

# NNCI Computation

Azad Naeemi

Georgia Institute of Technology

azad@gatech.edu



National Nanotechnology  
Coordinated Infrastructure



# Modeling and Simulation

- Modeling and simulation can enhance nanoscale fabrication and characterization:
  - guide experimental research
  - drastically reduce the required number of trial and error iterations
  - enable more in depth interpretation of the characterization results
  - help quantify the true potential value of the fabricated devices

# Current Status

- Abundance of resources and expertise at various sites even though few sites proposed any activities.
- Diverse funding sources for development and maintenance of these resources (inadequate in many cases).
- Ad hoc access and documentation.
- Many gaps and deficiencies.
- Duplicate efforts happen.

# NNCI Computation

## Objectives:

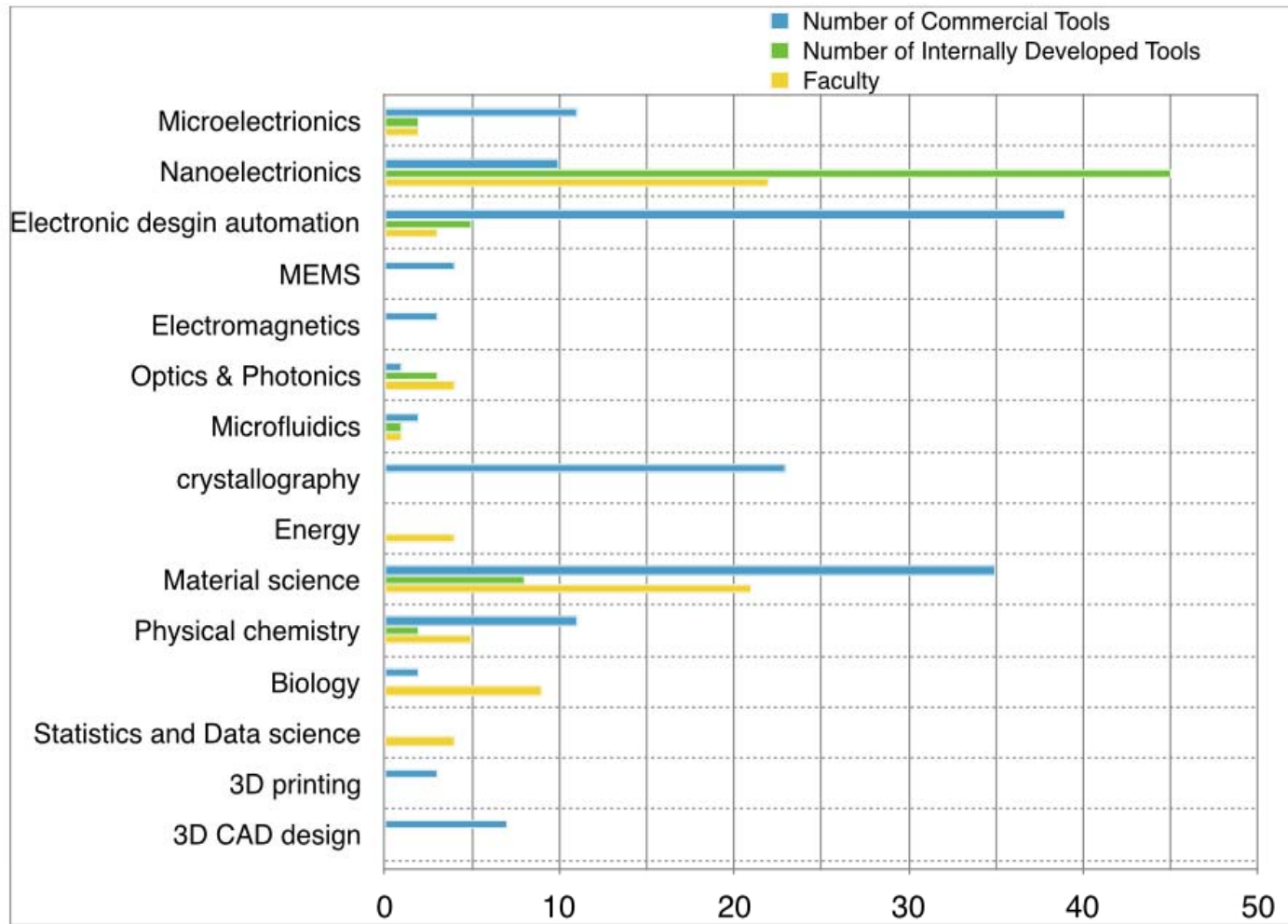
- To facilitate access to the modeling and simulation capabilities and expertise within NNCI sites.
- To identify the strategic areas for growth in modeling and simulation
- To promote and facilitate the development of the new capabilities.

An inventory of available modeling and simulation resources and expertise is being compiled. The directory is hosted by nanoHub.org.

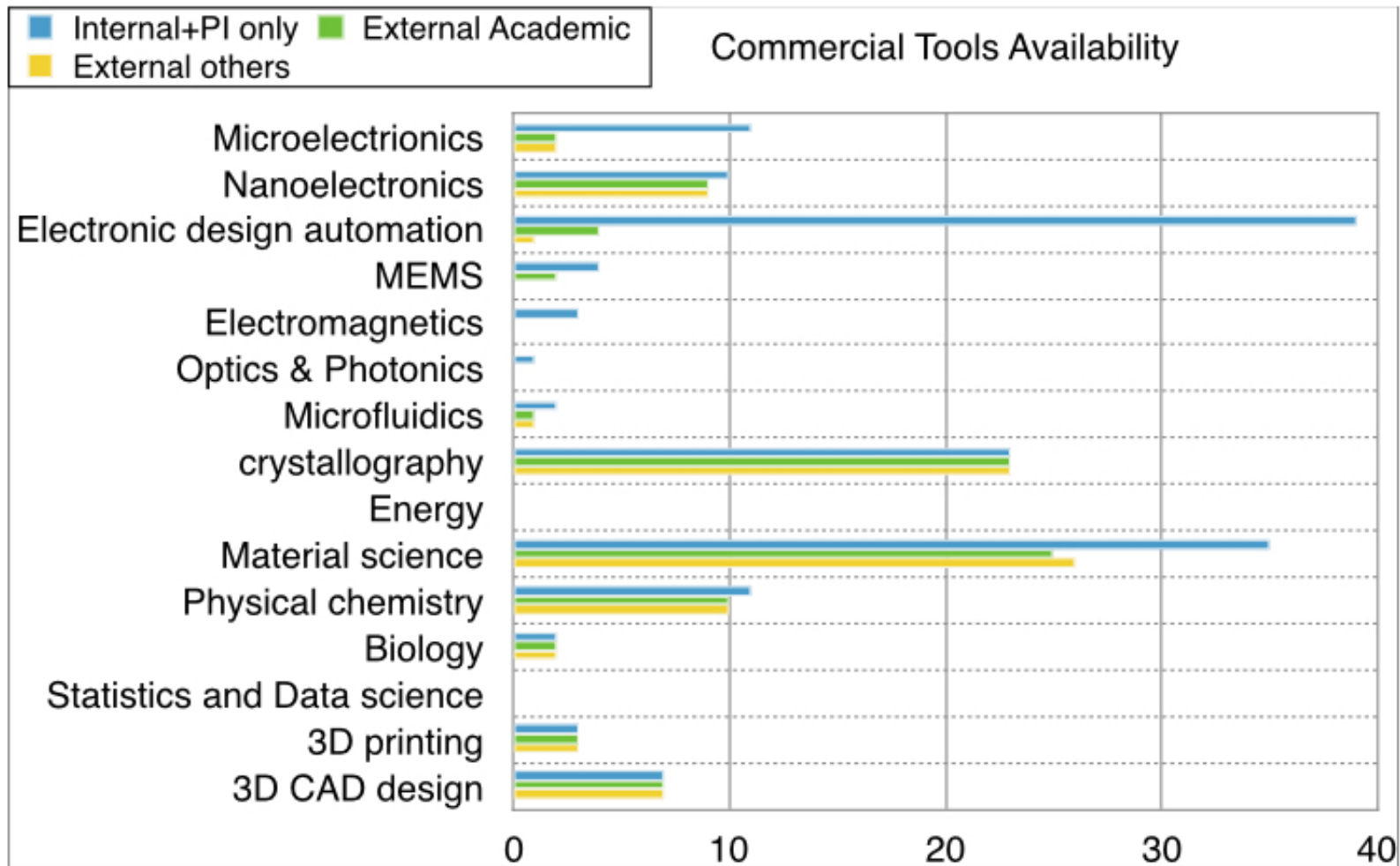
So far, 10 sites have reported collectively more than 65 commercial simulation tools and 40 internally developed simulation tools available for internal and/or external users (with and without fee).

8 supercomputers or major computing clusters are available in various sites.

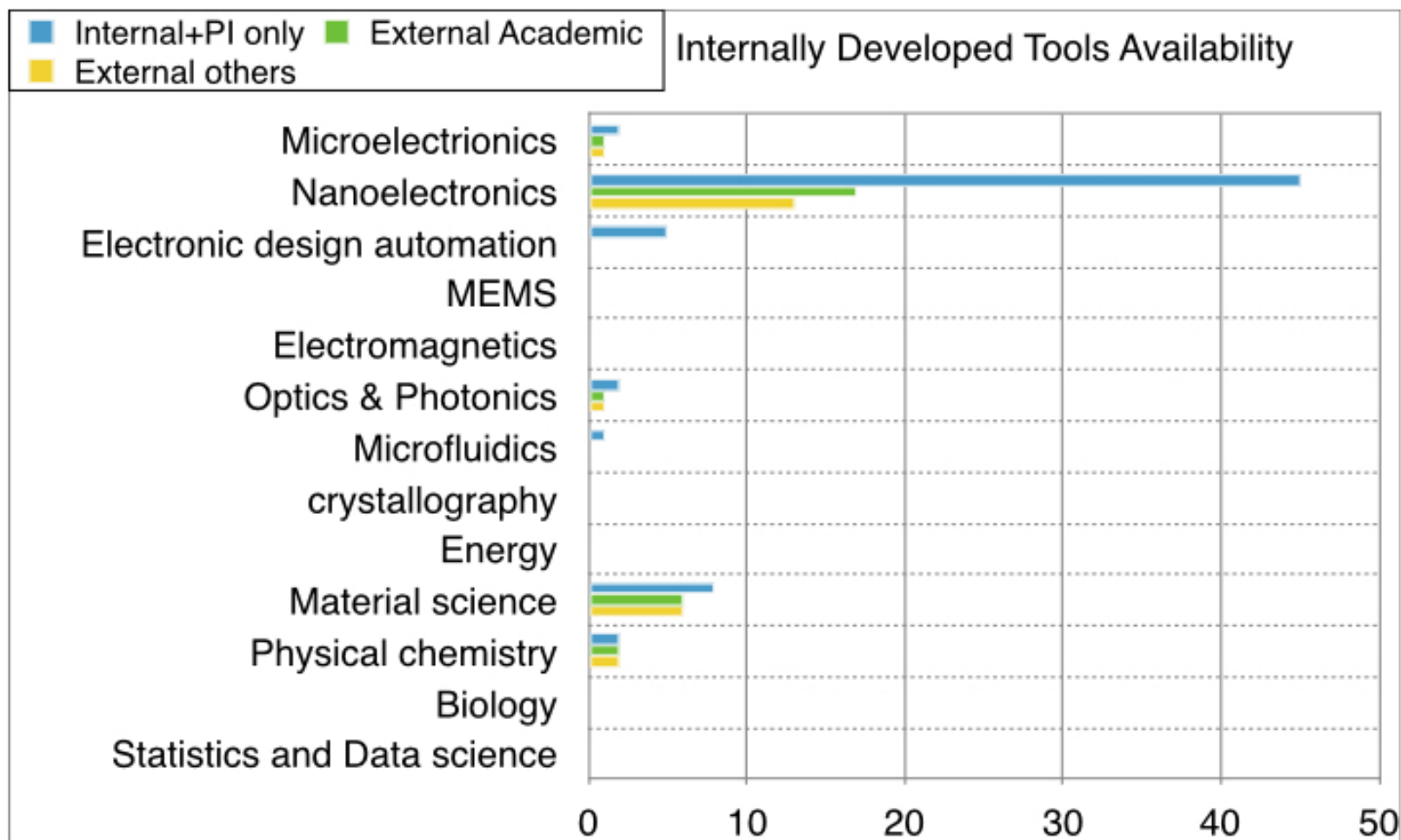
# Statistics by Disciplines



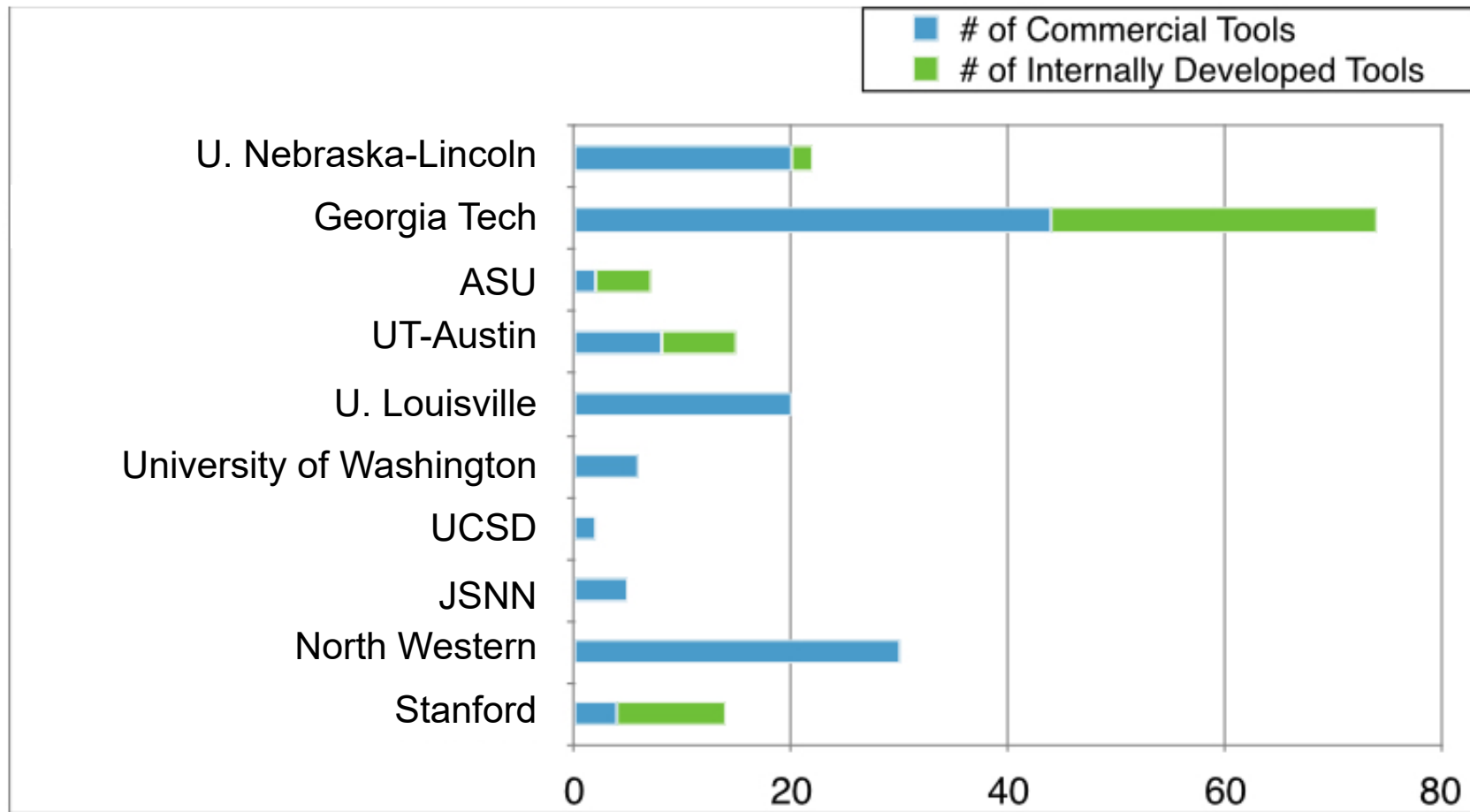
# Permission to Access: Commercial Tools



# Permission to Access: Internally Developed Tools

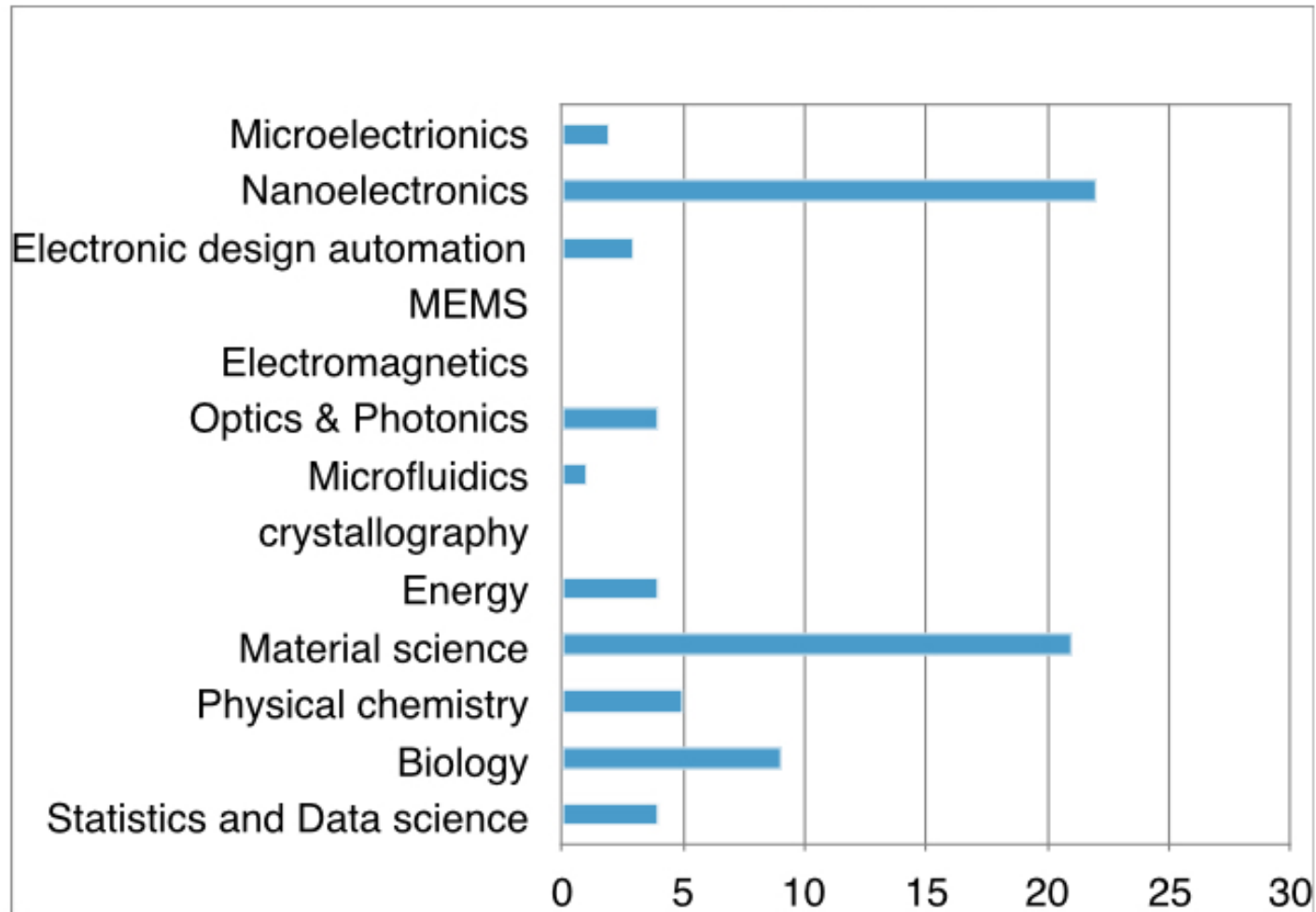


# Contributing Universities





# Modeling and Simulation Experts



# NNCI Computing Page on nanoHUB



Login

Overview

Software Packages

Computing Hardware Resources

People Expertise

Search for resources

## Software packages

Filter by Category Availability University/Research group Vendor

Showing 90 Software Packages

Name	Vendor	Category	University/Research Group	Availability
<b>3D Explorer</b> For processing of basic 2D data, pole figure and reciprocal maps	Rigaku	Crystallography	University of Texas, Austin	✓ Internal academic users ✓ External academic users ✓ Industry/Government users
<b>Apex 3 suite</b> Single crystal diffraction data analysis and structure solution)	Bruker	Crystallography	University of Texas, Austin	✓ Internal academic users ✓ External academic users ✓ Industry/Government users
<b>EVA</b> Rietveld, x-ray diffraction data processing	Bruker	Crystallography	University of Texas, Austin	✓ Internal academic users ✓ External academic users ✓ Industry/Government users
<b>Global fit 2</b> X-ray reflectivity and Rocking curve analysis of thin films	University of Texas, Austin	Crystallography	University of Texas, Austin	✓ Internal academic users ✓ External academic users ✓ Industry/Government users

1 2 END

Display # 15 Results 1 - 15 of 21




# NNCI Computing Page on nanoHUB

[nanohub.org/groups/nnci\\_computation](http://nanohub.org/groups/nnci_computation)

Title	PI	NNCI Site Name	Brief Description
CatApp	Norskov	Stanford	software for atomic-scale simulations to understand heterogeneous catalytic reactions
CNTmob	Pop	Stanford	calculates the mobility of semiconductor CNTs at various charge densities and temperatures
GFET Tool	Pop	Stanford	calculates I-V curves for graphene transistors
MSMBuilder	Pande	Stanford	software for understanding a molecule's conformational dynamics
nanoJoule	Pop	Stanford	calculates I-V curves for metallic single-wall carbon nanotubes
NEGF-BISFET	Frank Register	UT Austin	Quantum NEGF transport simulator for BisFETs and ITFETs
piezoD	Pruitt	Stanford	Tool for modeling the performance and optimizing the design of piezoresistive and piezoelectric sensors and
Stanford 2D Semiconductor (SZDS) Transistor Model	Pop	Stanford	a physics-based compact model for transistors based on two-dimensional semiconductors such as MoS2
Stanford Stratified Structure Solver (S4)	Fan	Stanford	open-source software to simulate and analyze photonic structures
Stanford Virtual-Source Carbon Nanotube Field-Effect Transistors Model	Wong	Stanford	a semi-empirical compact model that captures the scaling properties of CNFETs
SU RRAM Model	Wong	Stanford	a SPICE-compatible model that describes switching for bipolar metal-oxide RRAM
TMDMOSFET	Frank Register	-	Ballistic Transport simulator for 2D layered TMD materials using maximally localized Wannier function techni
TOMCAT	Sanjay Banerjee	UT Austin	General-purpose Monte Carlo simulator of particle transport in arbitrary 2-D structures. The main applicator
UT-Marlowe	Sanjay Banerjee	UT Austin	Neutron Transport Simulator which models scattering, electronic stopping, and damage accumulation
UT-QUANT	Sanjay Banerjee	UT Austin	CV Simulator for Silicon MOS Structures
UT-SCMC	Frank Register	UT Austin	Ensemble semi-classical Monte Carlo methods employing quantum corrections to address quantum confine
Macrosipin LLG Code	Sanjay Banerjee	UT Austin	C++ code for simulating stochastic magnetization dynamics, includes STT
Nanonet	Satish Kumar	Georgia Institute of Technology	A simulation tool for Thin films transistors based on network of nanotubes or nanowires
1D Monte Carlo code	Dragica Vasileska	ASU	calculates drift velocity, average carrier energy and the mobility of electrons in Q1D systems
2D Monte Carlo code	Dragica Vasileska	ASU	calculates drift velocity, average carrier energy and the mobility of electrons in Q2D systems
2D Particle-Based Device Simulator	Dragica Vasileska	ASU	IV Characteristics of n-channel MOSFETs and SOI devices
3D Particle-based Device Simulator	Dragica Vasileska	ASU	IV Characteristics of 3D devices, discrete impurity effects (RDF and RTN)
Bulk Monte Carlo Code	Dragica Vasileska	ASU	calculates drift velocity, average carrier energy and the mobility in bulk materials
Dzyaloshinskii-Moriya ferromagnets	Alexev Kovalev	Nebraska Nanoscale Facilities	spin wave theory in Wolfram and MATLAB
mumax3	Alexev Kovalev	Nebraska Nanoscale Facilities	micromagnetic modelling
Compact thermal model of Microgap flow cooling stacked chips for co-design	Yogendra Joshi	Georgia Institute of Technology	A compact multi-layer pin-fin liquid cooling model with high speed simulation has been established for stead
Power Delivery Network Analysis tool	Muhannad S. Bakir	Georgia Institute of Technology	This is a thermal electrical co-simulation framework especially for 2.5D and 3D Ics. Power Delivery Network C
Thermal Simulation tool for 2.5D and 3D Ics	Muhannad S. Bakir	Georgia Institute of Technology	This is thermal modeling tool which can perform both steady-state and transient thermal analysis Thermal r

# NSF Network for Computational Nanotechnology

POWERED BY [nanoHUB.org](http://nanoHUB.org)

 Azad Naeemi [azad@ece.gatech.edu](mailto:azad@ece.gatech.edu)

[Join Group](#)

[Help](#)



[NEEDS HOME](#)

[ABOUT US](#)

[RESOURCES](#)

[CONTACT US](#)

[NEEDS TEAM](#)

## Nano-Engineered Electronic Device Simulation Node

*NEEDS has a vision for a new era of electronics that couples the power of billion-transistor CMOS technology with the new capabilities of emerging nano-devices and a charter to create high-quality models and a complete development environment that enables a community of compact model developers.*

*NEEDS Team: Purdue, MIT, U.C. Berkeley, and Stanford.*

A short overview of the NEEDS initiative and several of the presentations and posters from the 2016 annual meeting are now available.

NEWEST COMPACT MODEL RELEASE: nMOSFET RF and noise model on standard 45nm SOI technology [See Compact Models Page](#)

NEEDS announces the public BETA testing of VALint, an automatic Verilog-A code quality checker.

Paper "Well-Posed Models of Memristive Devices" by Tianshi Wang and Jaijeet Roychowdhury



### COMPACT MODELS

SPICE-compatible Verilog-A format supporting resources



### COMPACT MODELS: TOOLS

Tools for developers including **MAPP** & **VALint**.

**new** VALint now in open BETA



### COMPACT MODELS: RESOURCES FOR DEVELOPERS

Seminars and tutorials for developing and publishing compact models

**new** Publish your compact model in NEEDS



### NANOSCIENCE TO SYSTEMS

Physically-detailed simulations system level tools

**new** Stanford script-based toolkit for system analysis



### NANOSCIENCE: SEMINARS, COURSES, ETC.

NEEDS Seminars, workshops, nanoHUB-U and more

**new** Seminar series on devices for 5 nm technology

# NSF Network for Computational Nanotechnology

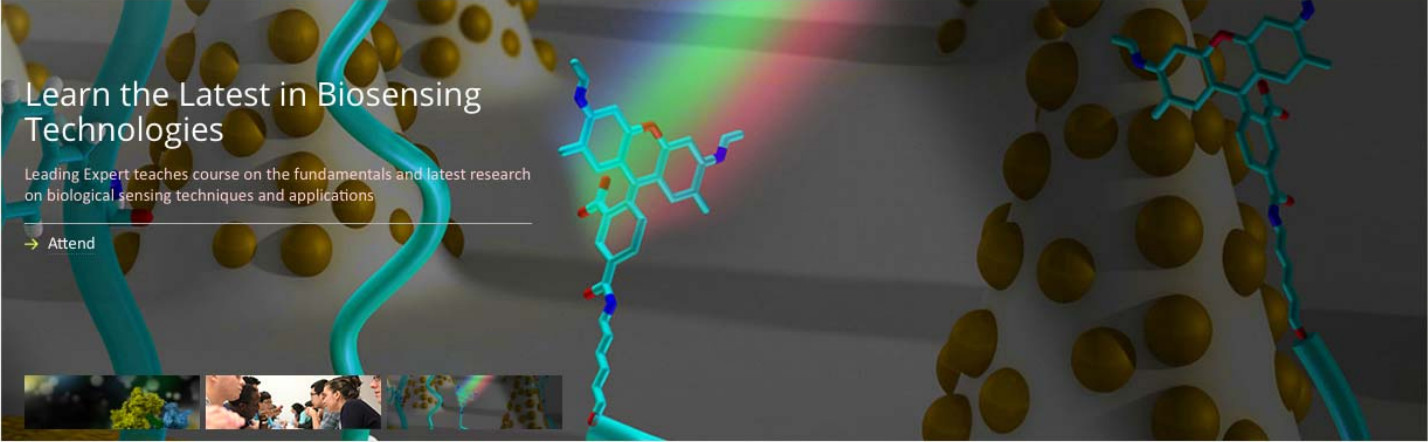
POWERED BY [nanoHUB.org](http://nanoHUB.org) Azad Naeemi [azad@ece.gatech.edu](mailto:azad@ece.gatech.edu) Group Closed Help

**nanoBIONODE** [SIMULATION TOOLS](#) [COURSES](#) [PRESENTATIONS](#) [COMMUNITY OPEN SOURCE](#) [ABOUT](#)

## Learn the Latest in Biosensing Technologies

Leading Expert teaches course on the fundamentals and latest research on biological sensing techniques and applications

[→ Attend](#)



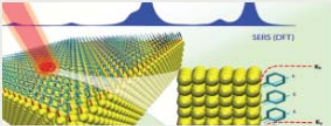
### CONTRIBUTE

- [How to Develop and Deploy a Tool](#)
- [How to Contribute Content](#)
- [nanoHUB Licensing Policies](#)

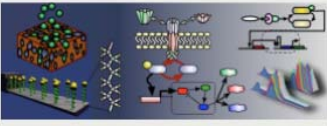
### EVENTS

- [NanoBIO Node Seminars](#)
- [Nanoindentation Workshop](#)
- [Beckman Director's Seminars](#)
- [Biongeering](#)
- [Mechanical Science and Engineering](#)

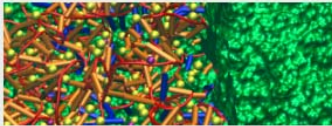
### SIMULATE



**Plasmonic Nanostructures**  
Plasmonic Nanostructures: Calculate scattering and absorption of electromagnetic waves by targets with arbitrary geometries and complex refractive index.



**Functionalization Workbench**  
Interact with simulations of surfaces functionalized with a variety of biomolecules.

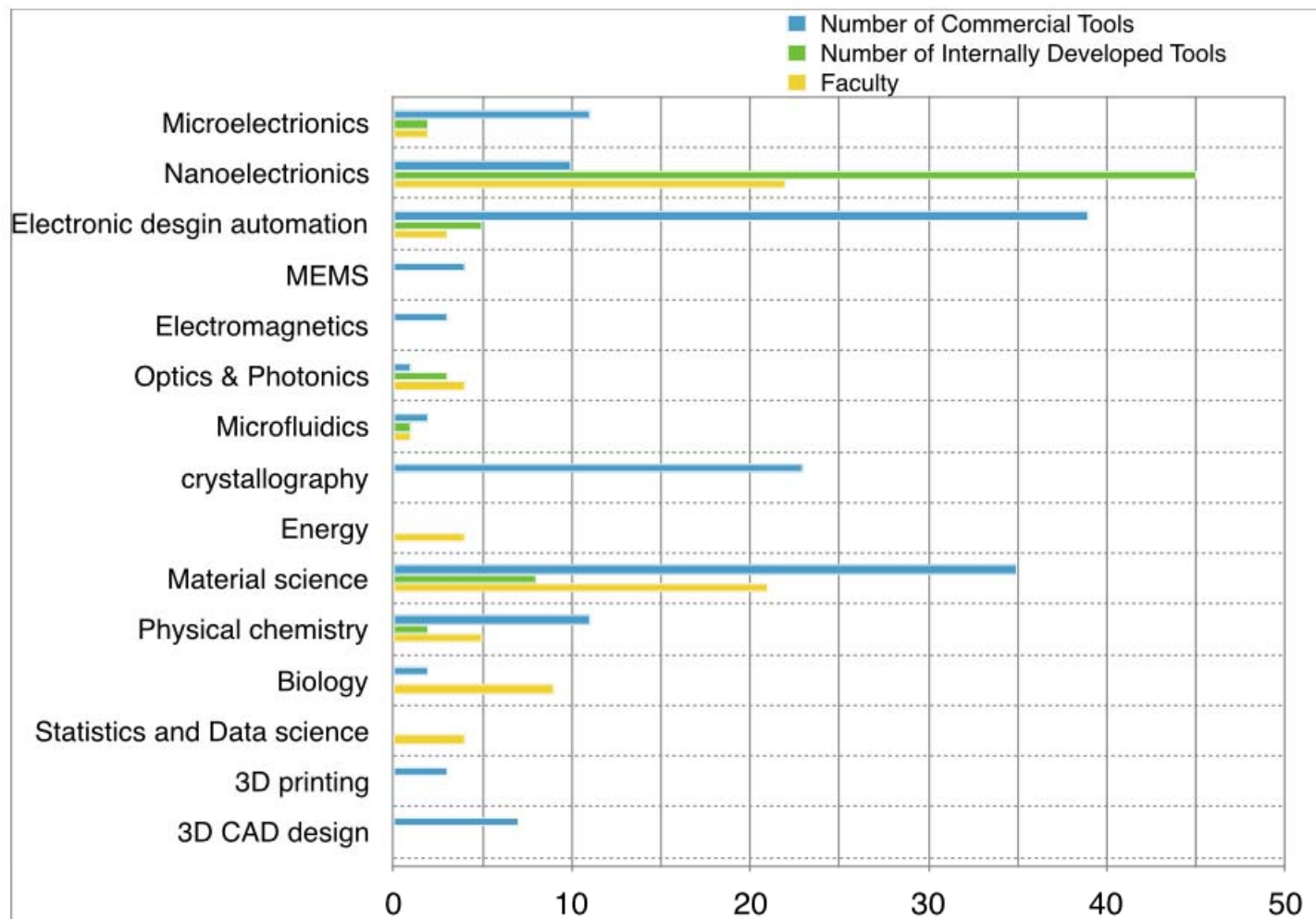


**Molecular Dynamics Showcase**  
Explore molecular dynamics simulations.

[Simulate more...](#)



# What are Major Gaps?



# Process Simulation Tools

- None of the sites have reported such tools.
- Can greatly help users and staff and cut cost.
- Fabrication complexity is growing and user experience is decreasing.
- Should NNCI invest in such tools?
- Buy commercial tools or develop its own sets of tools?

# Example: Electron Beam Lithography

- Job preparation is a key aspect:
  - CAD patterns must be converted to tool format and dose must be applied to correct for proximity effects.
  - Many other factors (resist, substrate, developer, accel. voltage, etc.) determine "proper" dose.
- Even with advanced knowledge and experience, it is common to do a dose test/skew. some iteration (hopefully  $< 3$  is required)
- Software provided by EBL vendors are very limited.
- Tools to simulate electron scattering are available but are expensive.
- These tools could be improved by have a more process/fabrication oriented outlook.



# Opportunities?

- Allow the user to iterate in the software rather than in the fab??
- Provide close to a "final answer" / "right condition"?
- Develop EBL conversion/proximity effect correction tool and share across NNCI network (reduce costs >\$100k/license)?
- Envision other process modules (etch, photolithography, etc.) to simulate?

**It will not be easy to develop such tools (Funding/resources).**

However, if we could create a tool to help users get "right" results faster and cheaper, the upside could be tremendous.

# Breakout Session Questions

- How can NNCI Computation can be most useful for the NNCI community?
- What should be the short term and long term goals?
- How can we facilitate tool development and access to the tools?
- Should NNCI identify some very important process simulation tools and invest in their development?
- What are the funding opportunities?