD firms (such as Synopsys) and make our product available as plug-ins to their well established TCAD tools that are used by all the semiconductor manufacturing industry. Again, we note that our device modeling tool is based atomistic first principles that does not rely on any phenomenological parameters which are difficult, time-consuming and expensive to extract from experiments; while the well established TCAD tools were all based on experimental parameters and semi-classical principles. Our plan is to quickly partner with one or a few large TCAD firms so that NAQEDA becomes an integrated and novel tool for electronic design automation. In this direction, the GUI of our product should be improved and interfacing with the TCAD software should be smoothed out. These works will be done in the immediate future.

2. We have produced an academic version of the NAQEDA software and will soon sale it through our usual marketing channels (web based). In academic research, researchers are highly specialized and technically involved people, our present version of the GUI is adequate, and hence the sale of this product will begin in the immediate future months.

3. NAQEDA was developed in the technical computing language Matlab© with numerical intensive parts in C. Matlab is the most widely used technical computing language in engineering and has extensive and widely used tool boxes (such as computational fluid dynamics). However, Matlab has no tool box for technical computing in nanotechnology and nanoelectronics. We will investigate the possibility to turn a version of NAQEDA to be that tool box which will then reach the huge user base of Matlab.

4. We were approached by customers and interested potential users of our products for possible service work. In fact we have indeed done such service work before for government labs using our products to generate some specific results. We are working on a service level NAQEDA software that a user can run on our own servers remotely through the web. There are a lot of R&D people in the world who may not wish to buy and install the software in their own computers and go through the learning curve of using it (especially experimental people), and this is actually a large market if we allow

them to use NAQEDA for a fee. The construction of this web based NAQEDA is underway already.

Commercialization is the key and is the first priority of our firm right now. Many discussions, meetings and consulting sessions were done in the past, but more are planned in the near future. We are also discussing with business executives in the TCAD market (people we know) about all the issues of bringing NAQEDA quickly to them.

7. How will this project's results influence your company's future plans?

This project has significant influence to our future plans. In particular, because it is a transformative technology, it has altered our firm's R&D directions. Before this project, our existing software products target largely academic researchers since these software can only handle small number of atoms and no approximate (but accurate enough) methods were implemented in our existing software that can get to a qualitative answer very quickly. With NAQEDA, this situation is changed in fundamental ways and our future development plan will focus on large scale industrial applications.

From the future product line point of view, NAQEDA is an overwhelming software package that encompasses our existing products in substantial ways. This helps us to streamline our product line to reduce overhead costs for maintaining many different products. NAQEDA provides an entirely new development platform for our new products.

In our original proposal to IRAP for the NAQEDA project, we had a discussion on our product lines as planned at that time. However, the NAQEDA project has completely changed that plan and our new product line is more innovative and targeting more urgent as well as larger markets. For example, based totally on the NAQEDA innovation, we will soon begin to develop a new software package called NASOLAR, stands for Nanoacademic Solar Cell Simulator that is specifically targeting the ever expanding renewable energy sector. Indeed, solar cells are made of semiconductors and the emerging generations of the solar cell (3^{rd} generation) are increasingly based on nanostructures. In addition, there is so far no specialized and atomic based nano-material modeling software in the solar cell sector and we plan to fill this void. The material structures in any solar cell have large number atoms thus requiring a tool like NAQEDA as its atomistic simulation engine.

Another example is our new plan to develop a specialized software tool based on NAQEDA to simulate chemical processes of capture, sequestration and storage of carbon dioxide (CO_2) from large point sources, using semiconductor nanowires. CO_2 can be chemically transformed into hydrocarbons such as methanol and other high energy density carbon-based fuels, which can be readily stored in the form of liquid or solid. More importantly, such value-added products have wide marketability and can significantly reduce, or even offset the cost associated with CO_2 capture. Again, there is no atomic based software simulator for the CO_2 chemical processes but such a tool is urgently needed by the hugely important environmental sector of the world.

In summary, NAQEDA allows us to open many doors for innovative and marketable software products in the near future so that we can occupy several strategically important industrial sectors. Finally, we wish to thank the NRC-IRAP organization and the people of IRAP for providing the extraordinary opportunity and financial support that allowed us to complete this most exciting R&D project.

Suite 256
7005 Blvd. Taschereau
Brossard QC J4Z 1A7 Canada
www.nanoacademic.com
Tel: (450)904-1626
Fax: (450)904-1555
email: guo@nanoacademic.ca