nanoHUB: How to create and maintain a successful national HUB

Michael Zentner, Gerhard Klimeck, Steve Snyder

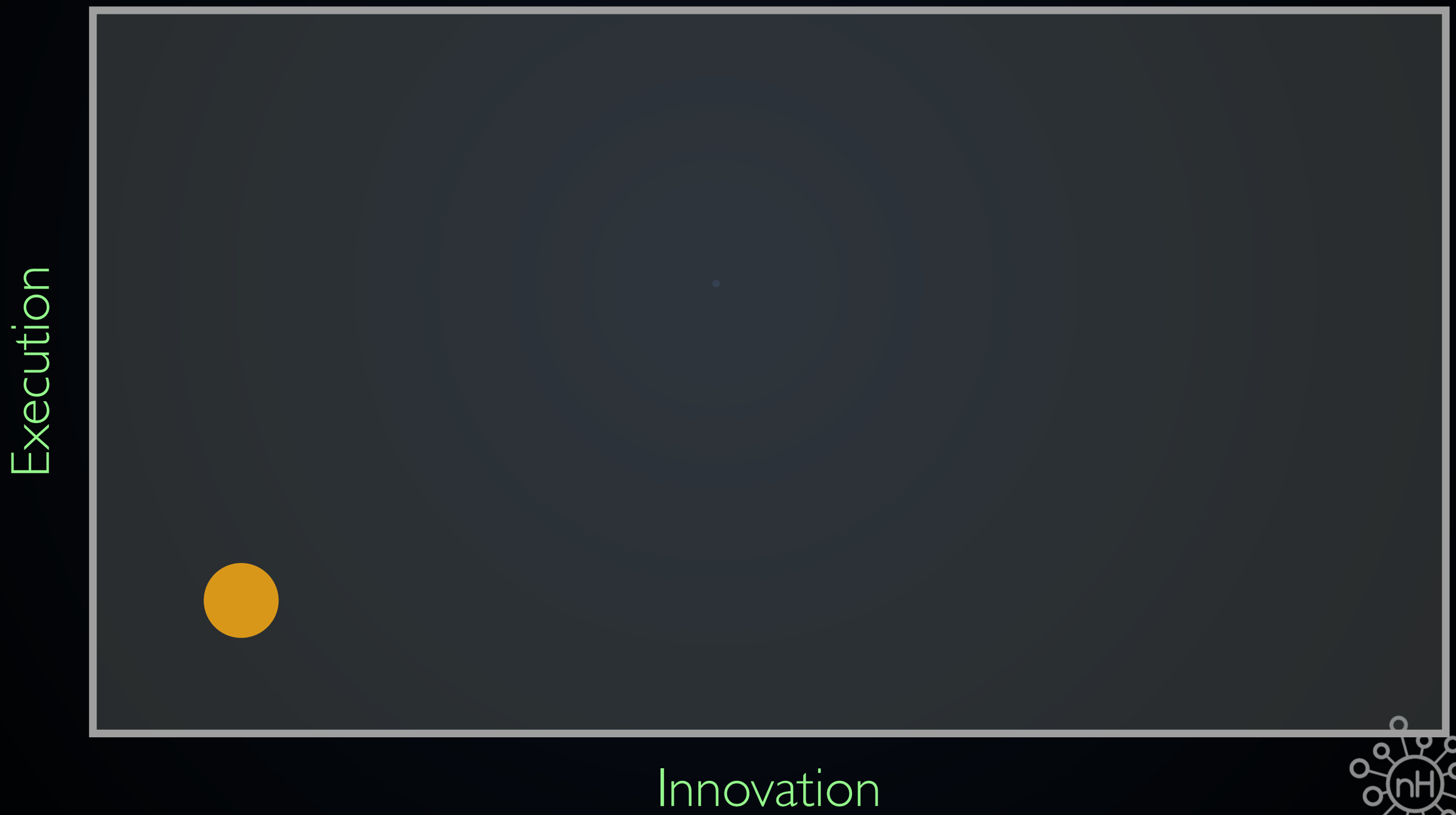
PURDUE UNIVERSITY

nanoHUB: (learning) how to create and maintain a successful (inter)national HUB

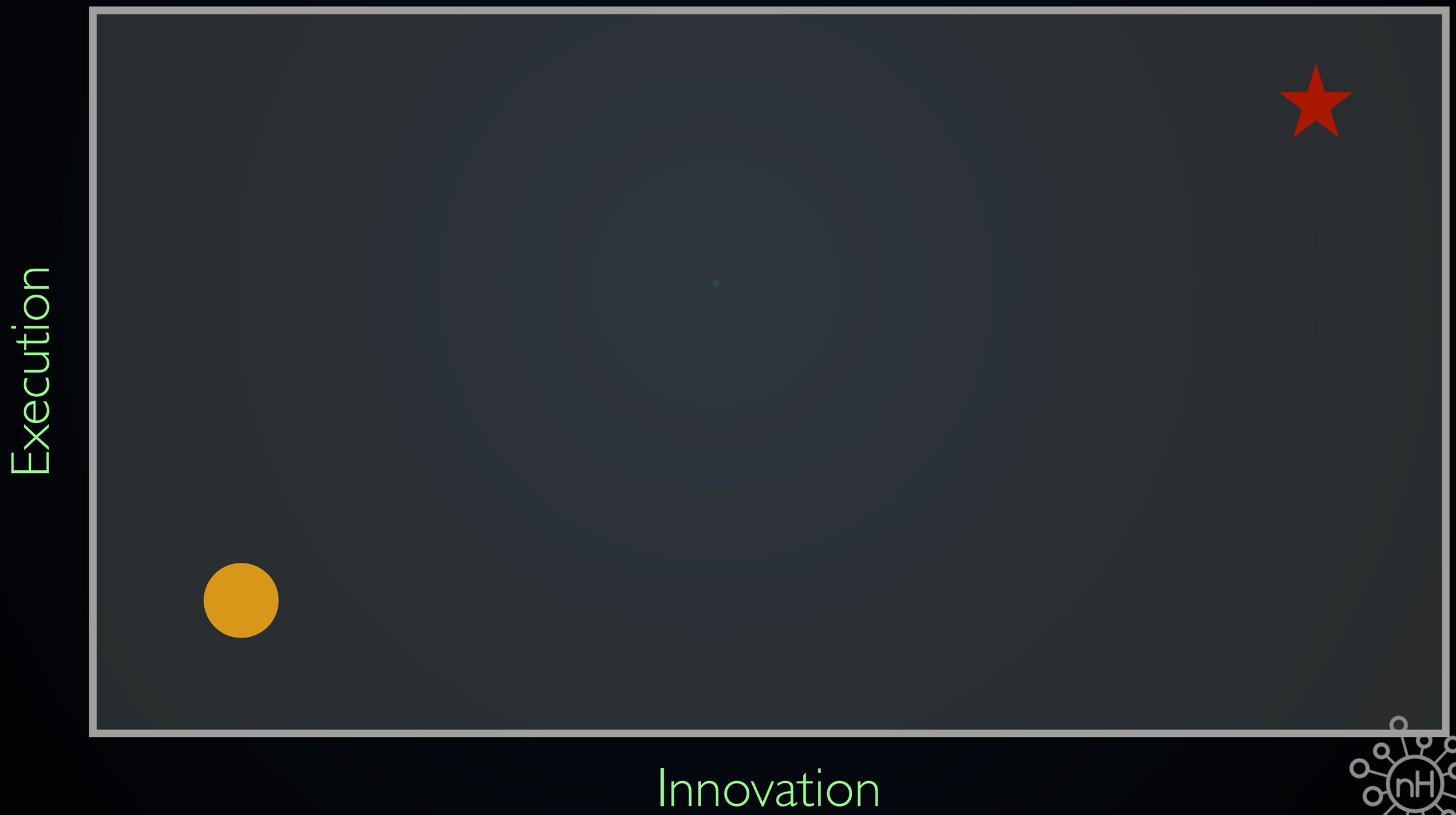
Michael Zentner, Gerhard Klimeck
Nathan Denny, Dwight McKay, Steve Snyder

PURDUE UNIVERSITY

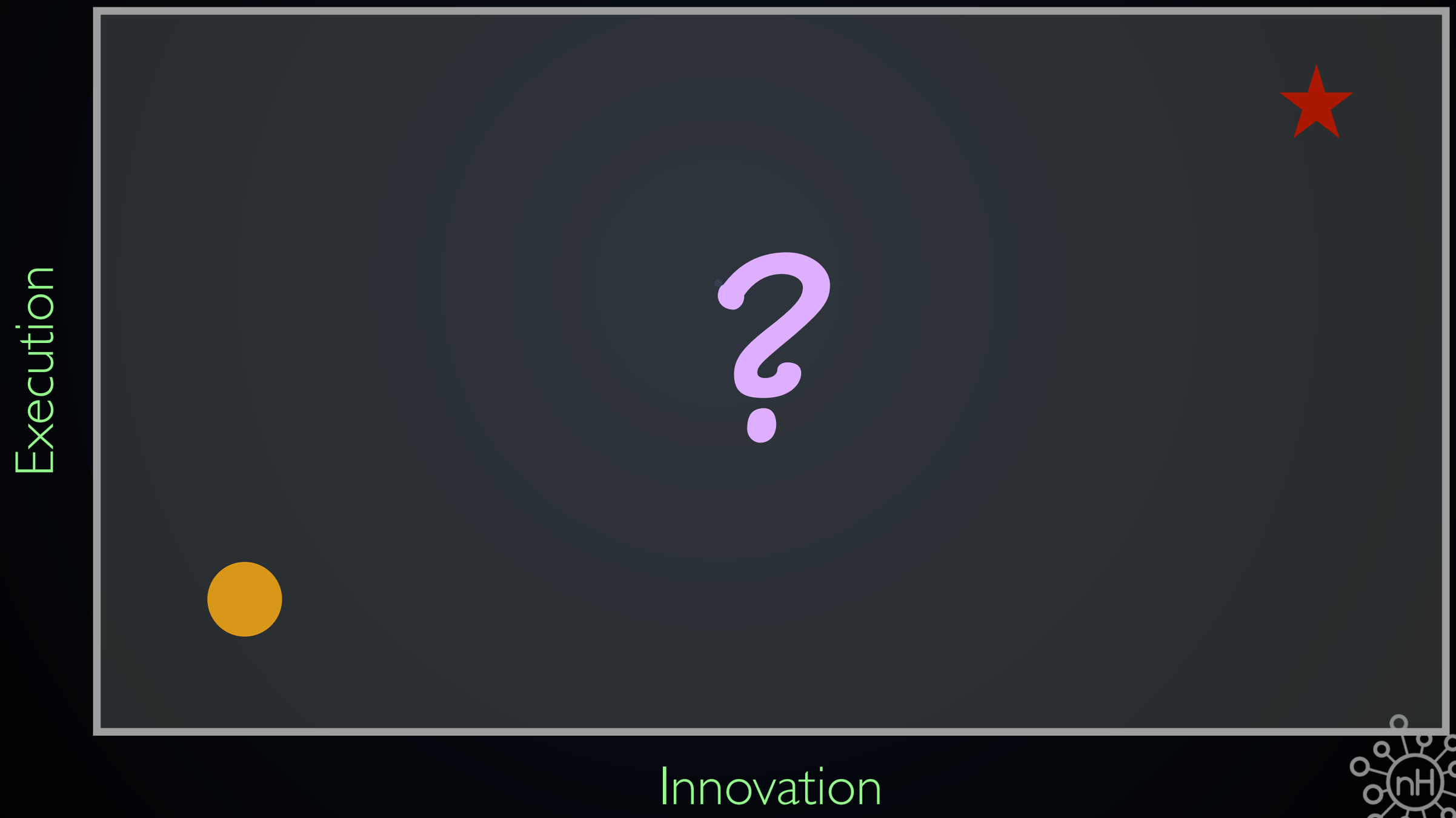
Situation



Situation ❖ Target



Situation ❖ Target ❖ Plan



Situation ❖ Target ❖ re-Plan

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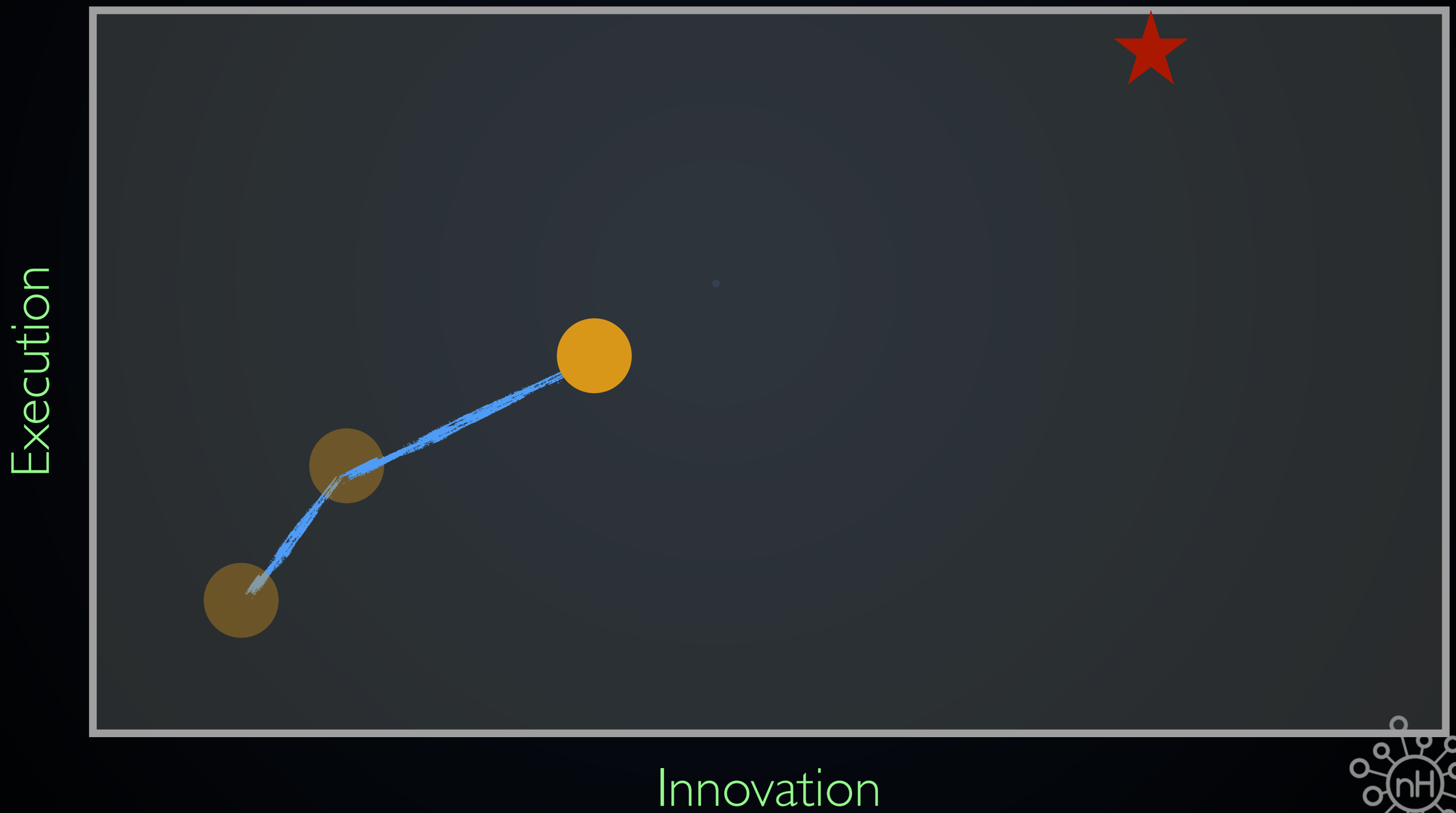
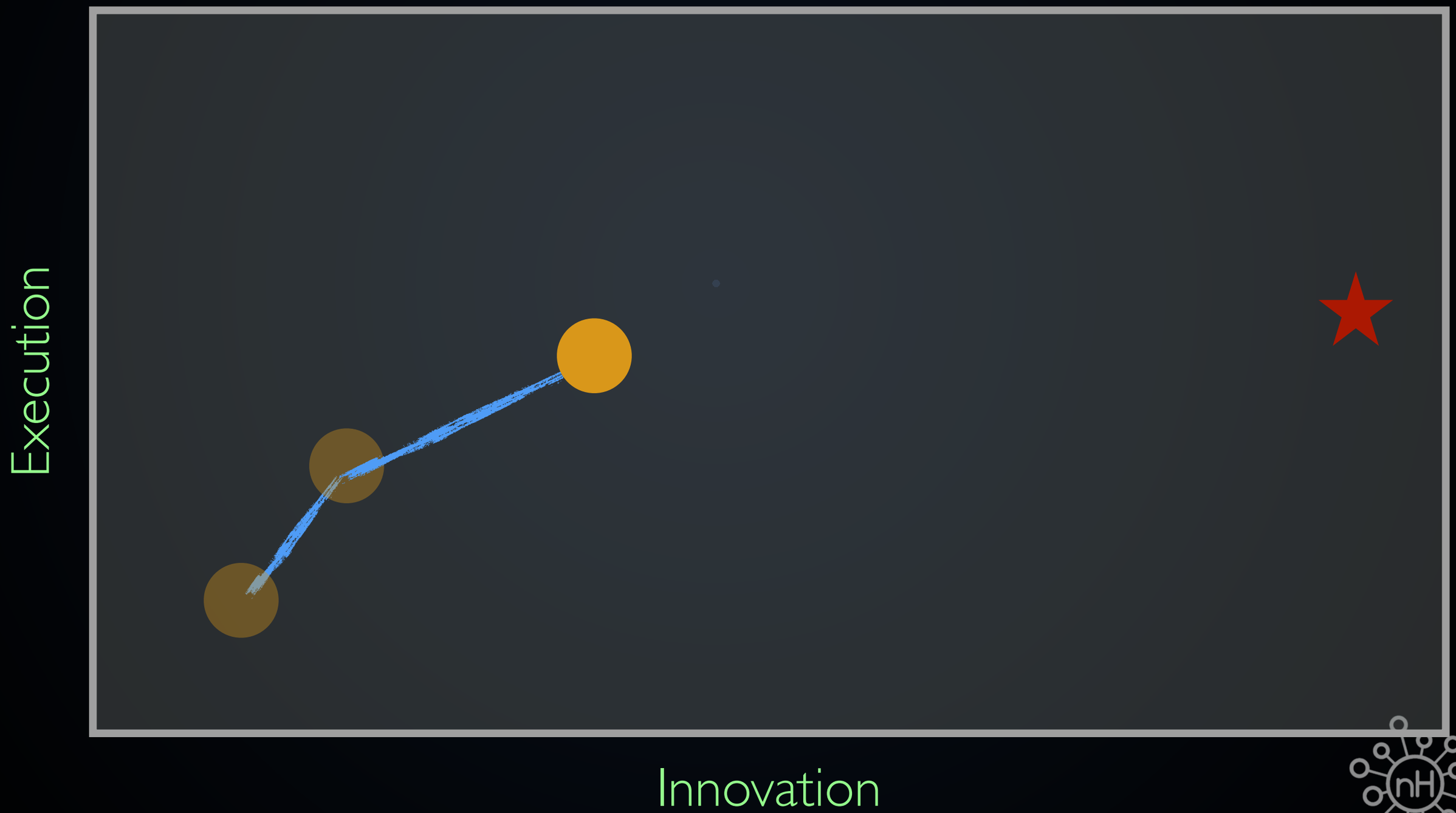
Situation ❖ Target ❖ re-Plan



Situation ❖ Target ❖ re-Plan



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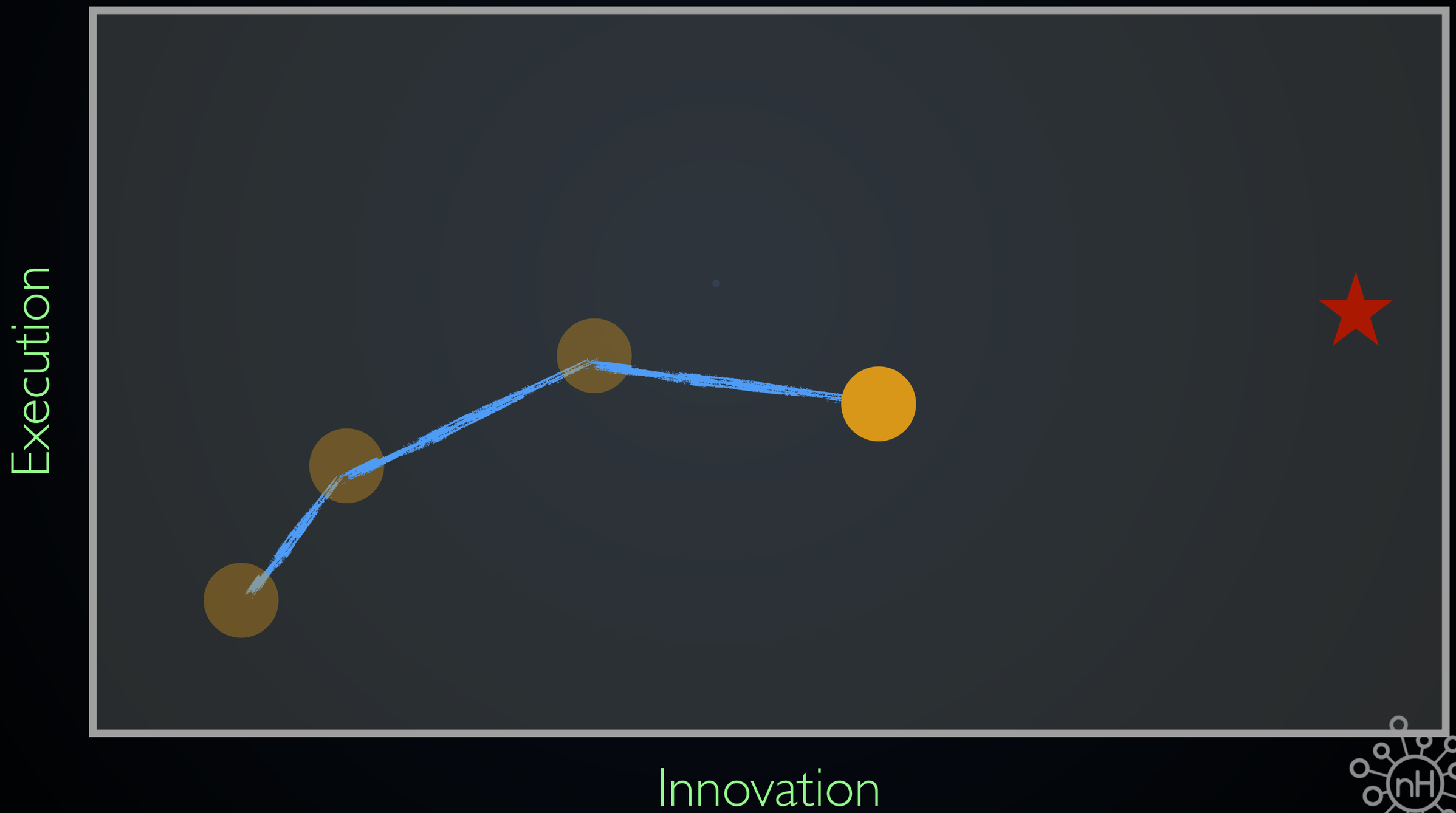
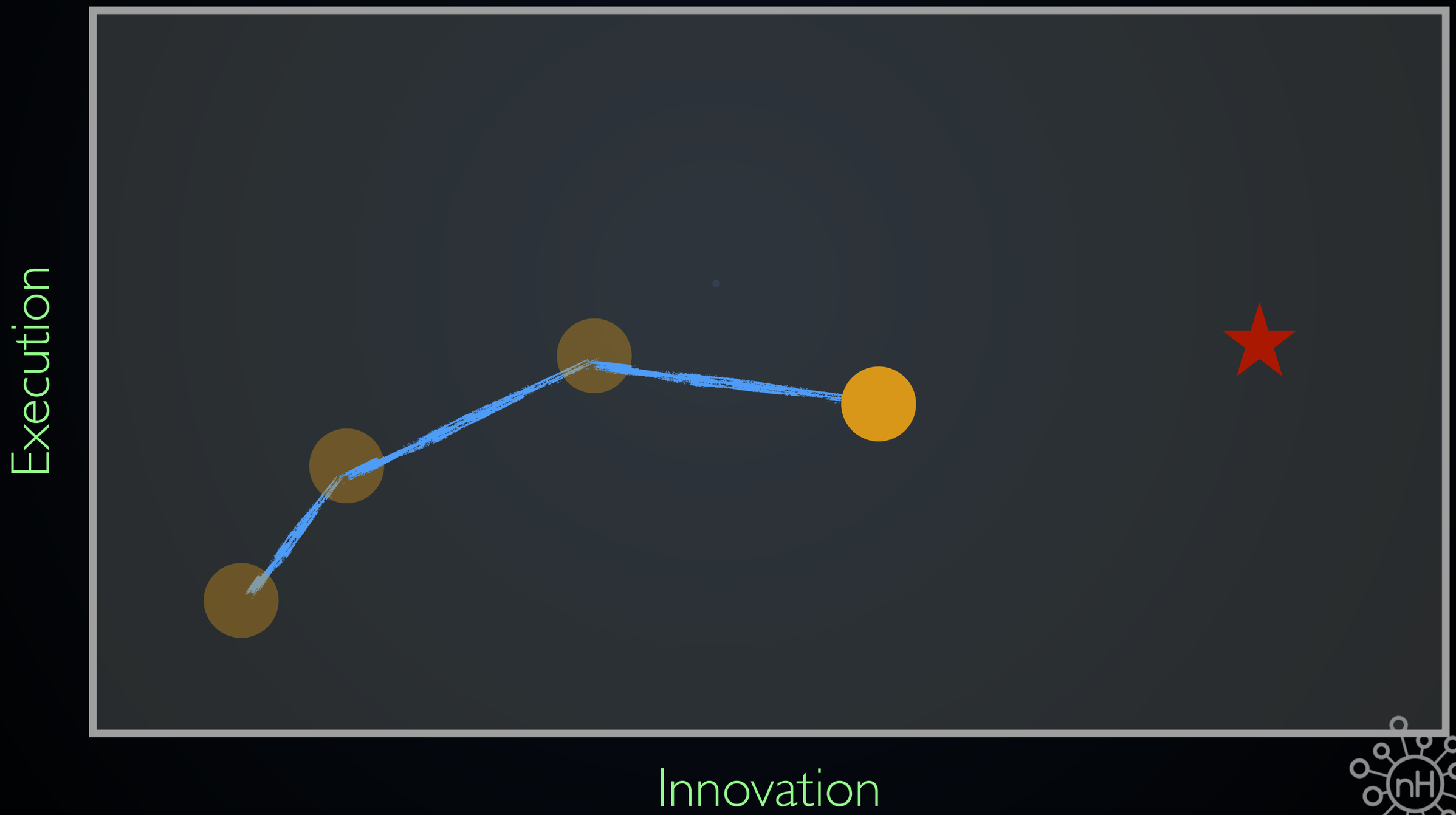
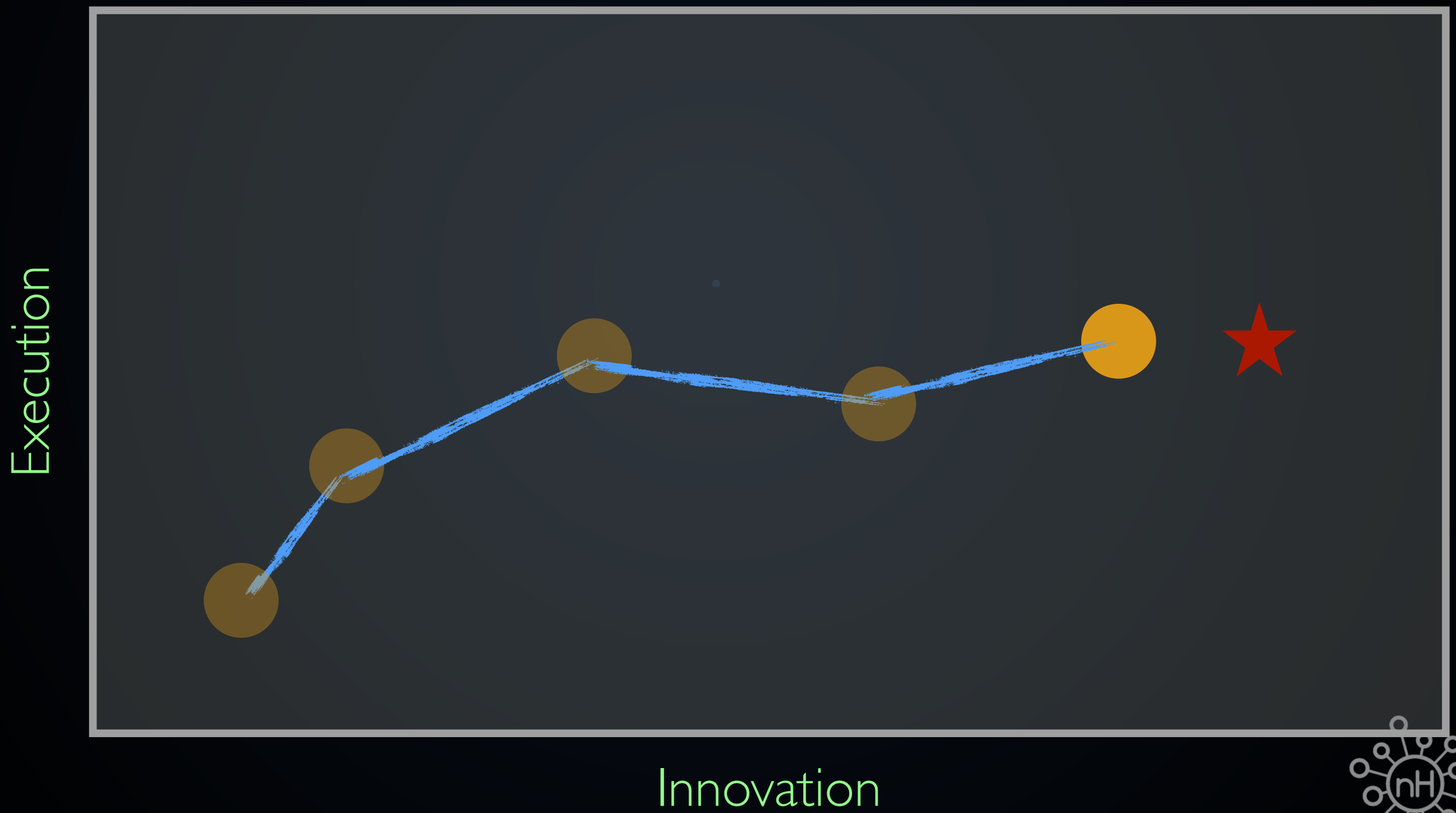


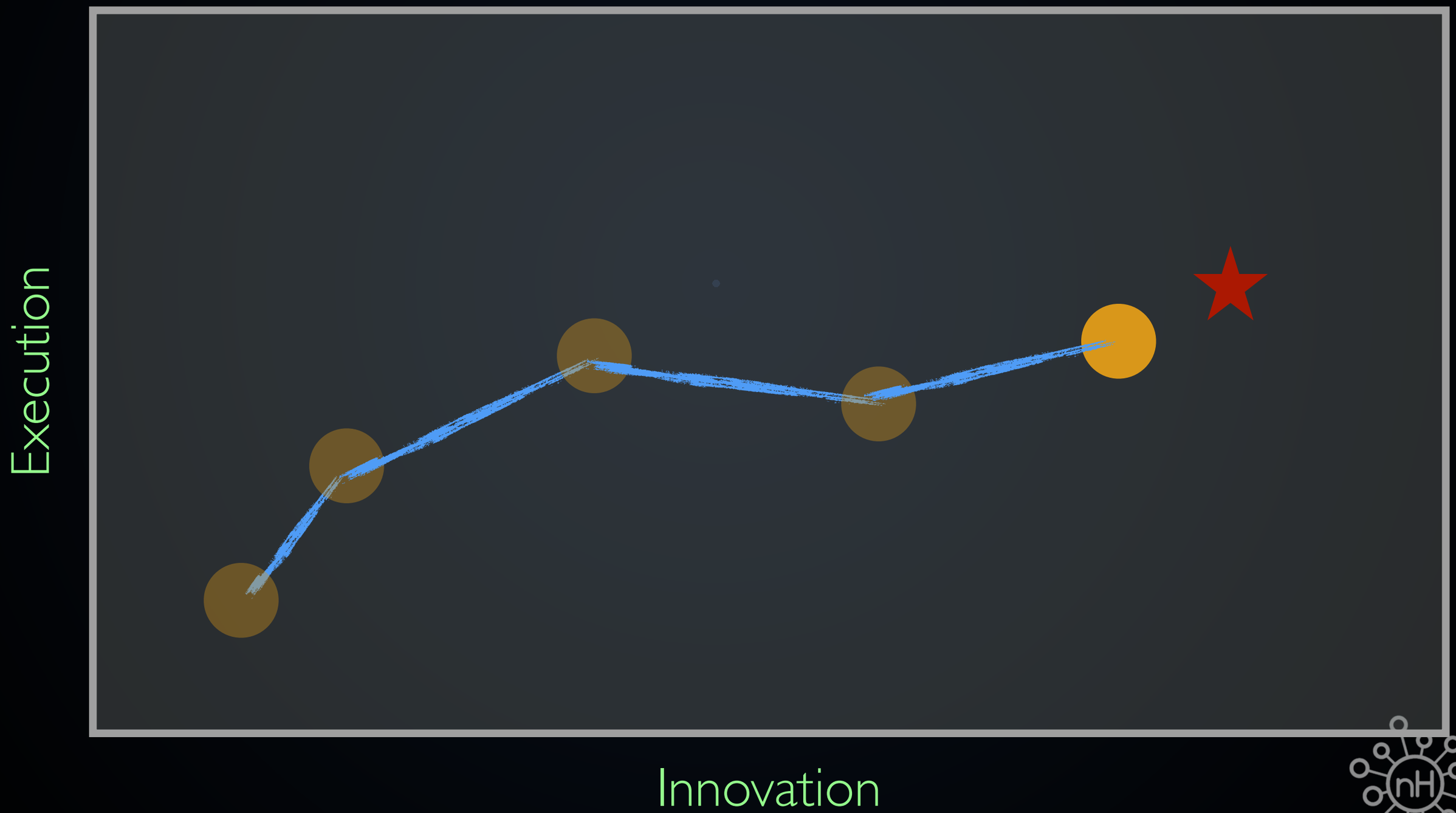
Situation ❖ Target ❖ re-Plan



Situation ❖ Target ❖ re-Plan



Situation ❖ Target ❖ re-Plan



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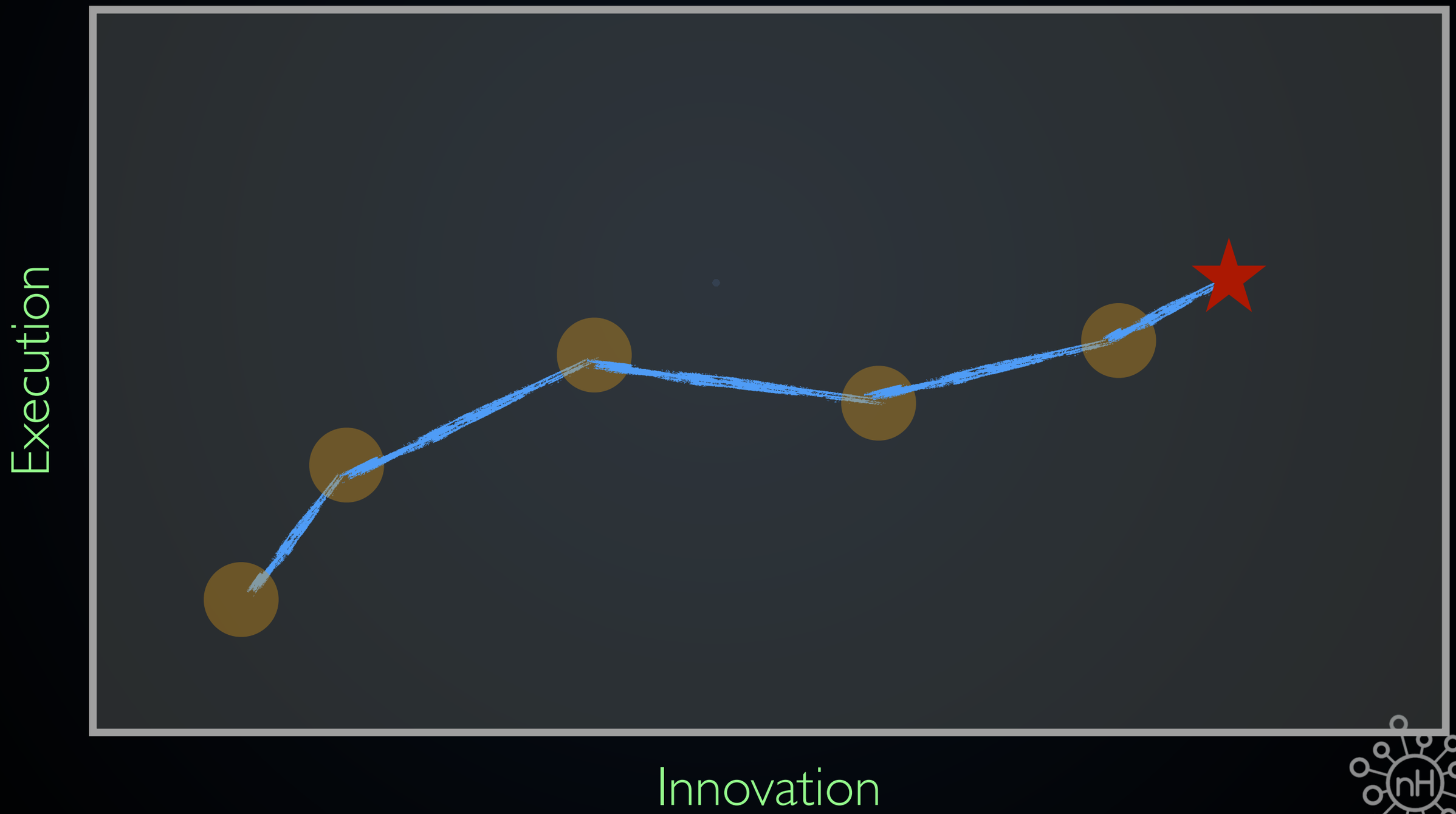
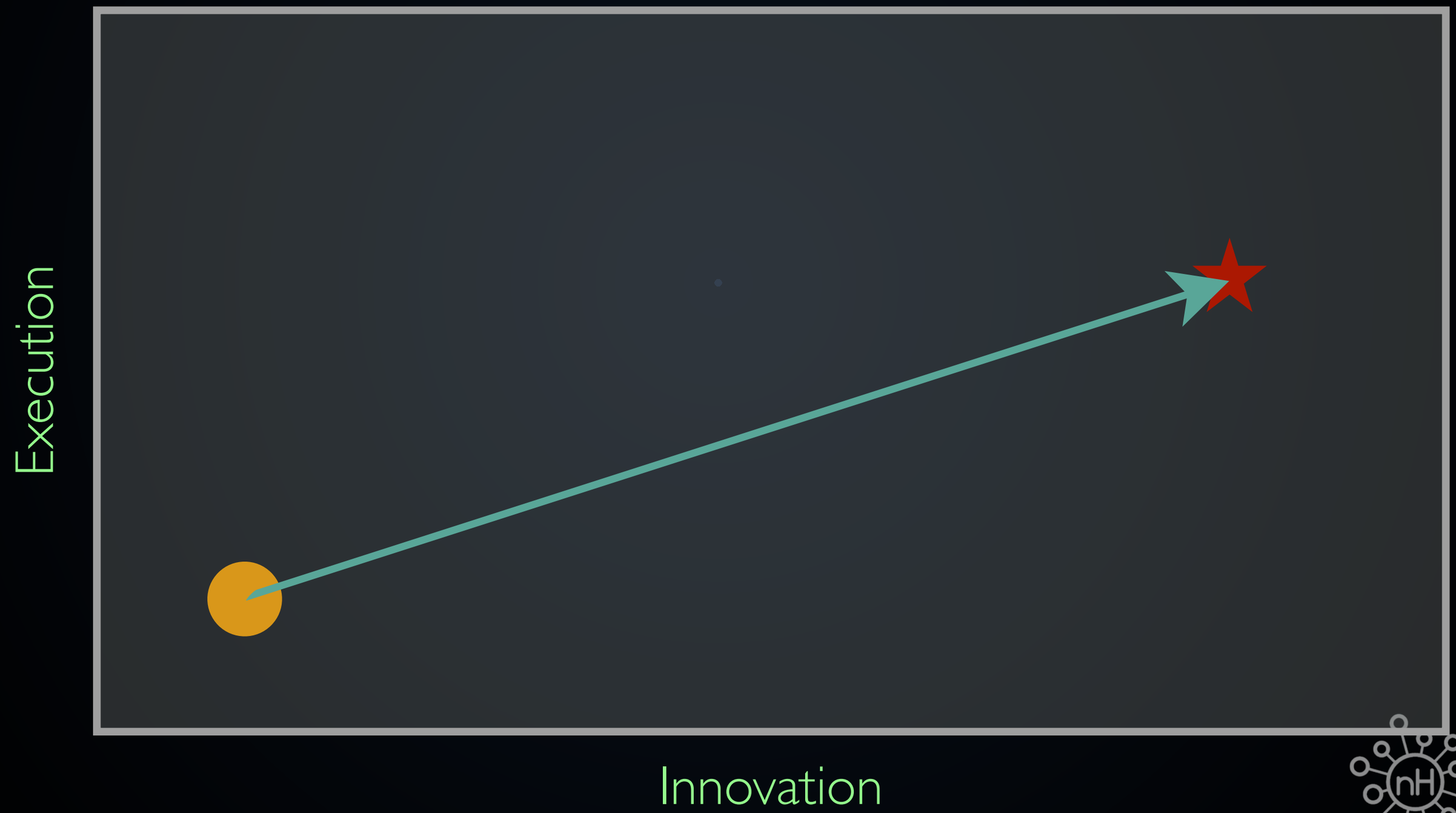
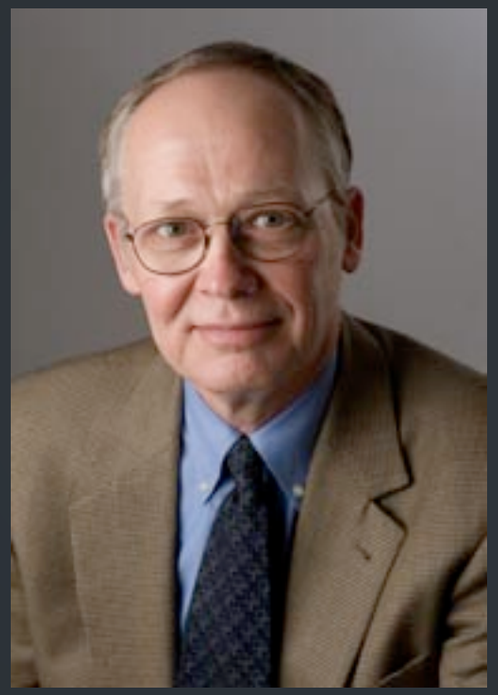


Not a Called Shot...
But It Looks Like One



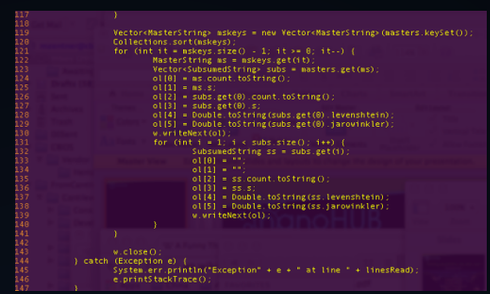
Situation

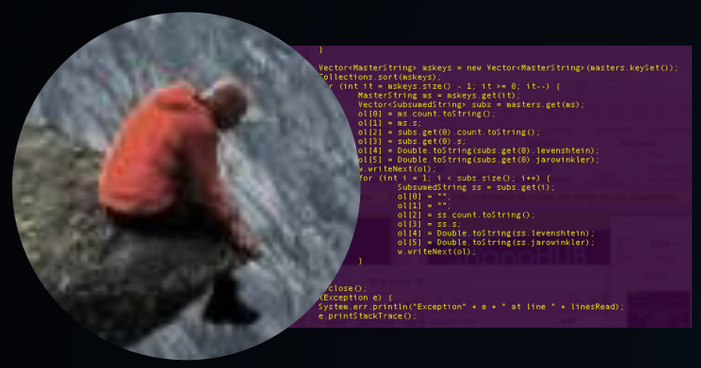


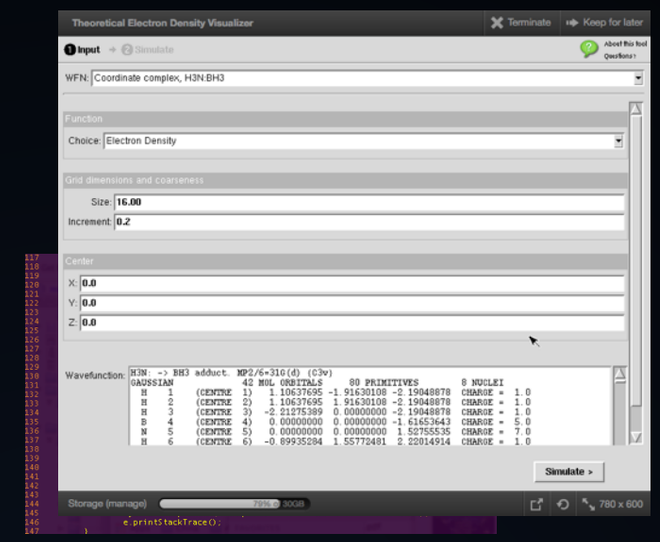
Execution

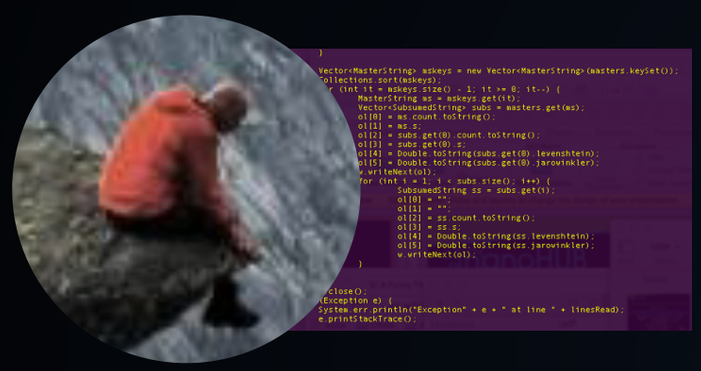
Innovation

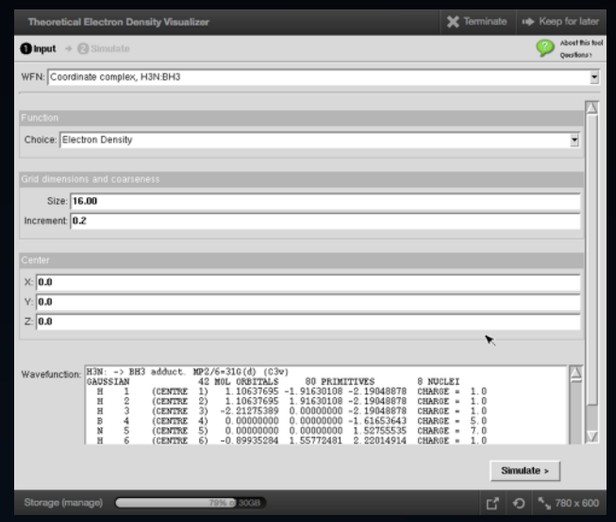
```
117                 }
118
119                 Vector<MasterString> mskeys = new Vector<MasterString>(masters.keySet());
120                 Collections.sort(mskeys);
121                 for (int it = mskeys.size() - 1; it >= 0; it--) {
122                         MasterString ms = mskeys.get(it);
123                         Vector<SubsumedString> subs = masters.get(ms);
124                         ol[0] = ms.count.toString();
125                         ol[1] = ms.s;
126                         ol[2] = subs.get(0).count.toString();
127                         ol[3] = subs.get(0).s;
128                         ol[4] = Double.toString(subs.get(0).levenshtein);
129                         ol[5] = Double.toString(subs.get(0).jarowinkler);
130                         w.writeNext(ol);
131                         for (int i = 1; i < subs.size(); i++) {
132                                 SubsumedString ss = subs.get(i);
133                                 ol[0] = "";
134                                 ol[1] = "";
135                                 ol[2] = ss.count.toString();
136                                 ol[3] = ss.s;
137                                 ol[4] = Double.toString(ss.levenshtein);
138                                 ol[5] = Double.toString(ss.jarowinkler);
139                                 w.writeNext(ol);
140                         }
141                 }
142
143                 w.close();
144         } catch (Exception e) {
145                 System.err.println("Exception" + e + " at line " + linesRead);
146                 e.printStackTrace();
147         }
```






Theoretical Electron Density Visualizer
Terminate
Keep for later
Input
Simulate
About this tool
Questions?
WFN: Coordinate complex, H3N-BH3
Function
Choice: Electron Density
Grid dimensions and coarseness
Size: 16.00
Increment: 0.2
Center
X: 0.0
Y: 0.0
Z: 0.0
Wavefunction: H3N: -> BH3 adduct. MP2/6-31G(d) (C3v)
GAUSSIAN 42 MUL ORBITALS 80 PRIMITIVES 8 NUCLEI
H 1 (CENTRE 1) 1.10637695 -1.91630108 -2.19048878 CHARGE = 1.0
H 2 (CENTRE 2) 1.10637695 1.91630108 -2.19048878 CHARGE = 1.0
H 3 (CENTRE 3) -2.21275389 0.00000000 -2.19048878 CHARGE = 1.0
B 4 (CENTRE 4) 0.00000000 0.00000000 -1.61653643 CHARGE = 5.0
N 5 (CENTRE 5) 0.00000000 0.00000000 1.52755535 CHARGE = 7.0
H 6 (CENTRE 6) -0.89935284 1.55772481 2.22014914 CHARGE = 1.0
Simulate >
Storage (manage)
780 x 600

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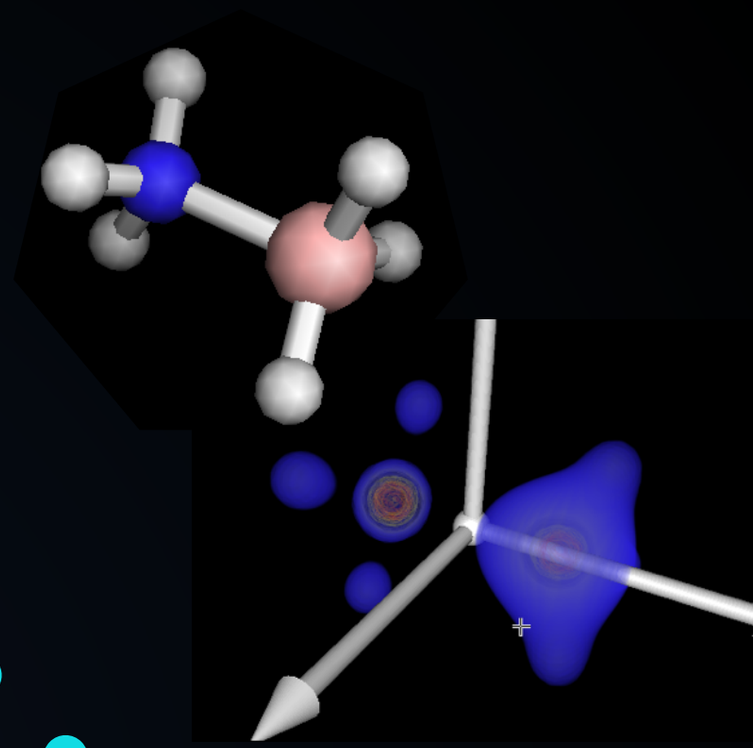

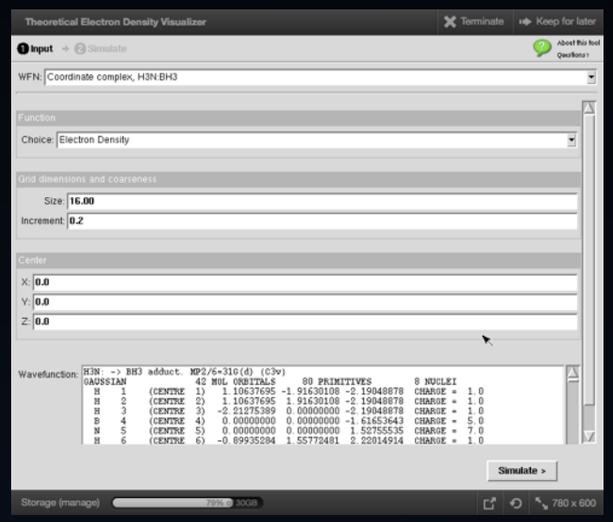
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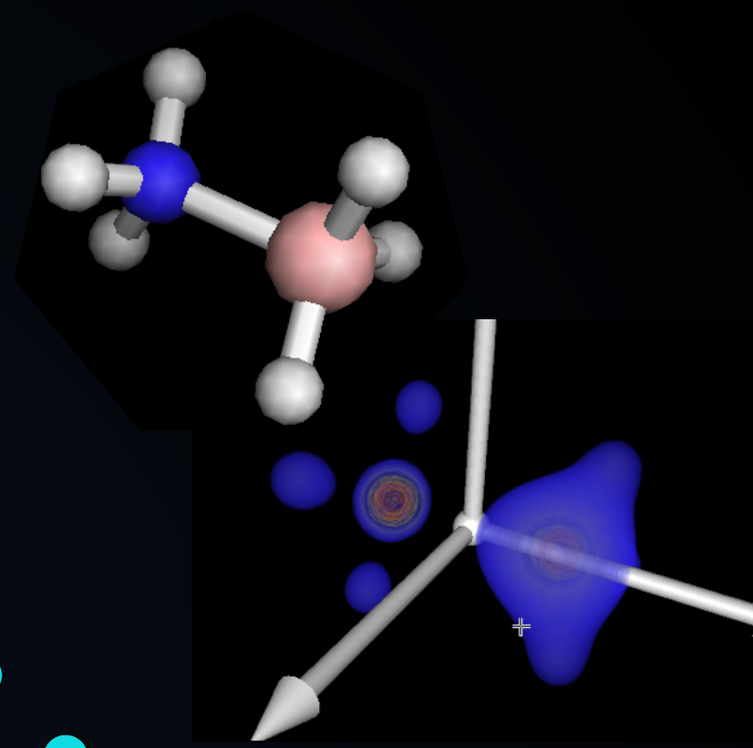
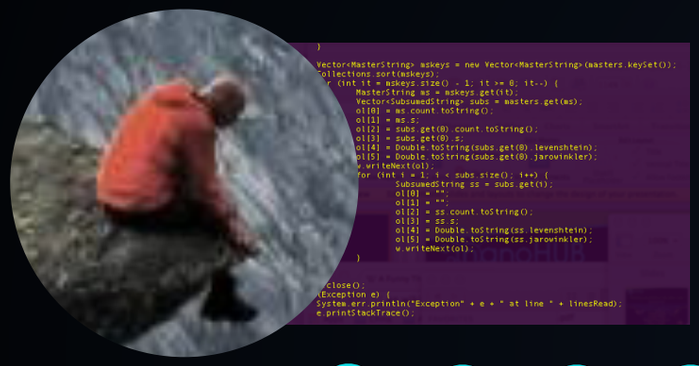
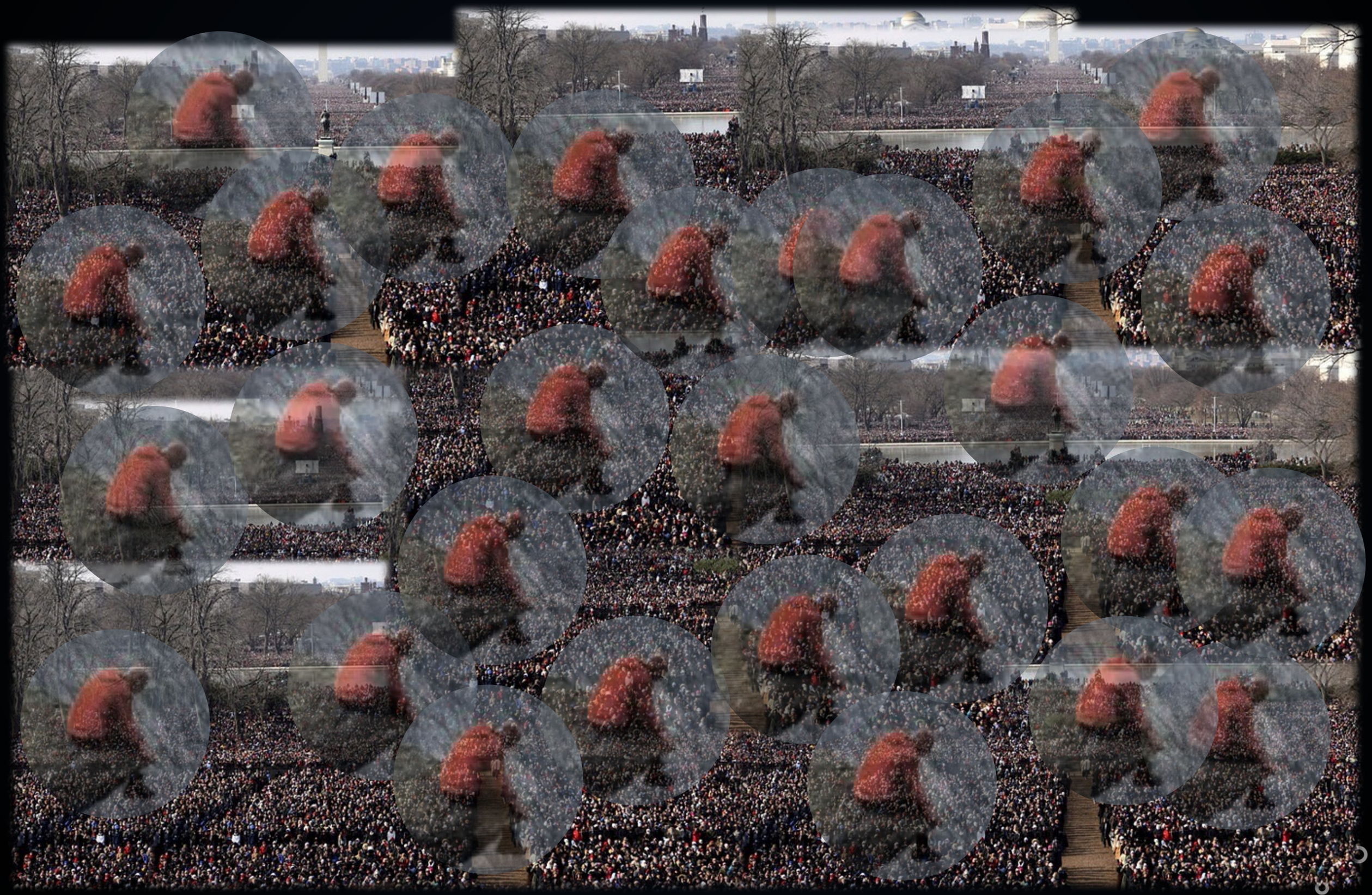




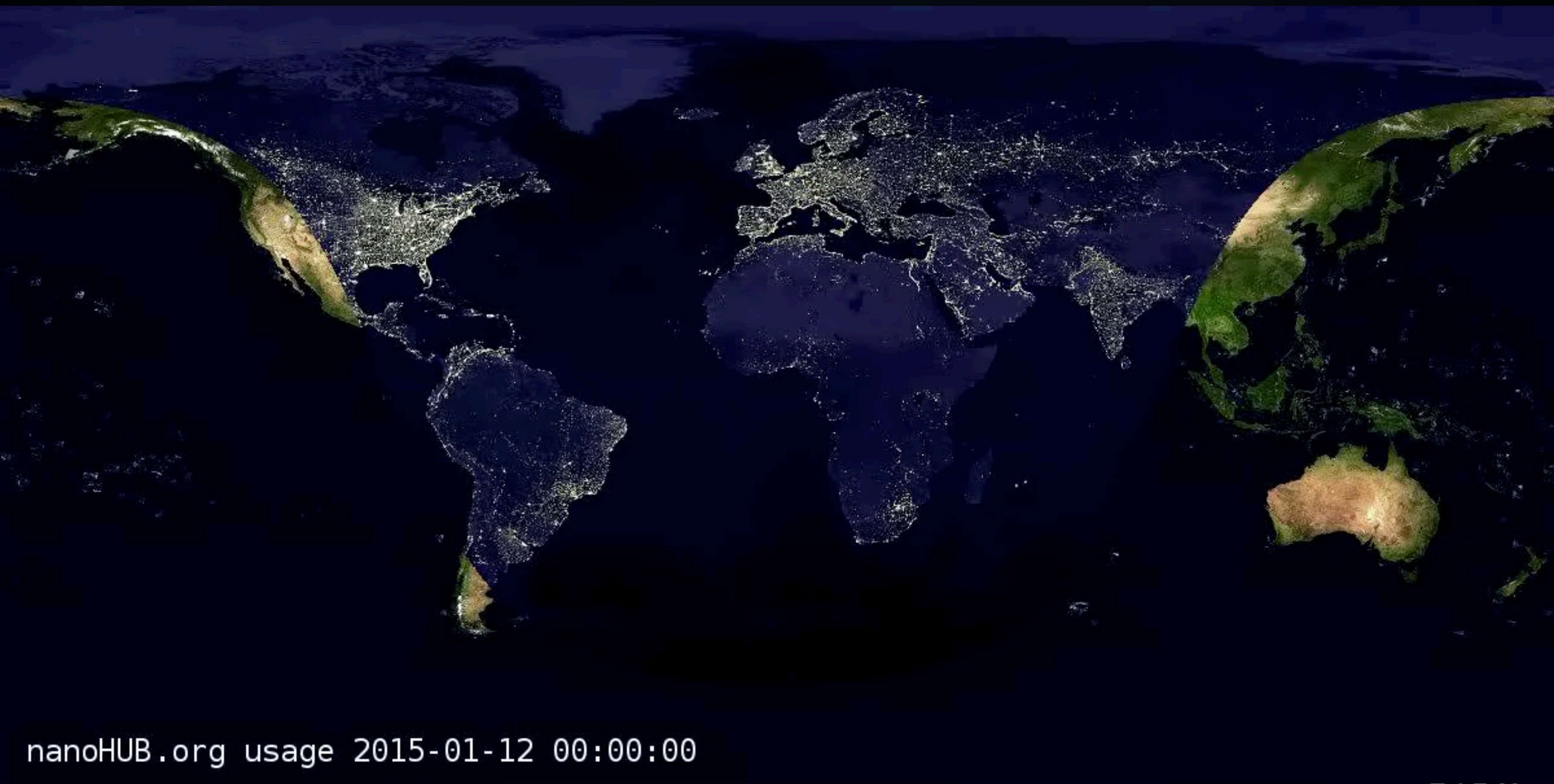


NANOHUB TODAY

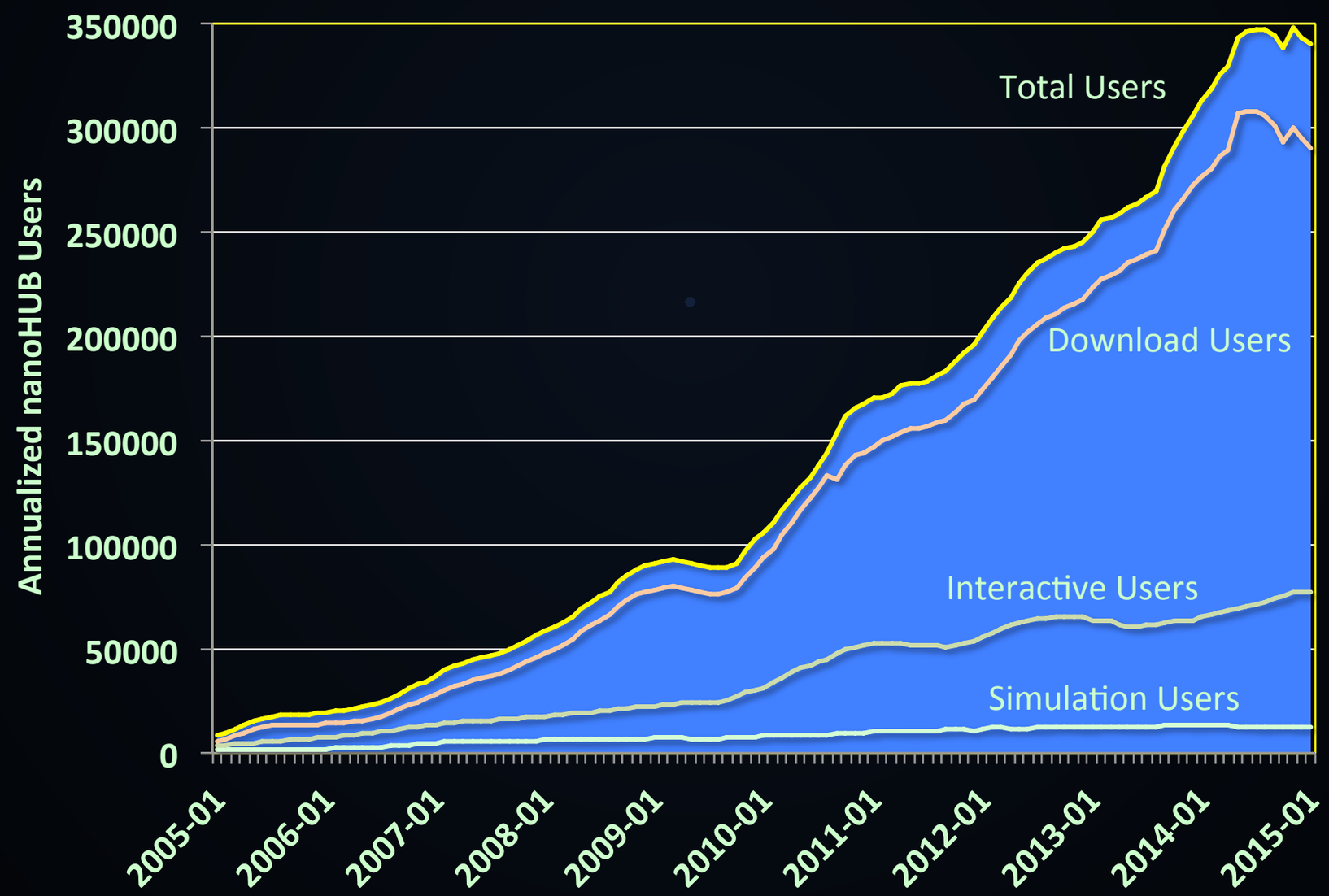
370+ Simulation Tools
4700+ Other Resources
3000+ Online Presentations
540+ Teaching Materials

At No Cost: nanohub.org

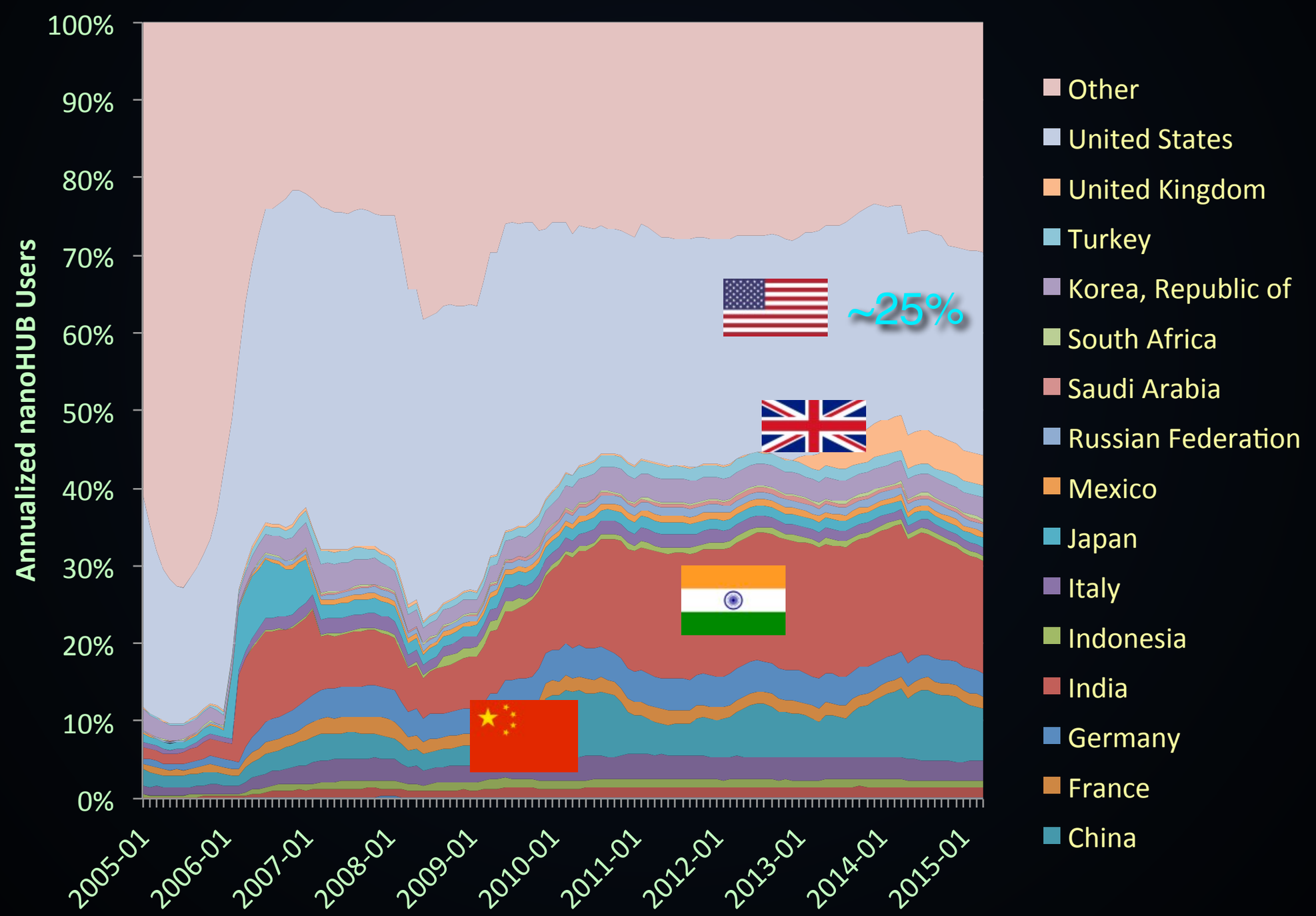
A Continuous User Base



A Large User Base



An International User Base



Lesson 1

Expand Vertically:

"The needs of the one outweigh the needs of the many"

More capabilities

More users

As the "market" informs you of its needs

Expertise Needed

- Domain Scientists
- HPC & Middleware
- Security
- Web Design / Programming
- Analytics
- Hardware
- Production Operations
- Databases

Expertise Needed

- Domain Scientists
- HPC & Middleware
- Security
- Web Design / Programming
- Analytics
- Hardware
- Production Operations
- Databases

Oh...and More Expertise Needed

- Domain Scientists
- HPC & Middleware
- Security
- Web Design / Programming
- Analytics
- Hardware
- Production Operations
- Databases
- Financial Management
- Project Management
- Outreach
- Administrative
- Educational Specialists

Lesson 2

Expand horizontally

You cannot afford the resources you need to do something like this.

Generalize and leverage across projects.

hubzero


NEEShub
George E. Brown, Jr. Network for
NCIP HUB
habricentral
Resources for the Study of the Human-Animal Bond
GLOBALHUB
PURR
ciHUB.org
BETA
PHARMAHUB
hubzero
iemHUB
a CIEM project
cceHUB
nH
nH

60+ HUBs
28 HUBzero Staff
10 NCN staff (7 FTE)
~2,000,000 Visitors Annually


NEEShub
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GLOBALHUB
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BETA
PHARMAHUB
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iemHUB
a CiEM project
cceHUB
nH

Lesson 3

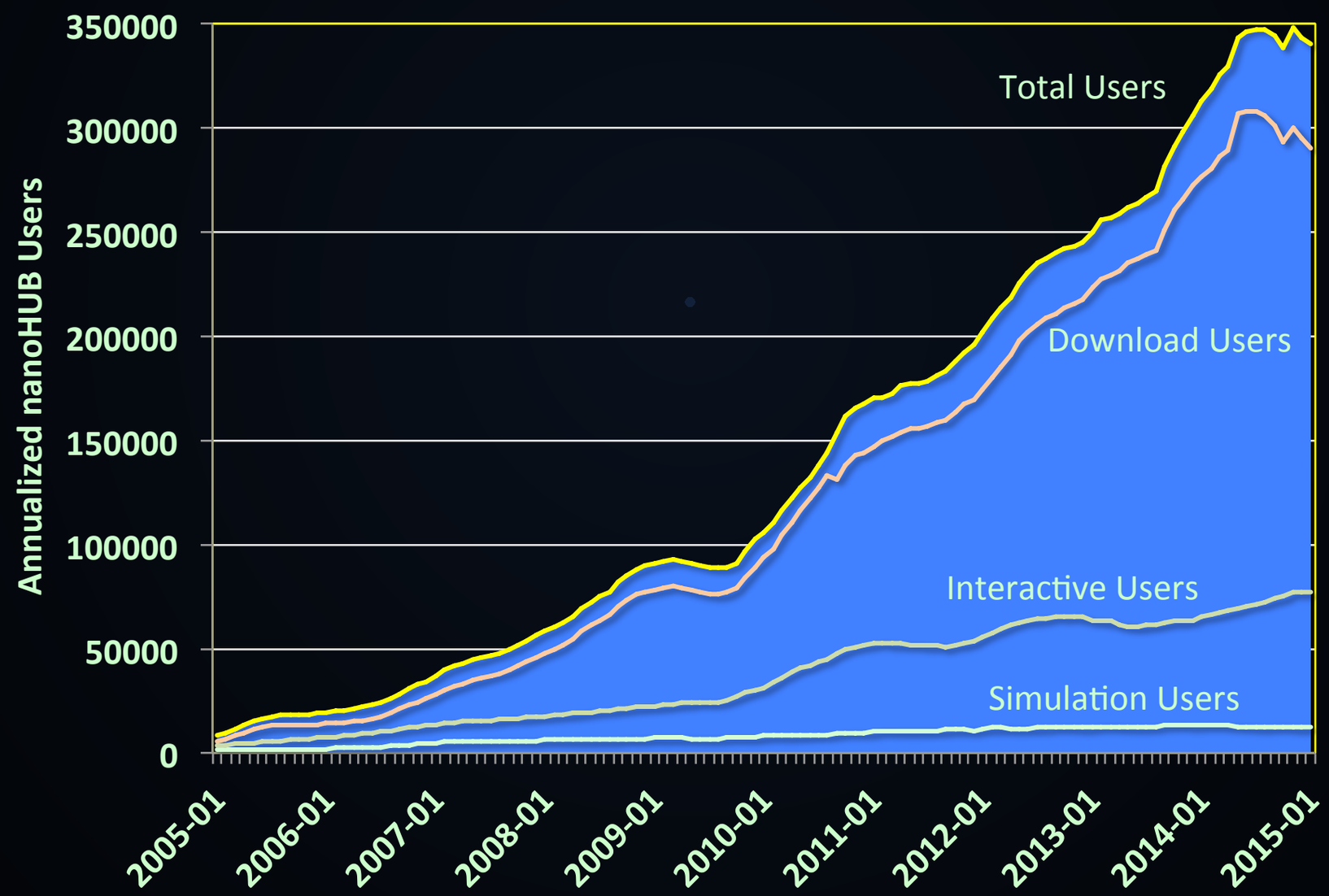
Justify Your Existence

Measure Impact, Not Just Users

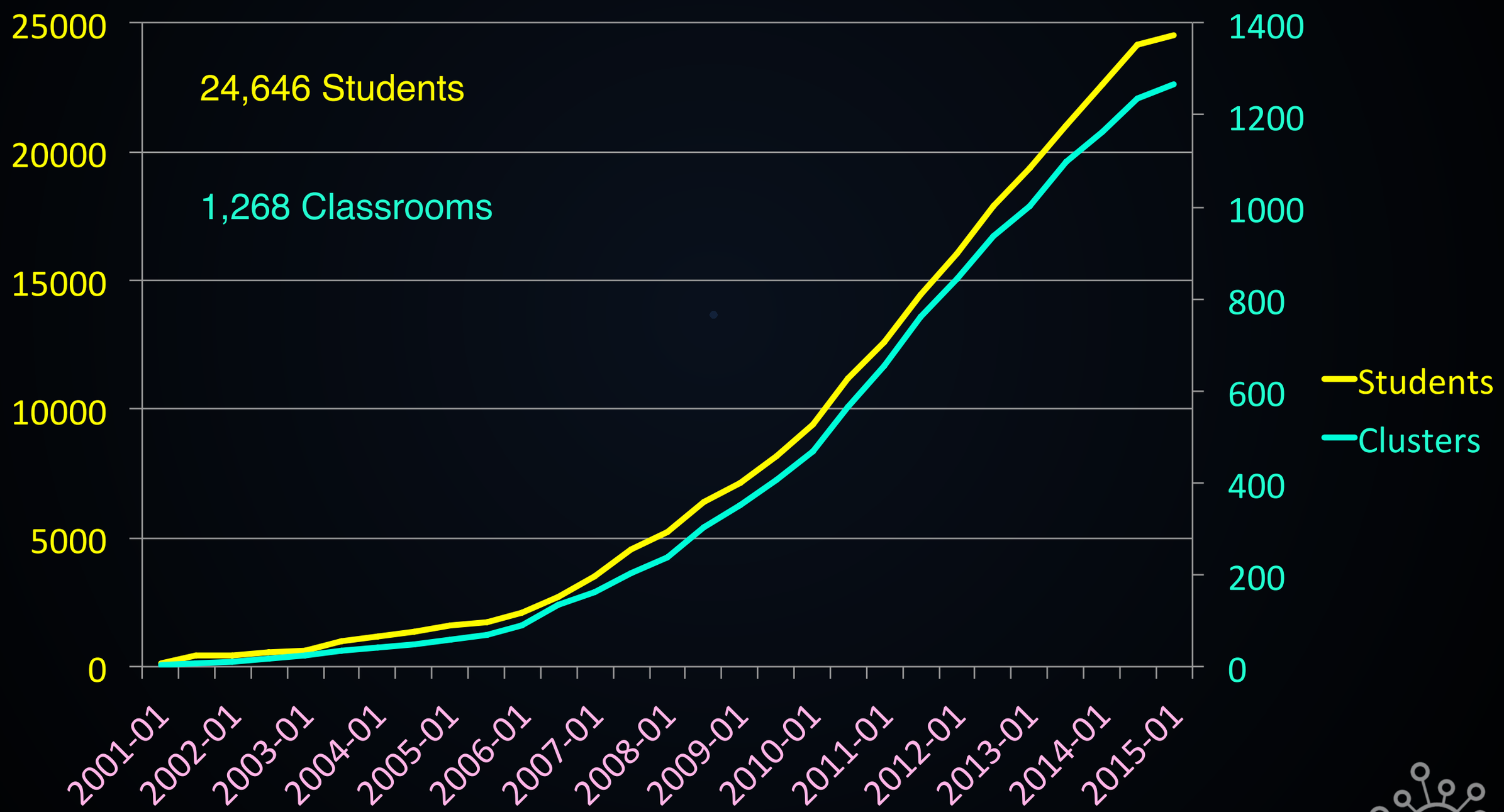
Make Your Contributors Want to Contribute

Learn from Users

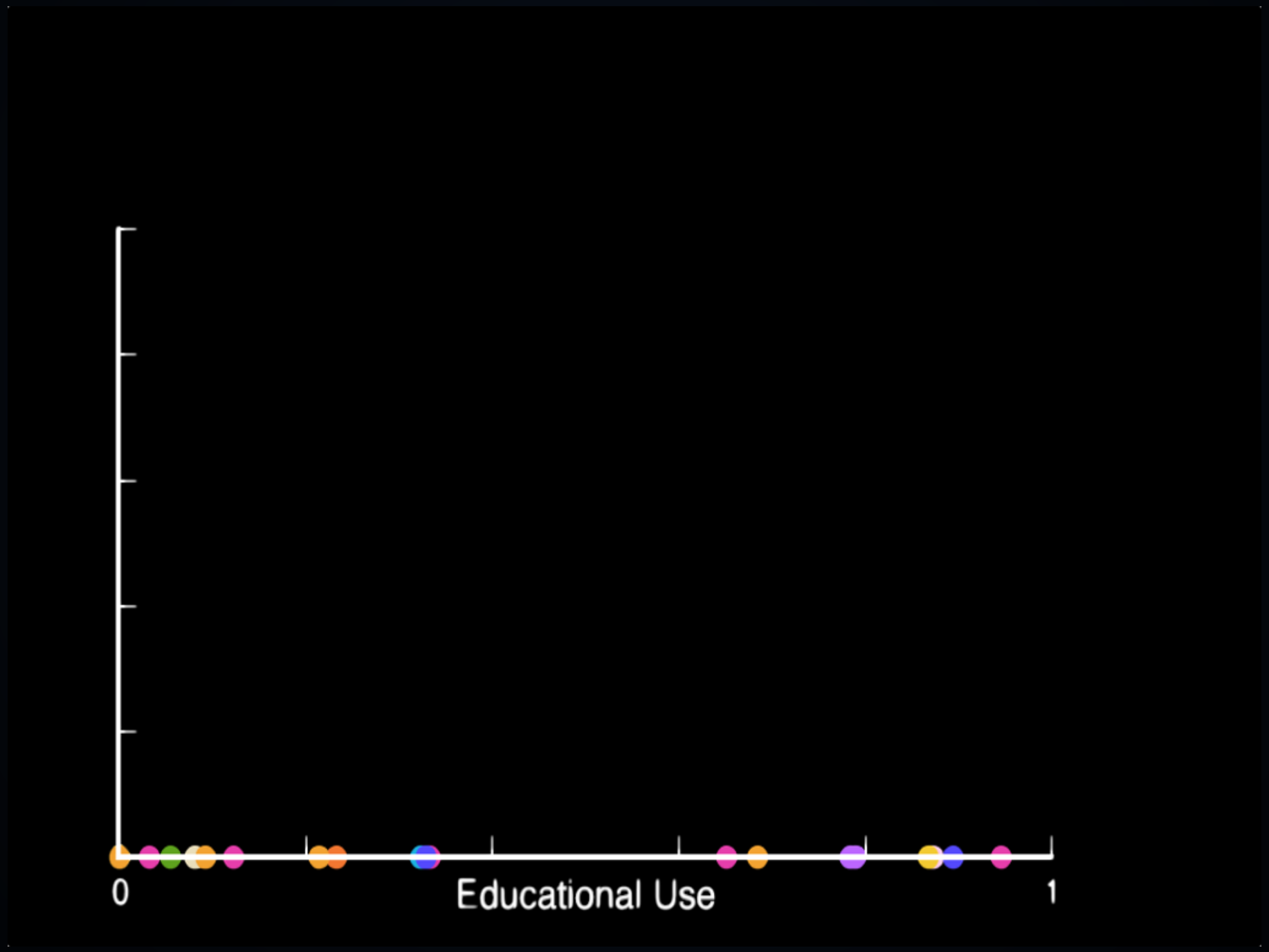
A Large User Base



Classroom Impact



Educational Migration



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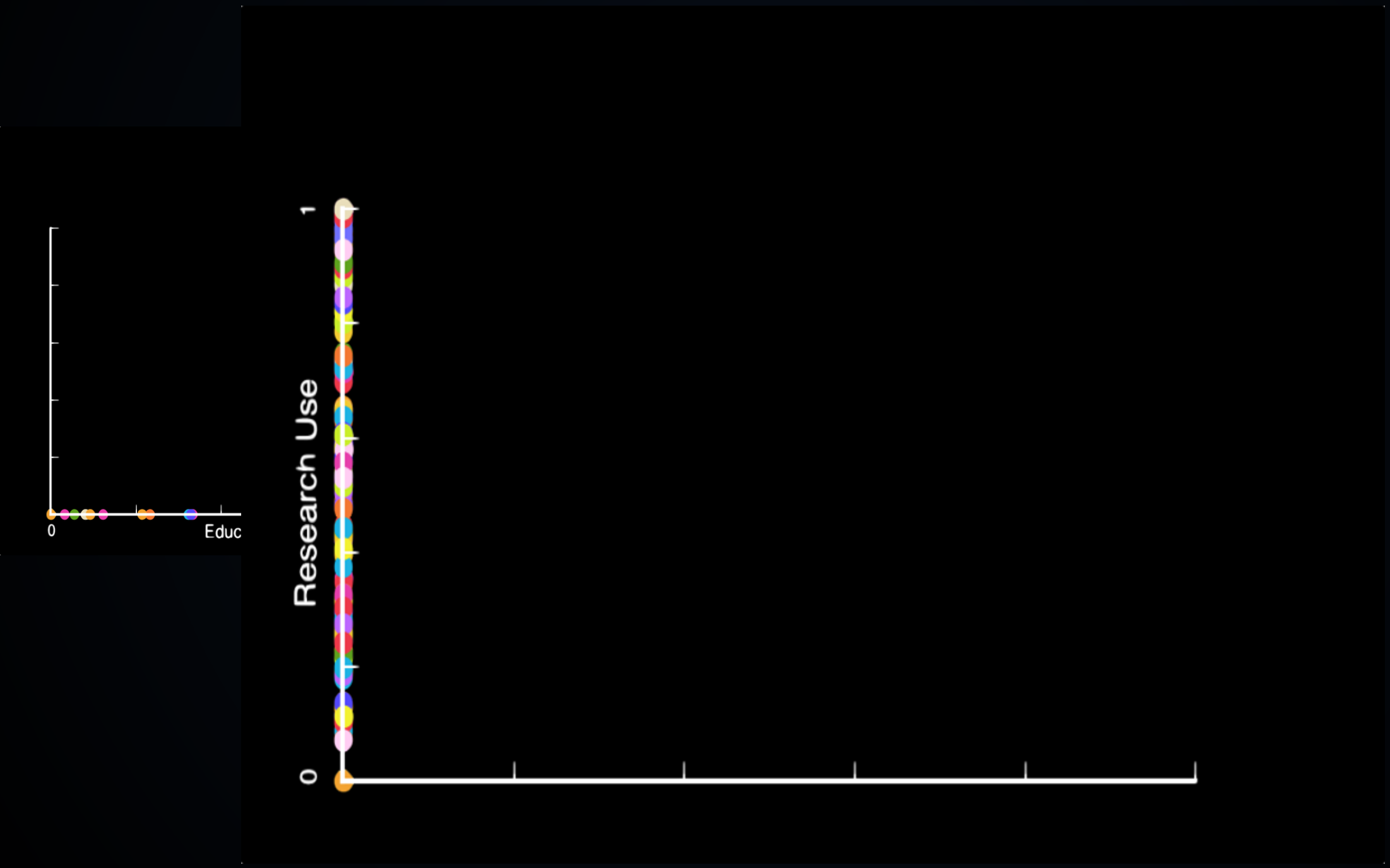
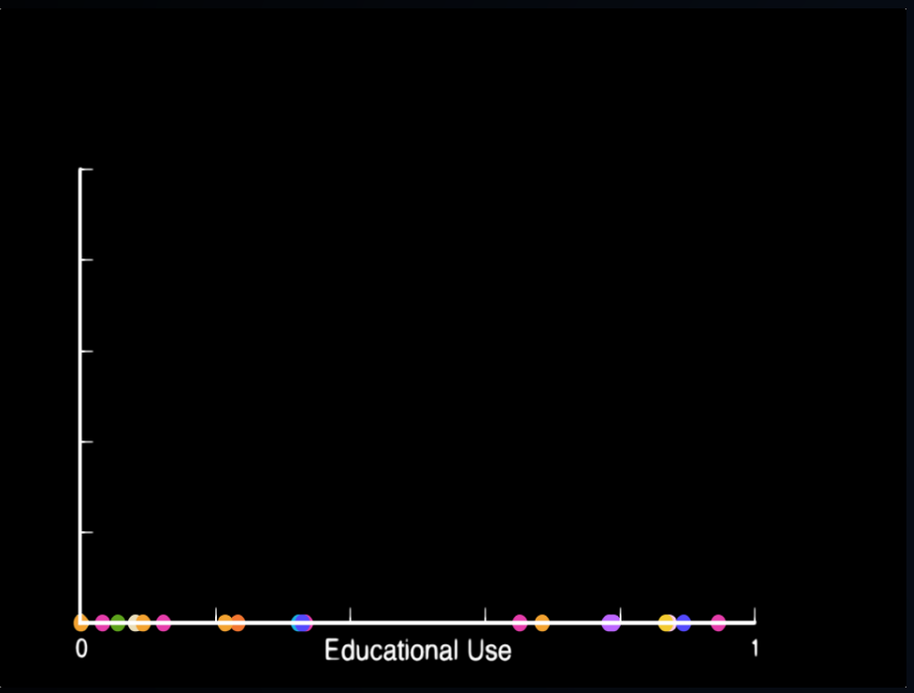
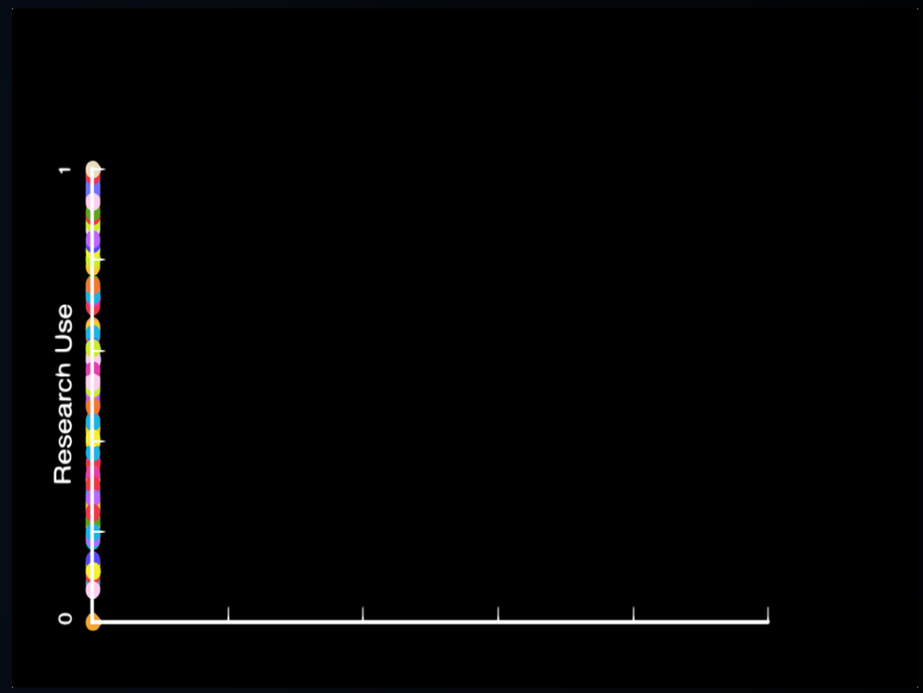
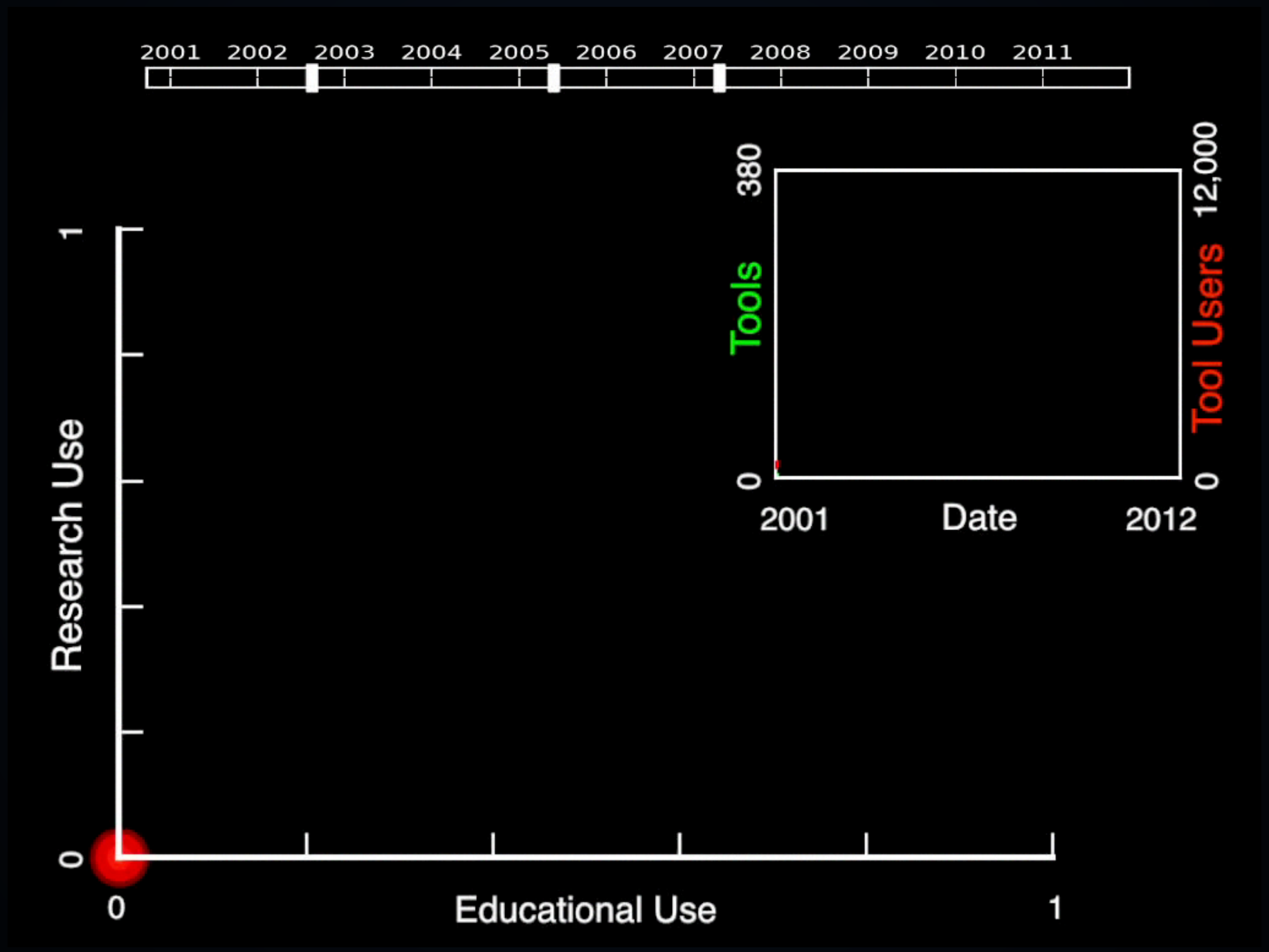


Educational Migration

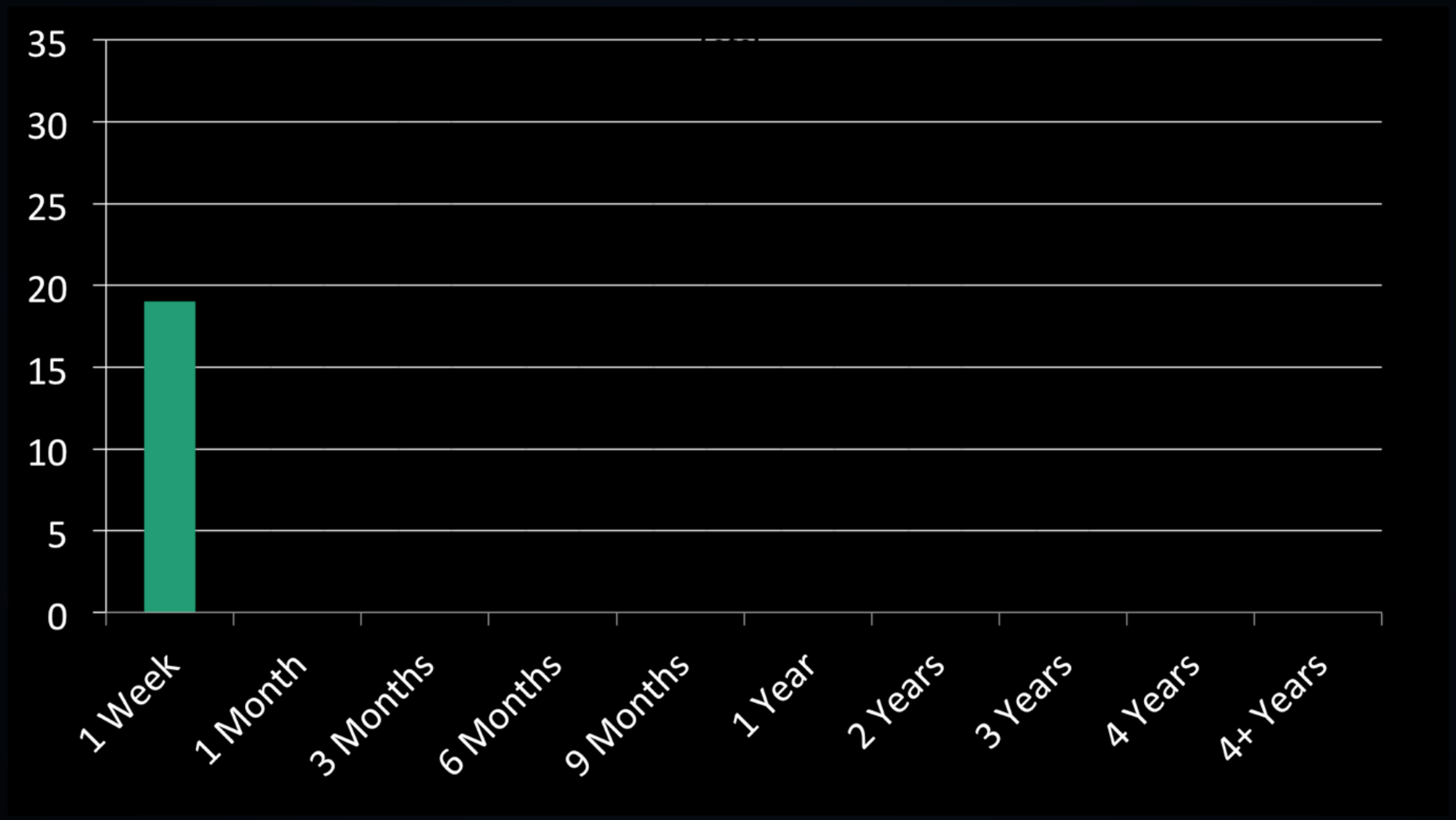




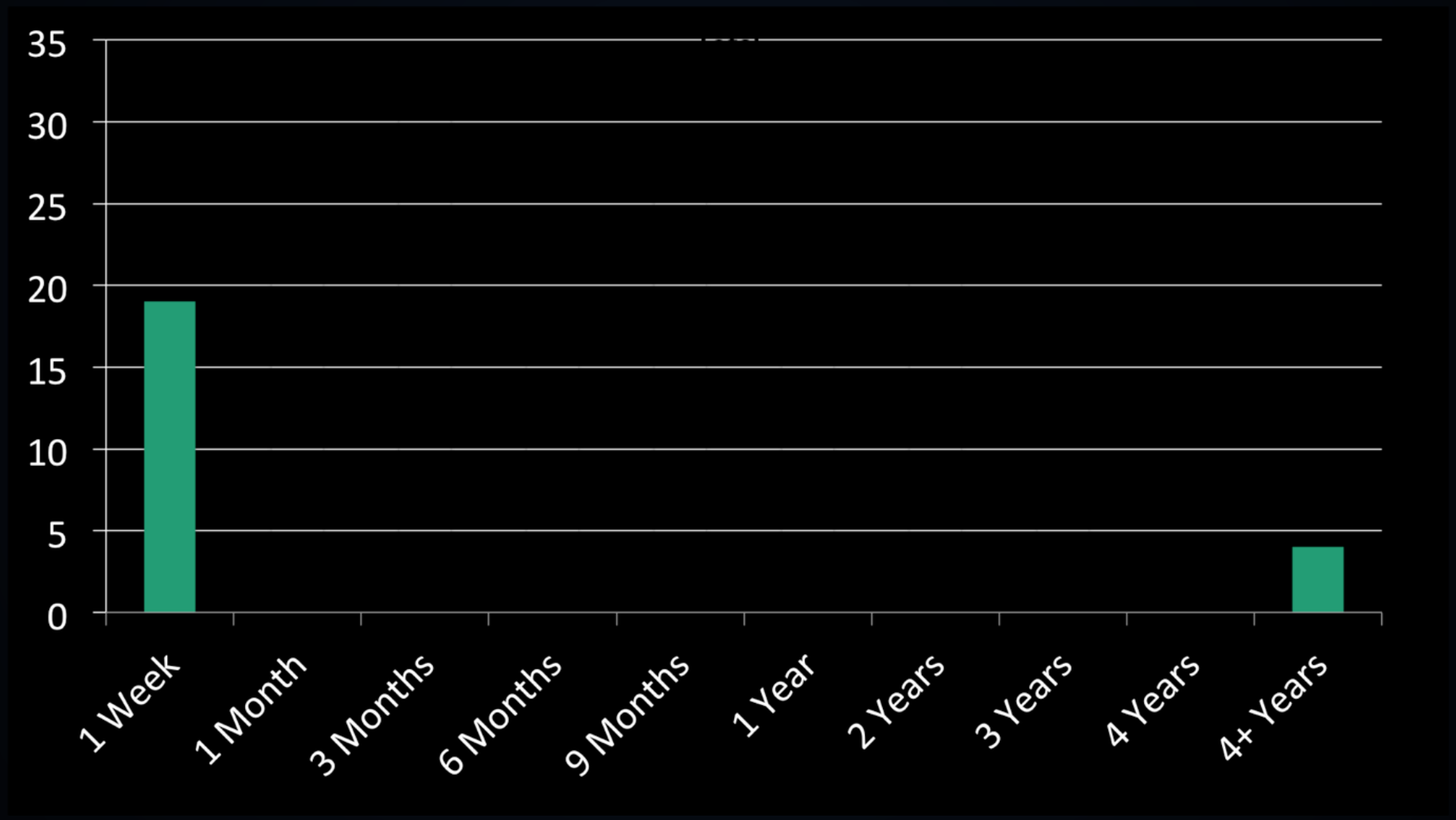
Educational Migration



Educational Adoption



Educational Adoption



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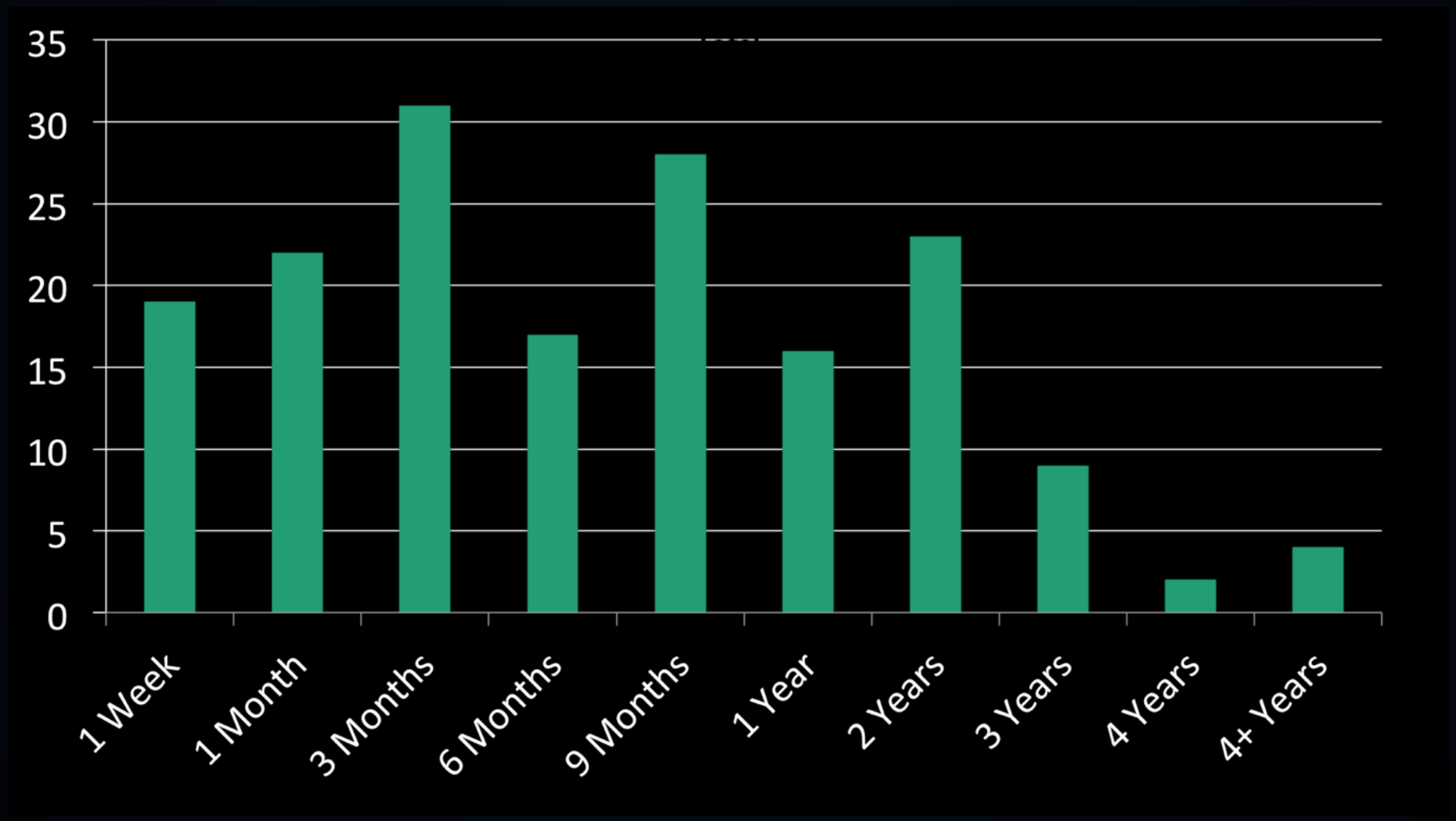
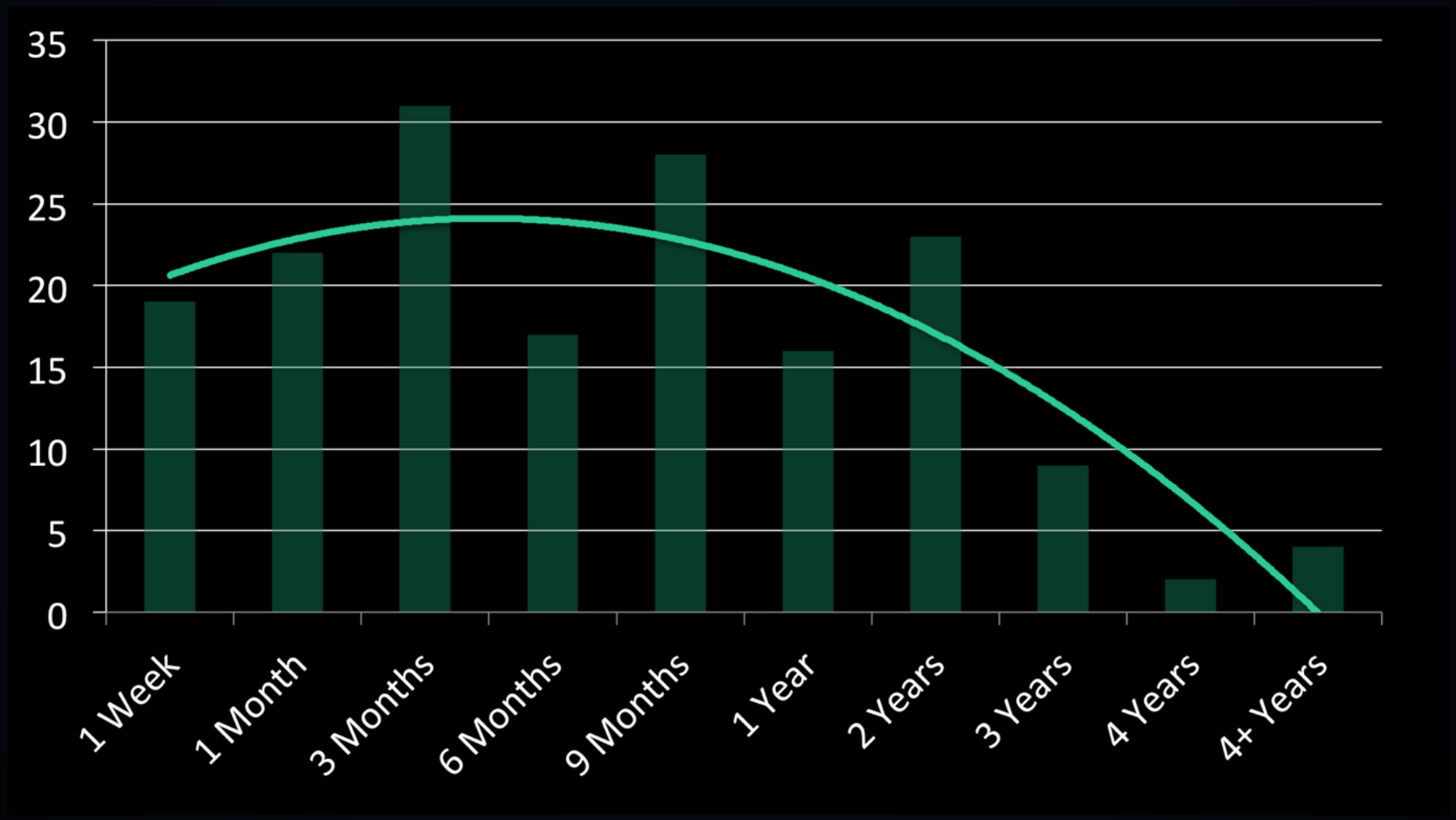


Educational Adoption



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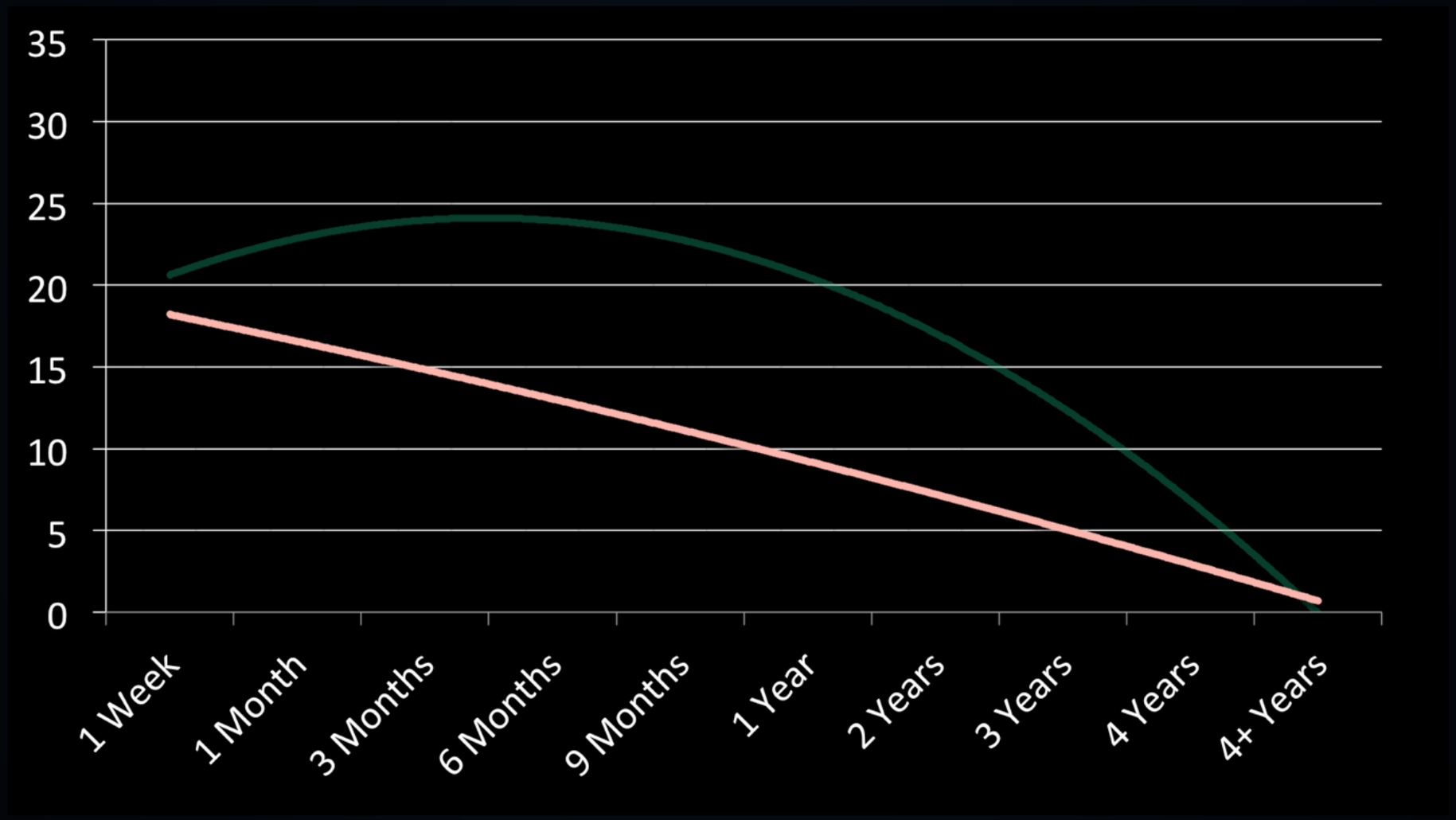

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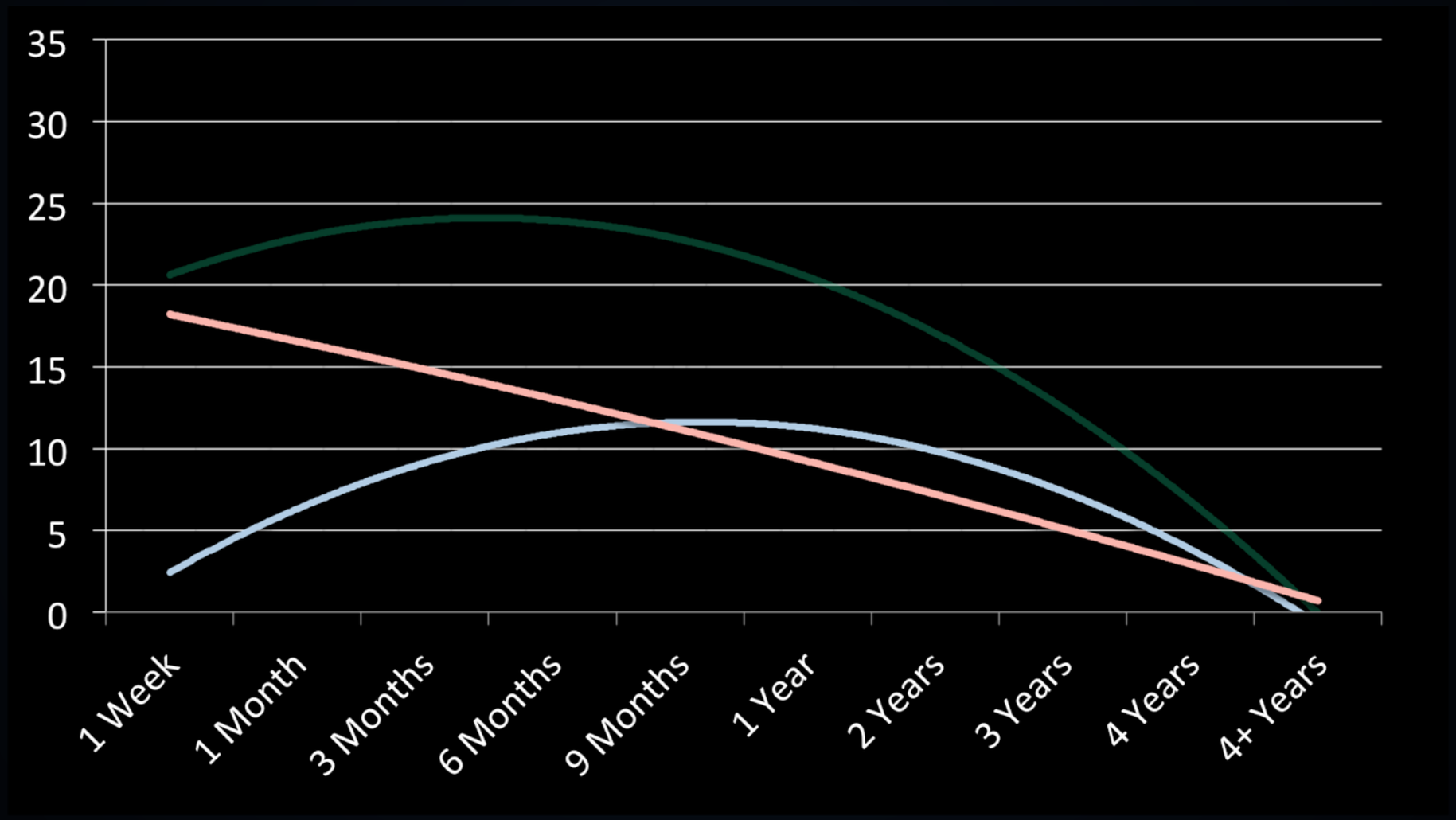
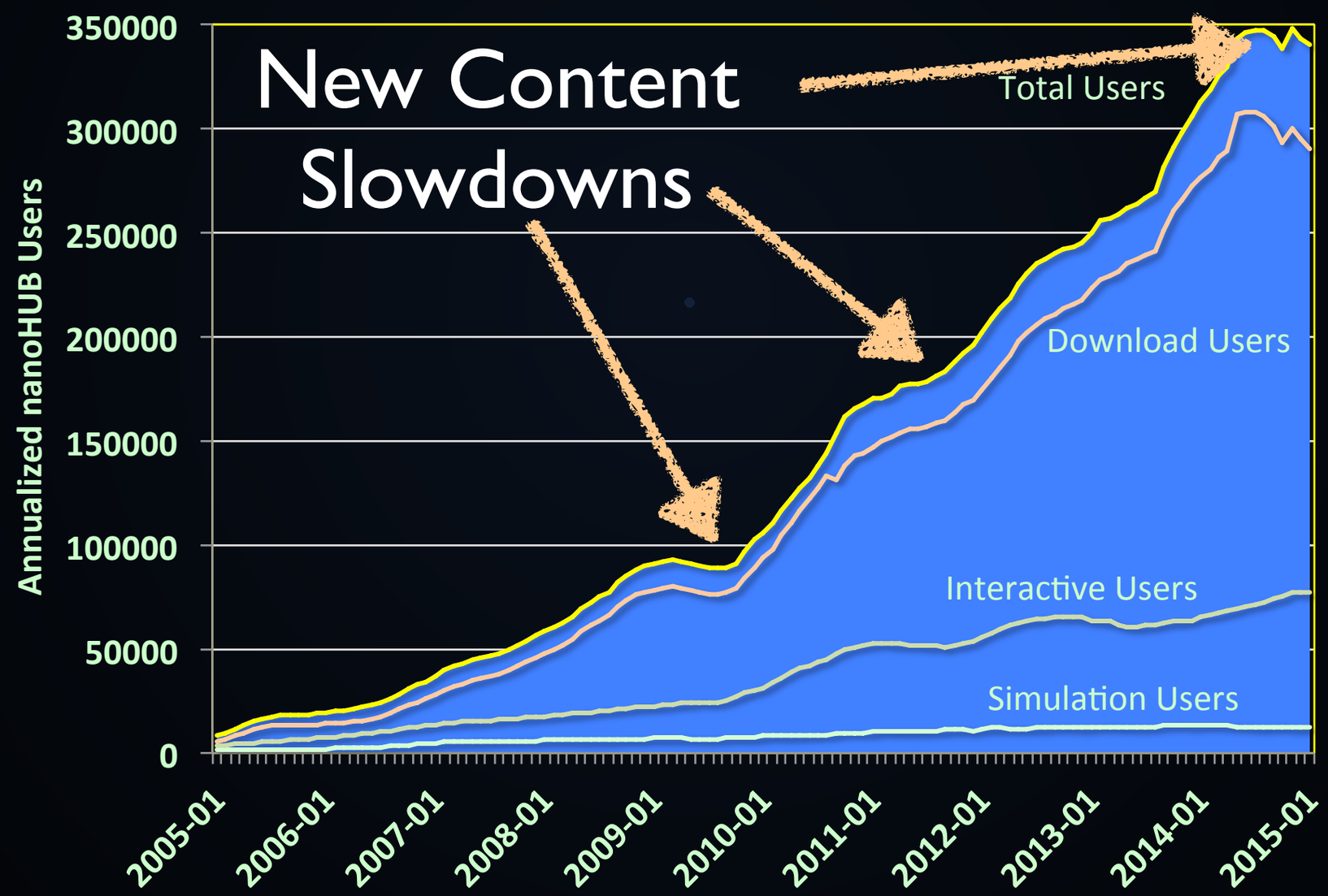


Lesson 4

Fresh and excellent content

Content - Growth Relationship



Lesson 5

Assemble the Right Team

Mark Lundstrom,
Core Science,
Visionary

Gerhard Klimeck,
Core Science,
Scale-up

Gerhard Klimeck,
Core Science,
Scale-up

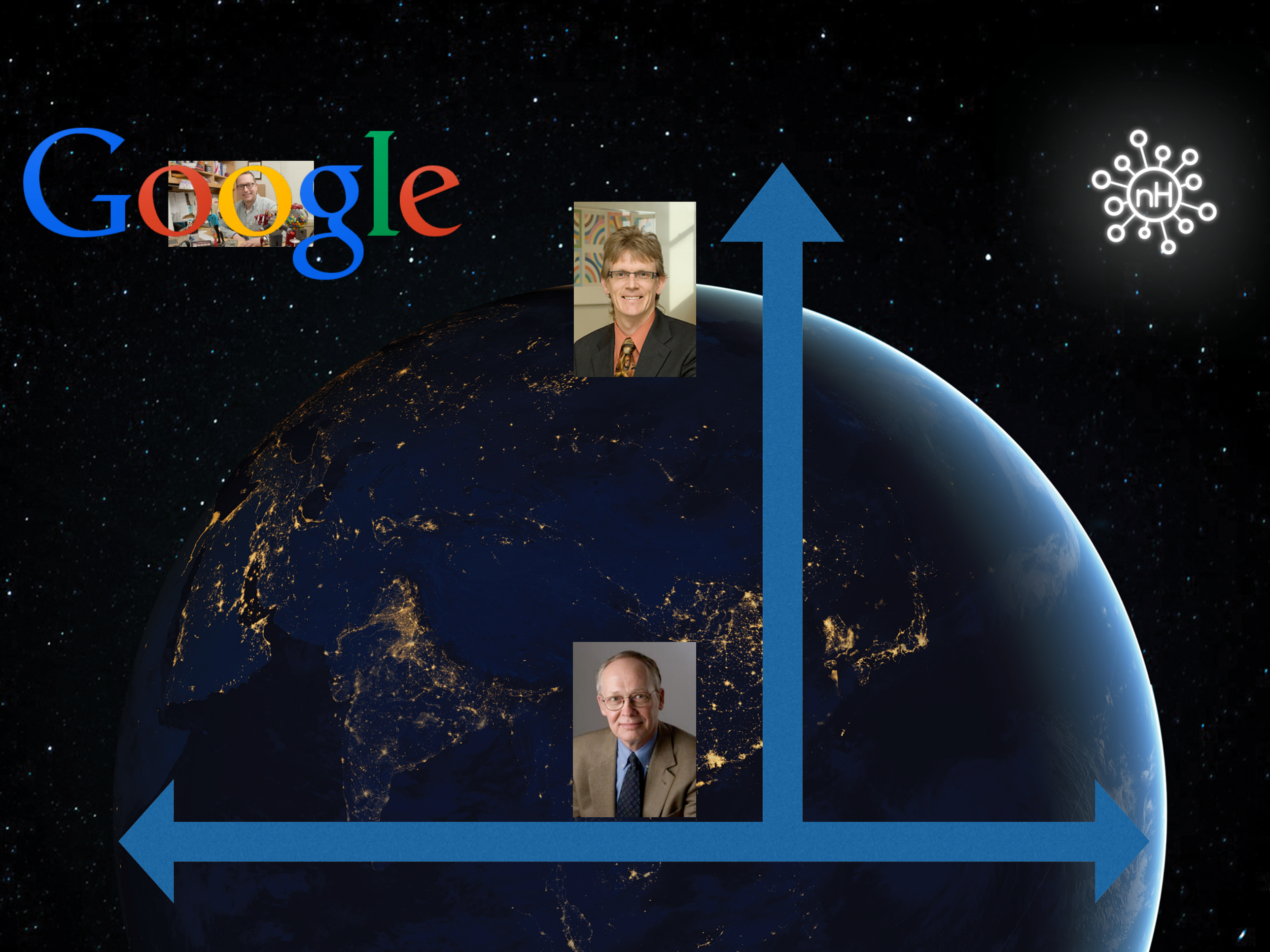
Content, Users

Michael McLennan,
Scale-out
(HUBzero)

Content, Users

Applications

Google


Google
nH

Lesson 6

You're never done!

How can we have the same impact for
people who work with data that
we did for people who simulate?

Publication with DOI & Journal Partners
Reputation with Thompson Reuters (Web of Science)
Uncertainty Quantification

Dense Data

Within Your Experiment, Your Knowledge is Somewhat Complete
(in your home you know what you own)

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 (you know many of the things your neighbors own)

Liver Uptake

Brain Uptake

Gold

?

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

Silver

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
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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

?

(more) Sparse Data

In Your Extended Community, Knowledge is Less Complete
(you know many of the things your neighbors own)

etc…

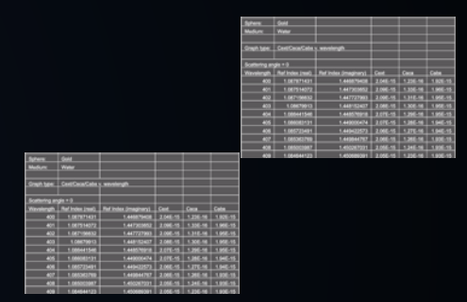
Environmental Measurements

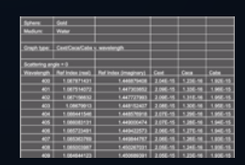
Biological Measurements

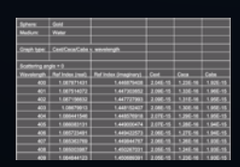
Gold

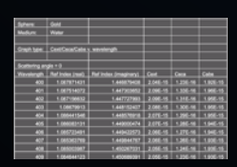
Silver

etc…









(very) Sparse Data

In A Wide Community, Knowledge is Very Incomplete
(you don't know what most people on earth own)

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

Wide

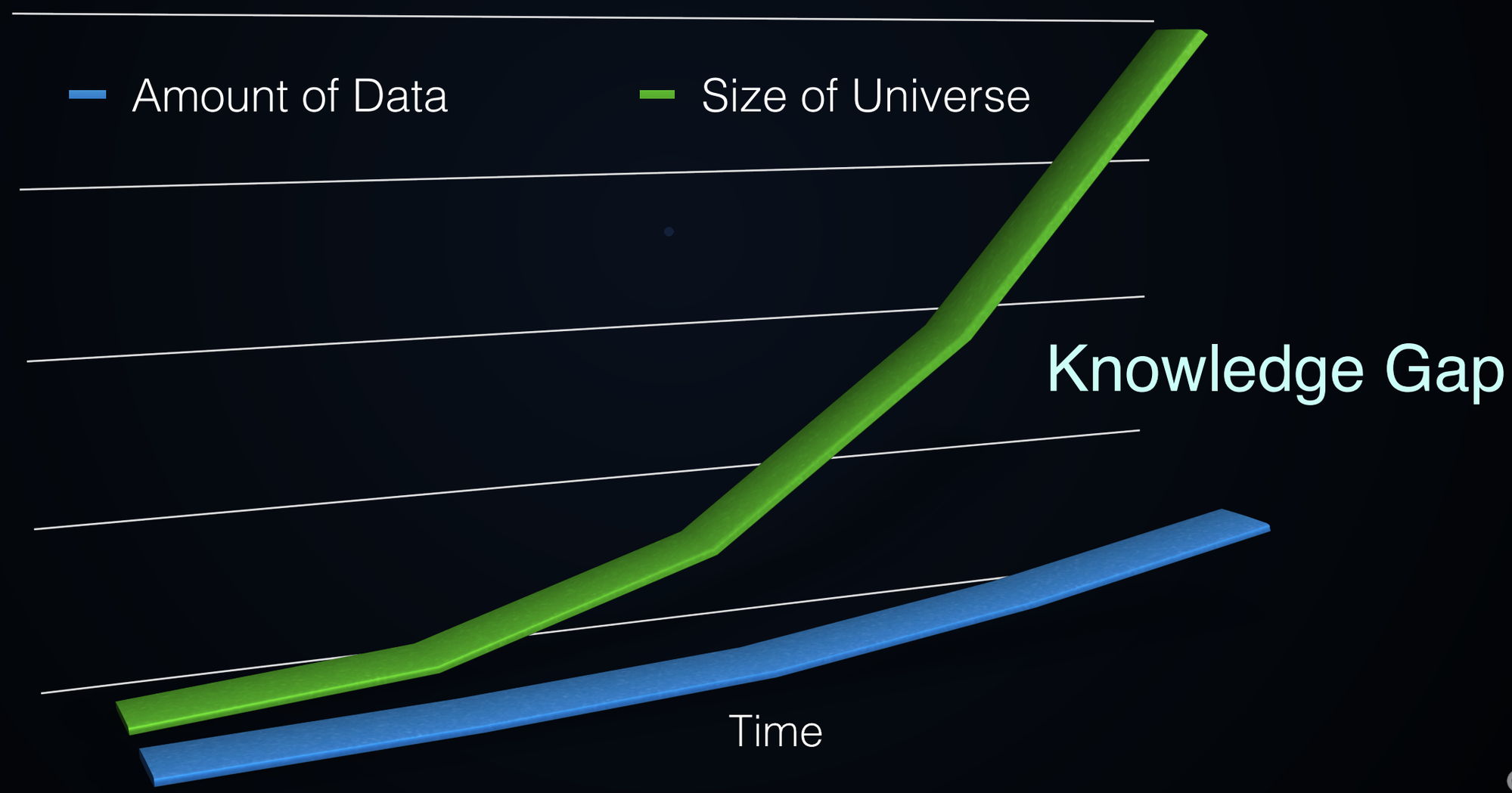
Variety

of

Materials

Knowledge vs Universe

The more we have, the less we know…



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

?

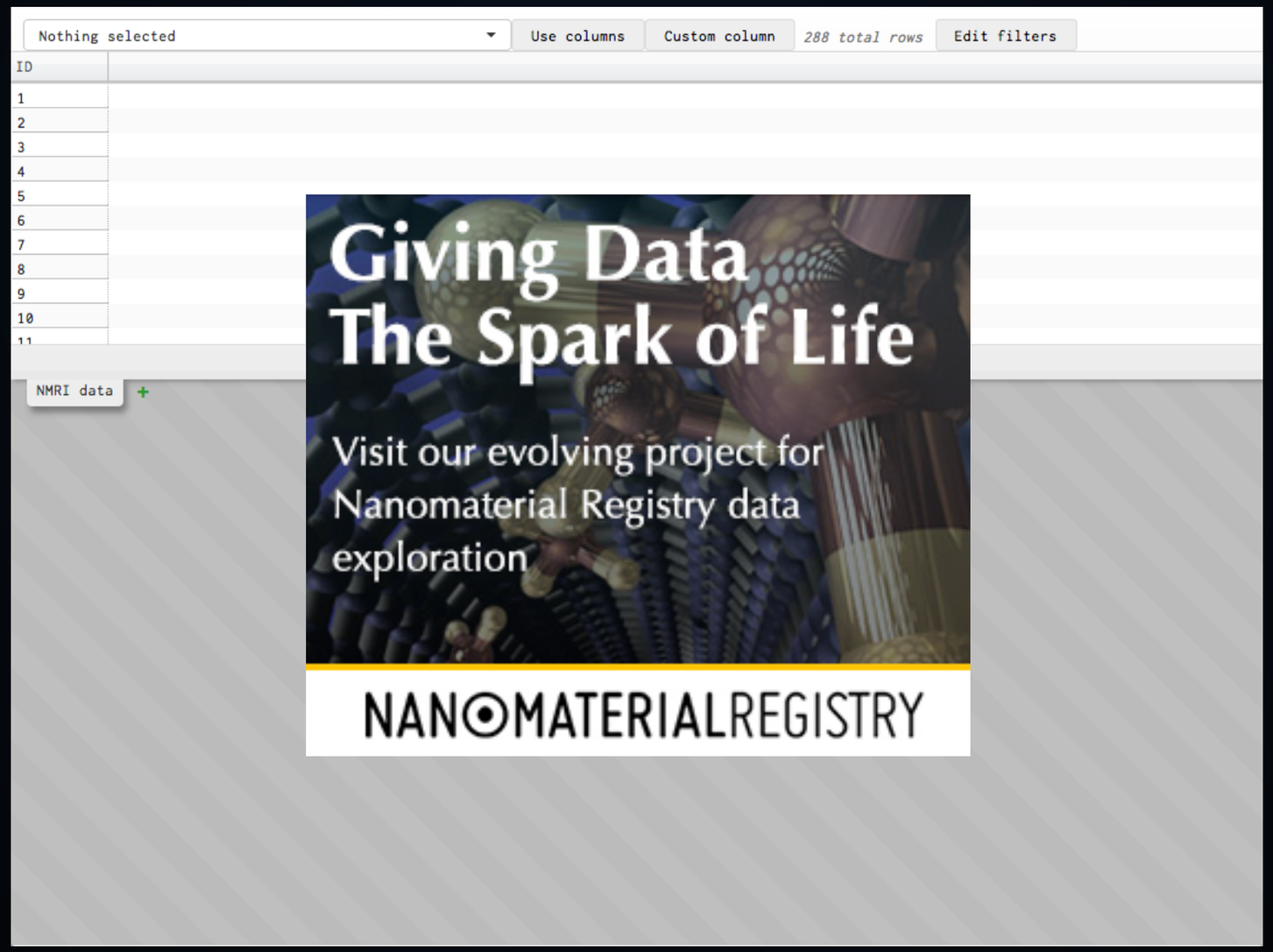
Exploration

Run Meta Data				Inputs				Outputs			
User	Time	Tool	etc.	I_1	I_2	I_3	etc	O_1	O_2	O_3	etc

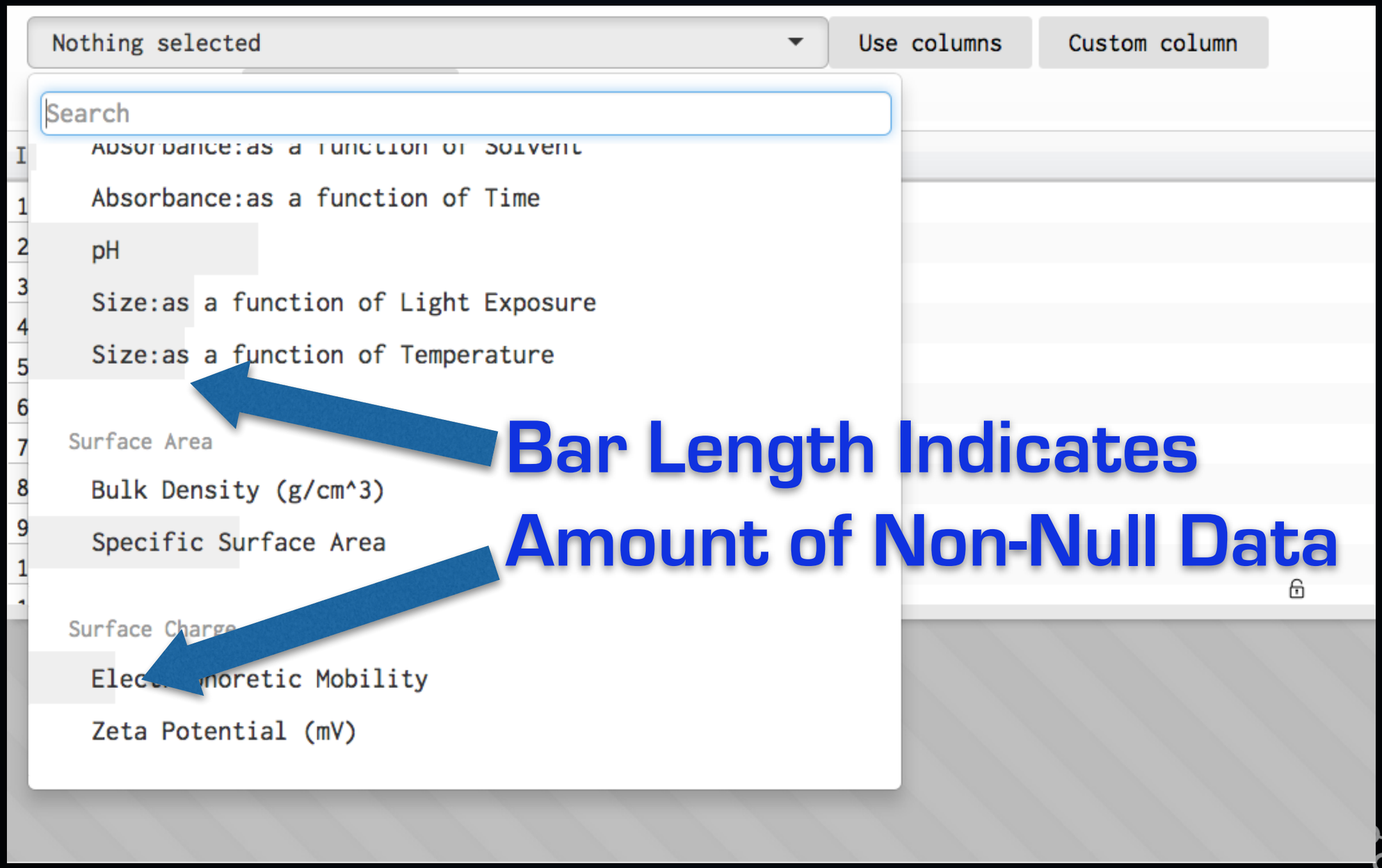
Exploration

IDENT: Partnership with Nanomaterial Registry

Interactive **D**ata **E**xploration & **N**avigation **T**ool for **N**ano **T**echnology



IDENT
Column Population Lookahead



IDENT
Column of Interest Selection

Nothing selected | Use columns | Custom column

288 total rows | Edit filters

Table of chosen data

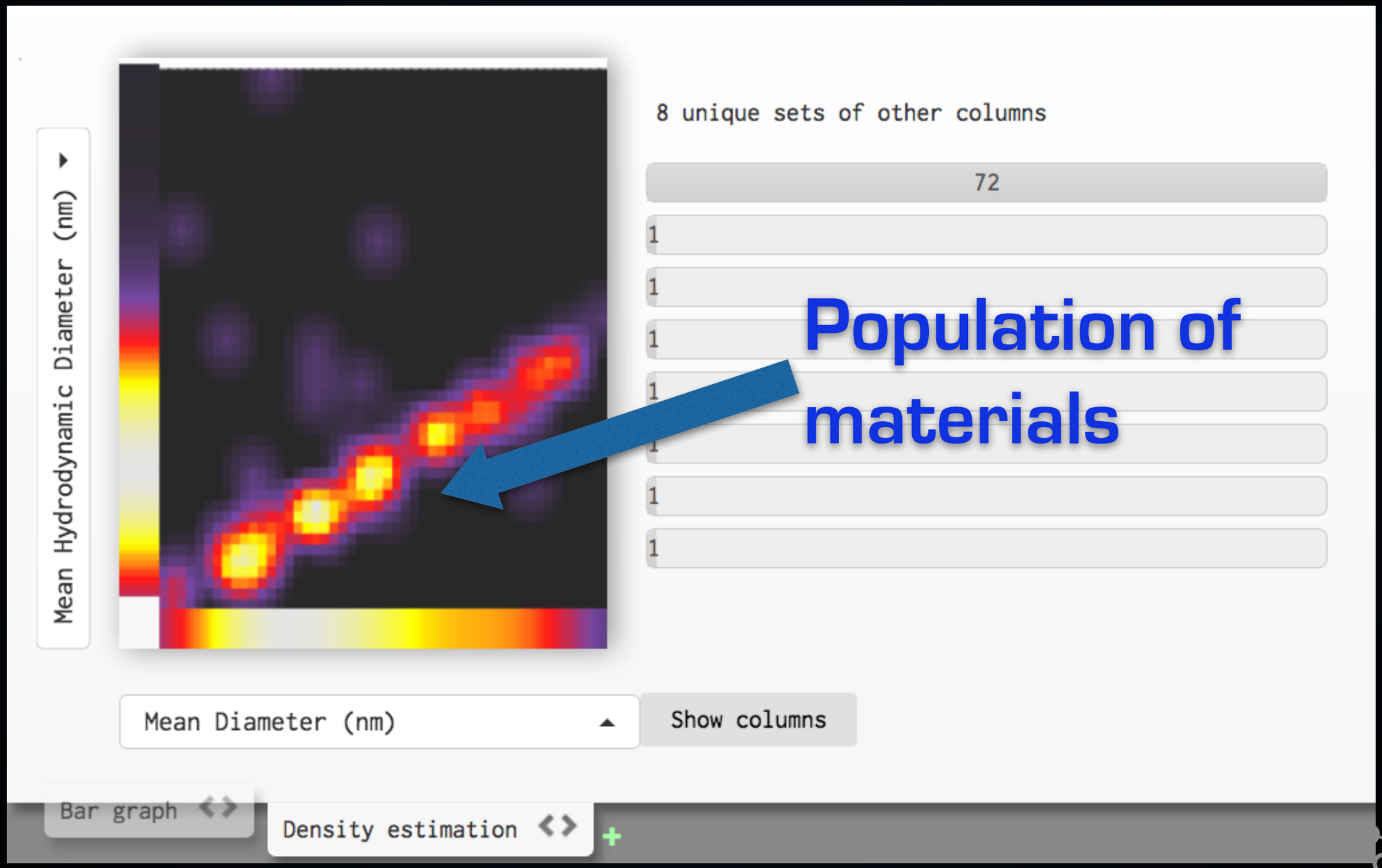
ID	Mean Diameter (nm)	Mean Hydrodynamic Diameter (nm)	DisplayName
6			Ag
7	7.2		Ag NP
8	20.8	32	Ag NP
9	29	39.6	Ag NP
10	43.4	47.6	Ag NP
11	41.9	43.1	Ag NP
12	49.1	59.2	Ag NP
13	53.5	57.1	Ag NP
14	57.7	68.3	Ag NP
15	8.2		Ag NP
16	19.2		Ag NP

Nanomaterials Registry Dataset

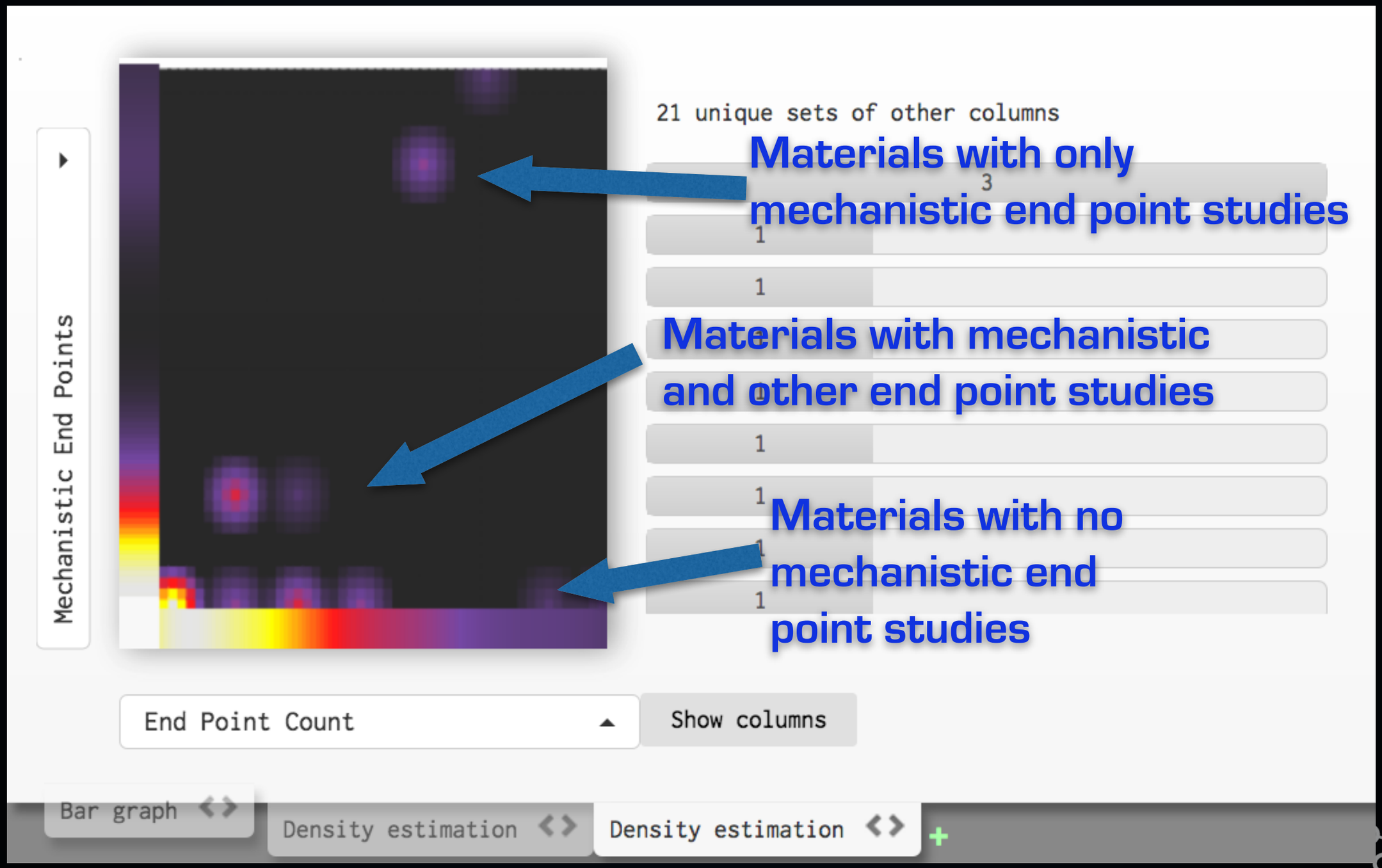
Visualize Content

Add a visualization +

IDENT
Visualization of Content



IDENT
Visualization of Knowledge

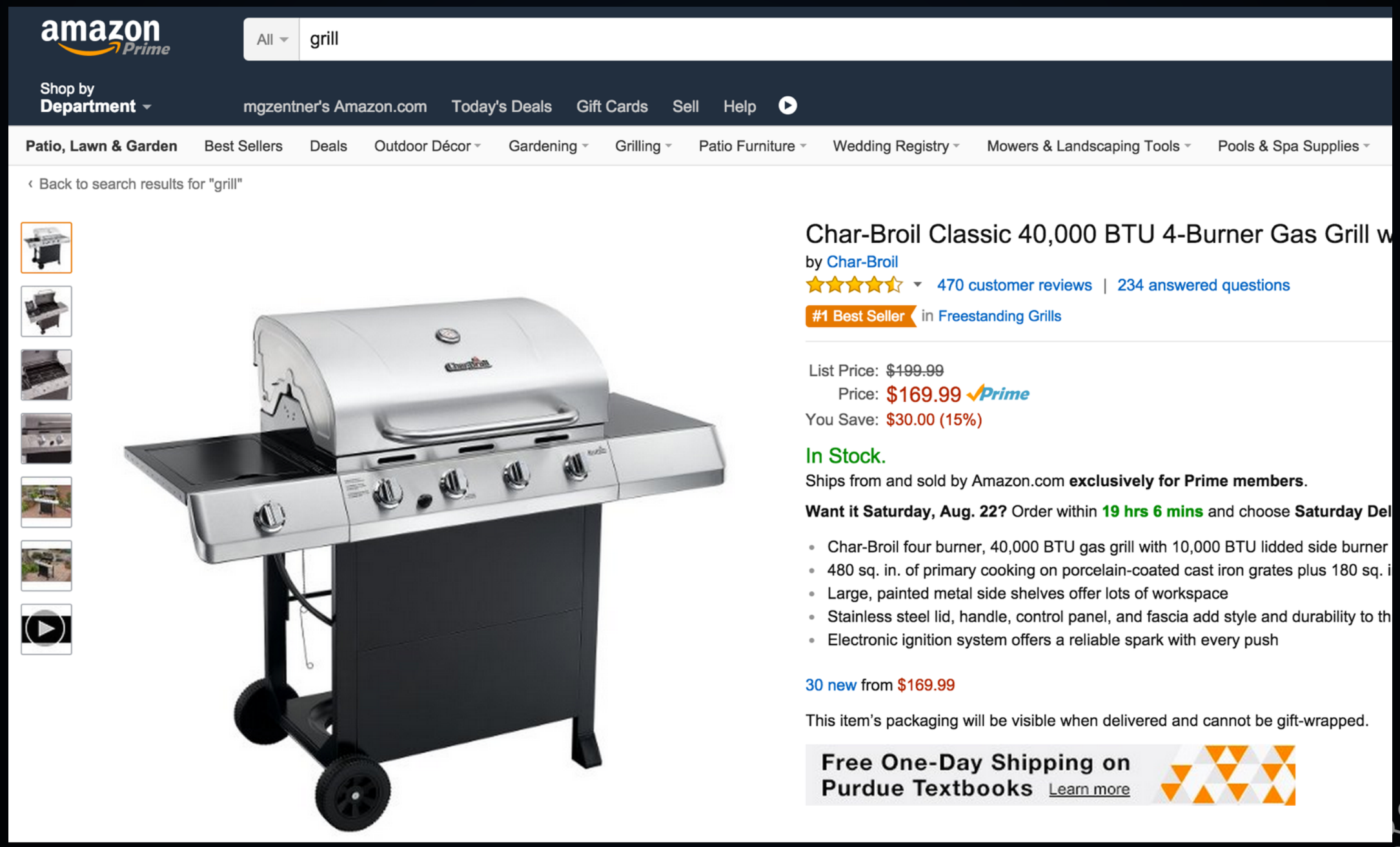


Lesson Digression

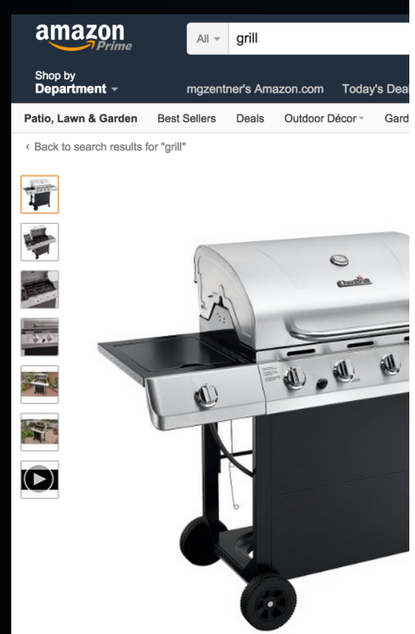
Ongoing Project:

Use Your Users to Help Each Other

Data About How People Use Data



Data About How People Use Data



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Coffee Coals Charcoal

by Coffee Coals

5 customer reviews

#1 New Release in Charcoal Starters

Price: $6.15 Prime

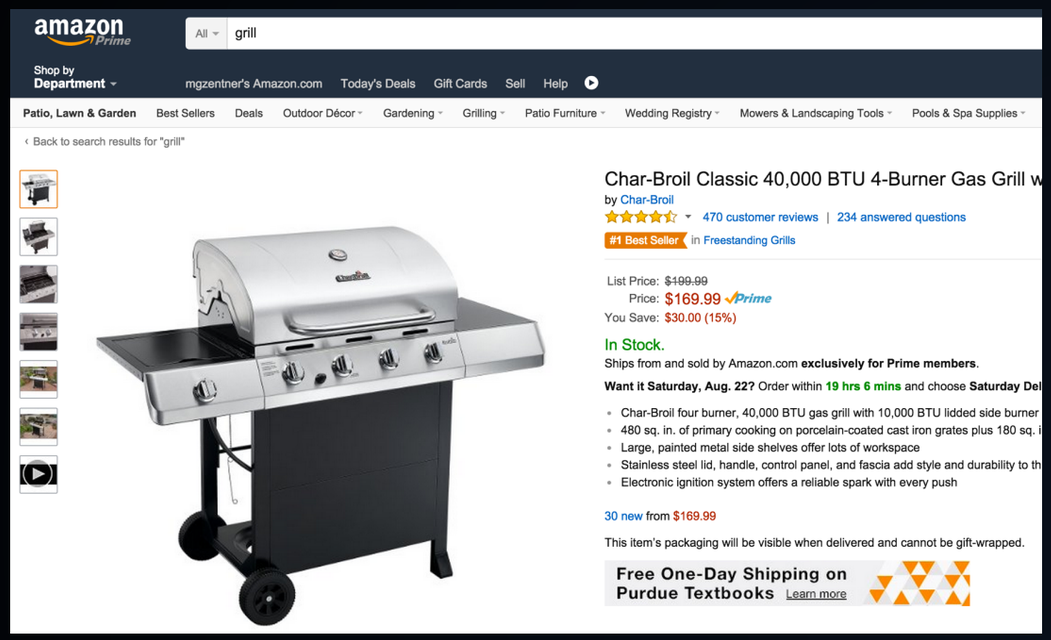
In Stock.

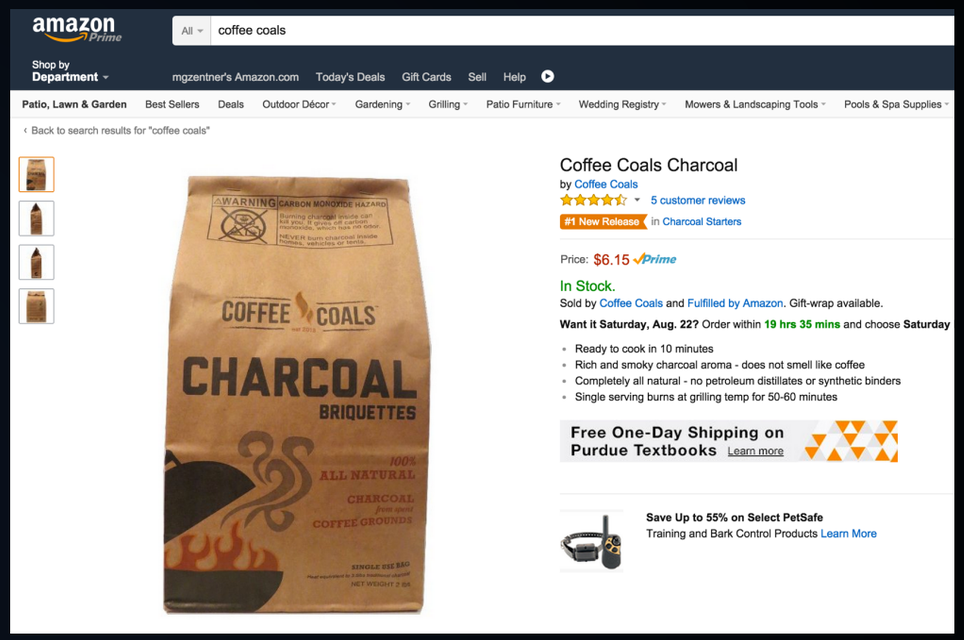
Sold by Coffee Coals and Fulfilled by Amazon. Gift-wrap available.

Want it Saturday, Aug. 22? Order within **19 hrs 35 mins** and choose **Saturday**

- Ready to cook in 10 minutes
- Rich and smoky charcoal aroma - does not smell like coffee
- Completely all natural - no petroleum distillates or synthetic binders
- Single serving burns at grilling temp for 50-60 minutes

Data About How People Use Data



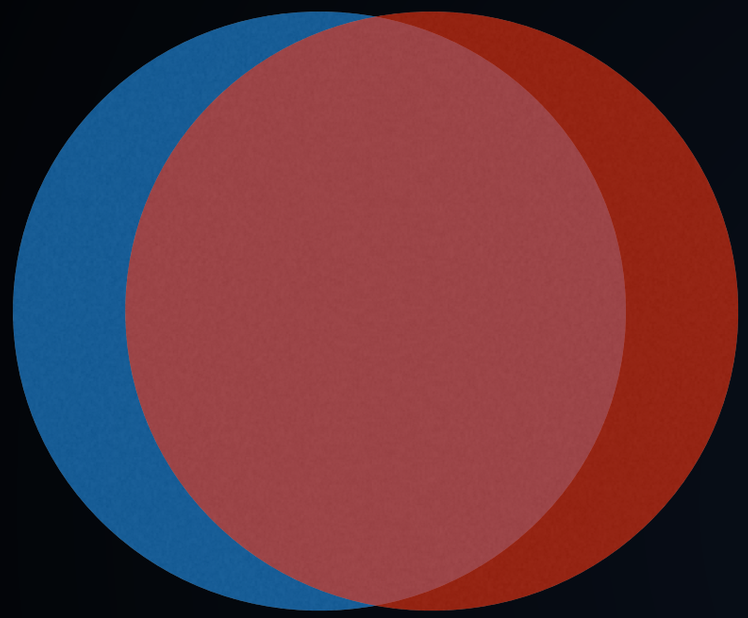


Pat LaFrieda Aged Ribeye,
500 F,
15g seasoning,
4 minutes on a side,
10 minute rest…

This is exactly the kind of information watching our users explore can tell us!

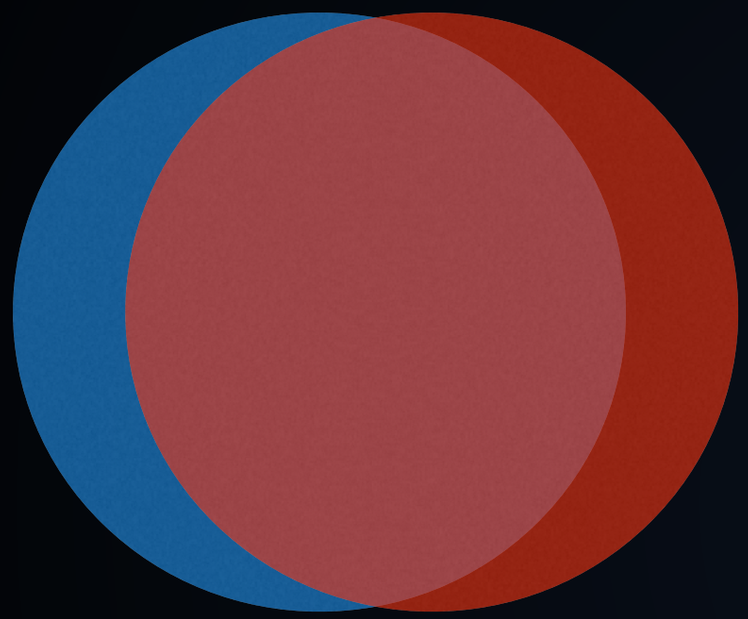
The Study of How People Study Data

The Study of How People Study Data

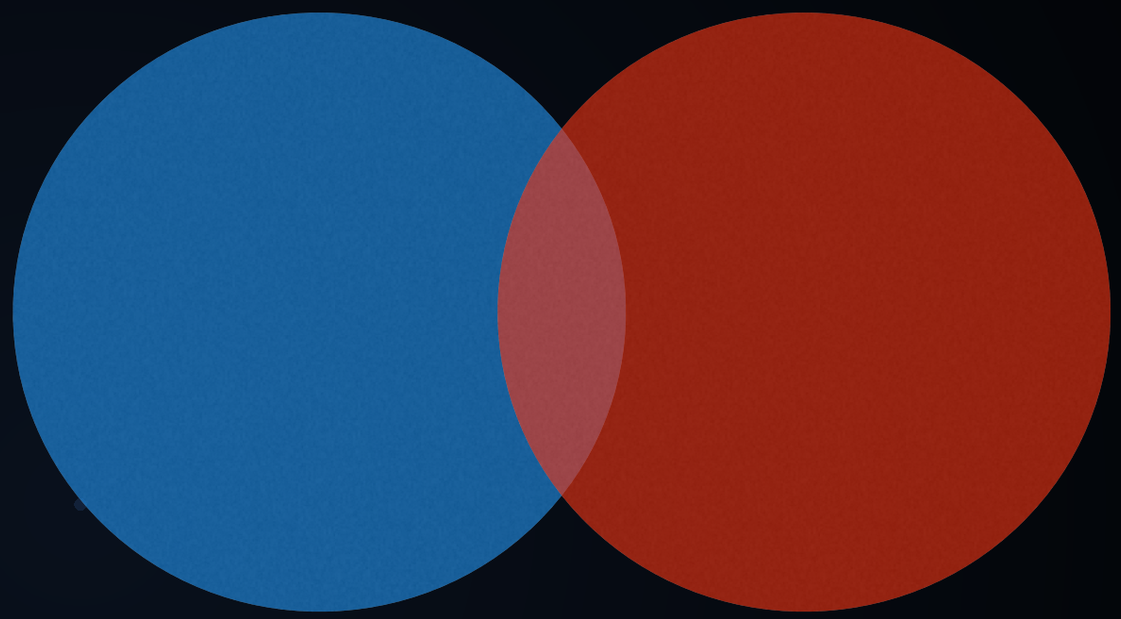


Small Digressions

The Study of How People Study Data

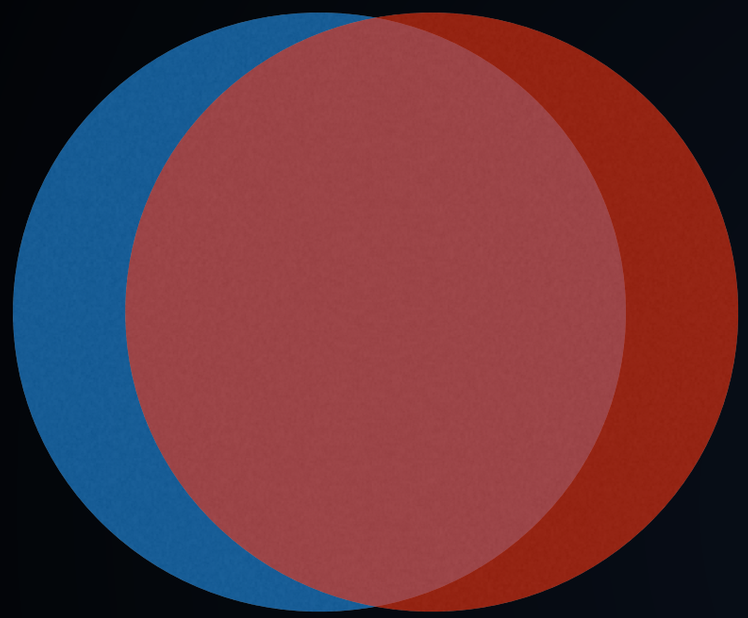


Small Digressions

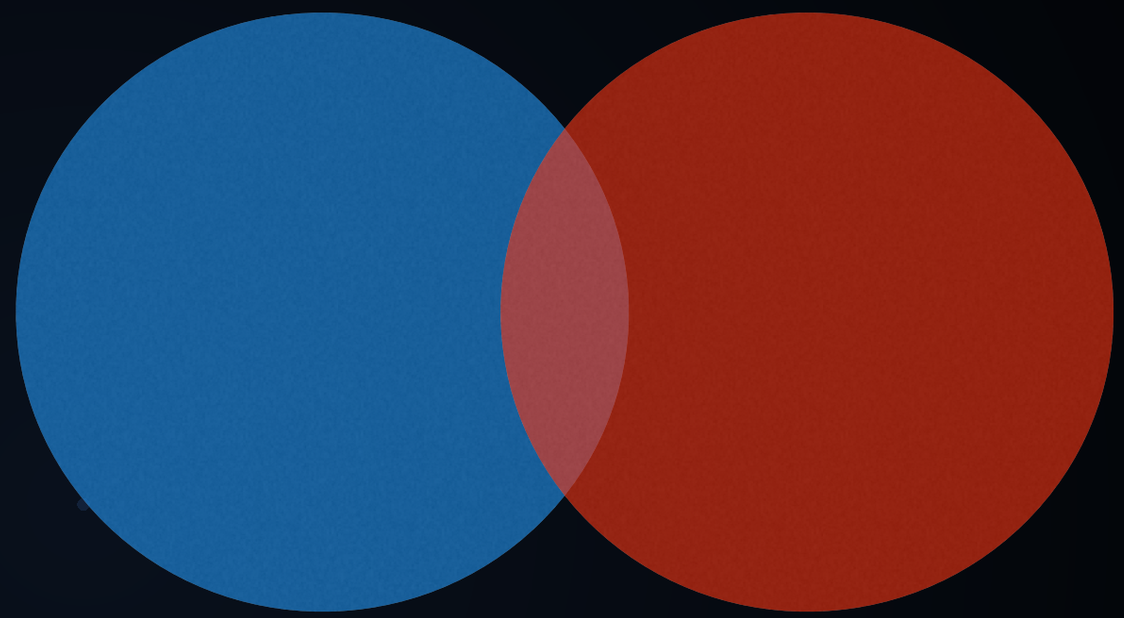


New Directions

The Study of How People Study Data



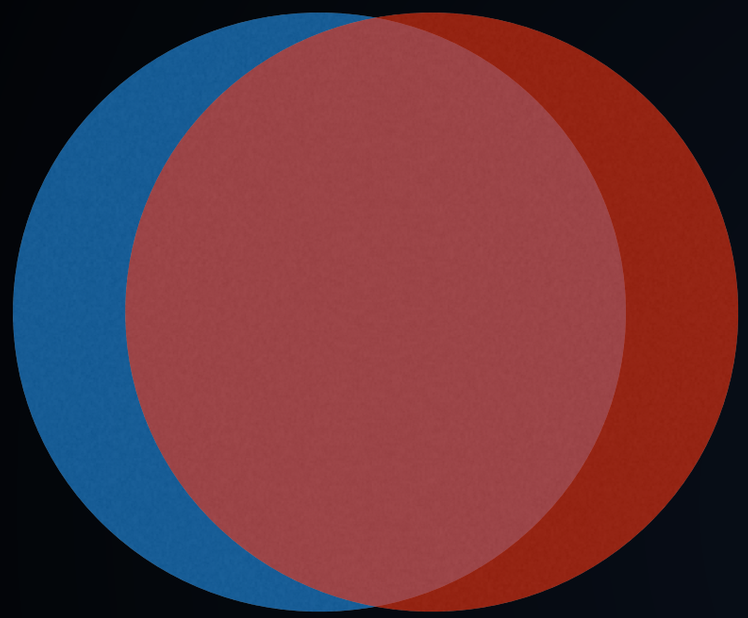
Small Digressions



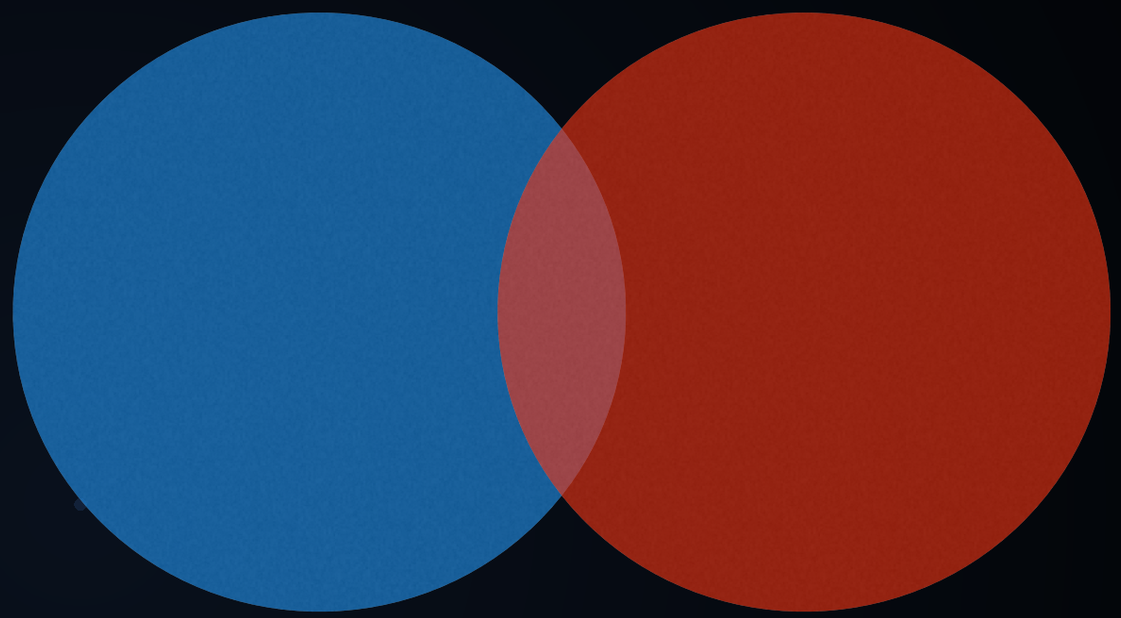
New Directions

New Fields

The Study of How People Study Data



Small Digressions



New Directions

New Fields

????

Lesson 7

Begin Thinking About Sustainability Early

The Difference a Year Makes

$Year_i$:

"We are working on the following for sustainability..."

"Why are you telling us about sustainability when you have N years left?"

(Experience from startups tells us that you have 2 years to try a business model. That's N/2 tries.)

$Year_{i+1}$:

"In the next N-1 years..."

"Why do you assume you have N-1 years? You should look at how to become sustainable."

Lesson 8

Assemble the Right Team

NSF: Lynn Preston, Eduardo Misawa, Keith Roper

- Mark Lundstrom
- Gerhard Klimeck
- Michael McLennan
- Gerry McCartney
- George Howlett
- Alejandro Strachan
- Shawn Rice
- Betsy Hillery
- Steve Clark
- Derek Kearney
- Ben Haley
- Chris Smoke
- Alissa Nedossekina
- Nick Kisseberth
- Steve Snyder
- Nathan Denny
- Dwight McKay
- Sam Wilson
- Rick Kennell
- David Benham
- Pascal Meunier
- Kevin Wojkovich
- Martin Hunt
- Ilya Shunko
- Lynn Zentner
- Tanya Faltens
- John Wright
- Vicky Johnson
- Israa Bukhari
- Swaroop Samek
- Jeff Turkstra
- Leslie Schumacher
- Emily Kayser
- Erich Huebner
- Nikki Huang
- Vicky Farnsworth

A Few Events

HUBbub 2015

14-16 Sept, 2015

Sheraton Indianapolis City Center Hotel

http://hubzero.org/hubbub

nanoHUB Users Conference

31 August - 1 September

Purdue University

In conjunction with International Workshop on Computational Electronics

https://nanohub.org/groups/conference

HUBzero - Sustainable Manufacturing Activities?