NNCI Computation

Azad Naeemi
Georgia Institute of Technology
azad@gatech.edu

National Nanotechnology Coordinated Infrastructure

NSF

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

National Nanotechnology Coordinated Infrastructure

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.

National Nanotechnology Coordinated Infrastructure

NSF

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.

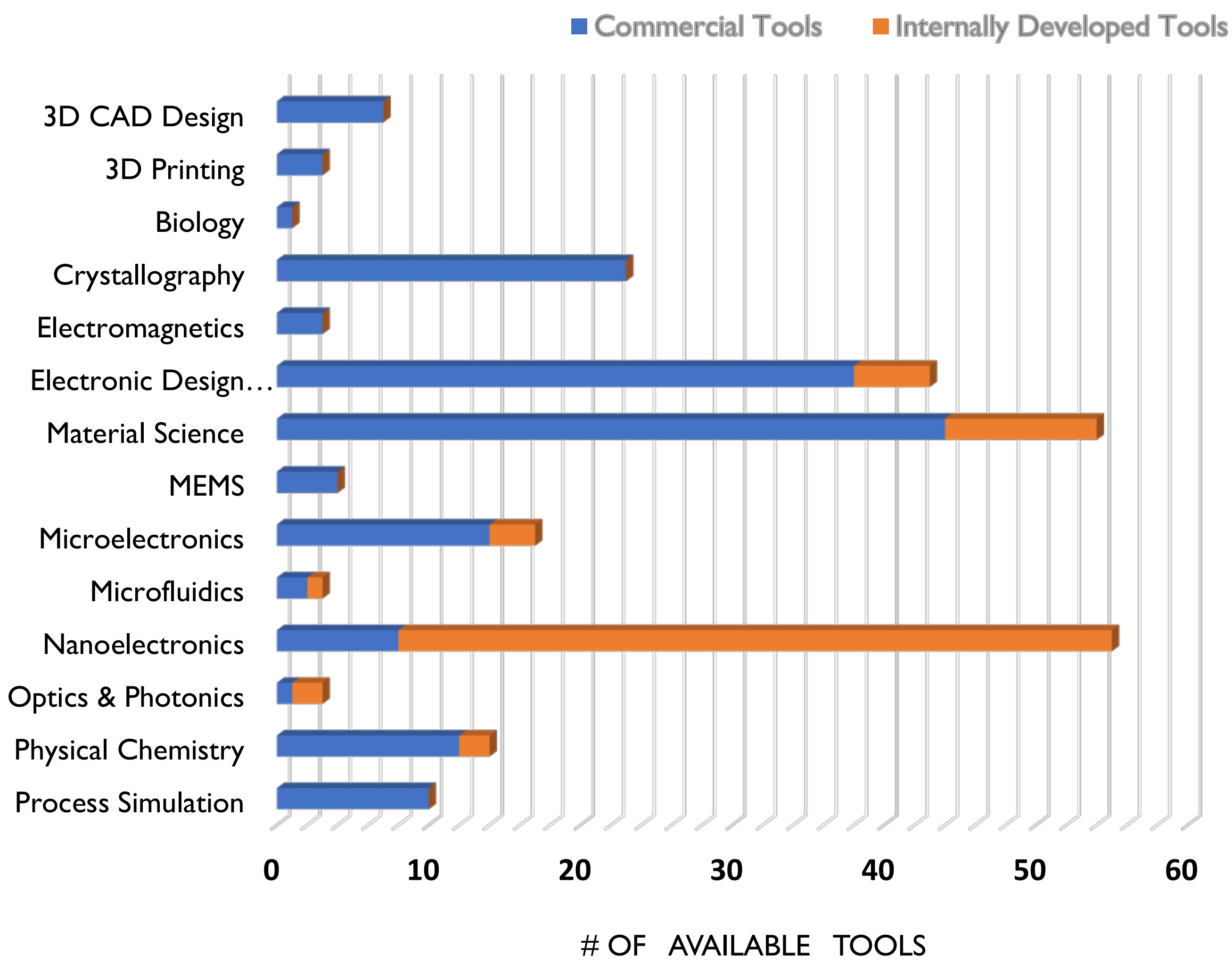
An inventory of available modeling and simulation resources and expertise is being complied. The directory is hosted by nanoHub.org.

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.

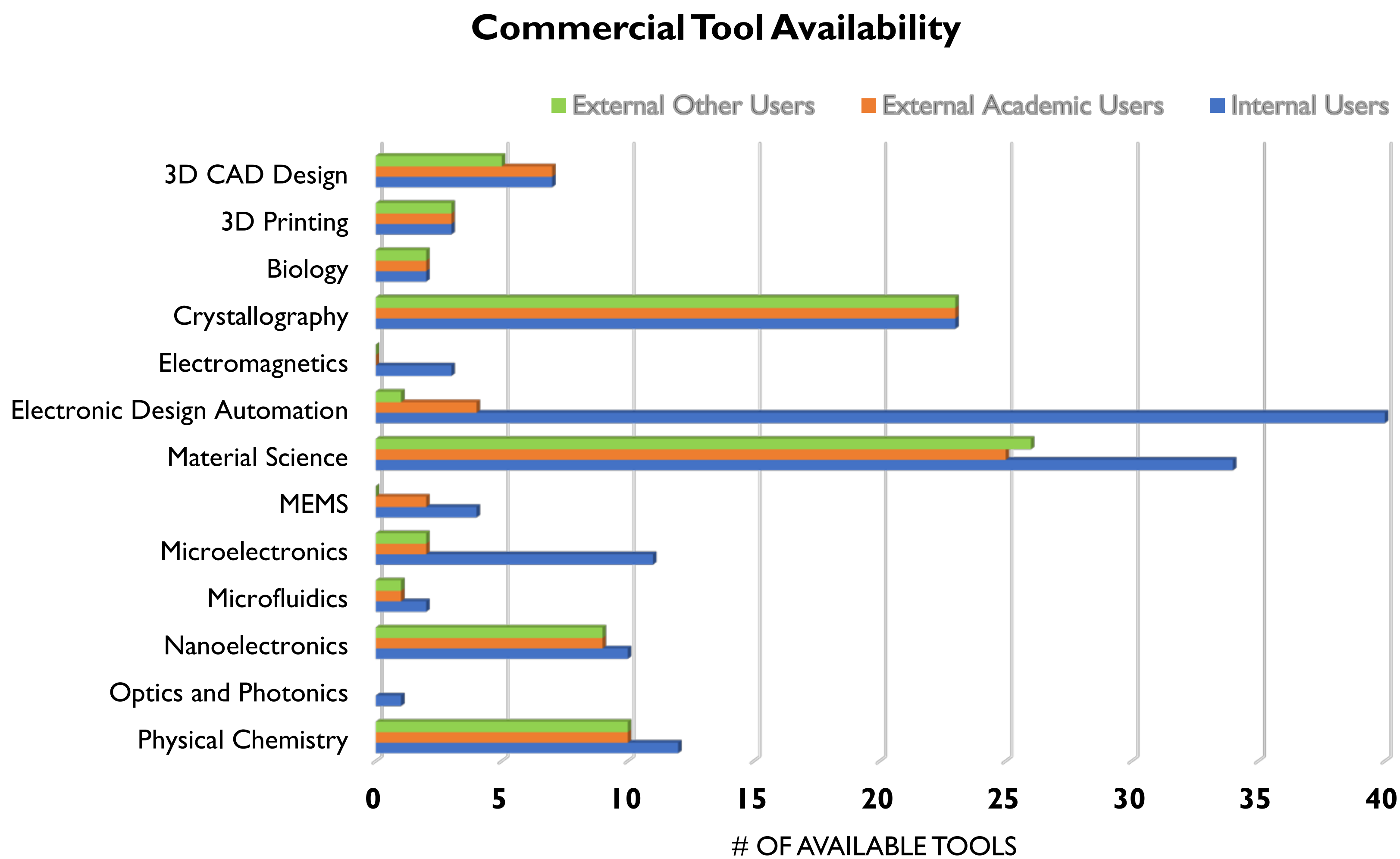
National Nanotechnology Coordinated Infrastructure

Statistics by Disciplines



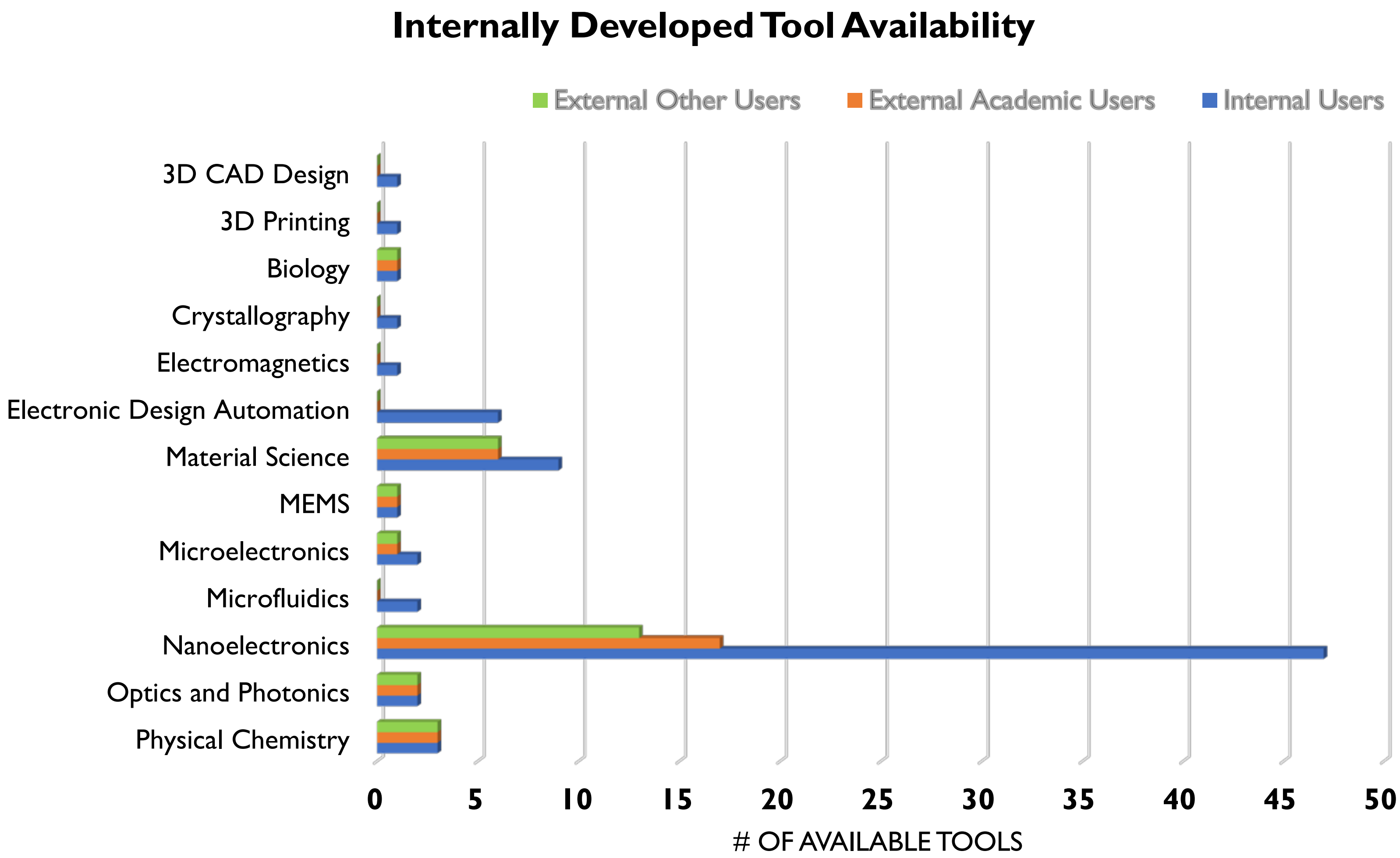
National Nanotechnology Coordinated Infrastructure

Permission to Access: Commercial Tools



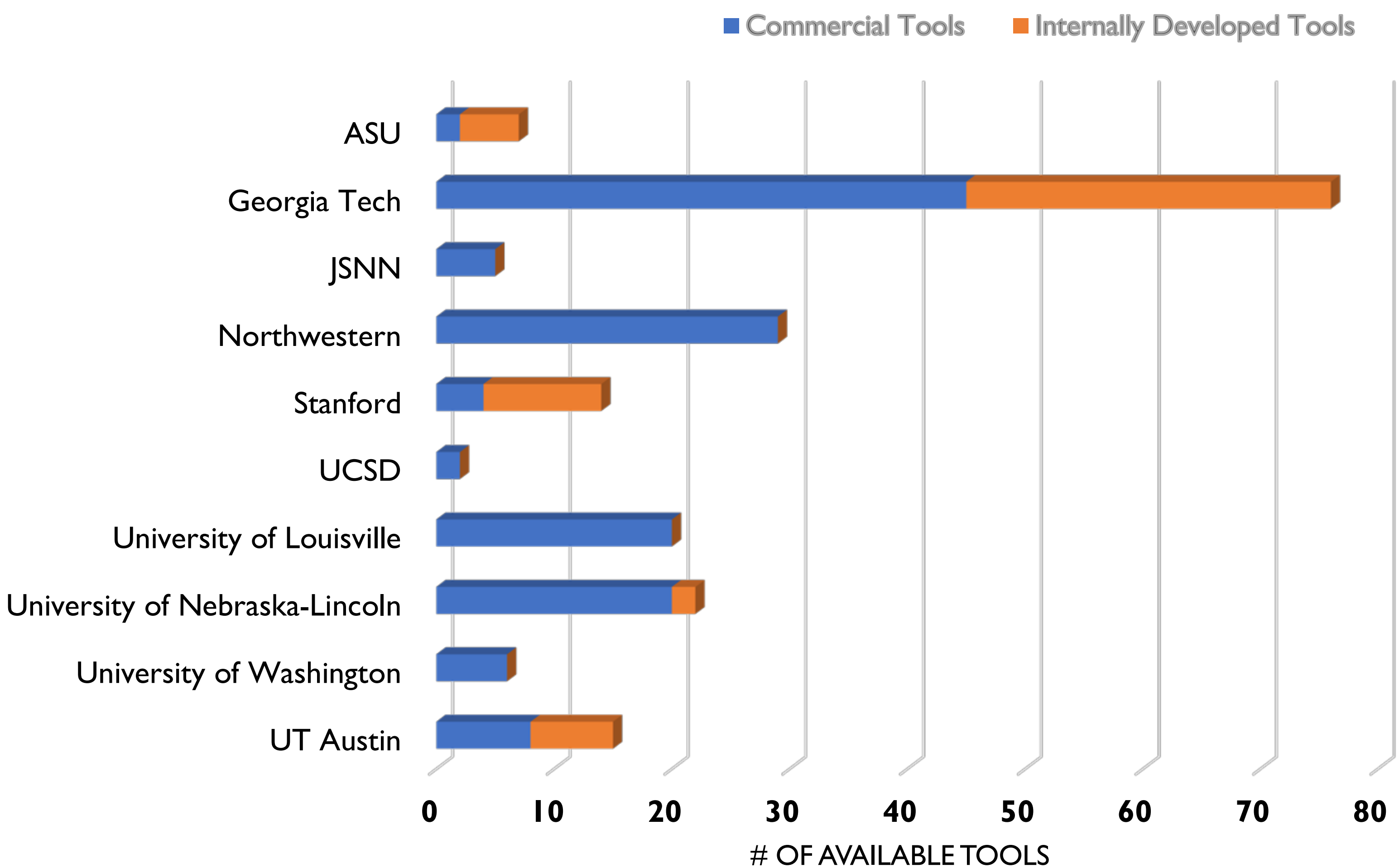
National Nanotechnology Coordinated Infrastructure

Permission to Access: Internally Developed Tools



National Nanotechnology Coordinated Infrastructure

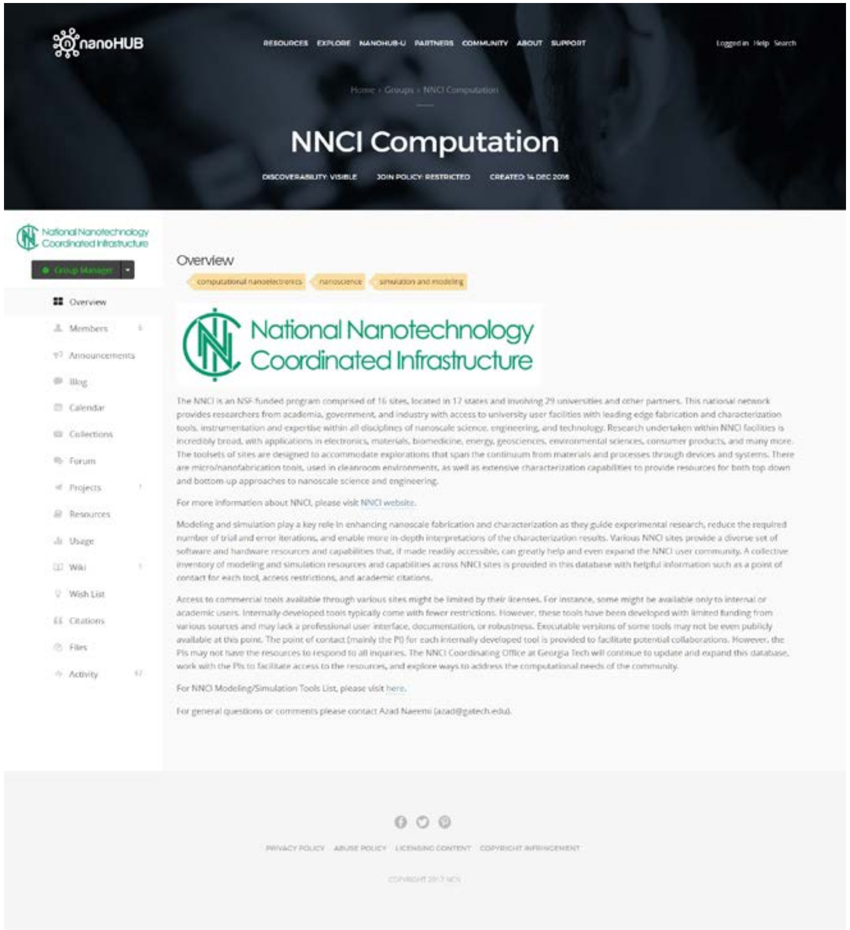
Contributing Universities



National Nanotechnology Coordinated Infrastructure

NNCI Computation Group Page on nanoHUB

nanohub.org/groups/nnci_computation



NNCI Modeling/Simulation Tools List

Download | Exit Fullscreen | Clear Filters | No-Wrap

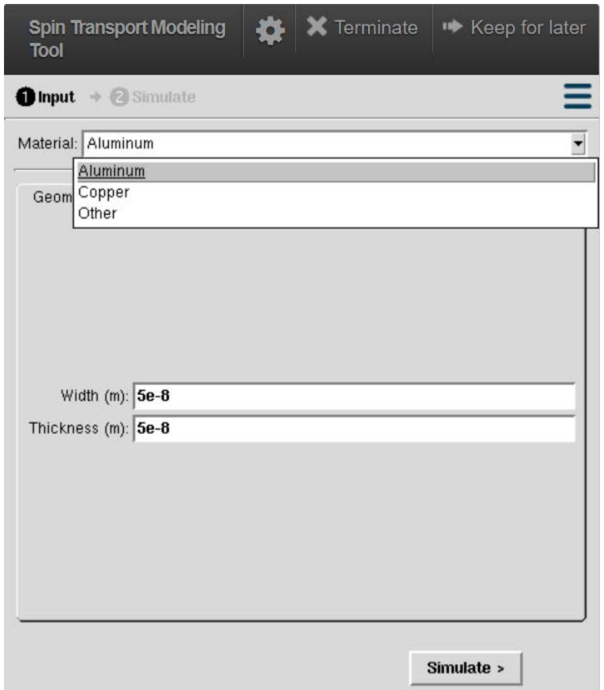
Show 50 entries — First Previous 1 2 3 4 Next Last

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, Physcial 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
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
Electronic design automation	SIWave	A specialized design platform for power integrity, signal integrity and EMI analysis of

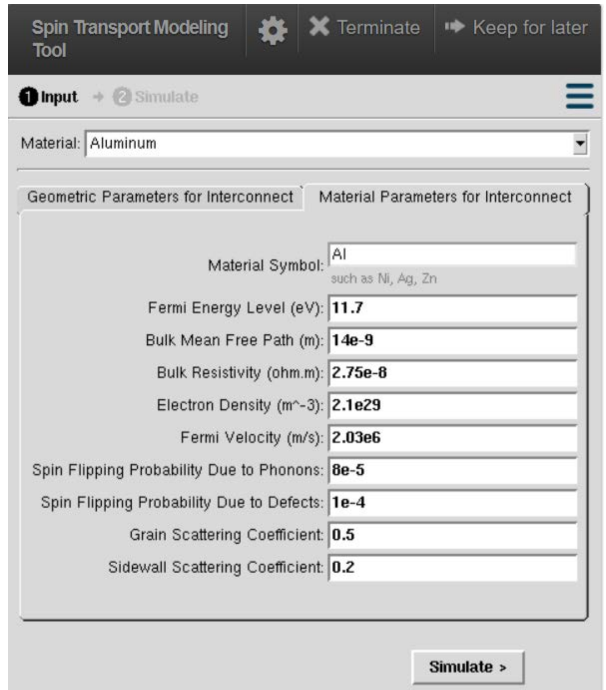
National Nanotechnology Coordinated Infrastructure

Spintronic Transport Modeling Tool

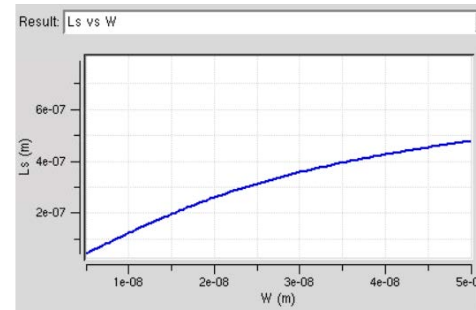
nanohub.org/tools/spintransport/

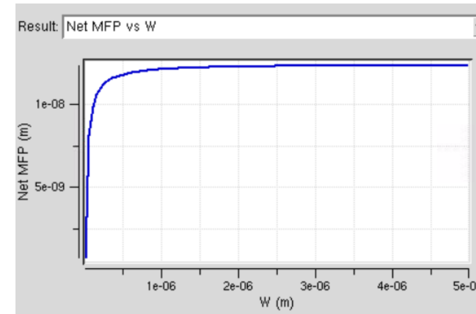


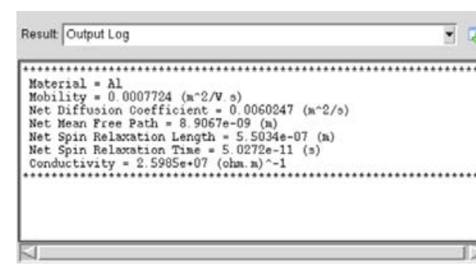
- Choose right material for your interconnect



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







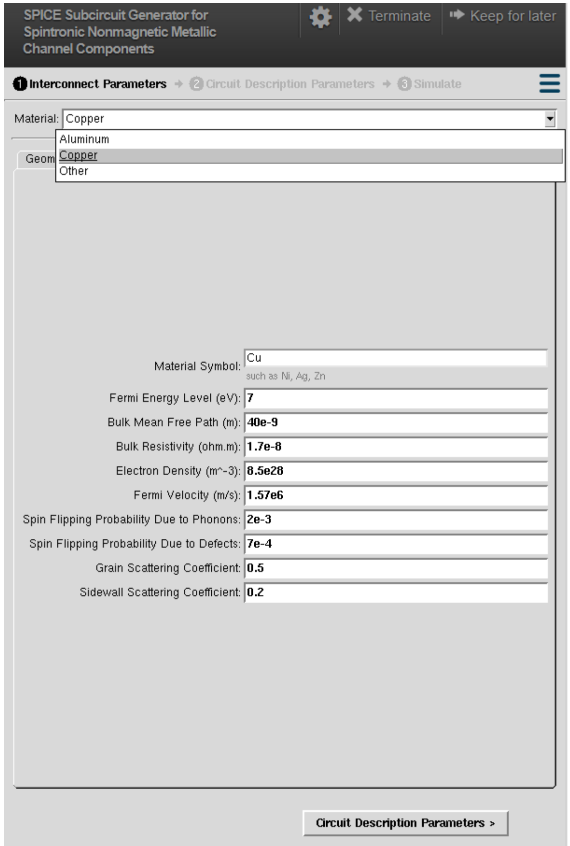
- Obtain electron-spin transport physics-based simulation results

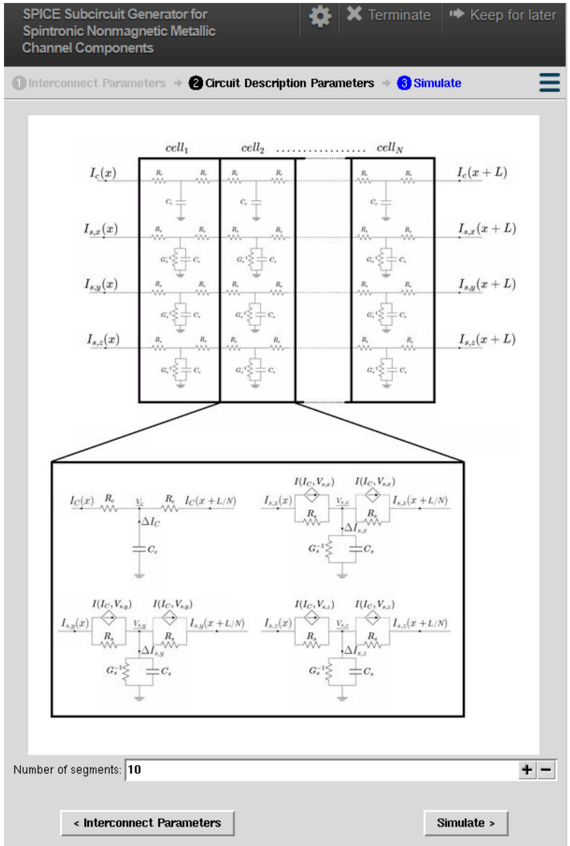
National Nanotechnology Coordinated Infrastructure

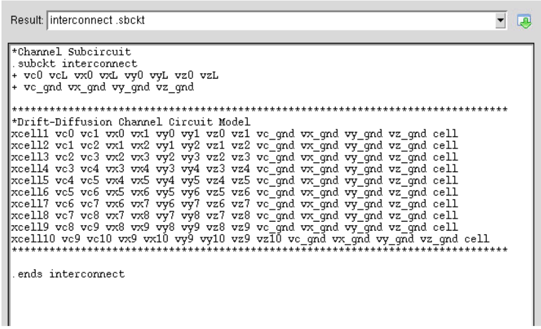
NSF

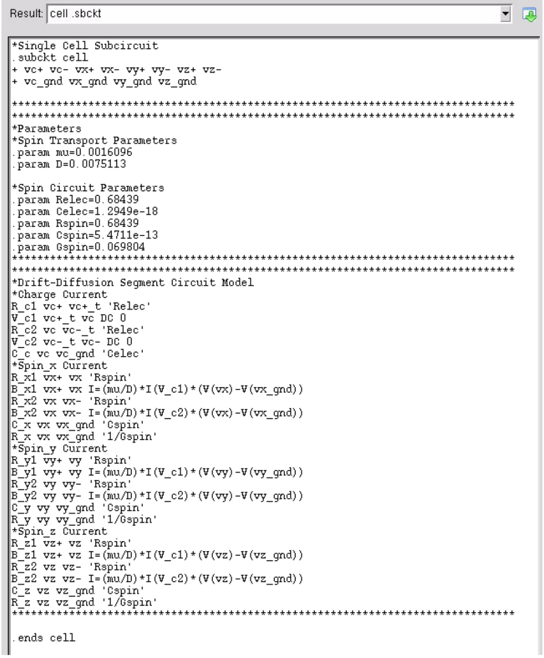
SPICE Subcircuit Netlist Generator for Spintronic Nonmagnetic Metallic Channel

nanohub.org/tools/spincircuit/









- Choose right material for your interconnect
- Use developed compact circuit model for spintronic transport
- Obtain SPICE subcircuit netlist describing spin&electron transport in channel

National Nanotechnology Coordinated Infrastructure

NSF

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

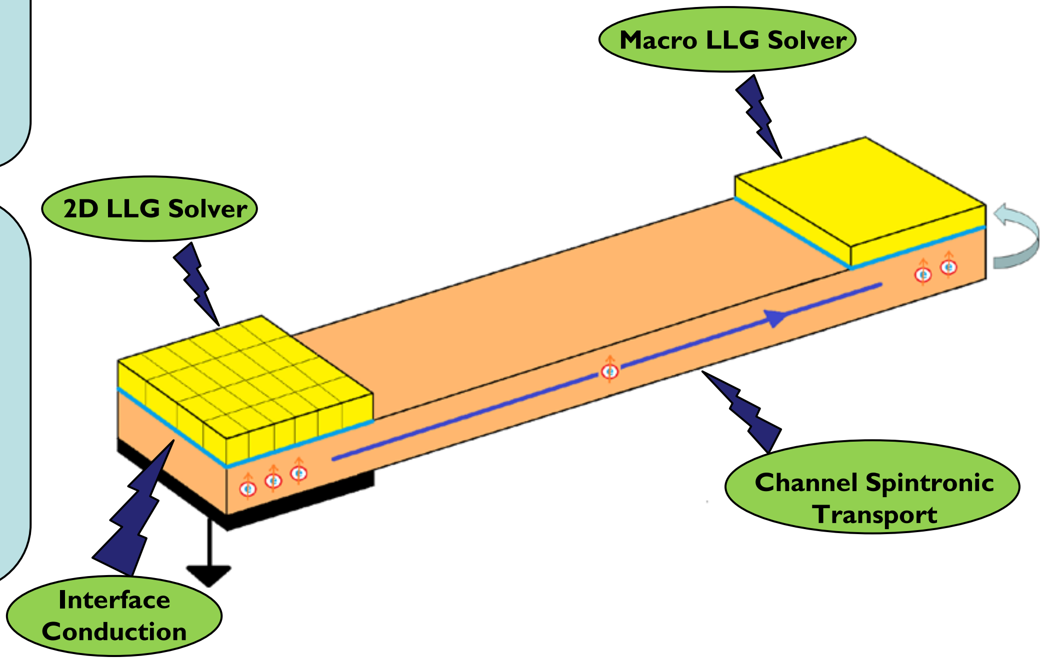
Interface Conduction Subcircuit Models

- Ferro – Nonmagnetic Metallic Interface

Channel Spintronic Transport Subcircuit Models

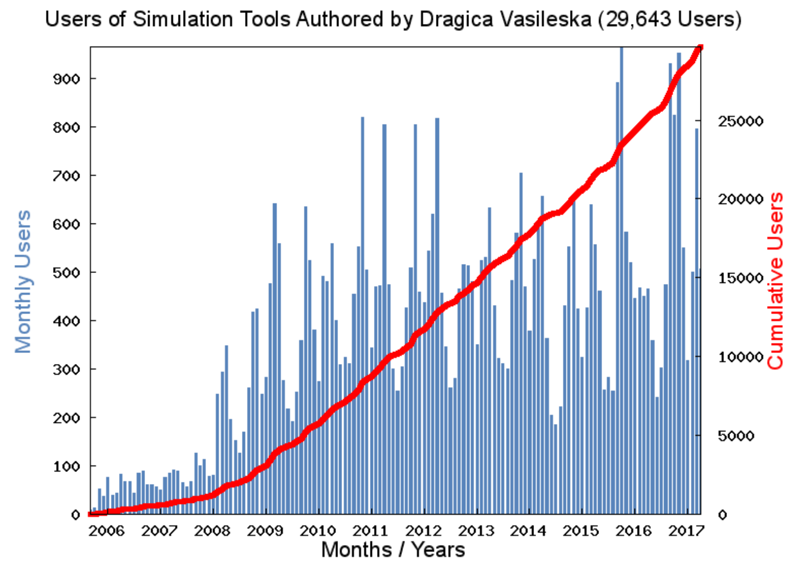
- Electron Transport
- Spin Transport
- Spintronic (both electron&spin) Transport

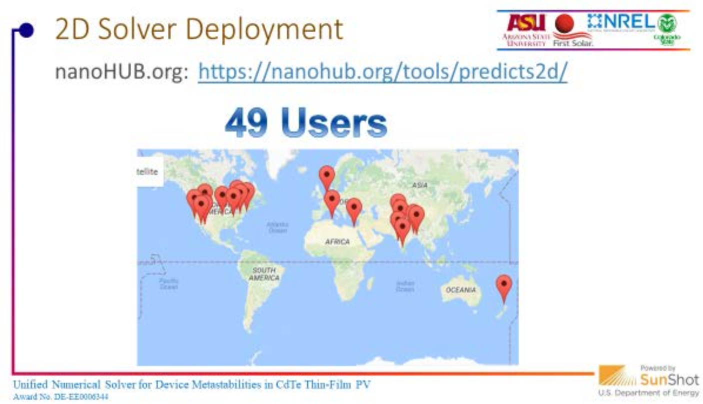
- Various modules to model and simulate various spintronic devices/circuits in SPICE.



National Nanotechnology Coordinated Infrastructure

Simulation Tools from ASU





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

National Nanotechnology Coordinated Infrastructure

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.

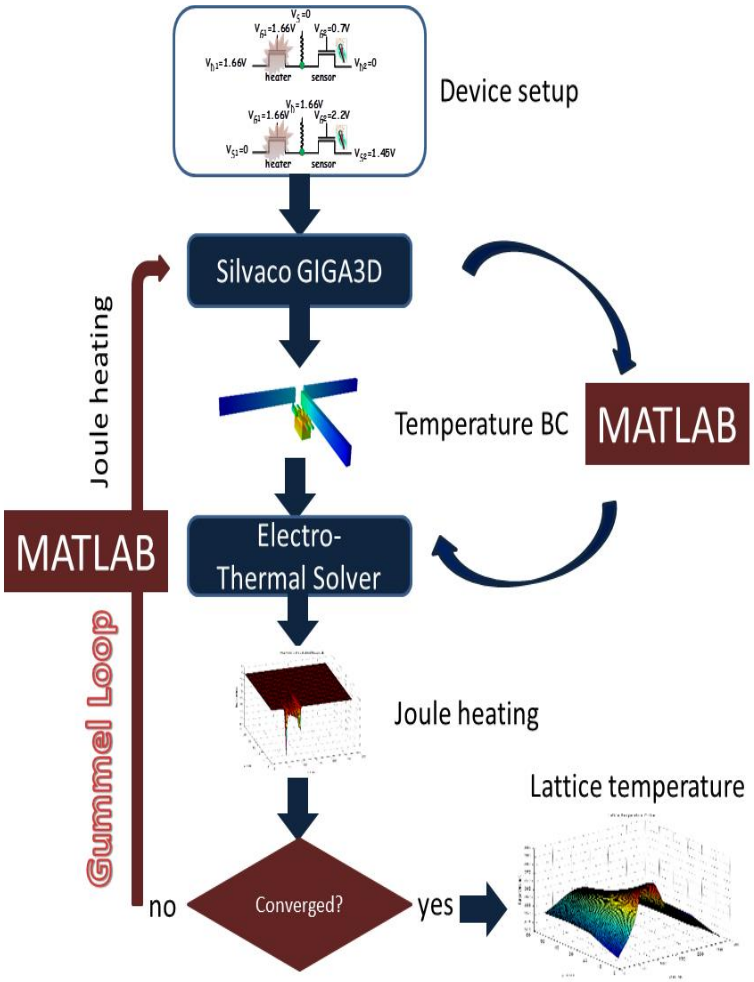
National Nanotechnology Coordinated Infrastructure

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

National Nanotechnology Coordinated Infrastructure

NSF

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.