



Platform for Scientific Exploration

*Michael Zentner
Director of HUBzero® Platform
Purdue University*

*Community
Interaction*

*Knowledge
Dissemination*



*Resource, Data, Analytics &
Application Sharing*



- Hosting 60+ online scientific communities
- 25 FTEs
- 2,000,000+ annual visitors



- Largest online nanotechnology facility
- 1,400,000 annual visitors

DENSE DATA

Within Your Experiment, Your Knowledge is Somewhat Complete

| Sphere: | Gold | | | | |
|----------------------|------------------------------|-----------------------|----------|----------|----------|
| Medium: | Water | | | | |
| Graph type: | Cext/Csca/Cabs v. wavelength | | | | |
| Scattering angle = 0 | | | | | |
| Wavelength | Ref Index (real) | Ref Index (imaginary) | Cext | Csca | Cabs |
| 400 | 1.087871431 | 1.446879408 | 2.04E-15 | 1.23E-16 | 1.92E-15 |
| 401 | 1.087514072 | 1.447303652 | 2.09E-15 | 1.33E-16 | 1.96E-15 |
| 402 | 1.087156632 | 1.447727993 | 2.09E-15 | 1.31E-16 | 1.95E-15 |
| 403 | 1.08679913 | 1.448152407 | 2.08E-15 | 1.30E-16 | 1.95E-15 |
| 404 | 1.086441546 | 1.448576918 | 2.07E-15 | 1.29E-16 | 1.95E-15 |
| 405 | 1.086083131 | 1.449000474 | 2.07E-15 | 1.28E-16 | 1.94E-15 |
| 406 | 1.085723491 | 1.449422573 | 2.06E-15 | 1.27E-16 | 1.94E-15 |
| 407 | 1.085363769 | 1.449844767 | 2.06E-15 | 1.26E-16 | 1.93E-15 |
| 408 | 1.085003987 | 1.450267031 | 2.05E-15 | 1.24E-16 | 1.93E-15 |
| 409 | 1.084644123 | 1.450689391 | 2.05E-15 | 1.23E-16 | 1.93E-15 |

 Dense



(SOMEWHAT) SPARSE DATA

In Your Immediate Community, Knowledge is Less Complete

Liver Uptake

Brain Uptake

Gold



| Sphere: | Gold | | | | |
|----------------------|------------------------------|-----------------------|----------|----------|----------|
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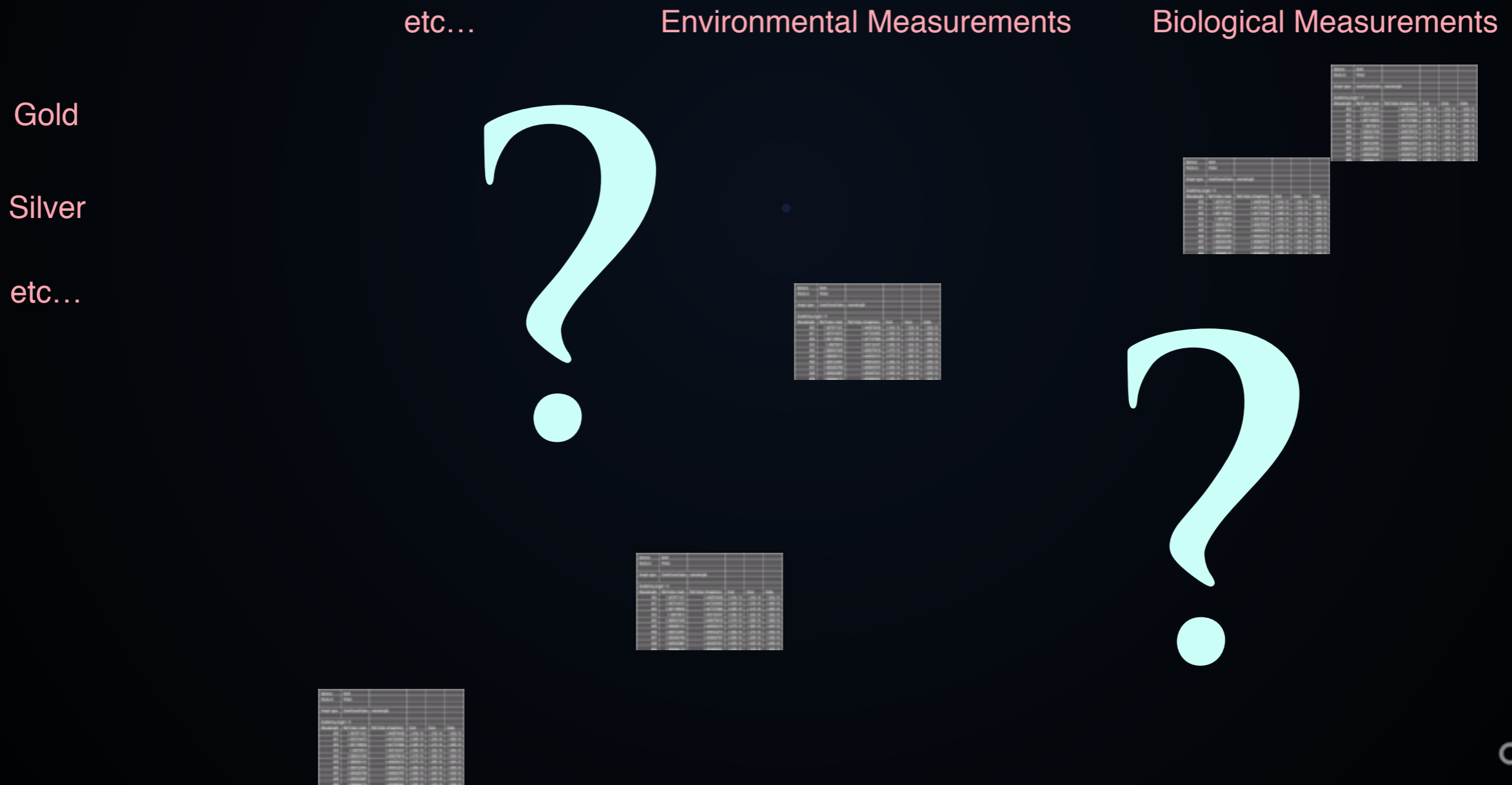
Silver

| Sphere: | Gold | | | | |
|----------------------|------------------------------|-----------------------|----------|----------|----------|
| Medium: | Water | | | | |
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| 409 | 1.084644123 | 1.450689391 | 2.05E-15 | 1.23E-16 | 1.93E-15 |



(MORE) SPARSE DATA

In Your Extended Community, Knowledge is Less Complete



(VERY) SPARSE DATA

In A Wide Community, Knowledge is Very Incomplete

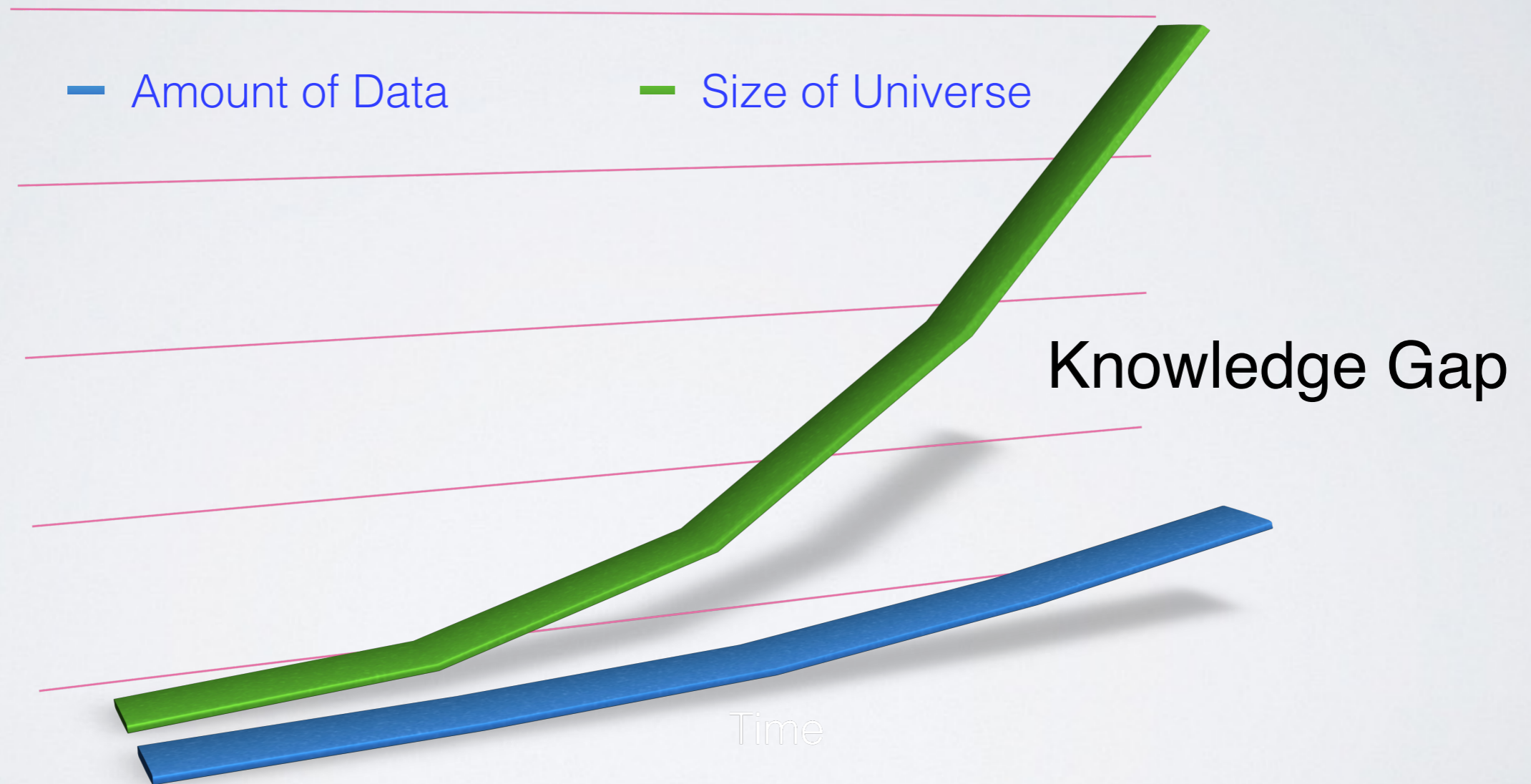
Electrical - Environmental - Medical - Physical - Financial - Interfacial - etc...

Wide
Variety
of
Materials



KNOWLEDGE VS UNIVERSE

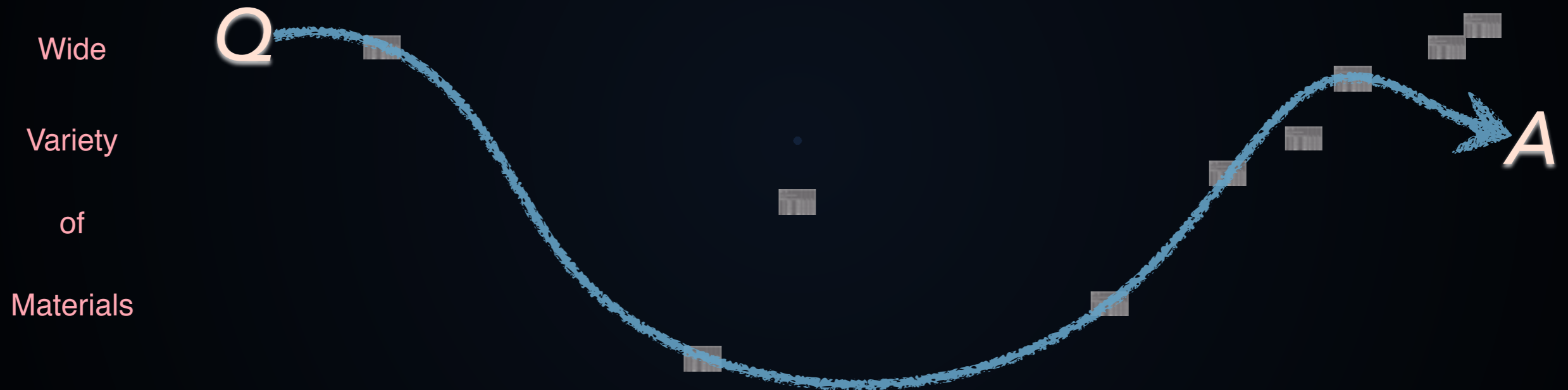
The more we have, the less we know...



INTEGRATION CHALLENGE

IF I DO X, WILL IT KILL ME?

Electrical - Environmental - Medical - Physical - Financial - Interfacial - etc...



THE TROUBLE WITH TABLES...

Dense tables are wonderful for sort, search, and filtration

| Run Meta Data | | | | Inputs | | | | Outputs | | | |
|---------------|------|------|------|----------------|----------------|----------------|-----|----------------|----------------|----------------|-----|
| User | Time | Tool | etc. | I ₁ | I ₂ | I ₃ | etc | O ₁ | O ₂ | O ₃ | etc |
| | | | | | | | | | | | |
| | | | | | | | | | | | |
| | | | | | | | | | | | |
| | | | | | | | | | | | |
| | | | | | | | | | | | |
| | | | | | | | | | | | |
| | | | | | | | | | | | |

Sparse tables are terrible for sort, search, and filtration

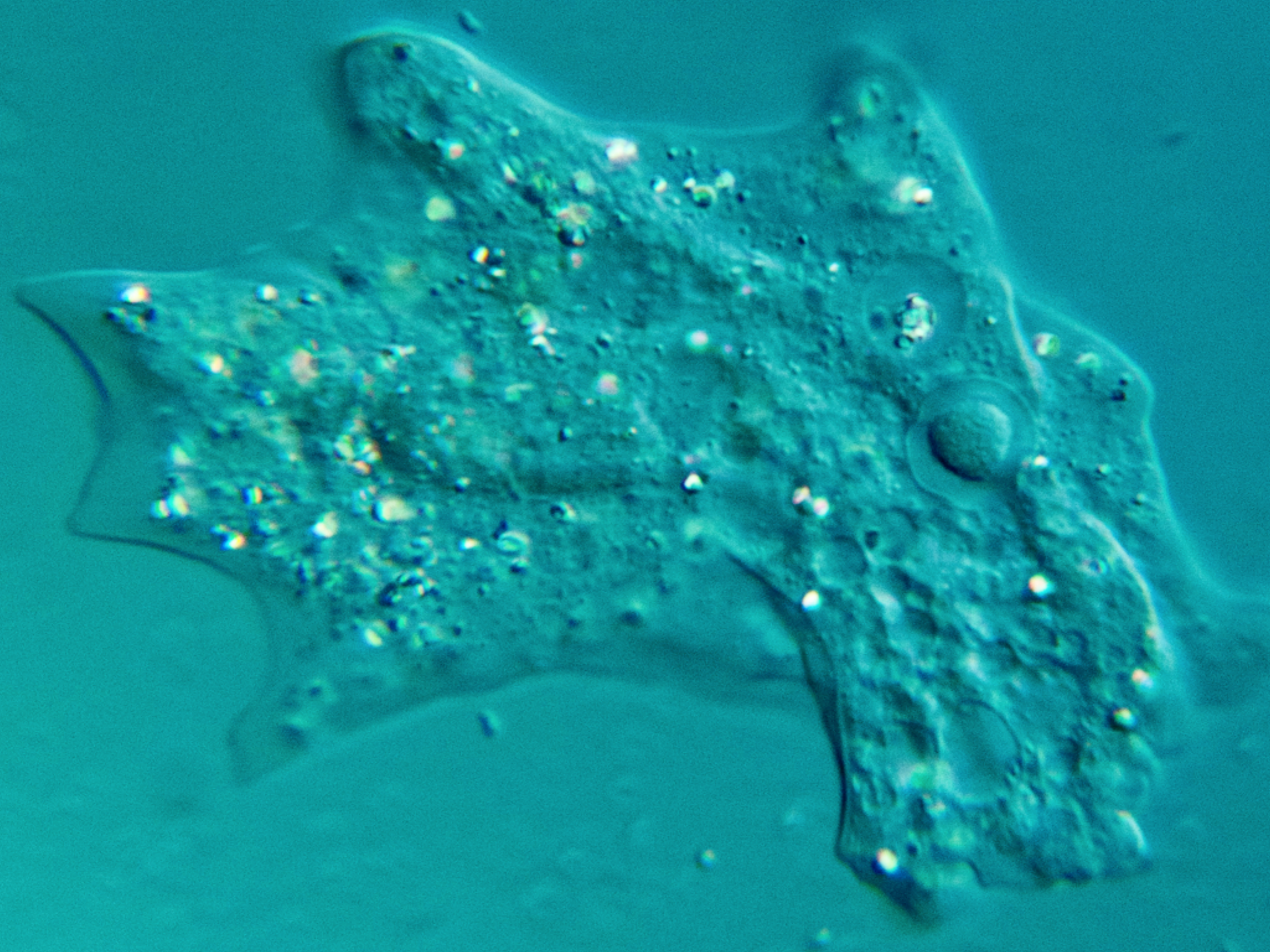


(PART OF) WHAT IS NEEDED TO
MEET THESE CHALLENGES:

A MODULAR TOOLKIT FOR
SPARSE DATA “MACROSCOPES”

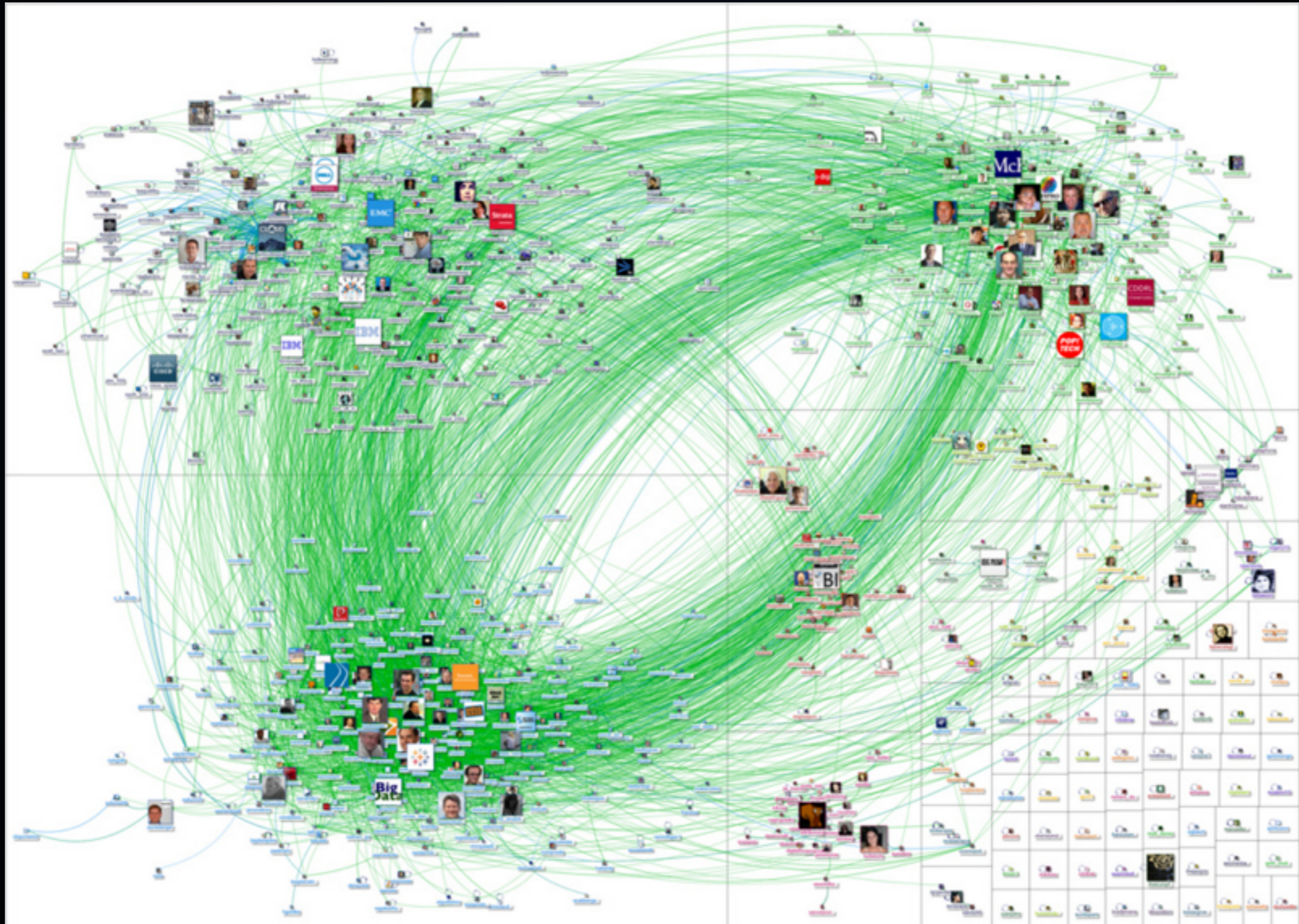
A microscopic image of a cell, likely a plant cell, showing a large, irregularly shaped nucleus on the right side. The nucleus contains a prominent, dark, spherical nucleolus. The cytoplasm is filled with various organelles, including numerous small, dark, granular structures and larger, clear, vacuolar spaces. The cell membrane is visible as a thin, dark boundary. The overall appearance is that of a complex, multi-organellar cell.

Needs A "Microscope"





EXAMPLE, VASTLY CONNECTED SOCIAL NETWORKS





IDENT: A SPARSE DATA MACROSCOPE

Interactive Data Exploration & Navigation Tool
for Nano Technology

Nothing selected Use columns Custom column 288 total rows Edit filters

| ID |
|----|
| 1 |
| 2 |
| 3 |
| 4 |
| 5 |
| 6 |
| 7 |
| 8 |
| 9 |
| 10 |
| 11 |

NMRI data +

**Giving Data
The Spark of Life**

Visit our evolving project for
Nanomaterial Registry data
exploration

NANOMATERIALREGISTRY

IDENT

COLUMN POPULATION LOOKAHEAD

Nothing selected Use columns Custom column

Search

| | | |
|---|--------------------------------------|--|
| 1 | Absorbance:as a function of Solvent | |
| 1 | Absorbance:as a function of Time | |
| 2 | pH | |
| 3 | Size:as a function of Light Exposure | |
| 4 | Size:as a function of Temperature | |
| 6 | Surface Area | |
| 8 | Bulk Density (g/cm ³) | |
| 9 | Specific Surface Area | |
| 1 | Surface Charge | |
| | Electrokinetic Mobility | |
| | Zeta Potential (mV) | |

Bar Length Indicates Amount of Non-Null Data

IDENT COLUMN OF INTEREST SELECTION

Nothing selected Use columns Custom column

288 total rows Edit filters

Table of chosen data

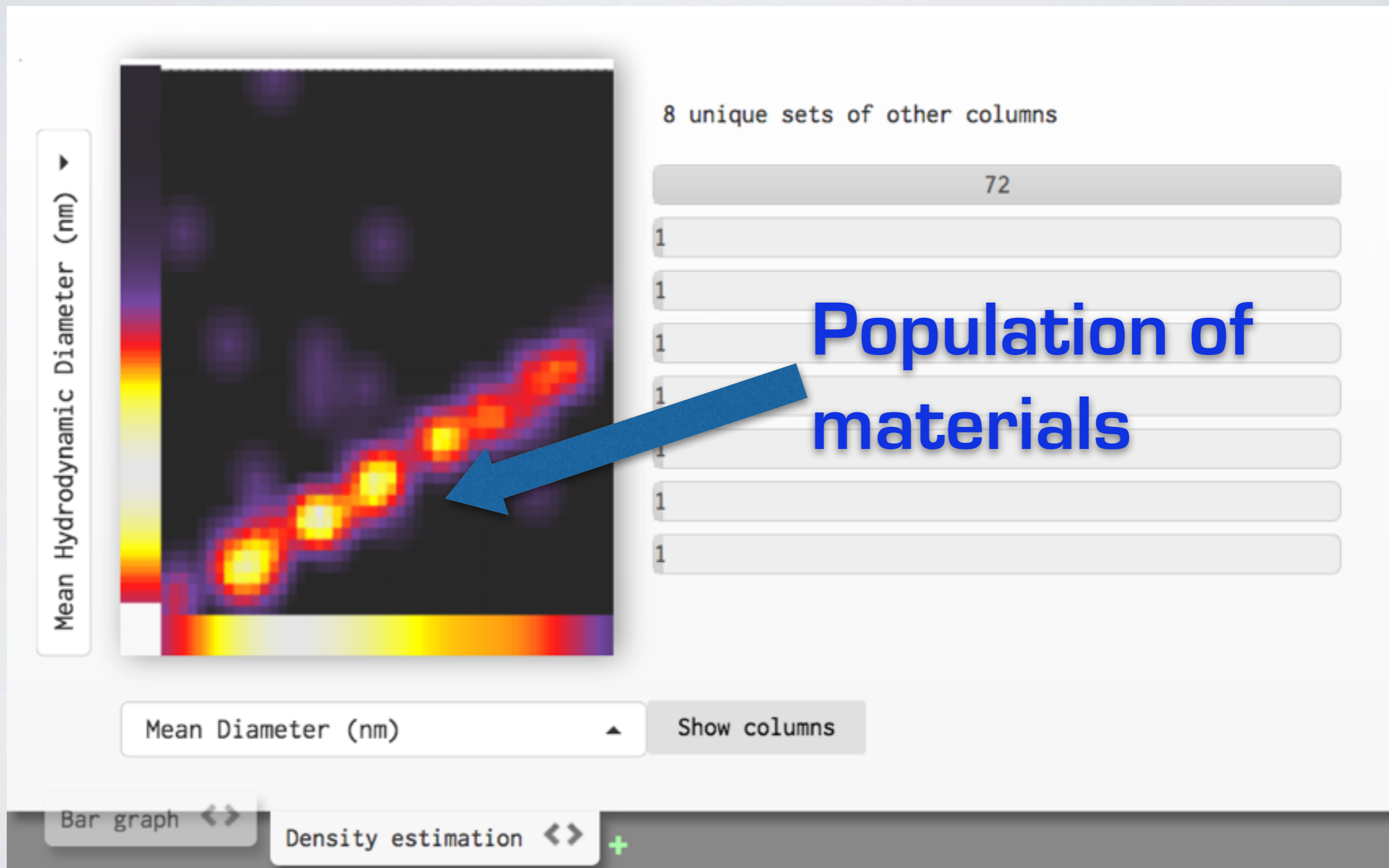
| ID | Mean Diameter (nm) | Mean Hydrodynamic Diameter (nm) | DisplayName | |
|----|--------------------|---------------------------------|-------------|---|
| 6 | | | Ag | |
| 7 | 7.2 | | Ag NP | |
| 8 | 20.8 | 32 | Ag NP | |
| 9 | 29 | 39.6 | Ag NP | |
| 10 | 43.4 | 47.6 | Ag NP | |
| 11 | 41.9 | 43.1 | Ag NP | |
| 12 | 49.1 | 59.2 | Ag NP | |
| 13 | 53.5 | 57.1 | Ag NP | |
| 14 | 57.7 | 68.3 | Ag NP | |
| 15 | 8.2 | | Ag NP | |
| 16 | 19.2 | | Ag NP | 🔒 |

Nanomaterials Registry Dataset

Visualize Content

Add a visualization +

IDENT VISUALIZATION OF CONTENT



IDENT: Graphical Tool Execution

III-V Strain Compensation Calculator

Settings Terminate Keep for later

Substrate Material

Substrate (III): Al_xGa_(1-x)

Substrate (V): As_yP_(1-y)

x: .03

y: .03

QD (III): In

QD (V): As

x: 1

y: 1

Strain Compensation Material

SC (III): Ga

SC (V): P

x: 1

y: 1

QD Diameter: 25nm

QD Height (or QW Thickness): 2nm

QD Density: 5e+10/cm²

Wetting Layer Thickness: 1nm

Simulate

Result: Output Log

Literature/Interpolated (i) Values =====

| Mat | lc [Å] | C11i [GPa] | C12i [GPa] | Poisson v | a_perp [Å] |
|-----|------------|------------|------------|------------|------------|
| Sub | 5.4571e+00 | 1.3973e+03 | 6.1892e+02 | 3.0697e-01 | |
| QD | 6.0583e+00 | 8.3290e+02 | 4.5260e+02 | 3.5208e-01 | 6.7117e+00 |
| SC | 5.4505e+00 | 1.4050e+03 | 6.2030e+02 | 3.0628e-01 | 5.4447e+00 |

Empirically Calculated (e) Values =====

| Mat | C11e [GPa] | C12e [GPa] | Poisson v | a_perp [Å] |
|-----|------------|------------|------------|------------|
| Sub | 1.3890e+03 | 6.2681e+02 | 3.1095e-01 | |
| QD | 8.9863e+02 | 4.5312e+02 | 3.3521e-01 | 6.6646e+00 |
| SC | 1.3960e+03 | 6.2916e+02 | 3.1068e-01 | 5.4446e+00 |

QD Volumes [nm³] =====

Sph. Cap: 4.9506e+02

Cylinder: 9.8175e+02

Obl. Sph.: 6.5450e+02

Strain Compensation =====

| Params Used | Req. SC Thick [nm] | Eff QD+WL Thick [nm ³ cm ⁻²] or [nm] | Max SL Method |
|-----------------------|--------------------|---|---------------|
| CET (QD Height as QW) | | | |

Find: Select All

1 result Clear

Storage (manage) 80% of 30 GB

980 x 600

IDENT: Graphical Tool Execution

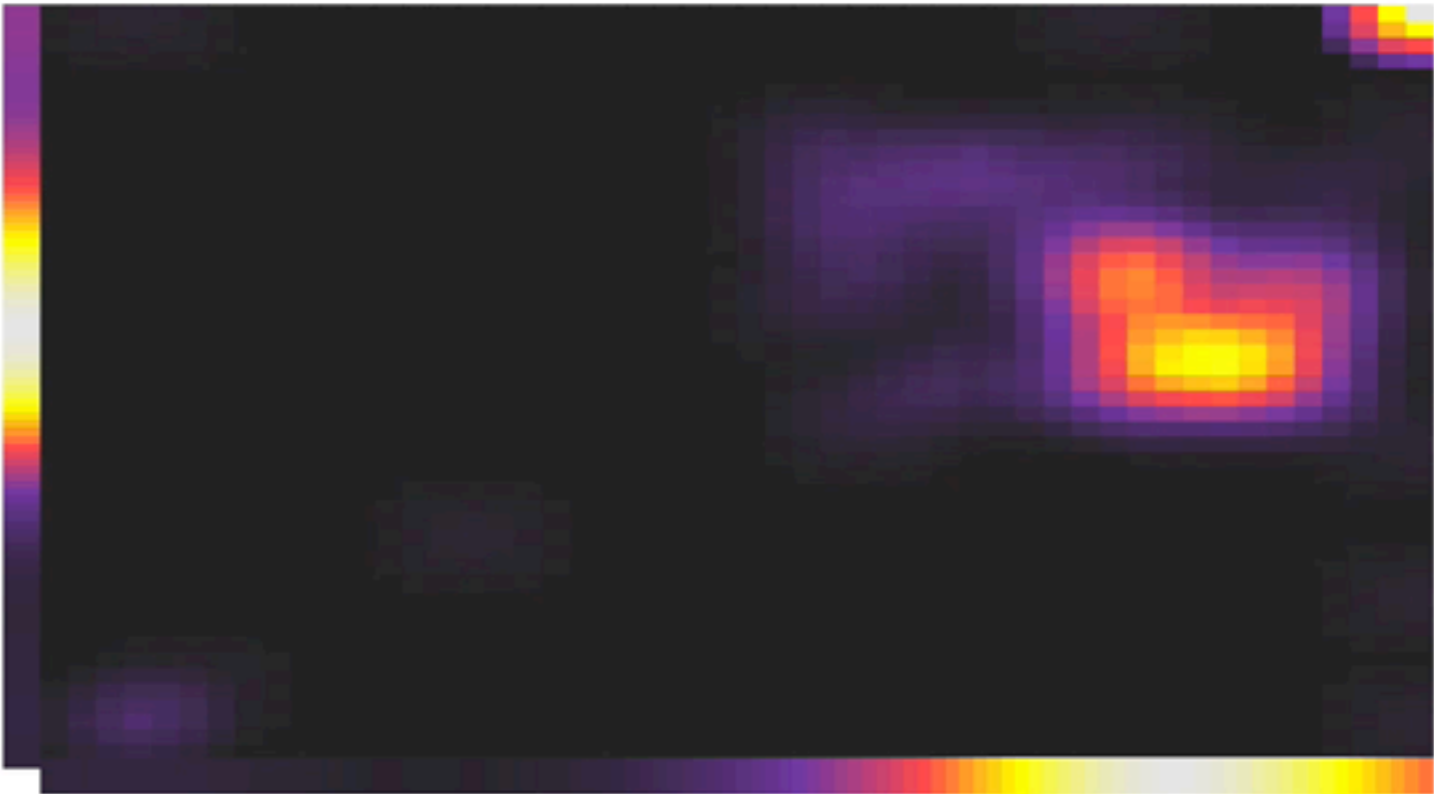
Nothing selected Use columns Custom column 202 total rows

| ID | Tool | Substrate x | Substrate y |
|----|------|--------------------|--------------------|
| 1 | | 0.7781874673773234 | 0.6599116204341688 |
| 2 | | 0.833543808403423 | 0.746030374446 |
| 3 | | 0.6543344226852987 | 0.6882546059375454 |
| 4 | | 0.6195678131023674 | 0.6306212655413835 |
| 5 | | 0.6486536880495332 | 0.7644257229555012 |
| 6 | | 0.7791129291856689 | 0.5979152983567378 |
| 7 | | 0.7231352091463779 | 0.721192957030748 |
| 8 | | 0.792529598930497 | 0.6681219371370225 |
| 9 | | 0.68554642297569 | 0.7644474175098513 |

III-V Strain Compensation Calculator

x:

y:



The heatmap displays a rectangular region with a color gradient from dark purple (low strain) to bright yellow (high strain). A prominent high-strain region is visible in the upper right quadrant, with a smaller, less intense region in the lower right. The rest of the area shows low to moderate strain levels.

IDENT: Graphical Tool Execution

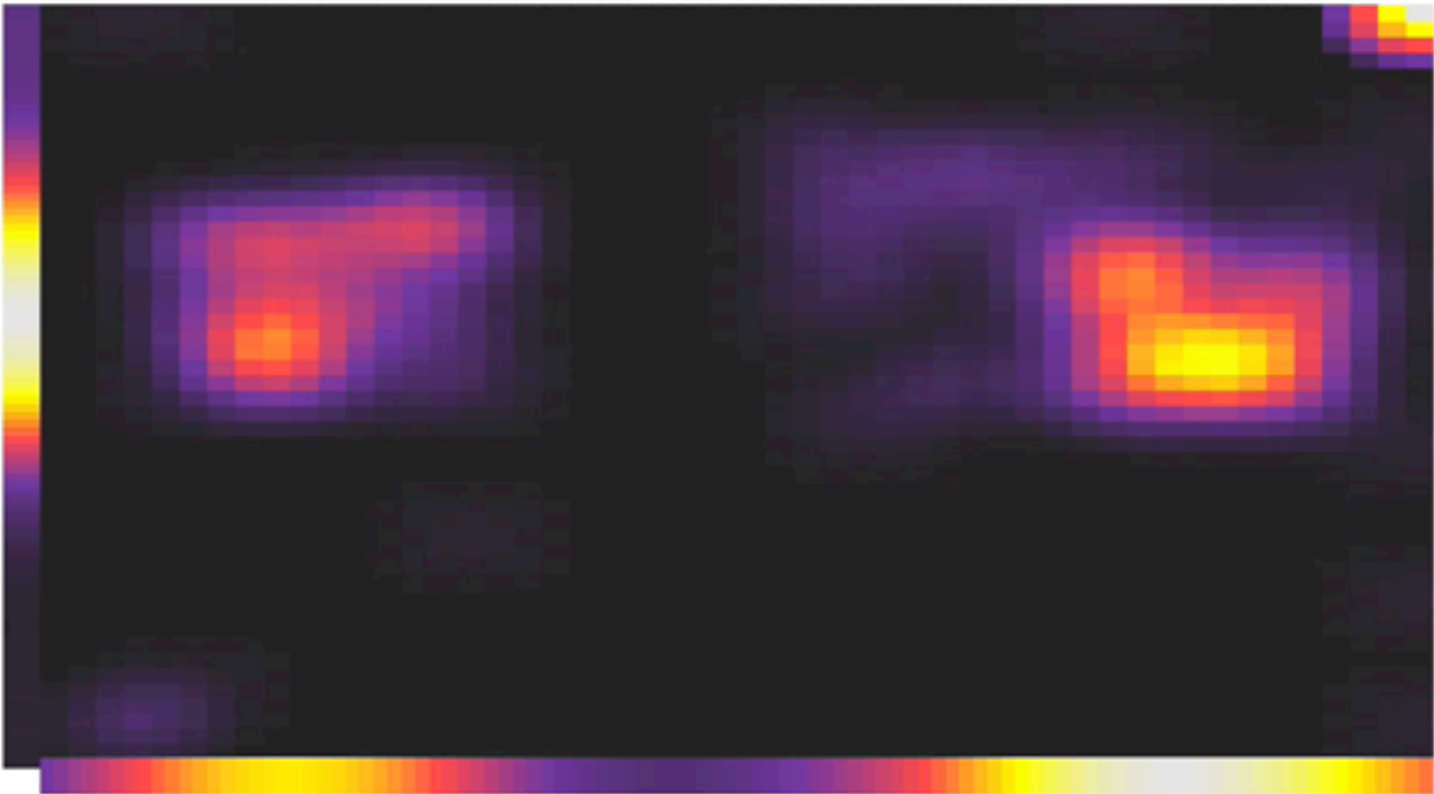
Nothing selected Use columns Custom column 302 total rows

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III-V Strain Compensation Calculator

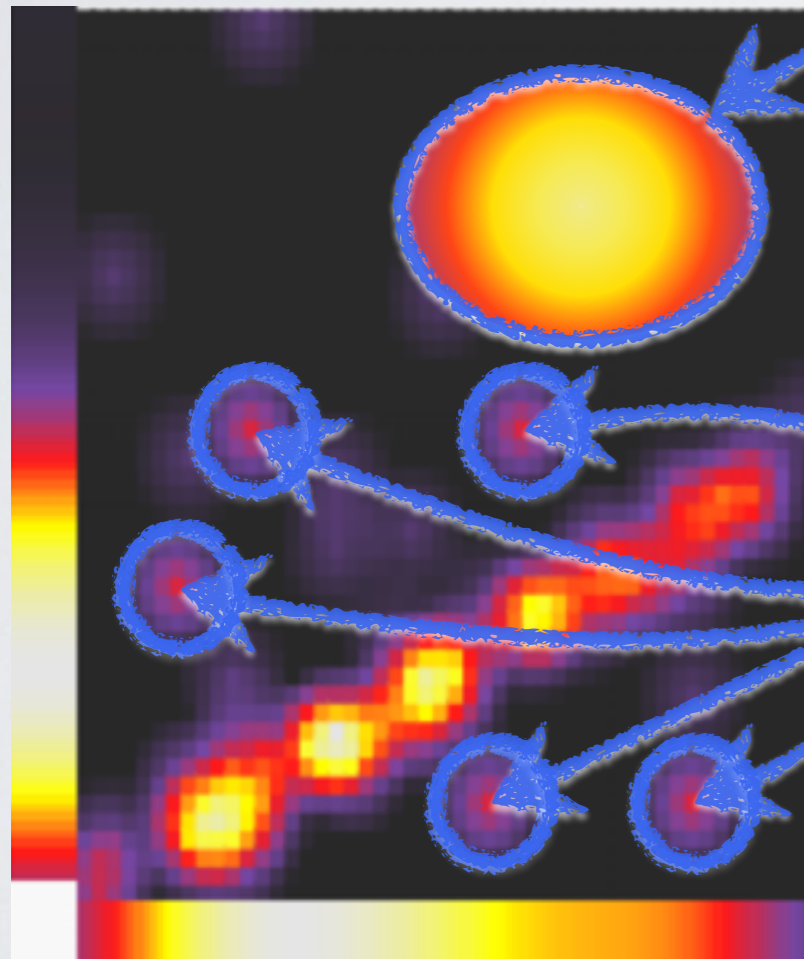
x:

y:



The heatmap displays a 2D distribution of strain values. The color scale ranges from dark purple (low strain) to bright yellow (high strain). Two distinct regions of high strain (yellow/red) are visible, corresponding to the substrate coordinates listed in the table above. The rest of the area is predominantly dark purple, indicating low strain.

EXPLORATION DRIVEN DATA POPULATION



*Exploration Driven
Simulation*



*Exploration Driven
Experimentation*



OUR (NANO)INFORMATICS CHALLENGES ARE:

- Storing Data

...and...

- Interacting with and Exploring Data
- Using Interactions as a Focal Point for Scientific Innovation and Collaboration