Theme 4:
(Device) Theory and Modeling

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NCN

www.nanohub.org

PURDUE UNIVERSITY

theme 4 team

1) James Raynolds (Albany)
   -electrically-based spin switching in hetero-dimen. quantum dot devices

2) Alex Xue (Albany)
   -quantum molecutronics

3) Michael Shur (RPI)
   -plasmonic devices

4) Azad Naeemi (Georgia Tech)
   -graphene interconnects and devices

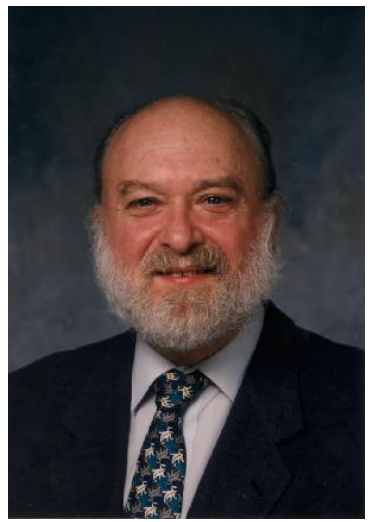
5/6) Mark Lundstrom / Supriyo Datta / NCN@Purdue
   -graphene electronics + NCN@Purdue leverage

“exploratory simulation”

“Excellent computer simulations are done for a purpose…

“exploratory simulation”

1) to **explore** uncharted territory
2) to **resolve** a well-posed scientific or technical question
3) to make a good **design** choice.”



L.P. Kadanov, “Excellence in Computer Simulation,” *Computing in Science and Engineering*, (Mar./Apr. 2004).

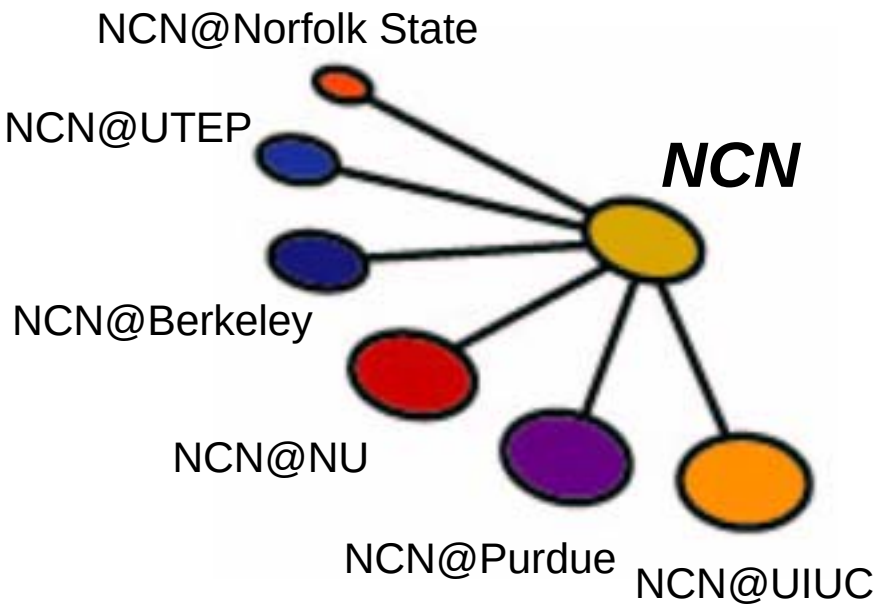
simulation philosophy

refine ideas
generate new ideas

develop sophisticated simulations step-by-step

bring understanding back

Network for Computational Nanotechnology



Mission:

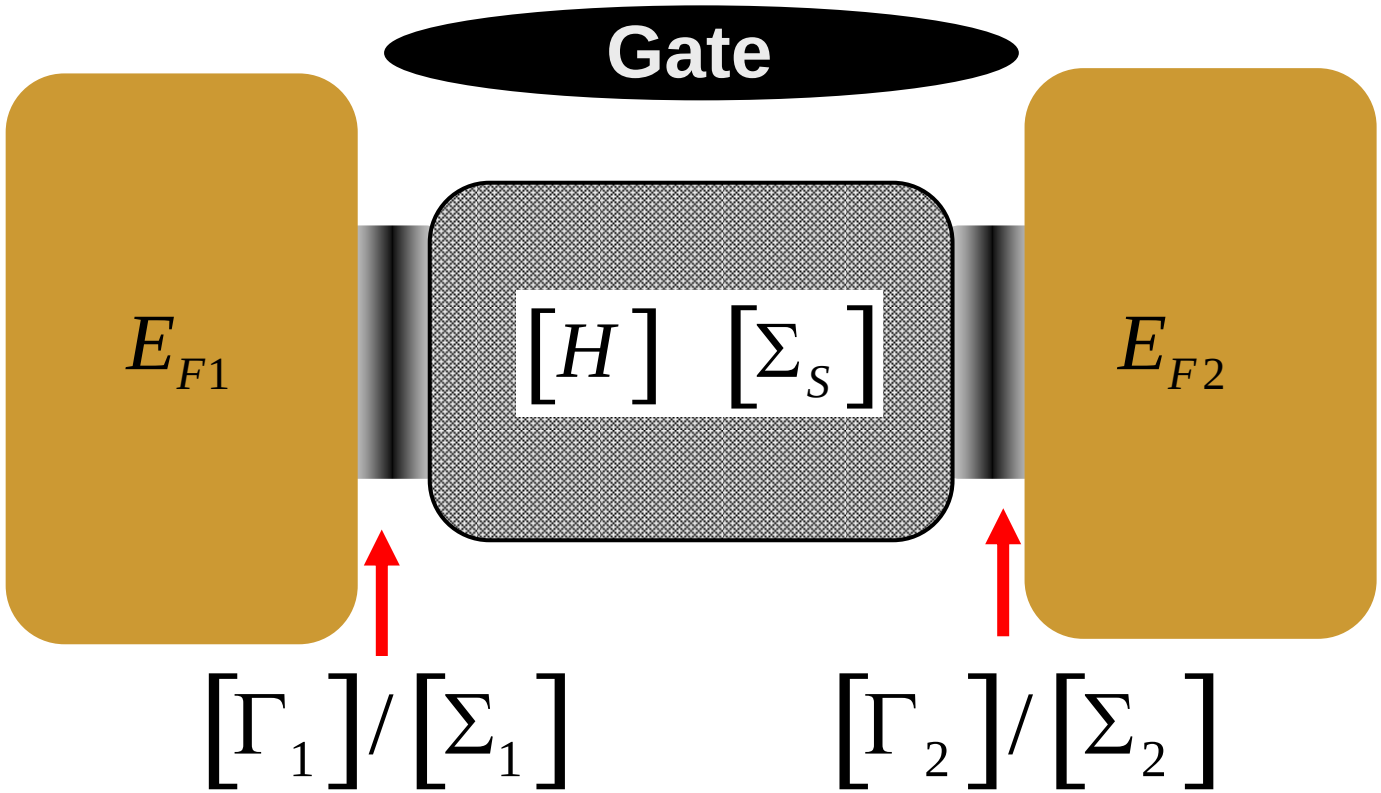
to connect those who develop simulations with those who use them in research

Key strategy:

cyberinfrastructure

an *'infrastructure and research network'*

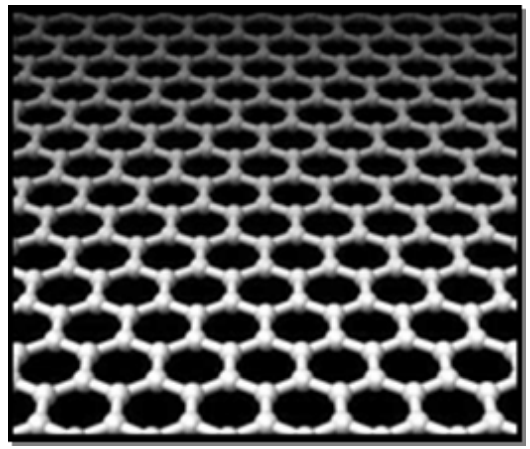
generic model to NEGF



S. Datta, *Quantum Transport: Atom to Transistor*, Cambridge, 2005
("Concepts of Quantum Transport" nanohub.org)

NEGF simulation

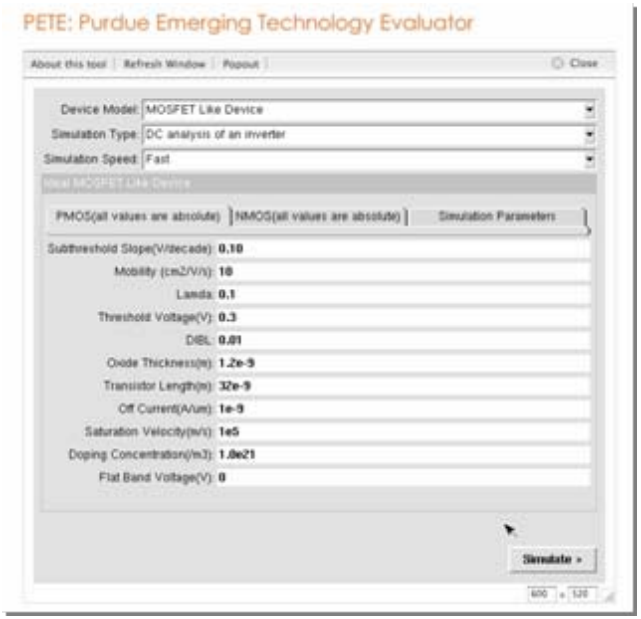
- molecular electronics
- semiconductor nanoelectronics
- spintronics
- electronic / magnetic devices



http://en.wikipedia.org/wiki/Graphene

graphene

benchmarking with PETE



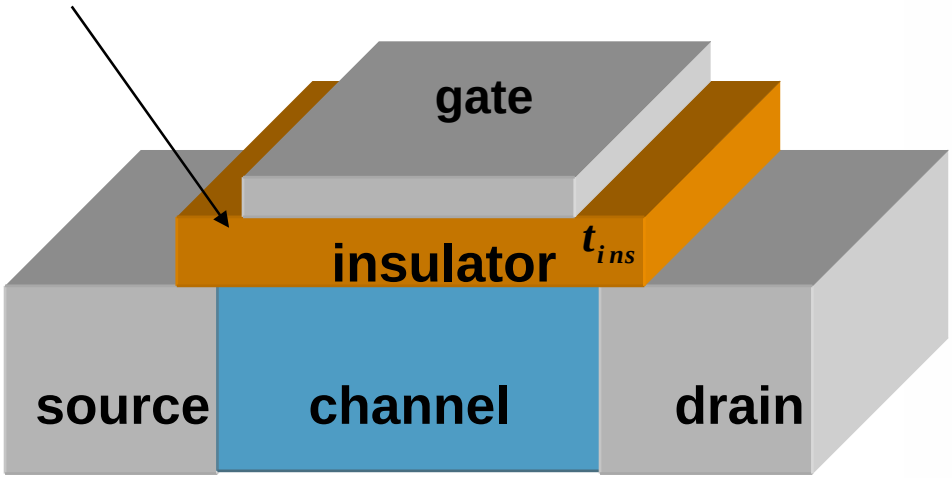
Purdue **E**xploratory **T**echnology **E**valuator

Kaushik Roy (Purdue)

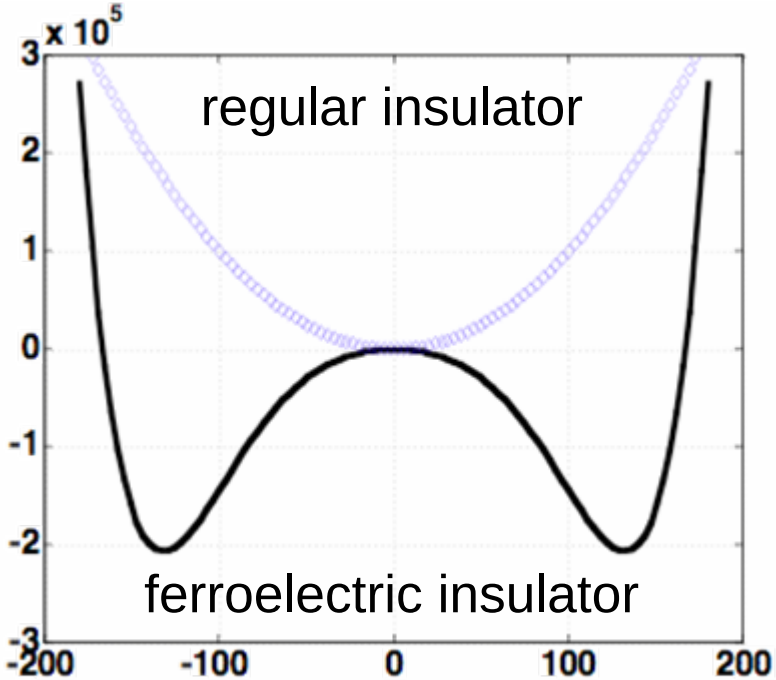
-table-based models
-validated against Spice
-speed / power assessment for benchmark circuits
-available on nanoHUB.org

FE FET

FE gate insulator



S. Salahuddin and S. Datta,
Nano Letters, Feb., 2008



$$U = \frac{Q^2}{2C}$$

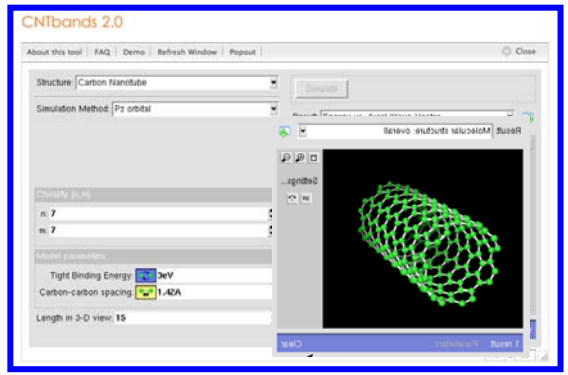
rappture.org and HUBzero.org

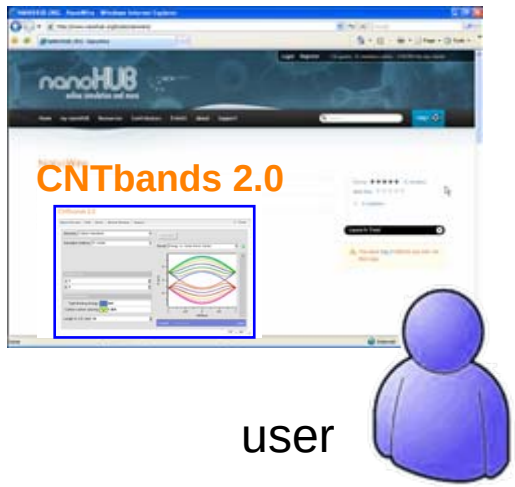
shared infrastructure

Rappture

Simulation Code

researcher





user

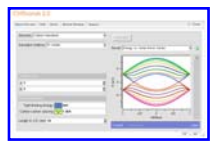
nanoHUB
online simulation and more
an NCN project

Content Database

Maxwell's Daemon

Physical Machine

Virtual Machine

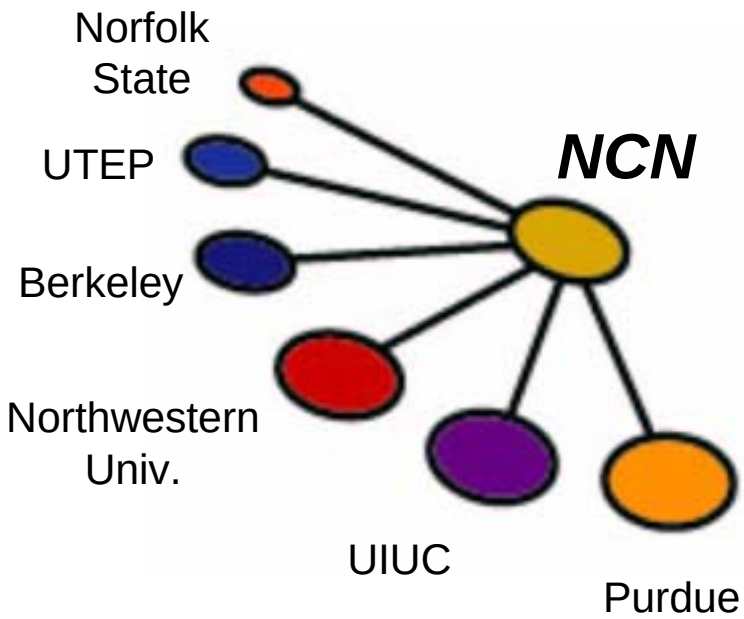


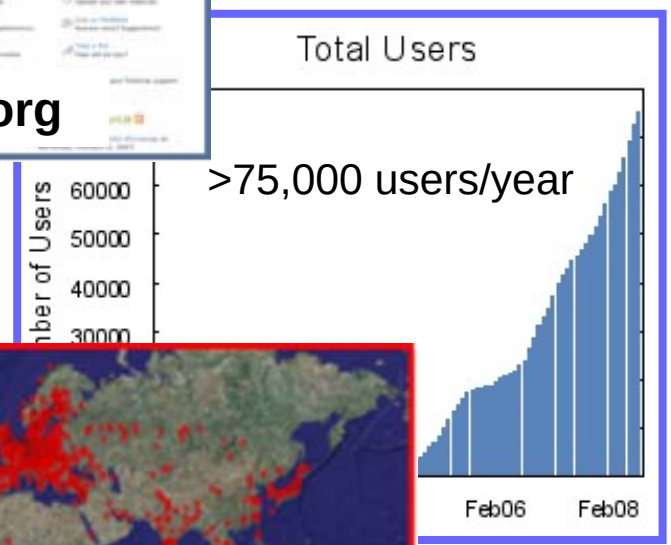
grid

rendering farm

INDEX
INSTITUTE FOR NANOELECTRONICS DISCOVERY AND EXPLORATION

Network for Computational Nanotechnology





NSF/NRI - NCN

- techniques for exploratory simulation
- new ideas for switching devices
- technology for dissemination and collaborations

theme 4 team

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James Raynolds

Technical focus: QD Spin Devices

Approach:
Finite-element based simulations of realistic devices

Key result:
Electrical spin switching/enhancement due to asymmetric confining potentials

INDEX Student:
Sanjay Prabhakar

Talk in QD Spin Device Session

Poster by: ***Sanjay Prabhakar***

Michael Shur

Technical focus: *THz plasmonic devices*

Approach:
Solving Maxwell equations and equations describing ballistic transport and THz characterization

Key result:
Si THz detection with nanoscale resolution

INDEX Student:
Bill Stillman

Poster by M. Shur: "Modeling and Characterization of THz Plasma Electronic Devices"

Yongqiang (Alex) Xue

Technical focus: Quantum Moletronics

Approach:

develop and apply density functional and Schwinger-Keldysh Green's function methods

Key result:

hydrogen passivation effect on silicon nanowires

INDEX Student:
Abraham Hmiel

Poster by: ***Abraham Hmiel***

Azad Naeemi

Technical focus: graphene interconnects and devices

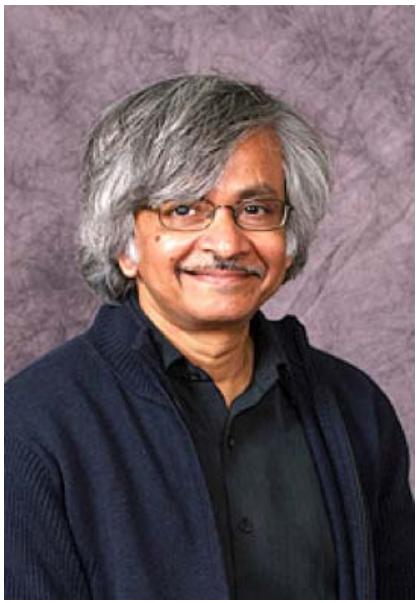
Approach:
quantify physical limits of various computational variables from interconnection point of view to identify the promising options

Key result:
quantum conductance modeling for GNRs

INDEX Student:
Shaloo Rakheja

***Talk in Graphene Session**

Supriyo Datta



Technical focus: Graphene

Approach:
extend and apply NEGF formalism

Key result:
role of MIGS states in graphene

***Talk in Graphene Session**

INDEX Students:
R. Golizadeh-Mojarad
Tony Low (pending)

***Posters by:**
Roksana Golizadeh-Mojarad
and ***Tony Low***

Mark Lundstrom

Technical focus: Graphene devices

Approach:
apply NEGF formalism, percolation theory, and assess and benchmark device concepts

Key result:
quantitative *understanding of graphene PN junction IV*

Students:
Tony Low (pending)
Dionisis Berbedes

Poster by: *Tony Low*

Summary

1) Focus on exploratory simulation and tight connections to experimental work.

2) NSF-NRI program provides additional leverage.

3) nanoHUB provides infrastructure support available to Theme 4 and the NRI program.