

# NNCI Computation

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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:

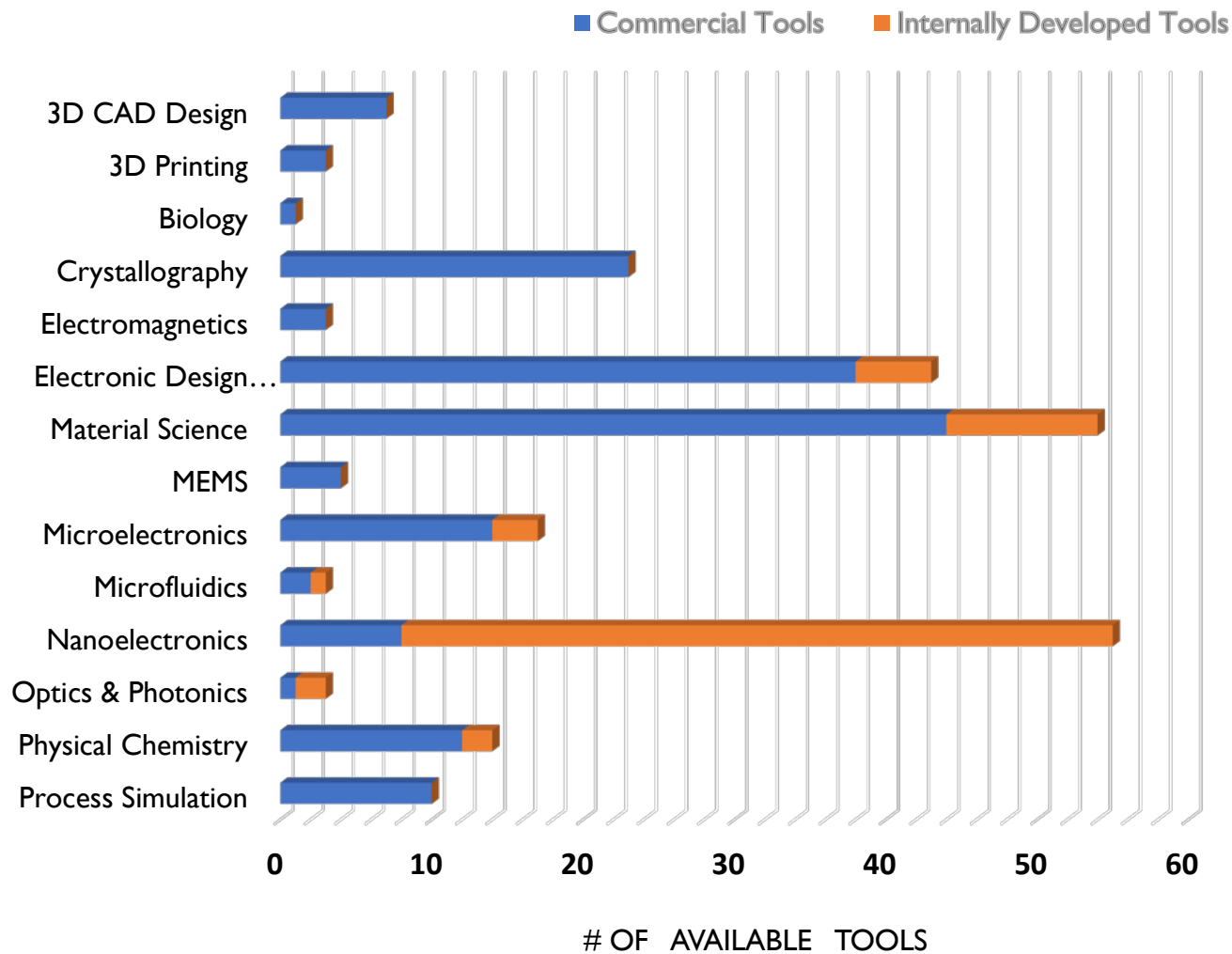
- To facilitate access to the modeling and simulation capabilities and expertise within NNCI sites.
- To identify the strategic areas for growth in modeling and simulation
- To promote and facilitate the development of the new capabilities.

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).

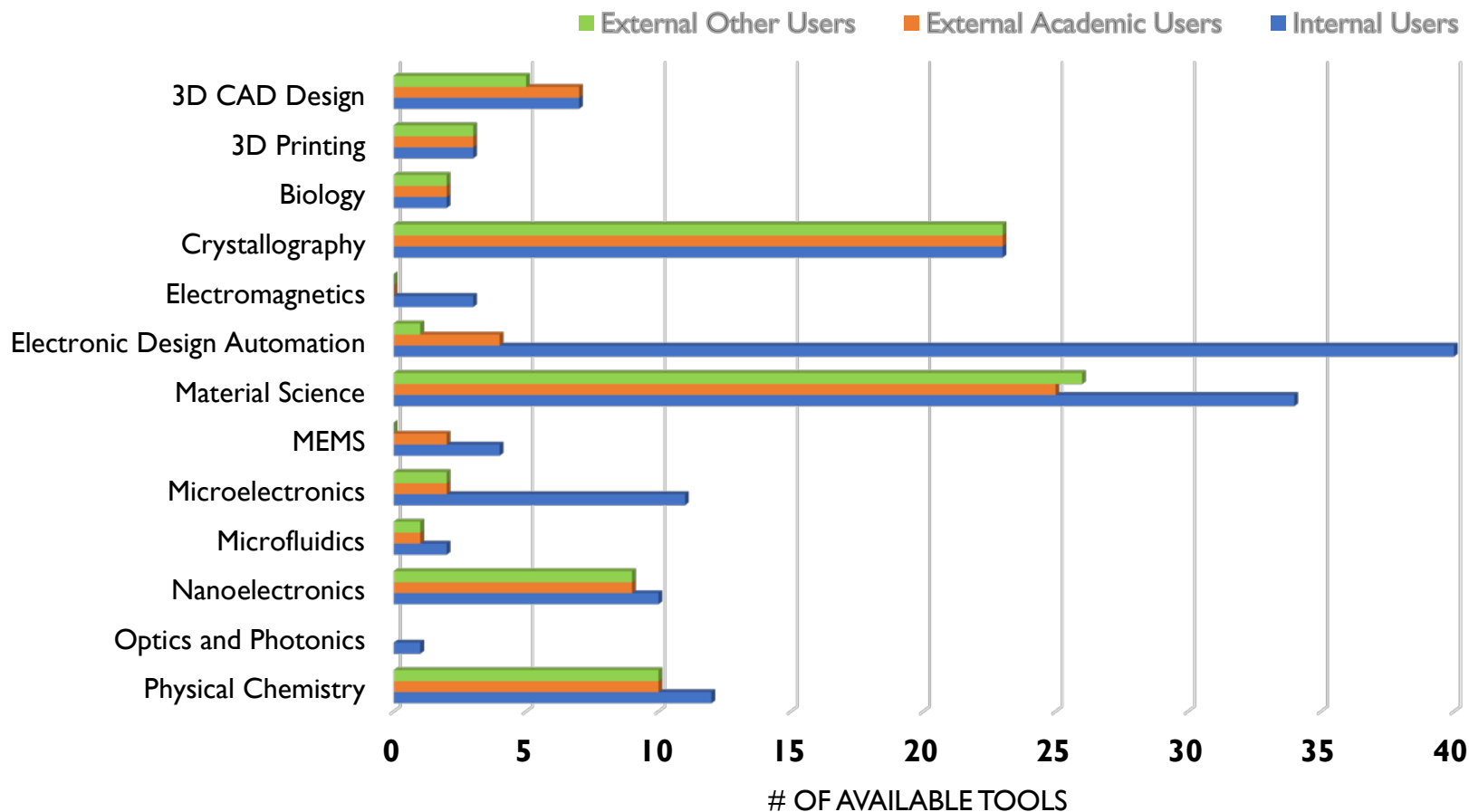
8 supercomputers or major computing clusters are available in various sites.

# Statistics by Disciplines



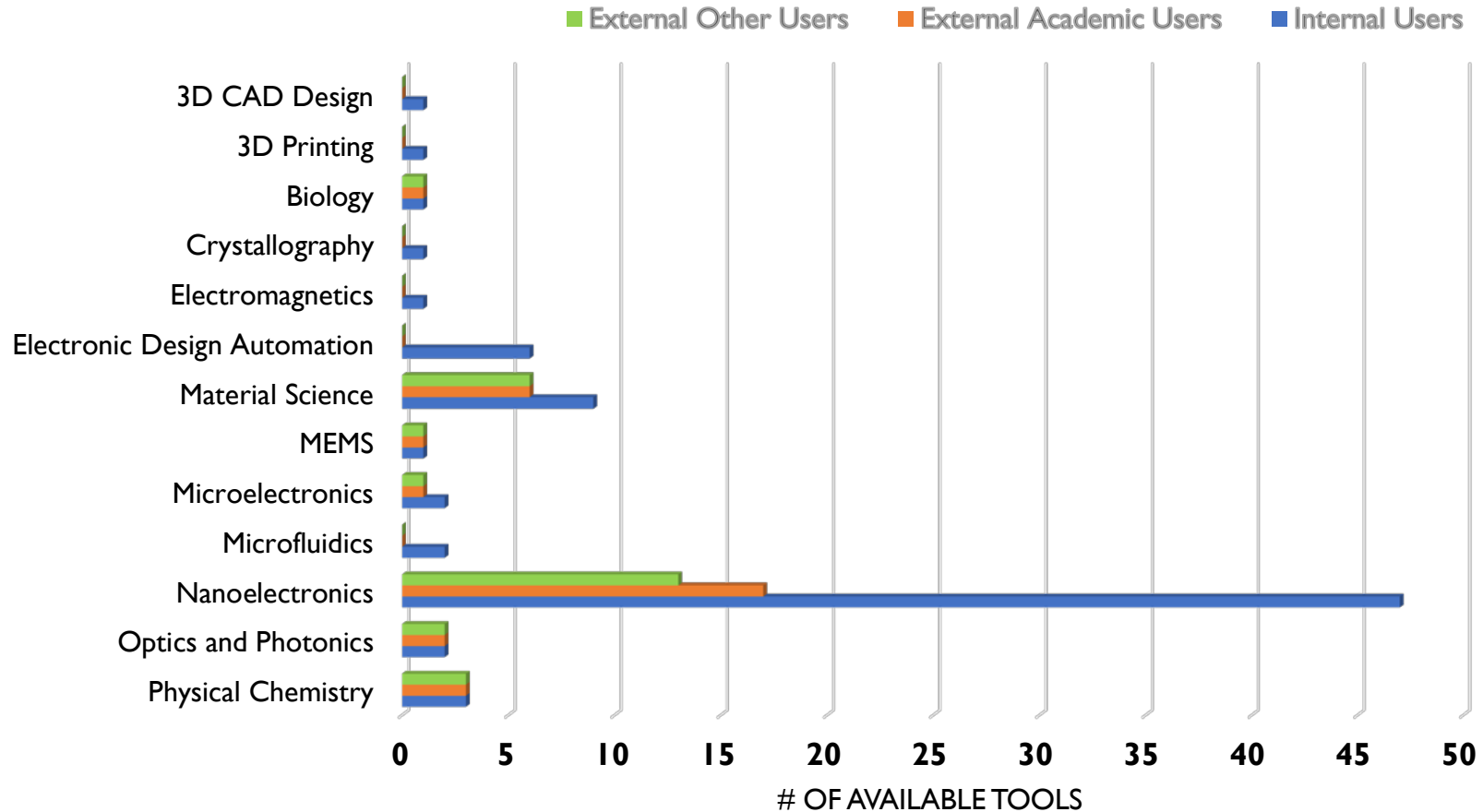
# Permission to Access: Commercial Tools

## Commercial Tool Availability

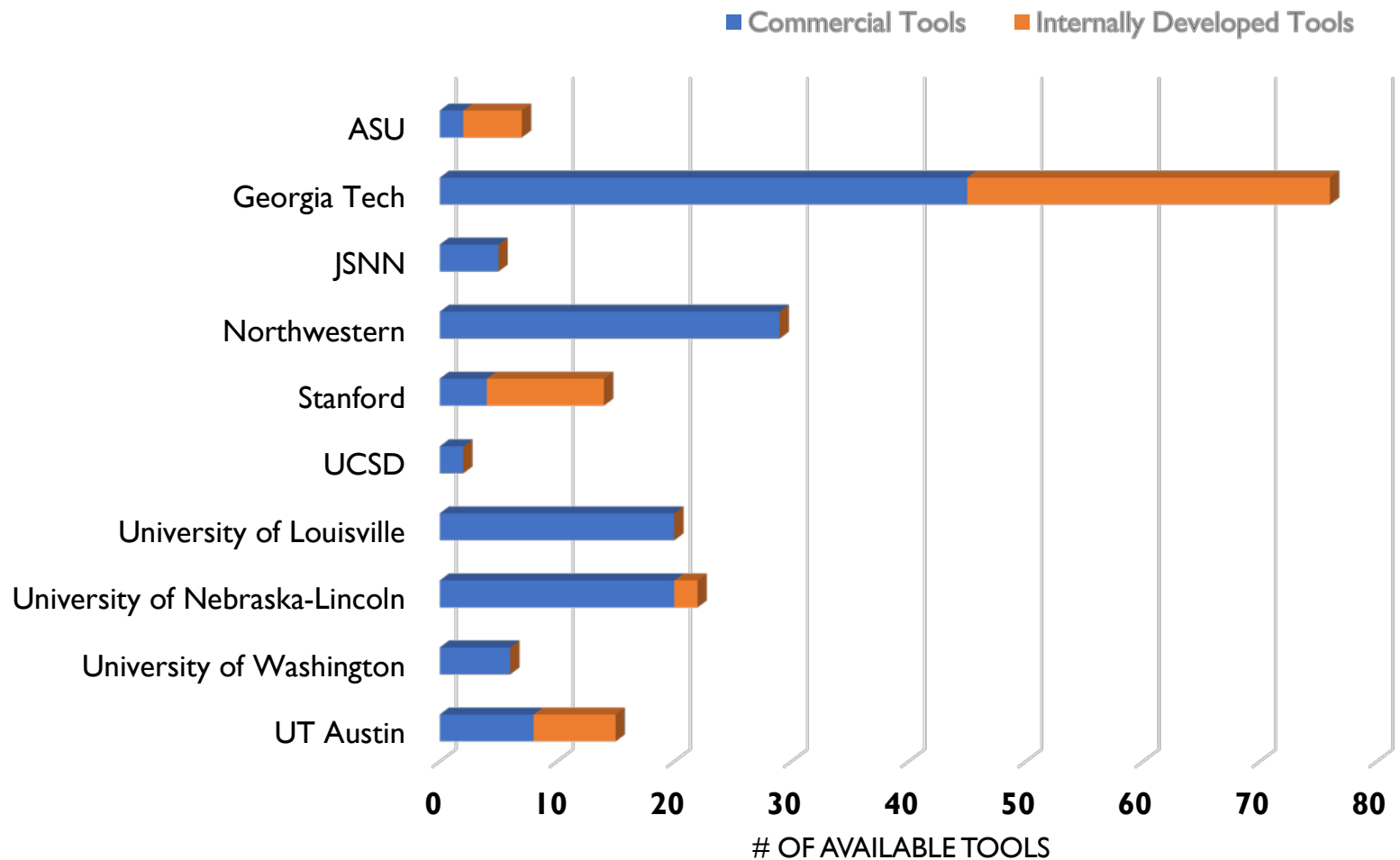


# Permission to Access: Internally Developed Tools

## Internally Developed Tool Availability



# Contributing Universities





# NNCI Computation Group Page on nanoHUB

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

**Overview**

computational nanoelectronics | nanoscience | simulation and modeling

**National Nanotechnology Coordinated Infrastructure**

The NNCI is an NSF-funded program comprised of 16 sites, located in 17 states and involving 29 universities and other partners. This national network provides researchers from academia, government, and industry with access to university user facilities with leading-edge fabrication and characterization tools, instrumentation and expertise within all disciplines of nanoscale science, engineering, and technology. Research undertaken within NNCI facilities is incredibly broad, with applications in electronics, materials, biomedicine, energy, geosciences, environmental sciences, consumer products, and many more. The toolsets of sites are designed to accommodate explorations that span the continuum from materials and processes through devices and systems. There are micro/manufacturing tools, used in classroom environments, as well as extensive characterization capabilities to provide resources for both top down and bottom up approaches to nanoscale science and engineering.

For more information about NNCI, please visit NNCI website.

Modeling and simulation play a key role in enhancing nanoscale fabrication and characterization as they guide experimental research, reduce the required number of trial and error iterations, and enable more in-depth interpretations of the characterization results. Various NNCI sites provide a diverse set of software and hardware resources and capabilities that, if made readily accessible, can greatly help and even expand the NNCI user community. A collective inventory of modeling and simulation resources and capabilities across NNCI sites is provided in this database with helpful information such as a point of contact for which tool, access restrictions, and academic citations.

Access to commercial tools available through various sites might be limited by their licenses. For instance, some might be available only to internal or academic users. Internally developed tools typically come with fewer restrictions. However, these tools have been developed with limited funding from various sources and may lack a professional user interface, documentation, or robustness. Executable versions of some tools may not be even publicly available at this point. The point of contact (mainly the PI) for each internally developed tool is provided to facilitate potential collaborations. However, the PIs may not have the resources to respond to all inquiries. The NNCI Coordinating Office at Georgia Tech will continue to update and expand this database, work with the PIs to facilitate access to the resources, and explore ways to address the computational needs of the community.

For NNCI Modeling/Simulation Tools List, please visit here.

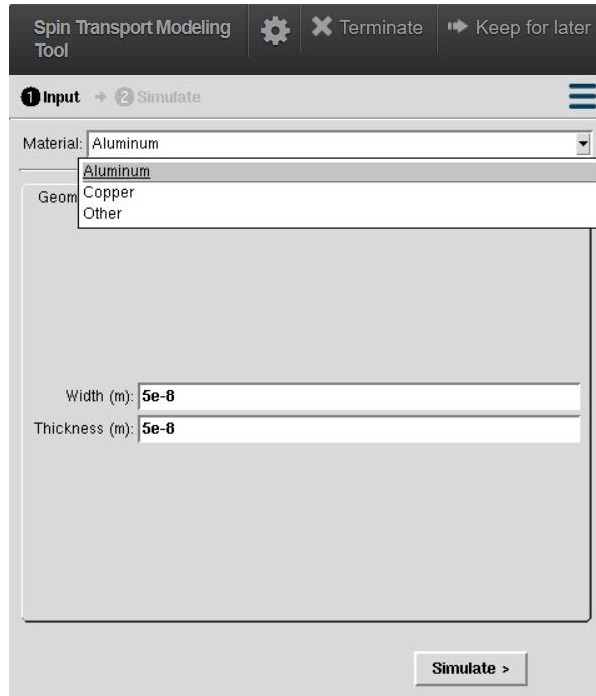
For general questions or comments please contact Arad Naremi (anaremi@gatech.edu).

## NNCI Modeling/Simulation Tools List

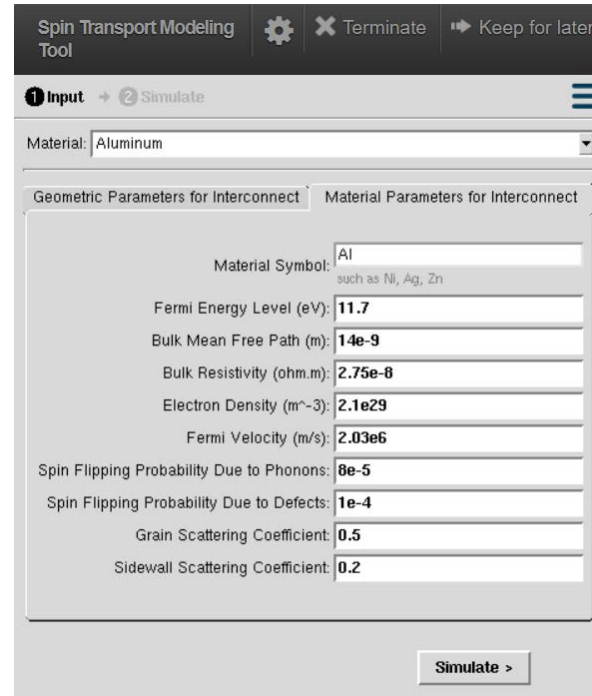
Category	Tool	Description
3D CAD design	Solidworks	Comprehensive solid modeling design and simulation software
3D CAD design	Rhino	Freeform modeling software
3D CAD design	Intralattice	Generative Lattice Design for Rhino
3D CAD design	Autodesk Fusion 360	Comprehensive solid modeling design and simulation software
3D CAD design	SolidThinking Inspire	Topology optimization
3D CAD design	Ansys	Computer-aided engineering software
3D printing	MAGICS	3D printing part manipulation and fixing
3D printing	Autodesk Meshmixer	3D printing file manipulation and fixing
3D Printing , Physical chemistry	Autodesk Within	Lattice/Cellular structure design and simulation for 3D printing
Biology, Physical chemistry	Lammps*	Opensource package for molecular dynamics simulations primarily designed for bio
Crystallography	TOPAS	Rietveld, XRD analysis
Crystallography	LEPTOS - old version	Rietveld, XRR analysis
Crystallography	MULTEX	Rietveld, pole figure analysis
Crystallography	EVA	Rietveld, x-ray diffraction data processing
Crystallography	PDXL 2	Rietveld, crystallite size and strain analysis, Residual stress, %Crystallinity, RIR quanti
Crystallography	NANO-Solver 3	SAXS analysis of nano particle/pore
Crystallography	Global fit 2	X-ray reflectivity and Rocking curve analysis of thin films
Crystallography	3D Explorer	For processing of basic 2D data, pole figure and reciprocal maps
Crystallography	Apex 3 suite	Single crystal diffraction data analysis and structure solution)
Crystallography	High Score Plus	Rietveld, Phase ID, phase quantification
Crystallography	Data Viewer	PANalytical, x-ray diffraction data processing, size
Crystallography	CaRine v 3.1	Molecular visualization and crystallography tools
Crystallography	Diamond v 3.2	Molecular visualization and crystallography tools
Crystallography	PROJECT/SAED2s	Simulation and analysis of electron diffraction (spot) patterns
Crystallography	PROJECT/PCED2s	Advanced simulation of PCED (ring) patterns and phase identification
Crystallography	PROJECT/SPICA	Stereographic projection for interactive crystallographic analysis
Crystallography	JECP/SVAT	Structural viewer and analytical tool
Crystallography	JECP/HOLZ2a	Simulation of HOLZ pattern, including dynamical correction
Crystallography	JECP/SAKI	Simulation analysis of Kikuchi lines and double diffraction effect
Crystallography	Reciprocal Net	Crystallographic information repository
Crystallography	Platon	Tool for crystallographic analyses
Crystallography	Encifer	Safely check and edit crystallographic information files (CIFs) without compromising t
Crystallography, Material science	Mercury	Visualization of structures/molecules
Electromagnetics	Antenna Magus	1. A software tool to help accelerate the antenna design and modelling process 2. Av
Electromagnetics	HFSS/Electromagnetic Suite	The industry standard for simulating 3-D, full-wave, electromagnetic fields
Electronic design automation	Power Delivery Network Analysis tool	Thermal electrical co-simulation framework especially for 2.5D and 3D ICs
Electronic design automation	Power Delivery Network Modeling	Power integrity analysis based on Huang Gang's work
Electronic design automation	Thermal Simulation tool for 2.5D and 3D ICs	Thermal modeling tool which can perform both steady-state and transient thermal a
Electronic design automation	Abaqus	A software package for Computer-aided engineering and Finite Element Analysis
Electronic design automation	Q3D Extractor	The premier 2-D and 3-D parasitic extraction tool for engineers designing electronic p
Electronic design automation	SIWave	A specialized design platform for power integrity, signal integrity and EMI analysis of

# Spintronic Transport Modeling Tool

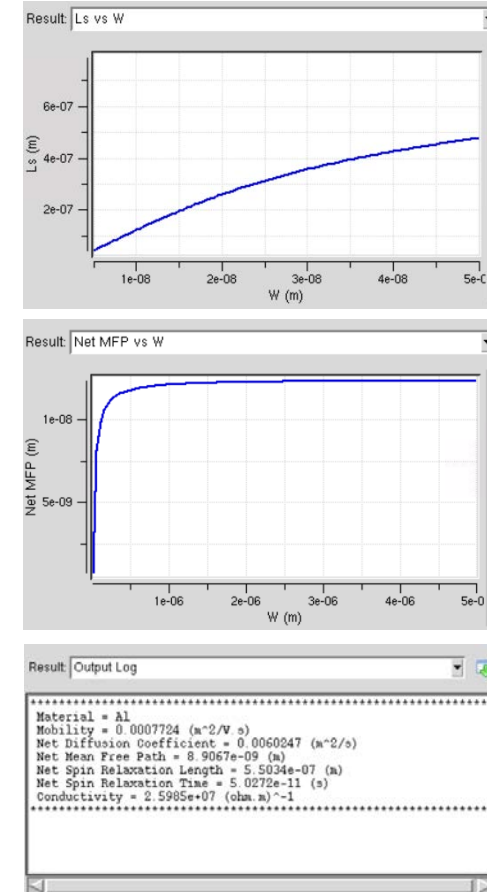
[nanohub.org/tools/spintransport/](http://nanohub.org/tools/spintransport/)



- Choose right material for your interconnect



- Use predetermined material parameters **OR** use your own



- Obtain electron-spin transport physics-based simulation results

# SPICE Subcircuit Netlist Generator for Spintronic Nonmagnetic Metallic Channel

[nanohub.org/tools/spincircuit/](http://nanohub.org/tools/spincircuit/)

SPICE Subcircuit Generator for Spintronic Nonmagnetic Metallic Channel Components

1 Interconnect Parameters → 2 Circuit Description Parameters → 3 Simulate

Material: Copper

Material Symbol: Cu

Fermi Energy Level (eV): 7

Bulk Mean Free Path (m): 40e-9

Bulk Resistivity (ohm.m): 1.7e-8

Electron Density (m<sup>-3</sup>): 8.5e20

Fermi Velocity (m/s): 1.57e6

Spin Flipping Probability Due to Phonons: 2e-3

Spin Flipping Probability Due to Defects: 7e-4

Grain Scattering Coefficient: 0.5

Sidewall Scattering Coefficient: 0.2

SPICE Subcircuit Generator for Spintronic Nonmagnetic Metallic Channel Components

1 Interconnect Parameters → 2 Circuit Description Parameters → 3 Simulate

Number of segments: 10

```
Result: interconnect.sbckt
*Channel Subcircuit
.subckt interconnect
* v0 vL vx0 vL vy0 vyL vz0 vzL
* vc_gnd vx_gnd vy_gnd vz_gnd
*****
*Drift-Diffusion Channel Circuit Model
pcell11 v0 v01 vx01 vy01 vz01 vc_gnd vx_gnd vy_gnd vz_gnd cell
pcell12 v01 v02 vx02 vy02 vz02 vc_gnd vx_gnd vy_gnd vz_gnd cell
pcell13 v02 v03 vx03 vy03 vz03 vc_gnd vx_gnd vy_gnd vz_gnd cell
pcell14 v03 v04 vx04 vy04 vz04 vc_gnd vx_gnd vy_gnd vz_gnd cell
pcell15 v04 v05 vx05 vy05 vz05 vc_gnd vx_gnd vy_gnd vz_gnd cell
pcell16 v05 v06 vx06 vy06 vz06 vc_gnd vx_gnd vy_gnd vz_gnd cell
pcell17 v06 v07 vx07 vy07 vz07 vc_gnd vx_gnd vy_gnd vz_gnd cell
pcell18 v07 v08 vx08 vy08 vz08 vc_gnd vx_gnd vy_gnd vz_gnd cell
pcell19 v08 v09 vx09 vy09 vz09 vc_gnd vx_gnd vy_gnd vz_gnd cell
pcell110 v09 v10 vx10 vy10 vz10 vc_gnd vx_gnd vy_gnd vz_gnd cell
*****
.ends interconnect
```

```
Result: cell.sbckt
*Single Cell Subcircuit
.subckt cell
* vc+ vc- vx+ vx- vy+ vy- vz+ vz-
* vc_gnd vx_gnd vy_gnd vz_gnd
*****
*Parameters
*Spin Transport Parameters
.param mu=0.0016096
.param D=0.0075113
*****
*Spin Circuit Parameters
.param Relec=0.68439
.param Gelec=1.2949e-18
.param Rspin=0.68439
.param Cspin=5.4711e-13
.param Gspin=0.069804
*****
*Drift-Diffusion Segment Circuit Model
*Charge Current
R_c1 vc+ vc- 'Relec'
W_c1 vc+ vc- DC 0
R_c2 vc- vc- 'Relec'
V_c2 vc- vc- DC 0
C_c vc vc_gnd 'Delec'
*Spin X Current
R_x1 vx+ vx- 'Rspin'
E_x1 vx+ vx- I=(mu/D)*I(V_c1)*(V(vx)-V(vx_gnd))
R_x2 vx vx- 'Rspin'
E_x2 vx vx- I=(mu/D)*I(V_c2)*(V(vx)-V(vx_gnd))
C_x vx vx_gnd 'Cspin'
R_x vx vx_gnd '1/Gspin'
*Spin Y Current
R_y1 vy+ vy- 'Rspin'
E_y1 vy+ vy- I=(mu/D)*I(V_c1)*(V(vy)-V(vy_gnd))
R_y2 vy vy- 'Rspin'
E_y2 vy vy- I=(mu/D)*I(V_c2)*(V(vy)-V(vy_gnd))
C_y vy vy_gnd 'Cspin'
R_y vy vy_gnd '1/Gspin'
*Spin Z Current
R_z1 vz+ vz- 'Rspin'
E_z1 vz+ vz- I=(mu/D)*I(V_c1)*(V(vz)-V(vz_gnd))
R_z2 vz vz- 'Rspin'
E_z2 vz vz- I=(mu/D)*I(V_c2)*(V(vz)-V(vz_gnd))
C_z vz vz_gnd 'Cspin'
R_z vz vz_gnd '1/Gspin'
*****
.ends cell
```

- Choose right material for your interconnect

- Use developed compact circuit model for spintronic transport

- Obtain SPICE subcircuit netlist describing spin&electron transport in channel

# Full Spintronic Device SPICE Netlist Generator on nanoHUB

## LLG Solver Subcircuit Models

- Macromagnetic Solver .subckt
- 1D Micromagnetic Solver .subckt
- 2D Micromagnetic Solver .subckt
- 3D Micromagnetic Solver .subckt

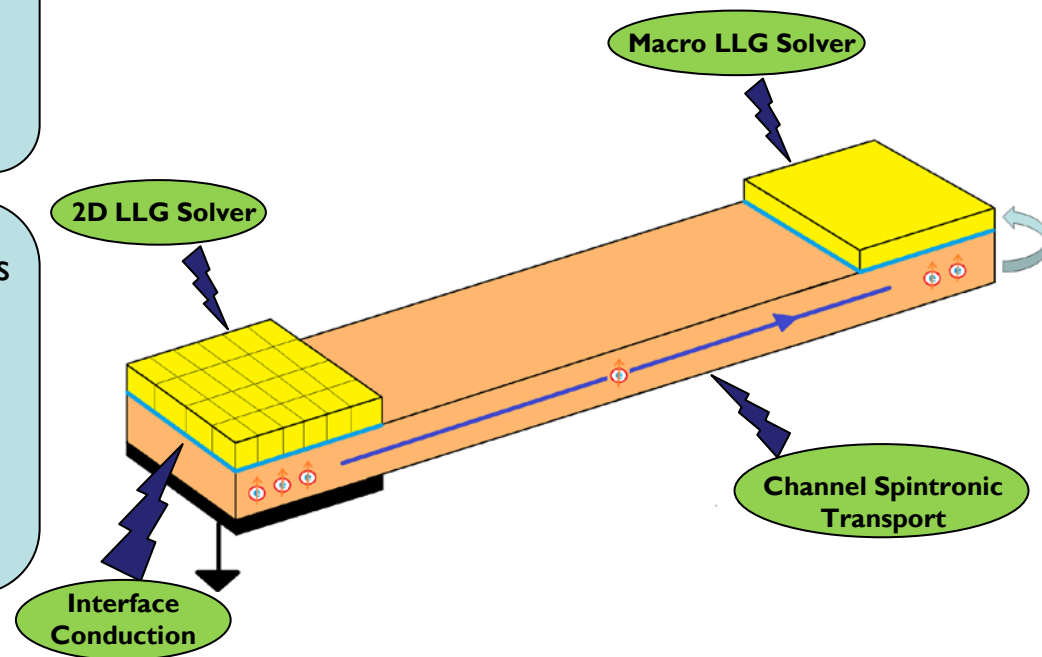
## Interface Conduction Subcircuit Models

- Ferro – Nonmagnetic Metallic Interface

## Channel Spintronic Transport Subcircuit Models

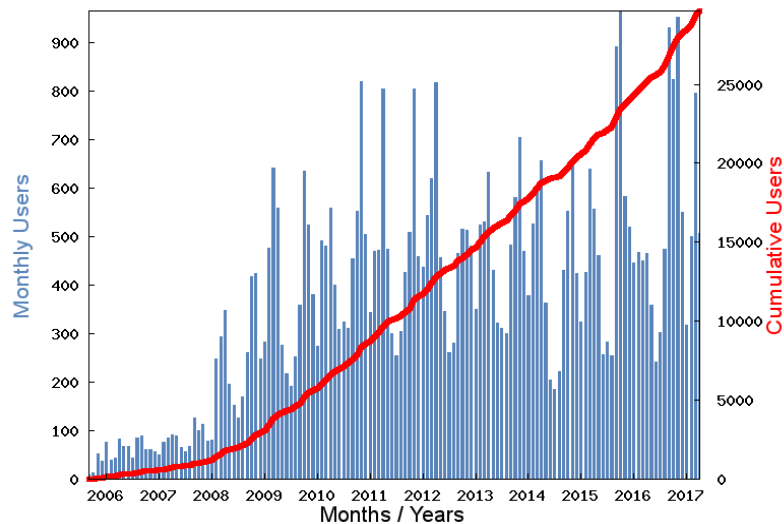
- Electron Transport
- Spin Transport
- Spintronic (both electron&spin) Transport

- Various modules to model and simulate various spintronic devices/circuits in SPICE.



# Simulation Tools from ASU

Users of Simulation Tools Authored by Dragica Vasileska (29,643 Users)



## 2D Solver Deployment

nanoHUB.org: <https://nanohub.org/tools/predicts2d/>



49 Users



Unified Numerical Solver for Device Metastabilities in CdTe Thin-Film PV  
Award No. DE-EE0006341



#	Tool Name	Users served in last 12 months	Simulation Runs in last 12 months	Total users served	Total Simulation Runs	Citations	Published On
1	<a href="#">Cu in CdTe Lab (2D Version)</a>	<u>39</u>	<u>152</u>	<u>50</u>	<u>214</u>	-	12 Jul 2016
2	<a href="#">Cu in CdTe Lab</a>	<u>14</u>	<u>35</u>	<u>53</u>	<u>204</u>	1	17 Feb 2015

# NNCI Hardware Resources

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

All serve internal uses only with the exception of the UT-Austin computing cluster.

Example :

Partnership for an Advanced Computing Environment (PACE).”  
at GT

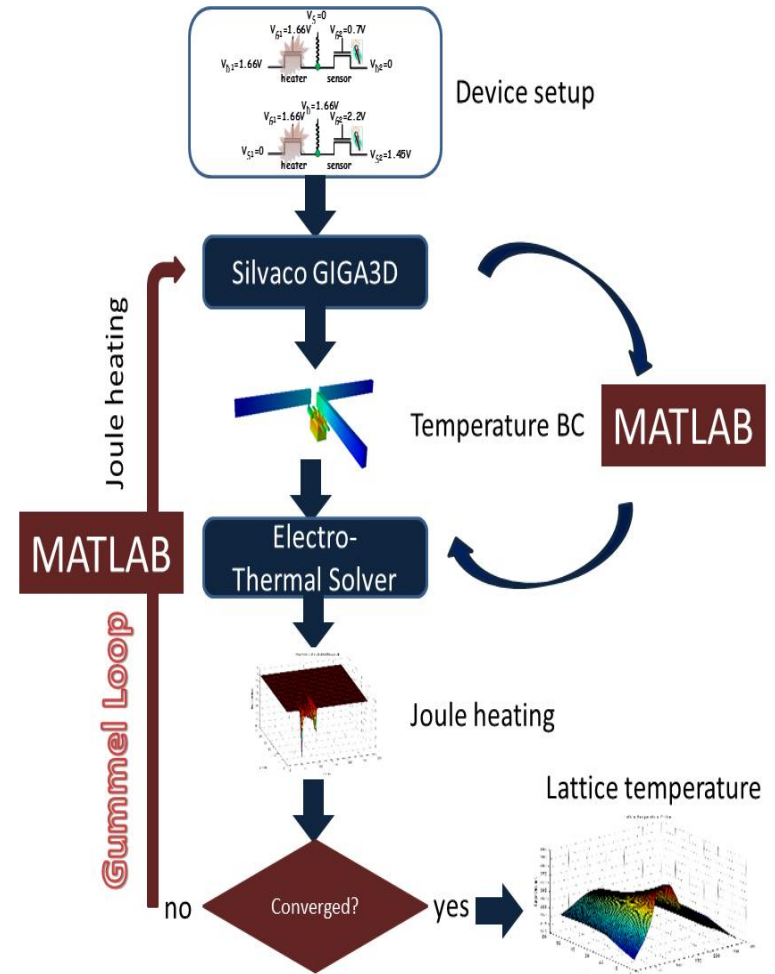
More than 50,000 cores and more than 8 Petabytes of storage used by approximately 3000 faculty and graduate students.

PACE is funded through a mix of central and faculty funding.

External users need to fund or collaborate with internal users.

# External Use of ASU Computing Cluster

- Two International Collaborations with Prof. Vasileska
- **Katerina Raleva** – UKIM, Macedonia: Multiscale modeling of self-heating effects in heater – sensor combination of MOSFETs
- **Gilson Wirth/Alan Rossetto** – UFRGS, Brazil: Modeling of NBTI in p-channel MOSFETs



Multi-scale thermal solver

# Process Simulation Tools

- Can greatly help users and staff and cut cost.
  - Enable in depth analysis and variability studies
  - Fabrication complexity is growing and user experience is decreasing.
  - Not widely used by users.
- 
- Plan to hold hands-on workshops to promote “Simulate before Fabricate”
  - Possible option:
    - Sentaurus TCAD: Fabrication steps: oxidation, diffusion, implantation, etc., Deposition Steps: PVD, CVD, PECVD, etc., Etching processes: Wet etch, RIE, CMP, etc.