

NanoElectronic Modeling with the NEMO toolkit on nanoHUB

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- nanoHUB
- Nanoelectronics modeling
- NEMO5 engine
- NEMO-powered nanoHUB tools
- Best practices

- 330,000 annual users
- 330 simulation tools
 - » Nanoelectronics, nanophotonics, materials science, molecular electronics, carbon-based systems
 - Microelectromechanical systems
- 4,200 resources (video lectures, presentations, tutorials, etc.)




RESOURCES

Keyword or phrase: Search

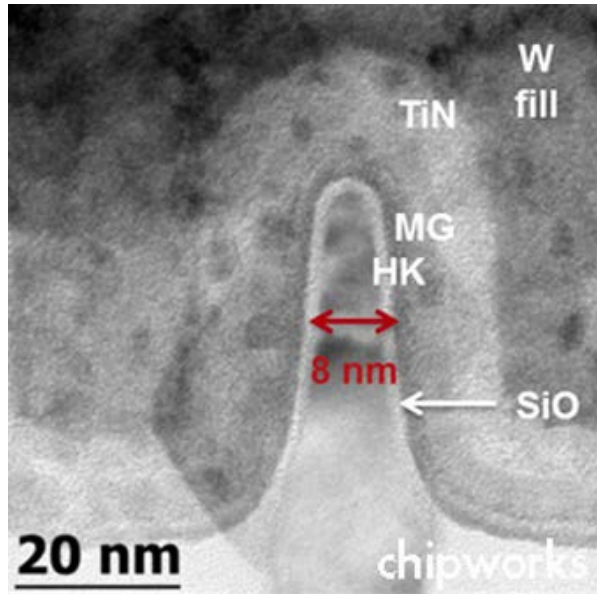
Popular Tags: [nanoelectronics](#) [course lecture](#) [Illinois](#) [materials science](#)
[NanoBio Node](#) [nano/bio](#) [nanotransistors](#) [UIUC](#) [research seminar](#) [devices](#)
[nanophotonics](#) [quantum transport](#) [transistors](#) [tutorial](#) [NEGF](#)
[carbon nanotubes](#) [nano electro-mechanical systems](#) [Simulation](#)

FEATURED

 nanoHUB-U: Your source for cutting-edge topics distilled into lectures with quizzes, homework, practice exams.

 NEEDS: The NSF-Funded Electronics Content Node.

- nanoHUB-U (online courses)
 - » Nanoscale transistors (Prof. Mark Lundstrom)
 - » Fundamentals of Nanoelectronics (Prof. Supriyo Datta)
 - » From Atoms to Materials: Predictive Theory and Simulations (Prof. Alejandro Strachan)
 - » Principles of Electronic Nanobiosensors (Prof. Ashraf Alam)

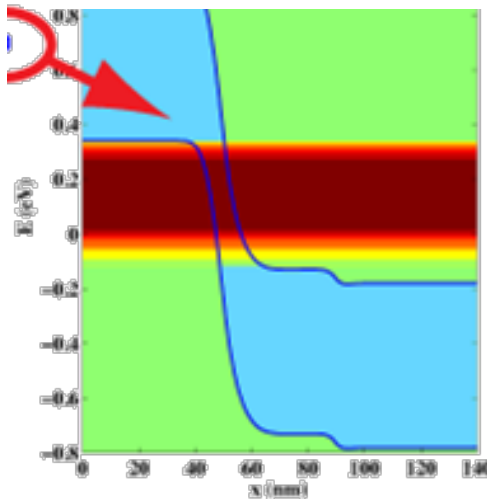


- \$300 billion semiconductor industry
- International Technology Roadmap for Semiconductors (ITRS)
- Moore's Law
- Countable number of atoms
- Quantum effects
- Devices (transistors)
 - Smaller, faster, more energy efficient
 - Designs, materials

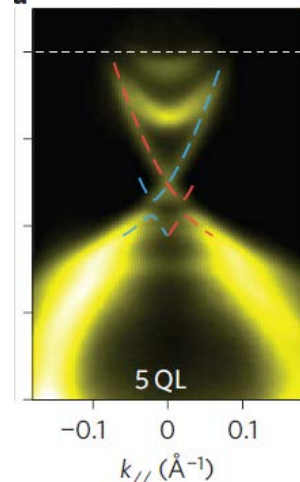
Band-to-band tunneling

Topological insulators

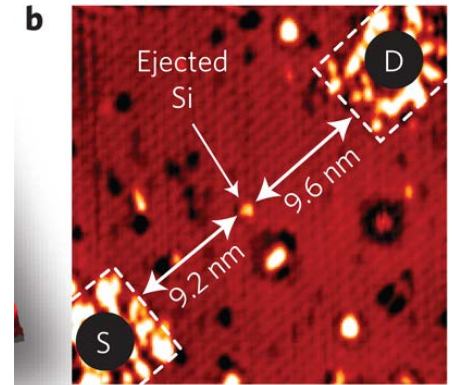
Single atom transistors



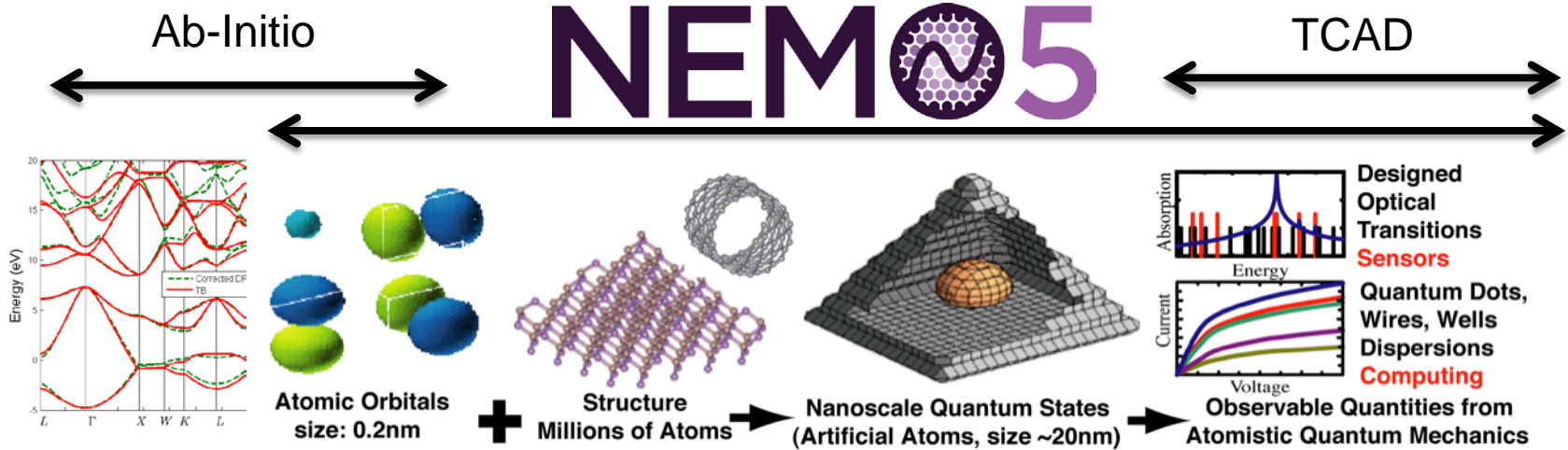
IEEE Elec. Dev. Lett. **30**, 602 (2009)



Nature Physics **6**, 584 (2010)



Nature Nanotechnology **7**, 242 (2012)



Goal:

- Device performance with realistic extent, heterostructures, fields, etc. for new / unknown materials

Problems:

- Need ab-initio to explore new material properties
- Ab-initio cannot model non-equilibrium.
- TCAD lacks real material physics

Approach:

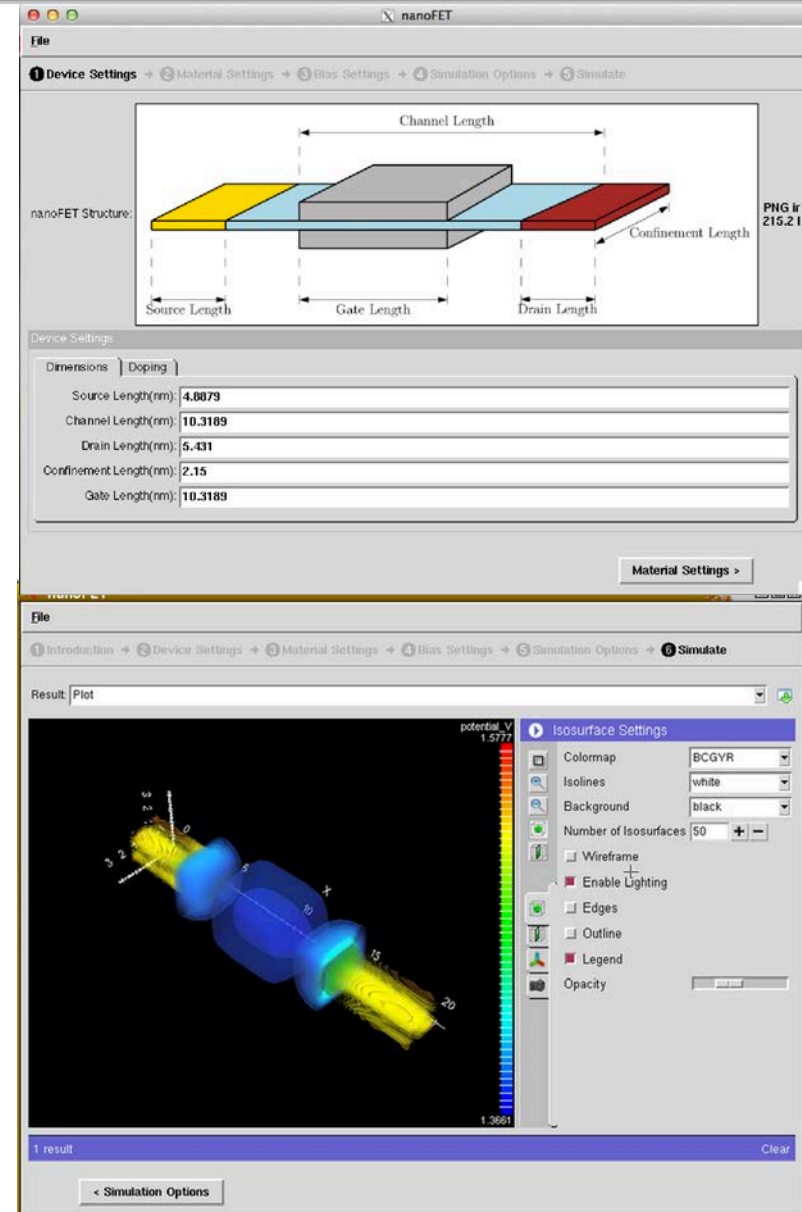
- Ab-initio:
 - Bulk constituents
 - Small ideal superlattices
- Map ab-initio to tight binding (binaries and superlattices)
- Current flow in ideal structures
- Study devices perturbed by:
 - Large applied biases
 - Disorder
 - Phonons

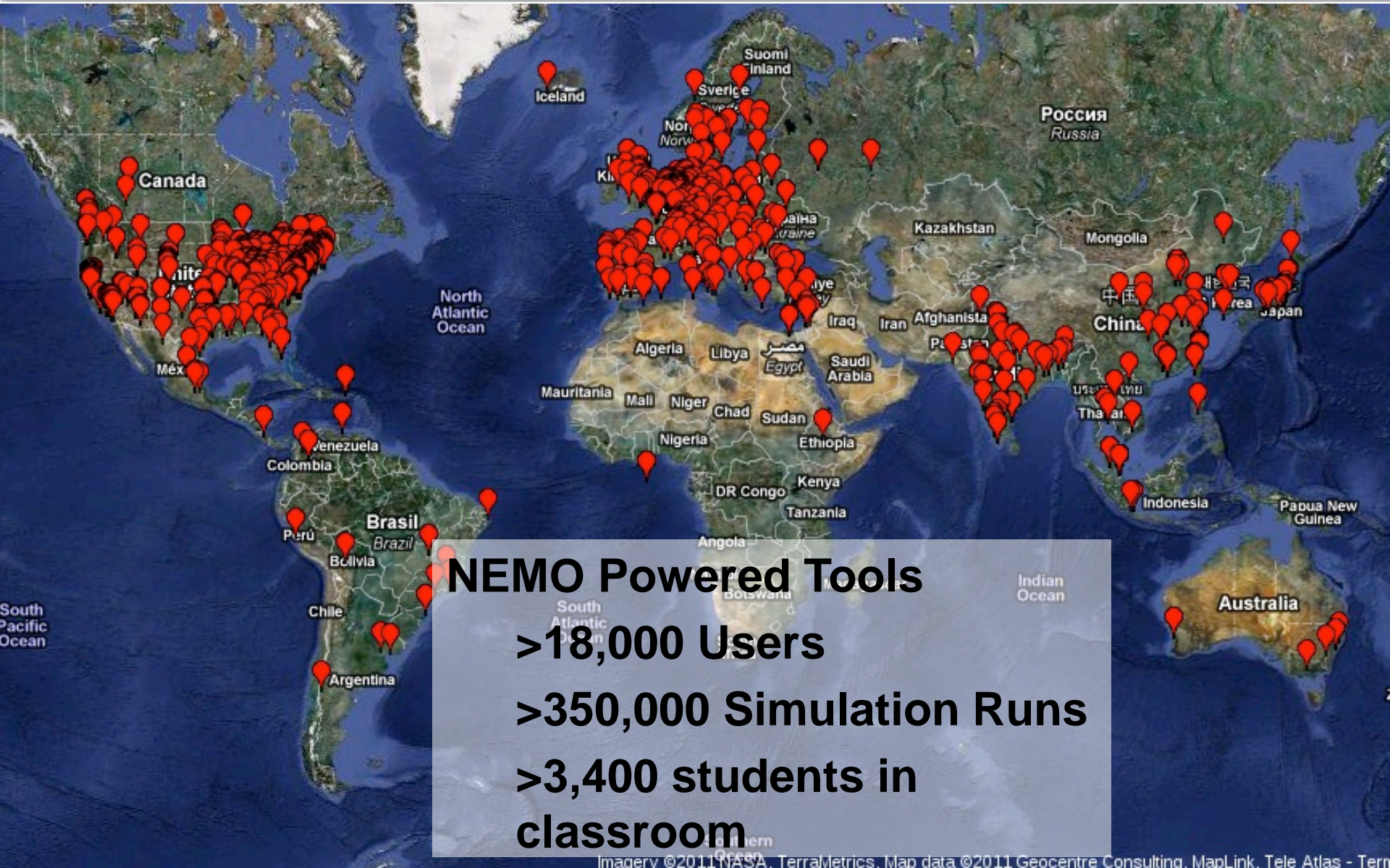
• NEMO5

- » Academic and industrial use
- » Free for academic use
- » ~30 developers currently
- » 500,000 lines of code
 - ✓ C++, python
 - ✓ 3rd party libraries
- » Input files 100s to 1000s of lines
- » 3 ways to use NEMO5
 - ✓ Distribution and support group on nanoHUB
 - Source code available
 - nanoHUB workspace → Purdue's RCAC clusters
 - ✓ nanoHUB tools

```
...
solver {
    name = QTBM:bands_source_mode_contact
    type = Schroedinger
    iterator {
        set {
            active_regions = (1,2,3)
            allow_reinit_k_points = true
            automatic_threshold = true
            charge_model = electron_hole
            convergence_limit = 1.e-10
            cutoff_distance_to_bandedge = 0.05
            domain = source_mode_contact
            eigen_values_solver = krylovschur
            job_list = (assemble_H,passivate_H,
calculate_band_structure)
            k_degeneracy = 1
            ...
        }
    }
}
solver {
    name = QTBM:bands_drain_mode_contact
    type = Schroedinger
    ...
```

- OMEN/NEMO5-based nanoHUB tools
 - » Brillouin Zone Viewer
 - ✓ Crystal theory
 - » Crystal Viewer
 - ✓ Visualize crystals, design your own
 - » Bandstructure Lab
 - ✓ Semiconductor fundamentals
 - » 1dhetero
 - ✓ Poisson-Schroedinger Solver for 1 dimensional heterostructures
 - » RTDNEGF –
 - ✓ Calculate current through resonant tunneling diodes
 - » Quantum Dot Lab
 - ✓ Eigenstates (energy levels) of particle in a box system
 - » nanoFET
 - ✓ Calculate transport properties of transistors
 - ✓ NEMO5 powered version of OMENwire, OMEN_FET
 - » ITRS tool OMEN/PADRE/NEMO5 powered - (coming soon)

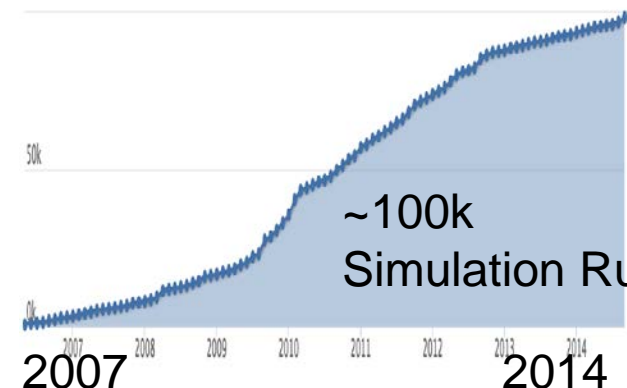
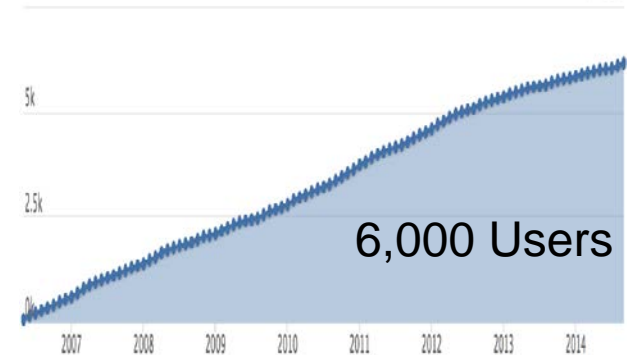
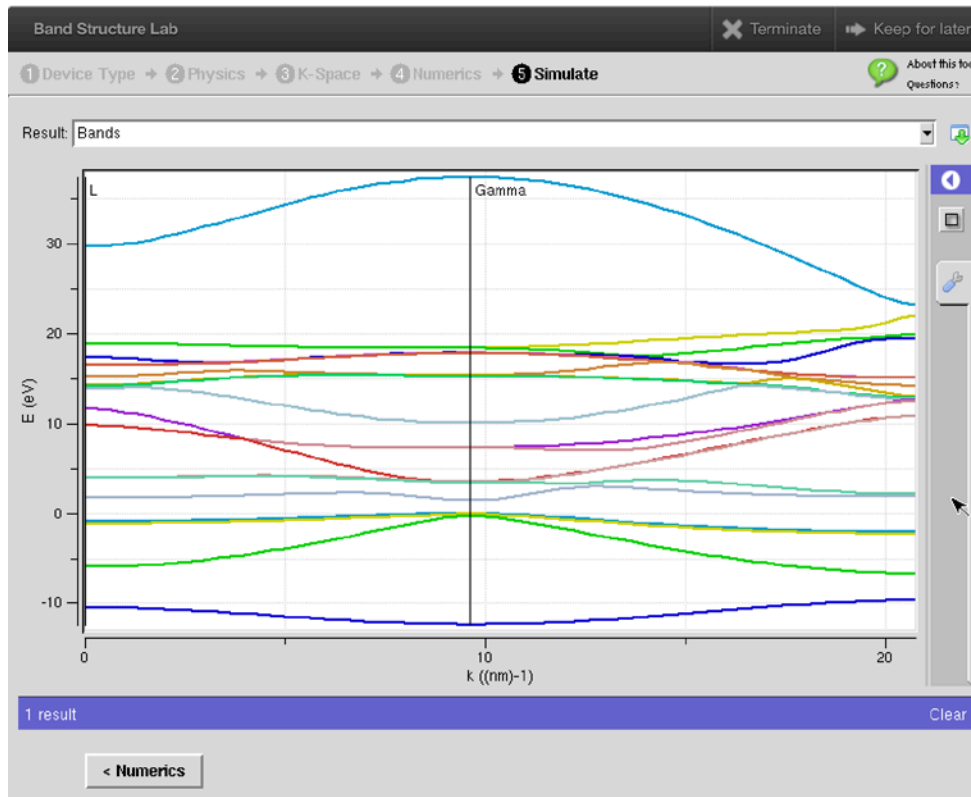


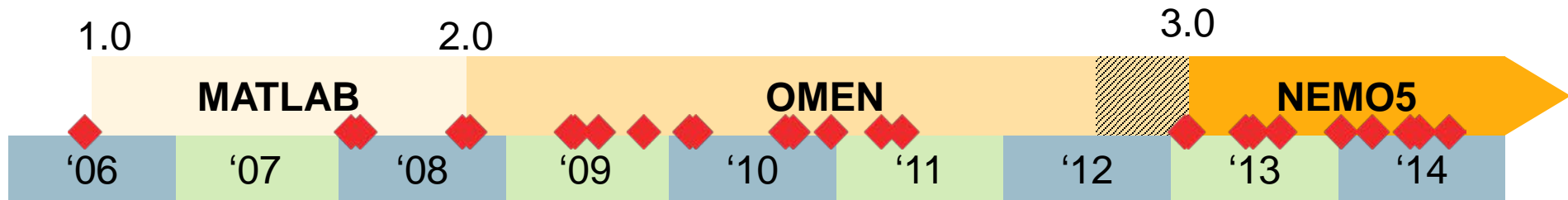


Imagery ©2011 NASA, TerraMetrics, Map data ©2011 Geocentre Consulting, MapLink, Tele Atlas - TerraMetrics

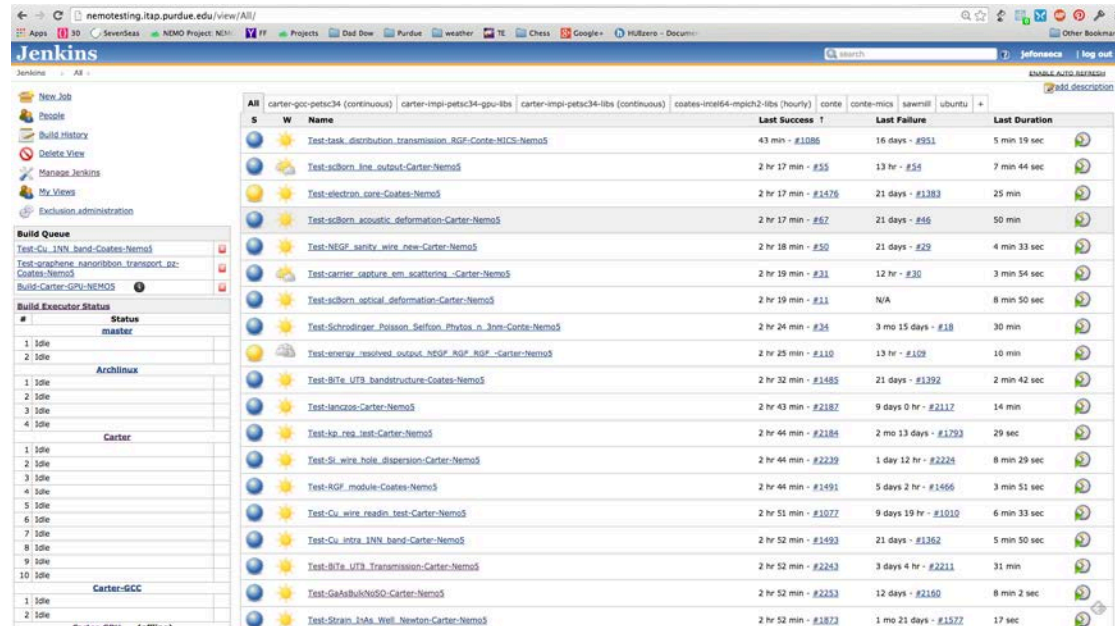
- Computes the electronic and phonon structure of various materials in the spatial configuration of bulk, quantum wells, and wires
- Various materials (Si, Ge, GaAs, etc.)

NEMO5
development --
Samik Mukherjee





- ~100 svn commits of Bandstructure Lab
- ~9200 commits of NEMO5 during development
- Jenkins
 - » <http://jenkins-ci.org/>
 - » Continuous integration and testing system
 - » Alerts developers / owners
 - ✓ Validity
 - ✓ performance
- 12 bandstructure lab regression tests



S	W	Name	Last Success	Last Failure	Last Duration
		Test-task_distribution_transmission_RGF-Coates-Nemo5	43 min - #1086	16 days - #951	5 min 19 sec
		Test-scborn_line_output-Carter-Nemo5	2 hr 17 min - #55	13 hr - #54	7 min 44 sec
		Test-electron_scare-Coates-Nemo5	2 hr 17 min - #1476	21 days - #1383	25 min
		Test-scborn_acoustic_deformation-Carter-Nemo5	2 hr 17 min - #67	21 days - #16	50 min
		Test-NEGf_sanity_wire_new-Carter-Nemo5	2 hr 18 min - #50	21 days - #29	4 min 33 sec
		Test-srangPhone_nacorbion_transport_uz-Coates-Nemo5	2 hr 19 min - #31	12 hr - #30	3 min 54 sec
		Test-scborn_optical_deformation-Carter-Nemo5	2 hr 19 min - #11	N/A	8 min 50 sec
		Test-Schrodinger_Poisson_Seifon_Phytos_n_3on-Corrie-Nemo5	2 hr 24 min - #34	3 mo 15 days - #18	30 min
		Test-energy_resolved_output_NEGf_RGF_Carter-Nemo5	2 hr 25 min - #110	13 hr - #109	10 min
		Test-BTe_UFB_bandstructure-Coates-Nemo5	2 hr 32 min - #1495	21 days - #1392	2 min 42 sec
		Test-lanczos-Carter-Nemo5	2 hr 43 min - #2182	9 days 0 hr - #2112	14 min
		Test-kp_res_test-Carter-Nemo5	2 hr 44 min - #2184	2 mo 13 days - #1793	29 sec
		Test-SI_wire_hole_dispersion-Carter-Nemo5	2 hr 44 min - #2239	1 day 12 hr - #2224	8 min 29 sec
		Test-RGF_module-Coates-Nemo5	2 hr 44 min - #1491	5 days 2 hr - #1466	3 min 51 sec
		Test-Cu_wire_readin_test-Carter-Nemo5	2 hr 51 min - #1072	9 days 19 hr - #1010	6 min 33 sec
		Test-Cu_intra_INN_band-Carter-Nemo5	2 hr 52 min - #1493	21 days - #1362	5 min 50 sec
		Test-BTe_UFB_Transmission-Carter-Nemo5	2 hr 52 min - #2243	3 days 4 hr - #2211	31 min
		Test-GaAsBulkNemo5-Carter-Nemo5	2 hr 52 min - #2253	12 days - #2160	8 min 2 sec
		Test-Strain_3As_Well_Newton-Carter-Nemo5	2 hr 52 min - #1873	1 mo 21 days - #1572	17 sec

- Multiple, noncurrent developers
 - » Testing
 - » activation Energy
- Development Guide and Resources
 - » Linux
 - » SVN
 - » NEMO5
 - » nanoHUB
 - » Rappture
 - » Wrapper code
 - ✓ Tcl, C
 - » HPC systems

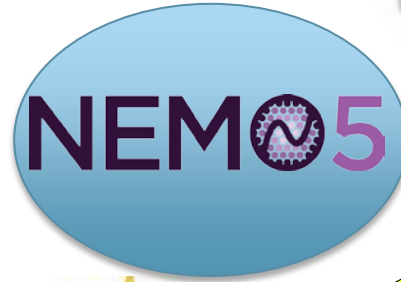
Industrial Use

Intel Samsung
TSMC Philips

Industrial Development



18,000 users



Tunneling Transistors
GaN, MoS₂



Contacts, HEMTs

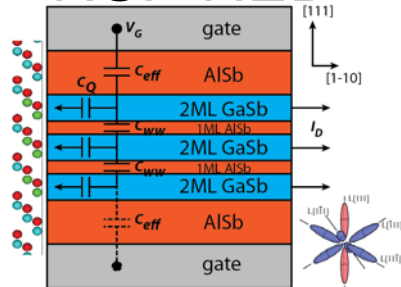
NSF-NCN
NSF-OCI



Peta-Scale Computing



NSF-NEB



Quantum Computing

A single-atom transistor

Martin Fuechsle¹, Jill A. Miwa¹, Suddhasatta Mahapatra¹,
Oliver Warschkow¹, Lloyd C. L. Hollenberg³, Gerhard Klimek¹

The ability to control matter at the atomic scale and build

- PI: Gerhard Klimeck
- 3 Research Faculty: Tillmann Kubis, Michael Povolotskyi, Rajib Rahman
- Research Scientist: Jim Fonseca
- 2 Postdocs: Bozidar Novakovic, Jun Huang
- Students: Kyle Aitken, **Tarek Ameen**, Yamini Bansal, James Charles, Chin-Yi Chen, **Fan Chen**, **Yuanchu (Fabio) Chen**, Rifat Ferdous, Jun Zhe Geng, Yu He, Yuling Hsueh, Jun Huang, Hesameddin Ilatikhameneh, **Zhengping Jiang**, Daniel Lemus, Pengyu Long, **Daniel Mejia Padilla**, Kai Miao, **Samik Mukherjee**, Ahmed kamal Reza, **Santiago Rubiano**, Harshad Sahasrabudhe, **Mehdi Salmani Jelodar**, **Prasad Sarangapani**, Saima Sharmin, Yaohua Tan, Yui Hong Tan, **Archana Tankasala**, **Daniel Valencia Hoyos**, KuangChung Wang, Yu Wang, **Evan Wilson**
- SURF Students: **Josef Borga**, **Woody Gilbertson**, **Kevin Margatan**, **Vincent Ntarugera**, **Travis Shepherd**, **Zach Schaffter**

