NEMO: From Esoteric Quantum Theory to Industrial Transistor Designs and Global Impact

Gerhard Klimeck
Network for Computational Nanotechnology and School of Electrical and Computer Engineering,
Purdue University, West Lafayette, IN 47907, USA
e-mail: gekco@purdue.edu

ABSTRACT

Today's nano-scaled transistor have been explored and designed with full quantum transport modeling tools utilizing an atomistic basis. The NEMO5 tool set has been integrated into the in-house Intel design suite [1] and is being commercialized by Silvaco [2]. Other technology leaders such as Samsung and TSMC have built their own in-house tools adopting NEMO approaches. Non-Equilibrium Green Functions (NEGF) for quantum transport with an atomistic basis (typically tight binding) are now the widely accepted standard. NEMO results were the basis for the 2004 rotated substrate technology at Texas Instruments [3] impacting chips in over a billion cell phones. Over 25,000 nanoHUB users have explored nanoscale devices such as nanowires, ultra-thin-body transistors, and quantum dots using NEMO/OMEN tools on nanoHUB.org. They use simple-to-use apps in the first end-to-end scientific computing cloud. Over half of nanoHUB's simulation users explore device and modeling concepts in formal classrooms in over 180 institutions globally. Atomistic device simulation, quantum transport with NEGF and million atom electronic structure simulations were deemed too expensive by the community. Dissemination of easy-to-use app versions of NEMO (and other codes) were deemed to be useless for research and for education. nanoHUB and NEMO have changed fundamental approaches and underlying assumptions: paradigm shifts. This presentation will highlight some of the key hurdles, insights, and developments that drove these paradigm shifts.

KEY INSIGHTS IN QUANTUM TRANSPORT

Today's 3D FinFETs [4] or nanosheet transistors have the same 5nm central length characteristics as 1D resonant tunneling diodes (RTDs). The quantitative and predictive modeling of 1D RTDs (1994-1997) has defined the standards needed for today's 3D nano-transistors.

Realistic devices are extended. It is not good enough to model a central component of a quantum device. Instead, the central component is embedded in large source and drain regions that have their own quantum and scattering physics that is just as important as the central device. We developed an approach to partition realistic devices for full quantum transport [5].

Incoherent scattering is critical in the source/drain regions. Decoherence and scattering effects are intellectually challenging and have been the focus of RTD models in the central device region. For high performance devices such scattering is much less important than the relaxation effects in the contacts [6].

Effective mass approaches are not predictive. At the 5nm scale a heterostructure does not only form a new device but a new composite material. Effects such as non-parabolicity, band-to-band coupling, crystal orientation, and quantization through geometry allow designers to create a new composite material with new bandgaps, effective masses that cannot be predicted by bulk effective mass approaches. Atomistic basis sets are critically needed, even though transport might just happen in the conduction band. Effective mass models can be tuned to specific atomistic representations but cannot be predictive [6-8]. The establishment of experimentally validated atomistic basis sets via genetic algorithms has been critical [9].

KEY INSIGHTS IN TOOL & DATA SHARING

The typical "products" of a research-oriented faculty member are the creation of new knowledge and graduate students. Papers usually just lead to other papers even in engineering departments. In general tools and data are not shared. As a result, most computational science or engineering papers cannot even be duplicated, calling into question their scientific merit. nanoHUB was created to share computational tools with the community such that others can duplicate results and use tools to drive new research or use in education.

Simplified user interfaces enable broad use. Most small research codes are written by one person for one person without any consideration of reuse or dissemination. Larger research codes and even commercial codes are often extremely complex that require months of tool training. nanoHUB has developed Rappture [10] and Sim2ls [11] environments that enable the encapsulation of such codes in simple-to-use user interfaces with reduced complexities. Over 2,600 research papers cite nanoHUB with over 68,000 secondary citations (h-index 121). Over 55% of nanoHUB simulation users are in formal classrooms.

nanoHUB tools – a new publication type. The Web-of-Science and Google Scholar have listed nanoHUB tools since 2017 creating an academic incentive to publish new tool & data artifacts. The US government has moved to federal requirements to share data if the research is funded by the government.

CONCLUSION

In the past 30+ years I have strived to create "products" that other researchers and educators can use. NEMO has created paradigm shifts in how people understand and model devices and has had impact on billions of people through chips in computing and communication devices since 2002. nanoHUB has created paradigm shifts by creating new types of publications and by enabling researchers and educators to use NEMO and hundreds of other tools.

ACKNOWLEDGMENT

This work would not have been possible without my hundreds of collaborators who helped to build, test drive, break, and rebuild NEMO/OMEN [5-9,12-14] and nanoHUB [10,11]. I have the deepest appreciation for their hard work, dedication and in most cases their personal friendship. The citations here just cover some of the fundamental developments. Citations to these papers lead to hundreds of application publications enabled by my collaborators and friends.

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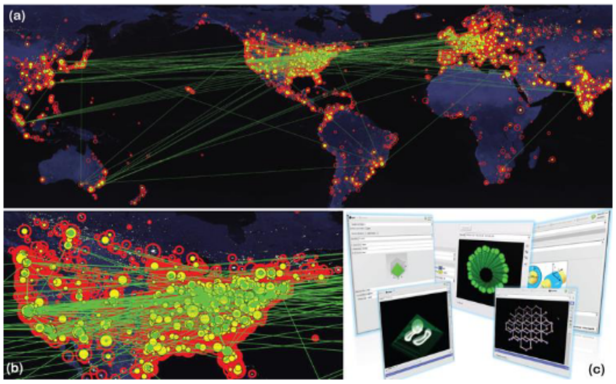

Fig. 1. nanoHUB user map representative of year 2016. Red circles designate users viewing lectures, tutorials, or homework assignments. Yellow dots are simulation users. Green dots indicate 4,100+ authors of 1,700+ scientific publications citing nanoHUB through 2016. Dot sizes correspond to number of users, and lines show author-to-author connections proving research collaboration networks. (b) U.S. enlarged. (c) a collage of typical nanoHUB interactive tool sessions and 3D-rendered interactively explorable results (quantum dots, carbon nanotubes, nanowires).