

**NEMO5**



# **NEMO5 on Blue Waters - A Flexible Package for Nanoelectronics Modeling Problems**

**Jim Fonseca**

**Network for Computational  
Nanotechnology**

**PURDUE**  
UNIVERSITY

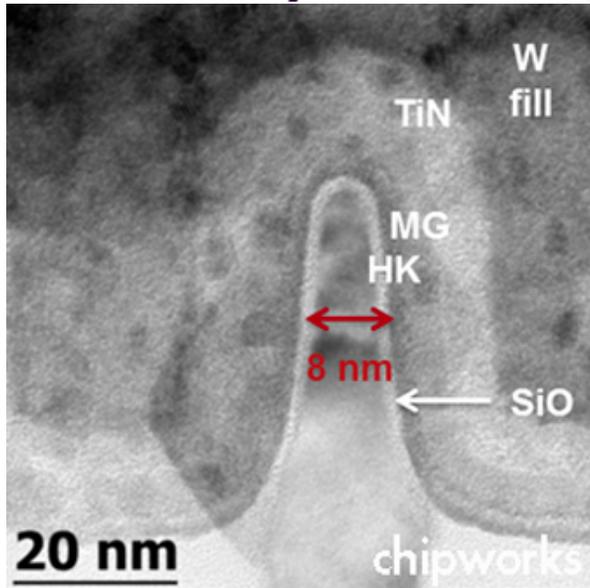
**PRAC - Accelerating Nano-scale Transistor  
Innovation**

**PI: Gerhard Klimeck**

**Blue Waters Symposium**

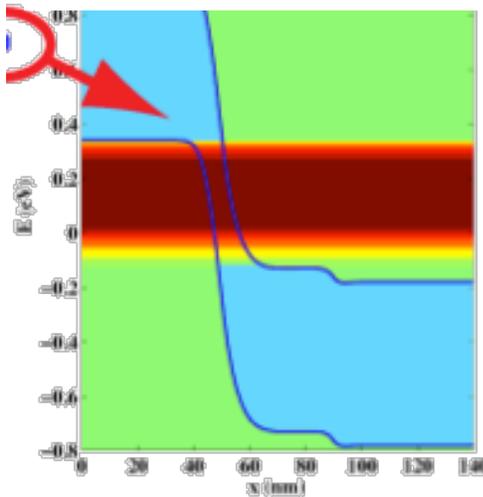
**June 2016**

- NEMO5
- nanoHUB
- NEMO5 Testing
- Science on Blue Waters
  - » Tunnel FET
  - » Time resolved
  - » Quantum Dots Compact Model
  - » Multi Quantum Well LEDs



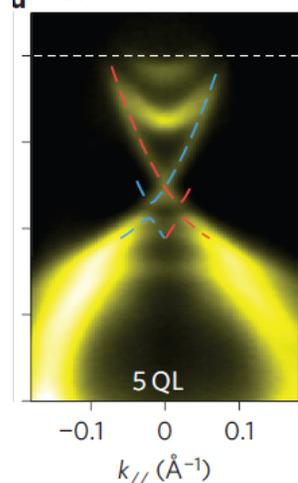
- \$300 billion semiconductor industry
- International Technology Roadmap for Semiconductors (ITRS)
- Moore's Law
- Countable number of atoms
- Quantum effects
- Devices (transistors)
  - Smaller, faster, more energy efficient
  - Designs, materials

Band-to-band tunneling



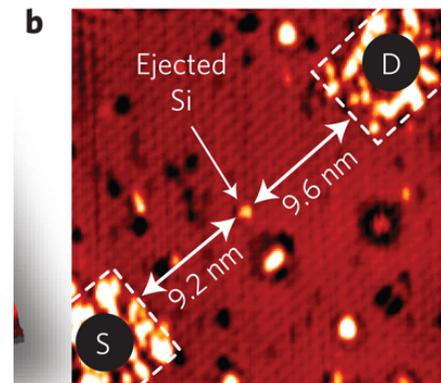
IEEE Elec. Dev. Lett. **30**, 602 (2009)

Topological insulators

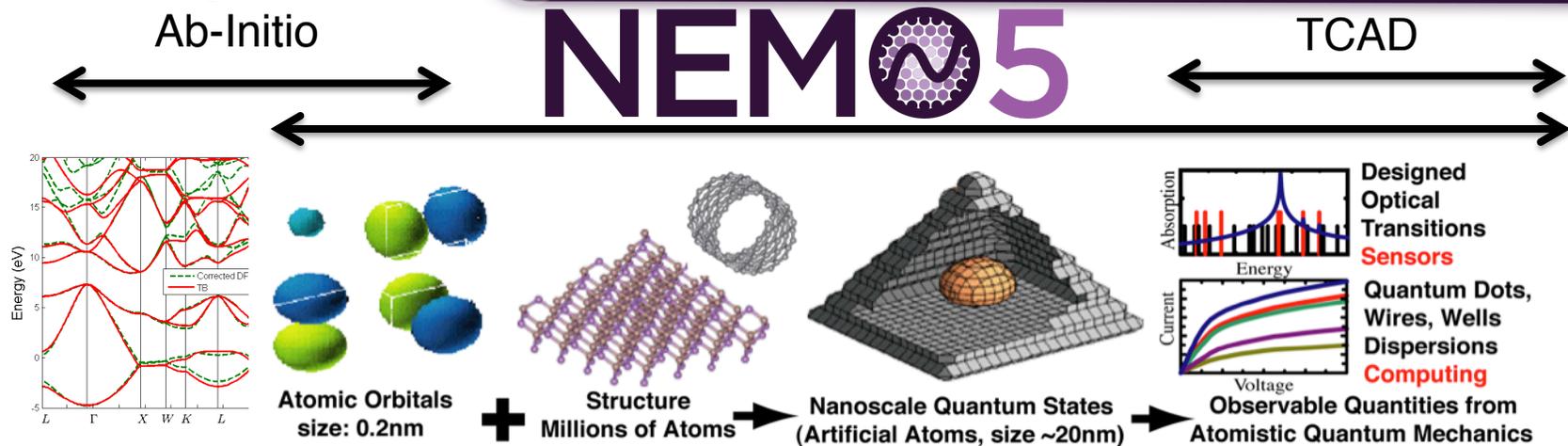


Nature Physics **6**, 584 (2010)

Single atom transistors



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 uses quantum corrections

### 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

- **Multiscale/multiphysics**

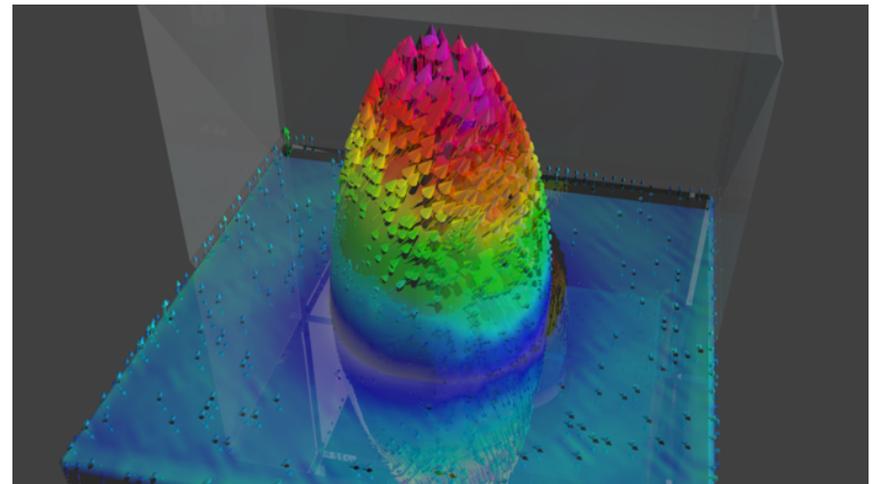
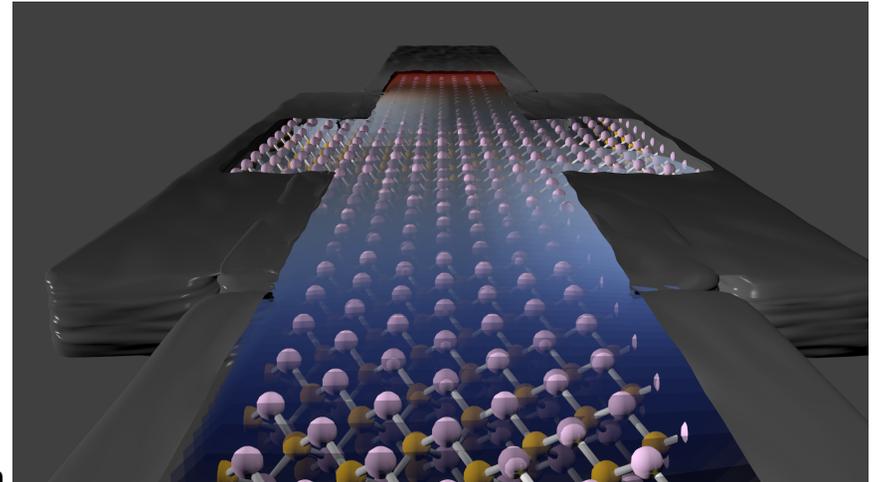
- Empirical tight binding
- NEGF, DD, QTBM, EM
- Electron core, k.p, mode space
- Ohmic and Schottky contacts
- Scattering optical and acoustic
- Phonons
- Strain models-VFF, Keating, Lazarenkova
- External magnetic fields

- **Solves**

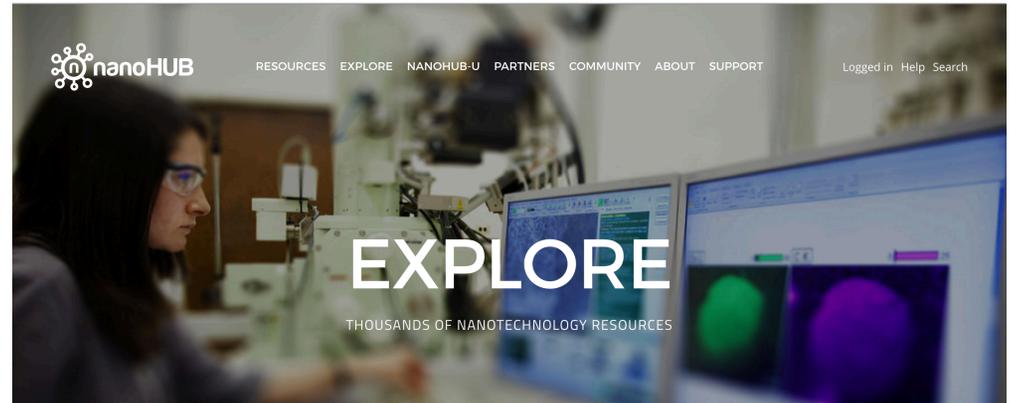
- Atomistic strain
- Electronic band structures
- Charge density
- Potential
- Current

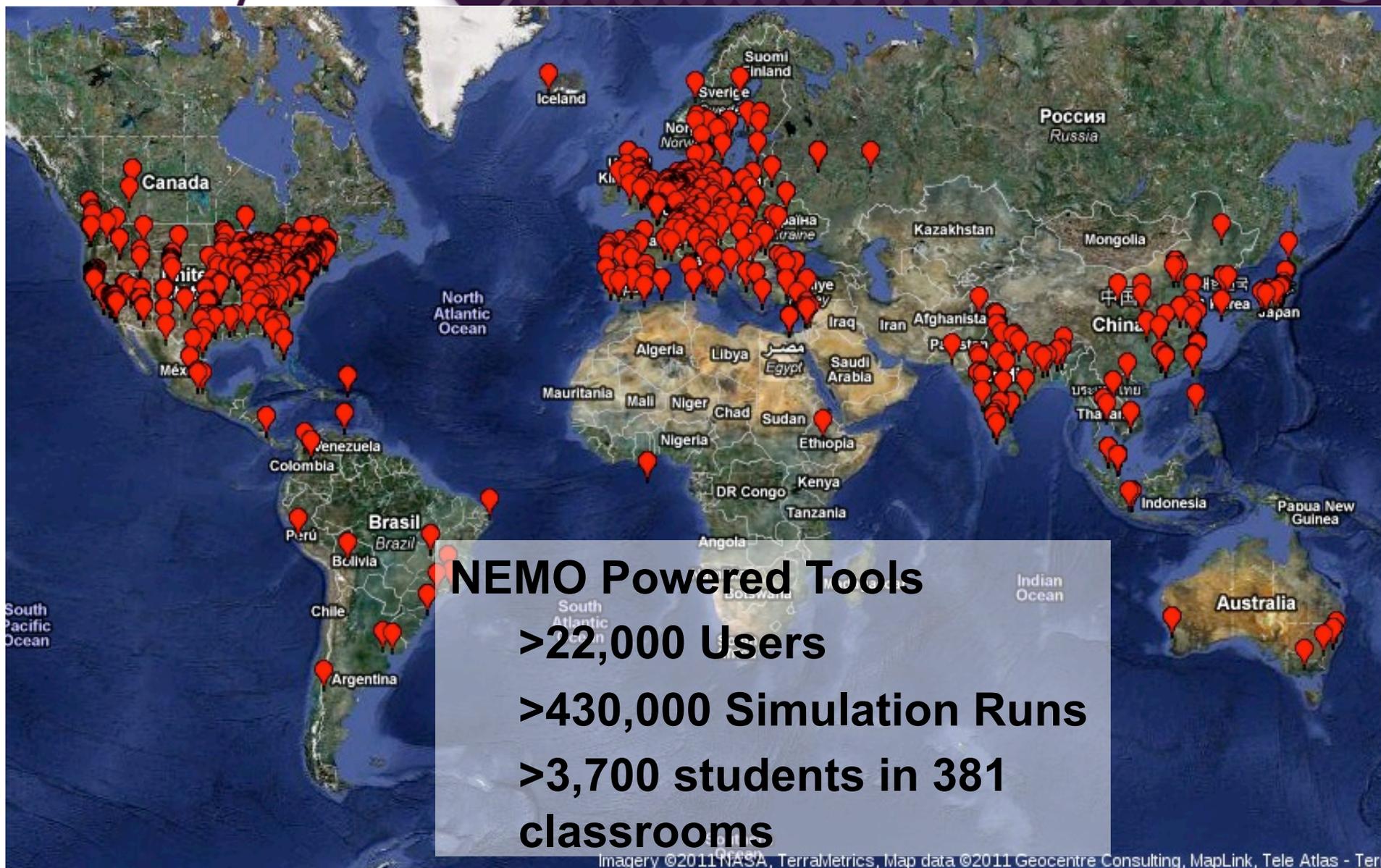
- **4-level MPI parallelization**

- bias, energy, momentum, space



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





### NEMO Powered Tools

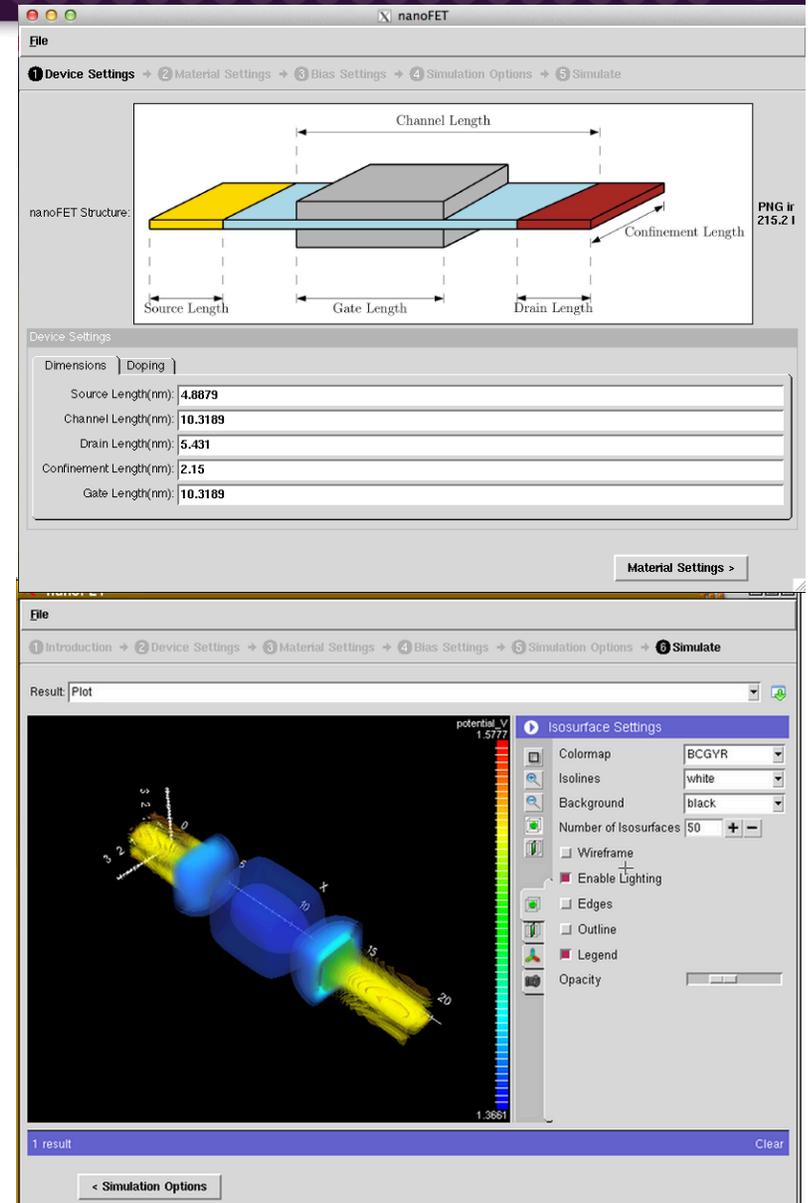
>22,000 Users

>430,000 Simulation Runs

>3,700 students in 381 classrooms

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

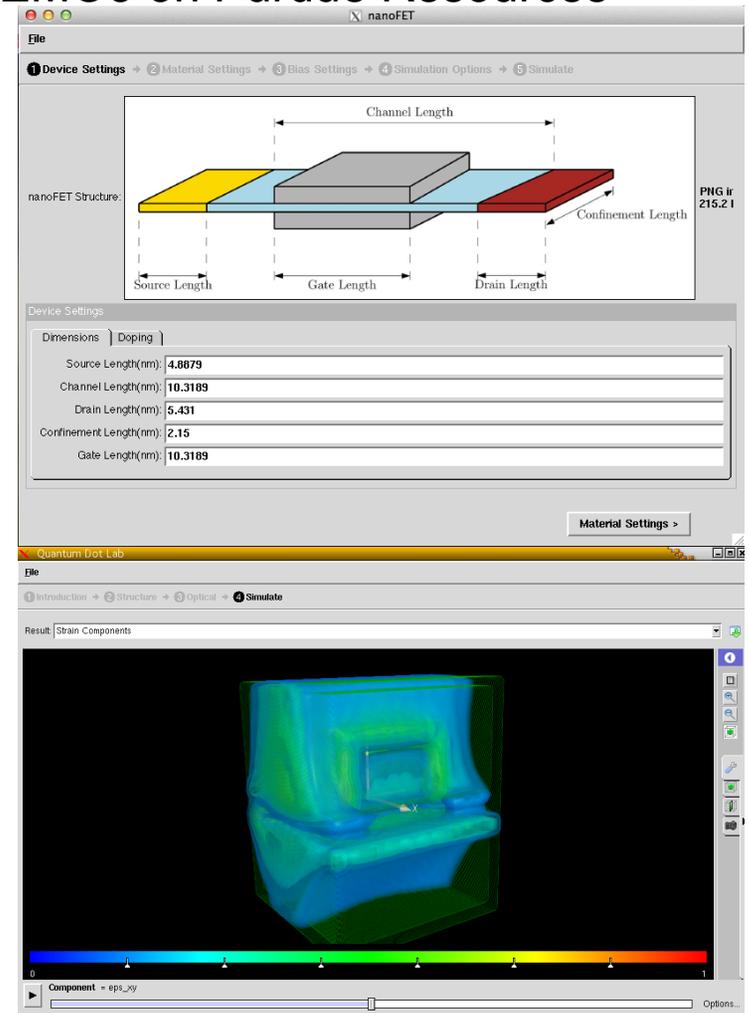
- OMEN/NEMO5-based nanoHUB tools
  - » Brillouin Zone Viewer
    - ✓ Crystal theory
  - » Crystal Viewer
    - ✓ Visualize crystals, design your own
  - » Bandstructure Lab
    - ✓ Semiconductor fundamentals
  - » 1dhetero
    - ✓ Poisson-Schroedinger Solver for 1 dimensional heterostructures
  - » RTDNEGF –
    - ✓ 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
- Distribution and Support Group on nanoHUB.org
  - » <https://nanohub.org/groups/nemo5distribution>
  - » Source code, example, discussion forum, run NEMO5 on Purdue Resources



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- nanoHUB.org

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- » Nanoelectronics, nanophotonics, materials science, molecular electronics, carbon-based systems, Microelectromechanical systems
- » 4,200 resources (video lectures, presentations, tutorials, etc.)
- » NEMO5 Tools
  - ✓ Quantum Dot Lab
  - ✓ Crystal Viewer
  - ✓ Bandstructure Lab



NEMO5



# NEMO5 Testing Jenkins and Launcher

S. Rubiano, J. Bermeo, Daniel Mejia, J.  
Fonseca, M. Povolotskyi, E. Wilson, Z. Jiang,  
D. Valencia, T. Ameen

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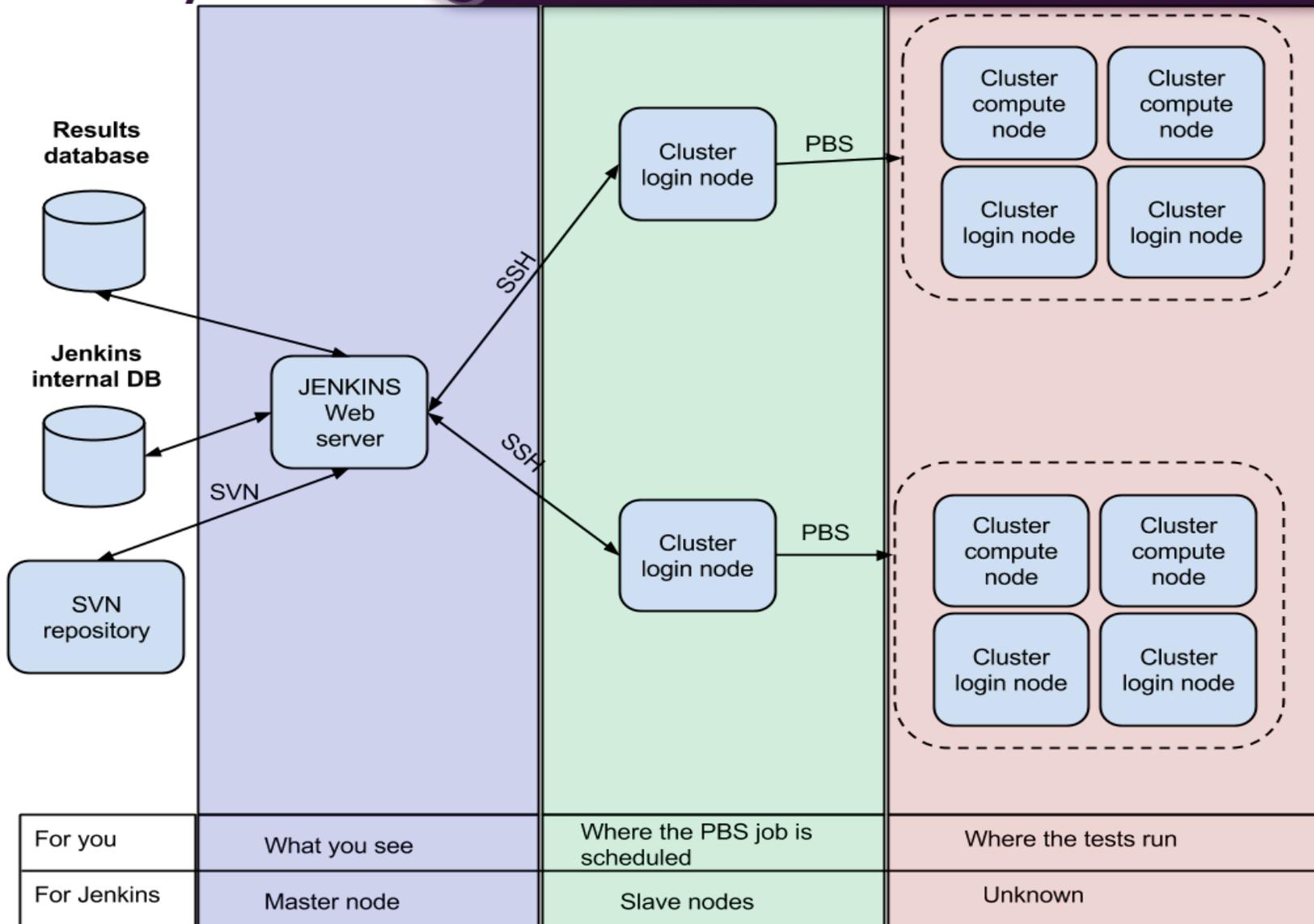
- Correctness
  - » Compare output files against reference data
- Performance
  - » Timing / memory history
  - » Can set thresholds and mark tests unstable under various conditions
- Compatibility
  - » Different machines, compilers, etc.
- Get Tests Fixed
  - » Alert test owner and other stakeholders
  - » Would like to know specific revision that caused issues
  - » Compiler, machine, library information
    - ✓ Everything needed to reproduce test by hand
  - » Tarball of all test data is provided

- Much better than nothing; left a lot to be desired
- Shell script started by cron job on local machine
- Run nightly
  - » Compile code
  - » Run regression tests
  - » Smart diff
  - » Email developers
- Problems
  - » 30-40 commits per day
  - » No tracking of memory or timing



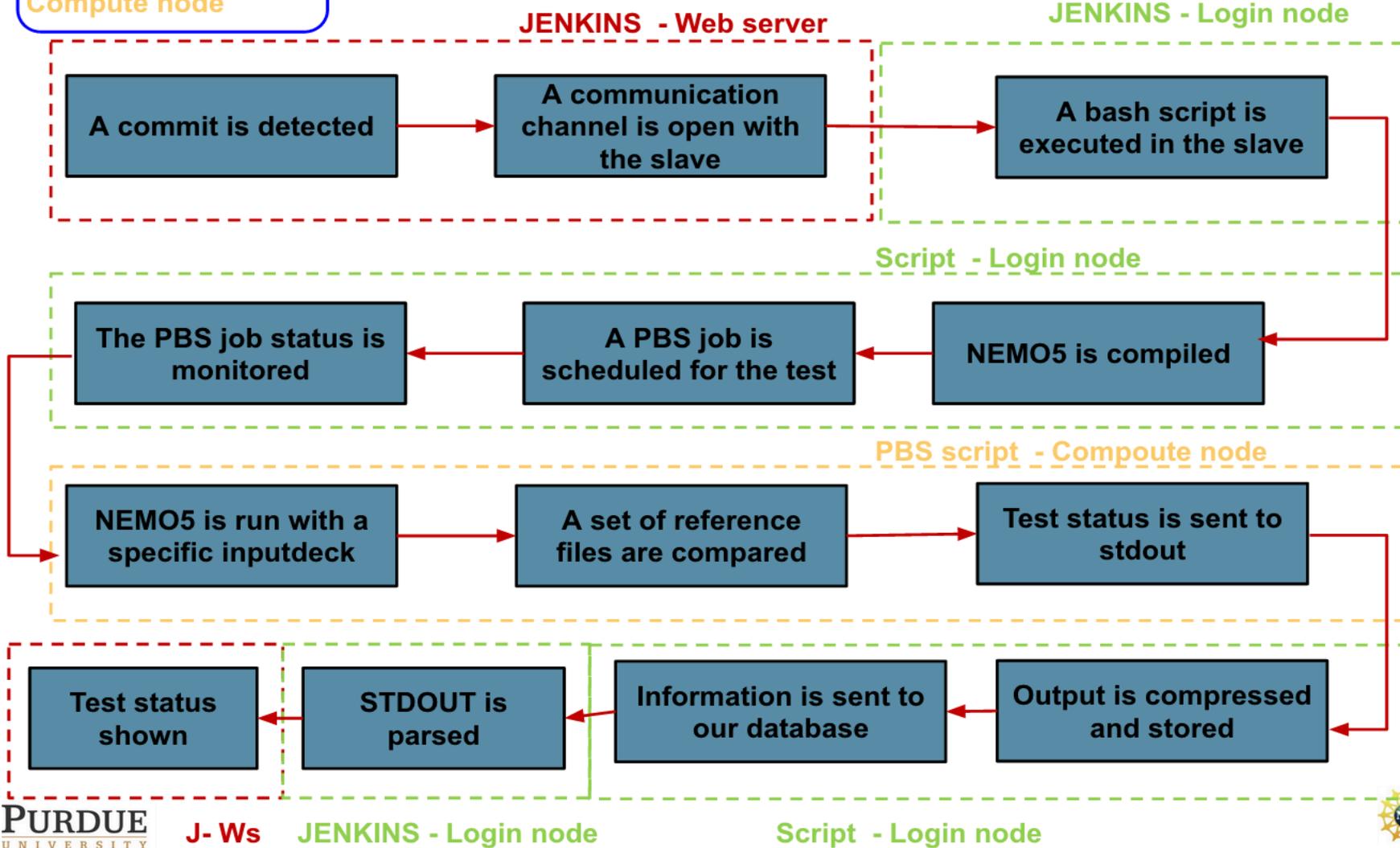
# Jenkins Architecture

<https://jenkins.io/>



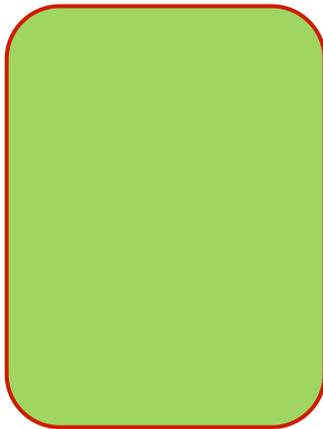
- Launcher
  - » Python script
  - » Facilitates running jobs through PBS
  - » Reads job requirements from a .res file
  - » Submits job; monitors queue for status
  - » Performs smart comparison of reference files and output
    - ✓ Essentially compares values within default 1% (can be customized)
  - » Closely coupled with Jenkins but can be used on its own
- Jenkins
  - » Continuous Integration Server
    - ✓ <https://jenkins-ci.org/>
  - » Run on a webserver hosted by Purdue's ITaP
  - » Also uses a mysql database for build information (pass/fail, timing, memory)

Web server  
Login node  
Compute node



A test is made from :

**INPUT**



**inputdeck.in**

**RESOURCES**



**resources.res**

**OUTPUT  
REFERENCE**



**out\_ref.dat**

```
$ module load python
$ cd prototype/bin/
$ ./launcher test ../../regression_test/numerical_tests/kp_reg_test/
QW_GaAs.in -out results -ranks 1
. . .
[INFO] This inputdeck will be run with the following resources :
Ranks : 1
[WARNING] The default testing script (comparison against reference files
in /home/srubiano/NEMO/regression_test/numerical_tests/kp_reg_test) will be
used instead with a tolerance of 1%
[INFO] Executing NEMO5
[INFO] Sending the job to the queue and waiting
[INFO] Waiting in queue for job 4251642
[INFO] Waiting in queue for job 4251642
. . .
[INFO] The job was allocated
[INFO] Waiting for the job 4251642 to finish. Current status : R
[INFO] Waiting for the job 4251642 to finish. Current status : R
. . .
[INFO] Waiting for the job 4251642 to finish. Current status : C
```

```
[INFO]      Waiting for the output files to get to the login node
```

```
[INFO]
```

```
===== The inputdeck was run =====
```

```
It generated the following files:
```

```
...
```

```
    /home/srubiano/NEMO/prototype/bin/results/
```

```
device_planes_2.vtk
```

```
...
```

```
[INFO]      ===== STDOUT (last 20 lines) =====
```

```
...
```

```
[INFO]      ===== END STDOUT (last 20 lines) =====
```

```
[INFO]      ===== STDERR (last 20 lines) =====
```

```
[INFO]      ===== END STDERR (last 20 lines) =====
```

```
[INFO]      ===== TEST RESULTS =====
```

```
[INFO]      Test : GaAs_well_k_points.dat passed. Details : The  
reference and generated files are equal up to 1.0%
```

```
[INFO]      Test : GaAs_well_energies.dat passed. Details : The  
reference and generated files are equal up to 1.0%
```

- 10 NEMO5 builds
  - » Intel/GNU compiler
  - » different RCAC (Purdue) machines
  - » PETSc 3.4/3.5, etc.
  - » Phi tests
  - » GPU tests
  - » optimized/debug
    - ✓ SVN polled every 3 minutes;

No Blue Waters-specific tests



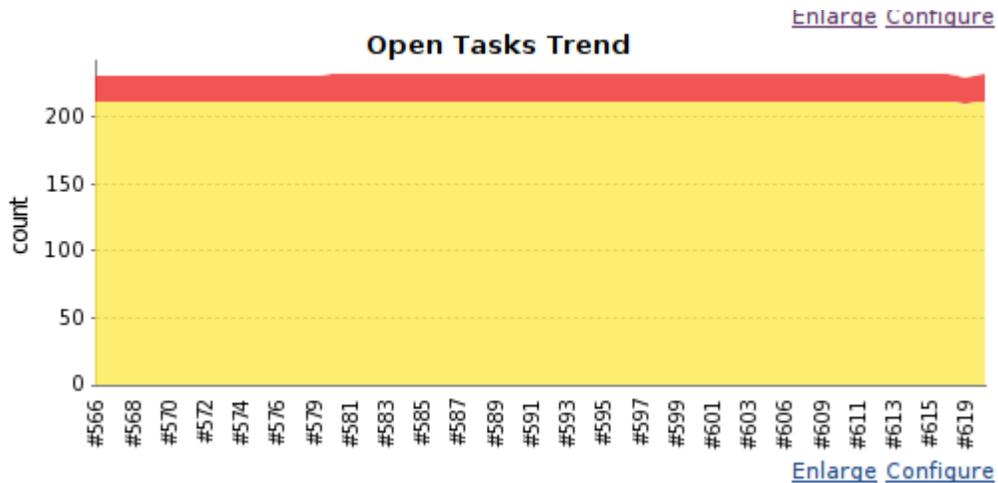
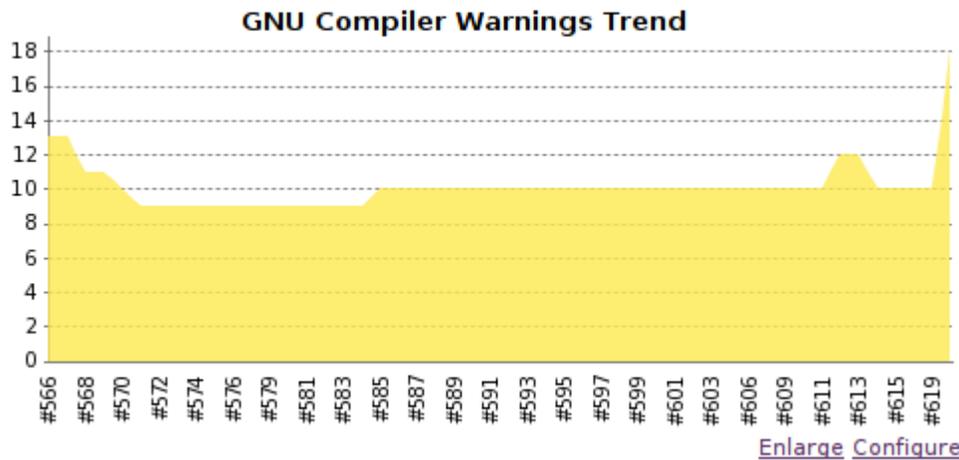
- ~500 active tests
  - » Ideally maximum requirements are 2 nodes for 10 minutes
  - » Some replicated on multiple builds
  - » Can be triggered by successful code build or on a timer
  - » Most tests are regression tests, but can support unit tests as well
- Tests are maintained by the owner
  - » Generally the student who has added the test or inherited it.

http://nemotesting.itap.purdue.edu/

The screenshot shows the Jenkins web interface. At the top, there is a search bar and a 'log In' link. Below the header, there are navigation links for 'People', 'Build History', and 'Exclusion administration'. The main content area displays a table of build jobs. The table has columns for 'S', 'LC', 'Name', 'LTR', 'FFR', 'LSR', and 'LFR'. The jobs listed include 'Build-Carter-NEMO5', 'Test-2nm\_si\_wire\_meta\_device-Carter-Nemo5', 'Test-5x\_111\_InGaAs-Carter-Nemo5', 'Test-BiTe\_UTB\_bandstructure-Carter-Nemo5', 'Test-BiTe\_UTB\_Transmission-Carter-Nemo5', 'Test-block\_lanczos-Carter-Nemo5', 'Test-brillouin\_zone\_viewer\_bcc\_cubic-Carter-Nemo5', 'Test-brillouin\_zone\_viewer\_bcc\_primitive-Carter-Nemo5', 'Test-brillouin\_zone\_viewer\_fcc\_cubic-Carter-Nemo5', 'Test-brillouin\_zone\_viewer\_fcc\_primitive-Carter-Nemo5', 'Test-brillouin\_zone\_viewer\_graphene\_primitive-Carter-Nemo5', 'Test-brillouin\_zone\_viewer\_hexagonal-Carter-Nemo5', 'Test-brillouin\_zone\_viewer\_rhombohedral-Carter-Nemo5', 'Test-brillouin\_zone\_viewer\_simplecubic-Carter-Nemo5', and 'Test-BSLAB\_Bulk\_Phonon\_Unfolding-Carter-Nemo5'. The table also includes a 'Build Queue' section on the left with a list of jobs and their status, and a 'Build Executor Status' section at the bottom left showing the status of the master node and the Carter node.

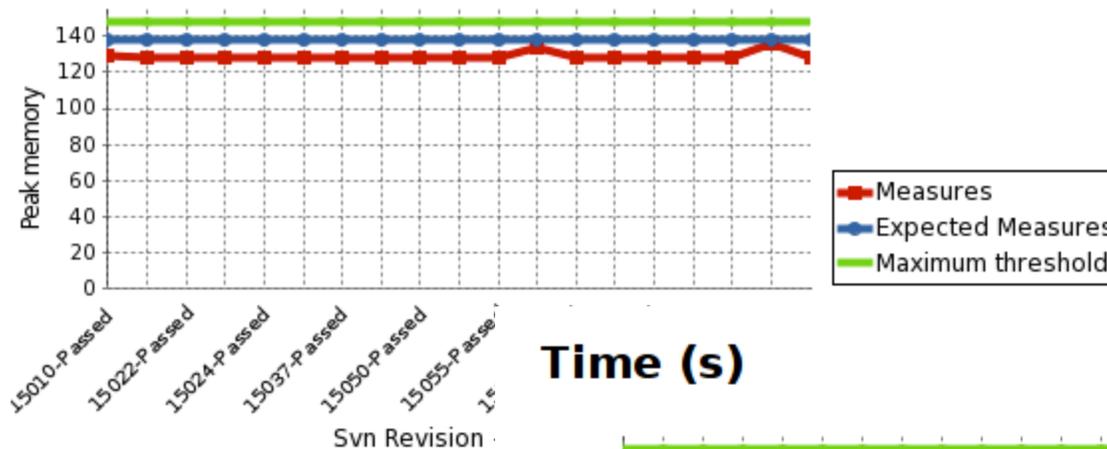
S	LC	Name ↓	LTR	FFR	LSR	LFR
		Build-Carter-NEMO5	15370	15370	15367	15370
		Test-2nm_si_wire_meta_device-Carter-Nemo5	n/a	13959	13948	13964
		Test-5x_111_InGaAs-Carter-Nemo5	n/a	n/a	15294	15157
		Test-BiTe_UTB_bandstructure-Carter-Nemo5	n/a	n/a	15262	13624
		Test-BiTe_UTB_Transmission-Carter-Nemo5	15366	n/a	15366	14914
		Test-block_lanczos-Carter-Nemo5	15312	n/a	15312	13606
		Test-brillouin_zone_viewer_bcc_cubic-Carter-Nemo5	15312	n/a	15312	n/a
		Test-brillouin_zone_viewer_bcc_primitive-Carter-Nemo5	15312	n/a	15312	n/a
		Test-brillouin_zone_viewer_fcc_cubic-Carter-Nemo5	15312	n/a	15312	n/a
		Test-brillouin_zone_viewer_fcc_primitive-Carter-Nemo5	15312	n/a	15312	n/a
		Test-brillouin_zone_viewer_graphene_primitive-Carter-Nemo5	15312	n/a	15312	n/a
		Test-brillouin_zone_viewer_hexagonal-Carter-Nemo5	15312	n/a	15312	n/a
		Test-brillouin_zone_viewer_rhombohedral-Carter-Nemo5	15312	n/a	15312	n/a
		Test-brillouin_zone_viewer_simplecubic-Carter-Nemo5	15312	n/a	15312	n/a
		Test-BSLAB_Bulk_Phonon_Unfolding-Carter-Nemo5	15312	n/a	15312	15294

»Keep track of code warnings, TODO items

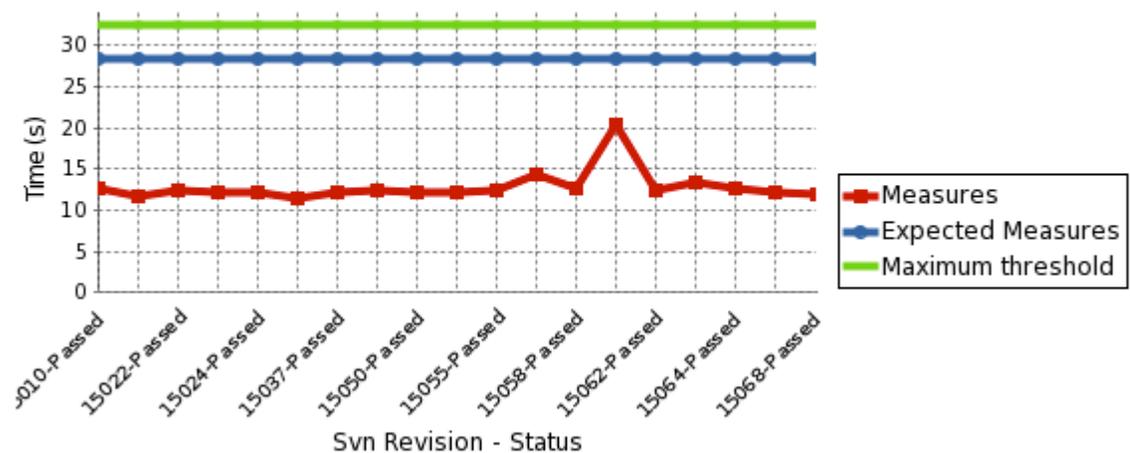


»Plot results: Plot time/memory consumption.

### Peak memory



### Time (s)



- » Provide the output of the execution
- » Show code changes that damaged a test

 **Build #392 (Apr 9, 2014 5:17:31 PM)**

**Svn revision number: 15062**

[Download all of NEMO5's output](#)

[Compare with previous revision](#)

[Compare last success with first failure.](#)



No changes.



Started by upstream project [Build-Carter-NEMO5](#) build number [1373](#) originally caused by:

- [Started by an SCM change](#)

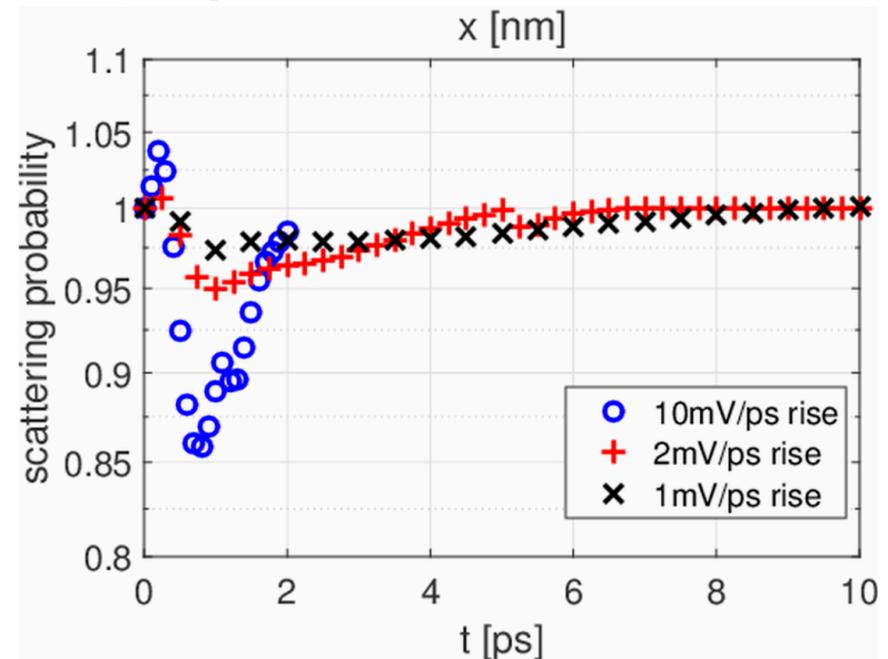
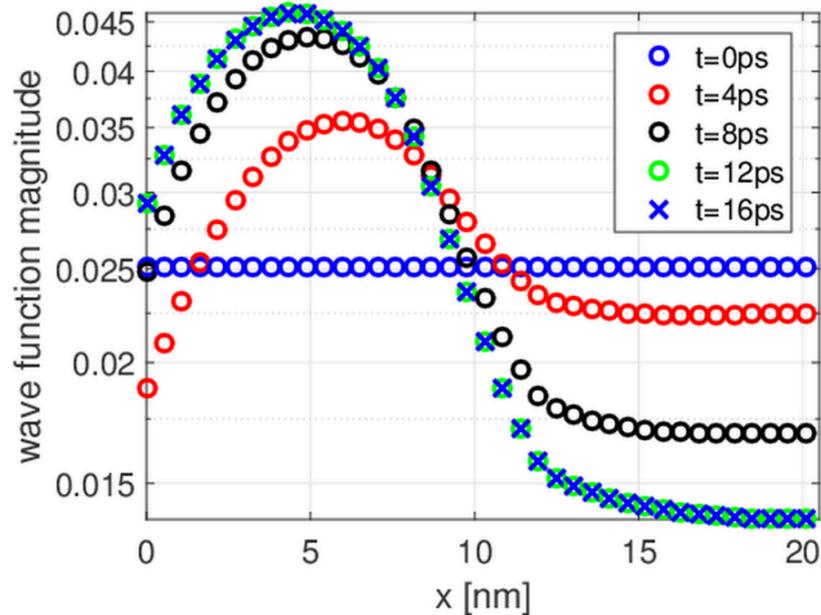
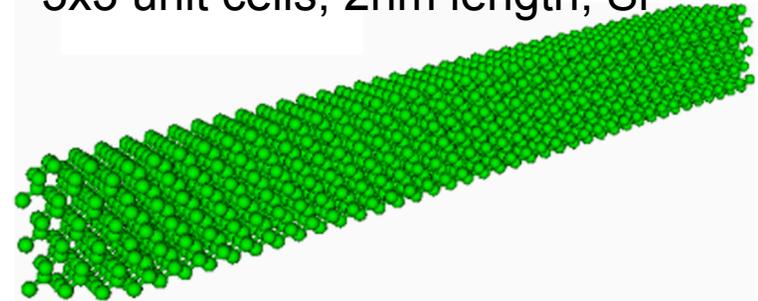
Reference File	Status
rgf_backward_module_eq2_GreenModule_eq2_result_Propagation_fulltransmission_ref.dat	Failed
rgf_total_density_ref.xyz	Failed

# Time Resolved Simulations

B. Novakovic and G. Klimeck

- Energy usage
- Time dependent Schrodinger
- Valid up to a few Ghz
- Working on GPU implementation

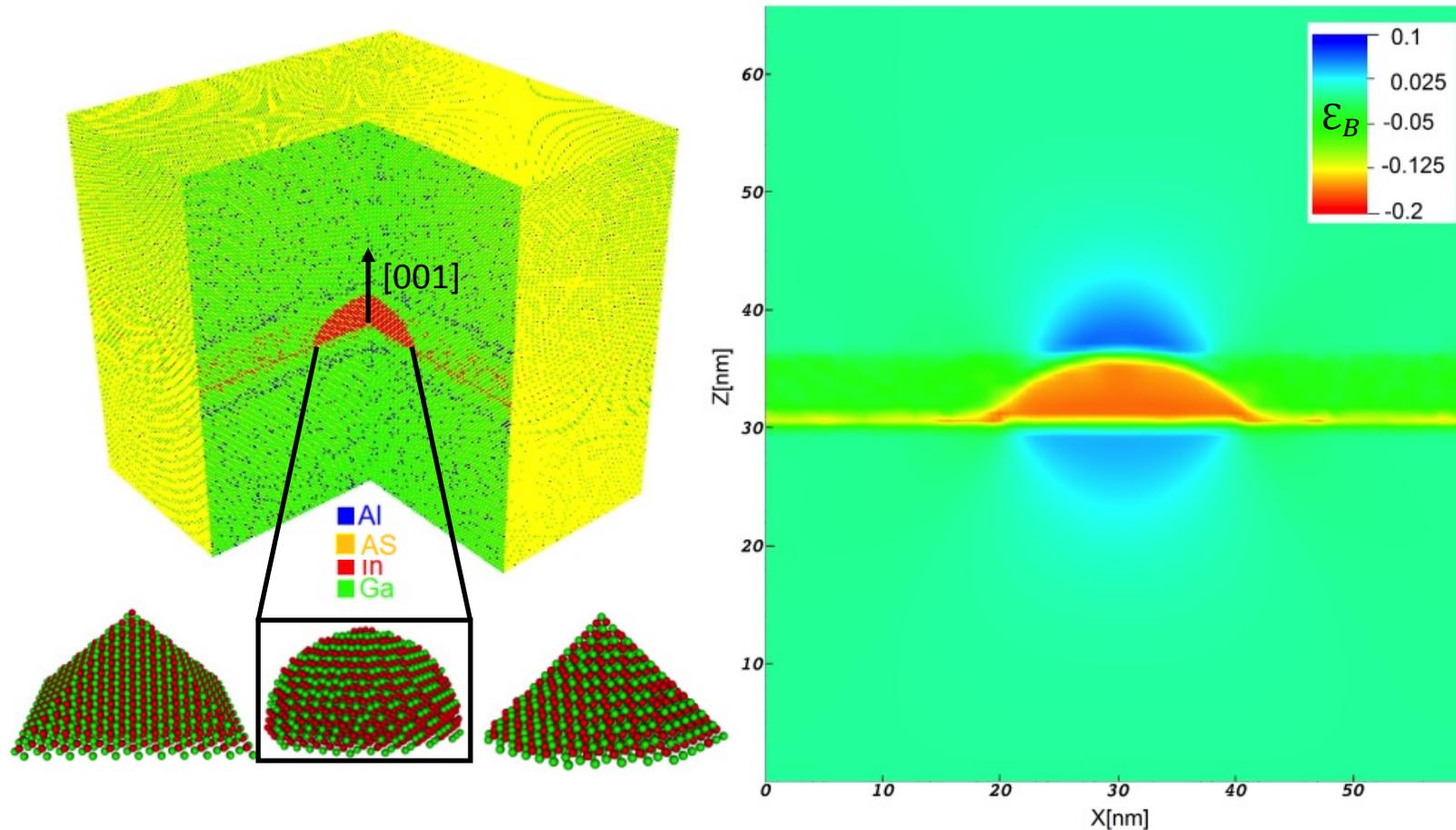
3x3 unit cells, 2nm length, Si



<http://ieeexplore.ieee.org/xpl/articleDetails.jsp?arnumber=7292245>

# Quantum Dot Compact Modeling

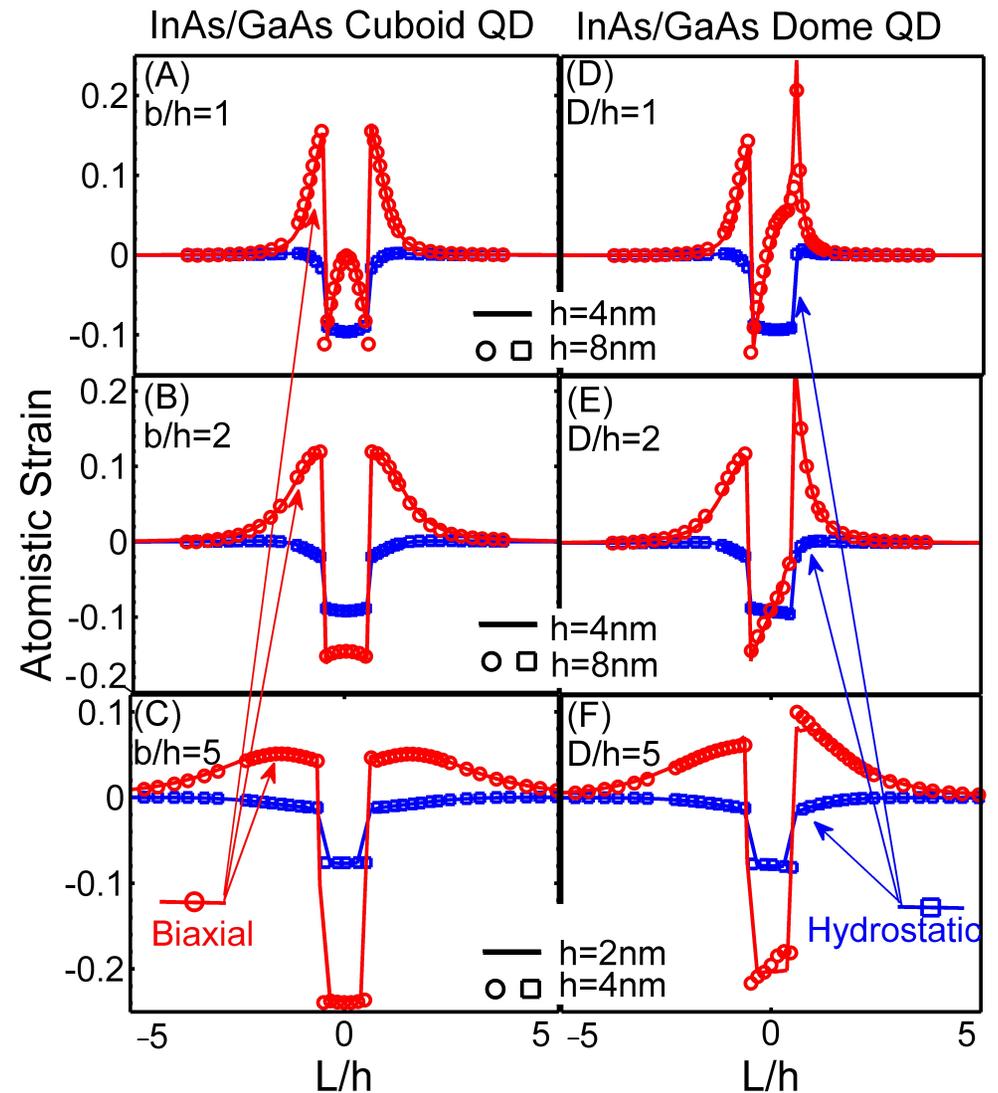
H. Ilatikhameneh, T. Ameen, G. Klimeck, and  
R. Rahman



Advanced QD simulations in NEMO5; Can simulate alloys (i.e. AlGaAs/InGaAs QD system) and different self-assembled QD shapes. Shown on the left atomistic structure of a 10 million atom system simulated using NEMO5. Shown on the right Biaxial strain distribution obtained by NEMO5 for a dome QD with 20X5nm.

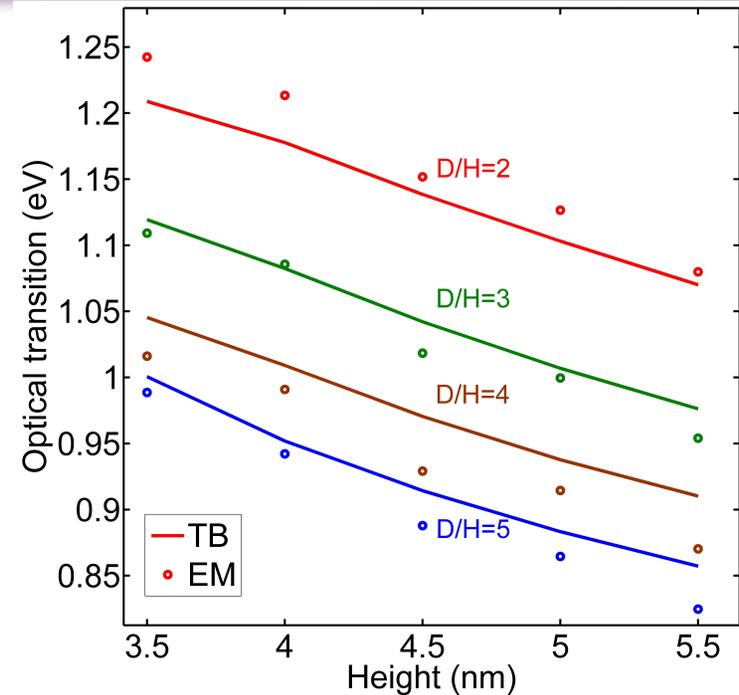
Solid lines and symbols correspond to strain distributions of QDs with different dimensions but same aspect ratios. Distributions overlay!

Atomistic strain distribution for a certain QD shape depends on aspect ratio not individual dimensions.



Universal strain + effective mass  
=
   
Very fast accurate model

- Error with atomistic (strain+sp3d5s\*\_SO) < 4%
- Computational cost is 20K less.



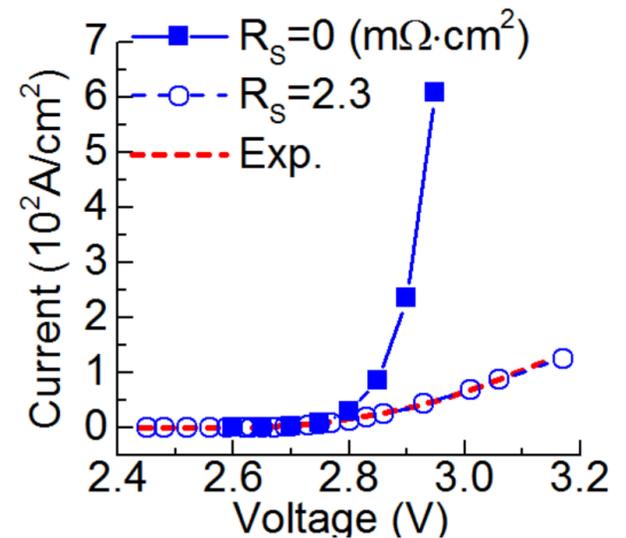
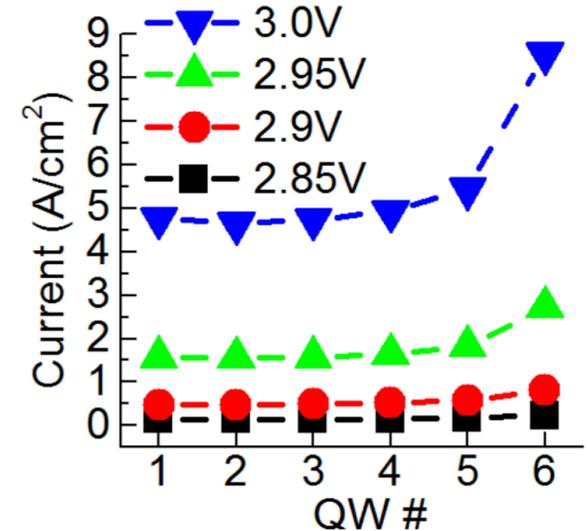
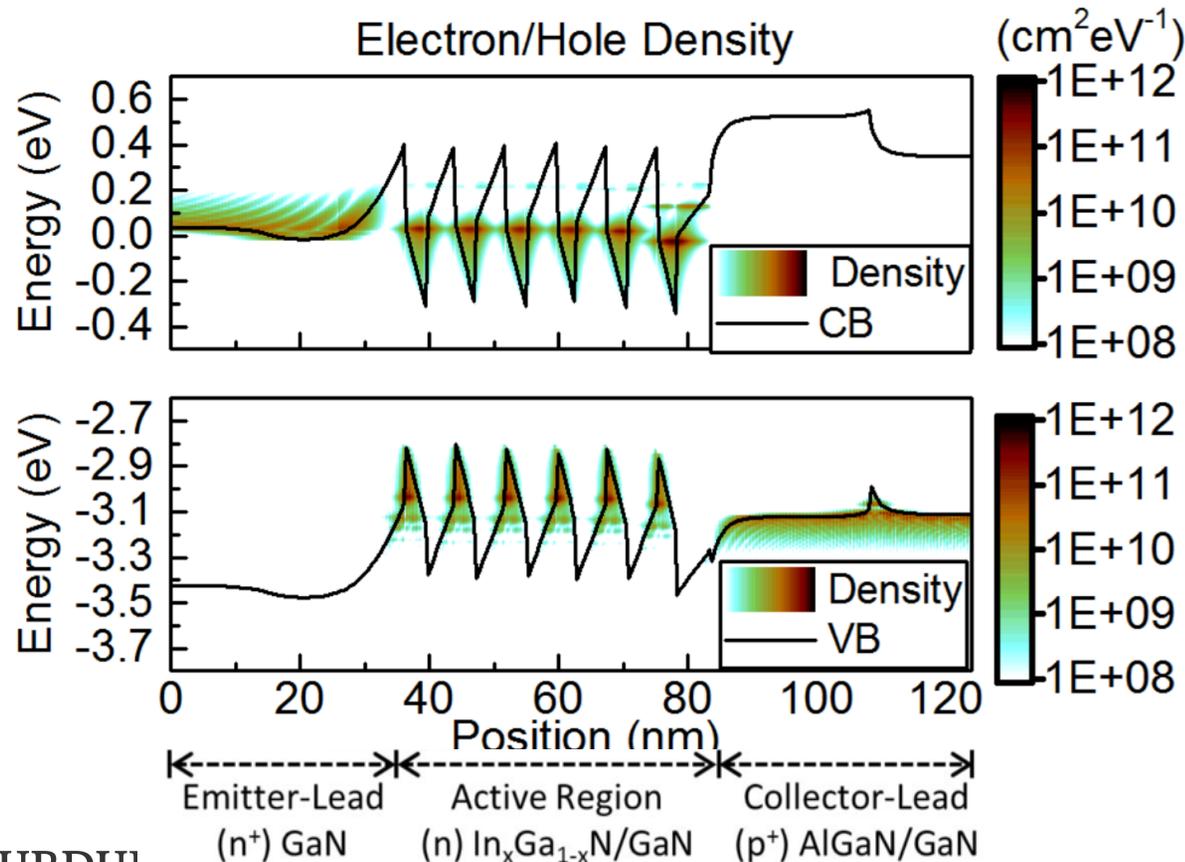
	EM no Strain	EM with Strain	TB Atomistic	Experimental*
Optical transition	0.7169 eV	0.9145	0.9377	0.976 - 0.93 eV
Error (VS 0.953 eV)	25%	4%	1.6%	
Processors	1	1	216	
Time/process (s)	80	81	7856	

\* J. Tatebayashi, M. Nishioka, and Y. Arakawa, "Over 1.5 m light emission from in as quantum dots embedded in ingaas strain-reducing layer grown by metalorganic chemical vapor deposition," Applied Physics Letters, vol. 78, no. 22, pp. 3469-3471, 2001

# Multi Quantum Well LEDs

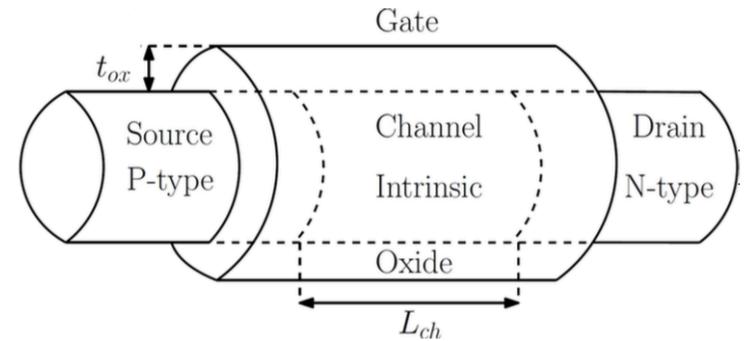
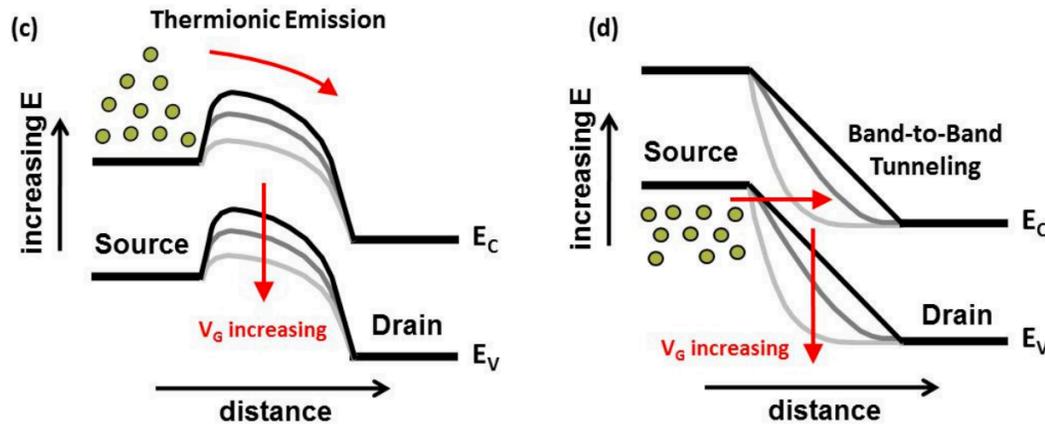
J. Geng, P. Sarangapani, E. Nelson, C.  
Wordelman, B. Browne, T. Kubis, and G.  
Klimeck

- Medium to high power blue light
- Multiphysics
  - » Barriers in equilibrium (red)
  - » Wells in nonequilibrium (green)
- Strong scattering

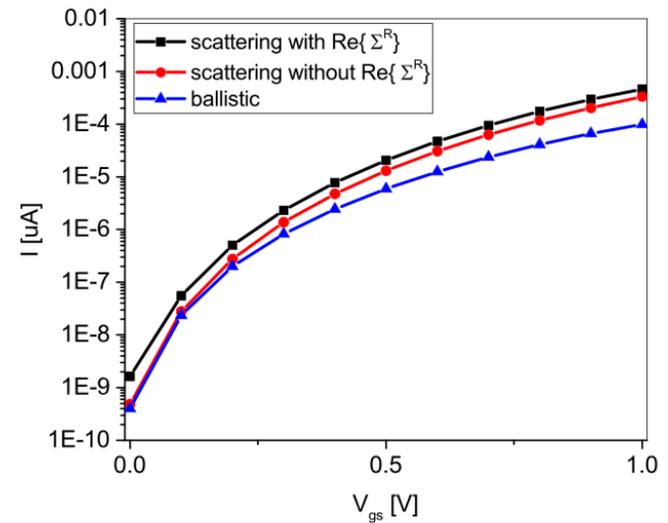
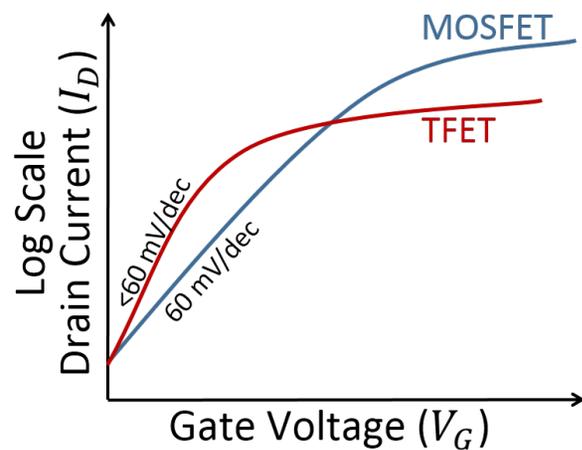


# Tunnel FETs

J. Charles, P. Sarangapani, R. Andrawis, D.  
Lemus, X. Guo, T. Kubis, G. Klimeck



<http://people.eecs.berkeley.edu/~tking/theses/shpkim.pdf>



J. Charles et al., Incoherent Transport in NEMO5: Realistic and Efficient Scattering on Phonons, *JCEL*, in press.

- PI: Gerhard Klimeck
- 3 Research Faculty: Tillmann Kubis, Michael Povolotskyi, Rajib Rahman
- Research Scientist: **Jim Fonseca**
- 2 Postdocs: **Bozidar Novakovic**, Jun Huang
- Students: **Tarek Ameen**, **James Charles**, Chin-Yi Chen, **Fan Chen**, Yuanchu Chen, Rifat Ferdous, Jun Zhe Geng, Xinchun Guo, Yuling Hsueh, **Hesameddin Ilatikhameneh**, Daniel Lemus, Pengyu Long, Daniel Mejia Padilla, Kai Miao, Samik Mukherjee, Harshad Sahasrabudhe, Prasad Sarangapani, Frederico Severgnini, **Archana Tankasala**, Gustavo Valencia, Daniel Valencia Hoyos, Kuang Chung Wang, Yu Wang, **Evan Wilson**
- SURF Students: Matt Bliss, Unmesha Kale, Jingbo Wu



- Ryan Mokos, Sharif Islam
- PRAC
- Intel, Samsung, Philips, TSMC