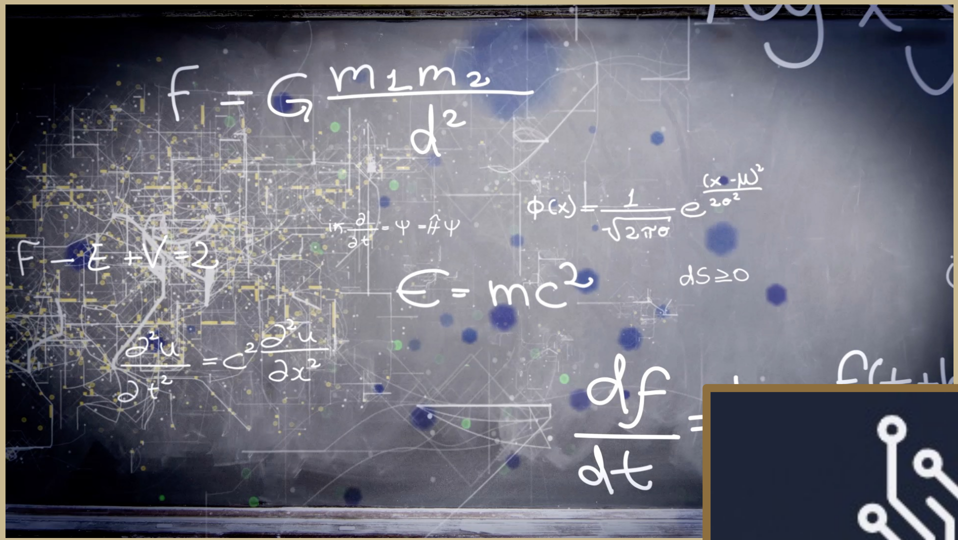

# Community Building: Global Translational Impact on Research and Education

chipshub by nanoHUB

PURDUE UNIVERSITY


**Gerhard Klimeck**
Director of nanoHUB
Deputy CIO for Academic IT
Fellow of APS, IOP, IEEE, AAAS

**Ale Strachan**
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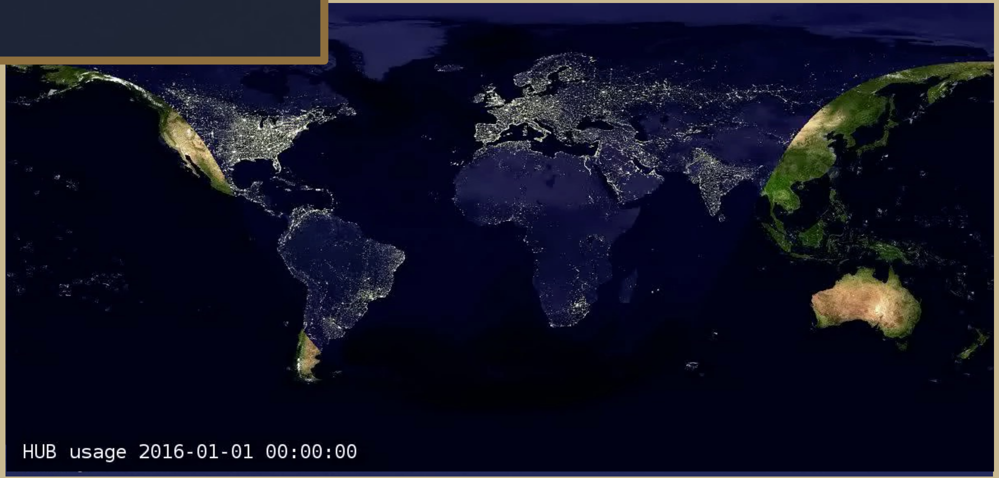
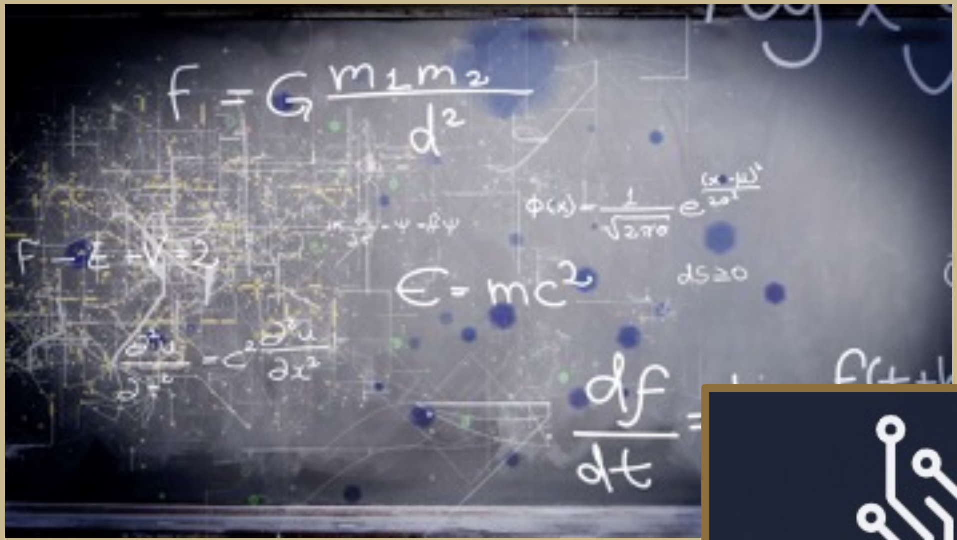



20+ years of "cloud" service – Software as a Service

**From Theory to Immersive Learning to Design (to Fabs)**



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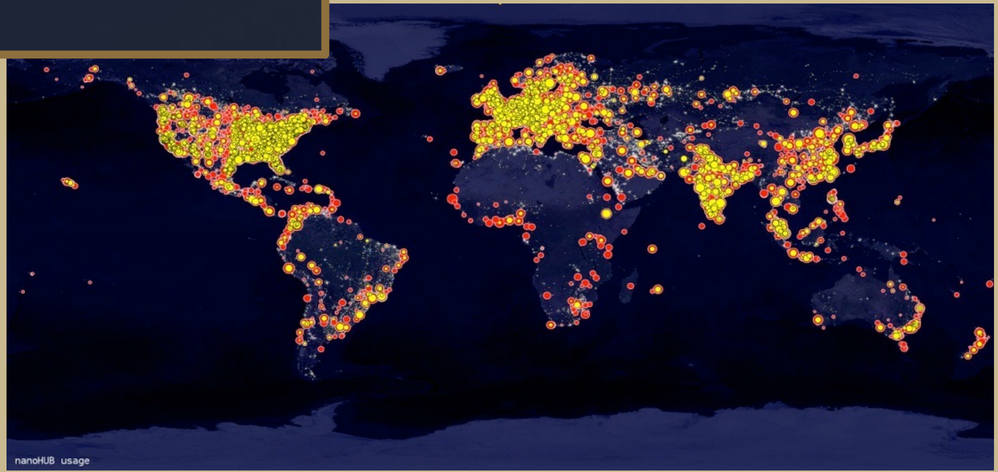


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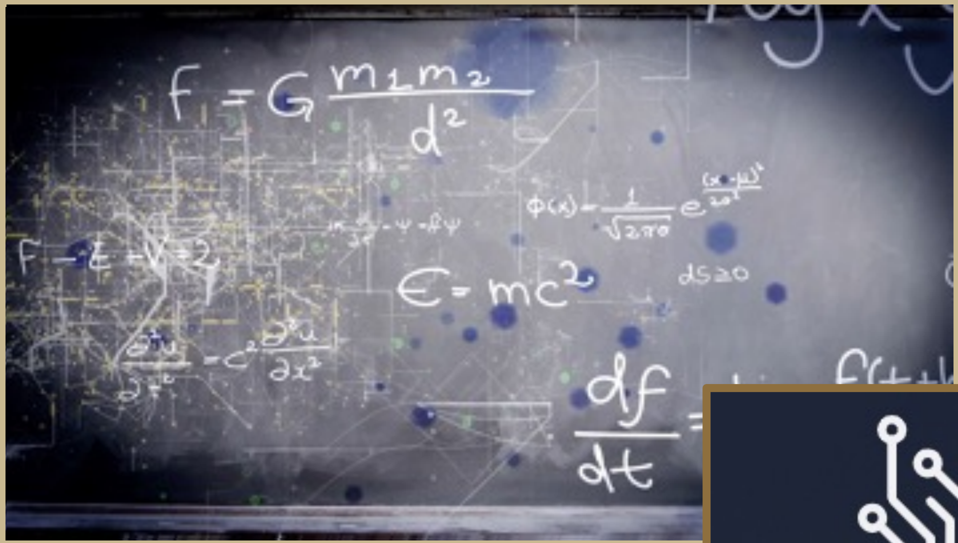

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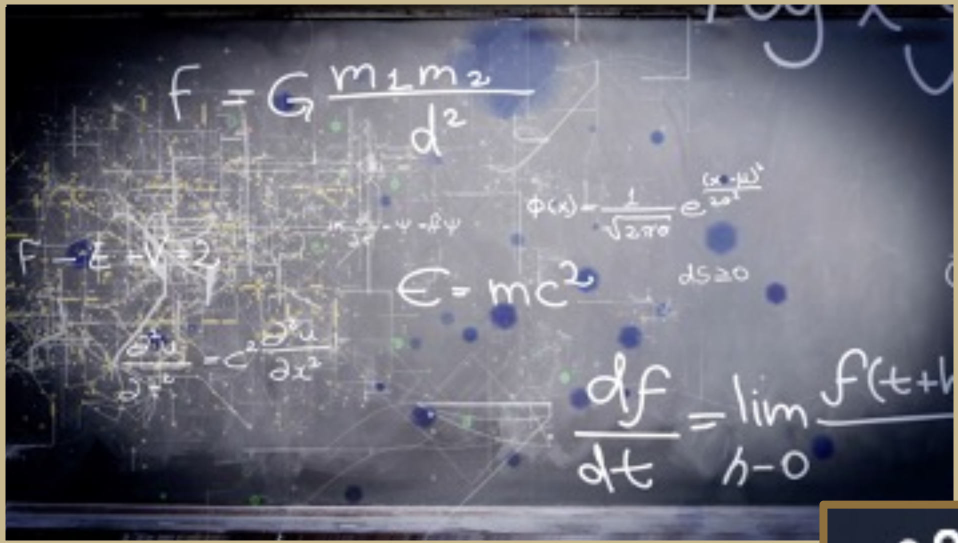

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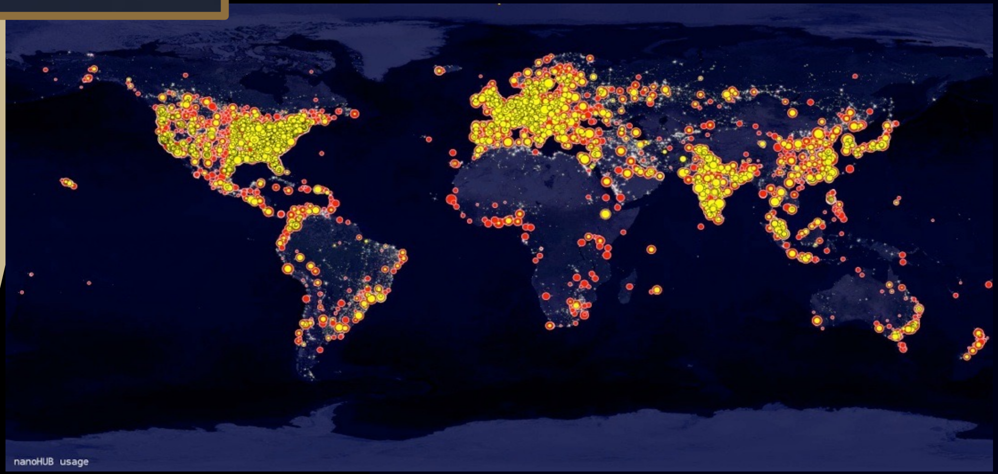


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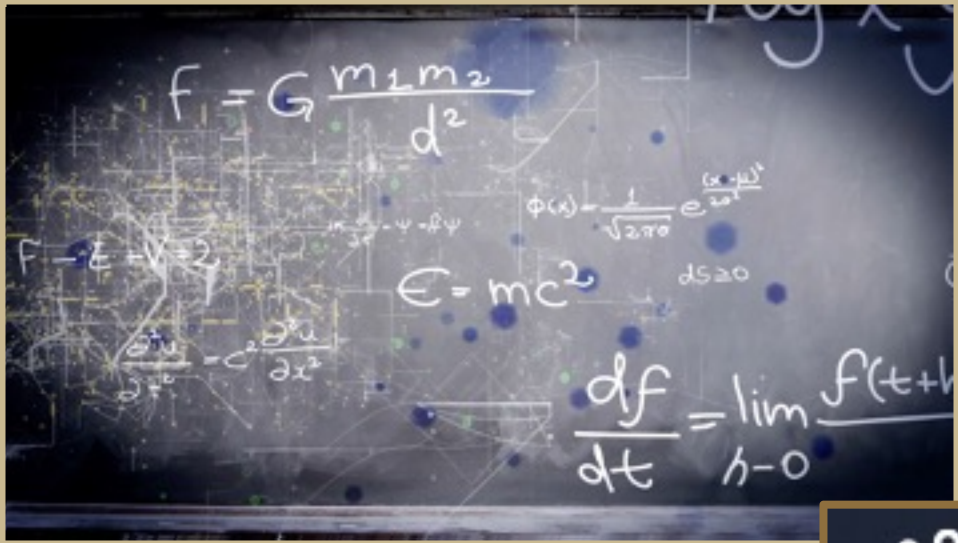

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"No experimentalist will ever use this!"

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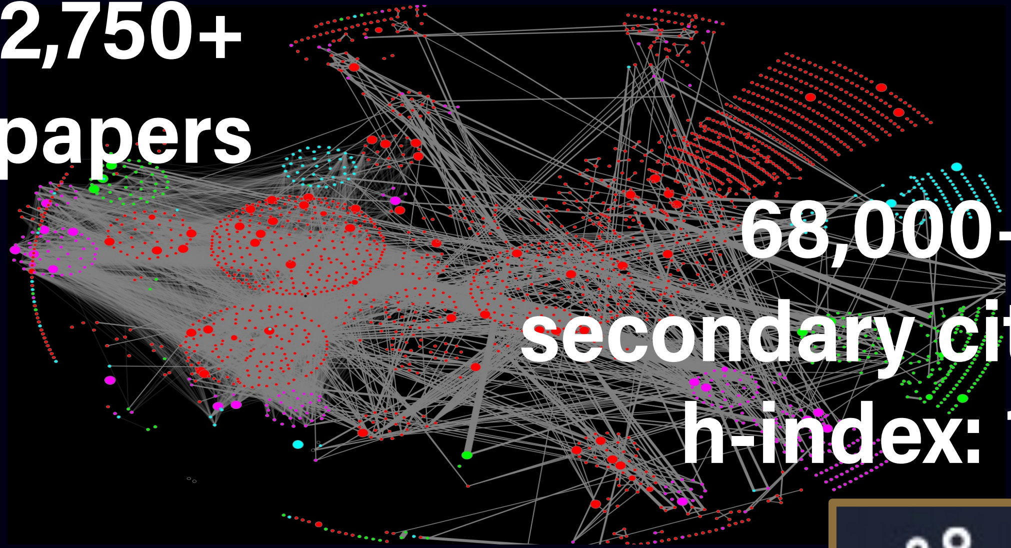

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68,000+ secondary citations

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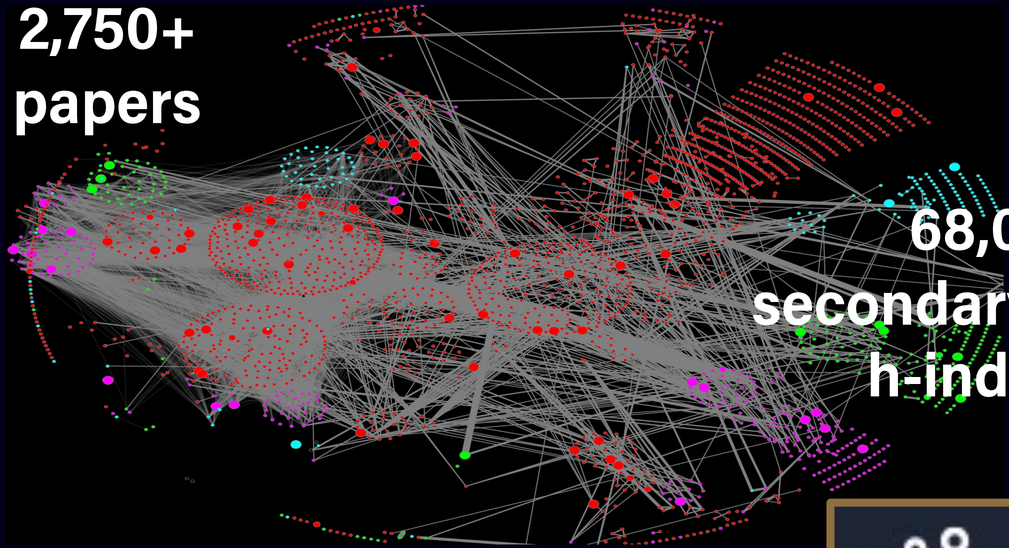

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949 papers w/ exp. data

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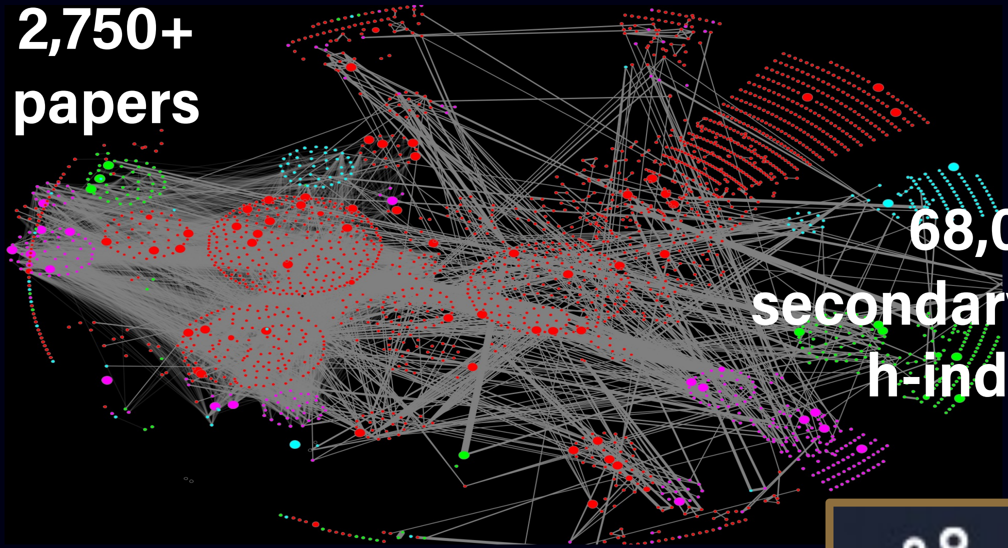

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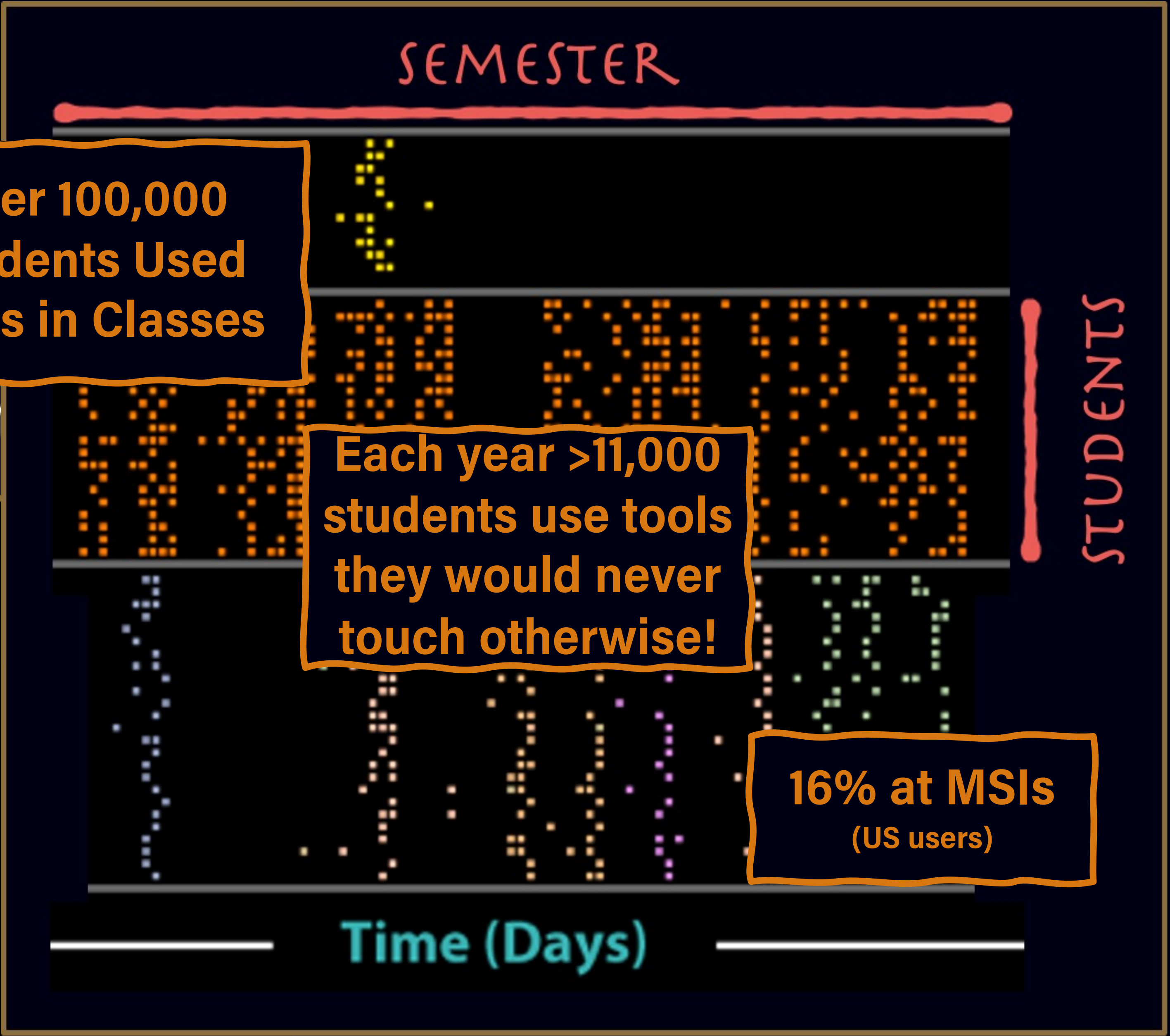

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**1 faculty => many students**

**Over 100,000 Students Used Tools in Classes**

**Community Building!**

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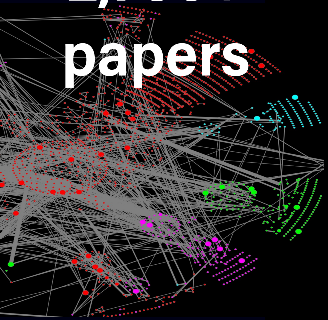

nanoHUB

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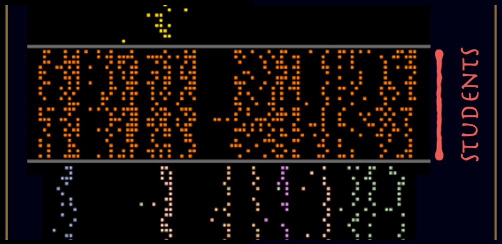


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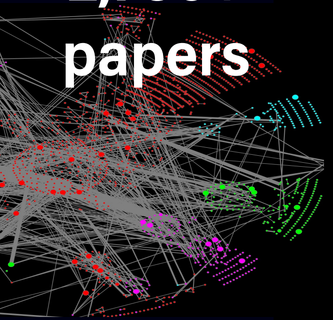

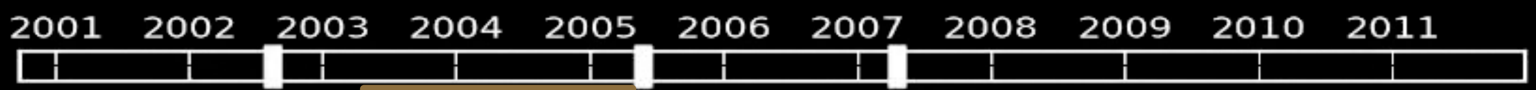


nanoHUB

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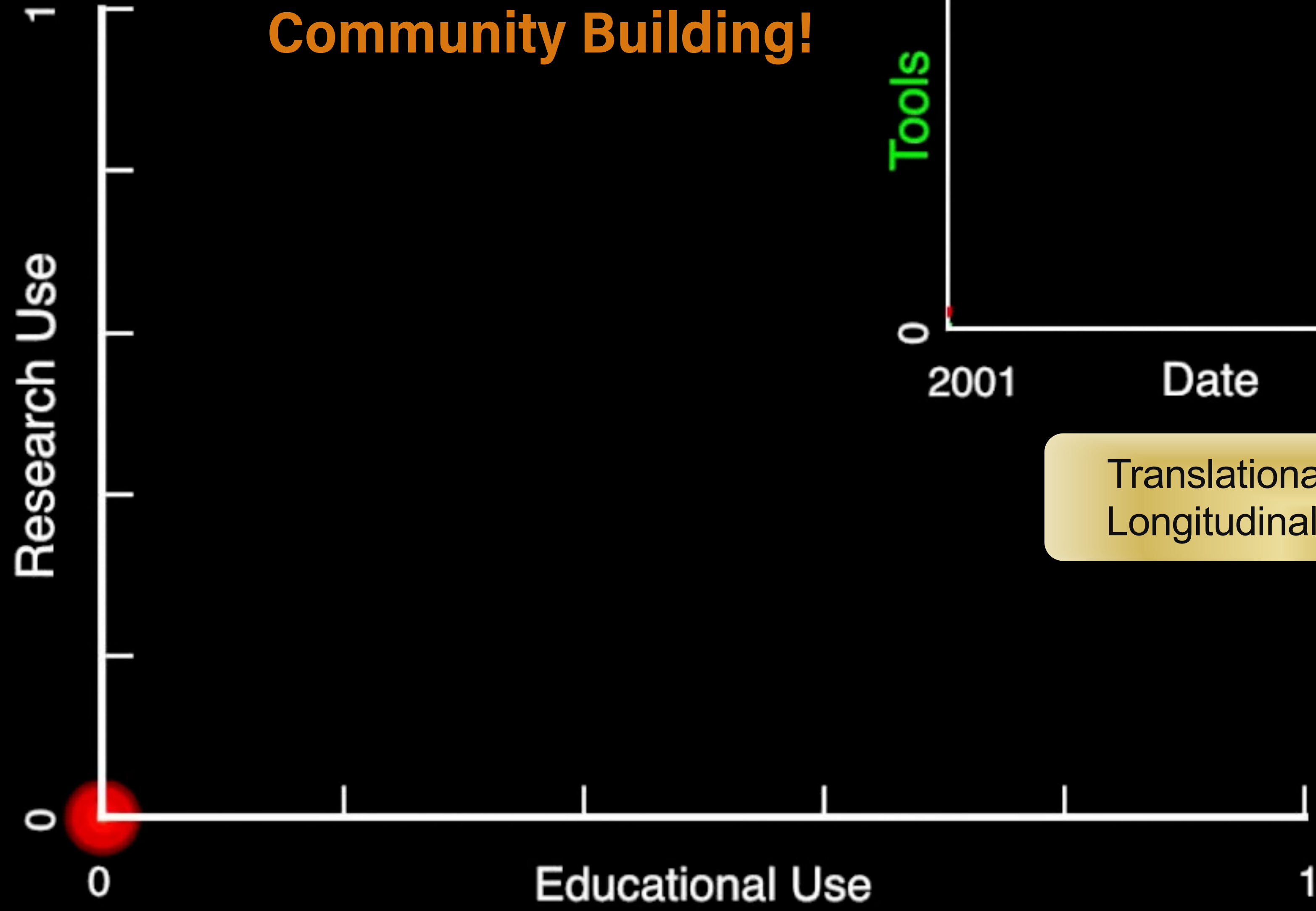
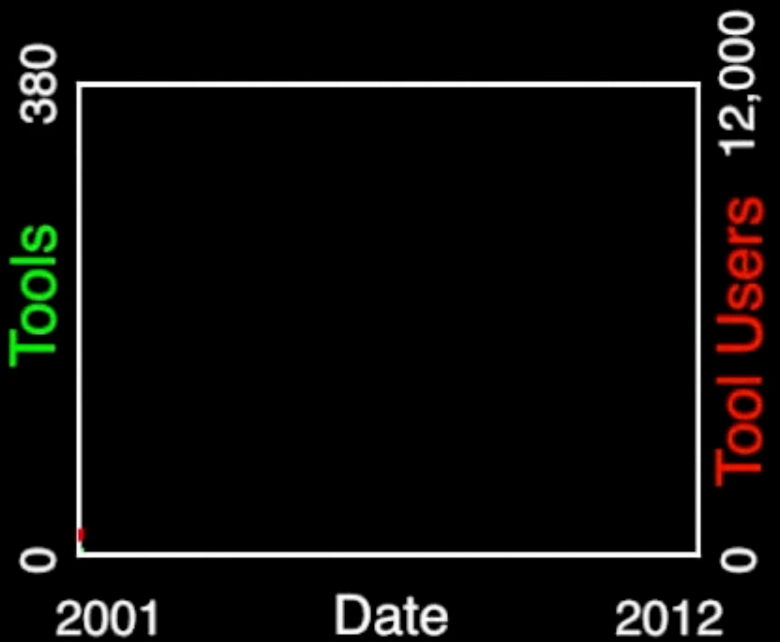
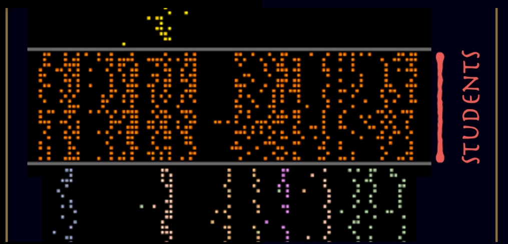



Translational with Longitudinal Data

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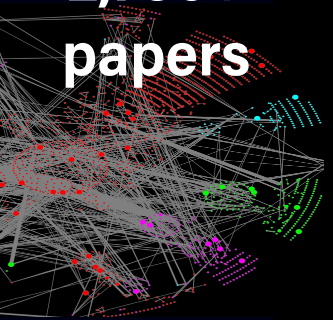


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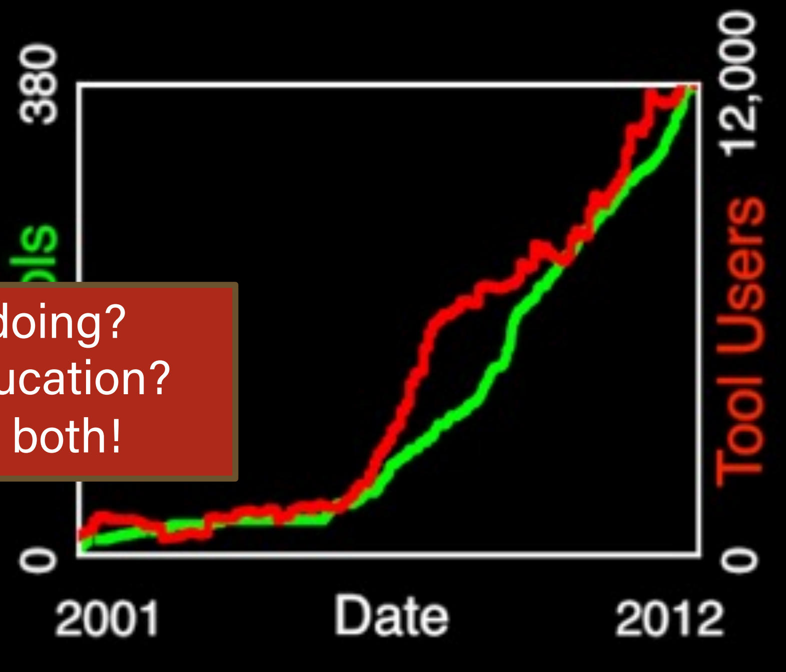


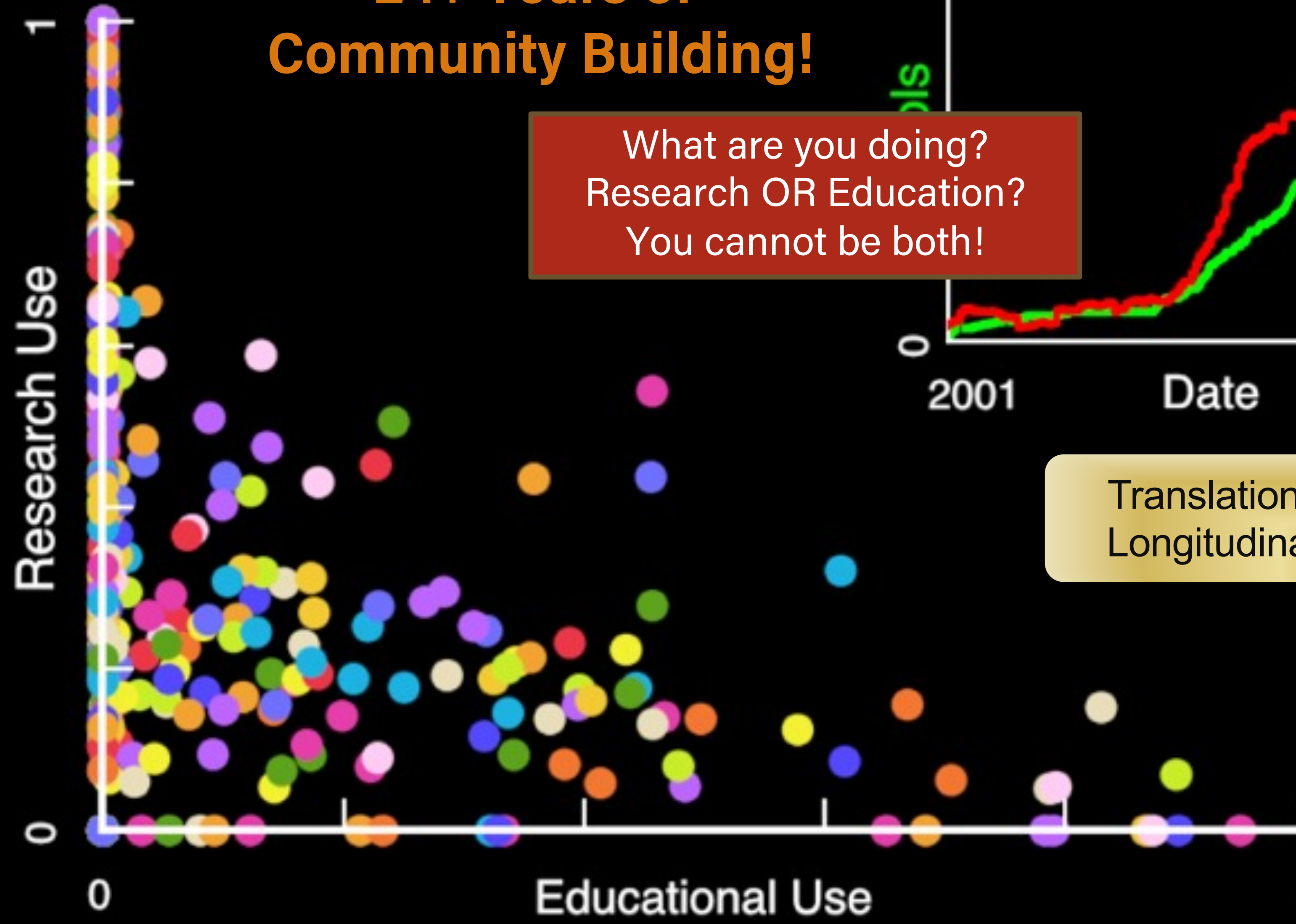


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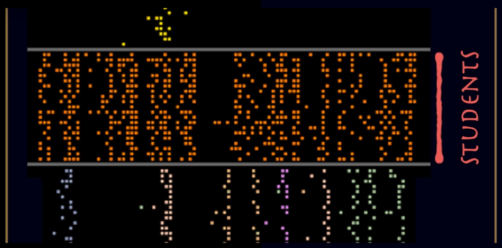


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nanoHUB

**Compact Models**

**FAIR Data**

**findable, accessible, interoperable, reusable**

**Couple nH Data to AI**

**We store all app-based simulation runs!**

**Community Building!**

**Ease of Use!**


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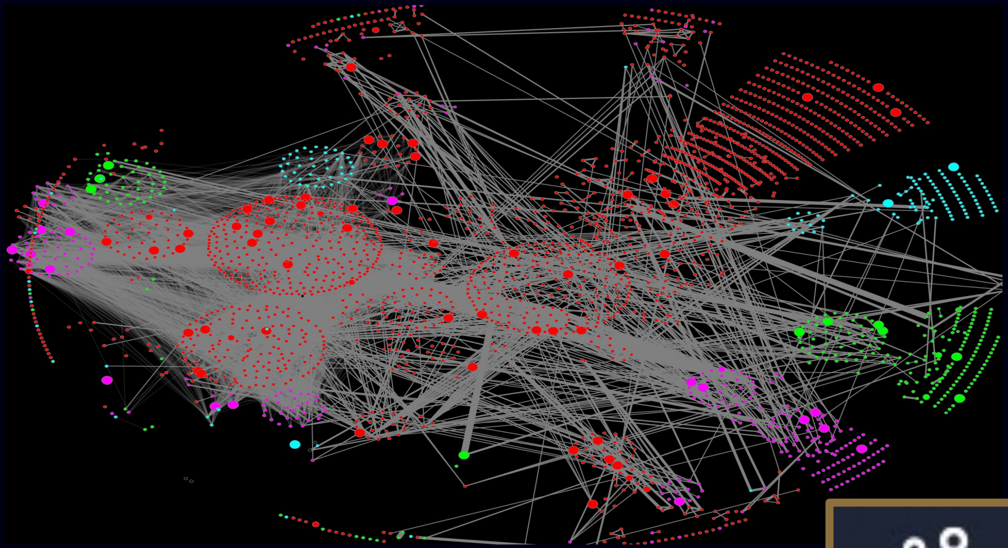

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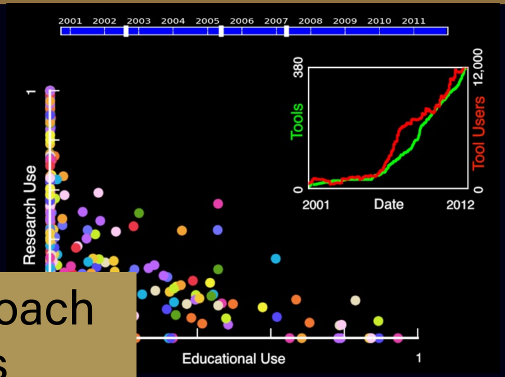


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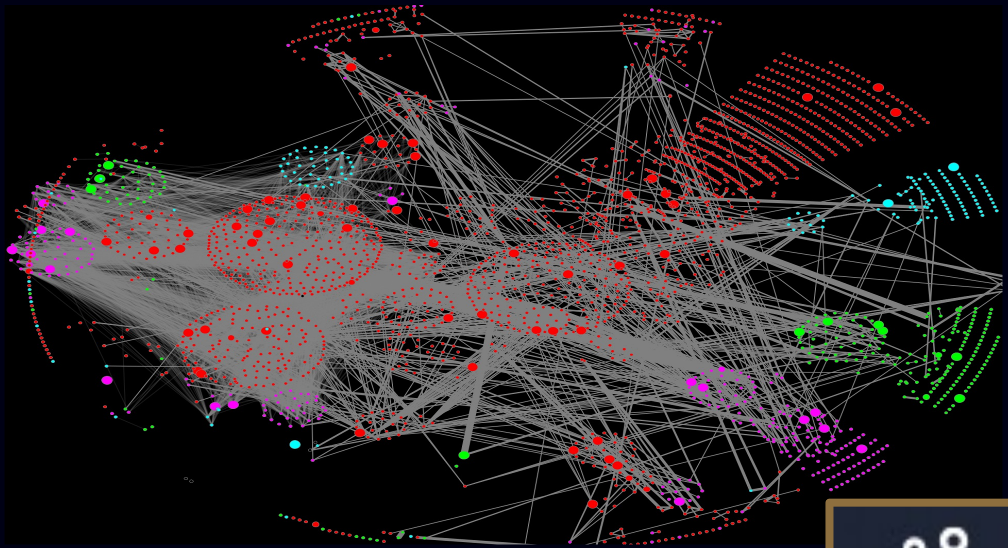

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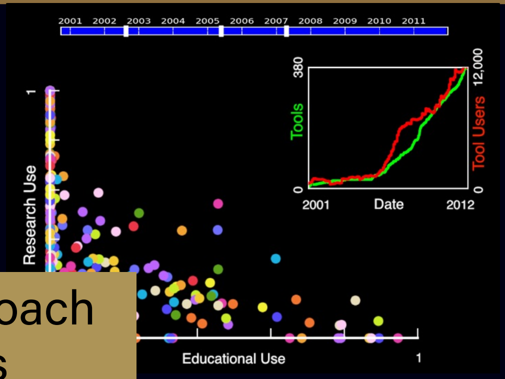


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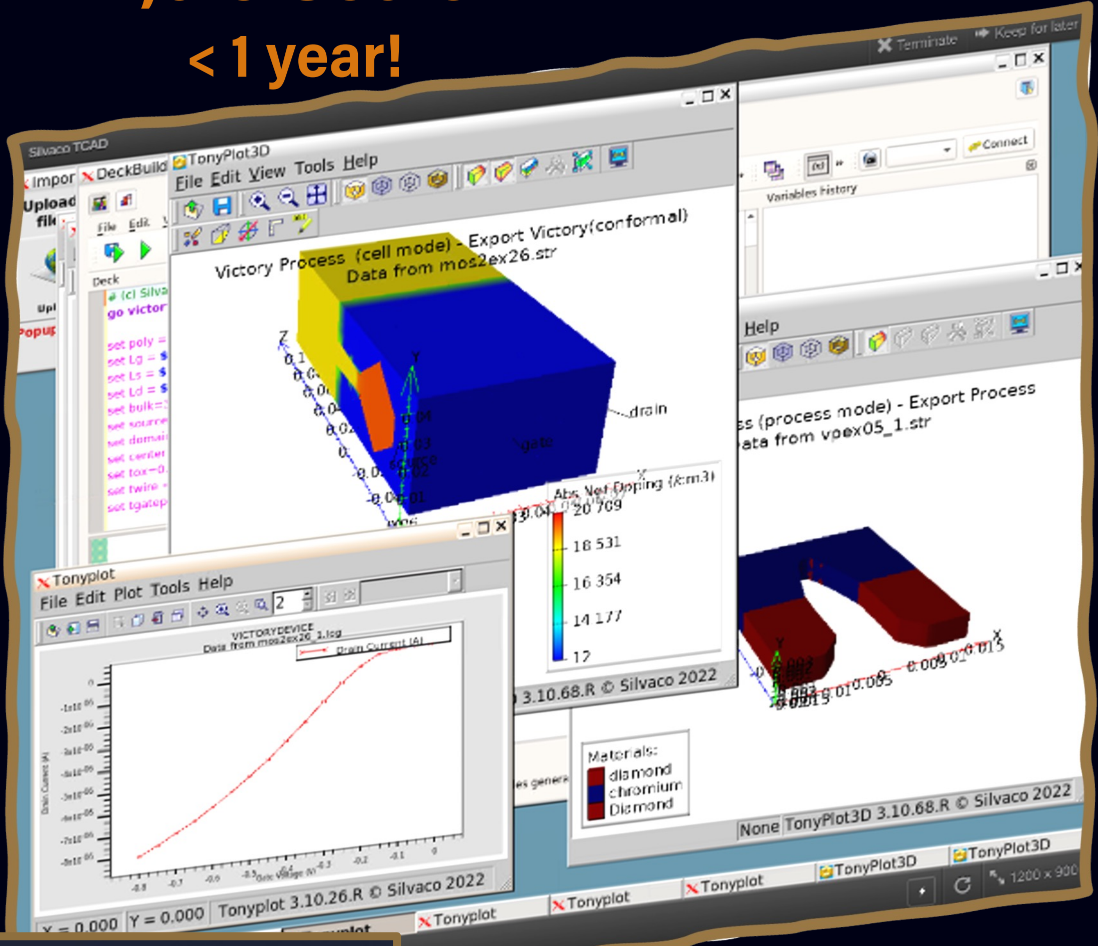
**SILVACO**

**1,015 Users**

**< 1 year!**



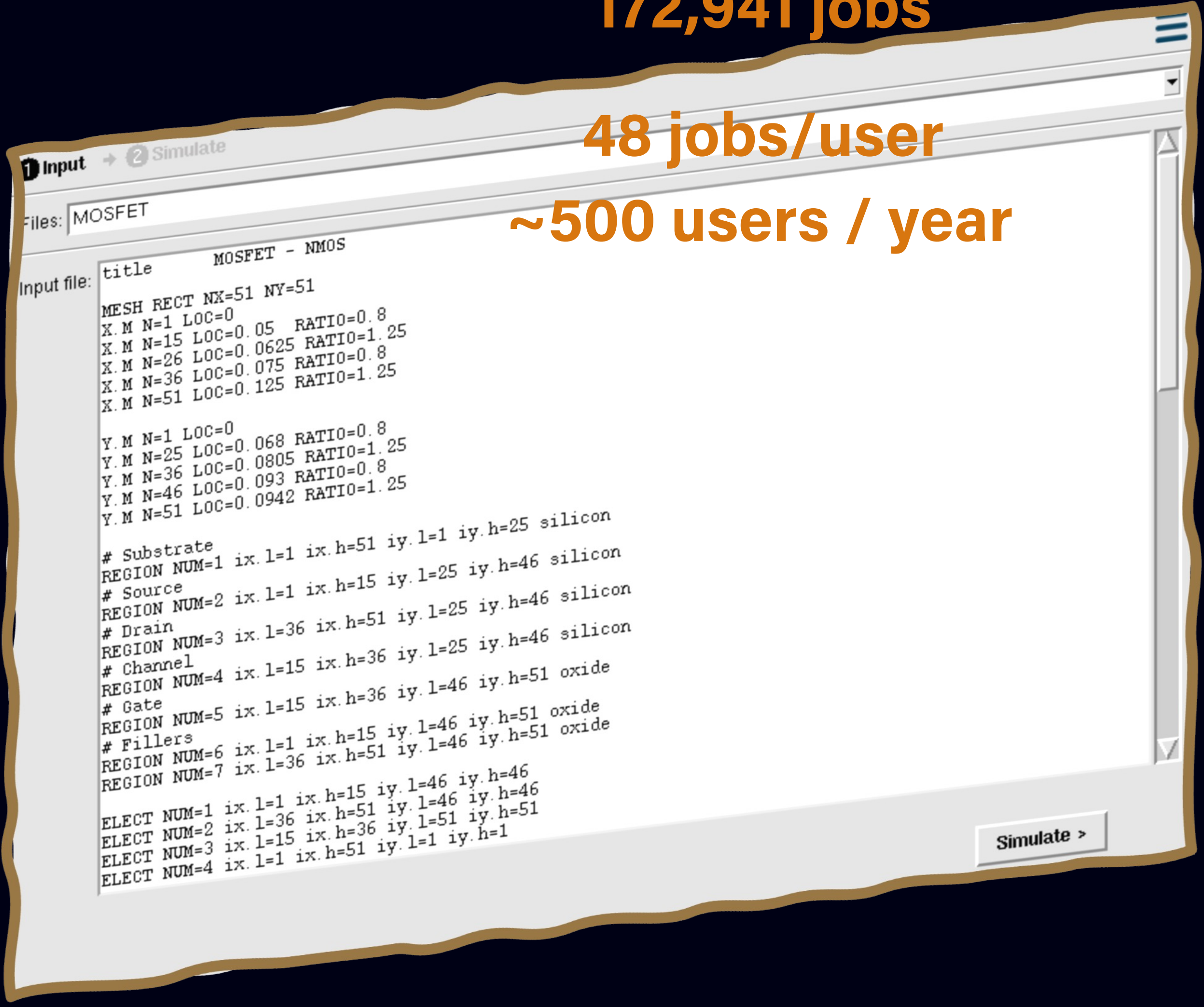

**PADRE / Bell Labs**

**3,566 Users,**

**172,941 jobs**

**48 jobs/user**

**~500 users / year**



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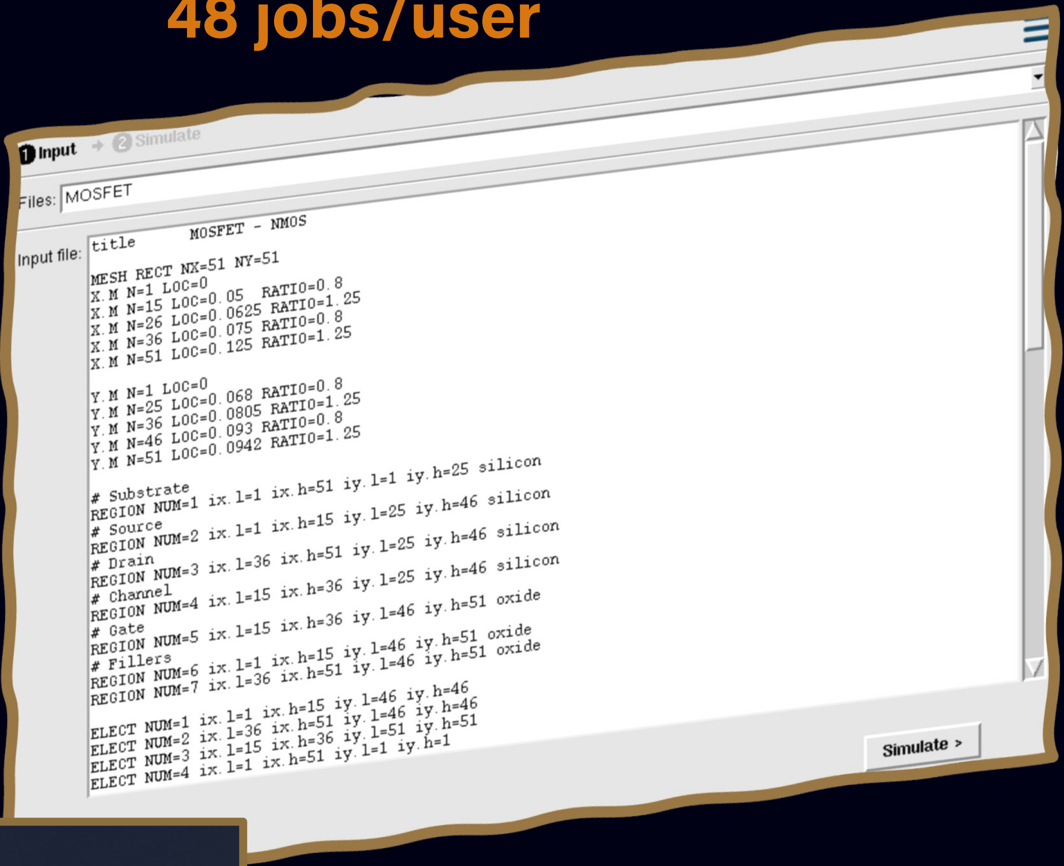
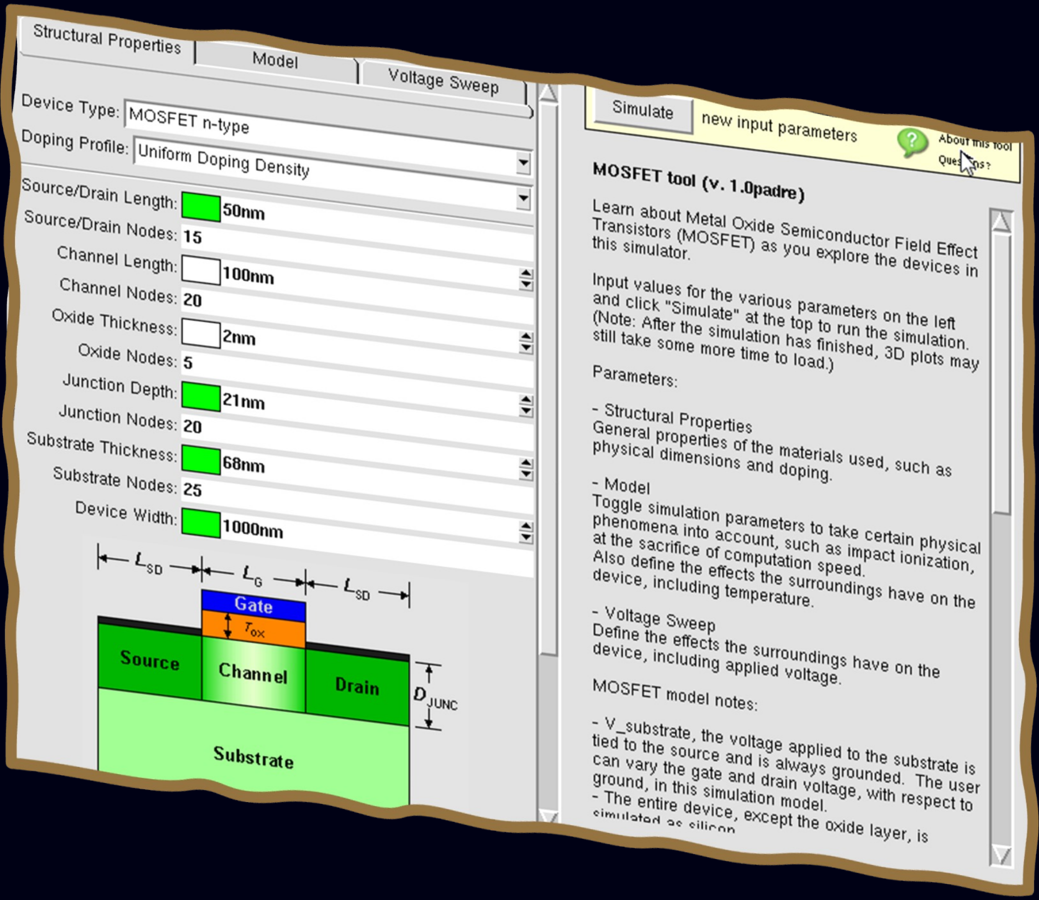



**MOSFET:**
**11,300 Users,**
**227,000 jobs**

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# Ease of Use!

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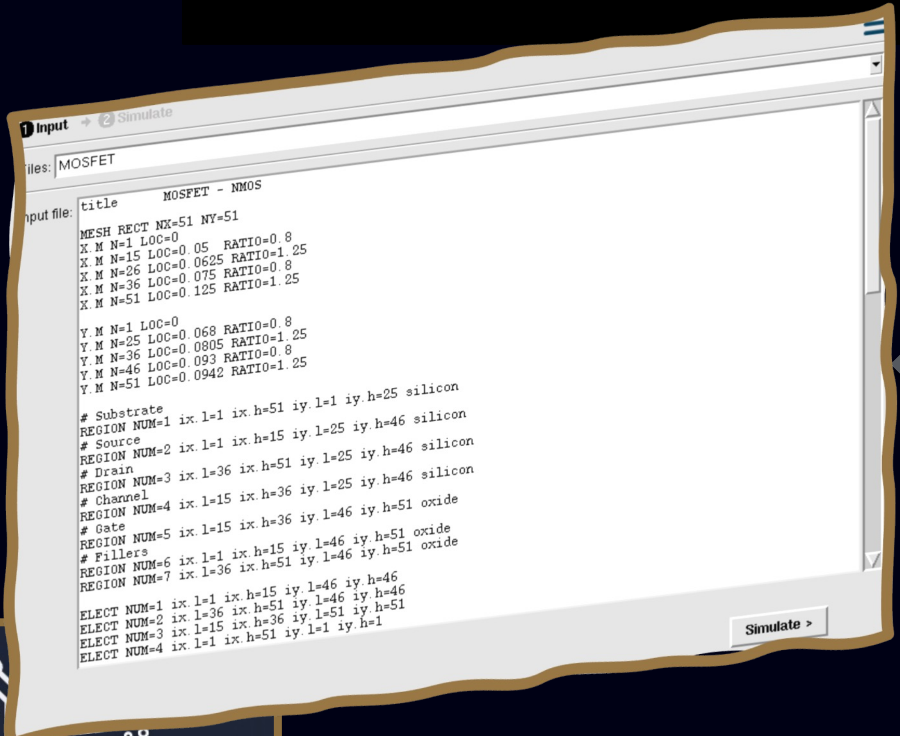
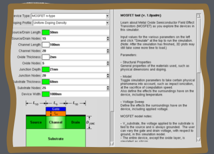
172,941 jobs

17x
4x

59,125 Users,
770,462 jobs



MOSFET:
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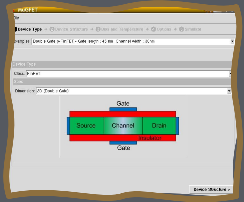
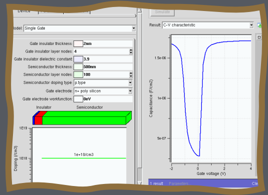
227,000 jobs

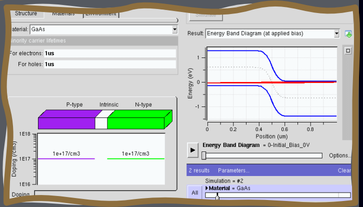
MUGfet:
3,846 Users,
52,619 jobs

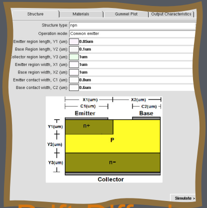




MOSCAP:
9,010 Users,
123,728 jobs

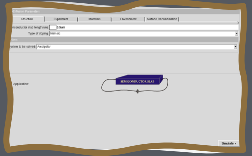
PN junction:
24,012 Users,
249,178 jobs





BJT:
5,084 Users,
41,433 jobs

Drift-Diffusion:
5,873 Users,
75,705 jobs



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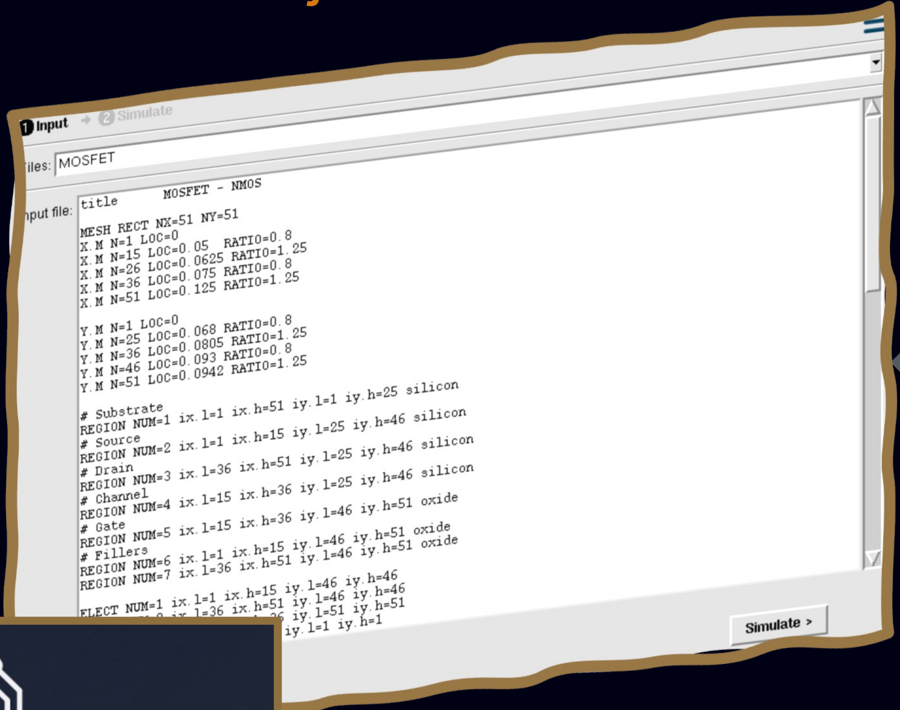
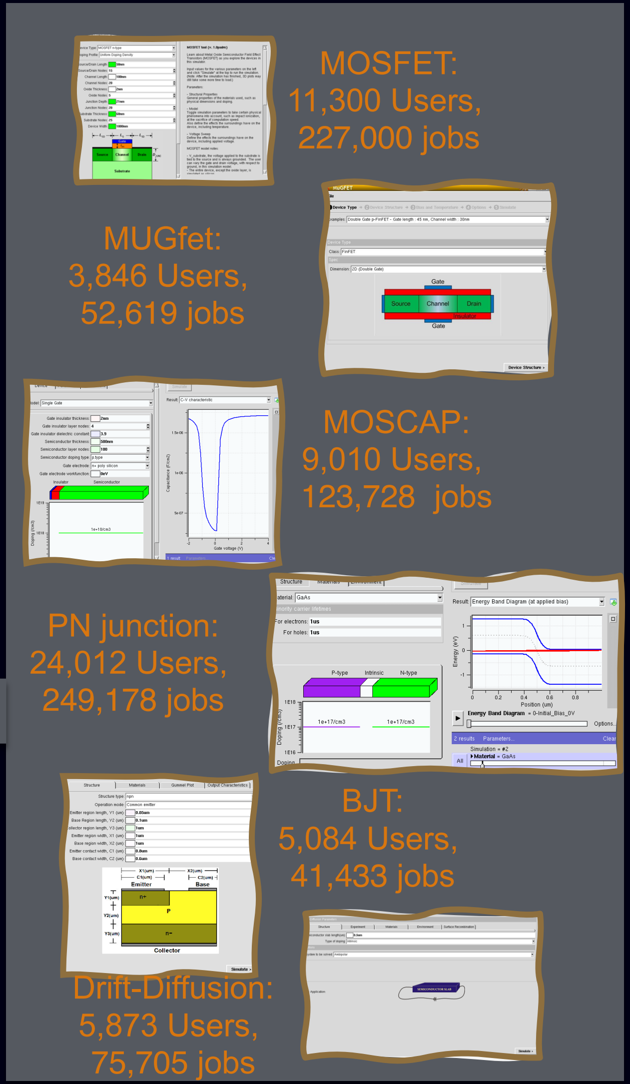
| --- | --- | --- |
| 48 jobs/user | 1/3.7x | 13 jobs/user |

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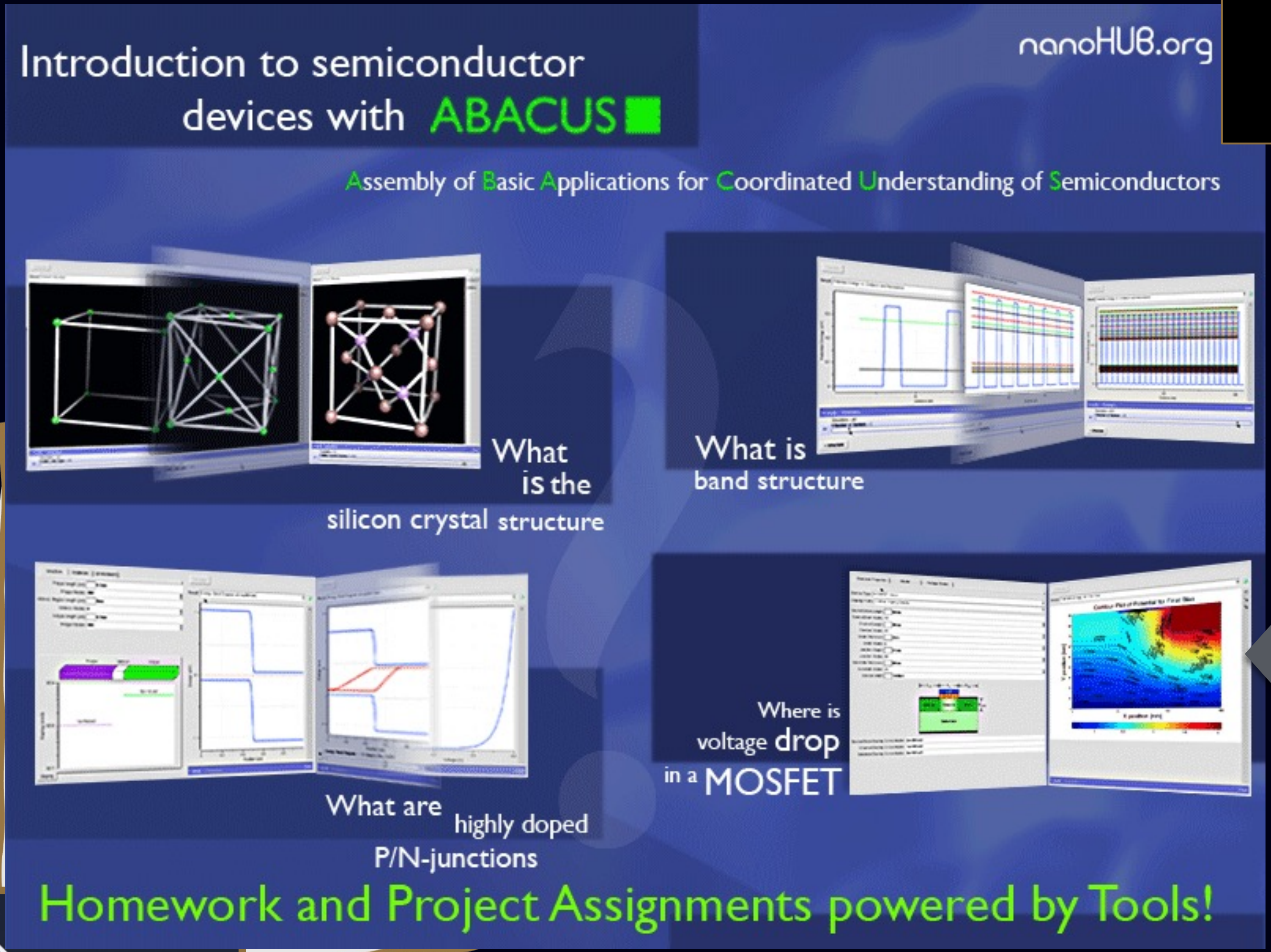
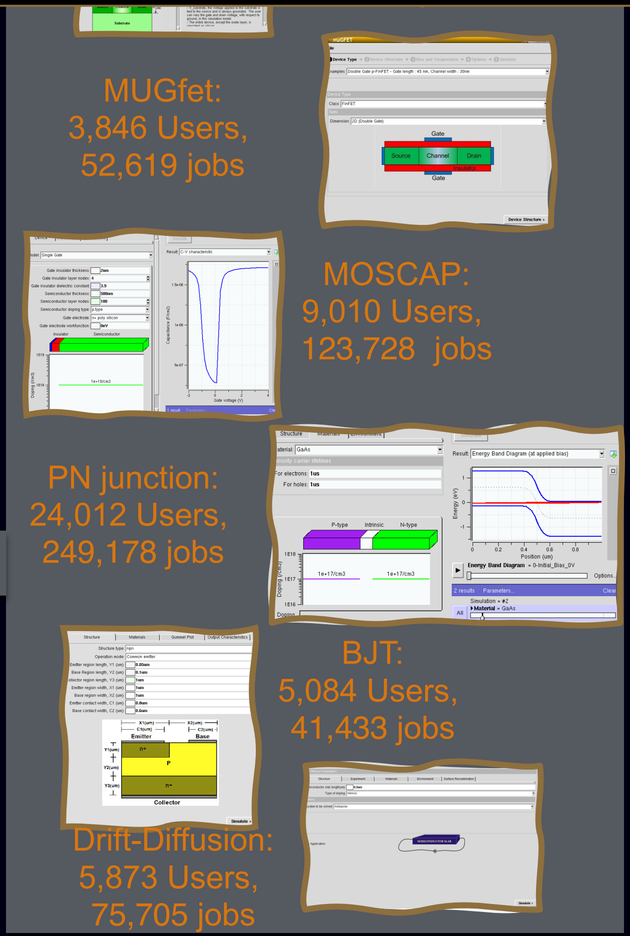
What can you do,
that no textbook does?

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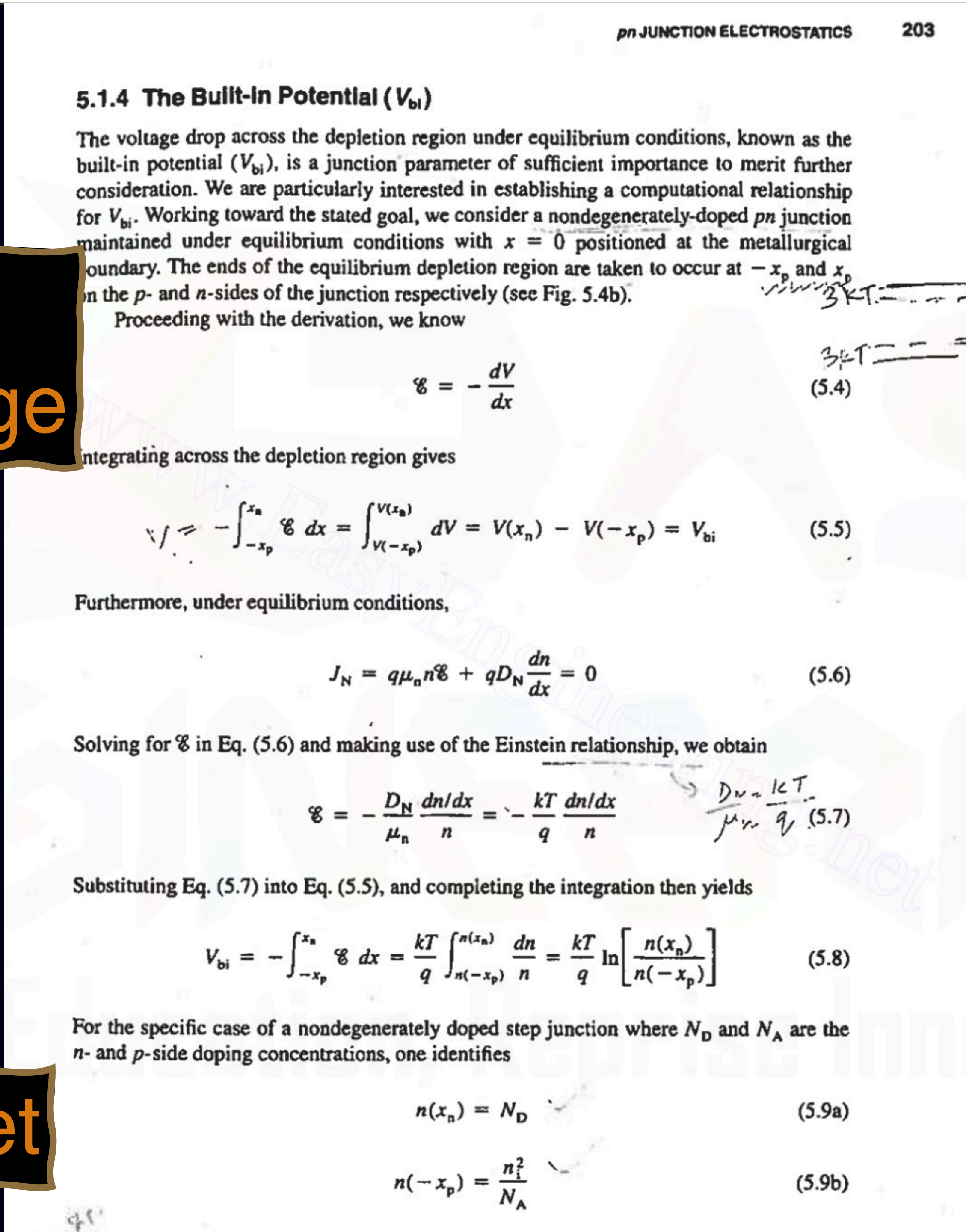
## A Typical Textbook Page





### 5.1.4 The Built-In Potential ($V_{bi}$)

The voltage drop across the depletion region under equilibrium conditions, known as the built-in potential ($V_{bi}$), is a junction parameter of sufficient importance to merit further consideration. We are particularly interested in establishing a computational relationship for $V_{bi}$. Working toward the stated goal, we consider a nondegenerately-doped *pn* junction maintained under equilibrium conditions with $x = 0$ positioned at the metallurgical boundary. The ends of the equilibrium depletion region are taken to occur at $-x_p$ and $x_n$ on the *p*- and *n*-sides of the junction respectively (see Fig. 5.4b).

Proceeding with the derivation, we know

$$\mathscr{E} = -\frac{dV}{dx} \tag{5.4}$$

Integrating across the depletion region gives

$$-\int_{-x_p}^{x_n} \mathscr{E}\, dx = \int_{V(-x_p)}^{V(x_n)} dV = V(x_n) - V(-x_p) = V_{bi} \tag{5.5}$$

Furthermore, under equilibrium conditions,

$$J_N = q\mu_n n\mathscr{E} + qD_N\frac{dn}{dx} = 0 \tag{5.6}$$

Solving for $\mathscr{E}$ in Eq. (5.6) and making use of the Einstein relationship, we obtain

$$\mathscr{E} = -\frac{D_N}{\mu_n}\frac{dn/dx}{n} = -\frac{kT}{q}\frac{dn/dx}{n} \tag{5.7}$$

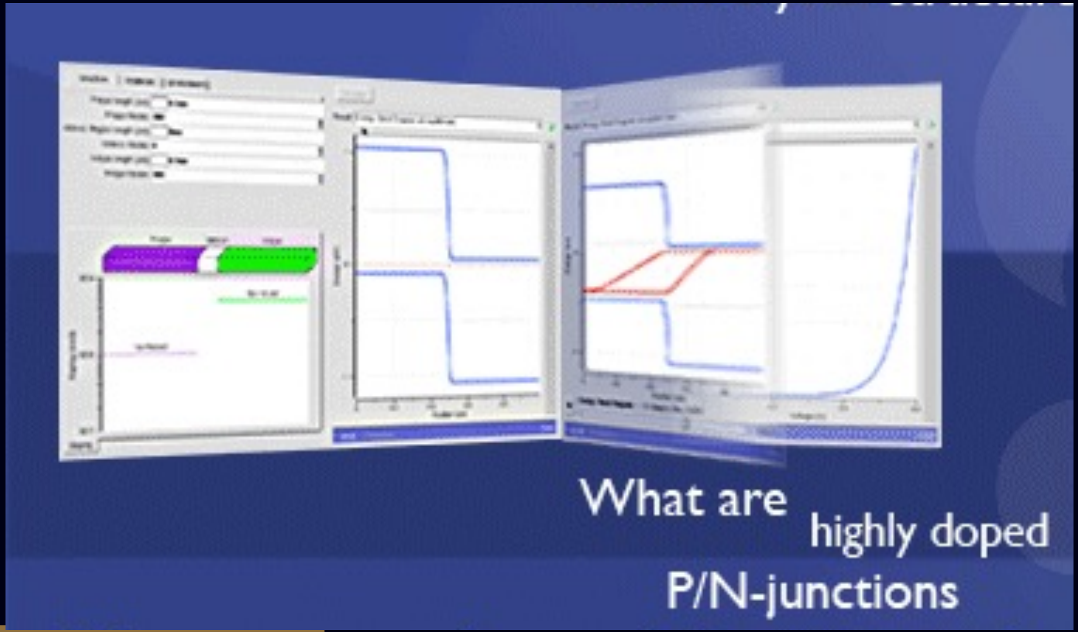
Substituting Eq. (5.7) into Eq. (5.5), and completing the integration then yields

$$V_{bi} = -\int_{-x_p}^{x_n} \mathscr{E}\, dx = \frac{kT}{q}\int_{n(-x_p)}^{n(x_n)} \frac{dn}{n} = \frac{kT}{q}\ln\left[\frac{n(x_n)}{n(-x_p)}\right] \tag{5.8}$$

For the specific case of a nondegenerately doped step junction where $N_D$ and $N_A$ are the *n*- and *p*-side doping concentrations, one identifies

$$n(x_n) = N_D \tag{5.9a}$$

$$n(-x_p) = \frac{n_i^2}{N_A} \tag{5.9b}$$




R.F. Pierret

chipshub by nanoHUB

# What can you do, that no textbook does?



### 5.1.4 The Built-in Potential ($V_{bi}$)

The voltage drop across the depletion region under equilibrium conditions, known as the built-in potential ($V_{bi}$), is a junction parameter of sufficient importance to merit further consideration. We are particularly interested in establishing a computational relationship for $V_{bi}$. Working toward the stated goal, we consider a nondegenerately-doped *pn* junction maintained under equilibrium conditions with $x = 0$ positioned at the metallurgical boundary. The ends of the equilibrium depletion region are taken to occur at $-x_p$ and $x_n$ on the *p*- and *n*-sides of the junction respectively (see Fig. 5.4b).

Proceeding with the derivation, we know

$$\mathscr{E} = -\frac{dV}{dx} \tag{5.4}$$

Integrating across the depletion region gives

$$-\int_{-x_p}^{x_n} \mathscr{E}\, dx = \int_{V(-x_p)}^{V(x_n)} dV = V(x_n) - V(-x_p) = V_{bi} \tag{5.5}$$

Furthermore, under equilibrium conditions,

$$J_N = q\mu_n n\mathscr{E} + qD_N\frac{dn}{dx} = 0 \tag{5.6}$$

Solving for $\mathscr{E}$ in Eq. (5.6) and making use of the Einstein relationship, we obtain

$$\mathscr{E} = -\frac{D_N}{\mu_n}\frac{dn/dx}{n} = -\frac{kT}{q}\frac{dn/dx}{n} \tag{5.7}$$

Substituting Eq. (5.7) into Eq. (5.5), and completing the integration then yields

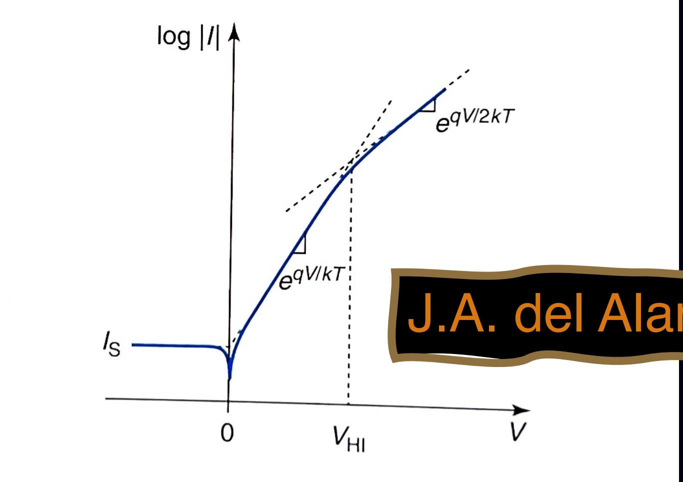
$$V_{bi} = -\int_{-x_p}^{x_n} \mathscr{E}\, dx = \frac{kT}{q}\int_{n(-x_p)}^{n(x_n)} \frac{dn}{n} = \frac{kT}{q}\ln\left[\frac{n(x_n)}{n(-x_p)}\right] \tag{5.8}$$

For the specific case of a nondegenerately doped step junction where $N_D$ and $N_A$ are the *n*- and *p*-side doping concentrations, one identifies

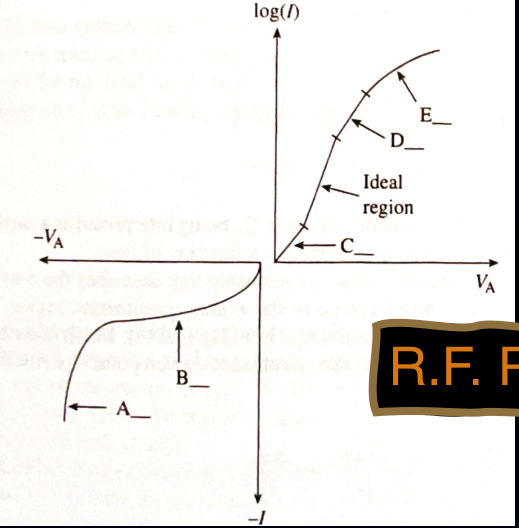
$$n(x_n) = N_D \tag{5.9a}$$

$$n(-x_p) = \frac{n_i^2}{N_A} \tag{5.9b}$$

# Real devices are non-ideal!




J.A. del Alamo




R.F. Pierret

**FIGURE 6.40**
Sketch of forward bias *I–V* characteristics of a PN diode. For strong forward voltage, the diode can go into high-level injection and the current grows as $e^{qV/2kT}$.

Fig. 6.40 that, in fact, for strong forward voltage, the *I–V* characteristics deviate from their ideal $e^{qV/kT}$ behavior into what appears more to be $e^{qV/2kT}$. Let us discuss why this happen…

First, let us estimate the voltage at which high-level injection occurs. This is simp… asymmetric diode, high-level injection occurs first in the lowly doped side of the di… us consider here a P$^+$N diode with a donor concentration $N_D$ (an entirely equivalen… obtained for a N$^+$P diode). Figure 6.41 shows the evolution of the minority and majori… concentrations (in a semilog scale) in the n region as the diode forward voltage increa… figure clearly shows that the location that is driven first into high-level injection is the e… SCR. For small forward voltages, the minority carrier concentration is much less than th… level and the majority carrier concentration is hence unaffected by minority carrier injectio… For a high enough forward voltage, the minority carrier concentration at the edge of the SCR

The prose gets dense

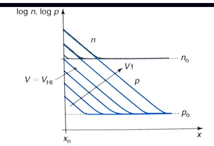



**FIGURE 6.41**
Minority and majority carrier concentrations in the n side of a P$^+$N diode as a function of forward bias. At $V_{HI}$, the n region goes into high-level injection.

reaches a value equal to the doping level. At this voltage, the majority carrier concentration at the edge of the SCR is twice the doping level. Clearly, it is not possible to assume any longer that the majority carrier concentration is unaffected as this would violate quasi-neutrality. The n side of the QNR has become high-level injected.

This is a reasonable definition for the onset of high-level injection. If we allow ourselves to "stretch" the low-level injection boundary condition, Eq. (6.29), up to this point, high-level injection occurs when

$$p(x_n) = \frac{n_i^2}{N_D}\exp\frac{qV_{HI}}{kT} = N_D \tag{6.124}$$

where $V_{HI}$ refers to the voltage at the onset of high-level injection. Solving for $V_{HI}$ in this equation, we get

$$V_{HI} = \frac{2kT}{q}\ln\frac{N_D}{n_i} \tag{6.125}$$

This result is reasonable. The higher the doping level (of the lowly doped side), the higher the voltage that it takes to drive the diode into high-level injection.

In microelectronic device operation, we are not interested in general in the high-level injection regime. This is something to be avoided. In PN junctions, for example, the *I–V* characteristics grow more slowly, as sketched in Fig. 6.40, something that is undesirable for many applications. In bipolar transistors, for example, high-level injection of the base brings with it a drop in gain. Unless one is working with devices that have been designed to operate in high-level injection, such as power diodes or certain kinds of solar cells, high-level injection is a syndrome to avoid all together. For this reason, we will not treat it in detail here.

It is of value, nevertheless, to understand the origin of the $e^{qV/2kT}$ dependence of the current in the high-level injection regime. This result can be easily derived from the expression of the *np* product inside the SCR given by Eq. (6.47). This equation remains valid in the high-level injection regime because it simply states that electrons and holes are in equilibrium among each other due to the fact that the SCR is very thin. At the edge of the SCR that goes into high-level injection first, $n \simeq p$, and

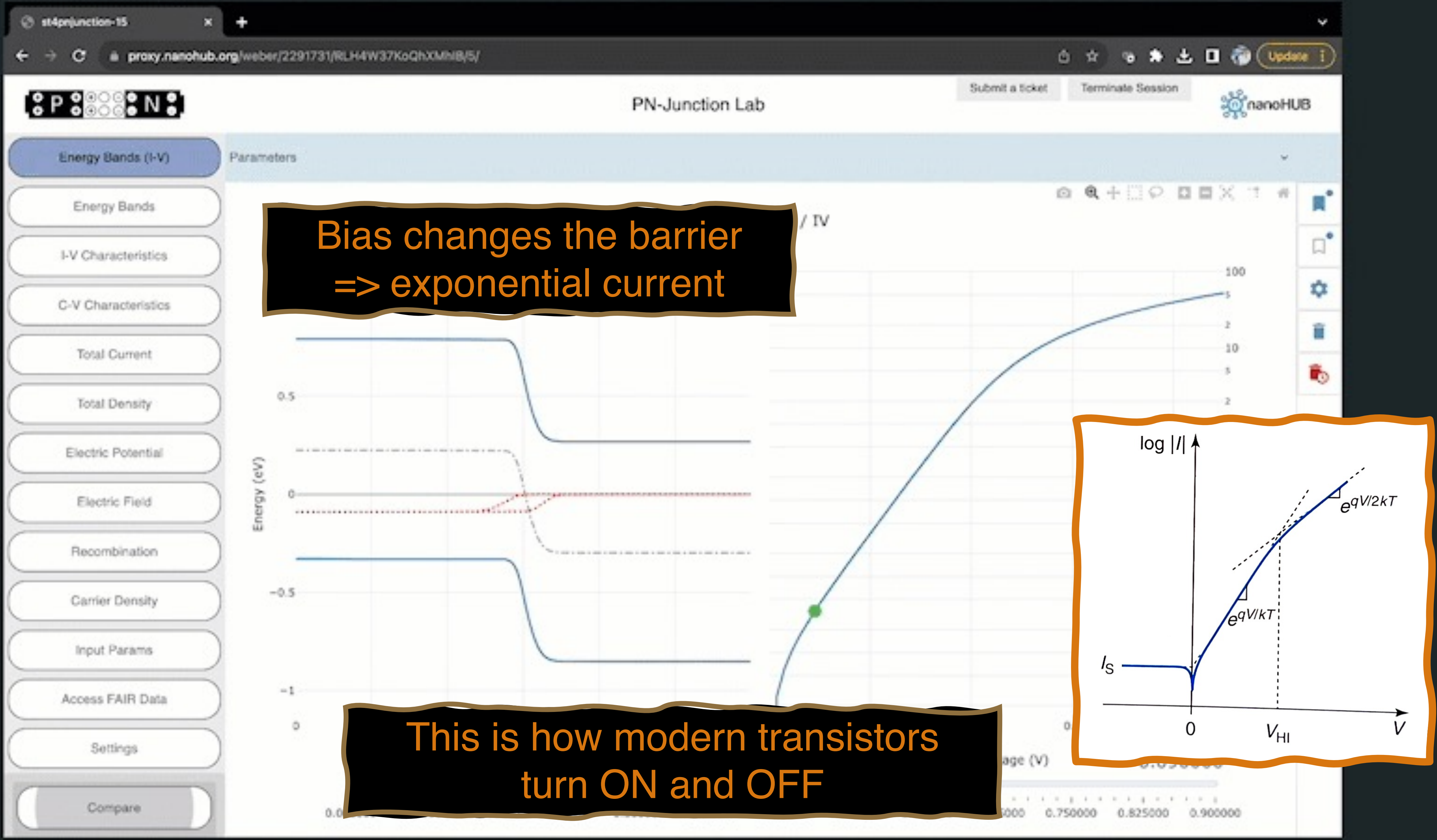
$$n \simeq p \simeq n_i \exp\frac{qV}{2kT} \tag{6.126}$$

The nature of the diode current is still carrier recombination in the QNRs. The boundary condition of Eq. (6.126) implies that the voltage dependence of the current will be of the form $e^{qV/2kT}$.

Physically, one can understand the origin of this result by examining the evolution of the energy band diagrams around the SCR as the voltage increases. This is sketched in Fig. 6.42. The key is to examine the dependence of the energy barrier that carriers face in crossing the junction. In the low-level injection regime, as the voltage increases, the energy barrier is reduced by exactly $qV$. This is because the majority carrier quasi-Fermi levels are "rigidly" tied up to the respective band edges. This results from the fact that in low-level injection, the majority carrier concentrations remain unchanged.

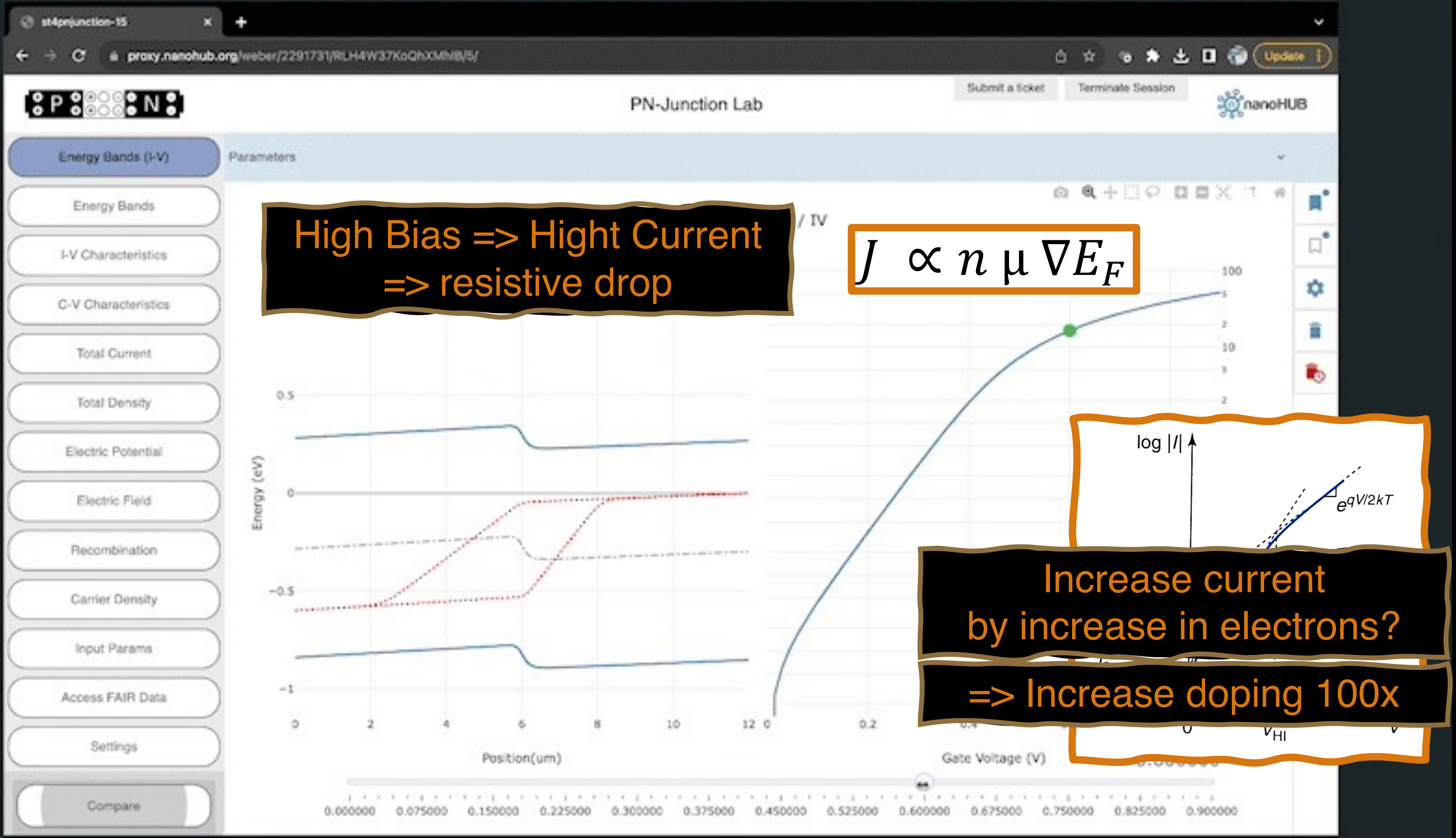
As one of the sides of the diode goes into high-level injection, this is not the case any longer. The large minority carrier injection forces an increase in the majority carrier concentration. As a consequence, in high-level injection, the majority carrier quasi-Fermi level on the high-level injected side gets closer and closer to the majority carrier band edge (conduction band for a p$^+$–n diode). After this happens, the energy barrier presented by the junction is only reduced at half the rate of the quasi-Fermi level splitting (always $qV$). This is sketched in Fig. 6.42.

References to "exact" solutions




Bias changes the barrier
=> exponential current

This is how modern transistors
turn ON and OFF



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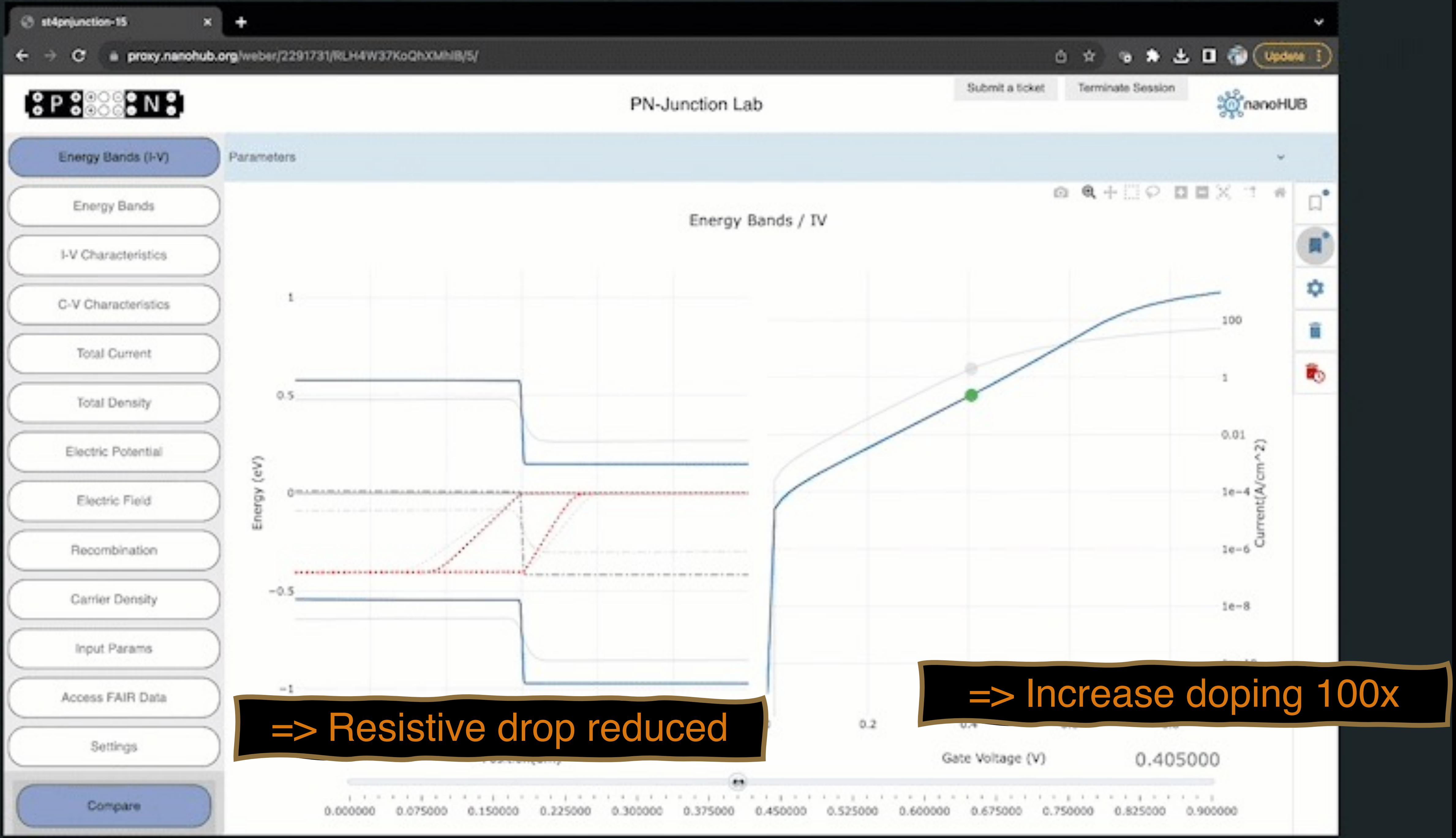
proxy.nanohub.org/weber/2291731/RLH4W37KoQhXMhIB/5/
PN-Junction Lab
Submit a ticket
Terminate Session
nanoHUB
Energy Bands (I-V)
Parameters
Energy Bands
I-V Characteristics
C-V Characteristics
Total Current
Total Density
Electric Potential
Electric Field
Recombination
Carrier Density
Input Params
Access FAIR Data
Settings
Compare
High Bias => Hight Current
=> resistive drop
$J \propto n\,\mu\,\nabla E_F$
Energy (eV)
Position(um)
Gate Voltage (V)
log |I|
$e^{qV/2kT}$
Increase current
by increase in electrons?
=> Increase doping 100x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proxy.nanohub.org/weber/2291731/RLH4W37KoQhXMhIB/5/
PN-Junction Lab
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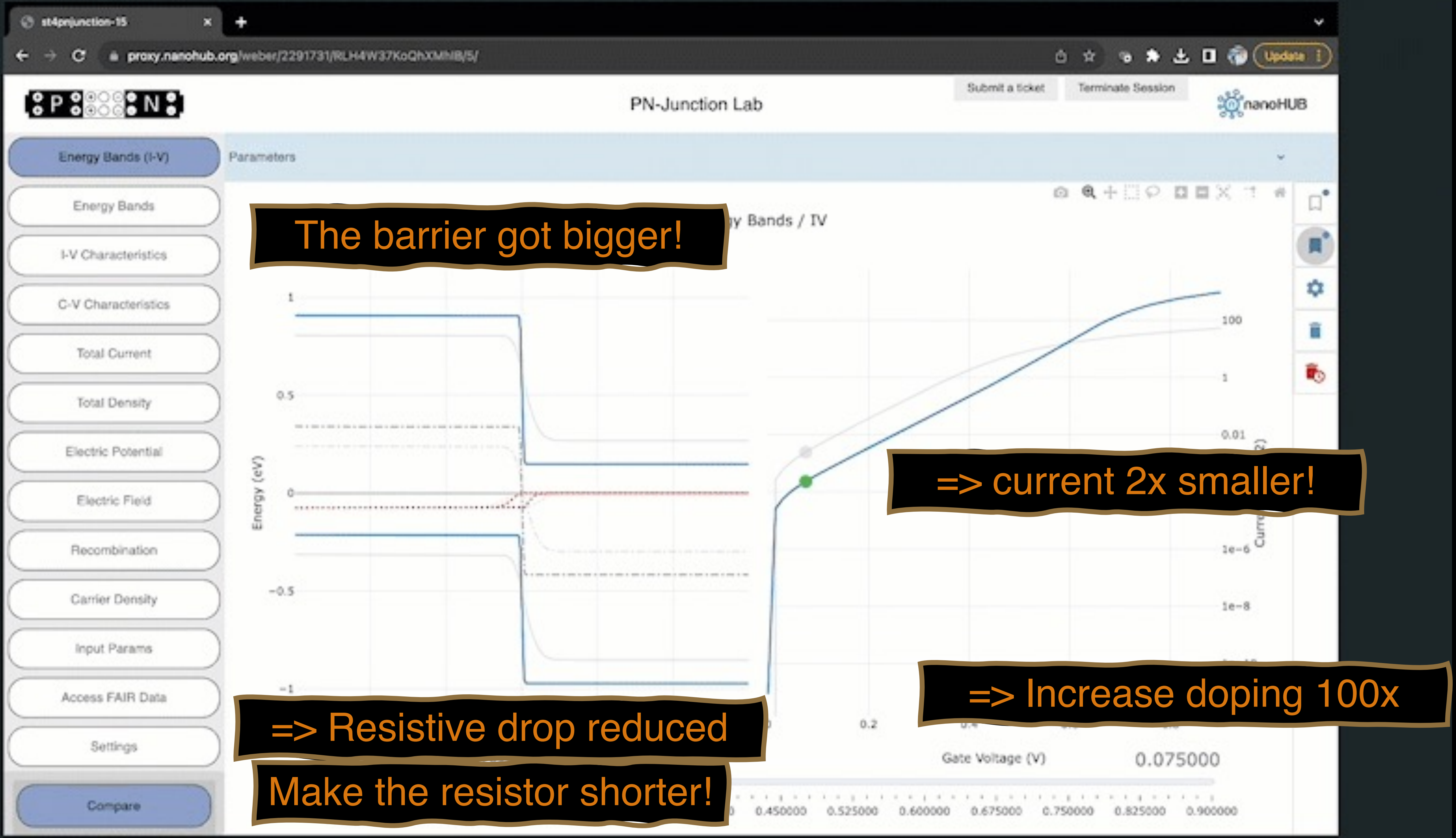
nanoHUB
Energy Bands (I-V)
Energy Bands
I-V Characteristics
C-V Characteristics
Total Current
Total Density
Electric Potential
Electric Field
Recombination
Carrier Density
Input Params
Access FAIR Data
Settings
Compare
Parameters
Energy Bands / IV
Energy (eV)
Current(A/cm^2)
Gate Voltage (V)
0.405000
=> Resistive drop reduced
=> Increase doping 100x



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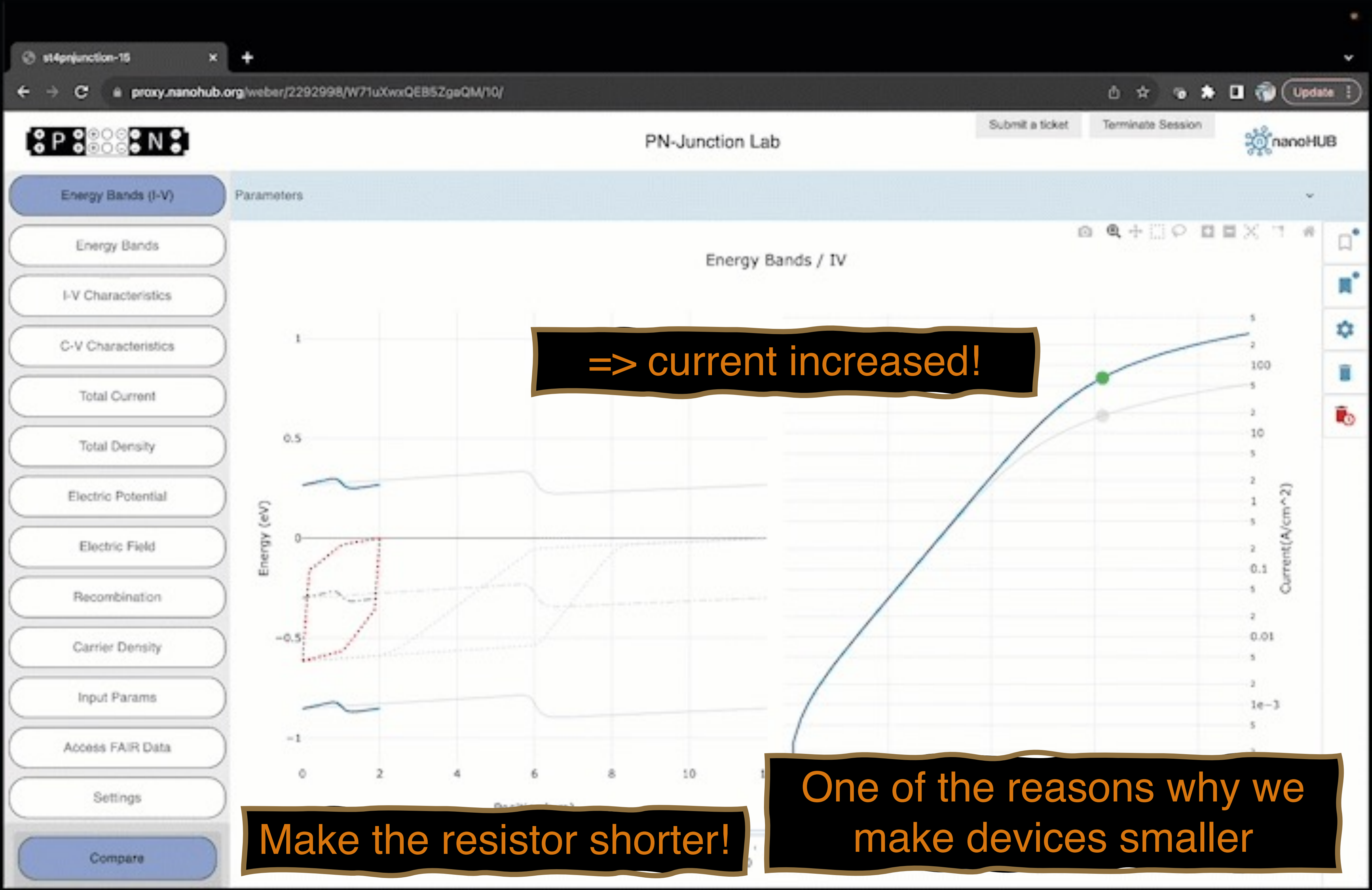
Update
PN-Junction Lab
Submit a ticket
Terminate Session
nanoHUB
Energy Bands (I-V)
Energy Bands
I-V Characteristics
C-V Characteristics
Total Current
Total Density
Electric Potential
Electric Field
Recombination
Carrier Density
Input Params
Access FAIR Data
Settings
Compare
Parameters
The barrier got bigger!
Energy (eV)
Gate Voltage (V)
0.075000
=> current 2x smaller!
=> Increase doping 100x
=> Resistive drop reduced
Make the resistor shorter!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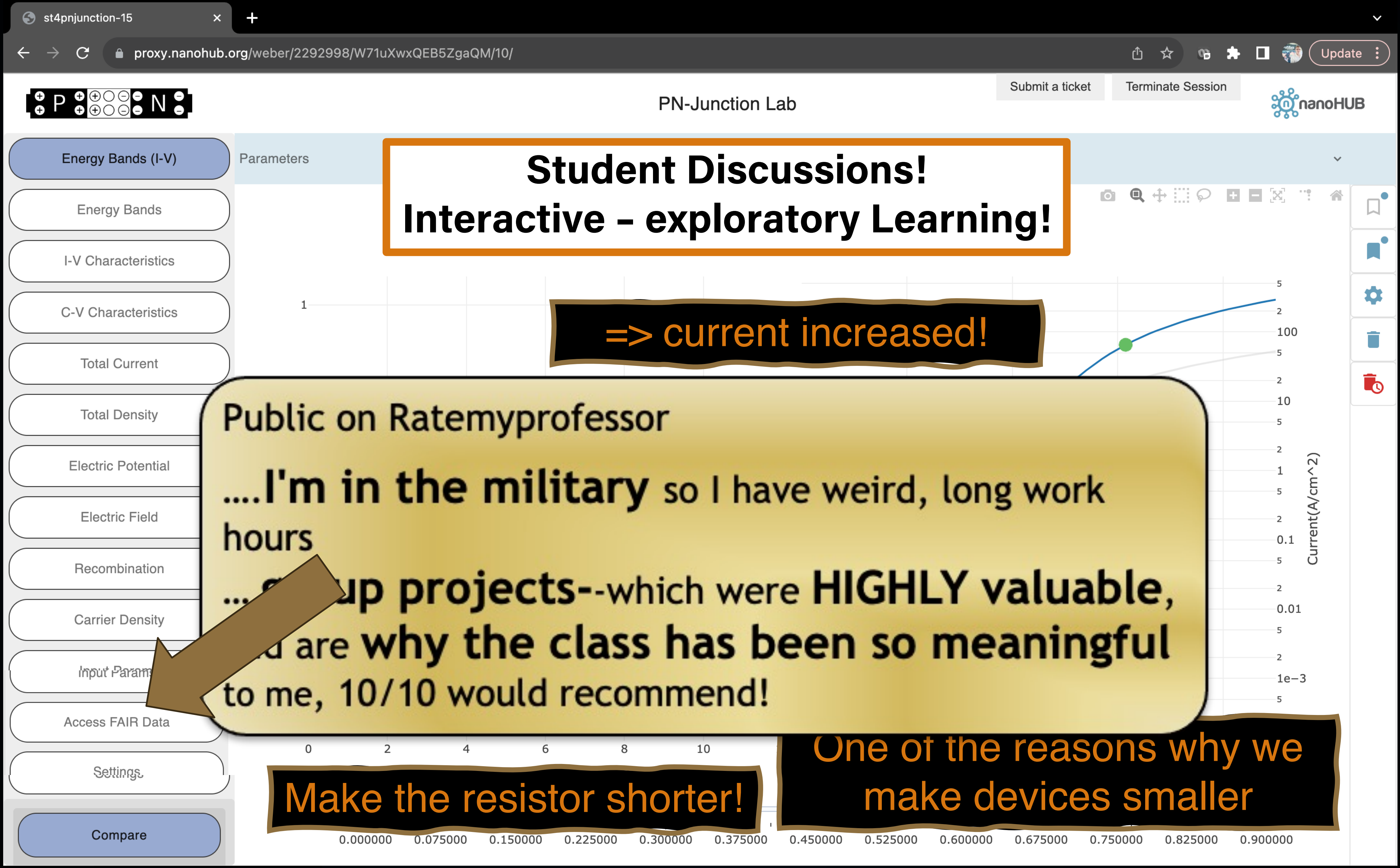
Terminate Session
PN-Junction Lab
nanoHUB
Energy Bands (I-V)
Energy Bands
I-V Characteristics
C-V Characteristics
Total Current
Total Density
Electric Potential
Electric Field
Recombination
Carrier Density
Input Params
Access FAIR Data
Settings
Compare
Parameters
Energy Bands / IV
Energy (eV)
Current(A/cm^2)
=> current increased!
Make the resistor shorter!
One of the reasons why we make devices smaller




# Student Discussions!
# Interactive – exploratory Learning!

=> current increased!

Public on Ratemyprofessor

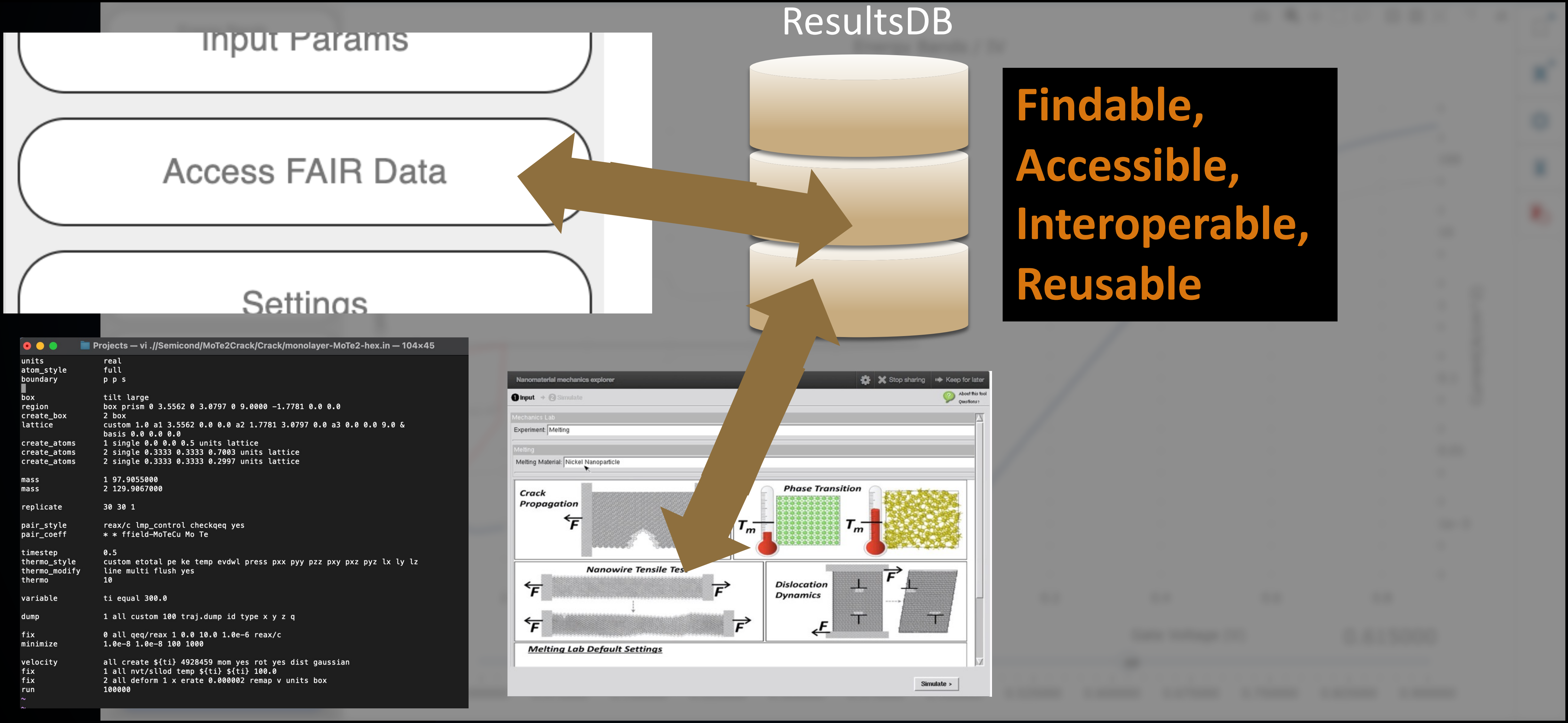
….**I'm in the military** so I have weird, long work hours

… **up projects-**-which were **HIGHLY valuable**, … are **why the class has been so meaningful** to me, 10/10 would recommend!

Make the resistor shorter!

One of the reasons why we make devices smaller

# Not just Devices!
# Materials, Photonics, Processing etc



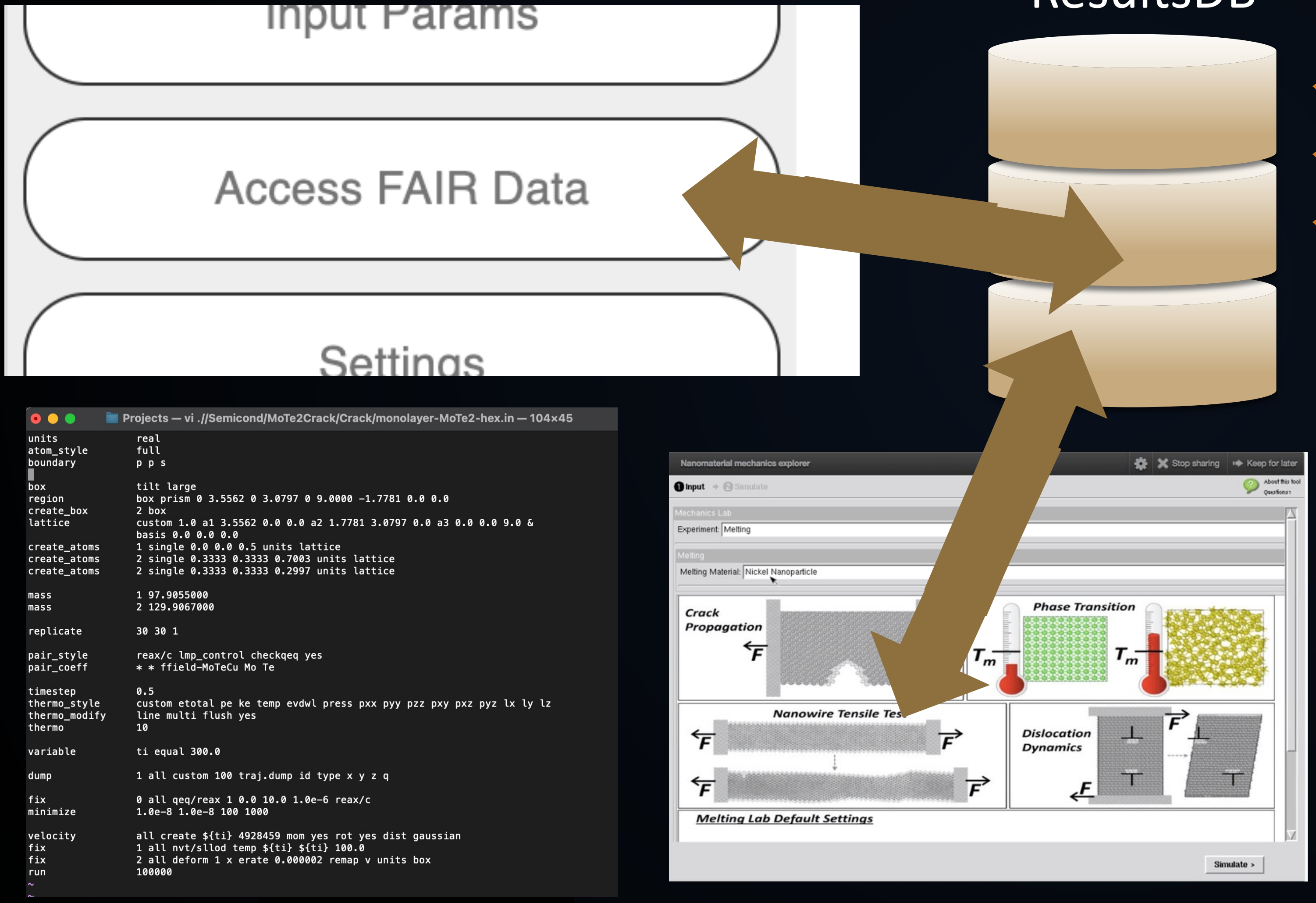

Projects — vi .//Semicond/MoTe2Crack/Crack/monolayer-MoTe2-hex.in — 104×45

```
units           real
atom_style      full
boundary        p p s

box             tilt large
region          box prism 0 3.5562 0 3.0797 0 9.0000 -1.7781 0.0 0.0
create_box      2 box
lattice         custom 1.0 a1 3.5562 0.0 0.0 a2 1.7781 3.0797 0.0 a3 0.0 0.0 9.0 &
                basis 0.0 0.0 0.0
create_atoms    1 single 0.0 0.0 0.5 units lattice
create_atoms    2 single 0.3333 0.3333 0.7003 units lattice
create_atoms    2 single 0.3333 0.3333 0.2997 units lattice

mass            1 97.9055000
mass            2 129.9067000

replicate       30 30 1

pair_style      reax/c lmp_control checkqeq yes
pair_coeff      * * ffield-MoTeCu Mo Te

timestep        0.5
thermo_style    custom etotal pe ke temp evdwl press pxx pyy pzz pxy pxz pyz lx ly lz
thermo_modify   line multi flush yes
thermo          10

variable        ti equal 300.0

dump            1 all custom 100 traj.dump id type x y z q

fix             0 all qeq/reax 1 0.0 10.0 1.0e-6 reax/c
minimize        1.0e-8 1.0e-8 100 1000

velocity        all create ${ti} 4928459 mom yes rot yes dist gaussian
fix             1 all nvt/sllod temp ${ti} ${ti} 100.0
fix             2 all deform 1 x erate 0.000002 remap v units box
run             100000
~
```

**Findable,**
**Accessible,**
**Interoperable,**
**Reusable**

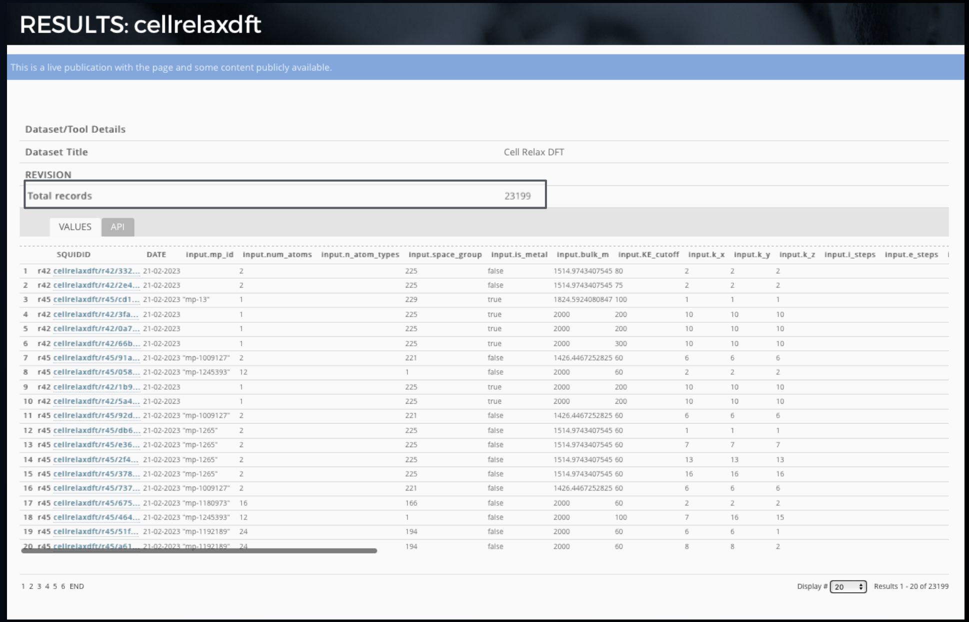
# FAIR Data

ResultsDB




- ✓ Inputs
- ✓ Outputs
- ✓ Metadata

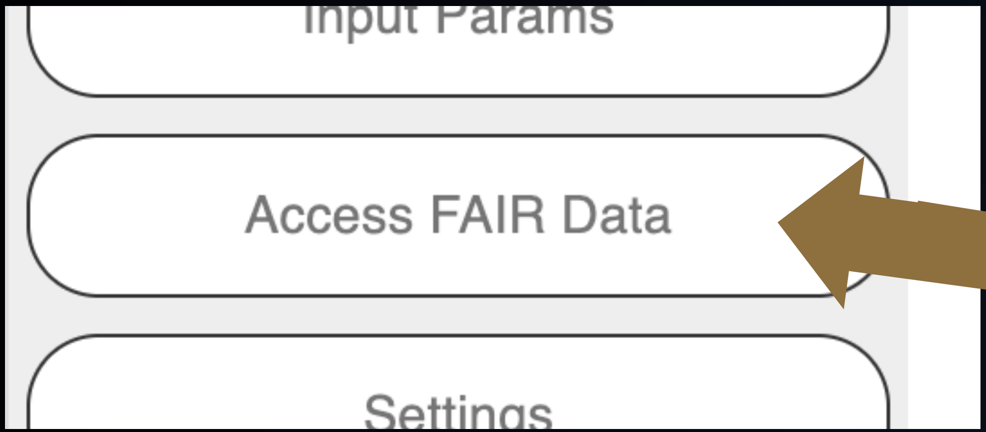
- DOIs for each dataset
- Unique identifier for each entry

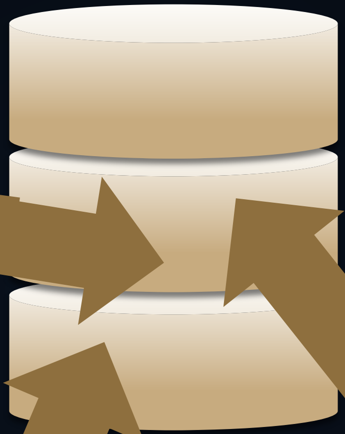


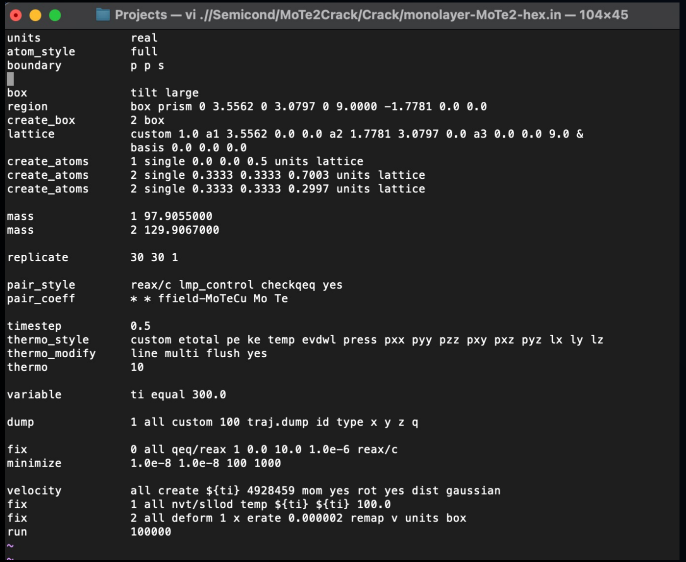
# Not just Our Own Data!

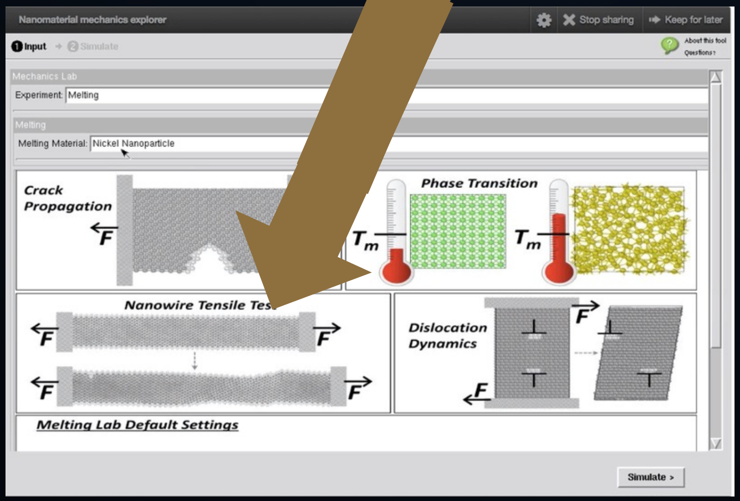
The Materials Project

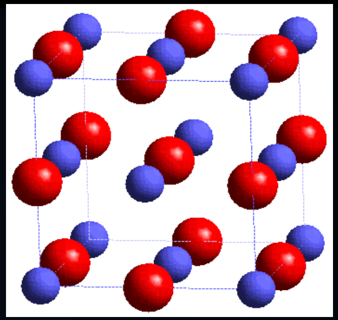
ResultsDB





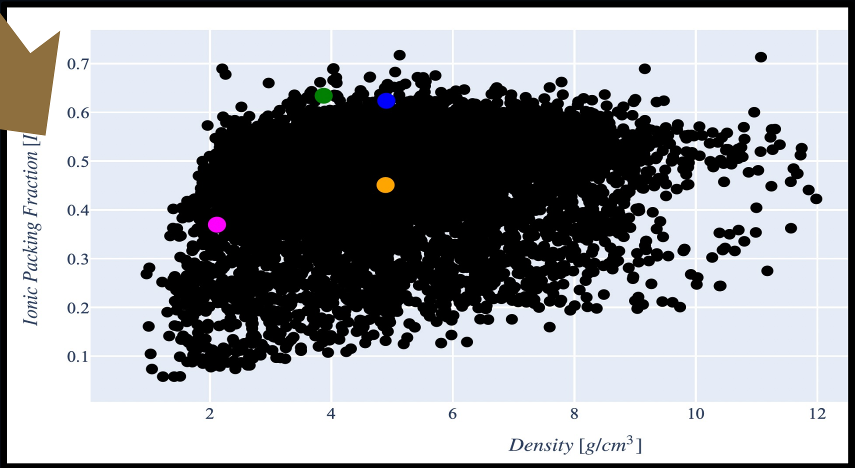
Ionic packing fraction:

$$IPF = \frac{\sum \frac{4}{3}\pi R_i^3}{(a \times b) \cdot c}$$

Sophomore-level class

Compute and visualize properties for 65,000 oxides

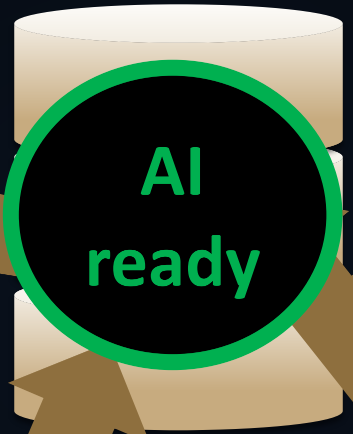
Materials discovery

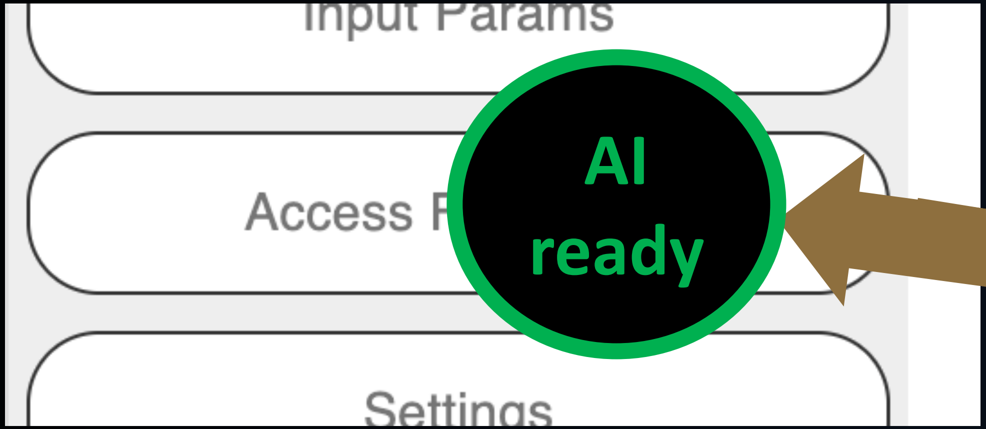


# FAIR Data & AI

The Materials Project

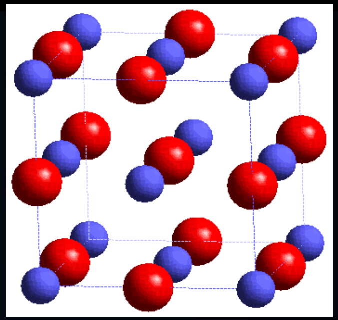
ResultsDB




Ionic packing fraction:

$$IPF = \frac{\sum \frac{4}{3}\pi R_i^3}{(a \times b) \cdot c}$$



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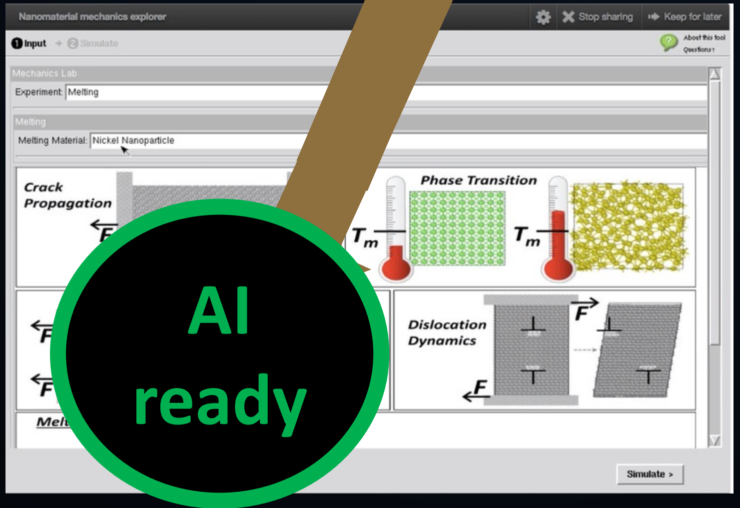
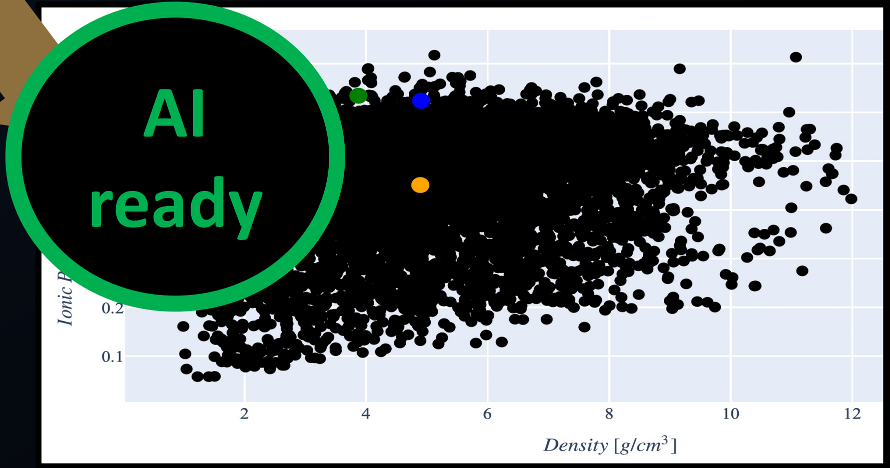
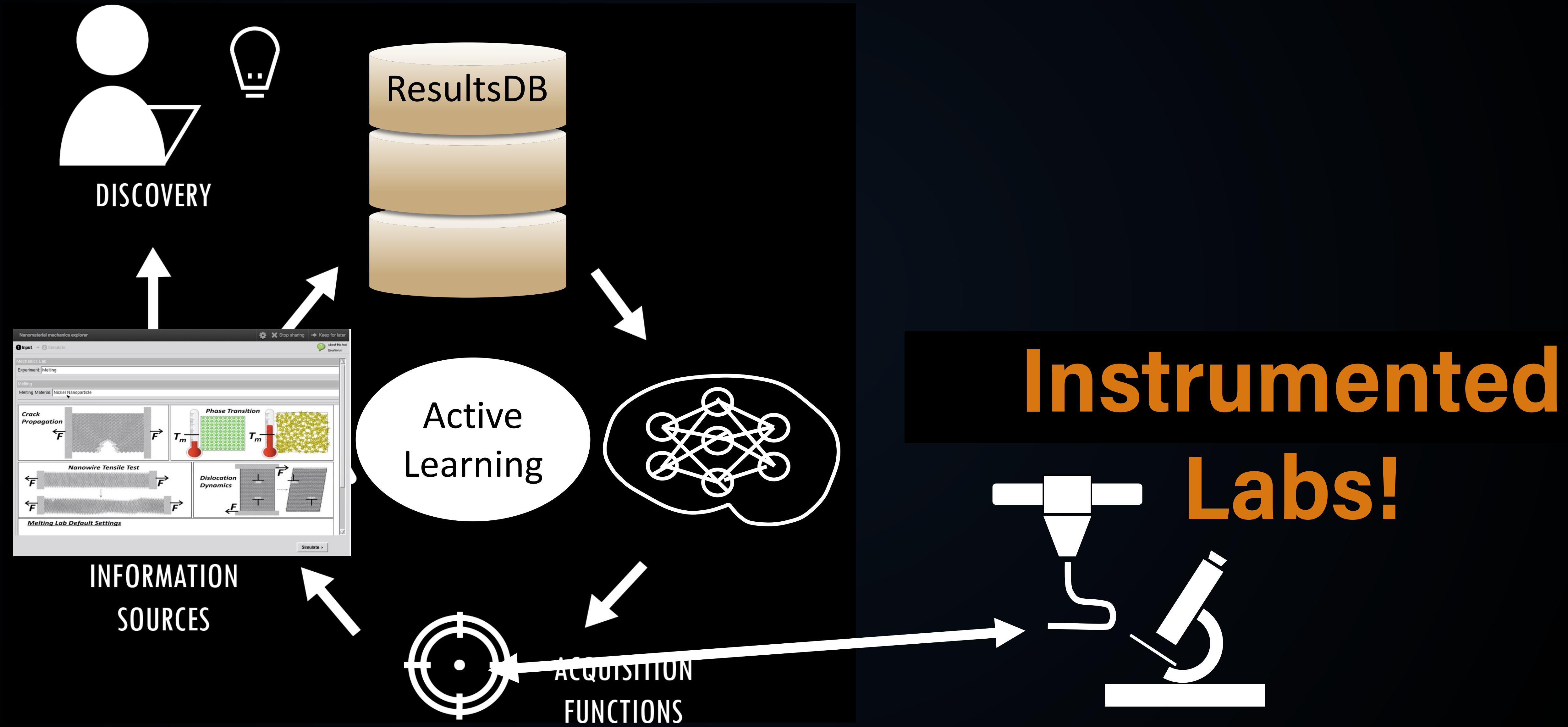
```
units           real
atom_style      full
boundary        p p s

box             tilt large
region          box prism 0 3.5562 0 3.0797 0 9.0000 -1.7781 0.0 0.0
create_box      2 box
lattice         custom 1.0 a1 3.5562 0.0 0.0 a2 1.7781 3.0797 0.0 a3 0.0 0.0 9.0 &
                basis 0.0 0.0 0.0
create_atoms    1 single 0.0 0.0 0.5 units lattice
create_atoms    2 single 0.3333 0.3333 0.7003 units lattice
create_atoms    2 single 0.3333 0.3333 0.2997 units lattice

mass            1 97.9055000
mass            2 129.9067000

replicate       30 30 1

pair_style      reax/c lmp_control checkqeq yes
pair_coeff      * * ffield-MoTeCu Mo Te

timestep        0.5
thermo_style    custom etotal pe ke temp evdwl press pxx pyy pzz pxy pxz pyz lx ly lz
thermo_modify   line multi flush yes
thermo          10

variable        ti equal 300.0

dump            1 all custom 100 traj.dump id type x y z q

fix             0 all qeq/reax 1 0.0 10.0 1.0e-6 reax/c
minimize        1.0e-8 1.0e-8 100 1000

velocity        all create ${ti} 4928459 mom yes rot yes dist gaussian
fix             1 all nvt/sllod temp ${ti} ${ti} 100.0
fix             2 all deform 1 x erate 0.000002 remap v units box
run             100000
~
```

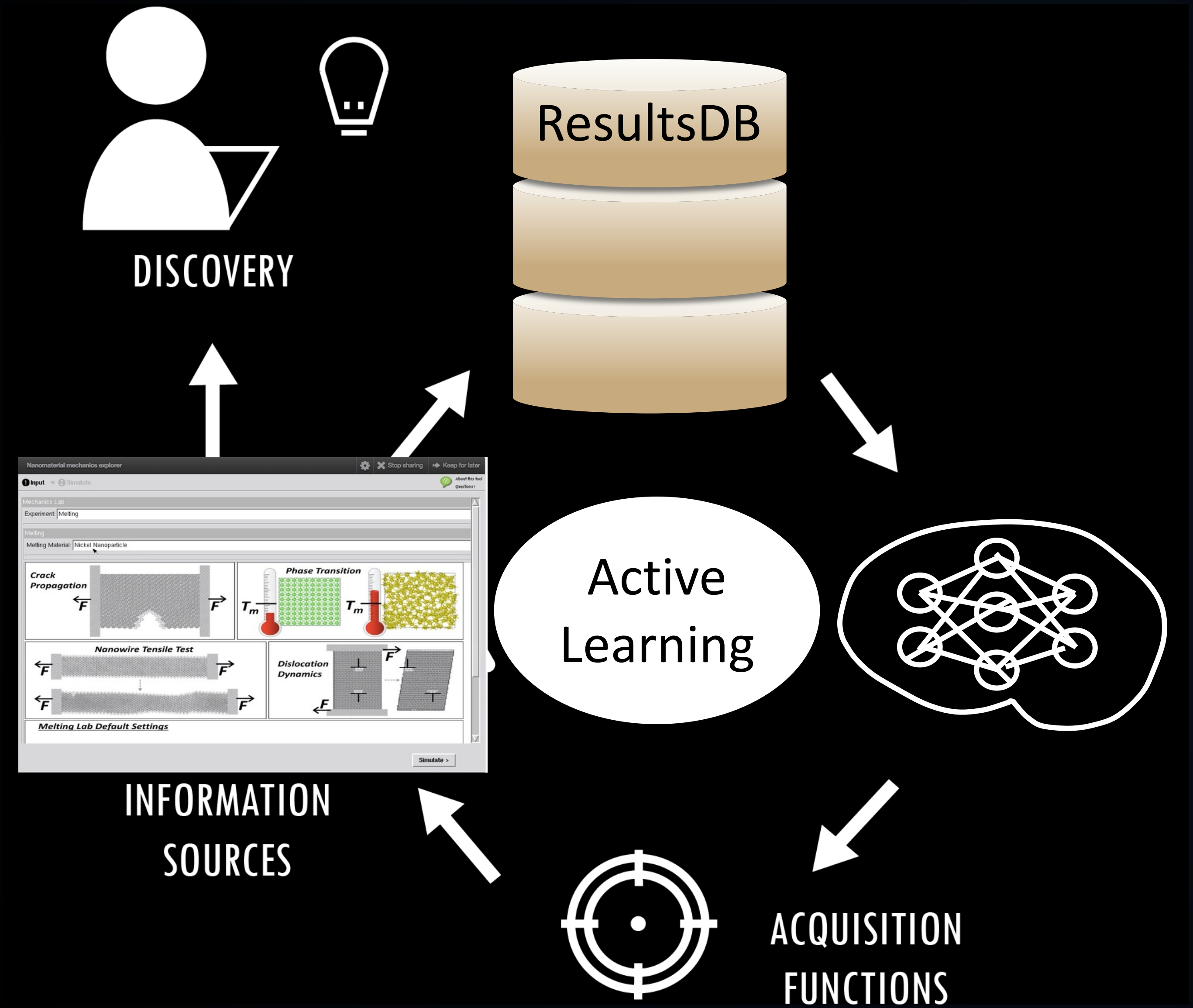


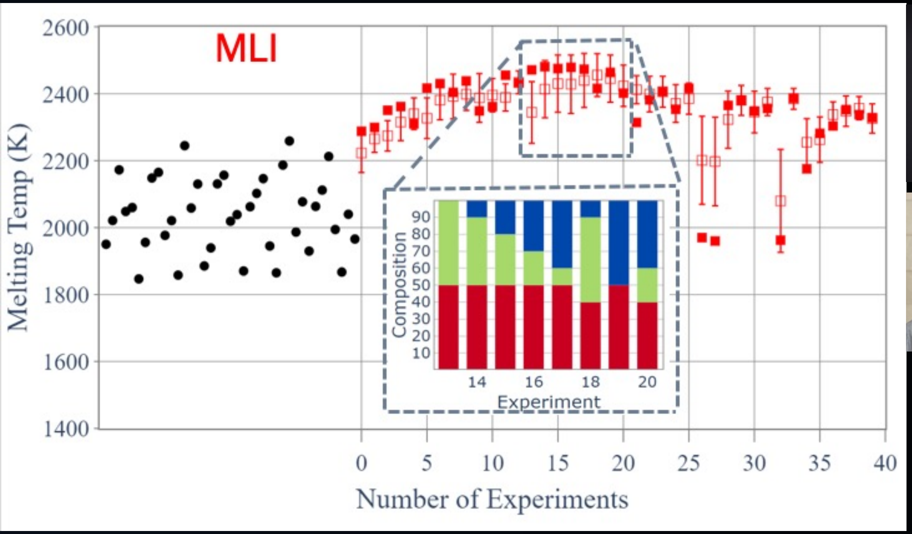
# FAIR Data & AI => the Lab of the Future



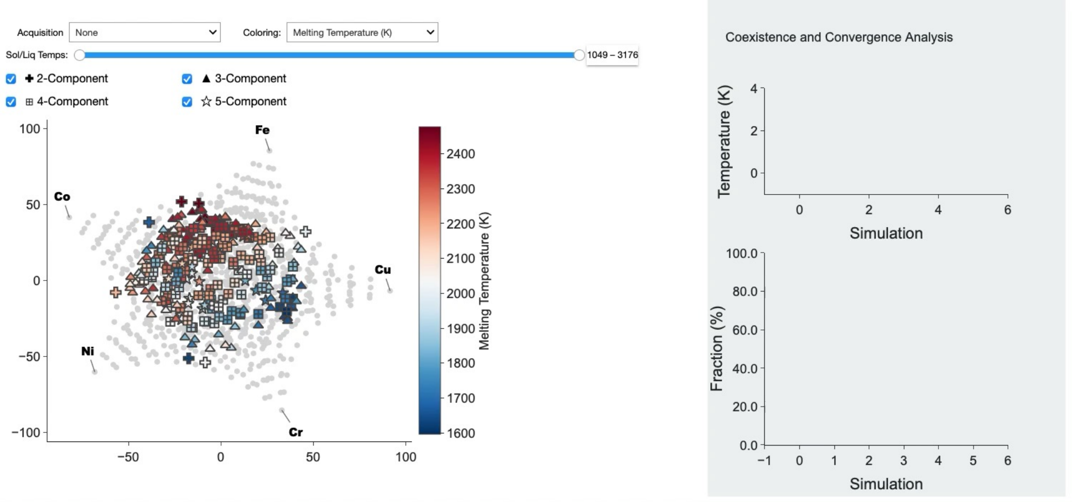
# FAIR Data & AI => the Lab of the Future



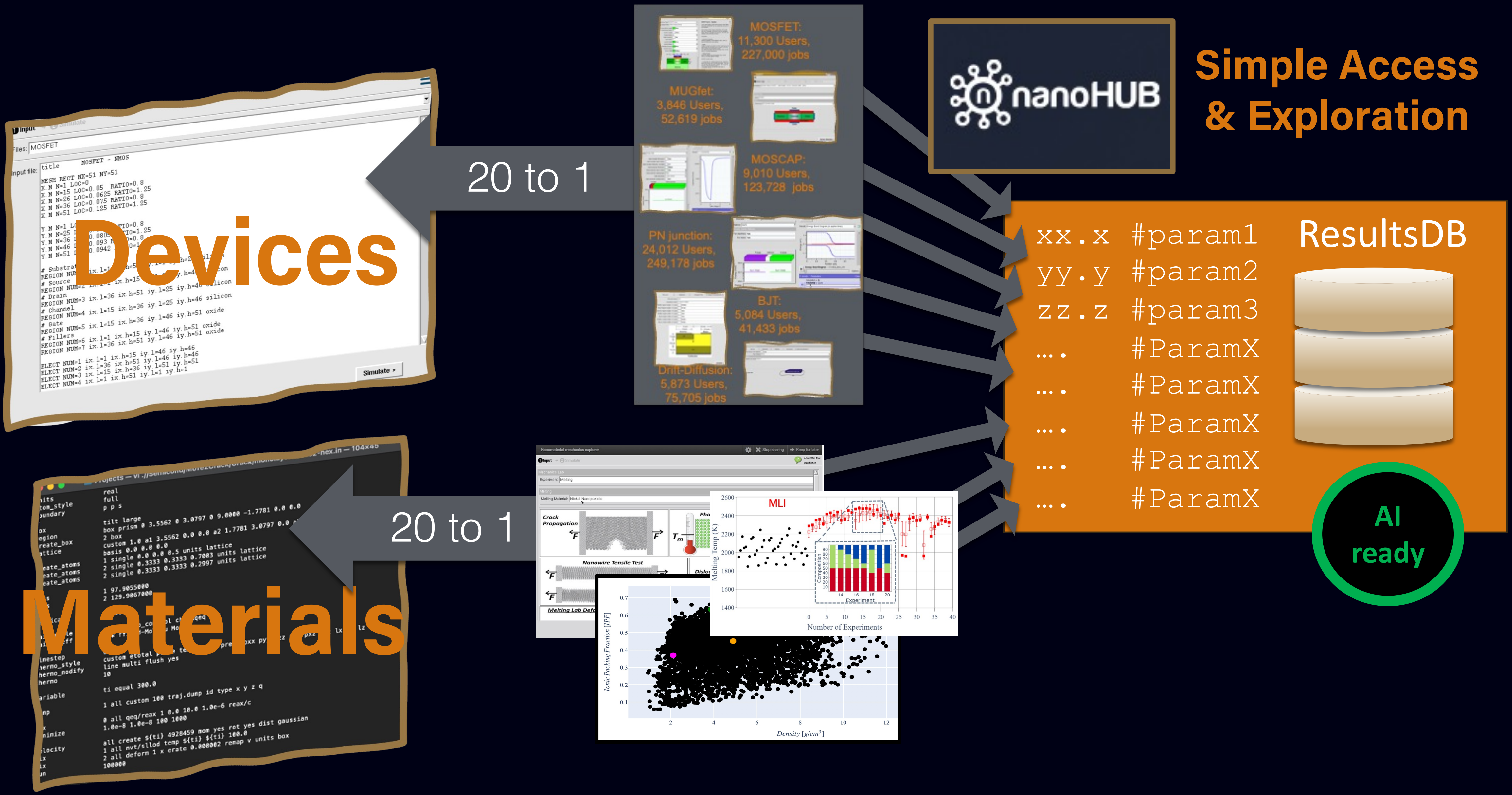

Discover the alloy with the highest melting temperature




Automatic FAIR data & data exploration tools



# Simple Access to Complex Tools



# Simple Access to Complex Tools

## Industrial Reality

### Simplified Optimization

SILVACO SYNOPSYS SIEMENS cadence

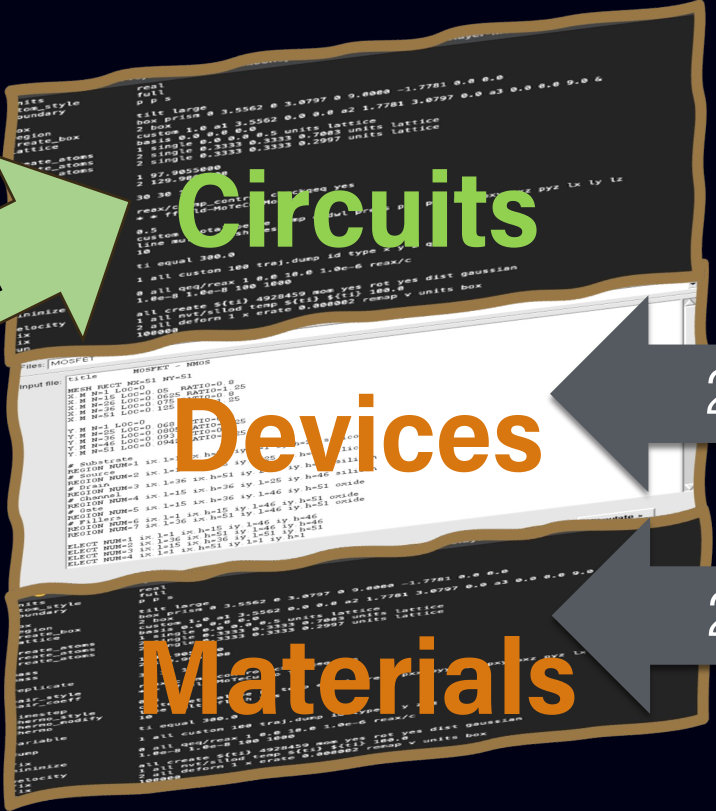
ResultsDB

1 engineer designs a “flow”

```
45.0 #param1
60.0 #param2
1.0  #param3
….   #ParamX
```

20 to 1

20 engineers optimize




20 to 1

20 to 1

nanoHUB

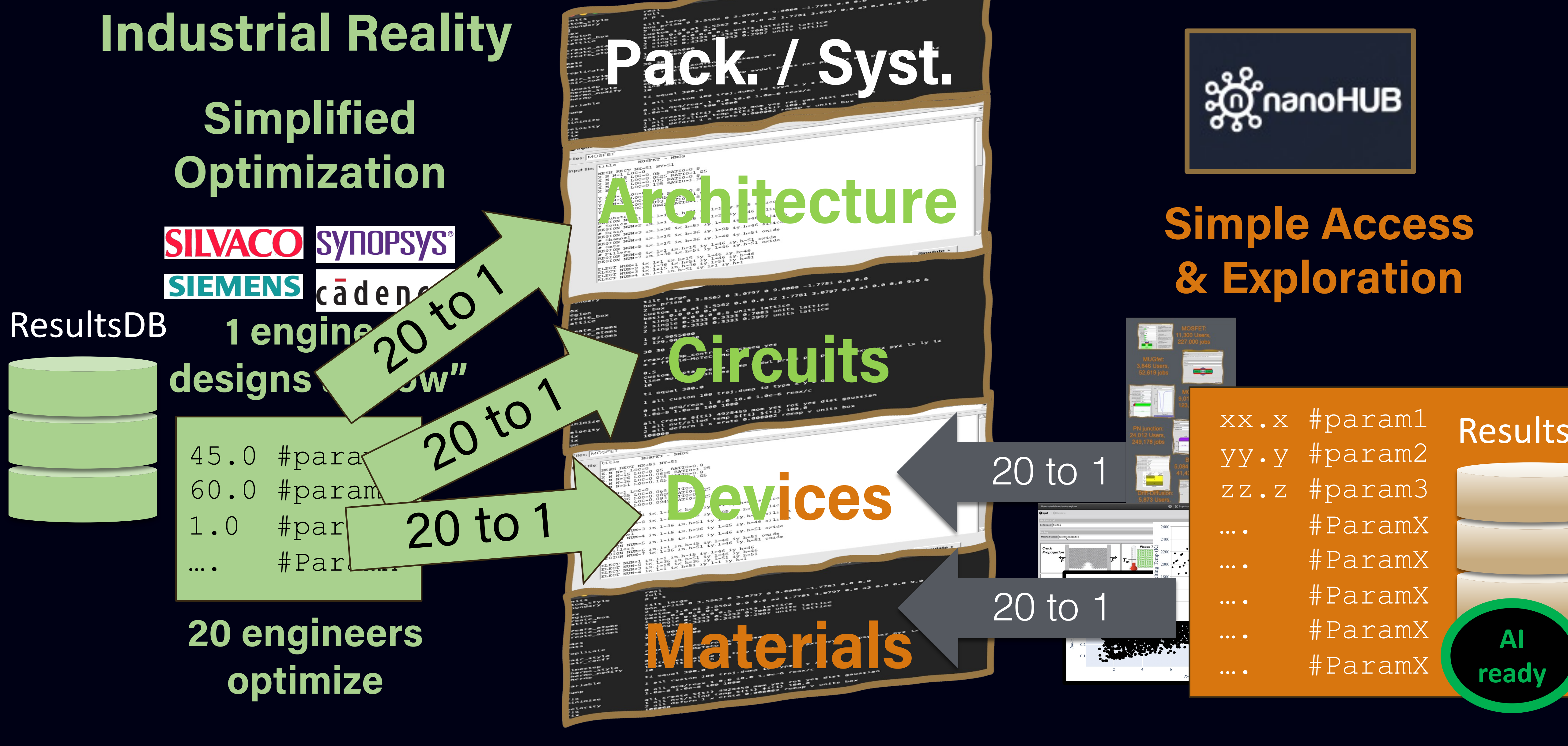
## Simple Access & Exploration

```
xx.x #param1
yy.y #param2
zz.z #param3
….   #ParamX
….   #ParamX
….   #ParamX
….   #ParamX
….   #ParamX
```

Results

AI ready

# Simple Access to Complex Tools

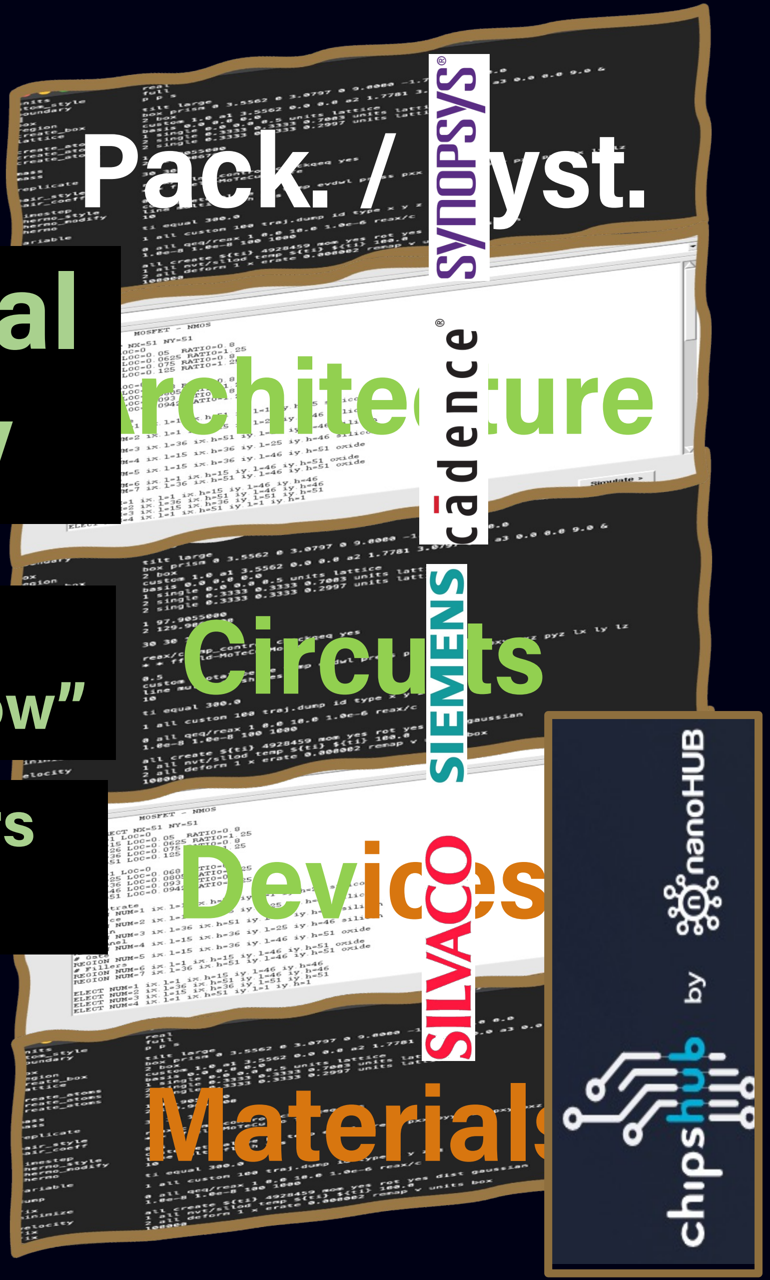


# 50,000 more Engineers Needed!

**Industrial Reality**

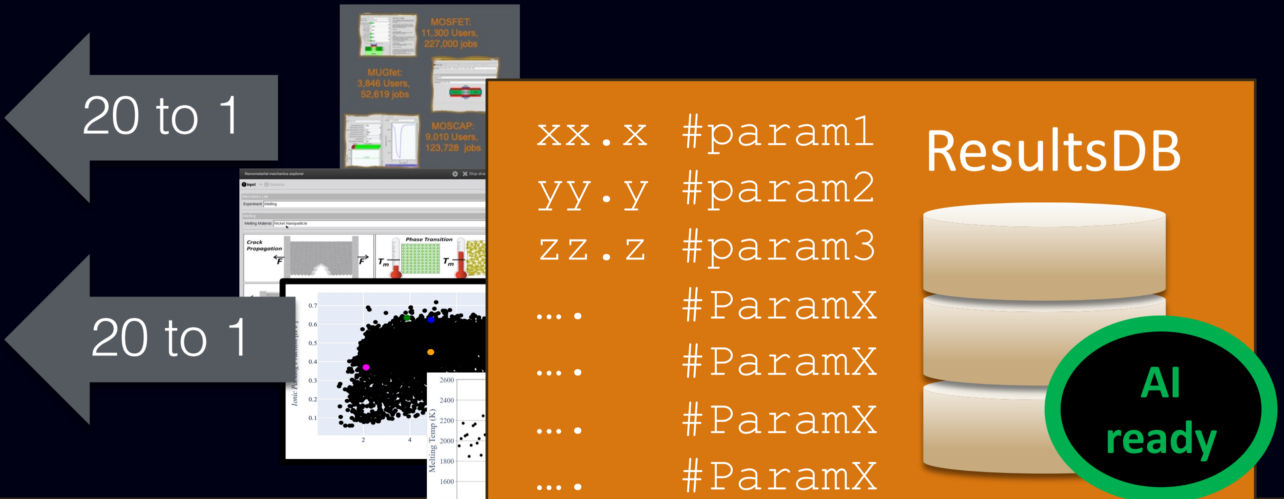
**1 engineer designs a “flow”**

**20 engineers optimize**




All need to understand the whole stack!

Not everyone must be a full design expert!



# 50,000 more Engineers Needed!

**Industrial Reality**

1 engineer designs a "flow"

20 engineers optimize

Pack. /

Archite

Circu

Devi

Mate

SYNOPSYS® cādence® SIEMENS SILVACO

Apps & Tools, & AI
& Lectures

chipshub by nanoHUB

20 to 1

20 to 1

20 to 1

20 to 1

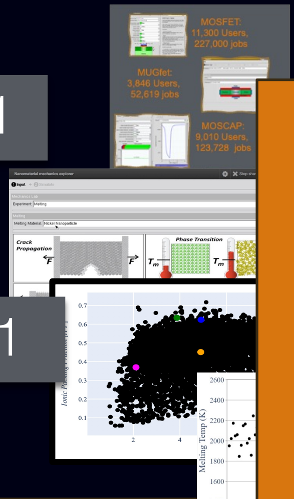
20 to 1

All need to understand the whole stack!

Apps & AI to teach:
Concepts & Optimization

Not everyone must be a full design expert!

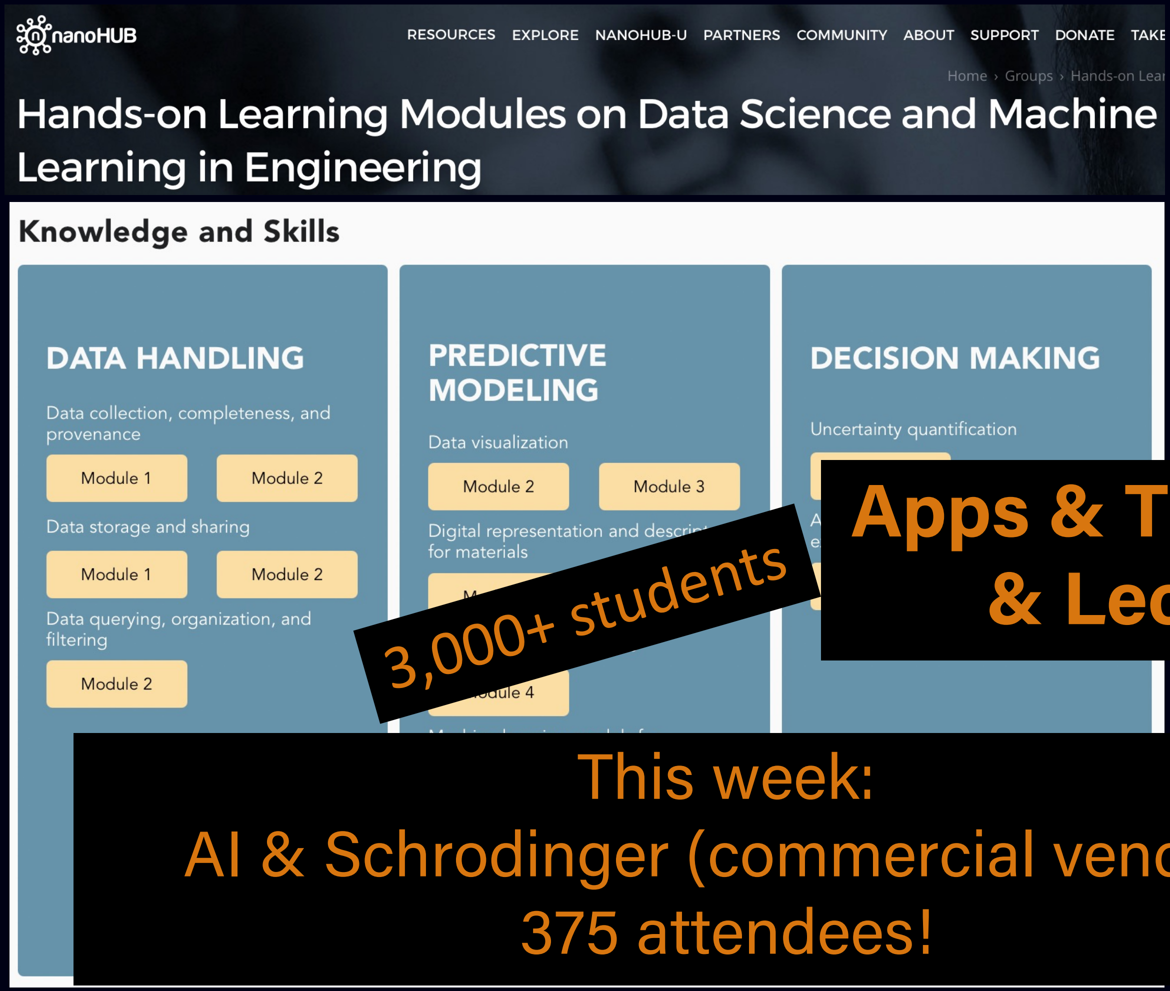
Tools to teach:
Detailed Design




| | | |
|---|---|---|
| xx.x | #param1 | ResultsDB |
| yy.y | #param2 | |
| zz.z | #param3 | |
| …. | #ParamX | |
| …. | #ParamX | |
| …. | #ParamX | |
| …. | #ParamX | |

AI ready

# Hands-on Data Science and Machine Learning Training Series

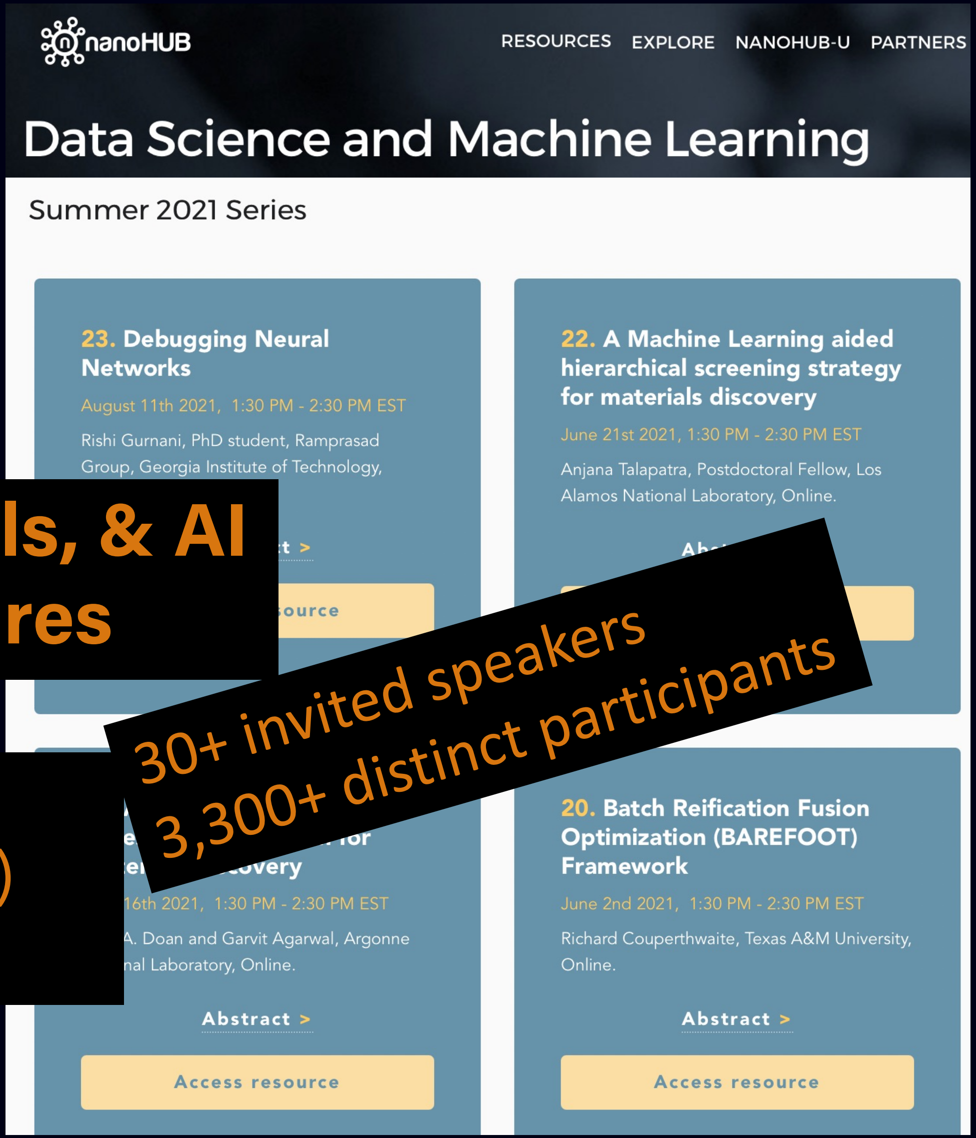



For undergraduate students
https://nanohub.org/groups/mlmodules

**3,000+ students**

**Apps & Tools, & AI & Lectures**

This week:
AI & Schrodinger (commercial vendor)
375 attendees!




**30+ invited speakers**
**3,300+ distinct participants**

For researchers
https://nanohub.org/groups/ml/handsontraining

# nanoHUB partners in workforce development

POWERED BY nanoHUB | Register | Login | Request Membership | Help

Home | About | Internships | Research Opportunities | Lecture Series | Courses | Simulation and CAD Tools | Calendar

SCALE
SCalable Asymmetric Lifecycle Engagement
Developing the U.S. Defense Microelectronics Workforce

## SCALE (Scalable Asymmetric Lifecycle Engagement)

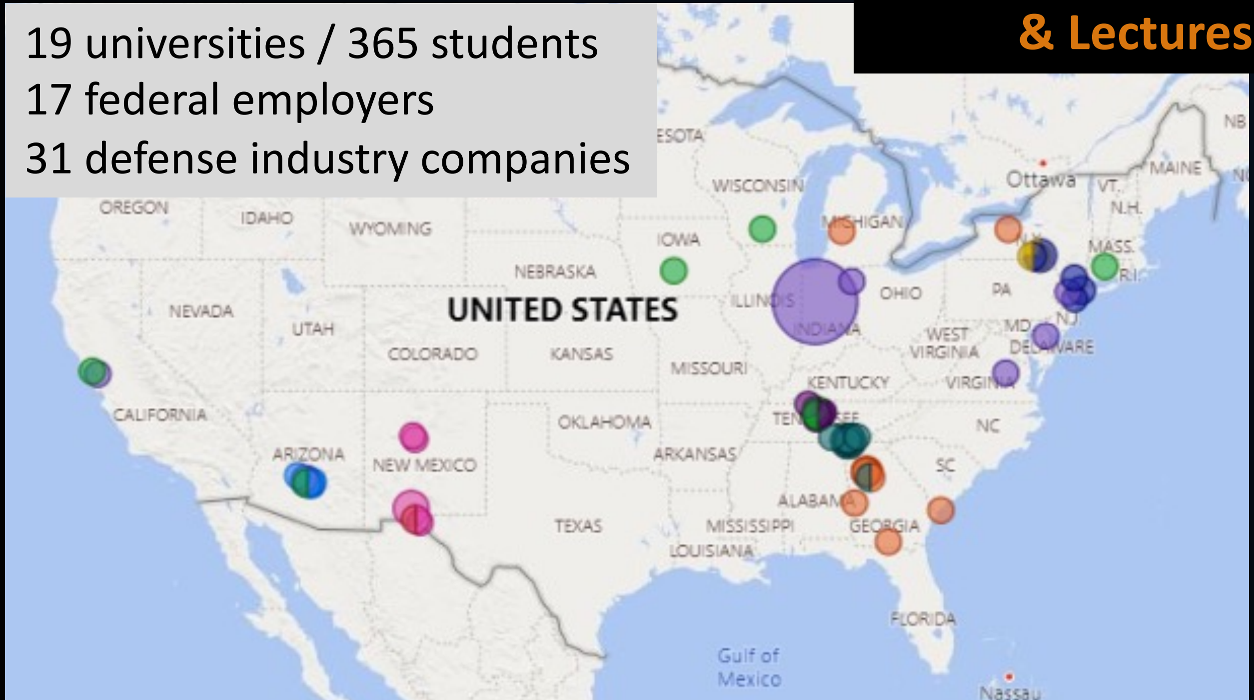
SCALE is the preeminent U.S. program for semiconductor workforce development in the defense sector.

Led by Purdue University, funded by the Department of Defense and managed by NSWC Crane, SCALE facilitates a different approach to training highly-skilled U.S. microelectronics engineers, hardware designers, and manufacturing experts, ensuring U.S. leadership in this important area.

300+ students have been impacted by SCALE.

**Apps & Tools, & AI & Lectures**

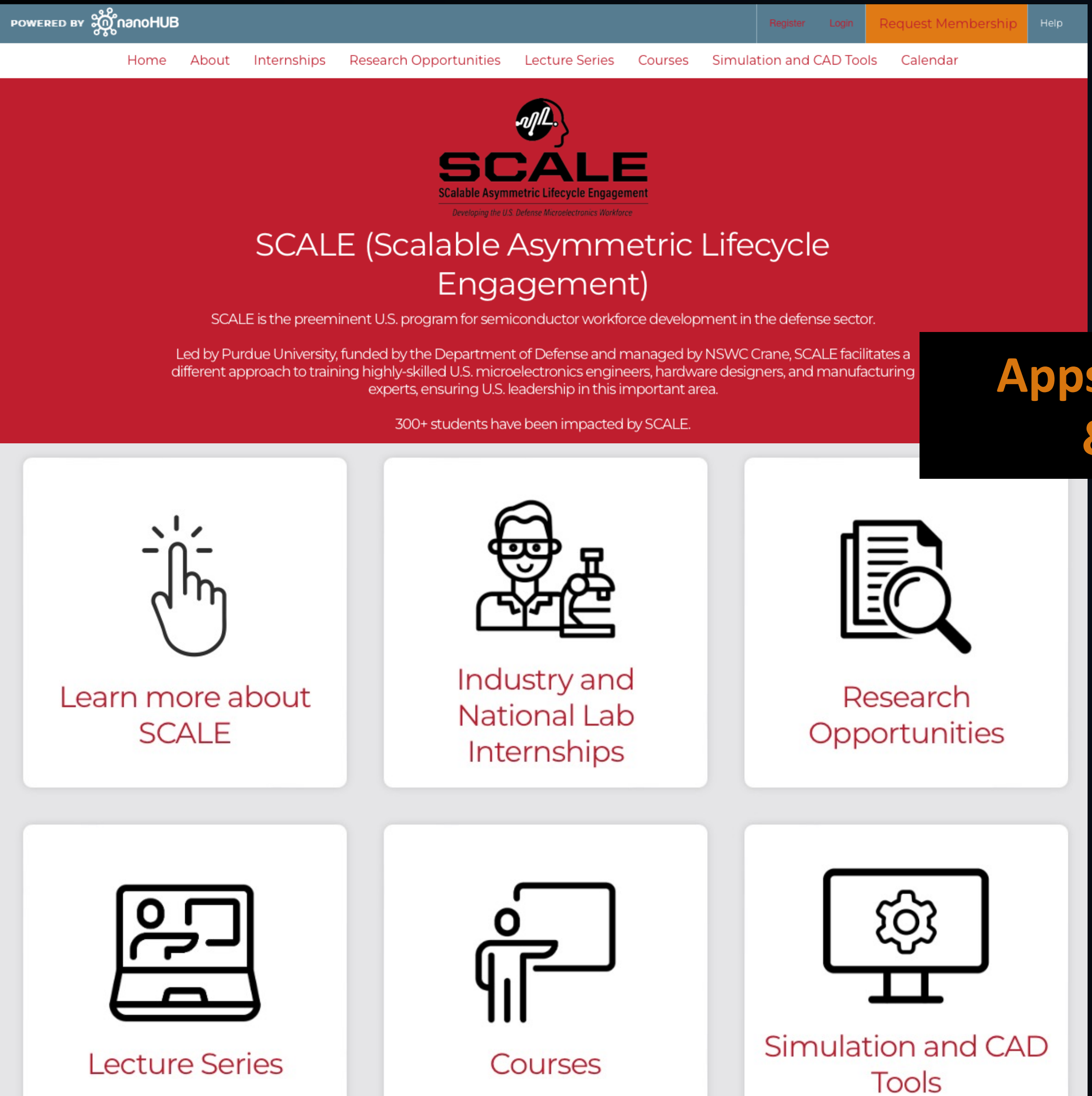
19 universities / 365 students
17 federal employers
31 defense industry companies




Undergraduate students + K-12

# nanoHUB partners in workforce development

## SCALE: Undergraduate students + K-12




## MEST: working professionals (government & contractors)

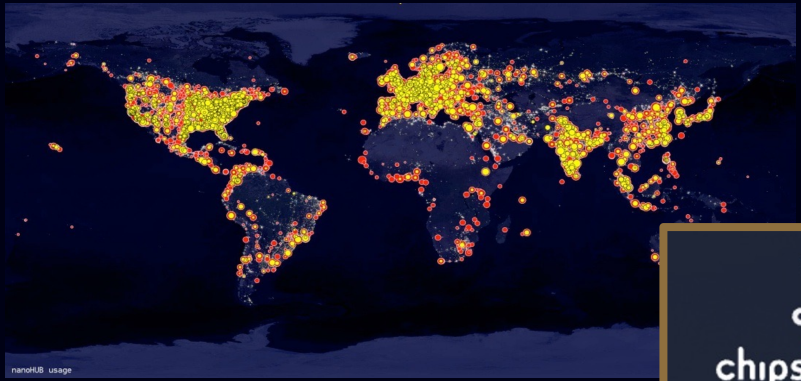
**Apps & Tools, & AI & Lectures**


**Ease of Use!**

**Community Building!**

With our technology, content & community:
We ...

- ... enable new groups of researchers!
- ... use research tools in education!
- ... publish  data & tools in a new way!
- ... changed expectations and approaches!
- ... built a global community!




chipshub by nanoHUB

170+ courses, 6500+ content items

15+ million visitors

700+ tools and apps

250,000+ simulation users

2,750 citations

55% in classes

WEB OF SCIENCE

SCALE
SCalable Asymmetric Lifecycle Engagement
Developing the U.S. Defense Microelectronics Workforce

MEST
NATIONAL MICROELECTRONICS SECURITY TRAINING CENTER

**Chipshub Questions - Can we ...**

- ... empower faculty and students?
- ... get from class to lab to fab?

# Chipshub approach:

**Ease of Use!**

**Community Building!**

https://chipshub.org

chipshub by nanoHUB

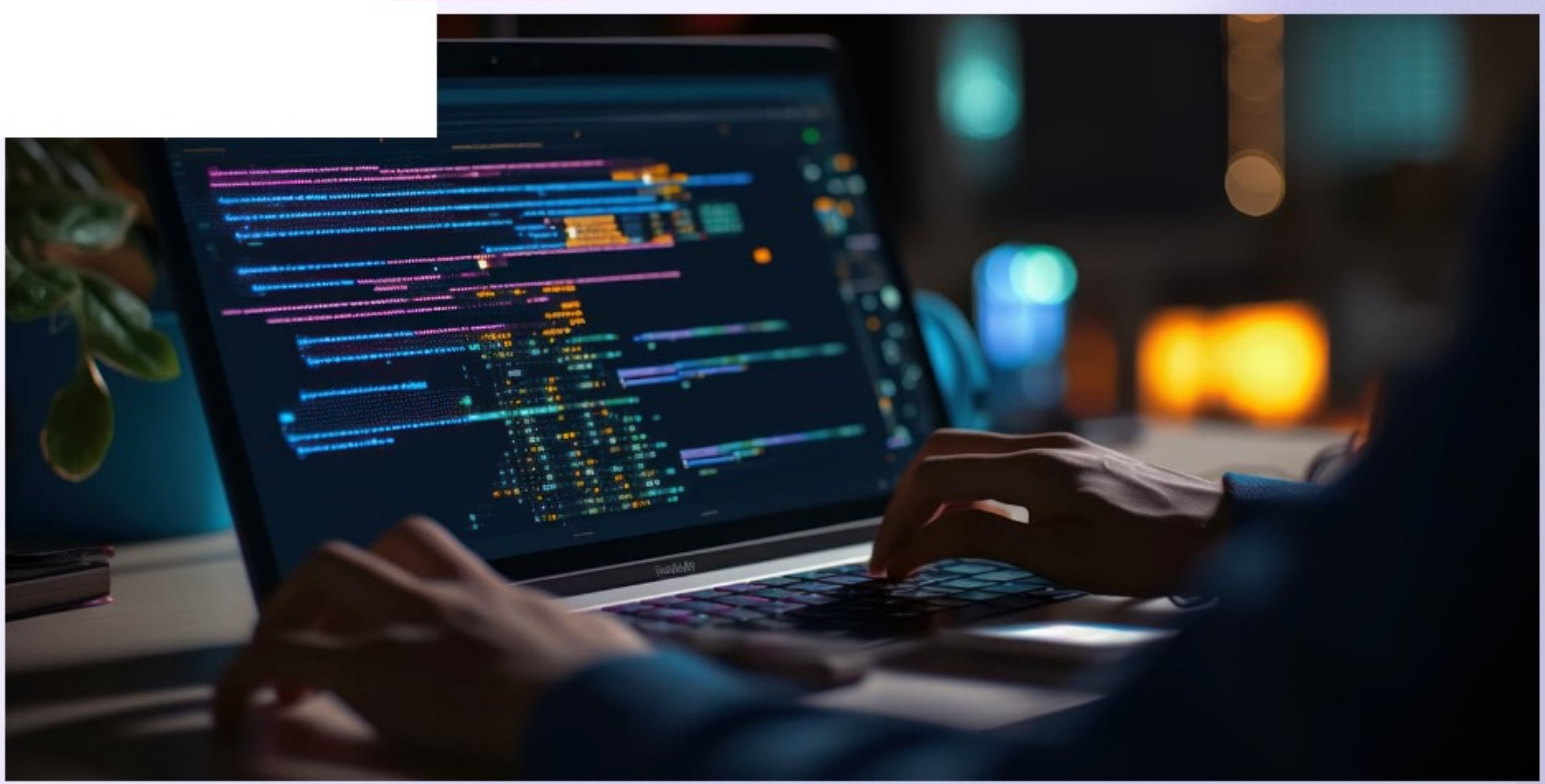
Login

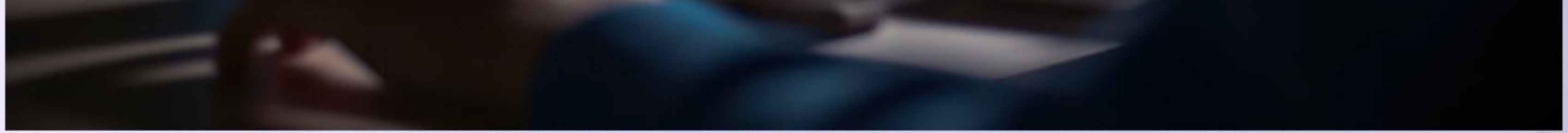
Tools Apps Courses & Textbooks Impact

# The future of chip design and manufacturing is here

# Tools that transform ideas into chips

Browse tools →



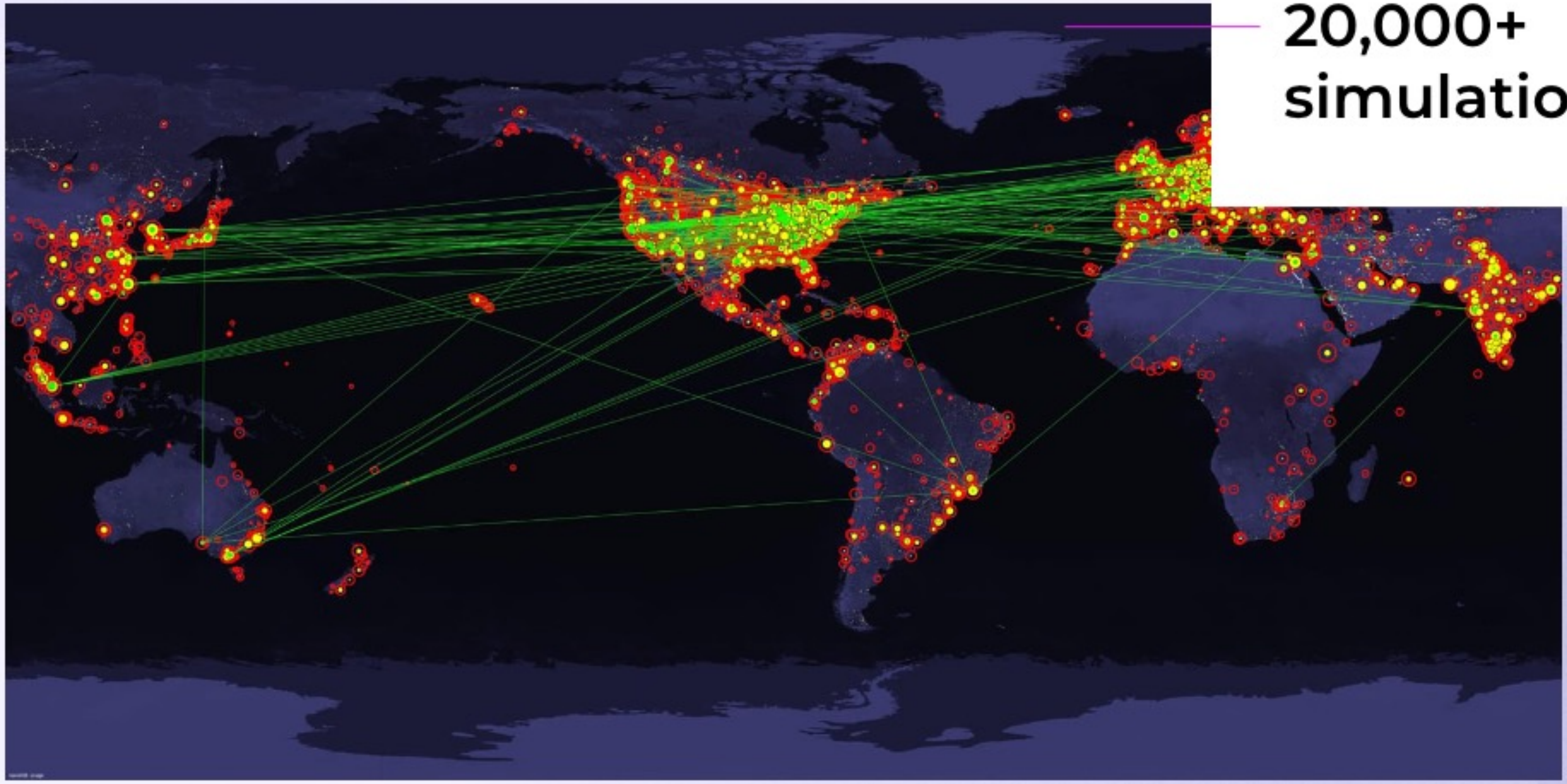


## Easy to use apps to learn and explore

← Get started with apps

## Free courses and textbooks

Explore courses →

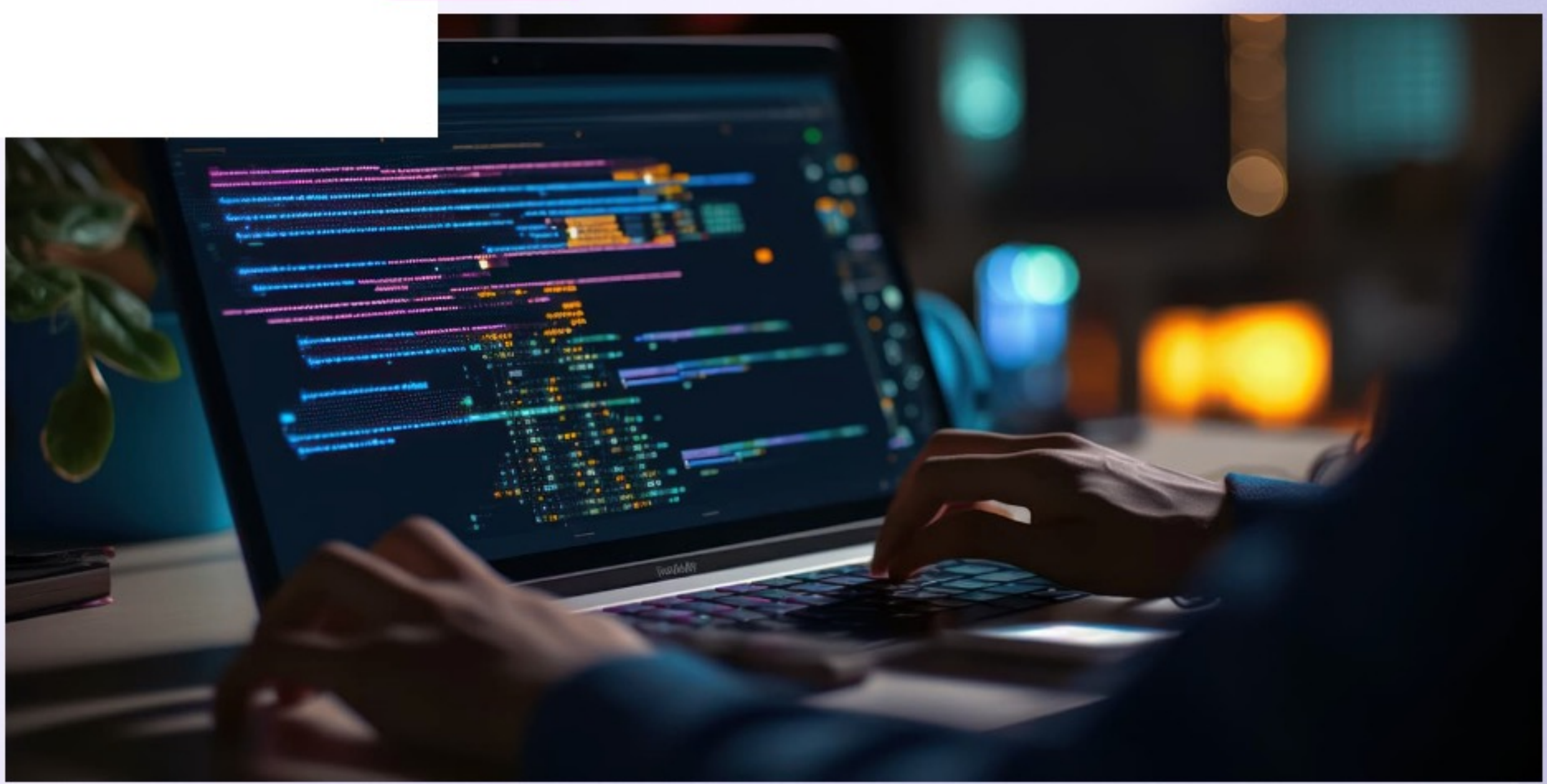


## A global platform serving 20,000+ simulation users per year

View our impact

# Tools that transform ideas into chips

Browse tools →



## Easy to use apps

chipshub.org/tools-chips

chipshub by nanoHUB

Login

Tools Apps Courses & Textbooks Impact

# Tools that transform ideas into chips

Chipshub is a central place with access to a variety of expert-level tools that can be used in the chip design process. Spend your time working rather than struggling with code installation.

### Available now:

SILVACO

SILVACO Semiconductor Process and Device Simulation for Educational Purposes Only

Thermo-Calc Software

The Thermo-Calc Software Educational Package is intended for teaching and learning basic thermodynamics and kinetic theory at an undergraduate level. This is achieved through a cooperation with Professors Mats Hillert and Malin Selleby from the department of Materials Science and Engineering at KTH Royal Institute of Technology, Stockholm, Sweden and Thermo-Calc Software AB.

Schrödinger

Schrödinger's Materials Science platform integrates predictive physics-based simulation with machine learning techniques to accelerate materials design and Schrödinger's AutoQSAR for Machine Learning educational tool is implemented on nanoHUB.

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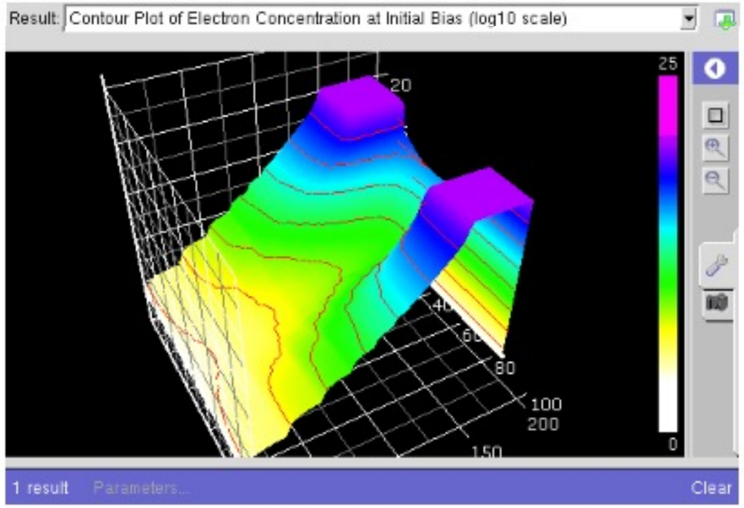
Schrödinger's Materials Science platform integrates predictive physics-based simulation with machine learning techniques to accelerate materials design and Schrödinger's AutoQSAR for Machine Learning educational tool is implemented on nanoHUB.

**From Bell Labs -**

- Padre is a 2D/3D simulator for electronic devices
- Prophet provides a framework to solve systems of partial differential equations (PDEs) in time and 1, 2, or 3 space dimensions




## Forthcoming tools:

SILVACO

SILVACO Semiconduc
for Educational Purpo

Thermo-Calc

Schrödinger

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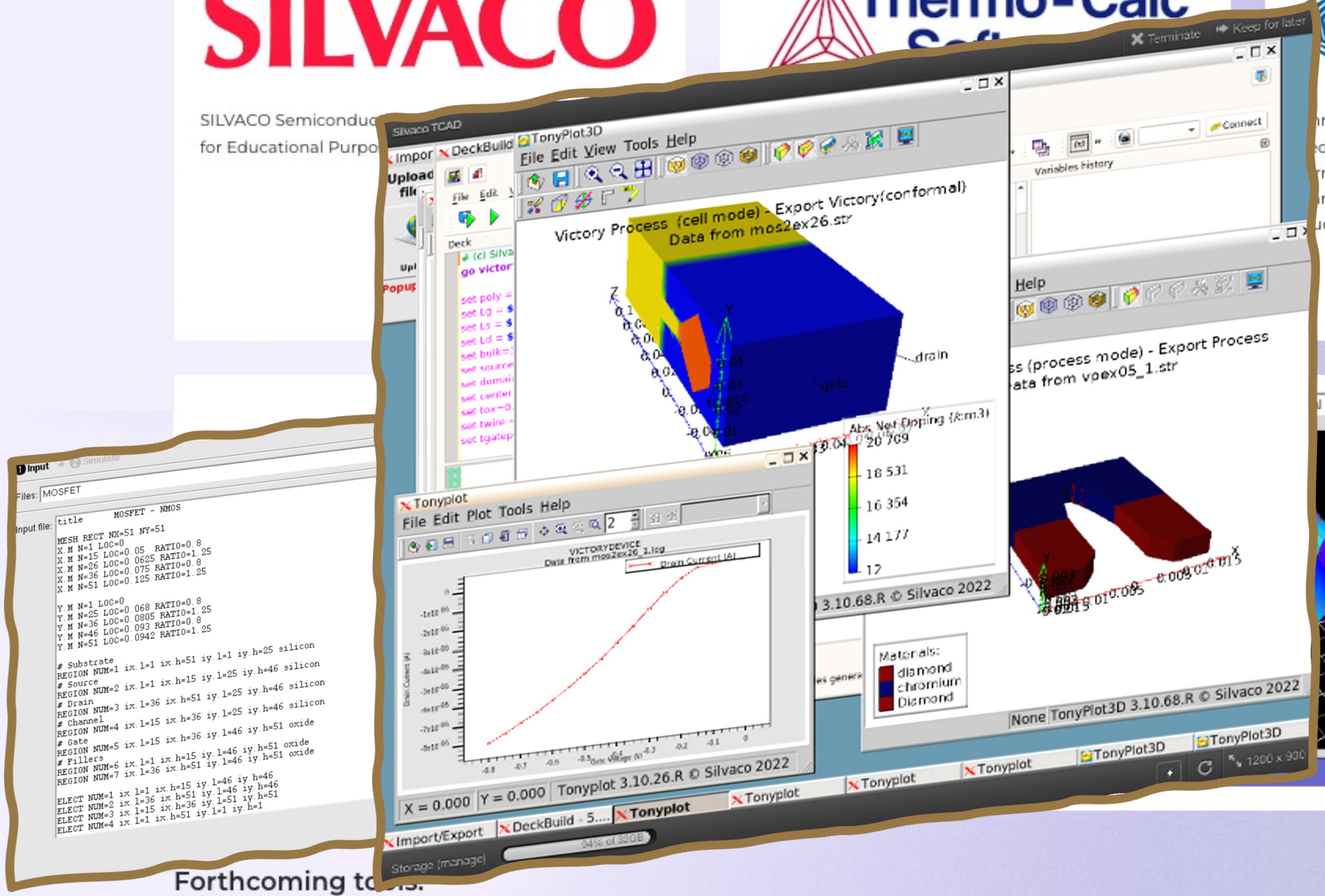
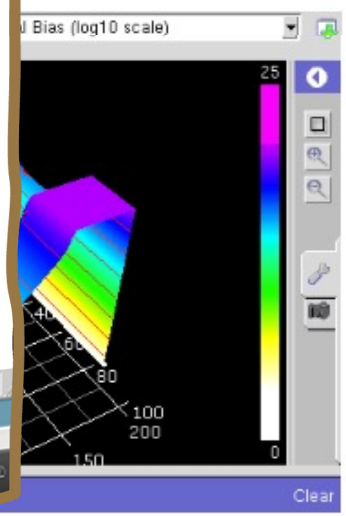


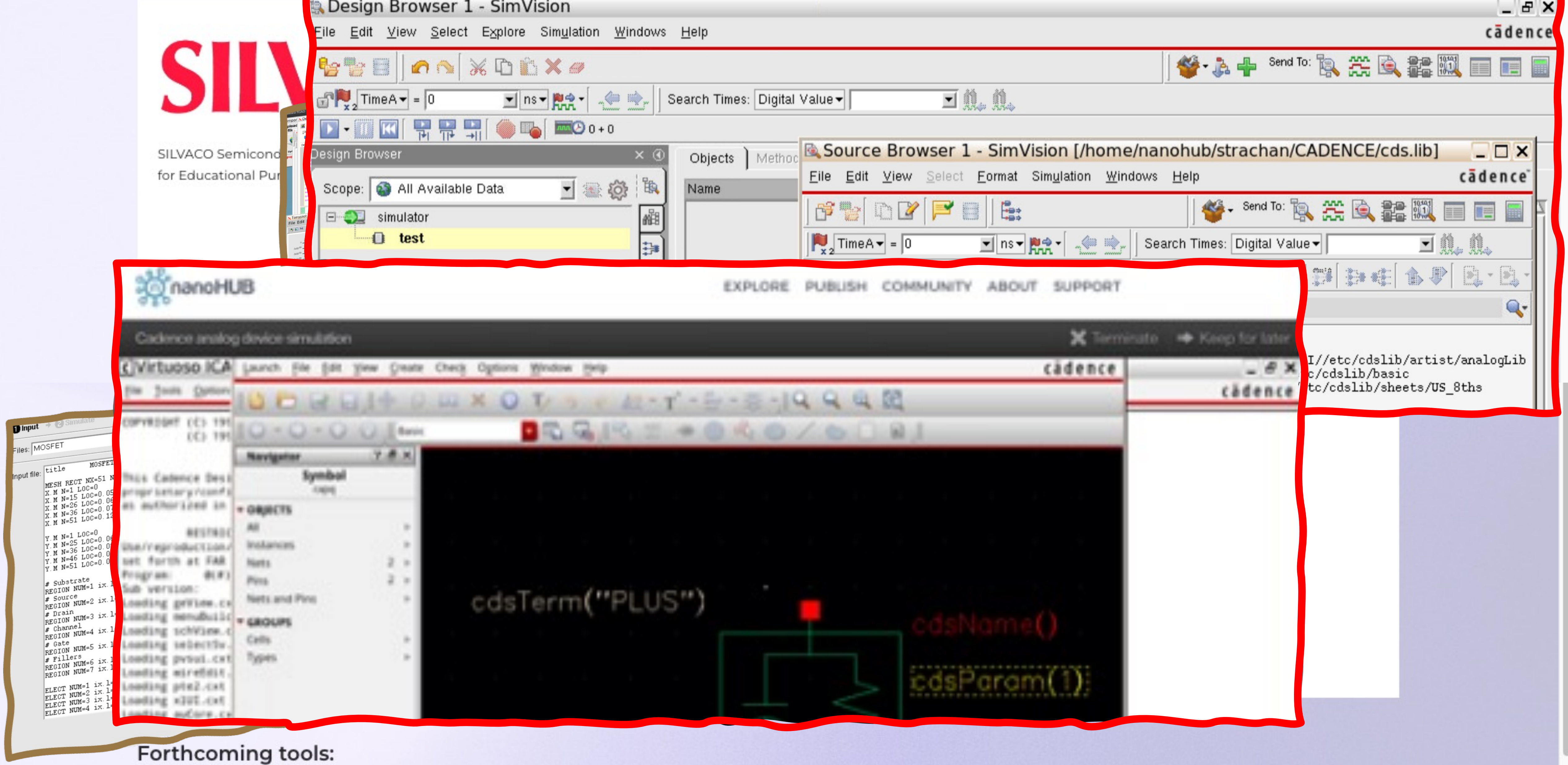

Forthcoming to...

cādence

CHIPYARD

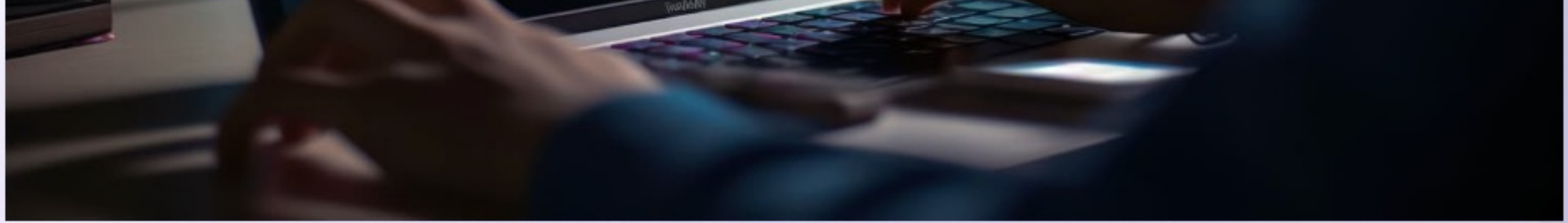
efabless.com

SYNOPSYS




Forthcoming tools:

cadence CHIPYARD efabless synopsys



## Easy to use apps to learn and explore

Get started with apps

chipshub.org/apps

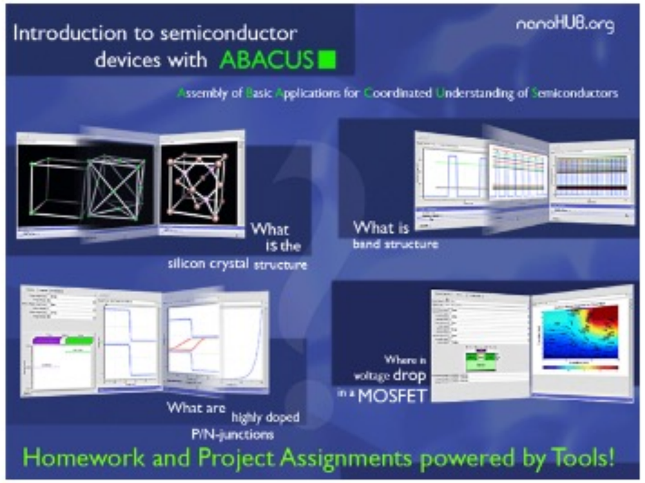
chipshub by nanoHUB

Login

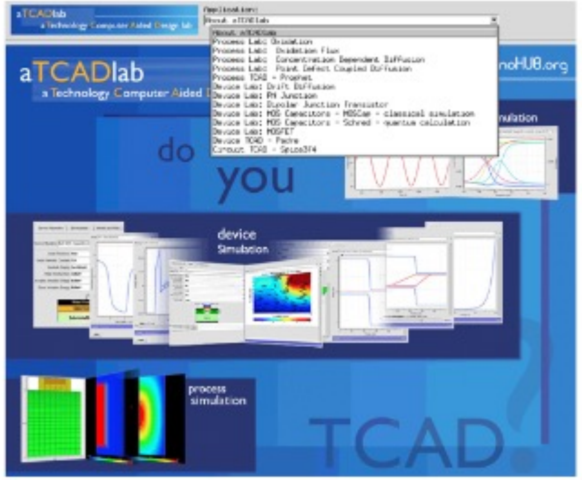
Tools Apps Courses & Textbooks Impact

# Easy to use apps to learn and explore

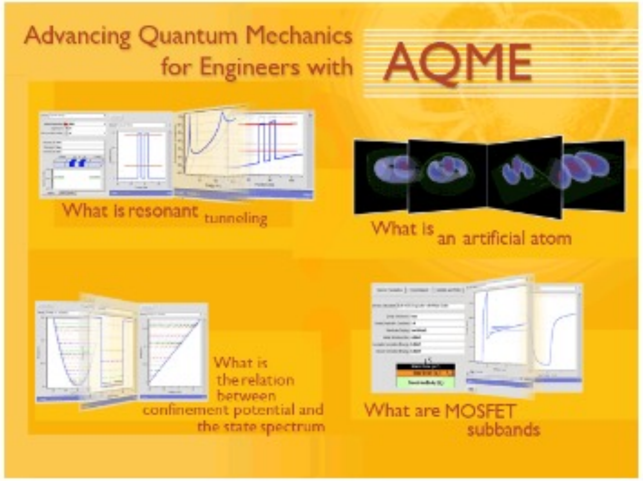
Simple apps that focus on user experience and delivery of modeling results.
No software installation needed and a gentle learning curve.
Used by 90,000+ students around the world.



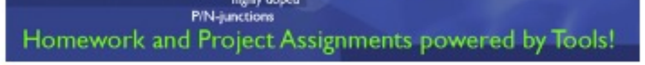

## Semiconductor Device Fundamentals with ABACUS




## Introduction to TCAD Simulation with aTCADlab




## Advancing Quantum Mechanics for Engineers with AQME




### Semiconductor Device Fundamentals with ABACUS

ABACUS is a set of tools that have been used by hundreds of classes to enable students to explore the fundamental devices that are taught in typical undergraduate and graduate level courses.


### Introduction to TCAD Simulation with aTCADlab

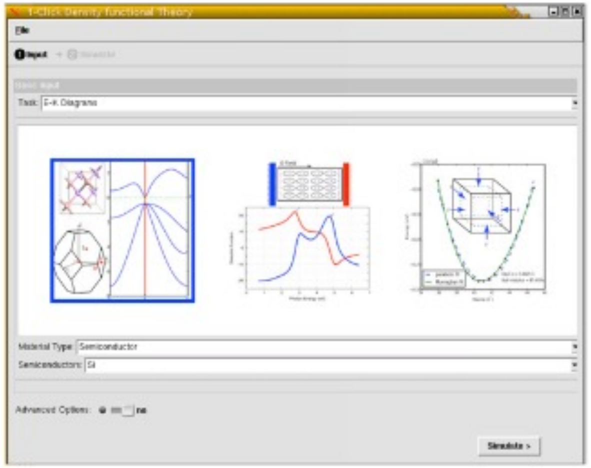
nanoHUB tools ranging from process simulation, over device simulation to circuit simulation.


### Advancing Quantum Mechanics for Engineers with AQME

The AQME toolbox holds a set of easily employable tools appropriate for teaching a quantum mechanics class in either engineering or physics.

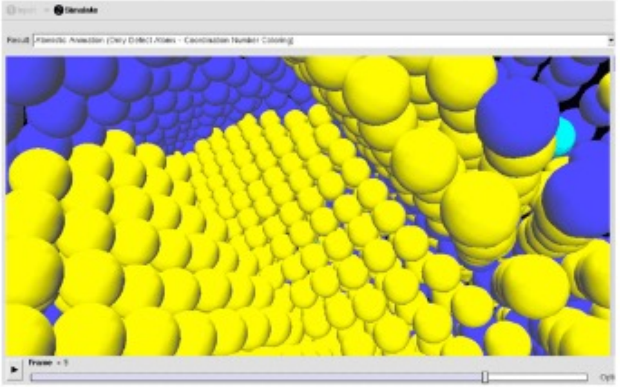
### Virtual Reality Immersive Learning in vFabLab™

nanoHUB is partnering with vFabLab™ to enable students at all educational levels to learn about real semiconductor device processing tools. Currently vFabLab™ users have to sign up separately from a nanoHUB account.



### DFT Material Properties Simulator

Materials modeling provides a cost and time efficient method for studying their properties, especially in nanotechnology where length and time scales are not accessible experimentally. The tool relies on density functional theory (DFT) calculations to compute specific properties for a wide range of materials including semiconductors, insulators, and metals. The tool can compute electronic band structures, density of states, bulk modulus, dielectric constants and other properties of the material. The user can select from various pre-set materials or create one of their own by specifying the atomic structure.



### Nanomaterial Mechanics Explorer

This tool enables users to explore properties of materials from the atomistic scale including dislocation motion, crack propagation, plastic deformation, melting, and martensitic transformation. The tool uses molecular dynamics simulations with pre-built examples and full control of individual simulation parameters for experienced users within advanced options. The tool runs the LAMMPS molecular dynamics code and connects to OpenKIM, a database of interatomic models, enabling simulation of over 30 elements and 50 alloys from more than 180 models, primarily of the embedded-atom method type.



Homewo

Semicond
ABACUS

ABACUS is a
classes to en
that are taug
courses.

Advancing Quantum Mechanics for Engineers

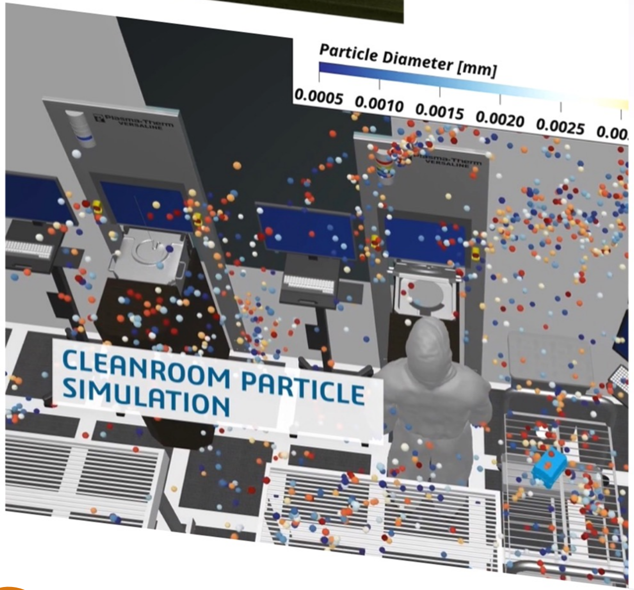
Virtual Re
vFabLab™

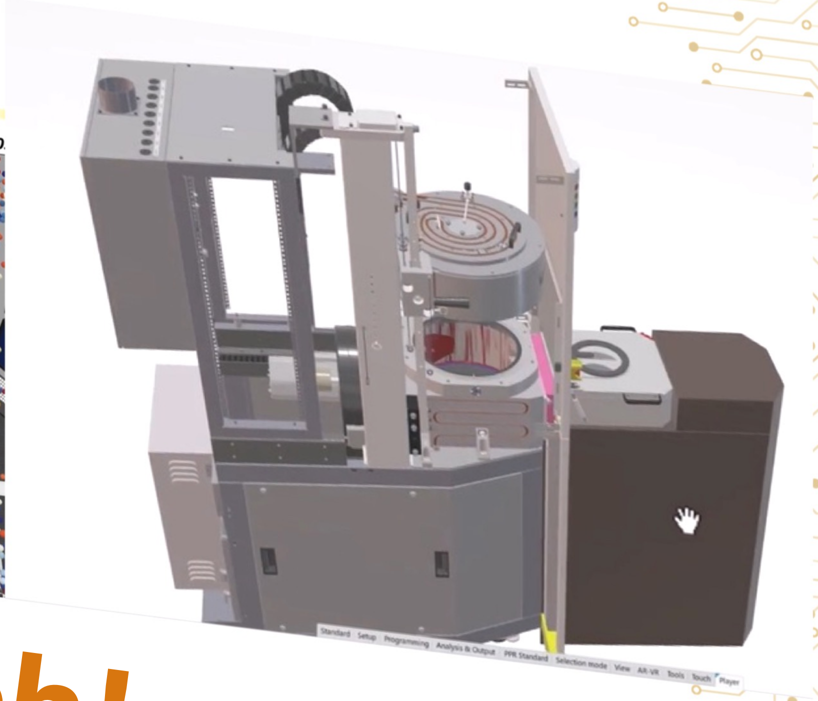
nanoHUB is
educational
processing to
separately fr

# Virtualization of Birck Nanotechnology Center

PURDUE UNIVERSITY

DASSAULT SYSTEMES



Video at Lunch!

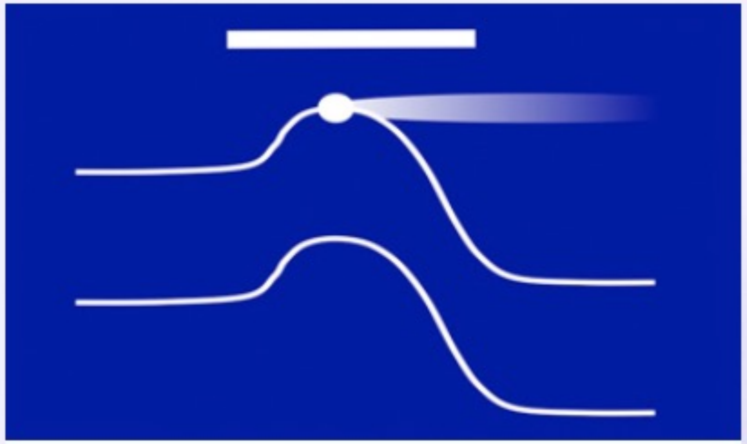
## Free courses and textbooks

Explore courses →

# Free courses and textbooks

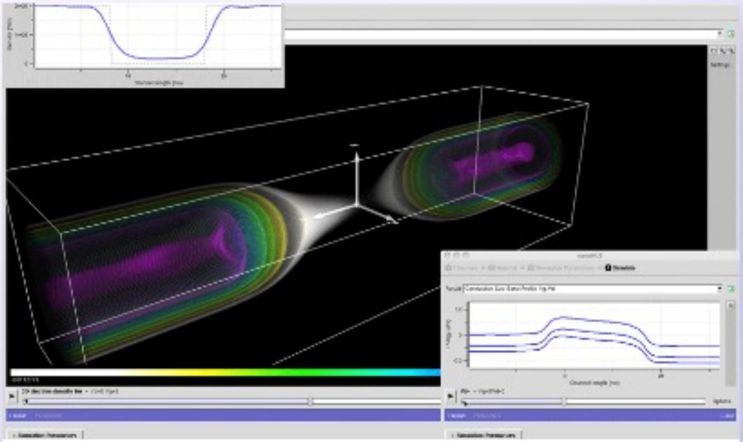
Millions of users annually access our open courseware and experience the next generation of textbooks from leading faculty through a partnership with World Scientific Publishing.

## Open courses



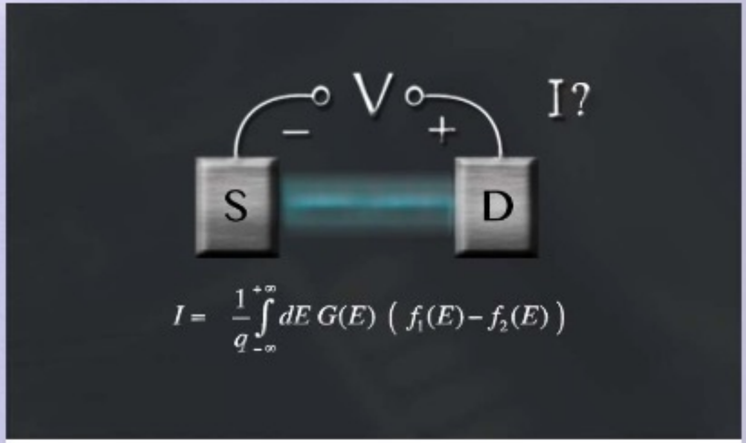
### Fundamentals of Nanotransistors, 2nd Edition

by Mark Lundstrom



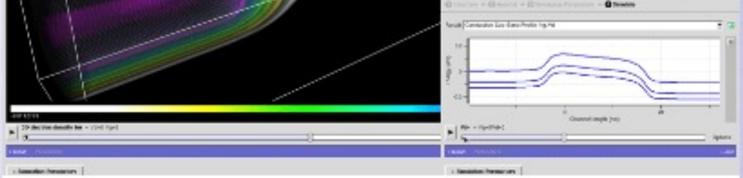
### Solid State Devices I

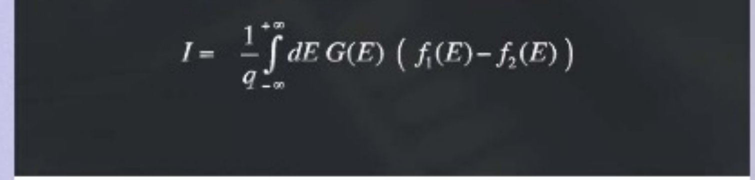
by Gerhard Klimeck




### Fundamentals of Nanoelectronics - Part A: Basic Concepts, 2nd Edition

by Supriyo Datta






### Fundamentals of Nanotransistors, 2nd Edition

by Mark Lundstrom

Nanotransistors is a self-paced nanoHUB-U offering by Prof. Mark Lundstrom. This course features video lectures, quizzes, and exams. Prof. Lundstrom also provides background resources on the essential physics of nanoscale transistors.

### Solid State Devices I

by Gerhard Klimeck

Semiconductors are everywhere in human activities, from your credit card to space exploration. This graduate-level introduction brings aspects of physics, chemistry, and engineering together to understand, analyze, and design transistors and solar cells.

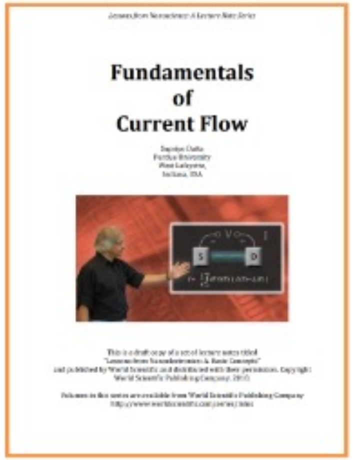
### Fundamentals of Nanoelectronics - Part A: Basic Concepts, 2nd Edition

by Supriyo Datta

Basic Concepts presents key concepts in nanoelectronics and mesoscopic physics and relates them to the traditional view of electron flow in solids.

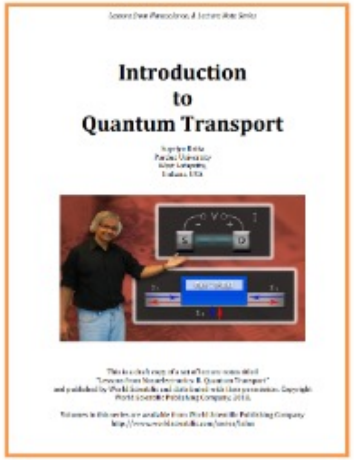
More courses

## Downloadable textbooks



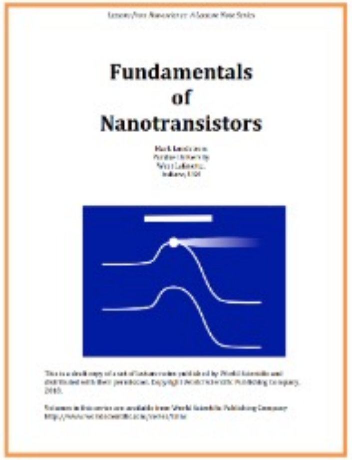

### Fundamentals of Current Flow

by Supriyo Datta




### Introduction to Quantum Transport

by Supriyo Datta




### Fundamentals of Nanotransistors

by Mark Lundstrom

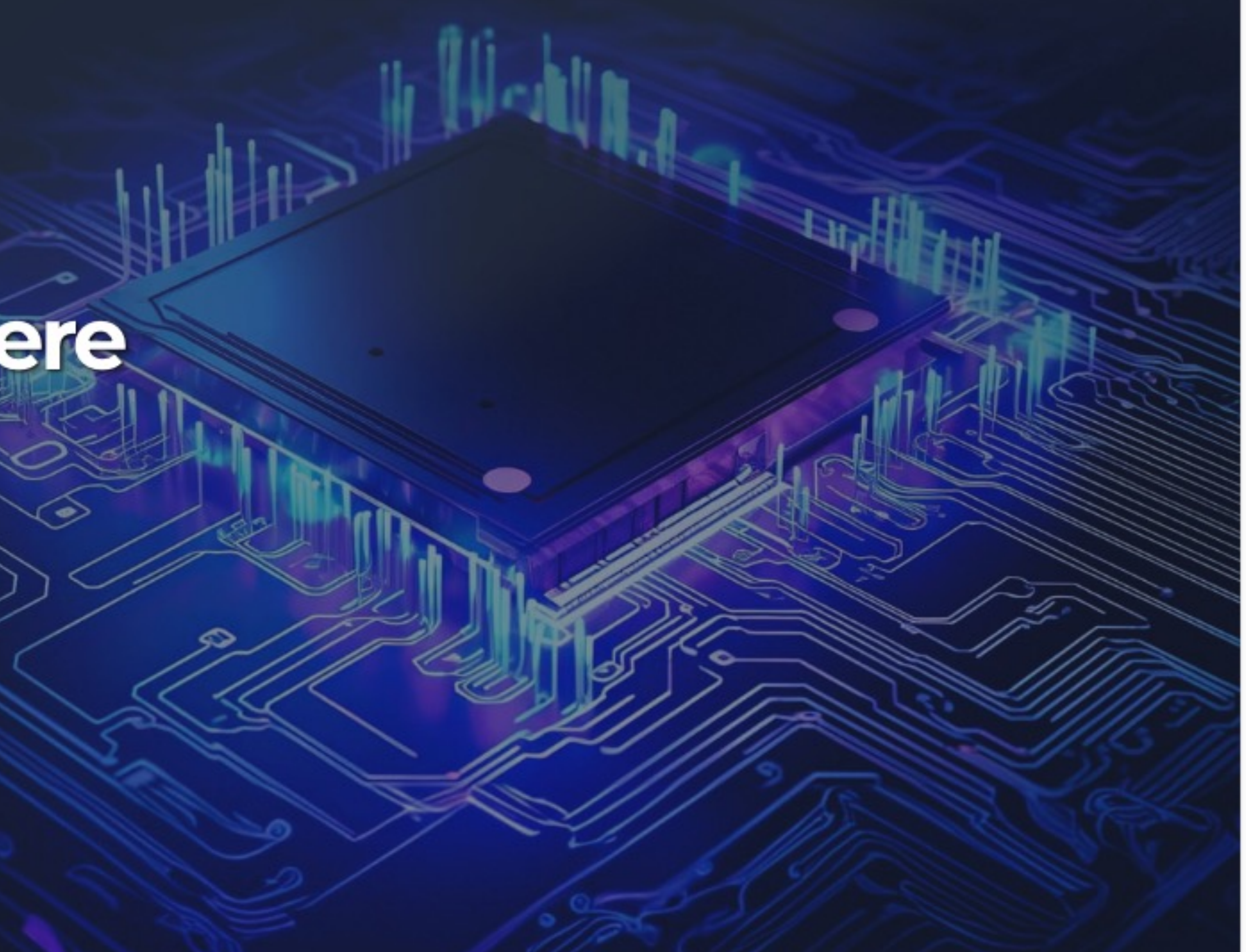
We have ...

- ... 700+ tools and Apps.
- ... 170+ courses, 6500+ content items

# The future of chip design and manufacturing is here

We ...

- ... enable new groups of researchers!
- ... use research tools in education!
- ... publish  data & tools in a new way!
- ... changed expectations and approaches!
- ... built a global community!



https://chipshub.org

chipshub by nanoHUB

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## We are not done yet. We need ...

- ... deeper support
  SILVACO, SYNOPSYS, CHIPYARD, cādence, SIEMENS, OpenLane
- ... PDK vendor engagement
  intel, tsmc, gf, skywater
- ... scalable licensing management
- ... tape out partners & "white glove"
  efabless.com, imec IC-link, CMC MICROSYSTEMS, THE MOSIS SERVICE
- ... commercial cloud partners
  Microsoft Azure

https://chipshub.org

chipshub by nanoHUB

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## We are not done yet. We need ...

## So... How can we get there?

## history / background:

~1996 Software Portals Emerge
Serving small expert groups
Not reaching "different" users
=>begin to have a bad reputation

2002 NSF funds nanoHUB
2005 nanoHUB cloud
2005 nanoHUB apps

Largest academic end-to-end scientific user cloud

https://chipshub.org

chipshub by nanoHUB

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2002 NSF funds nanoHUB
2005 nanoHUB cloud

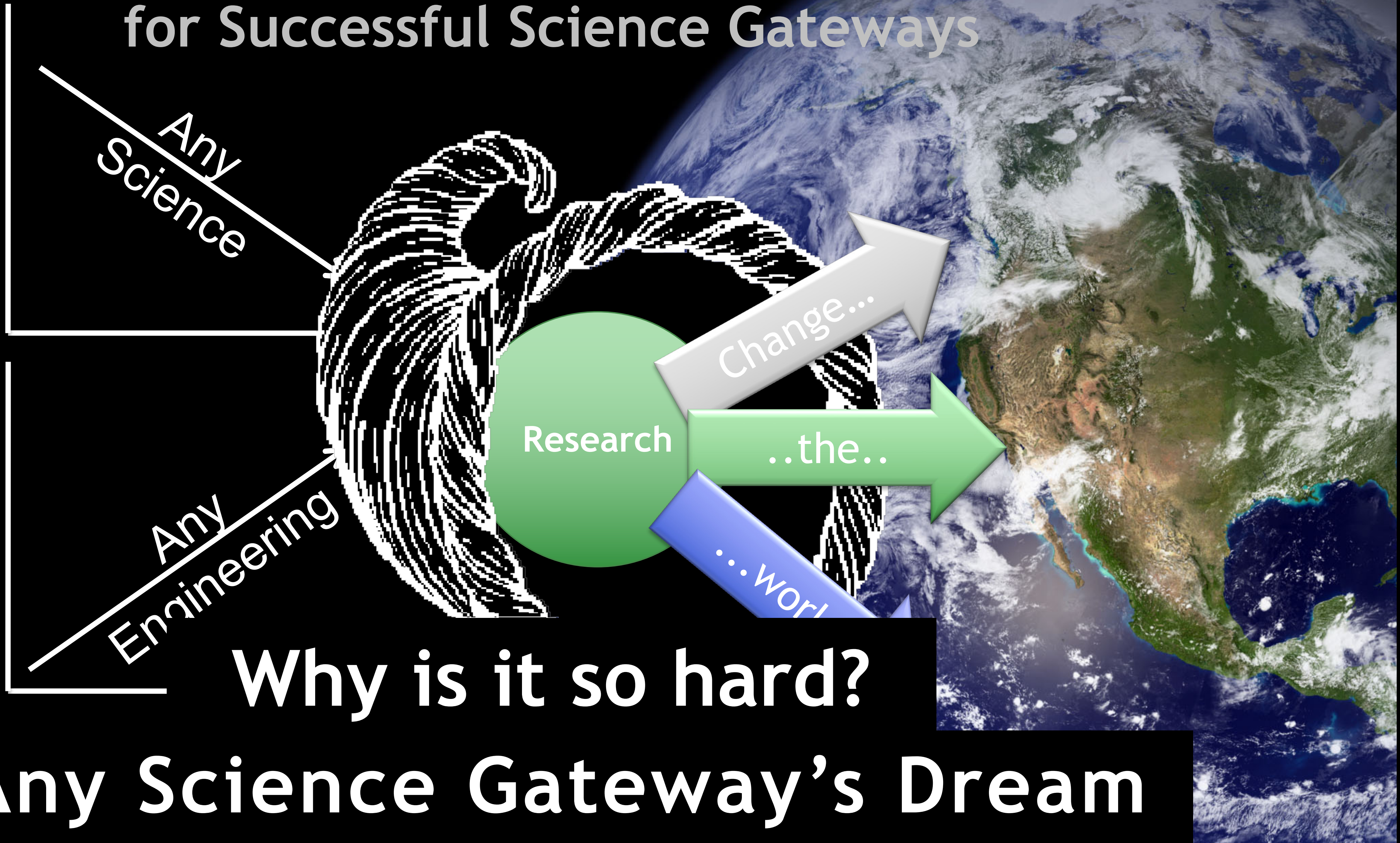
Largest academic end-to-end scientific user cloud

**Just hosting software is not enough!**

**7 Criteria for Successful Science Gateways**

# 7 Criteria

## for Successful Science Gateways



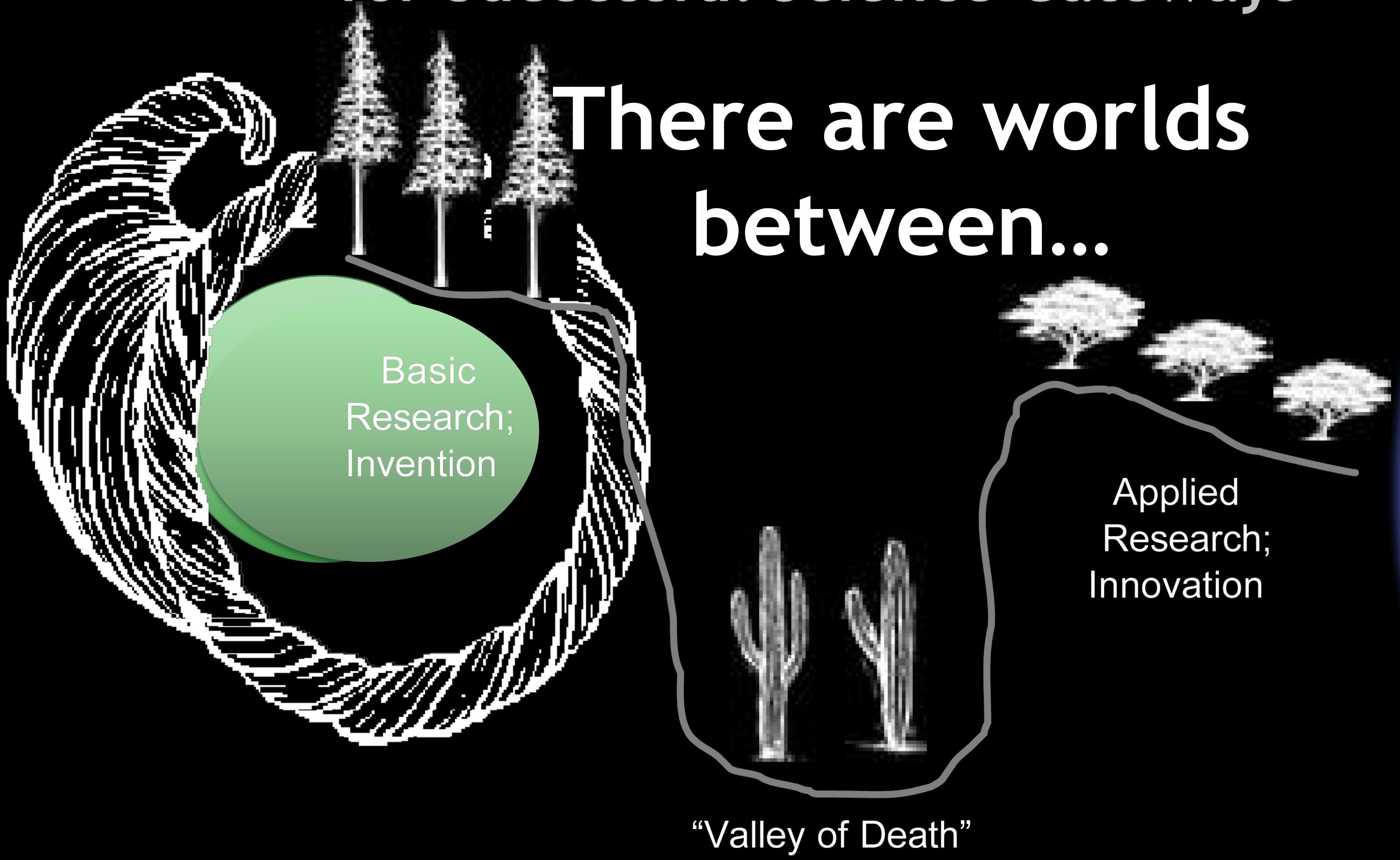

## Why is it so hard?

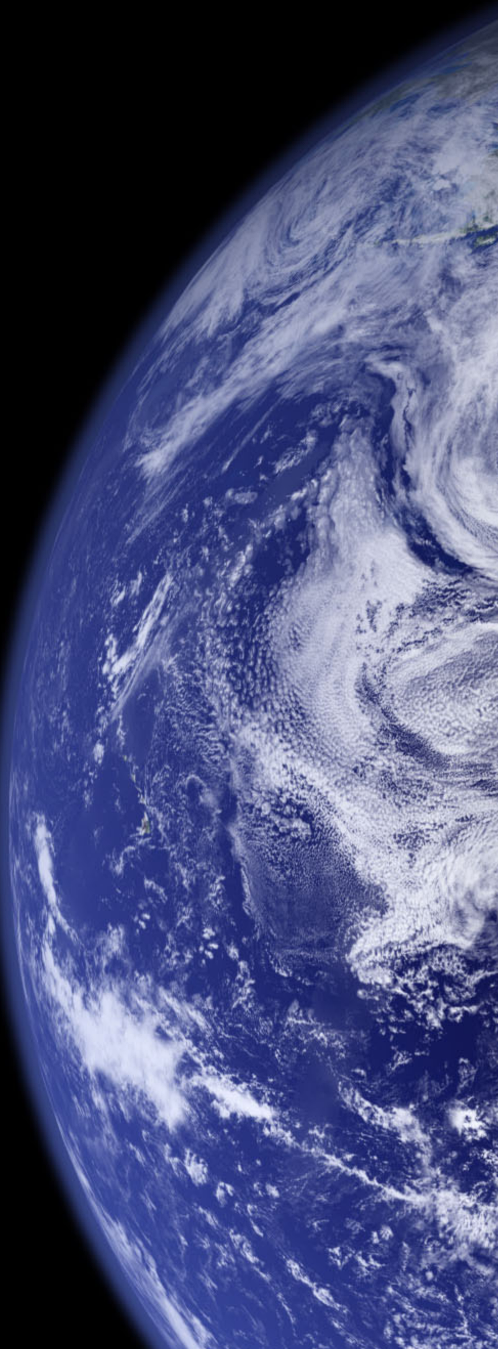
## Any Science Gateway’s Dream

# 7 Criteria

## for Successful Science Gateways

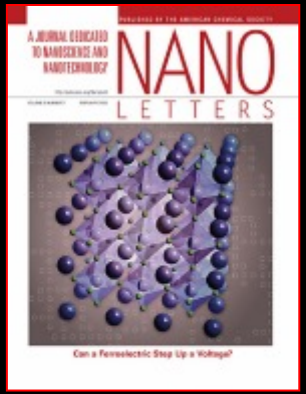
## There are worlds between…

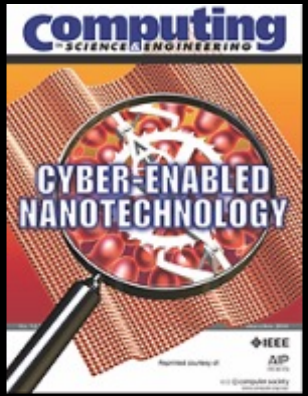


# 1: Outstanding Science / Quality

"Stuff the world wants"




Leveraged Research

**$5.1M**

NRI anoelectronics RESEARCH INITIATIVE

SRC Semiconductor Research Corporation

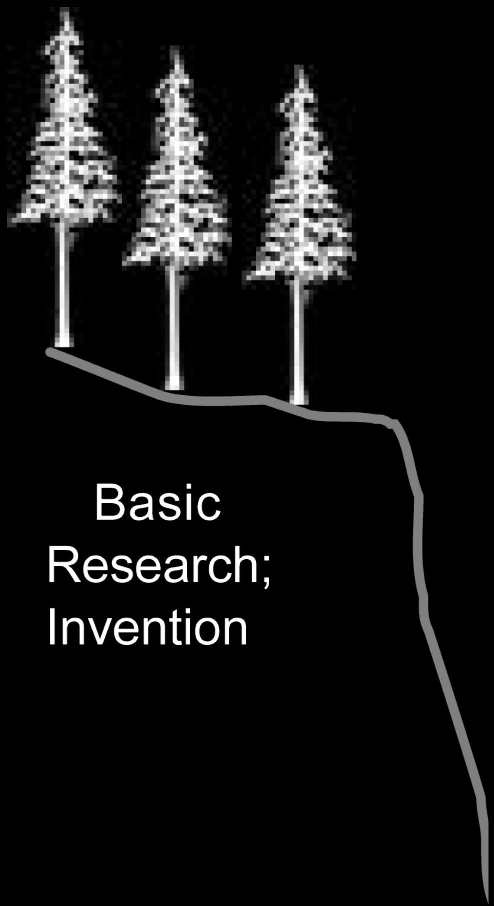
intel

MARCO

IBM

INDEX Institute For Nanoelectronics Discovery And Exploration

2011 Data



ncn

Basic Research; Invention

"Stuff you would use yourself!"

# 2: Commitment to Dissemination

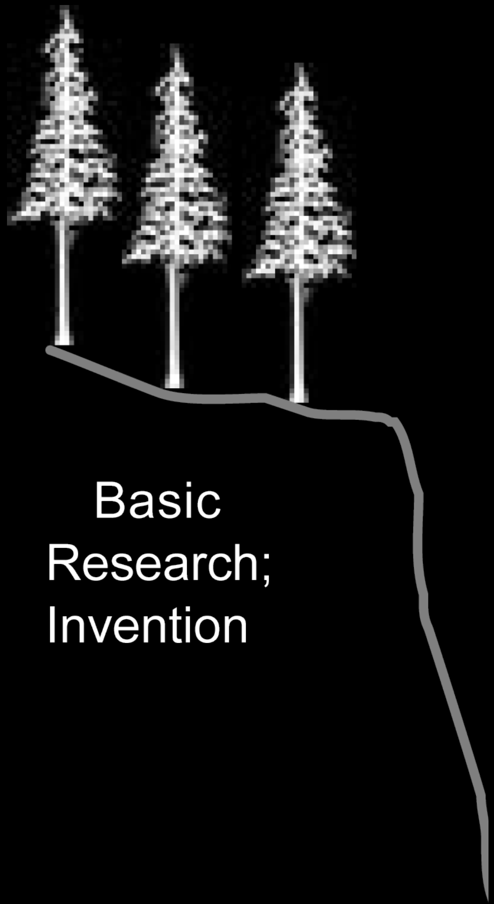
"faculty that want to give it away"

**Building Faculty Incentives**

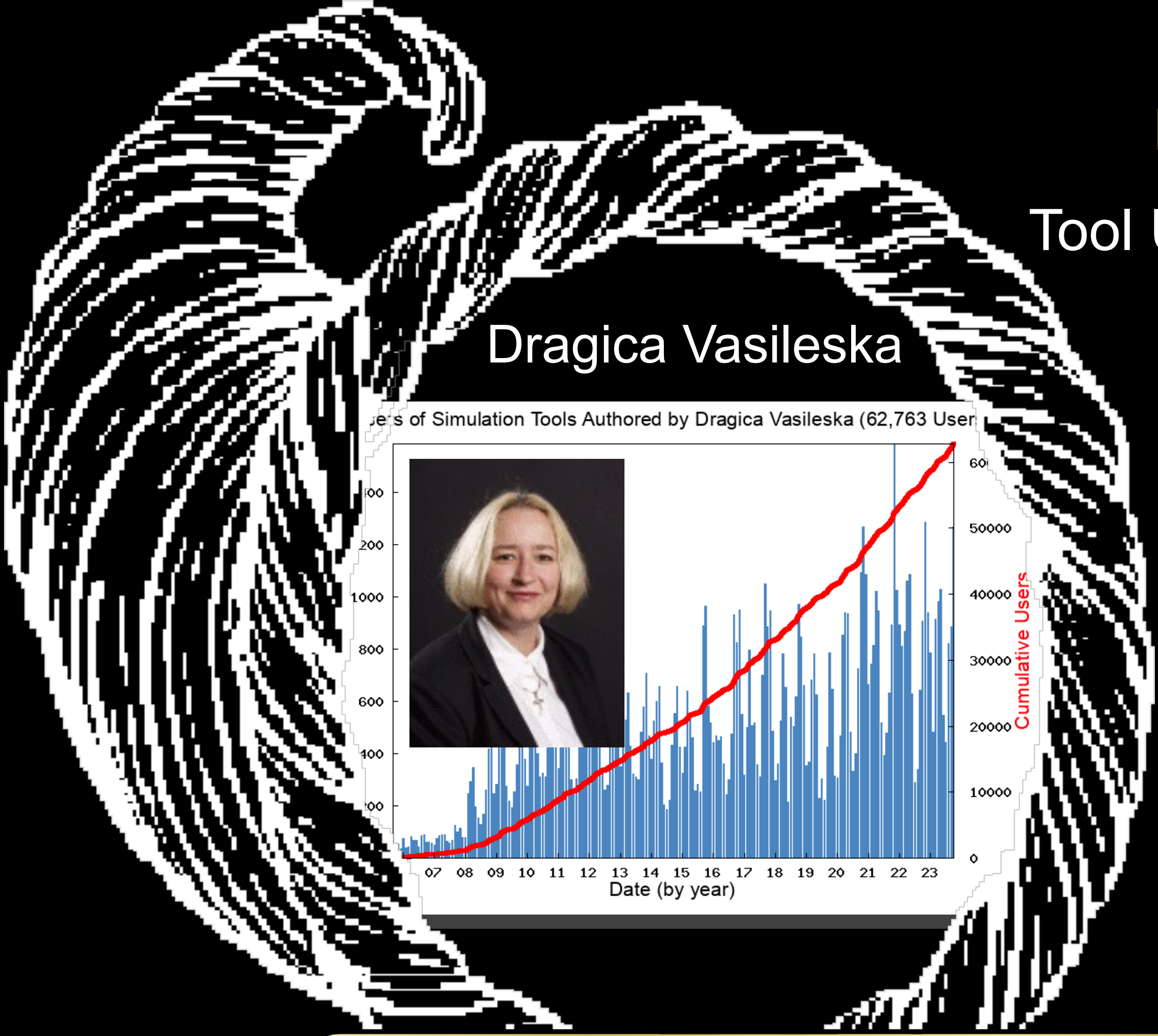
46 faculty

+ 6 site leads

106 grad students




2011 Data



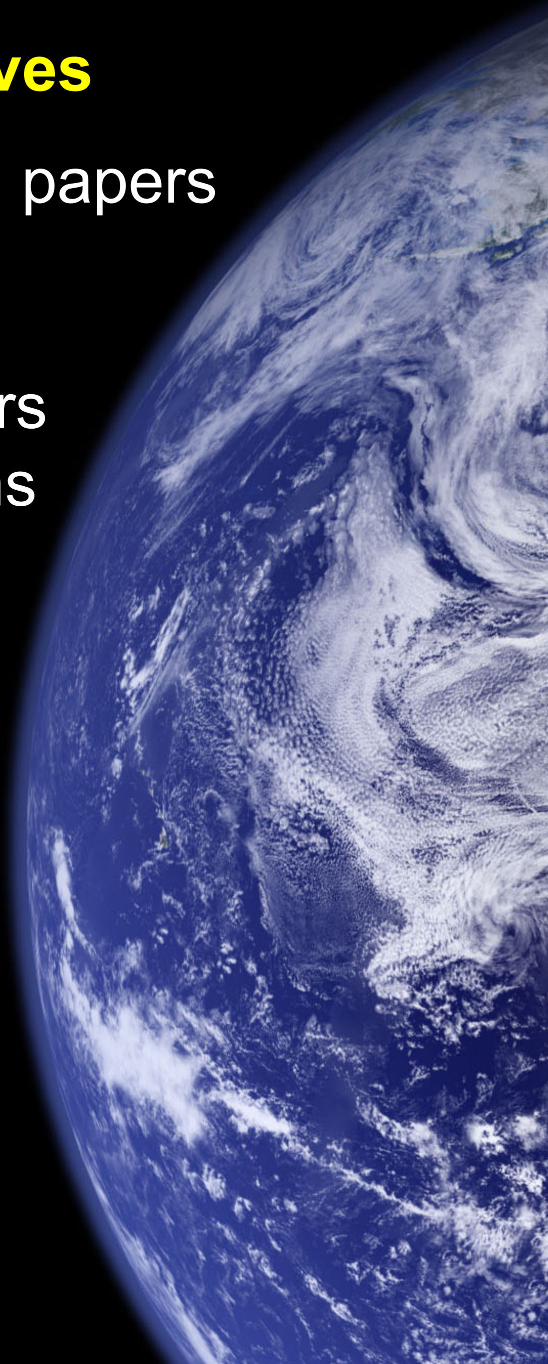

## Faculty Incentives

Tool Usage ≈ reading papers

**20 tools**

➔ 62,763 users

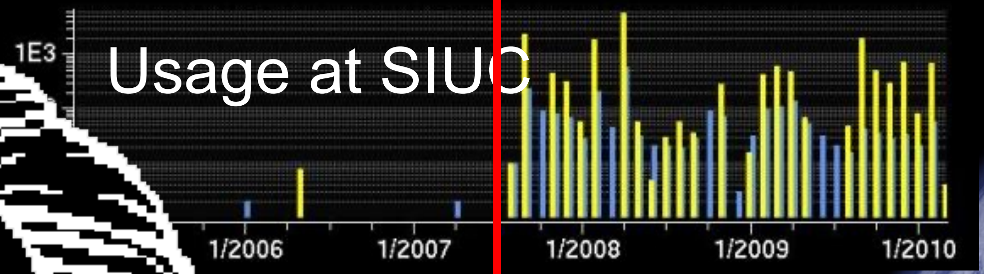
➔ 192 citations



Proof of Impact!

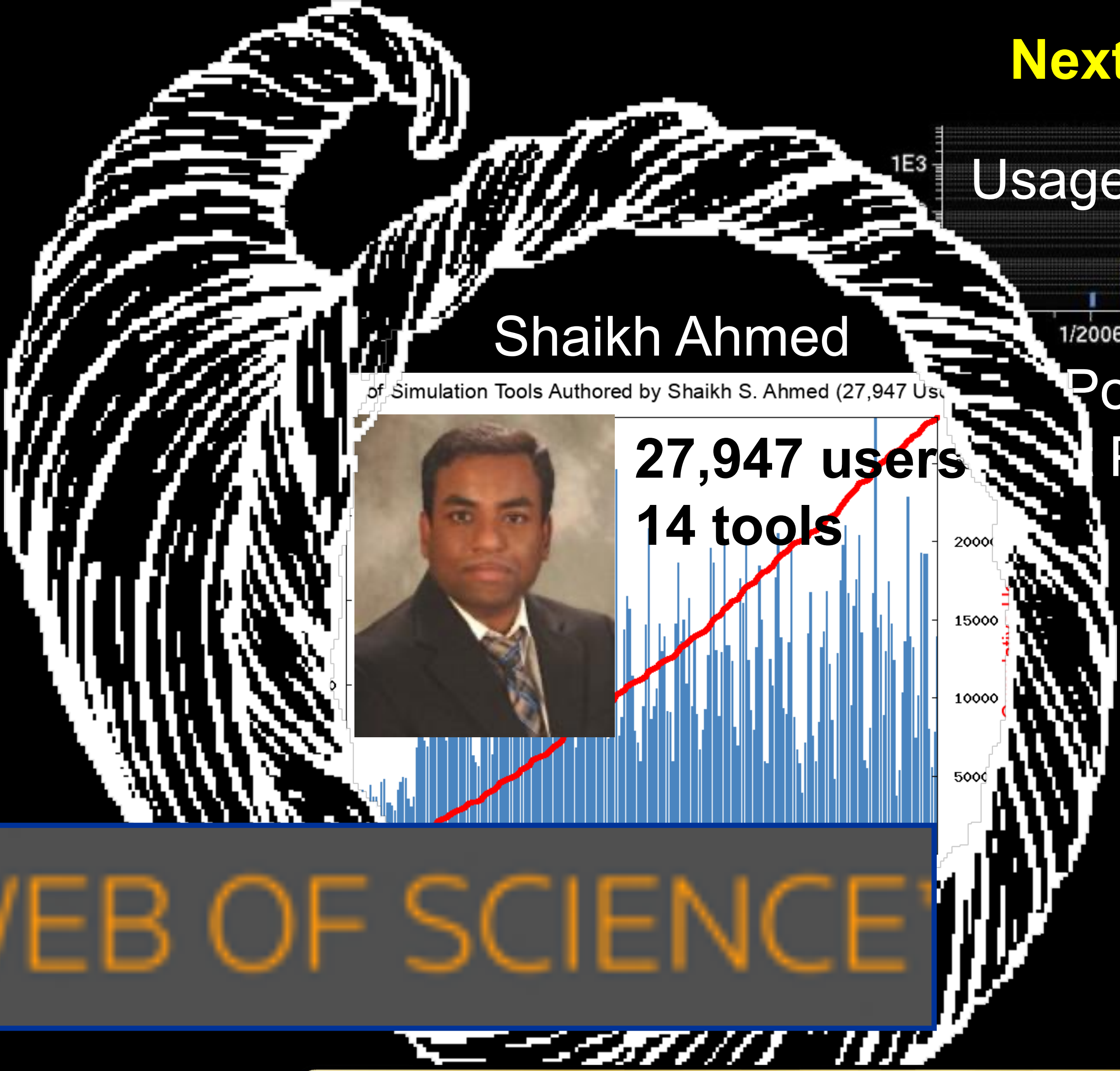
Great in Proposals!

## Next Generation Faculty:




Post Doc Purdue | Faculty at SIUC

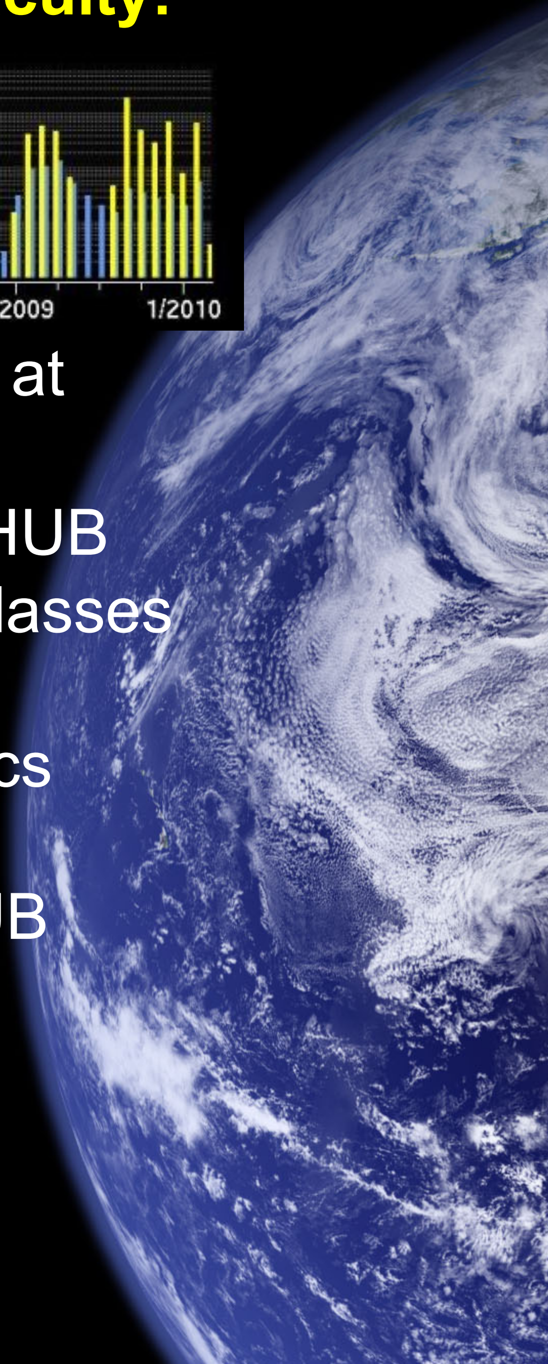
Shaikh Ahmed



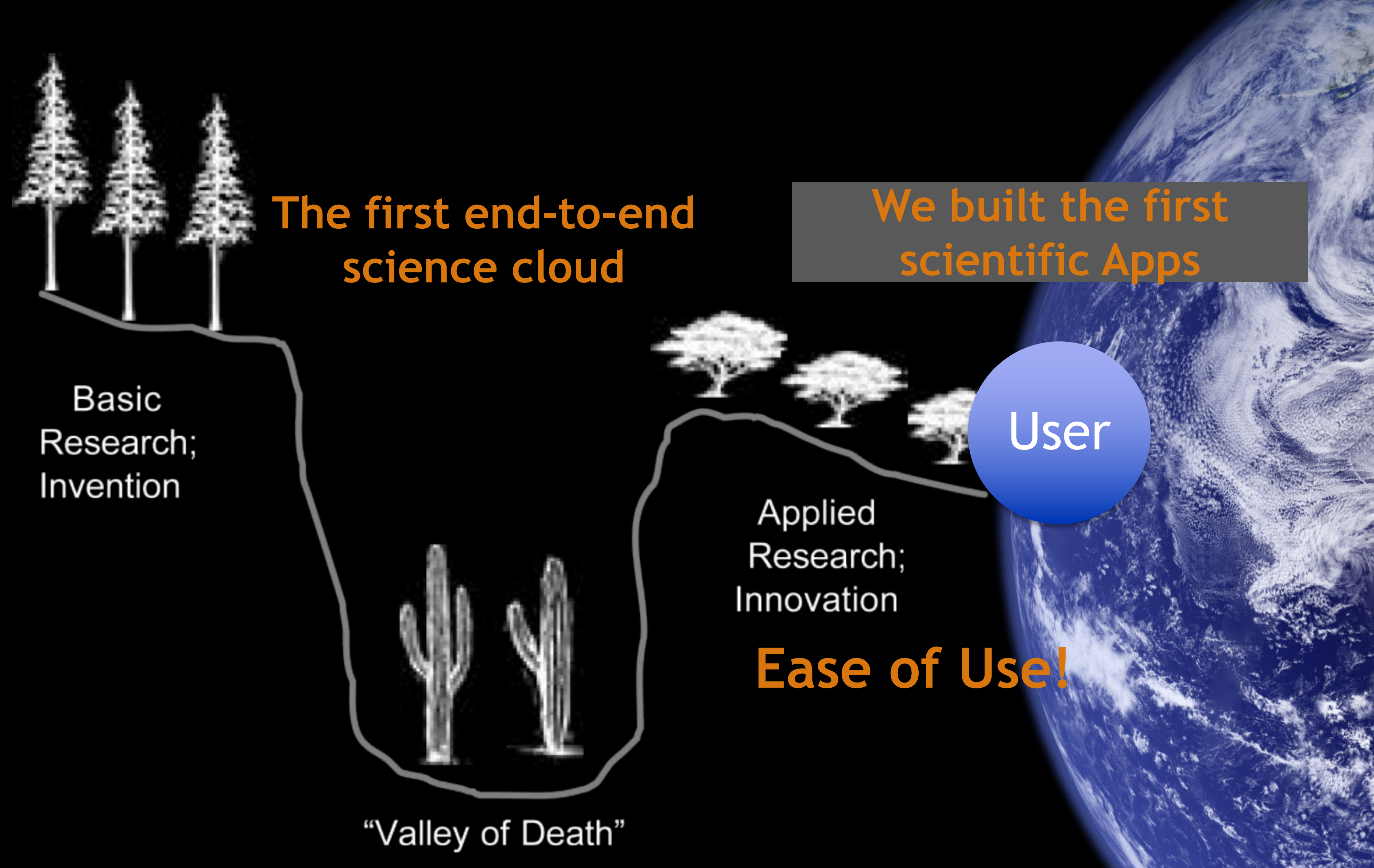

- Infused nanoHUB into existing classes
- Built a new nanoelectronics curriculum
- Used nanoHUB for research

WEB OF SCIENCE

Early Tenure Promotion



# 3: Technology for Dissemination

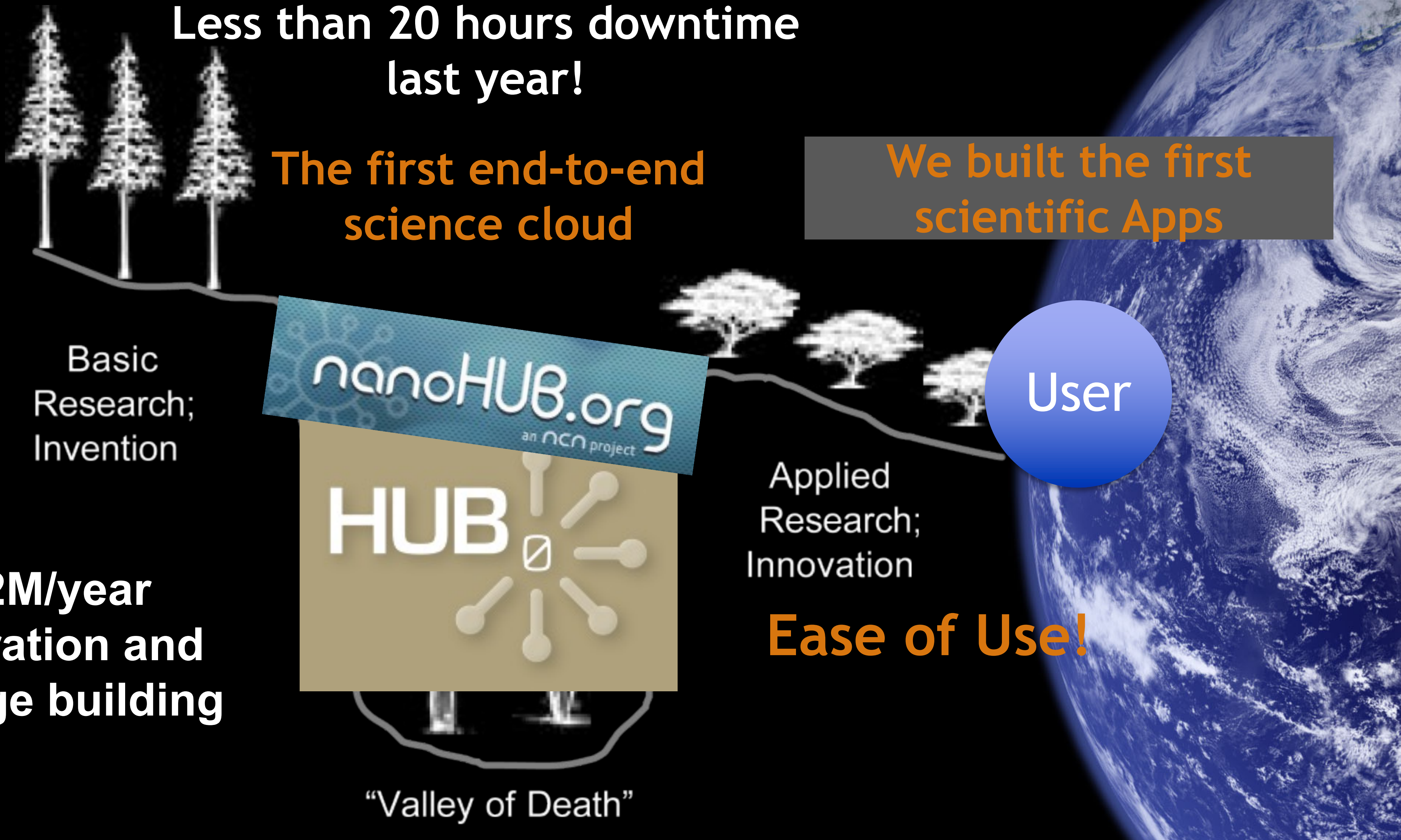


# 3: Technology for Dissemination

**"simple and utterly dependable"**
**Less than 20 hours downtime last year!**

The first end-to-end science cloud

We built the first scientific Apps

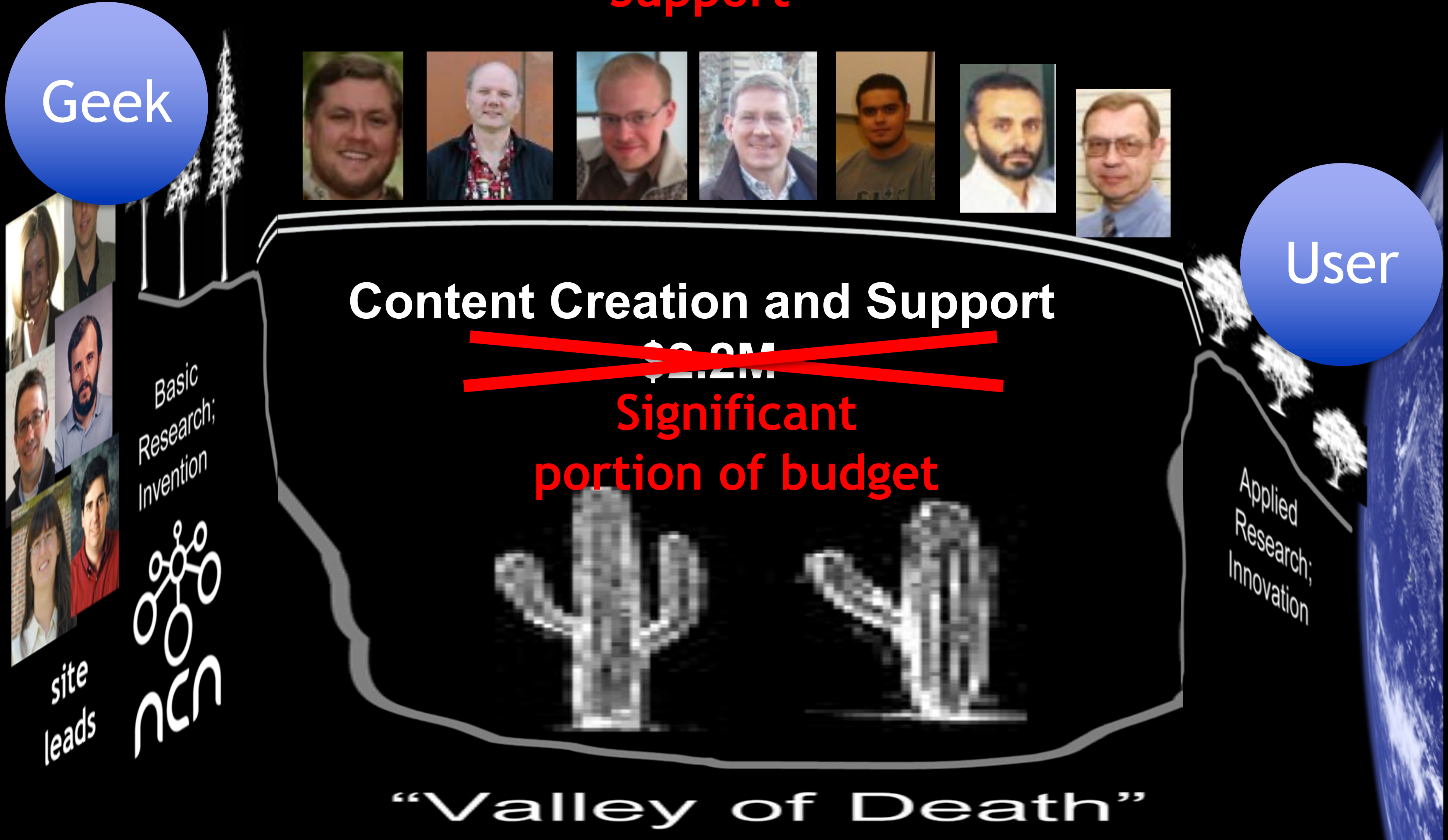



Ease of Use!

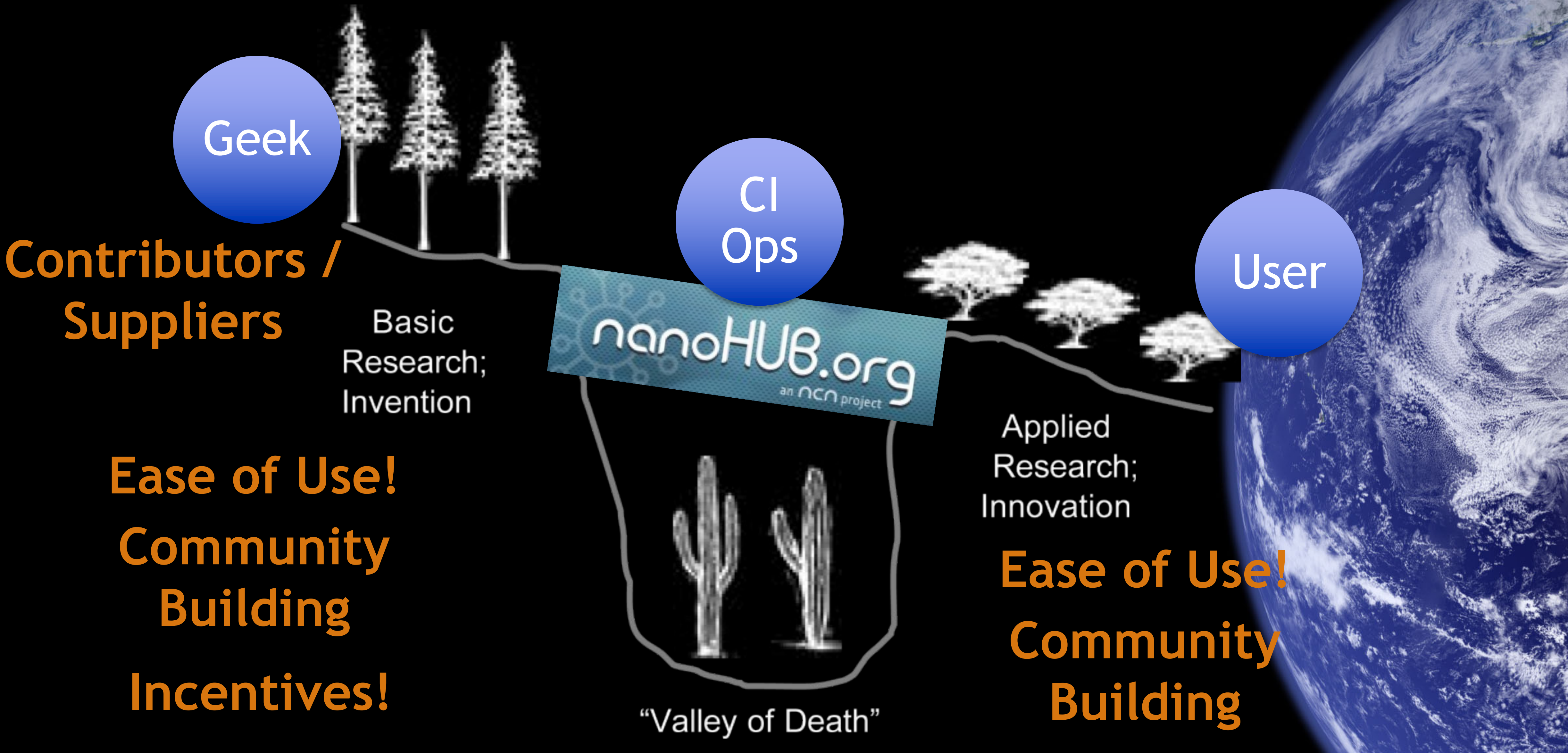
**$2M/year operation and bridge building**

# 4: Tech Transfer Processes

“~~dedicated technical site leads~~”
Consultants -
Support

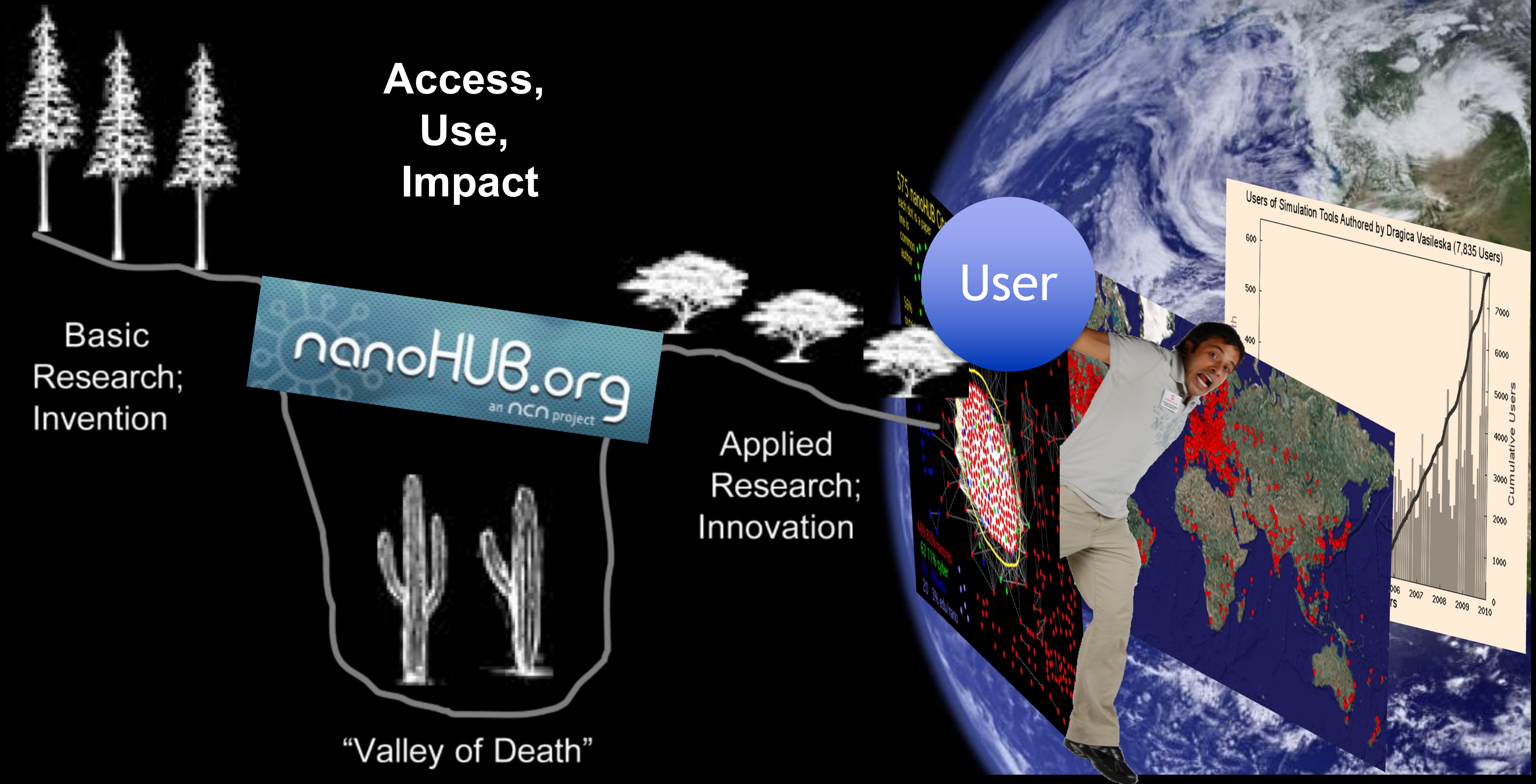


# 5: Understanding Stakeholders



# 6: Open Assessment / Incentives

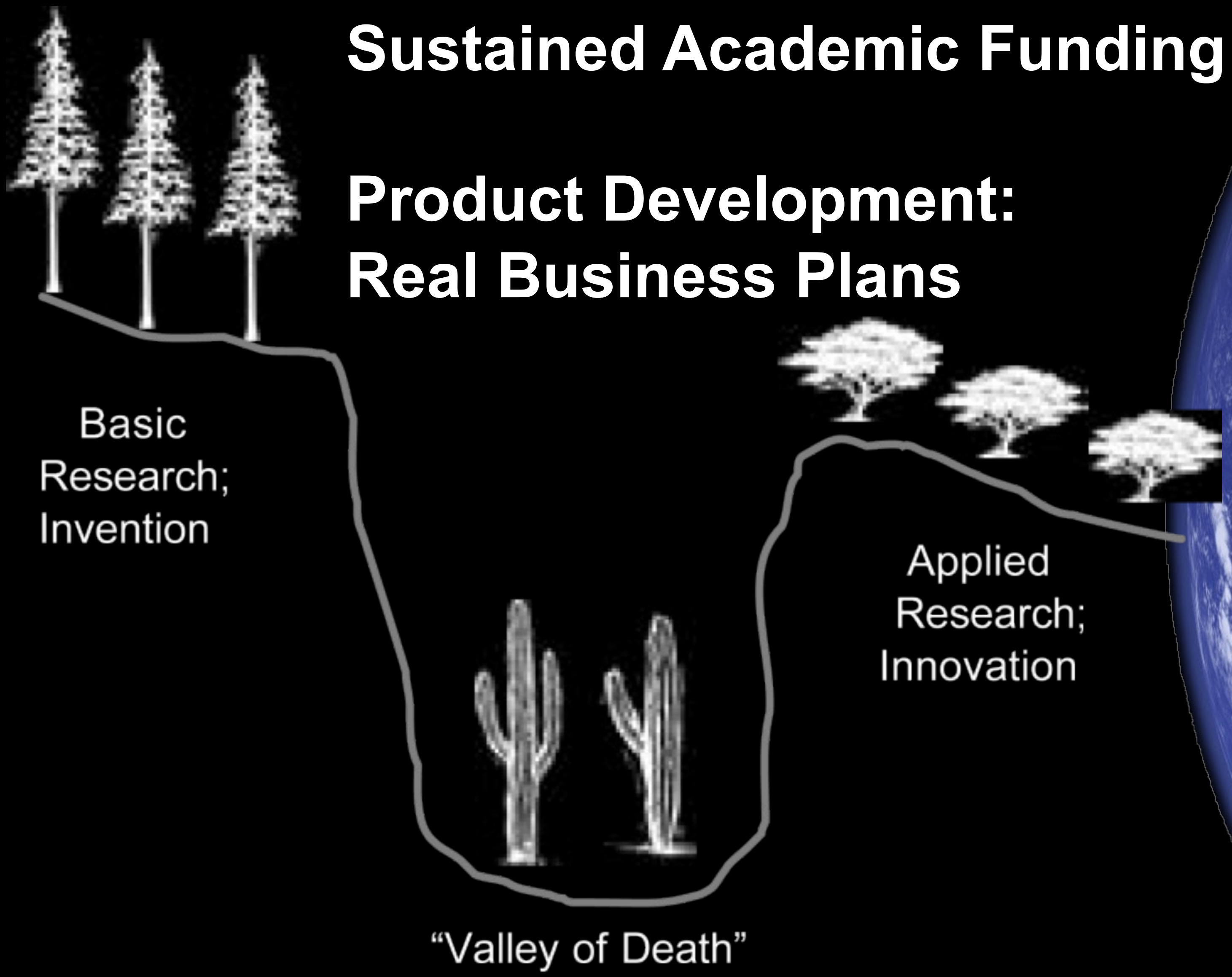
"gather, understand, disseminate stats"

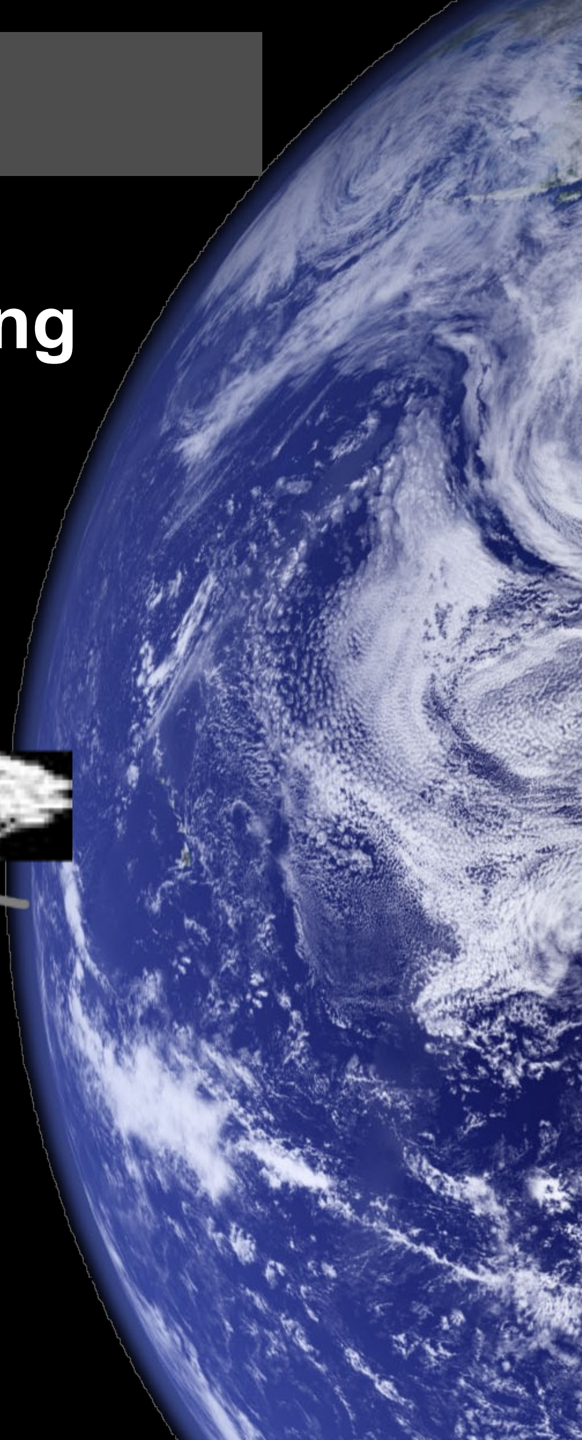


# 7: Business Model

**Research:**
**Sustained Academic Funding**

**Product Development:**
**Real Business Plans**



# 7 Criteria

## for Successful Science Gateways

1: Outstanding Science / Quality

2: Commitment to Dissemination

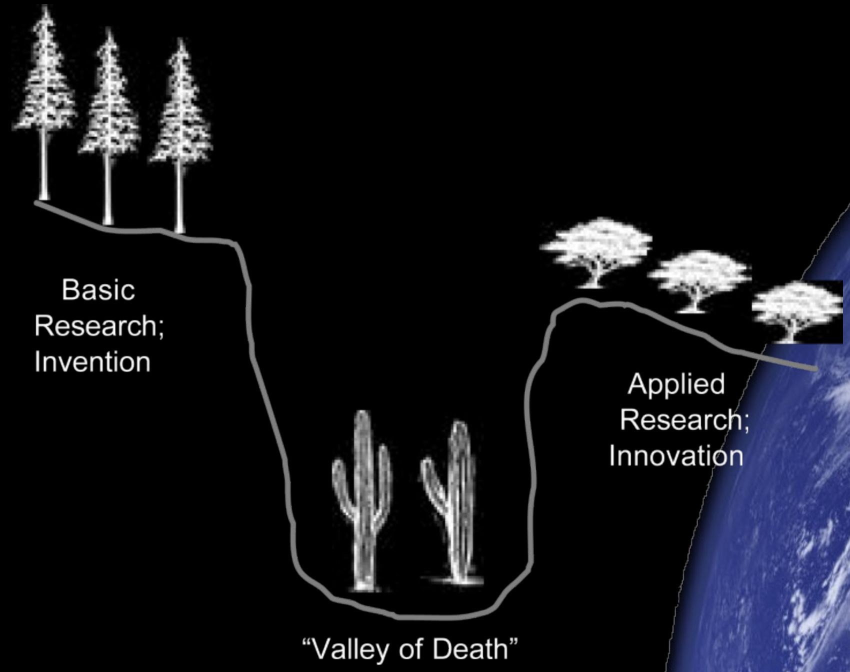
3: Technology for Dissemination

4: Tech Transfer Processes

5: Understanding Stakeholders

6: Open Assessment / Incentives

7: Business Model




chipshub by nanoHUB

**Just hosting expert software is not enough!**

https://chipshub.org

12,000 students using tools each year in classes!

16 % at MSIs

## Just hosting expert software is not enough!

# The future of chip design and manufacturing is here

Public on Ratemyprofessor

....**I'm in the military** so I have weird, long work hours

... **group projects**--which were **HIGHLY valuable**, and are **why the class has been so meaningful** to me, 10/10 would recommend!

## We work with partners ...

SILVACO, SYNOPSYS, CHIPYARD, cadence, SIEMENS, OpenLane, intel, tsmc, skywater, CMC MICROSYSTEMS, efabless.com, THE MOSIS SERVICE, imec IC-link, Microsoft Azure

## We re-envision access to tools...

- We mimic industrial implementations!
- Across the whole stack
- Apps for freshmen and
- Scripts for optimization
- Lectures and tutorials

for everyone

From class to Lab to Fab

**Thank You !**