EDISON Project in Nanophysics/electronics

- Current status of contents and service -

Hoon Ryu, Ph.D.

National **I**nstitute of **S**upercomputing and **N**etworking,
Korea **I**nstitute of **S**cience and **T**echnology **I**nformation.

elec1020@gmail.com

국가슈퍼컴퓨팅연구소 National Institute of Supercomputing and Networking
한국과학기술정보연구원 Korea Institute of Science and Technology Information
KiSTi www.kisti.re.kr

Technology-Computer-Aided-Design

TCAD?

- Group of tools
  - Predict “real world” by computing, critical to save time/money/manpower etc.
- Large-scale problems in various fields of science
  - With aids of HPC. “Computational Science” now “an area of research”

If you are a developer and a scientist - OK. I know you’re great, BUT

- Should a person know everything to do modeling/simulation-based research?

```
//+-------------------------------------------------------------------------
//
//  Copyright ( C ) Microsoft, 1994 - 2002.
//
//  File:       regexpr2.cpp
//
//  Contents:   implementation for rpattern methods, definitions for all the
//              subexpression types used to perform the matching, the
//              charset class definition .

#include <stdio.h>
#include <float.h>

int main()
{
    // Open the data file
    FILE* pFile = fopen( "data.dat", "rb" );
    if( pFile == NULL )
    {
        assert( false );
        return 1;
    }

    /* Read data from file */
    if( fread(szBuf, 100, 1, pFile) != 1 )
    {
        fclose( pFile );
        return 1;
    }

    /* Close file */
    fclose( pFile );
    return 0;
}
```

Technology-Computer-Aided-Design

TCAD?

- Group of tools
  - Predict “real world” by computing, critical to save time/money/manpower etc.
- Large-scale problems in various fields of science
  - With aids of HPC. “Computational Science” now “an area of research”

If you are a developer and a scientist - OK. I know you’re great, BUT

- Should a person know everything to do modeling/simulation-based research?

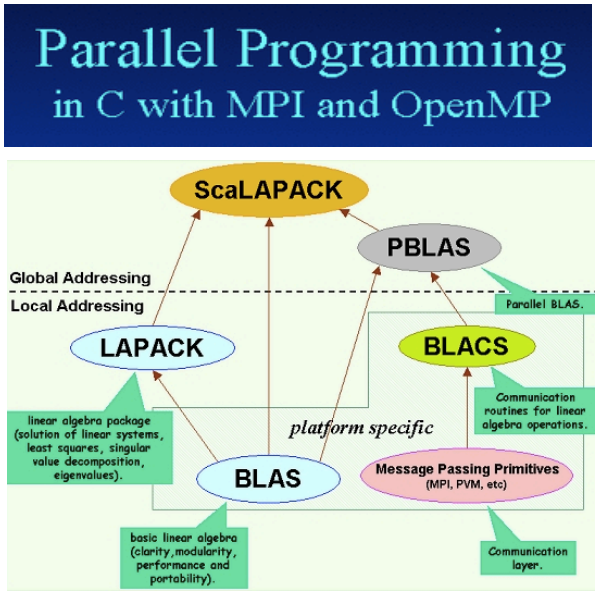
```
//+-------------------------------------------------------------------------
//
//  Copyright ( C ) Microsoft, 1994 - 2002.
//
//  File:       regexpr2.cpp
//
//  Contents:   implementation for rpattern methods, definitions for all the
//              subexpression types used to perform the matching, the
//              charset class definition .

#include <stdio.h>
#include <float.h>

int main()
{
    // Open the data file
    FILE* pFile = fopen( "data.dat", "rb" );
    if( pFile == NULL )
    {
        assert( false );
        return 1;
    }

    /* Read data from file */
    if( fread(szBuf, 100, 1, pFile) != 1 )
    {
        fclose( pFile );
        return 1;
    }

    /* Close file */
    fclose( pFile );
    return 0;
}
```



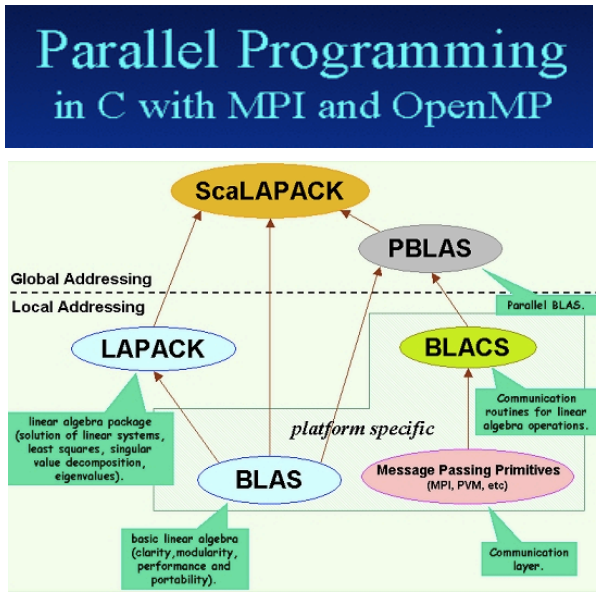
Technology-Computer-Aided-Design

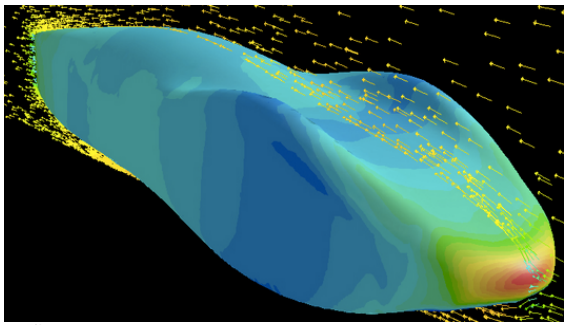
TCAD?

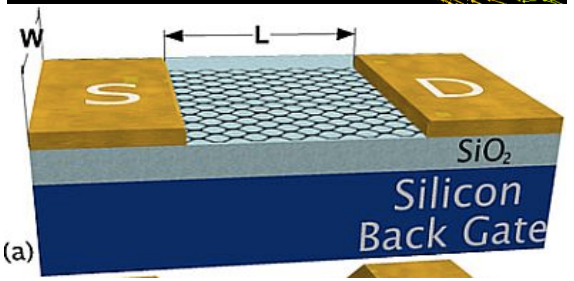
- Group of tools
  - Predict “real world” by computing, critical to save time/money/manpower etc.
- Large-scale problems in various fields of science
  - With aids of HPC. “Computational Science” now “an area of research”

If you are a developer and a scientist - OK. I know you’re great, BUT

- Should a person know everything to do modeling/simulation-based research?







Technology-Computer-Aided-Design

TCAD?

- Group of tools
  - Predict “real world” by computing, critical to save time/money/manpower etc.
- Large-scale problems in various fields of science
  - With aids of HPC. “Computational Science” now “an area of research”

If you are a developer and a scientist - OK. I know you’re great, BUT

- Should a person know everything to do modeling/simulation-based research?

Why don’t we make people a bit happier?

- Easy Access to Simulations
- Efficiency of Learning – Let people experience interactively!
- Strong motivation to “Take the pain” for learning all the technical details

Science Gateway: The EDISON Project

"Easy Simulation" is the keyword for increasing efficiency in EDU/Research!!

Initiation of the EDISON Project
(EDucation-research **I**ntegration through **S**imulation **O**n the **N**et**)**

- Started in 2011 July under governmental support
- Initiative domain: Computational Fluids Dynamics (CFD)

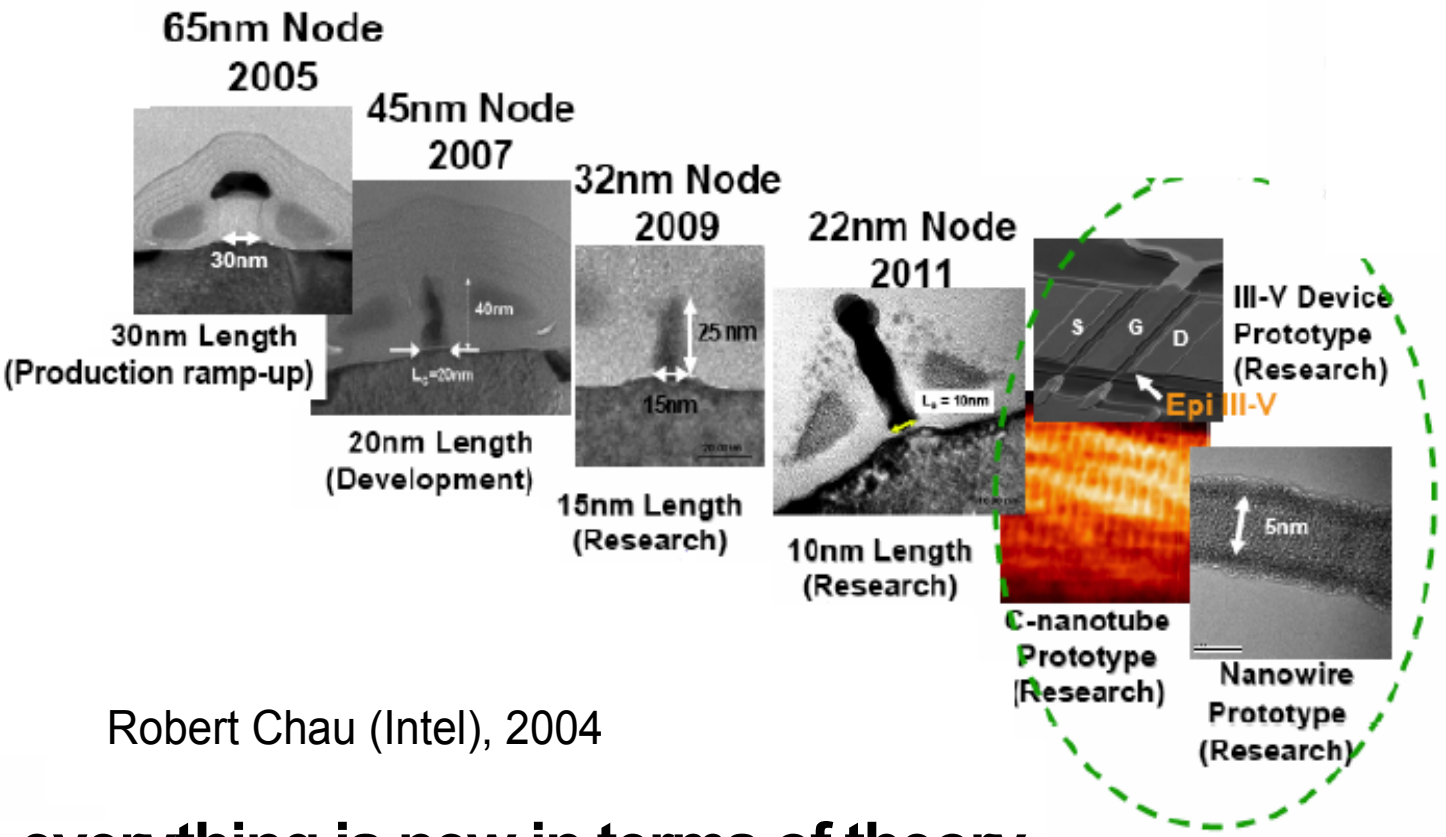
Moving to the 2nd step: Towards "new" scientific domains.

- 2012 July, we have started to support two new domains
  - Computational Chemistry and **Computational Nanophysics**

Objective of remaining talk – Focusing on the nanophysics

- A brief Introduction of EDISON_Nanophysics
  - Motivation and Objectives
  - Current Status of Services
  - Summary of available TCAD software

Nano + Physics + Electronics?



Robert Chau (Intel), 2004

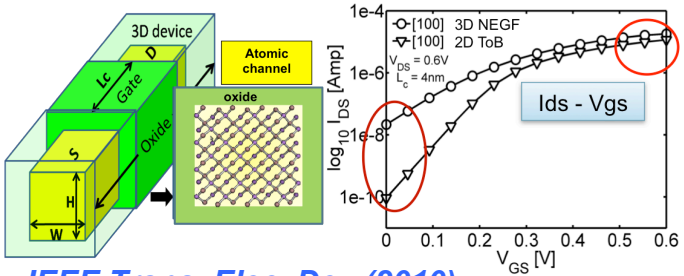
Small – everything is new in terms of theory

- **Nanoscale Materials**
- **Nanoscale Devices**
- **Fundamentals of Theory**
  * Solid-state, Quantum Physics, Semiconductors Crystalline ETC

Nano+Physics+Electronics - Research

Si Devices: Transport in FETs

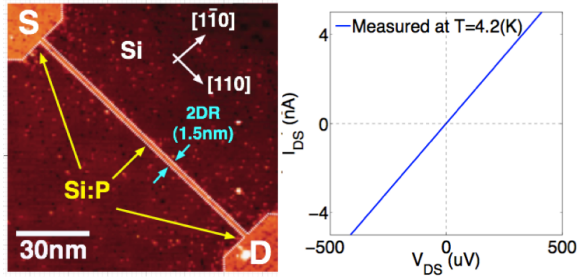
- Performance-degradation in nanoscale FETs.
- Needs for 3-D NEGF simulation.



IEEE Trans. Elec. Dev (2010)
IEEE Trans. Nanotech. (2012)
IEEE Elec. Dev. Lett. (Under Review)

New Material: Si:P Devices

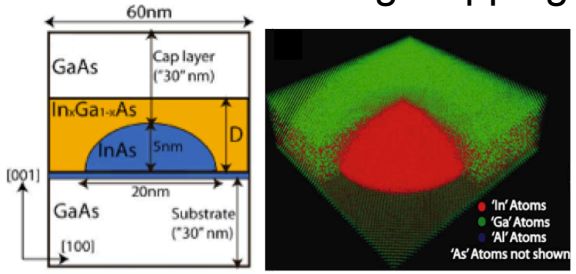
- Metallic Property of P δ-doped Nanowires.
- Sensitivity to channel dopant distributions.



Phys. Rev. B (2011), Science (2012),
Nat. Nanotech. (2012, 2014) Nanoscale (2013)

III-V Devices: Optoelectronics - Photodetectors

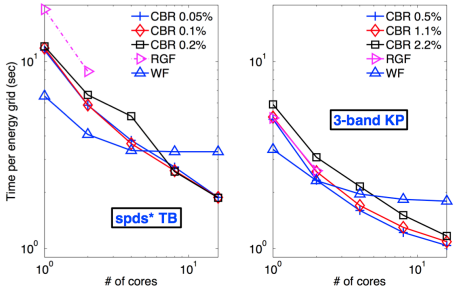
- Engineering of III-V Quantum Dot Optical Gaps with Strain-reducing Capping Layers.



IEEE Trans. Nanotech. (2009)
Math. Comp. Model. (2013)

Algorithm: Parallel Solver

- Quantum Transport: Contact Block Reduction vs. Recursive Green's Function.



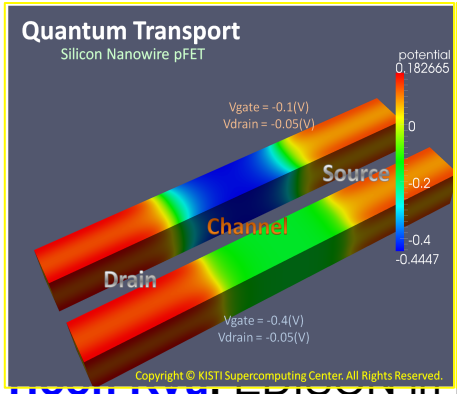
J. Appl. Phys. (2012)
Math. Comp. Model. (Under Review)

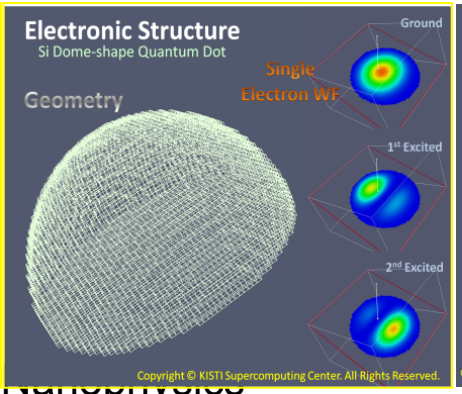
- Electronic Structure: Deflation LANCZOS for calculation of spin-degenerate states.

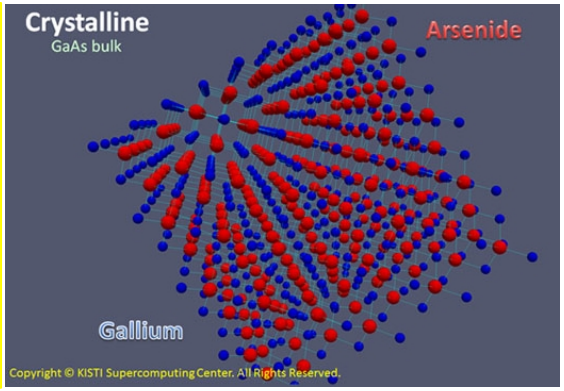
Nano+Physics+Electronics - Education

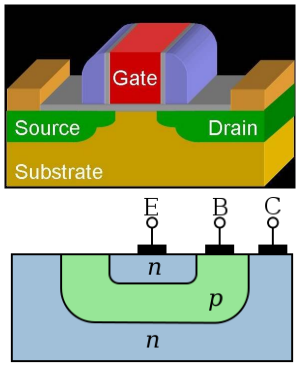
EDISON_Nanophysics

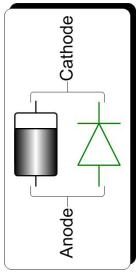
Physics Fundamentals	Advanced Materials	Advanced Devices
Electronic/Electrical Engineering	Semiconductor Fundamentals	Device Electronics	CMOS and Non-CMOS Devices
Materials Science and Engineering	Semiconductor Crystalline	Structure Relaxations	Nanocrystals, Advanced Materials
Physics	General Physics Fundamentals	Solid-state Physics	Semiclassical and Quantum Physics











EDISON_Nanophysics: Available TCAD SWs

- **As of today, a total of 45 TCAD Tools are available**
- **Tools are categorized by a set of problem filters**
  - **Five big categories:** Geometry/Material/Device/Problem/Structure Representation

Geometry	Material	Device Type	Problem Type	Structure Rep.
1D	Si	Bulk Devices	Drift-Diffusion	Ab-initio
2D	Si/Ge	Nanowires	Quantum Transport	Effective Mass
3D	III-V	Quantum-wells	Electronic Structure	*k.p*
	C	Quantom-dots	Boltzmann Transport	Tight-binding
	Others	Others	Optical Properties	Semi-classical
			Crystal Structures	Others
			Physics Education	
			Others	

(a) Geometry Description	Number of Tools
1D	24
2D	9
3D	12

(c) Device Type	Number of Tools
Bulk Devices	10
Nanowire	9
Quantum-well	5
Quantum-dot	1
Others	25

(b) Device Material	Number of Tools
Si	14
SiGe	0
III-V	10
Carbon	4
Others	34

(d) Problem Type	Number of Tools
Drift-Diffusion	4
Quantum Transport	4
Electronic Structure	10
Optical Properties	1
Crystal Structure	4
Physics Education	5
Others	21

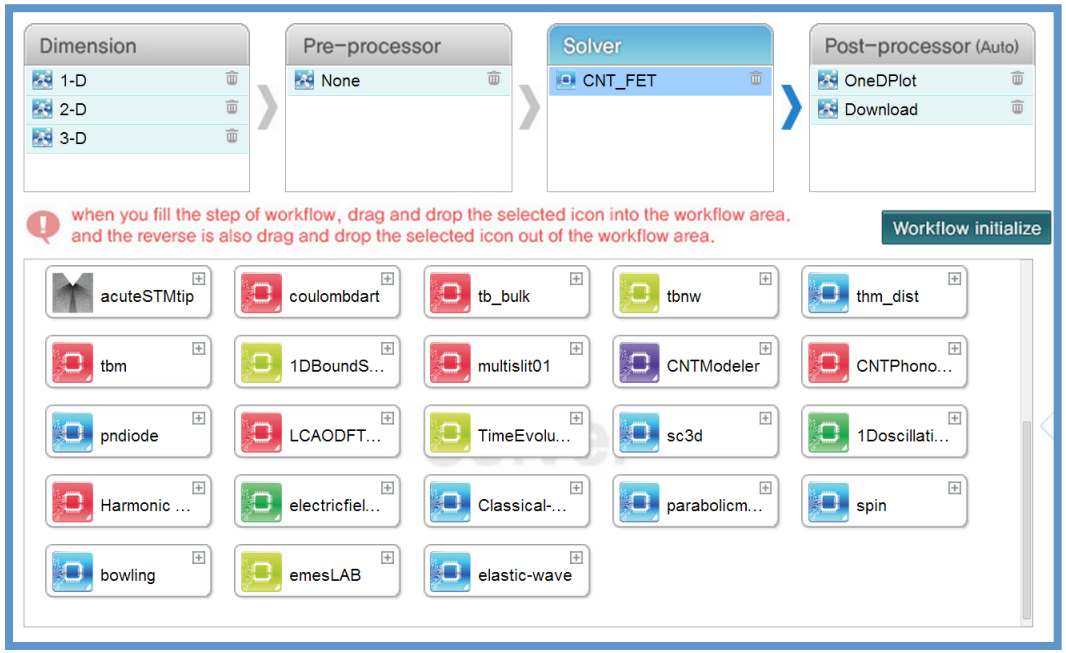
(e) Structure Representation	Number of Tools
Ab-initio	3
Effective Mass	6
k.p	1
Tight-binding	4
Semi-classical	5
Others	26

EDISON Nanophysics: Web-based Service

- **Remarks**

- **Native-web interface**: Do not invoke GUIs through X-term. Light - a clear strength in resource overhead for supporting multiple job requests.
- **Job monitoring**: Submitted jobs runs in the backend HPC. Provides a control interface of submitted jobs – In the case of X-term GUIs?
- **Easy Postprocessing**: Simple, intuitive ways of visualizations and data-downloading

- **Four steps to support "easy simulations"**



Users can select preferred tools either by:

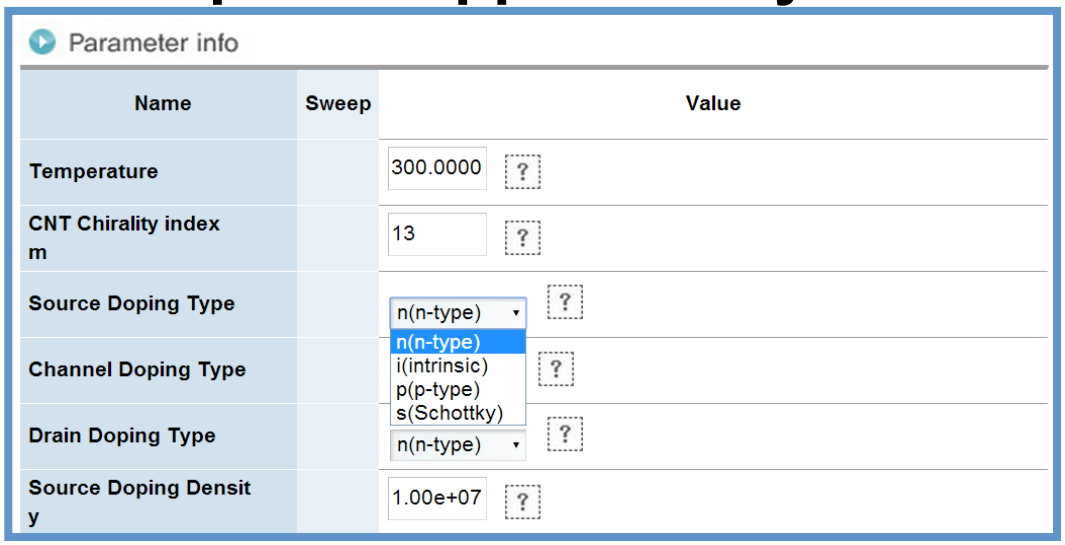
- combine workflow components
- combine problem filtering conds. (Will show later again)

EDISON Nanophysics: Web-based Service

- **Remarks**

- **Native-web interface**: Do not invoke GUIs through X-term. Light - a clear strength in resource overhead for supporting multiple job requests.
- **Job monitoring**: Submitted jobs runs in the backend HPC. Provides a control interface of submitted jobs – In the case of X-term GUIs?
- **Easy Postprocessing**: Simple, intuitive ways of visualizations and data-downloading

- **Four steps to support "easy simulations"**



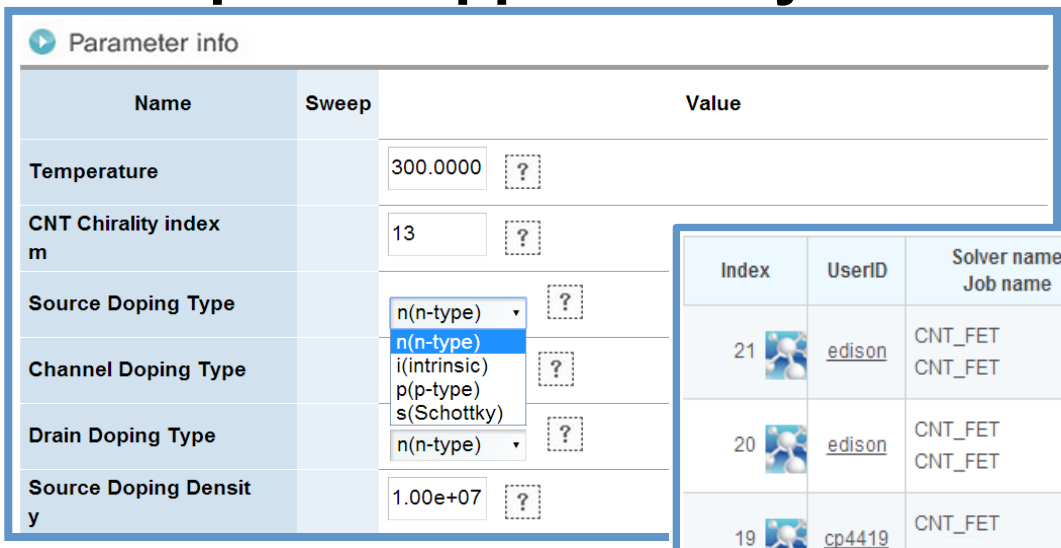
Control simulation parameters

EDISON Nanophysics: Web-based Service

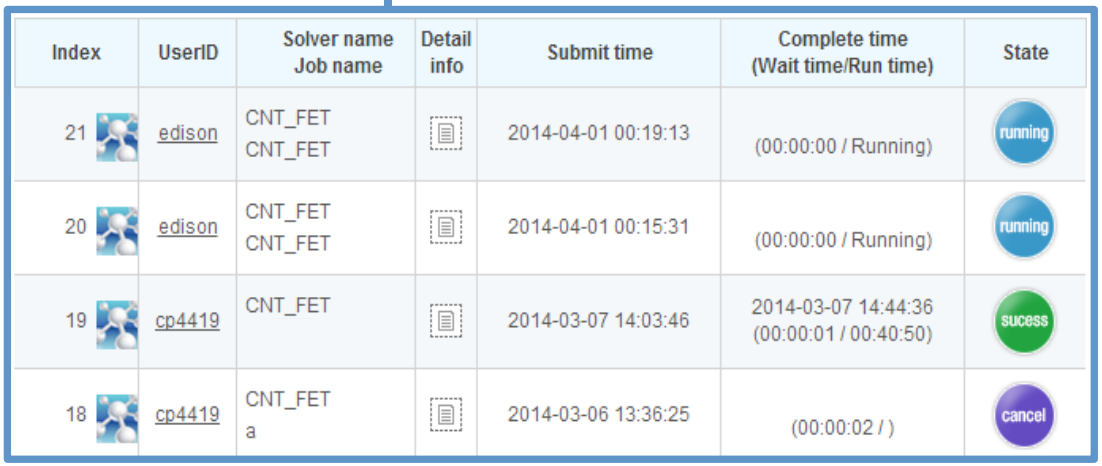
- **Remarks**

  - **Native-web interface**: Do not invoke GUIs through X-term. Light - a clear strength in resource overhead for supporting multiple job requests.
  - **Job monitoring**: Submitted jobs runs in the backend HPC. Provides a control interface of submitted jobs – In the case of X-term GUIs?
  - **Easy Postprocessing**: Simple, intuitive ways of visualizations and data-downloading

- **Four steps to support "easy simulations"**



Control simulation parameters



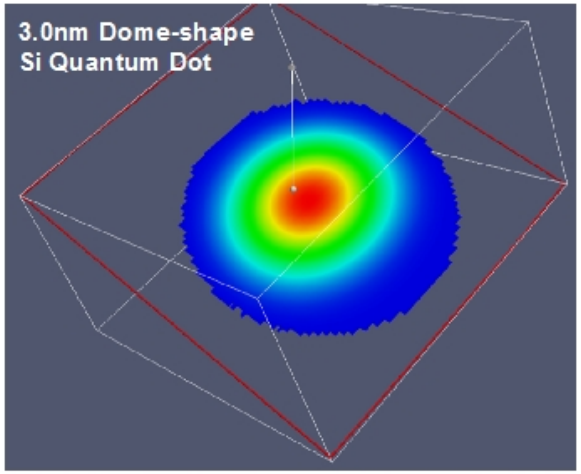
Check the status of submitted simulation jobs

EDISON Nanophysics: Web-based Service

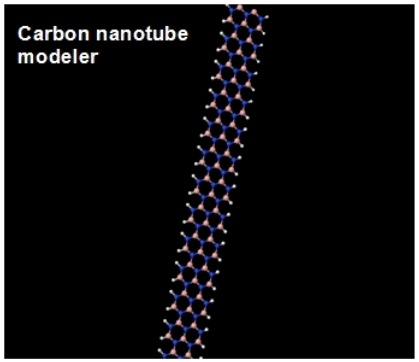
- **Remarks**
  - **Native-web interface**: Do not invoke GUIs through X-term. Light - a clear strength in resource overhead for supporting multiple job requests.
  - **Job monitoring**: Submitted jobs runs in the backend HPC. Provides a control interface of submitted jobs – In the case of X-term GUIs?
  - **Easy Postprocessing**: Simple, intuitive ways of visualizations and data-downloading

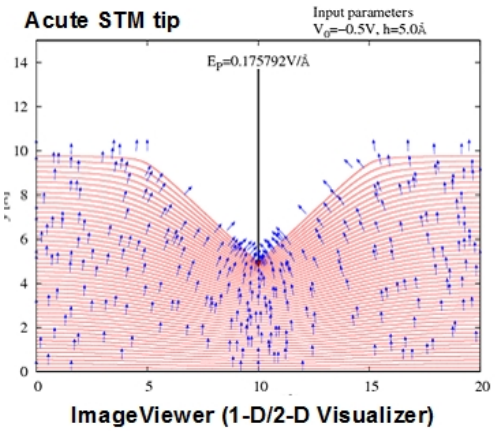
- **Four steps to support "easy simulations"**

OneDplot (1-D Visualizer)



Paraview (2-D/3-D Visualizer)





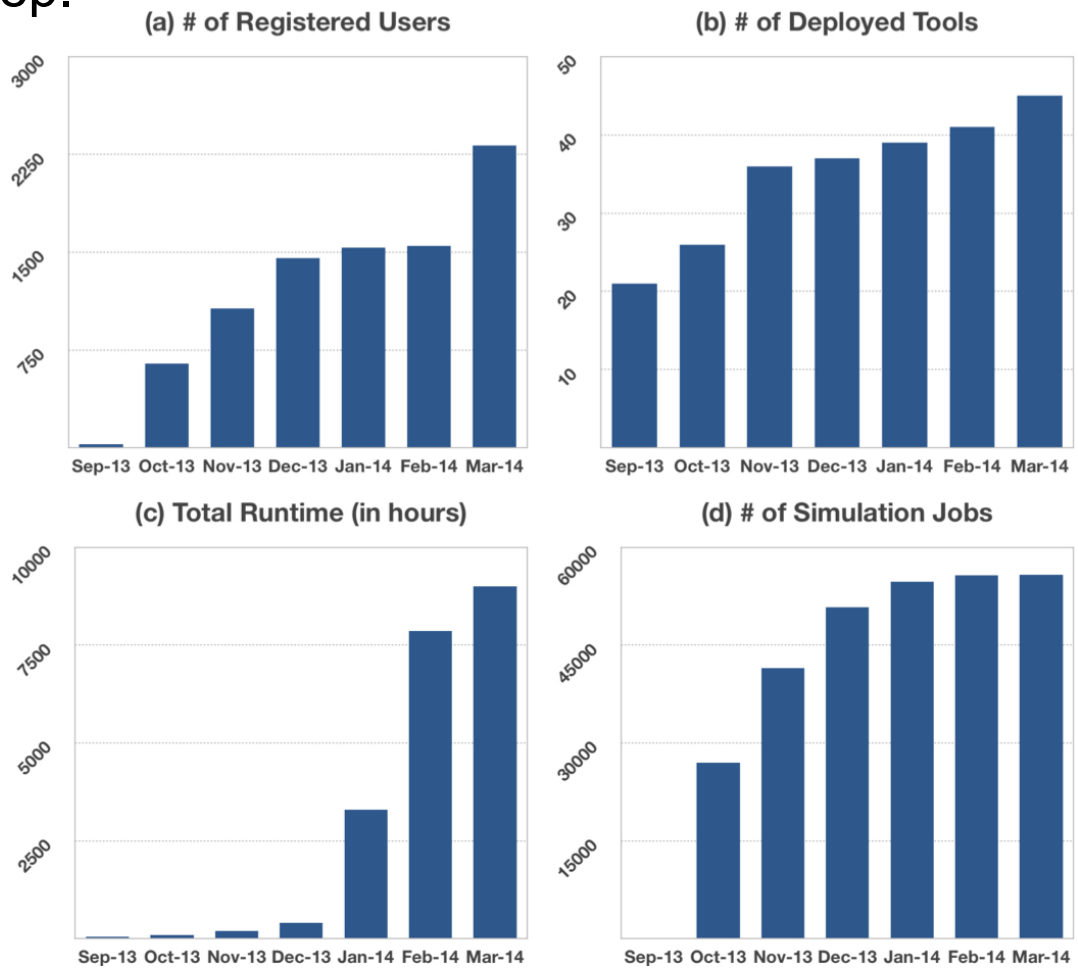
ImageViewer (1-D/2-D Visualizer)

- 4 Vis. Interf.: oneDplot, Paraview (VTK), Jmol, Imageviewer
- Directly downloadable for local processing

Current Status of Service Utilizations

- **Service Statistics**
  - Full service opened in 2013-Sep.
  - 2300 domestic users.
  - 45 TCAD Tools
  - 50K jobs with wall-time of ~8K hours

- **Remarks**
  - 60 classes in 30 domestic universities.
  - "Open universities" have joined our customers
    **** Korea National Open Univ.**
    - Biggest and Oldest National Universities.
  - We want to hear from you now!



EDISON_Nanophysics GLOBAL

- **EDISON_Nanophysics for global users (~ 2014.Mar)**
  - 8 most popular tools are currently available. (Tool migration is ongoing)
  - http://nano.edison-project.org - Migration will be completed soon.

Tool Description
1D Harmonic Oscillator Problem Simulation LAB
Particle-in-a-box Problem Simulation LAB
P/N Junction Diode Simulation LAB
Nano-MOS Device Simulation LAB
Carbon NanoTube FET Simulation LAB
Nanowire FET Simulation LAB
Electric-field and Potential-energy Simulation LAB
Parabolic-motion Problem Simulation LAB

Physics Fundamentals | Semiconductor Fundamentals | Advanced Nanoscale Devices

- User-guides to support self-study
- Further Details: Demo Tomorrow!

Conclusions

- **A brief Introduction of EDISON_Nanophysics is given**
  - Motivation and Objectives
  - Current Status of Services
  - Summary of available TCAD software
- **Please consider EDISON for teaching and learning nanoscience in your school/institutes**
  - http://nano.edison-project.org
  - Will give you further details about service tomorrow
- **Inquiries/Questions**
  - Dr. Ruth Lee (jsruthlee@kisti.re.kr) or Me (elec1020@gmail.com)
  - Any fruitful comments would be appreciated
- **Do we have more time?**
  - Yes! then next.
  - Thank you otherwise. ☺

P/N Junction Diode Simulation LAB

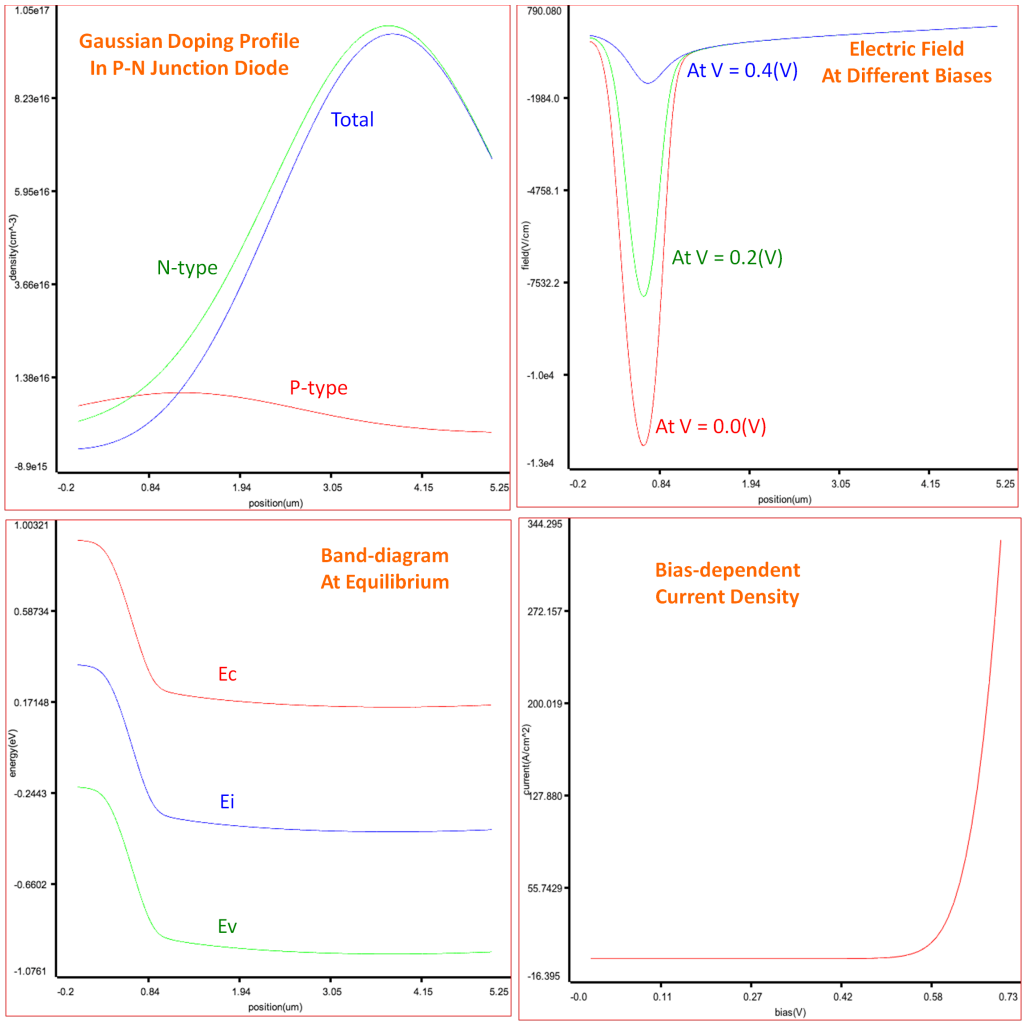
Objective:
- Diode: 2-terminal devices
- Electronic performance of P/N junction diode – Design guide-line.

Platform of Development:
- C++, ARPACK - Serial runs only

Features:
- Calculate I-V characteristic of 2-terminal diode devices
- Drift-diffusion equation
- Support various doping profiles with which the I-V characteristic is hard to be computed with hands

Target of classes:
- Fundamentals of semiconductors
- Electronic Circuits

P/N Junction Diode: Gaussian doping profile



Carbon NanoTube Simulation LAB

Objective:

- Simulate the electronic performance of CNT using a full quantum mechanical approach

Platform of Development:

- C++, PETSc – Support parallel runs

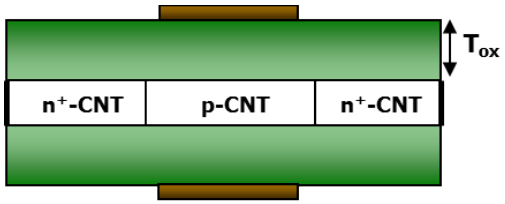
Features:

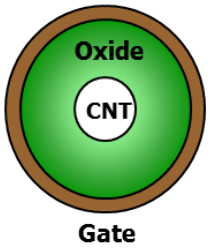
- I-V calculations using Non-Equilibrium Green's Function (NEGF)
- Ballistic Transport

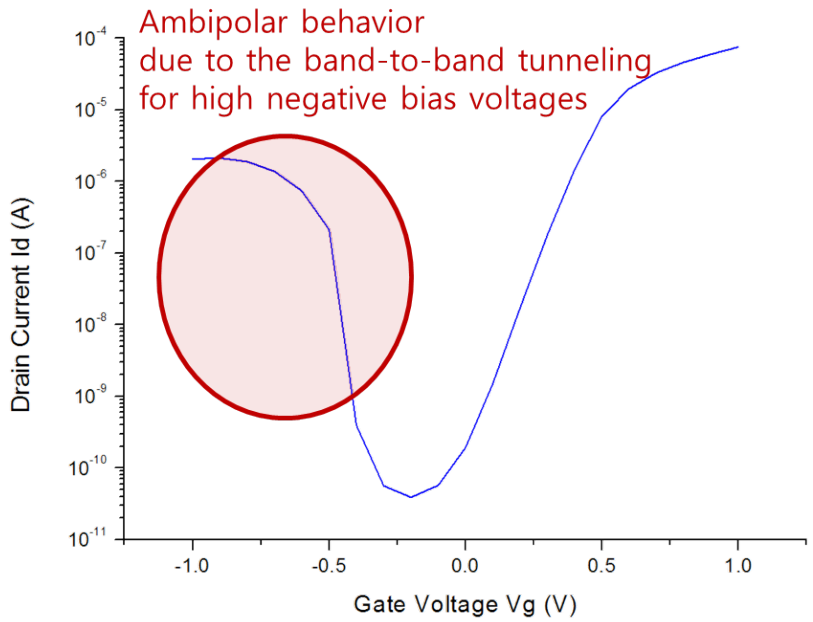
Target of classes:

- Advanced nanoscale devices
- Research purpose

R=1nm, (13, 0) zig-zag pattern CNT







Electric-field and Potential-energy Sim. LAB

Objective:

- Simulate the field and potential profiles for arbitrarily placed point charges

Platform of Development:

- C++ and FDM/Aztec Linear Solver

Features:

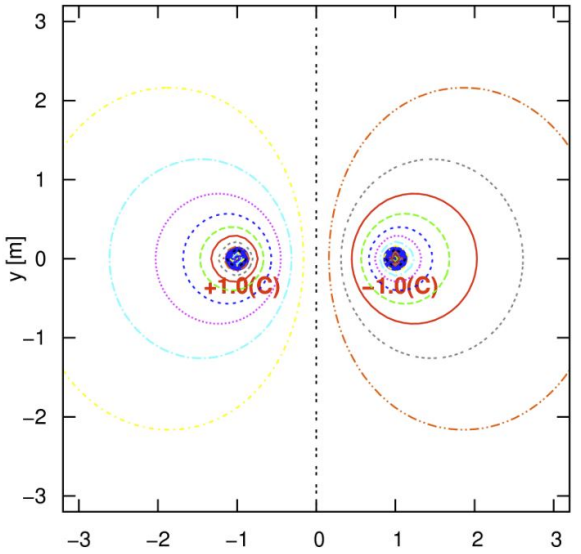
- Solve 2D Poisson Equations

Target of classes:

- Fundamentals of Physics
- Fundamentals of Electromagnetic

Two point charges: +1/-1 (C)

Equi-potential Contours



Electric Fields