

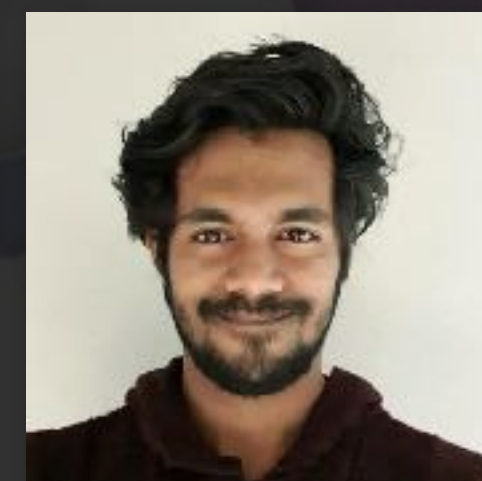
SFO in Advanced Functional Materials (AFM)
at LiU

SMALL CELLS ON LARGE GPUS:

SCALING SMALL CELL CALCULATIONS EFFICIENTLY ON MODERN GPUS

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Head of the Physics at Extreme Conditions Unit
Honorary Fellow of the University of Edinburgh



**Abhijith S
Parackal**



**Rickard
Armiento**



**Dominique
Laniel**

Experimental
Collab.

2026-10-07

We need new sustainable materials with advanced functionalities for many applications !

Hydrides

Chemical hydrogen storage
High-T superconductors

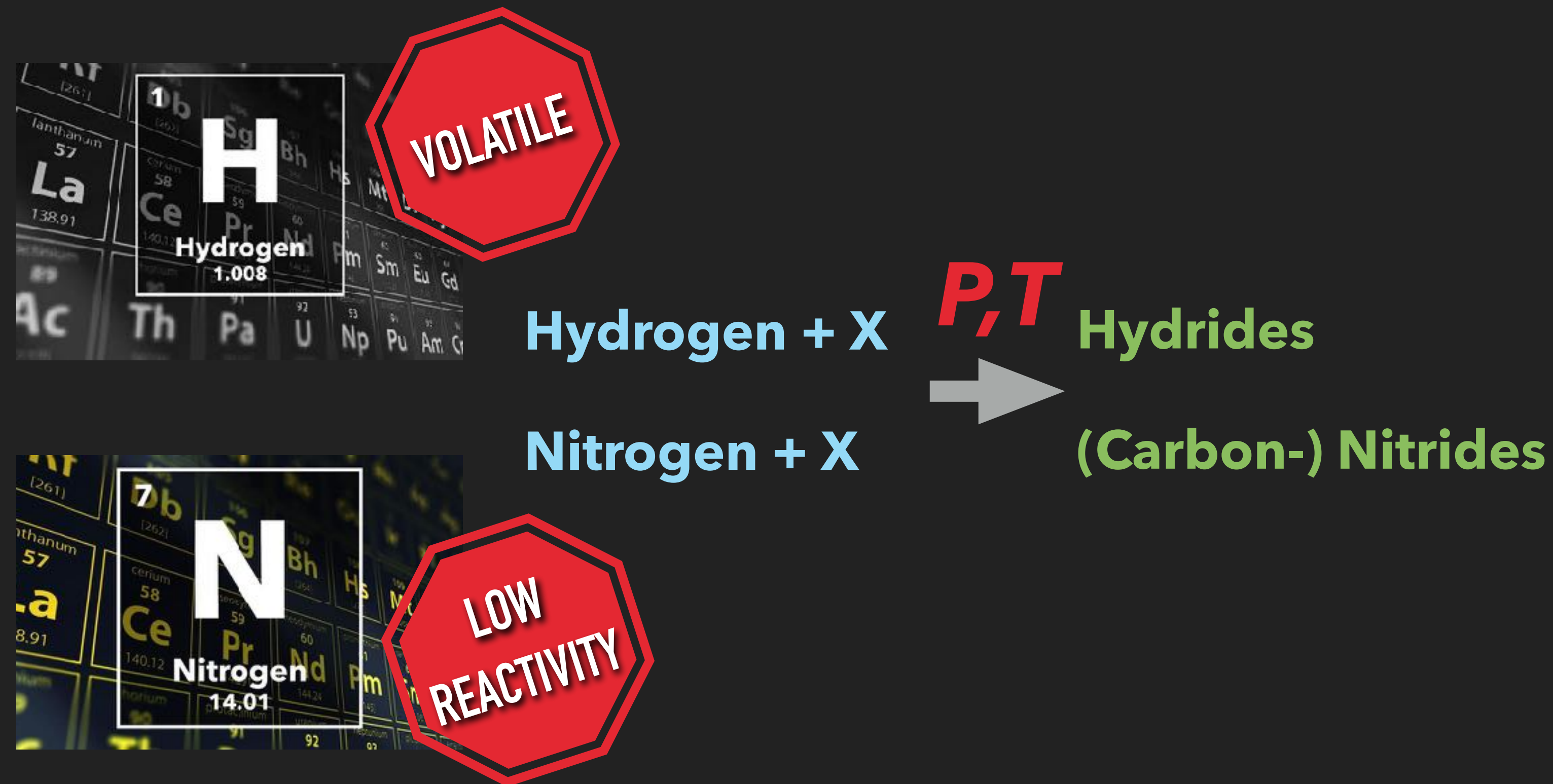
**ONLY
LIMITED NUMBER
OF COMPOUNDS
KNOWN!**

(Carbo-) Nitrides

Superhard materials
Wide bandgap semiconductors

High melting temperature
High energy density (HED)
Piezoelectric
Photovoltaics
Optical applications

CREATING NEW COMPOUNDS?



Complex chemistry

Small amounts
synthesized at high- P

Limited experimental
analysis possible after
synthesis

**SYNERGY BETWEEN
THEORY AND
EXPERIMENT!**

NITRIDES:C-N

1989

Science

Prediction of New Low Compressibility Solids

AMY Y. LIU AND MARVIN L. COHEN [Authors Info & Affiliations](#)

SCIENCE • 25 Aug 1989 • Vol 245, Issue 4920 • pp. 841-842 • DOI: 10.1126/science.245.4920.841

“[...] we suggest that it may be possible to synthesize a **covalent C-N solid** such as $\beta\text{-C}_3\text{N}_4$ with compressibility comparable to diamond.”

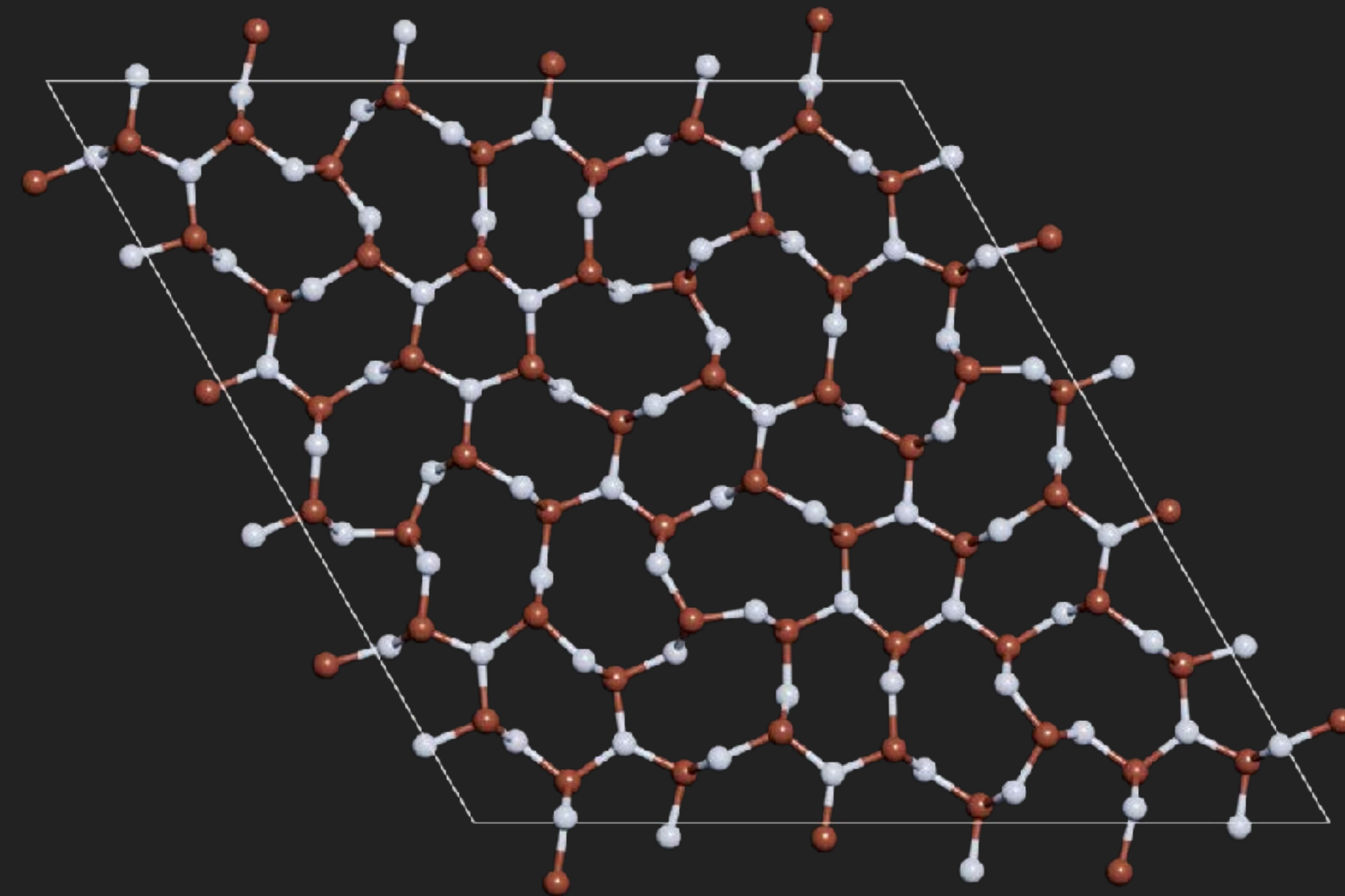
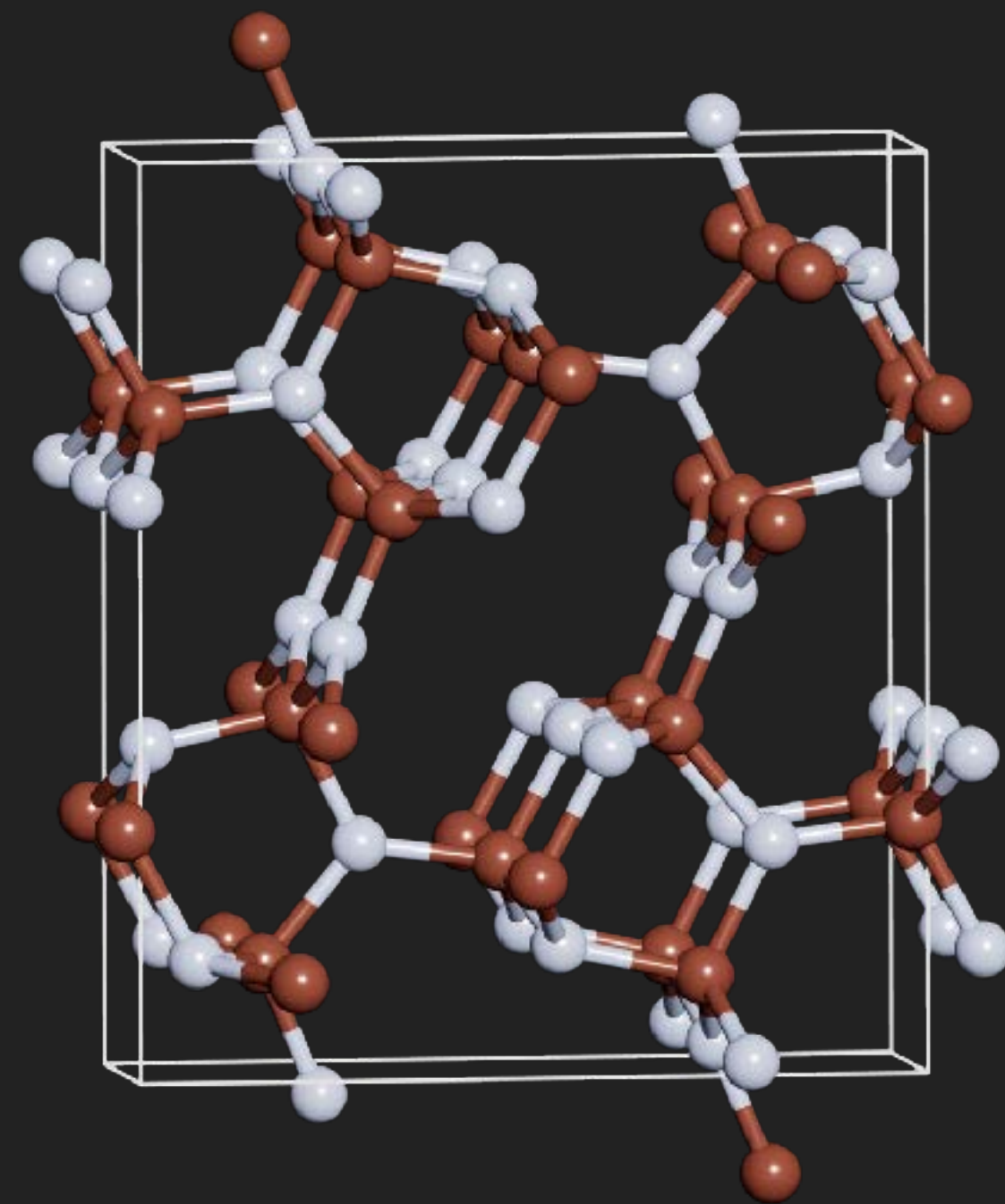
No synthesis until 2016. Compound decomposed <11 GPa

Very different predictions!

SYNTHESIS OF POLYMERIC CARBON NITRIDES

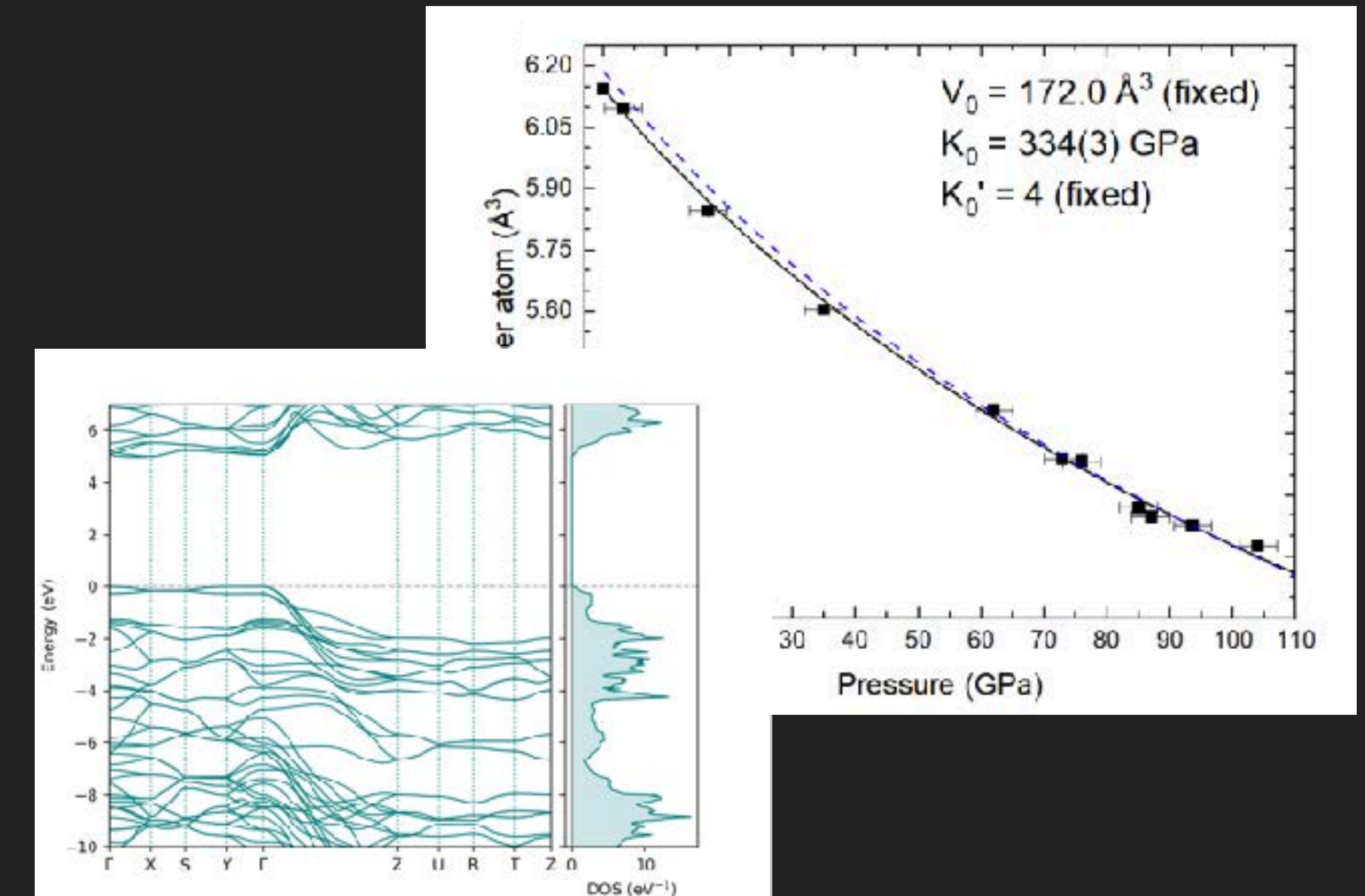
Synthesis and characterization of **five recoverable polymeric C-N compounds** at high P!

*t*l14-C₃N₄, *h*P126-C₃N₄, *t*l24-CN₂, *o*P28-C₃N₄ and *o*P8-CN

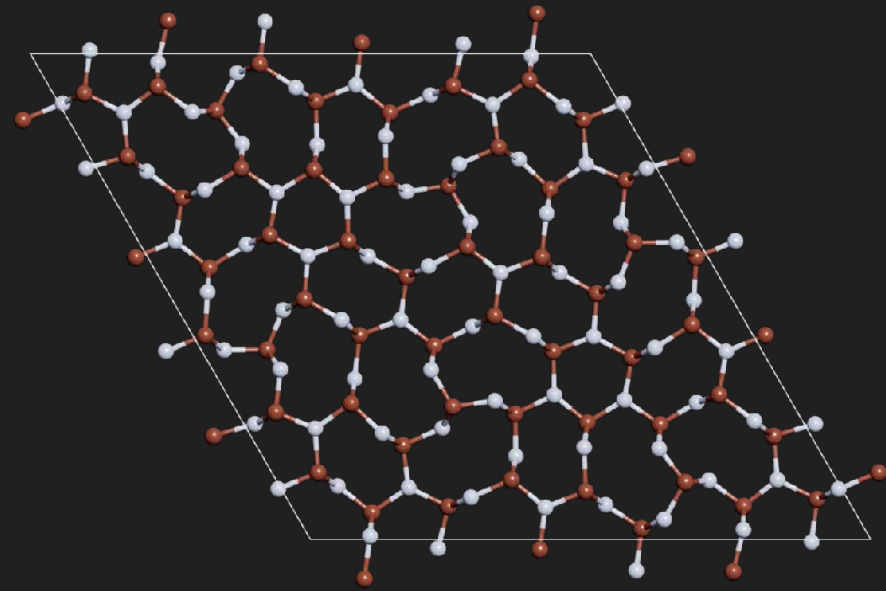


MULTIPLE PROMISING PROPERTIES

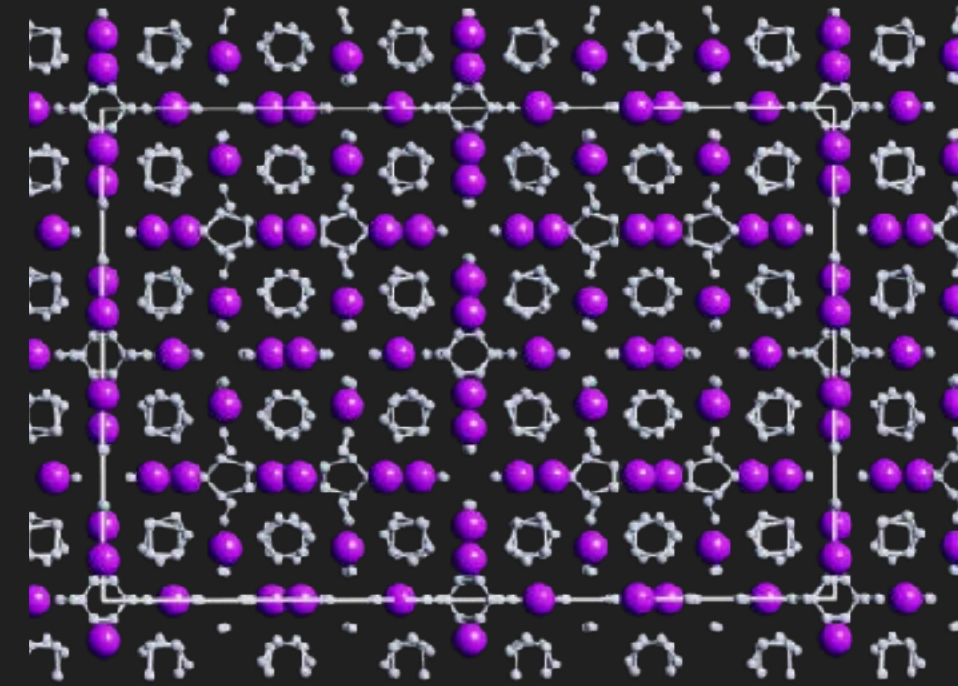
	K (GPa)		Microscopic hardness (GPa)	Macroscopic hardness (GPa)	Bandgap HSE (eV)
	Exp.	Calc.			
c-BN	395(2)	398	63.2	63.1 – 68.3	6.1
Diamond	446(1)	440	89.2	92.9	5.5
oP8-CN	365(9)	344	78.0	53.4	5.3
t/24-CN ₂	419(8)	401	86.8	50.0	5.4
t/14-C ₃ N ₄	383(9)	377	80.4	52.9	4.3 (d)
hP126-C ₃ N ₄	417(6)	383	80.8	49.9	4.4 (d)
oP28-C ₃ N ₄	334(3)	323	79.7	47.5	5.0 (d)



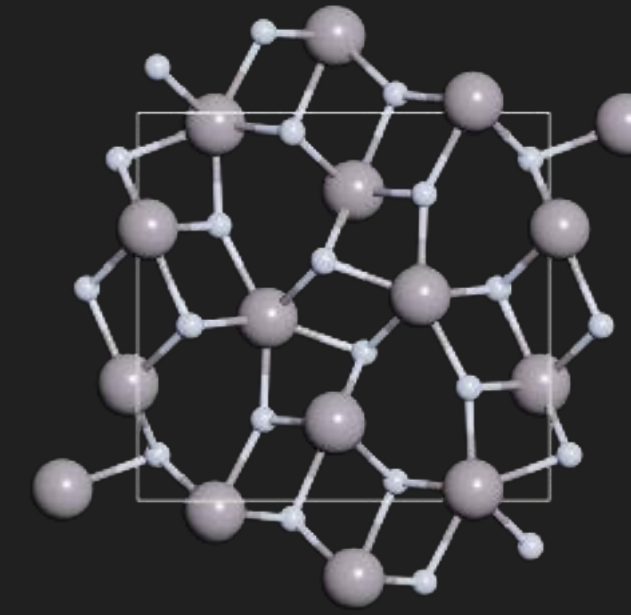
- (1) High incompressibility
- (2) High calculated hardness
- (3) High calculated fracture toughness
- (4) Wide (direct) bandgap
- (5) Piezoelectric response

$hP126-C_3N_4$


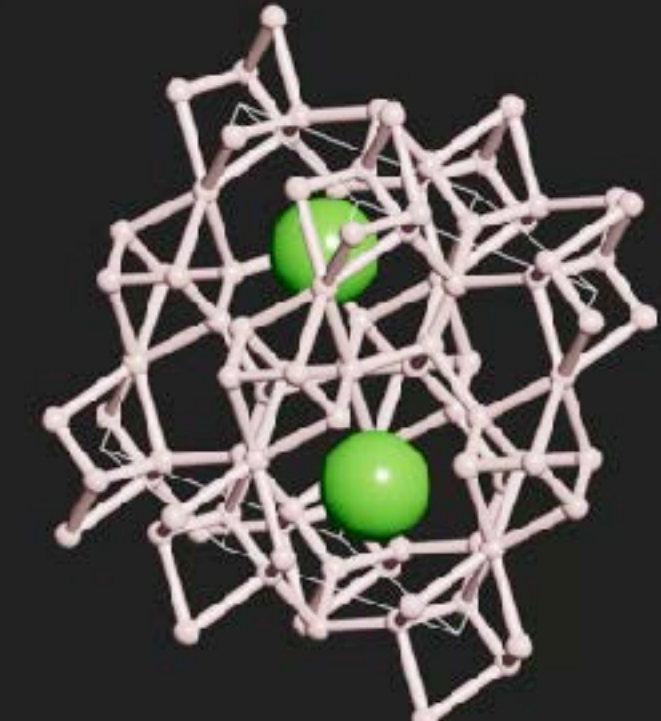
Laniel, Trybel, et al. (2024).
Advanced Materials, 36(3), 2308030.

 K_9N_{56}


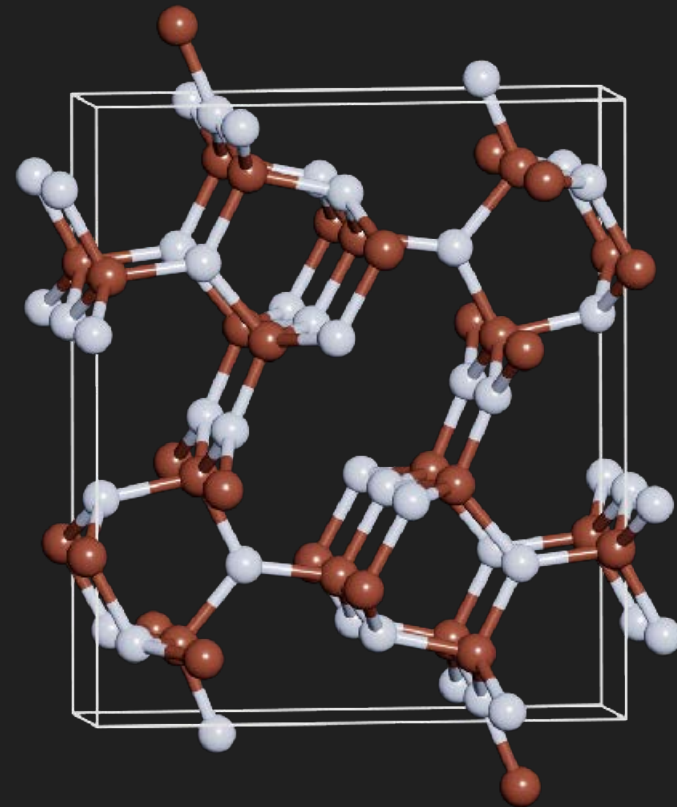
Laniel, Trybel et al. (2023). *Nat. Chem.* **15**, 641–646 (2023)

 W_2N_3


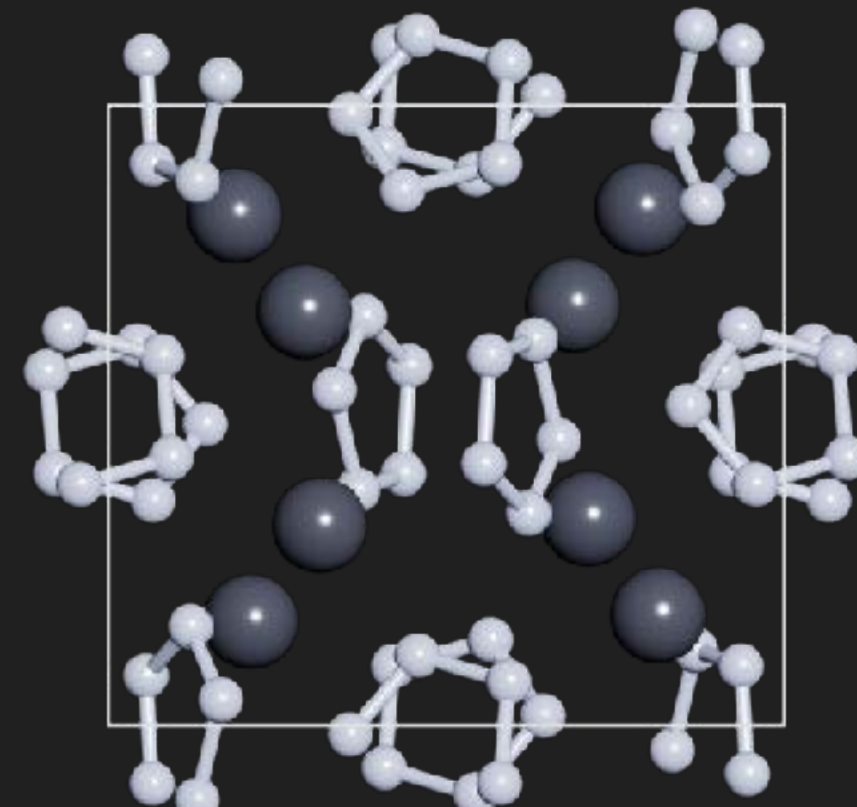
Liang, ..., Trybel & Laniel (2024).
Advanced Functional Materials, 2313819.

 LaH_9


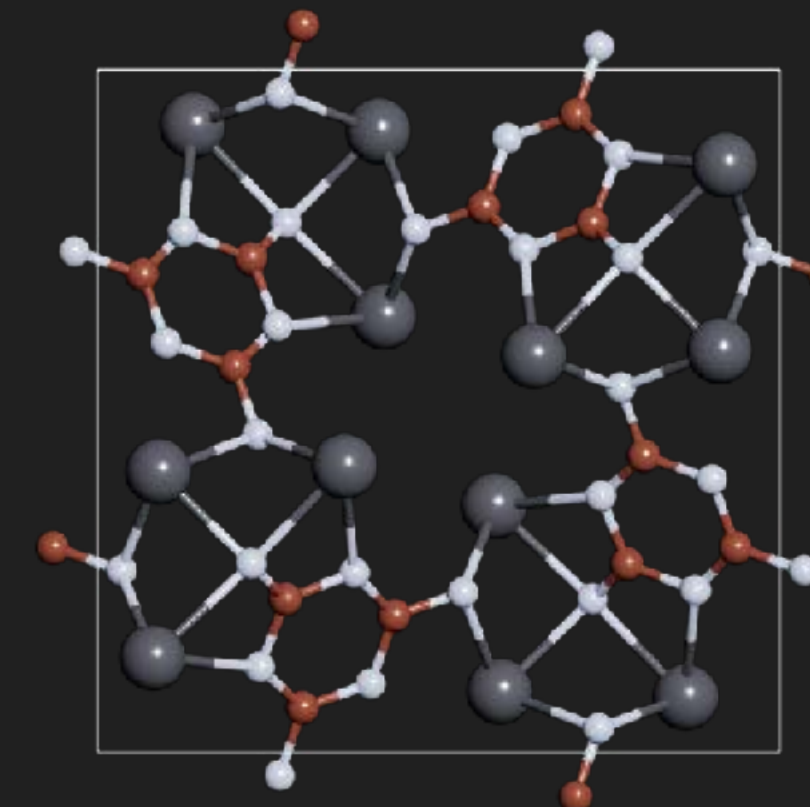
Laniel, Trybel, et al. (2022).
Nat. Comm., 13(1), 6987.


 $oP28-C_3N_4$

Laniel, Trybel, et al. (2024).
Advanced Functional Materials, 2416892.


 AgN_5

Liang, Trybel & Laniel (2026).
JACS Au, 6(1), 193–199.


 $hP72-Pb_3(C_3N_6)$

Ranieri,..., Trybel & Laniel (2025).
JACS, 147(39), 35431–35437.

and many more...

Enabled by
NAISS
resources!

Once we know the crystal
structure DFT
(& MLIPs) is in great agreement!

One clear “failure” was to restrict lattice
ratios and assume global minima!



Using what we learn
from high-pressure
experiments...

... for the
development of new
computational methods



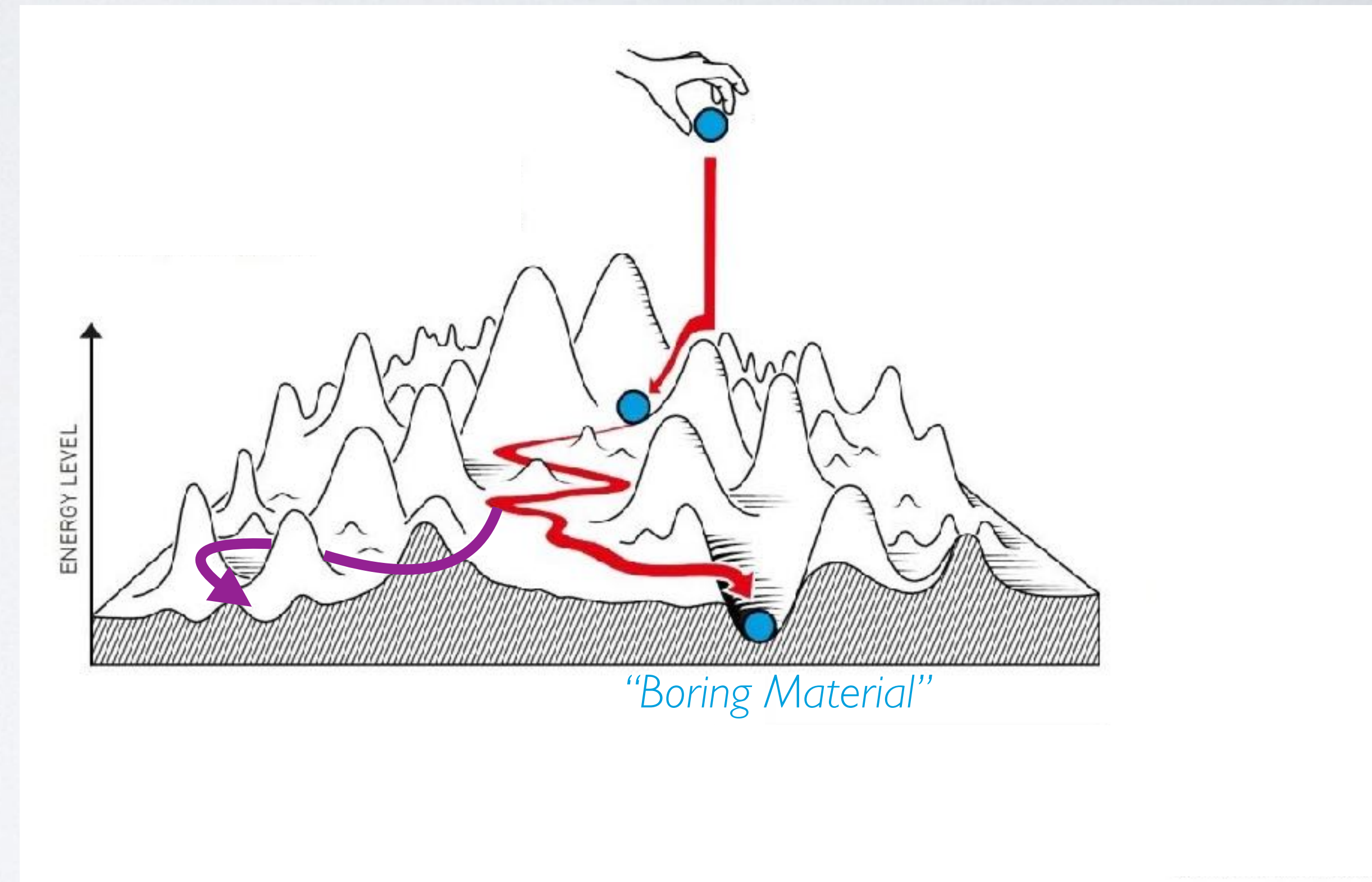
COMPUTATIONAL GOAL



COMPUTATIONAL GOAL



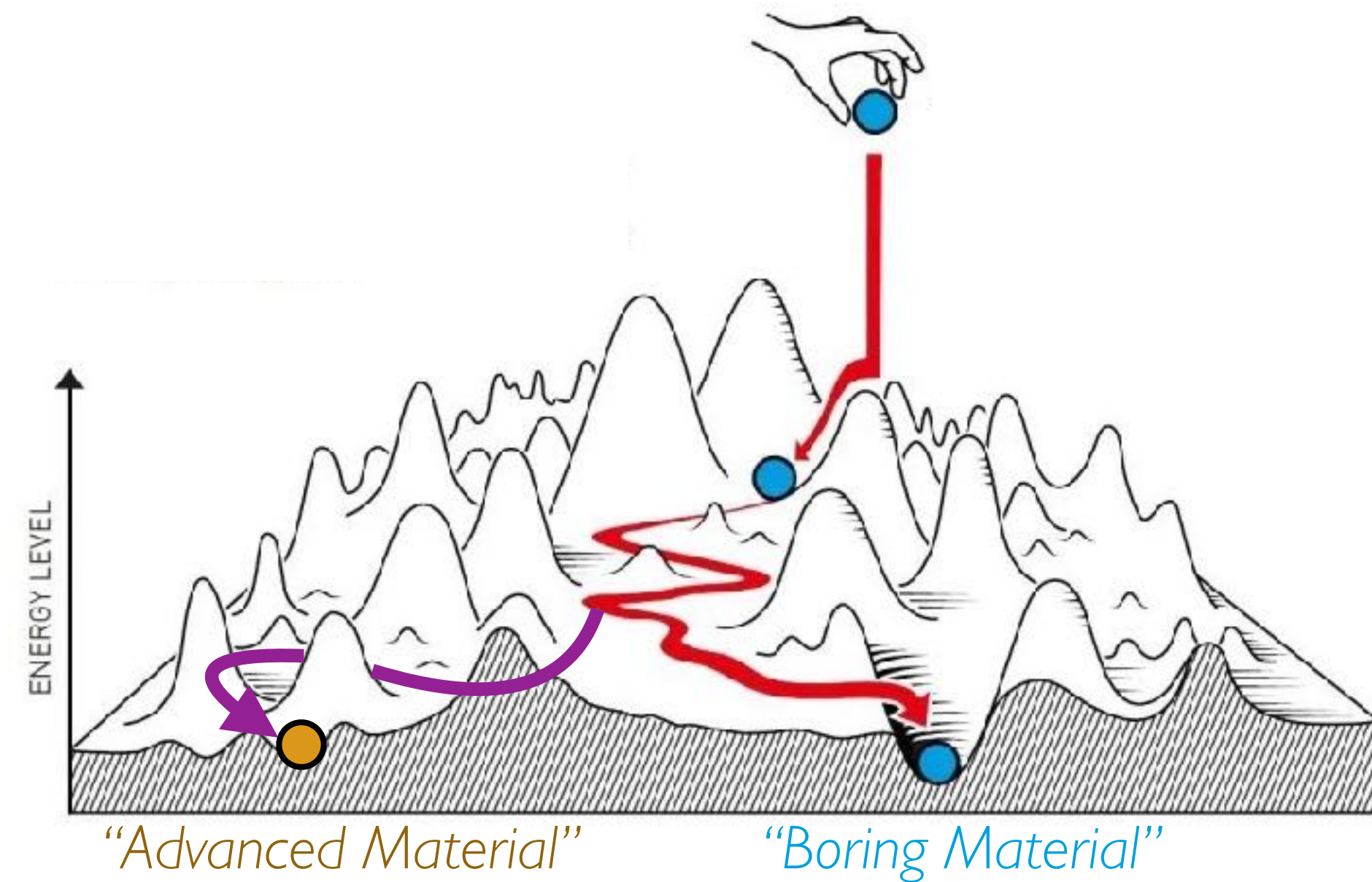
<https://www.nobelprize.org/prizes/physics/2024/popular-information/>



COMPUTATIONAL GOAL



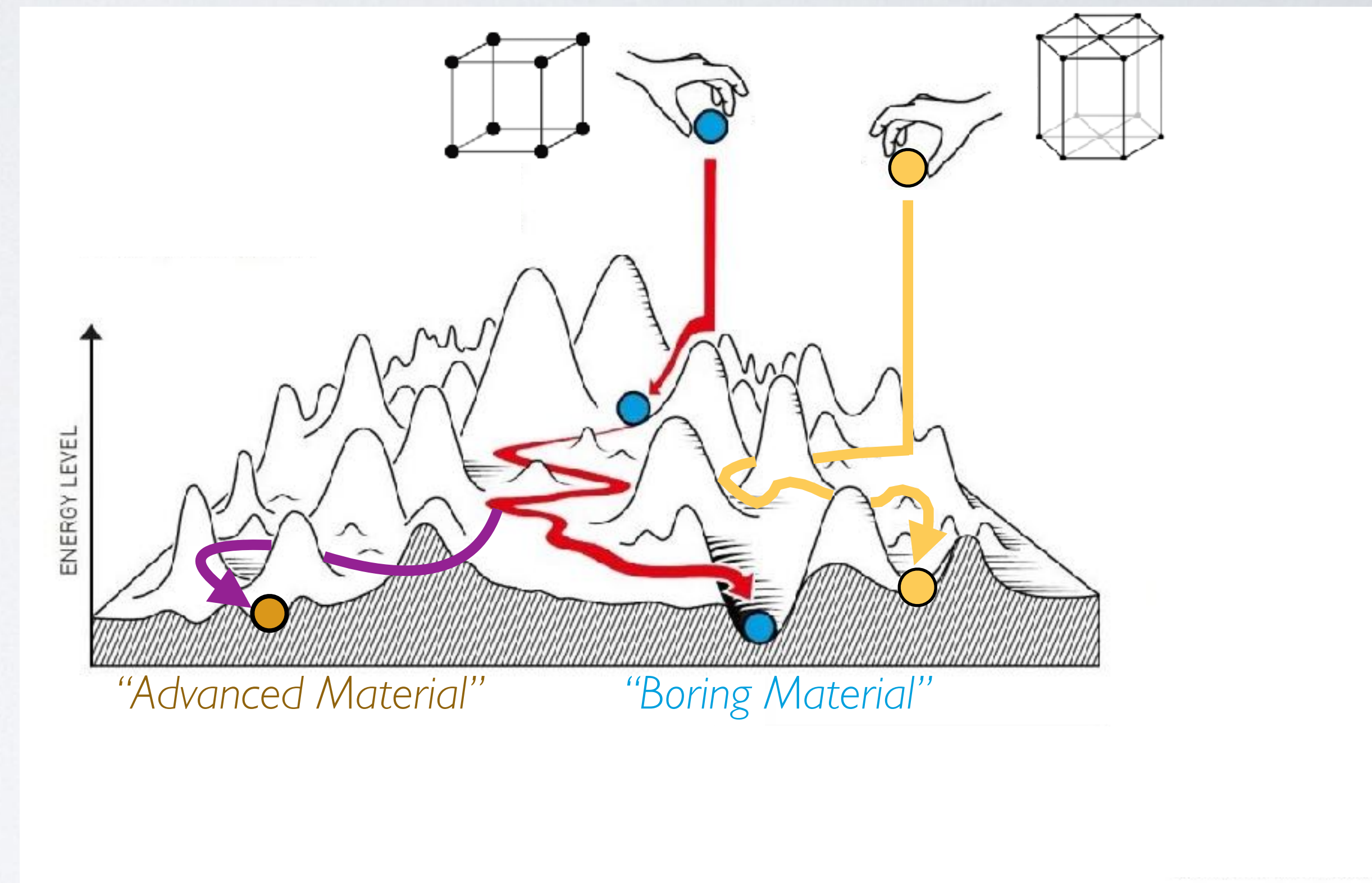
<https://www.nobelprize.org/prizes/physics/2024/popular-information/>



COMPUTATIONAL GOAL



<https://www.nobelprize.org/prizes/physics/2024/popular-information/>

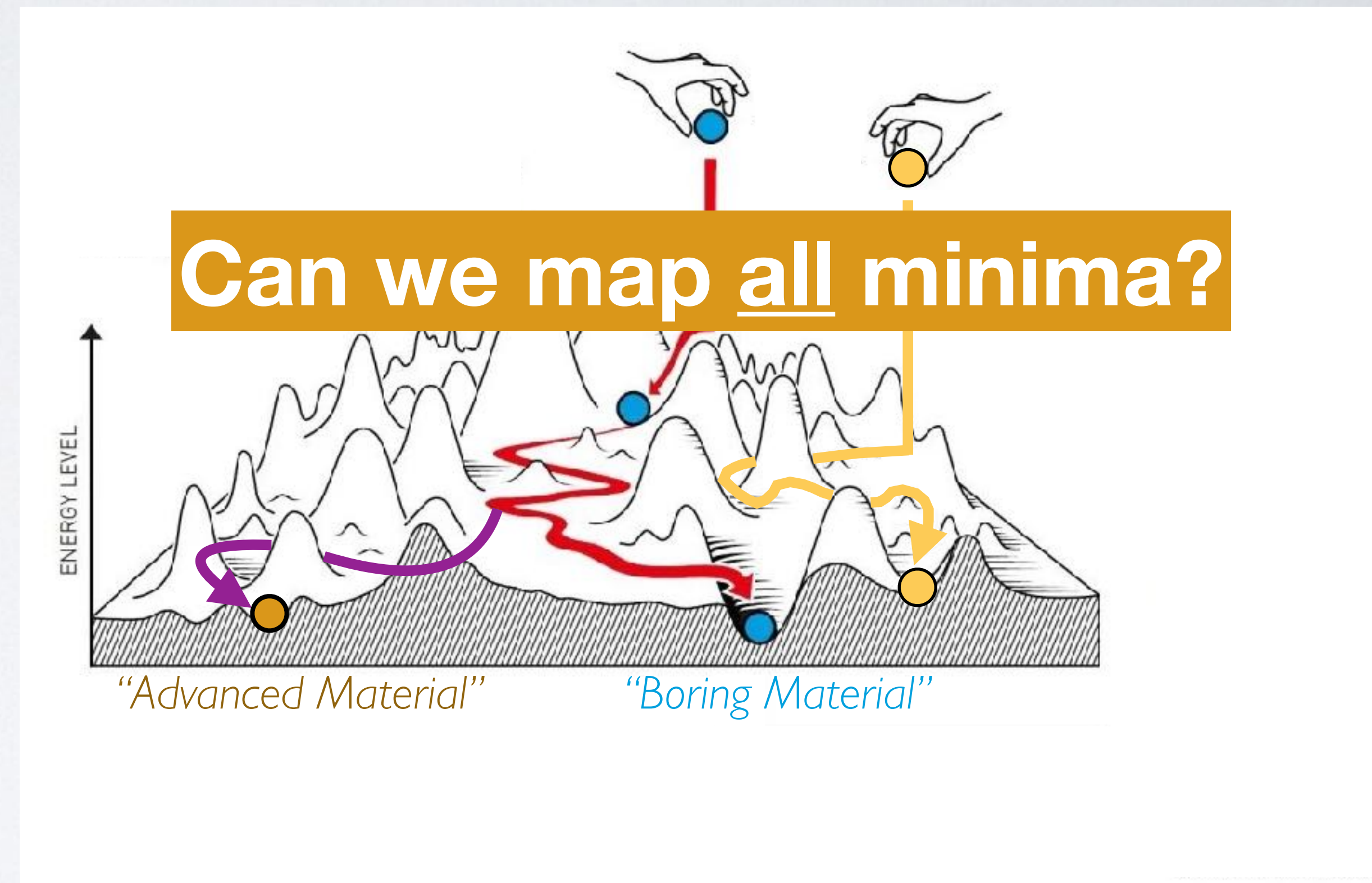


The path is important!
(All?) local minima are important

COMPUTATIONAL GOAL



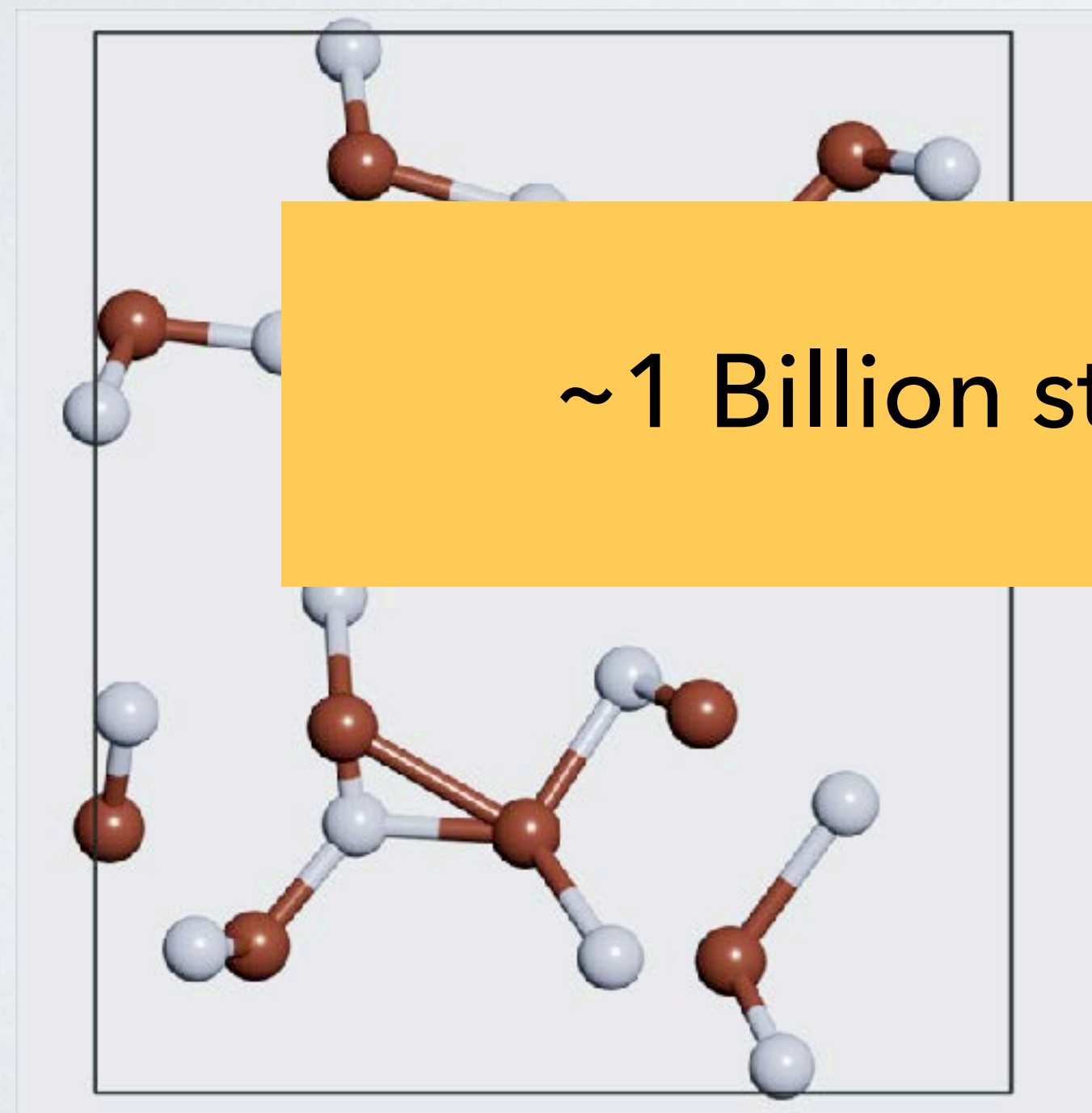
<https://www.nobelprize.org/prizes/physics/2024/popular-information/>



Start and path are important!
(All?) local minima are important

COMPUTATIONAL GOAL

Replace DFT with Machine learned interatomic potentials



Real Time!

<https://www.nobelprize.org/prizes/physics/2024/popular-information/>

Can we map all minima?

~1 Billion structure evaluations per day/per node

"Advanced Material"

"Boring Material"

Start and path are important!
(All?) local minima are important

SCREENING WYCKOFF POSITIONS SPACE

10 Atoms in the unit cell $\rightarrow 10 \cdot 3 + 6 = \underline{36 \text{ DOF}}$

Space group 84 (P4/m)

4 Wyckoff positions

Atomic Positions

Wyckoff	Element	x	y	z
1a	Na	0	0	0
1d	Na	1/2	1/2	1/2
4j	Cl	0.595425	0.79749	0
4k	Na	0.326112	0.885098	1/2

0 DOF

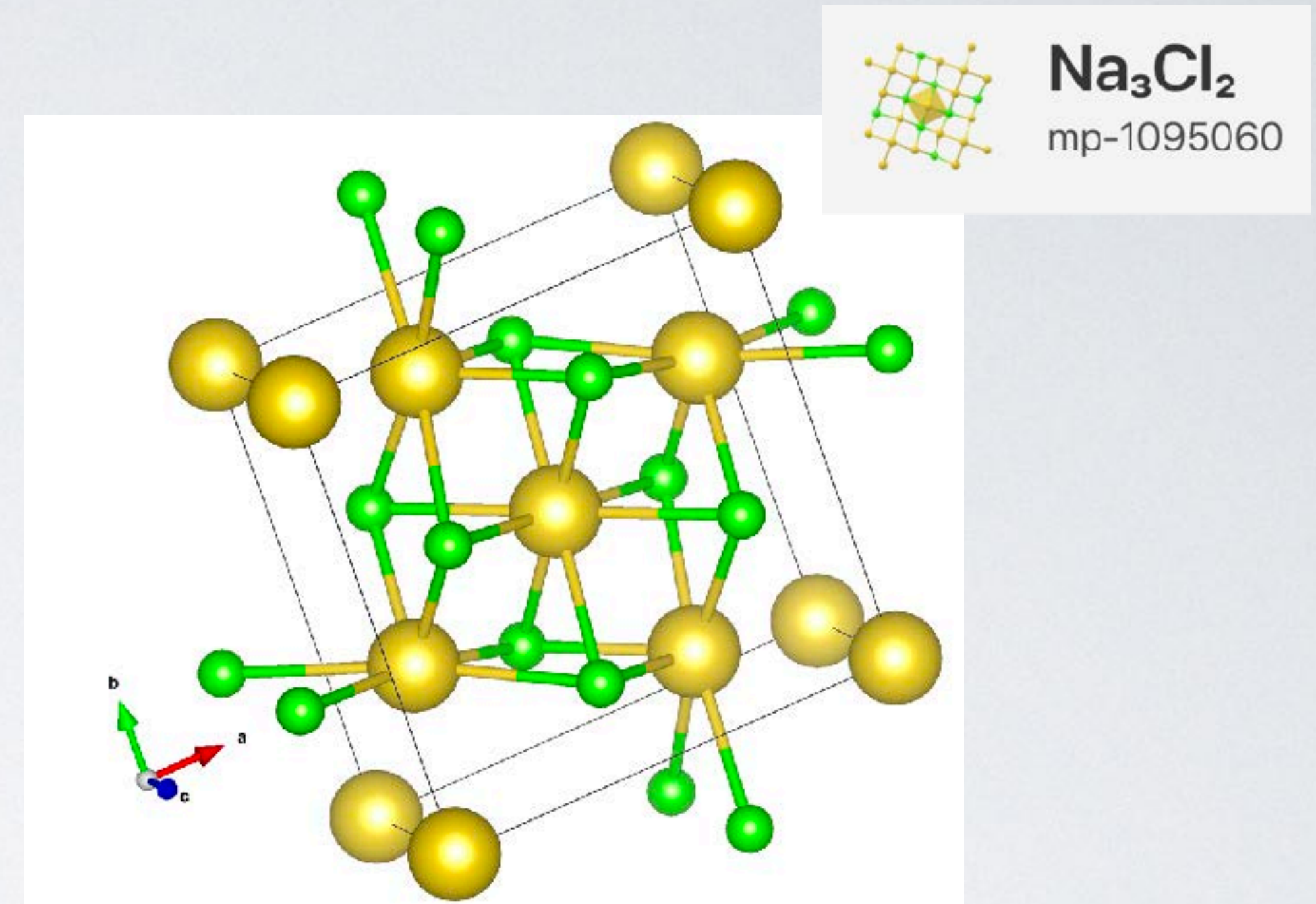
0 DOF

2 DOF

2 DOF

4+2 (tetragonal) DOF = 6 DOF

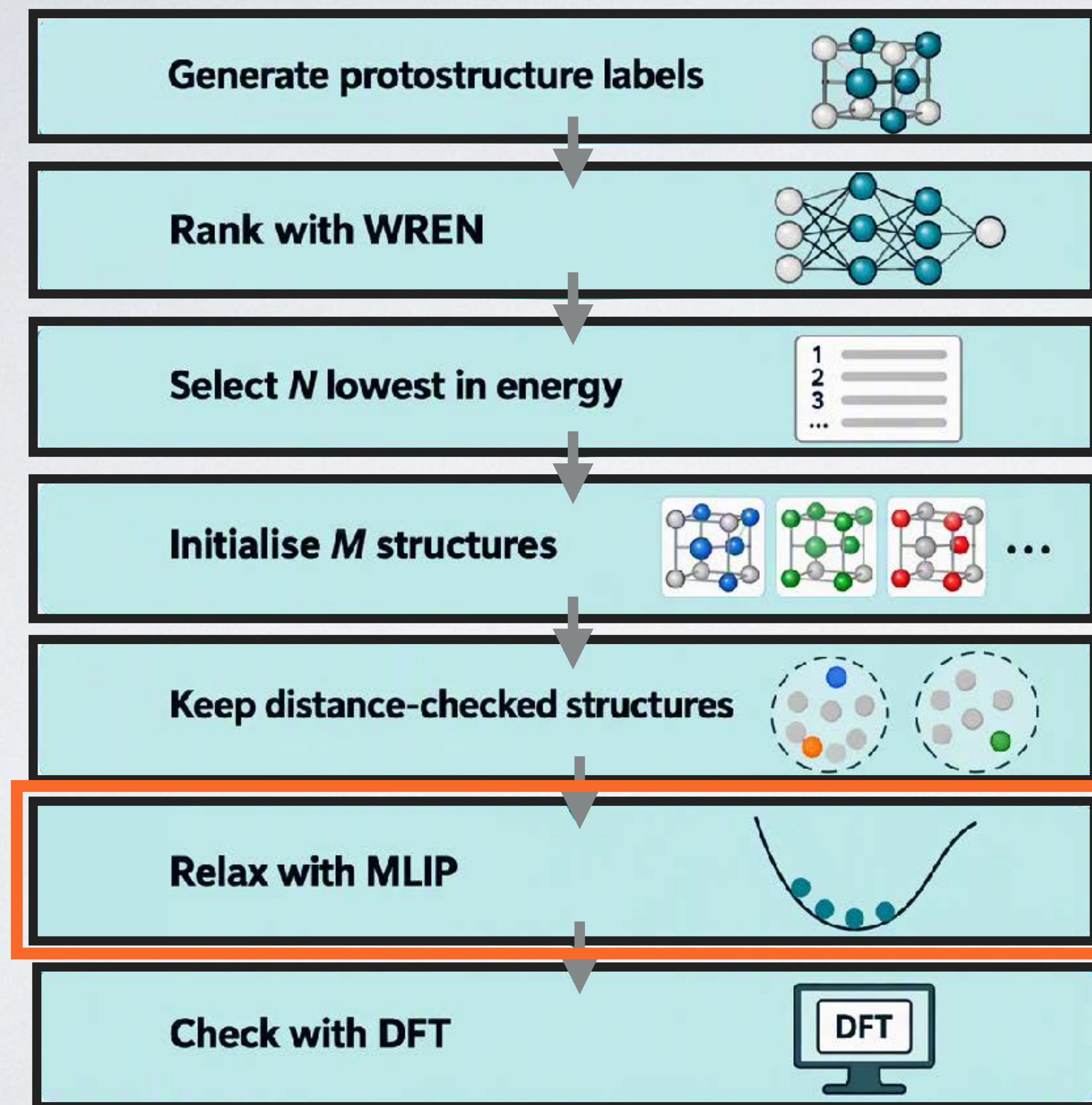
Reduce number of degrees of freedom (DOF) by sampling Wyckoff DOF instead of atomic



- **Anonymous chemical formula** (e.g., A₂B₃)
- **Pearson symbol** (e.g., oP28)
- **Spacegroup number** (e.g., 58)
- **Sequence of occupied Wyckoff letters** (e.g., ad_jk)

A₃B₂_oP28_58_jk_ad:Cl-Na

Enumerable coarse graining in
symmetry space



Precompute!

Very fast!

$N \gg 1000/\text{chemical system}$

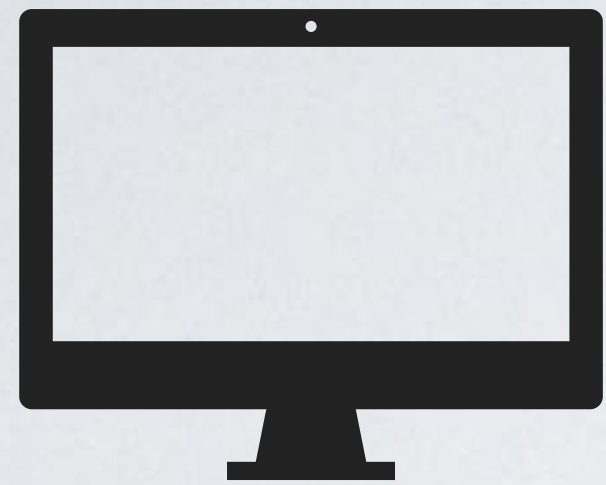
$M > 50000!$

$X > 100/\text{Protostructure}$

Suddenly
slow at scale

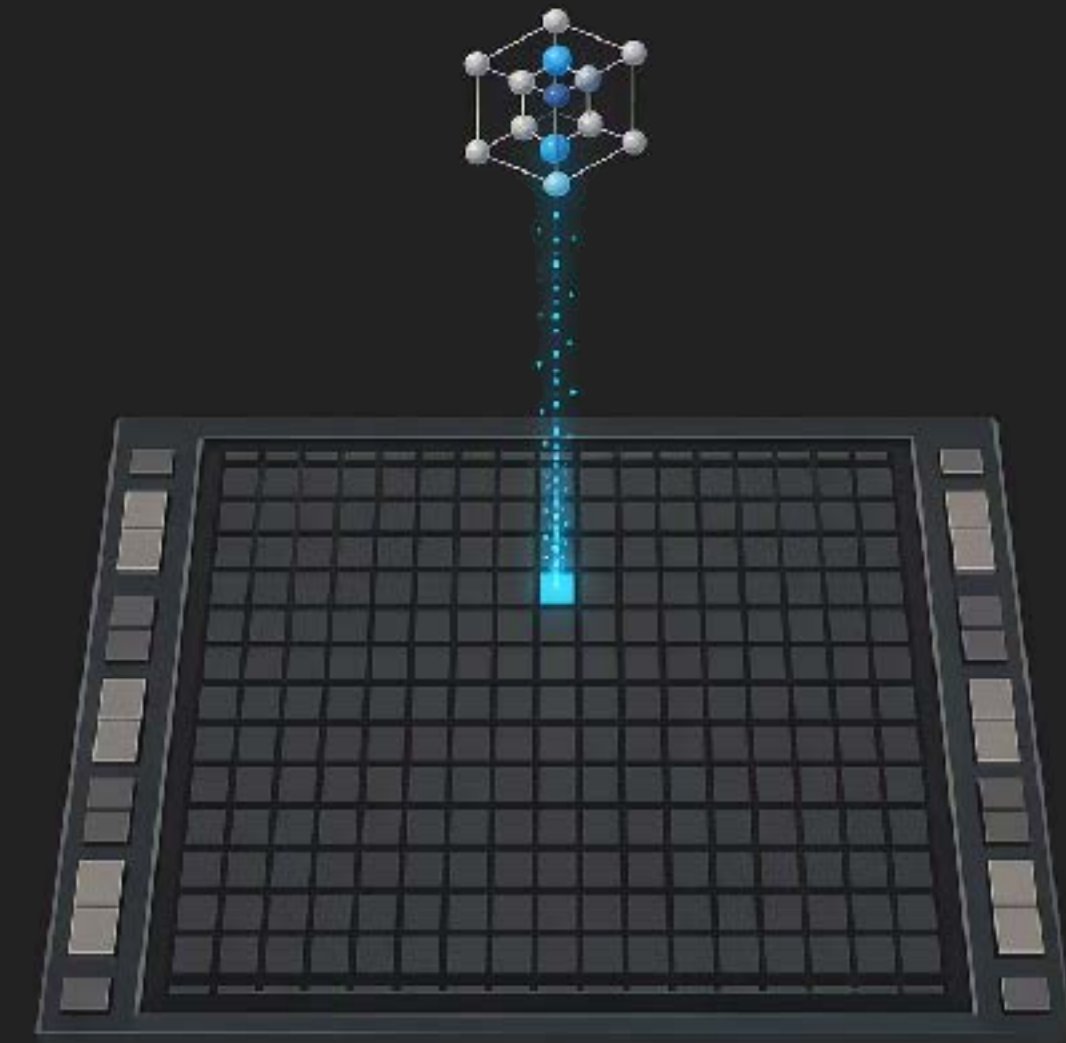


[github.com/
jax-ml/jax](https://github.com/jax-ml/jax)



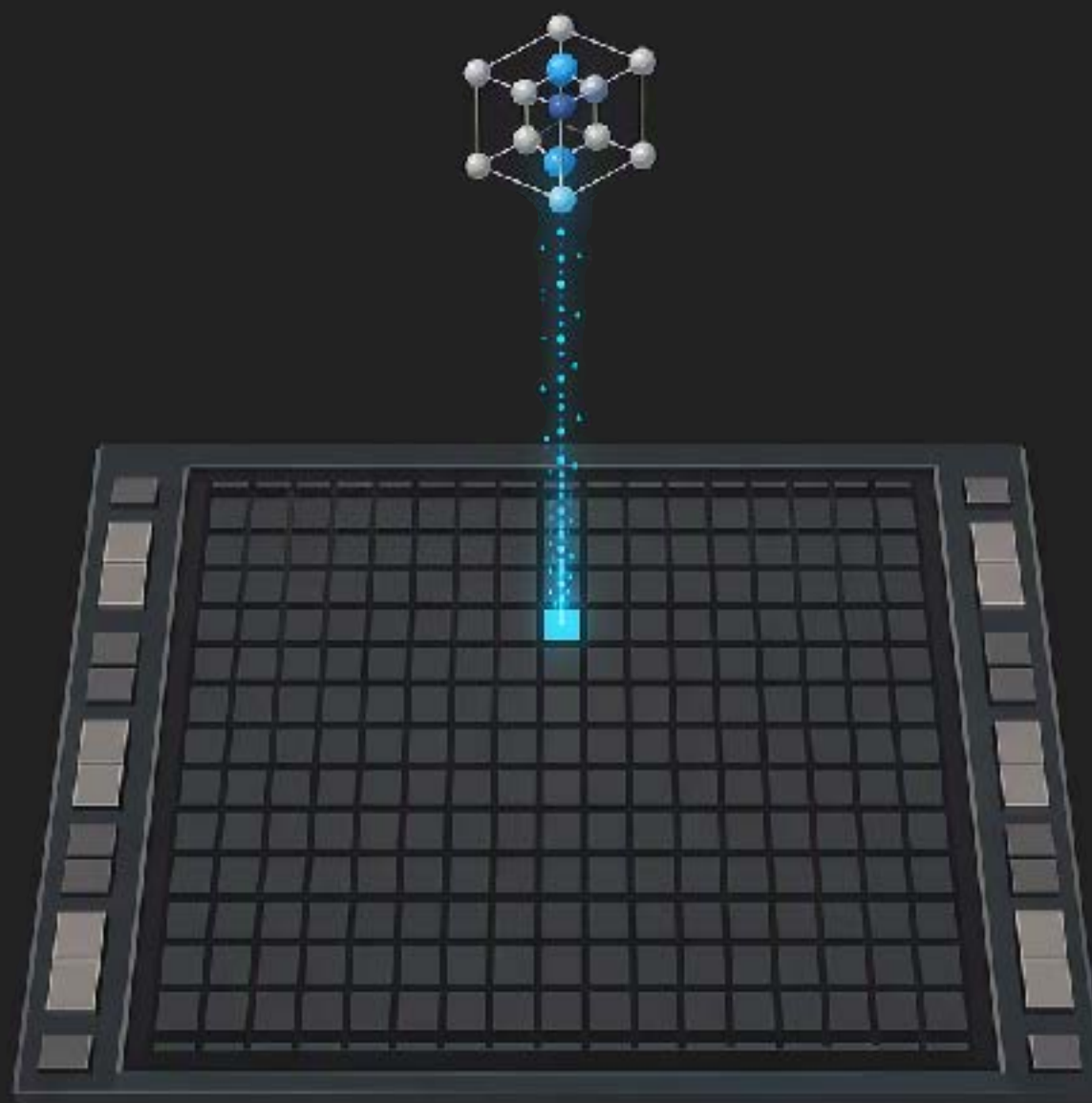
Fast and cheap
numerics

... at scale
on GPUs.

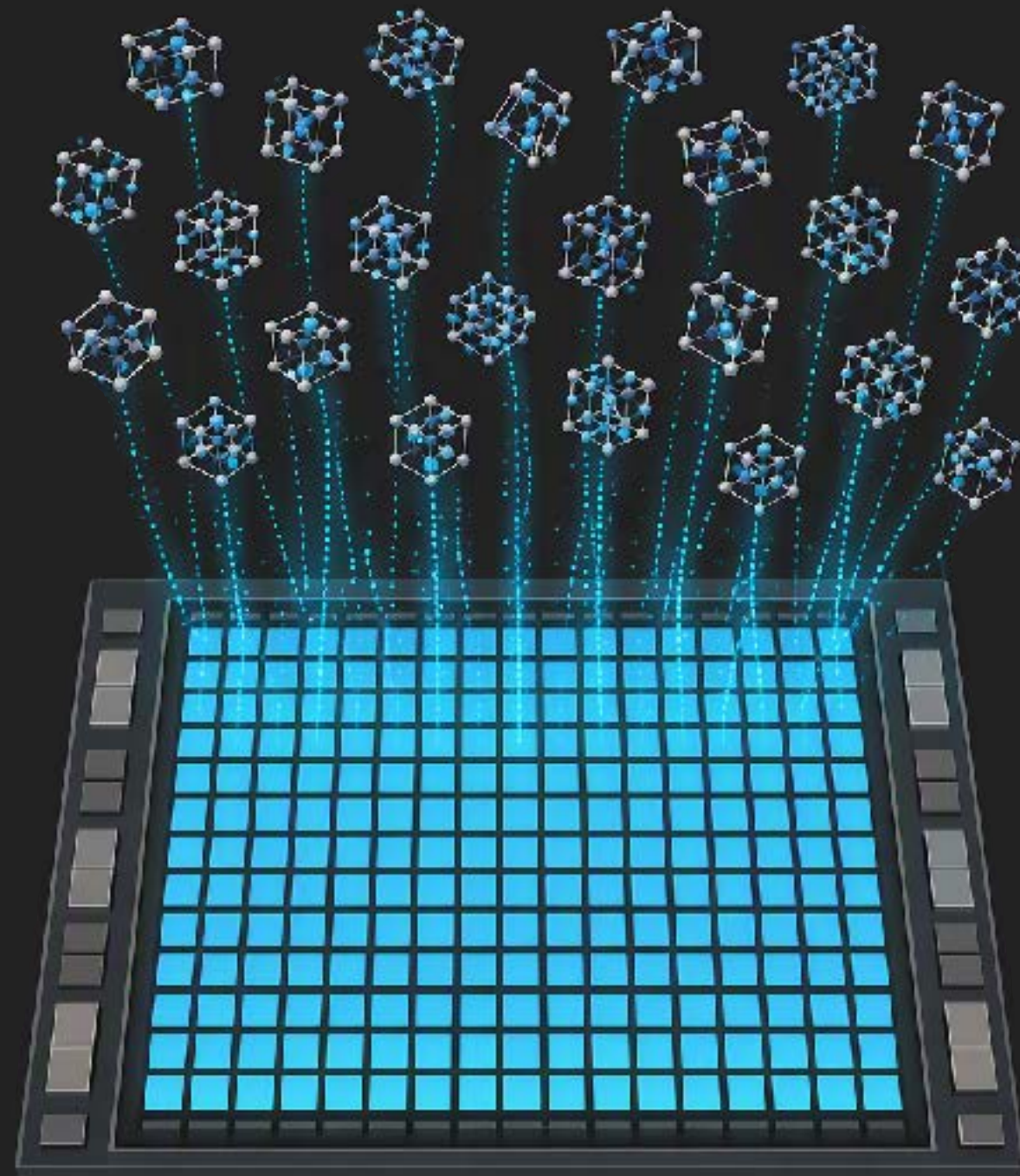


How do we stick as many small structures as
possible into one GPU?

Single Structure

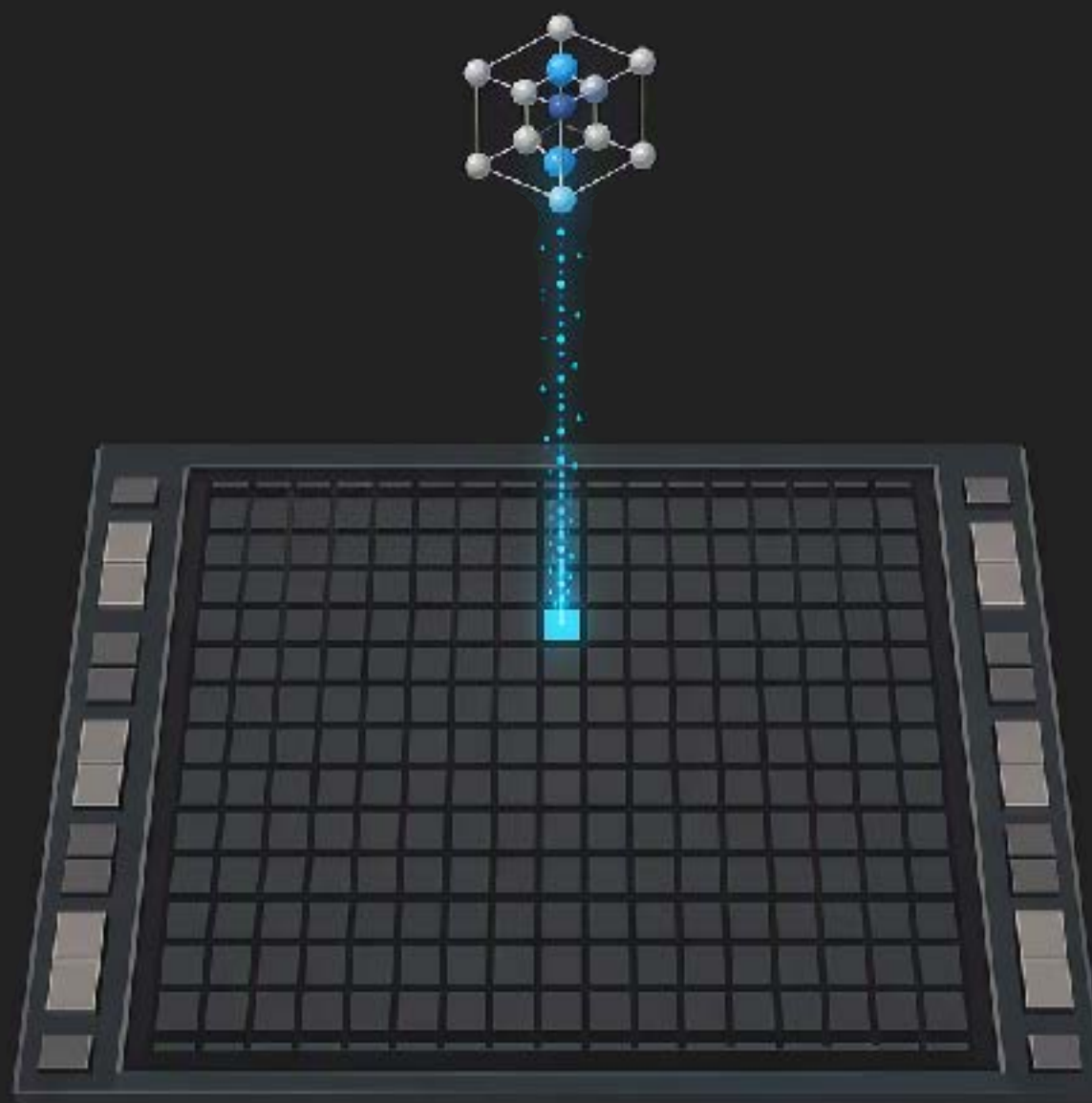


Batches of Similar Structure



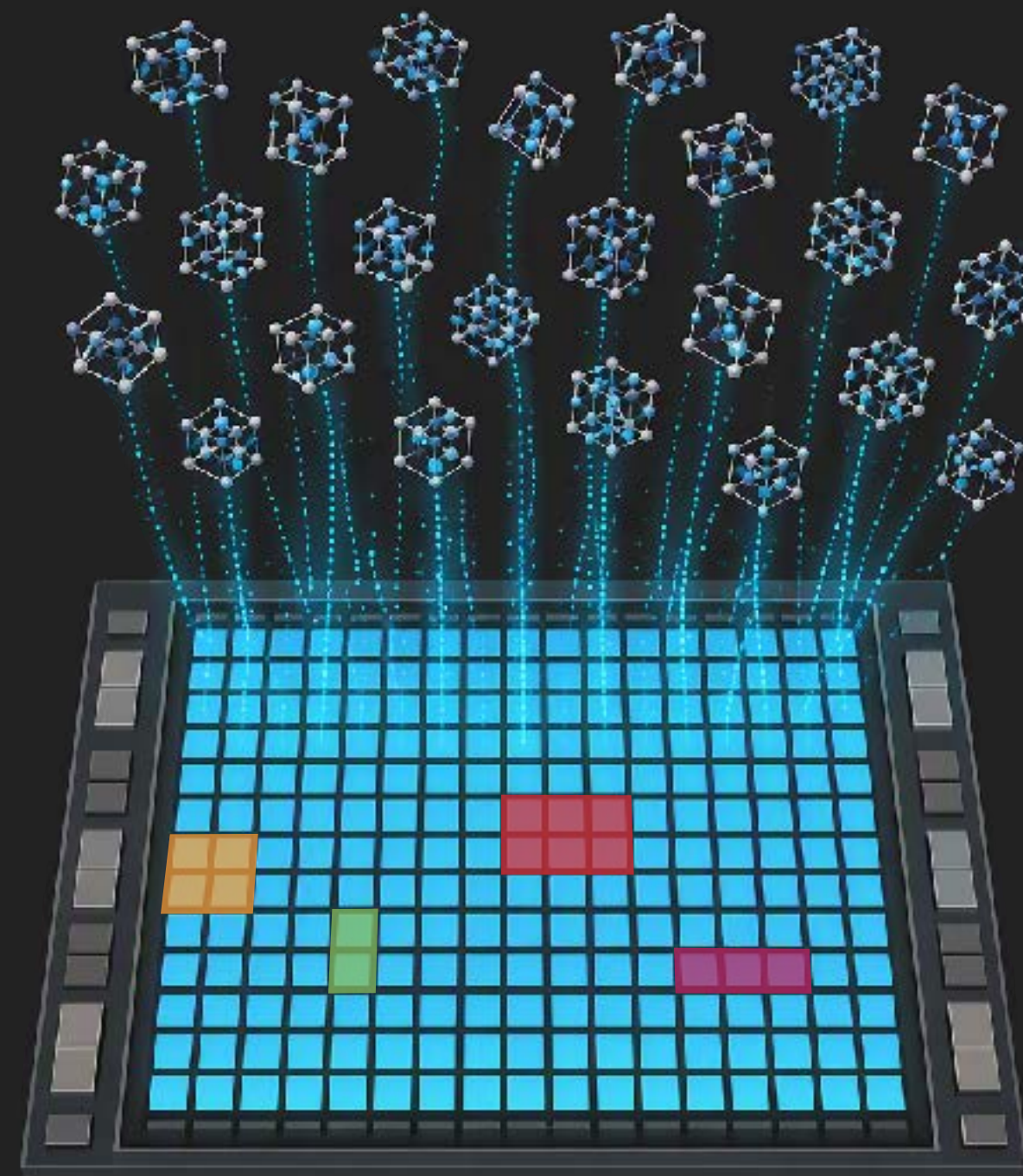
■ Occupied
■ Unoccupied

Single Structure



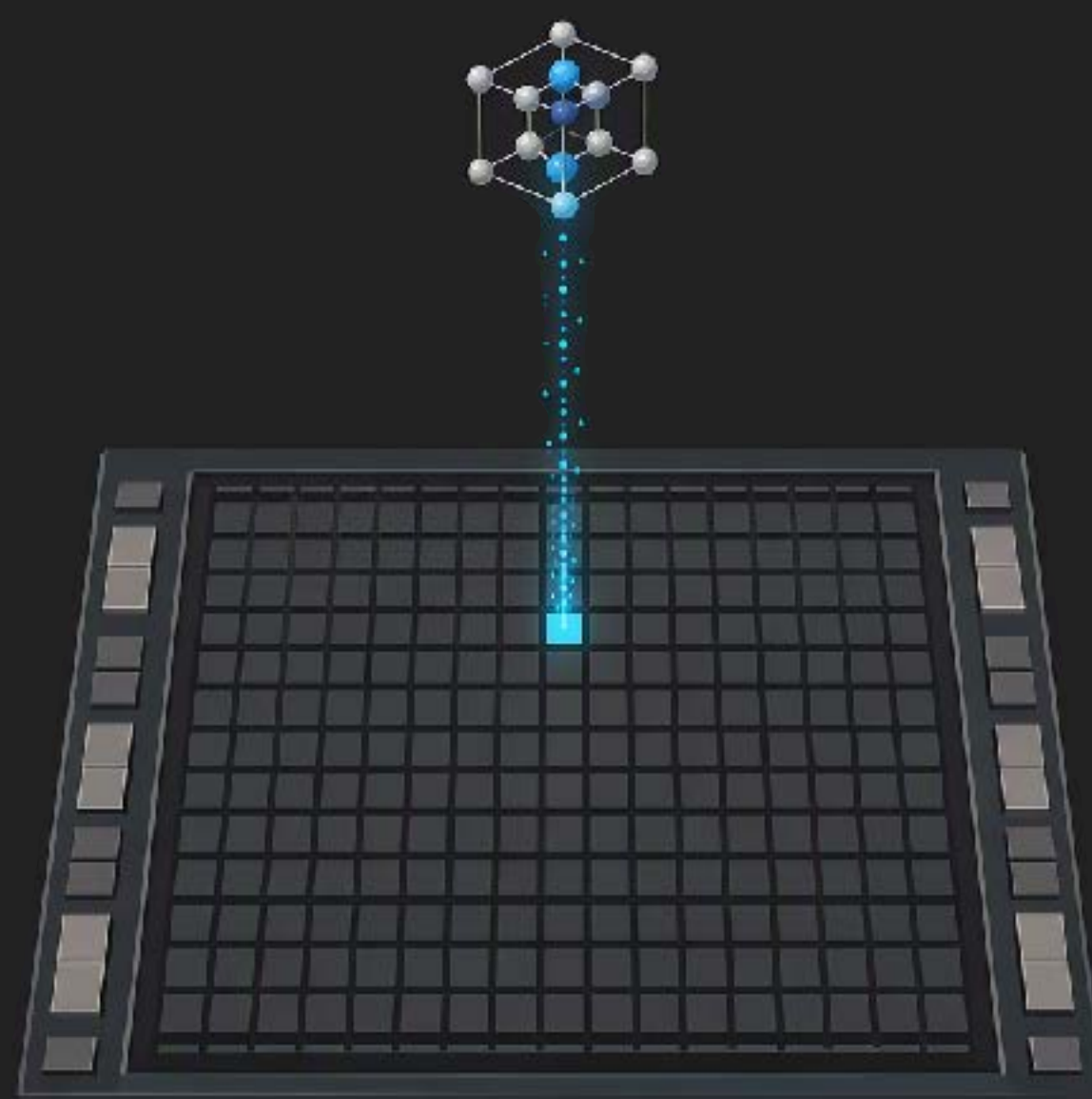
■ Occupied
■ Unoccupied

Batches of Similar Structure



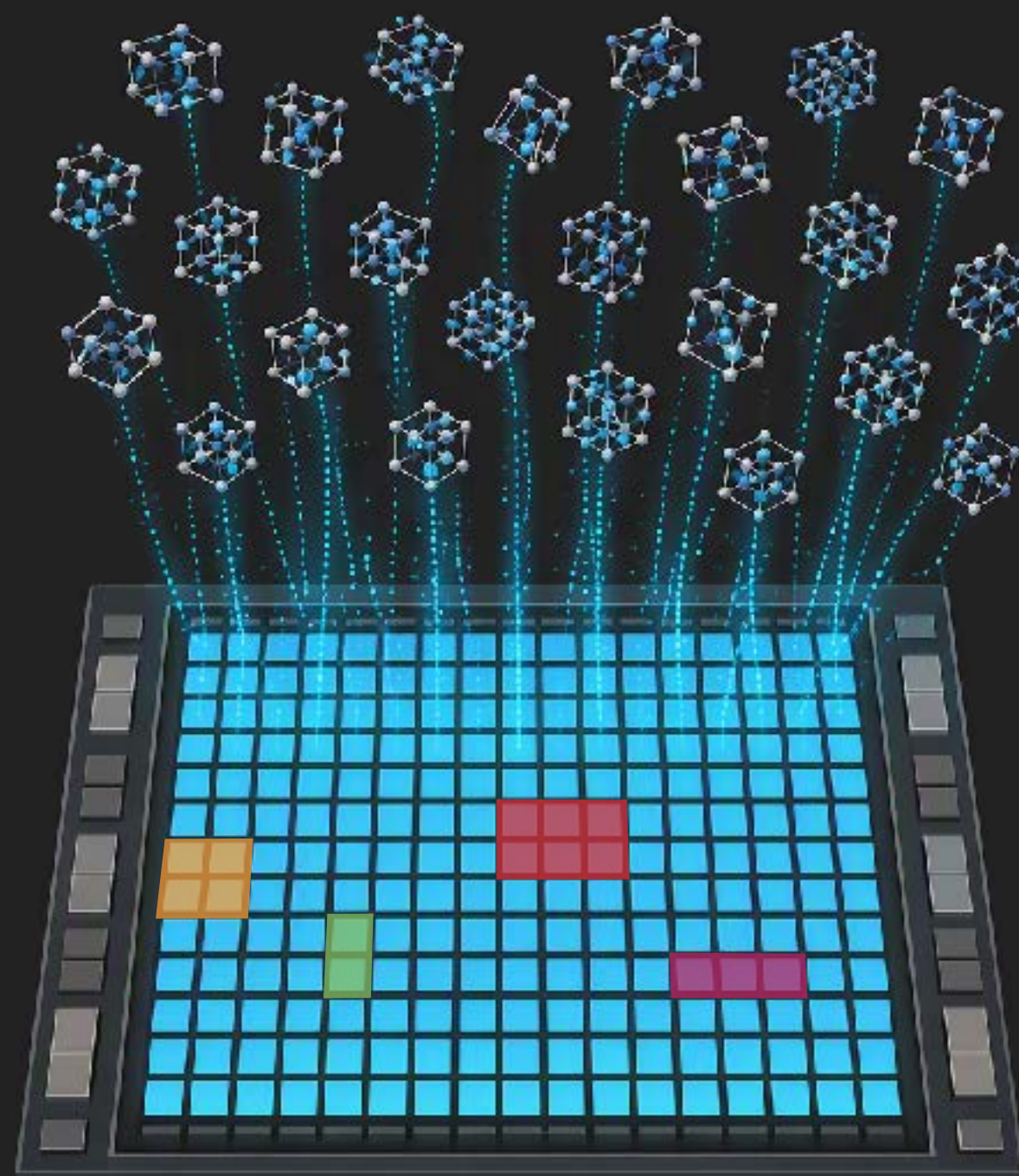
■ ■ ■ ■
Different size of crystal structures

Single Structure



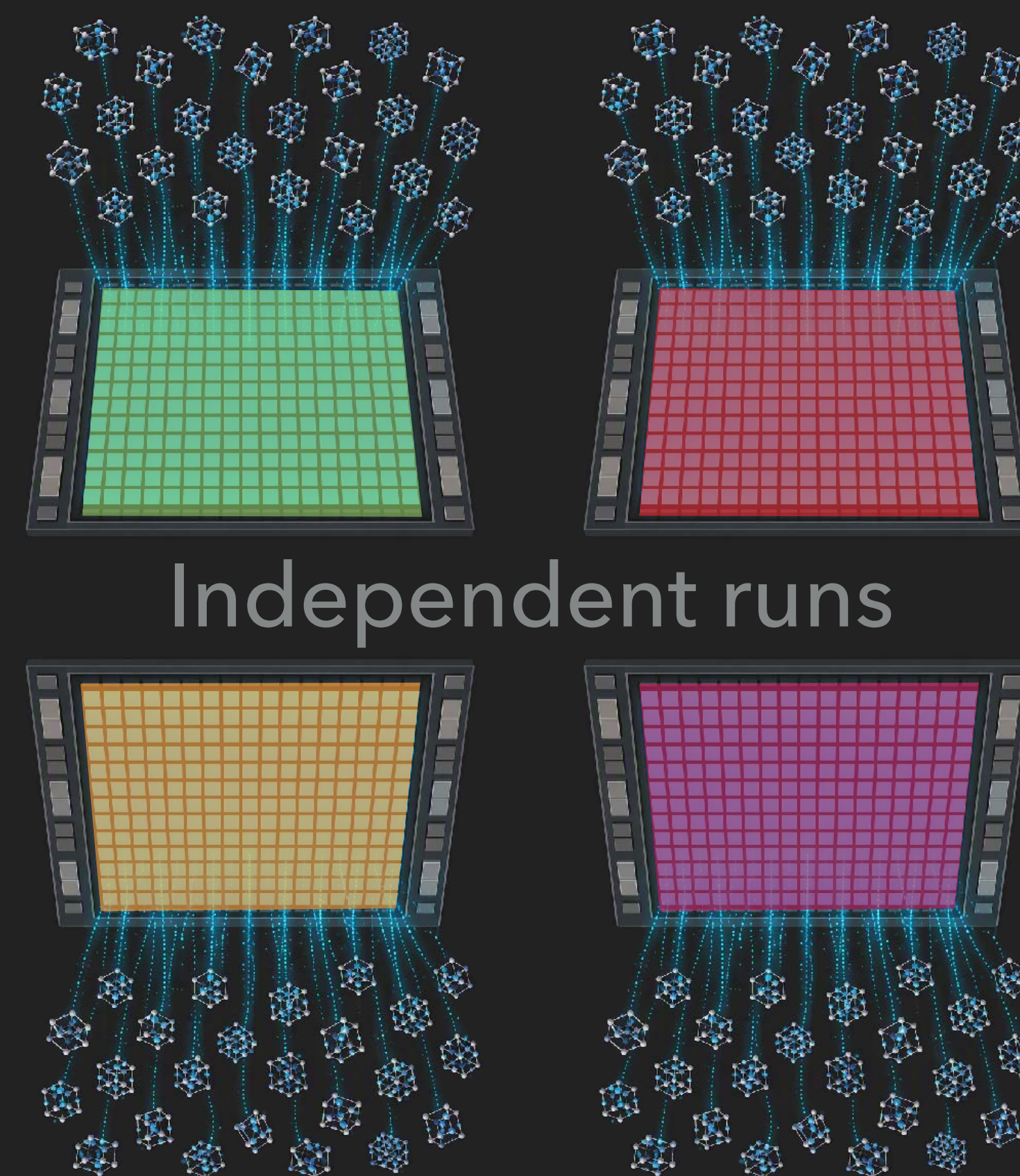
■ Occupied
■ Unoccupied

Batches of Similar Structure



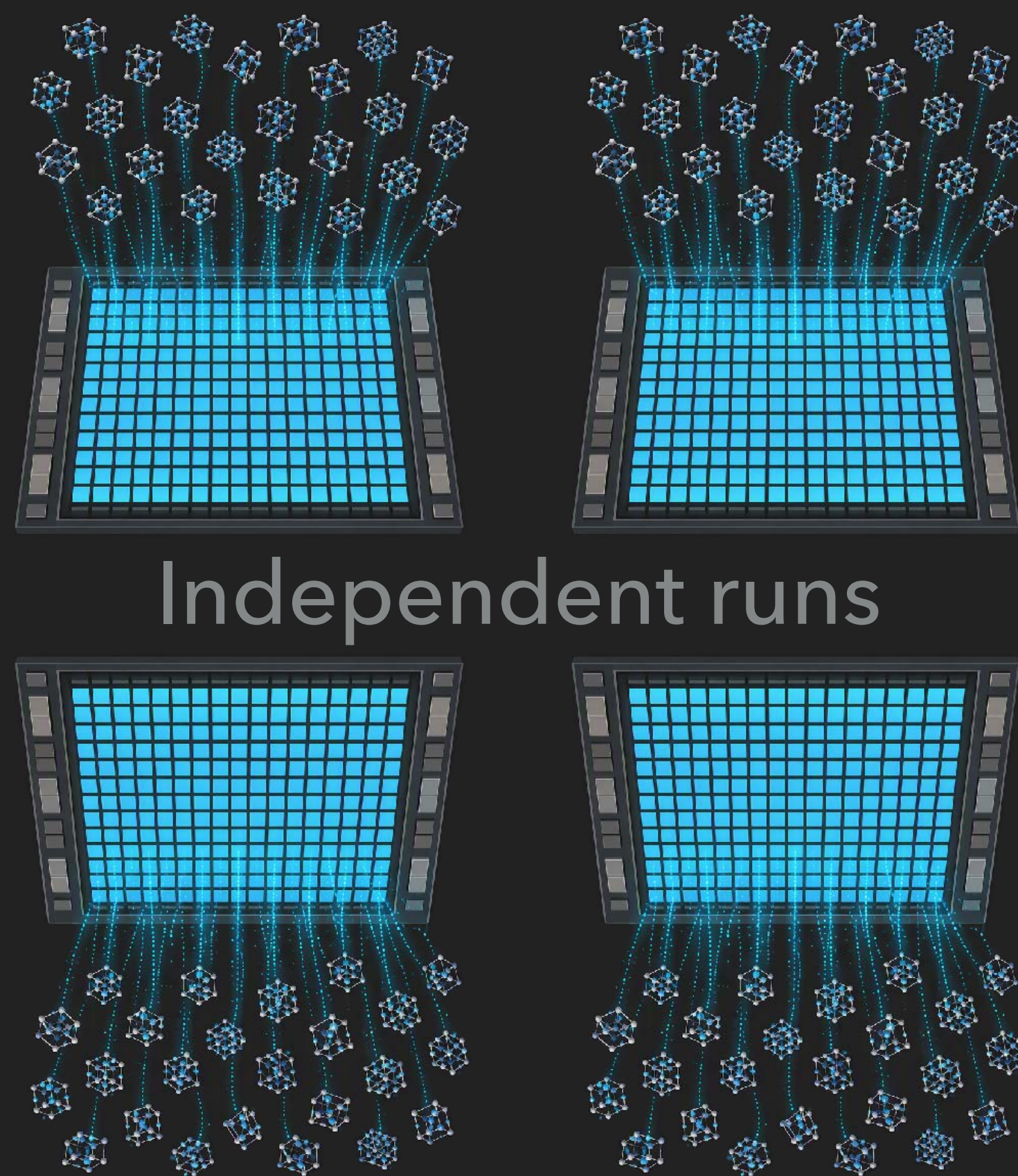
■ ■ ■ ■
Different size of crystal structures

Batches of Similar Batches



Independent runs

Batches of Similar Batches

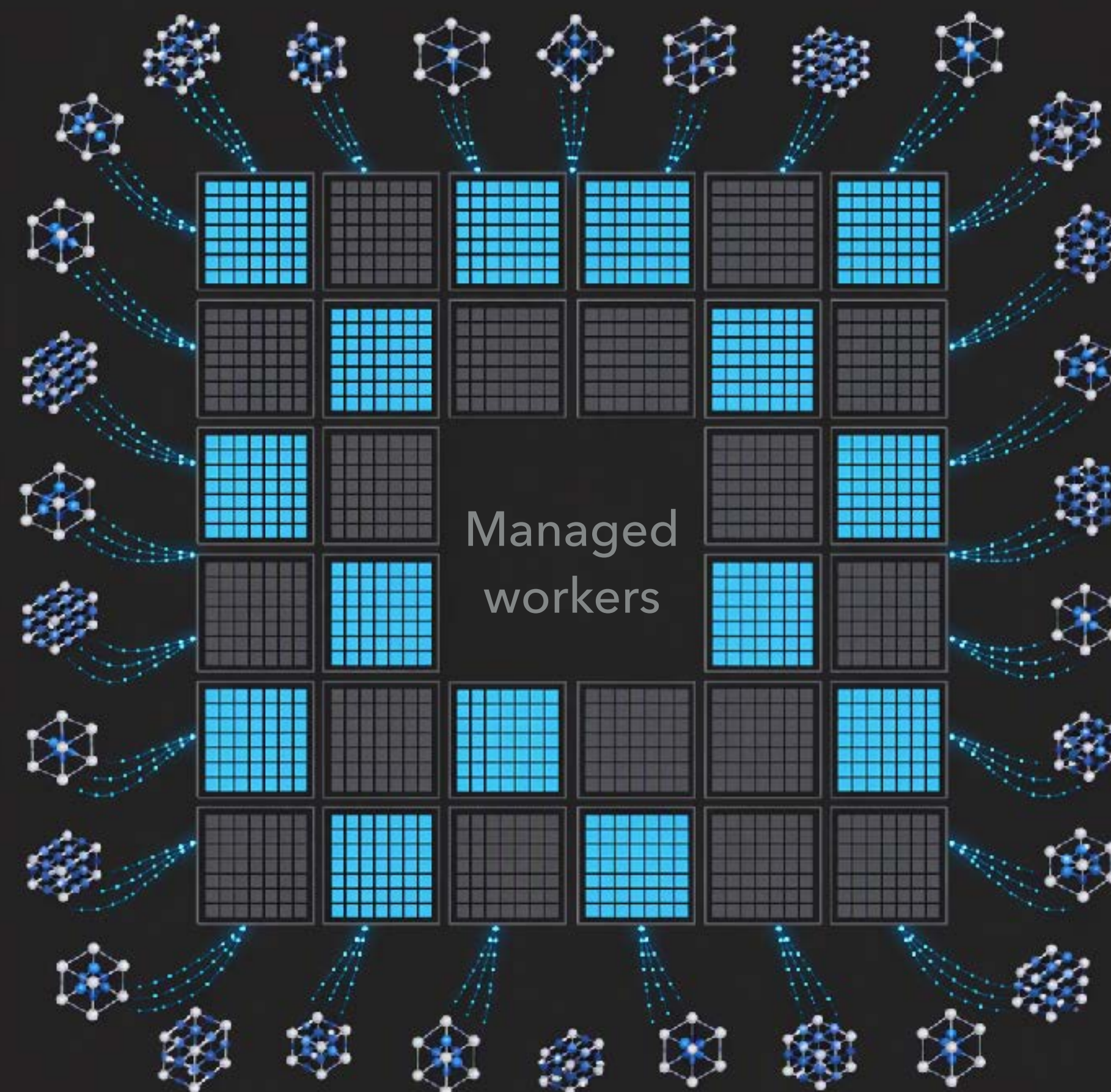


Independent runs

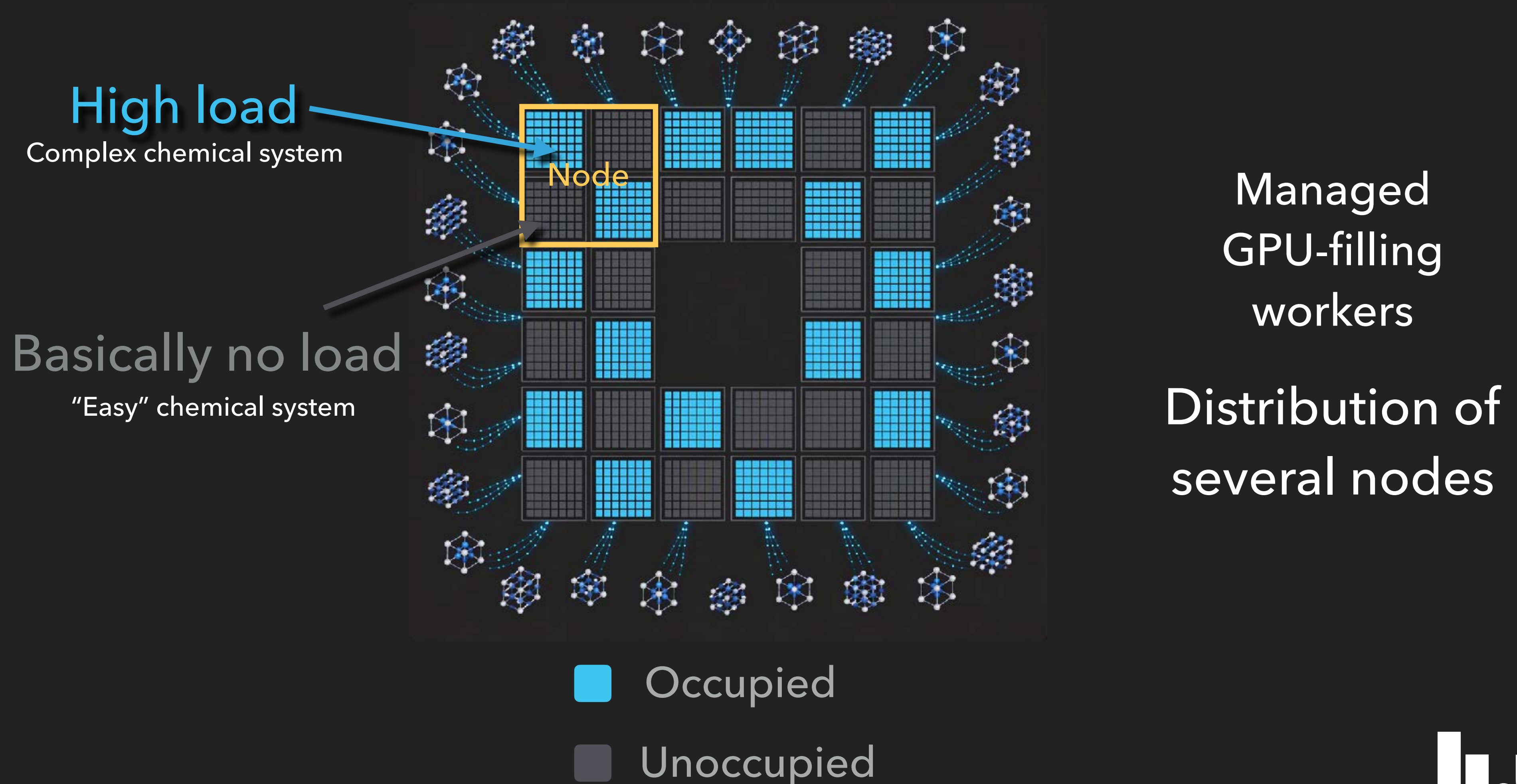
■ Occupied

■ Unoccupied

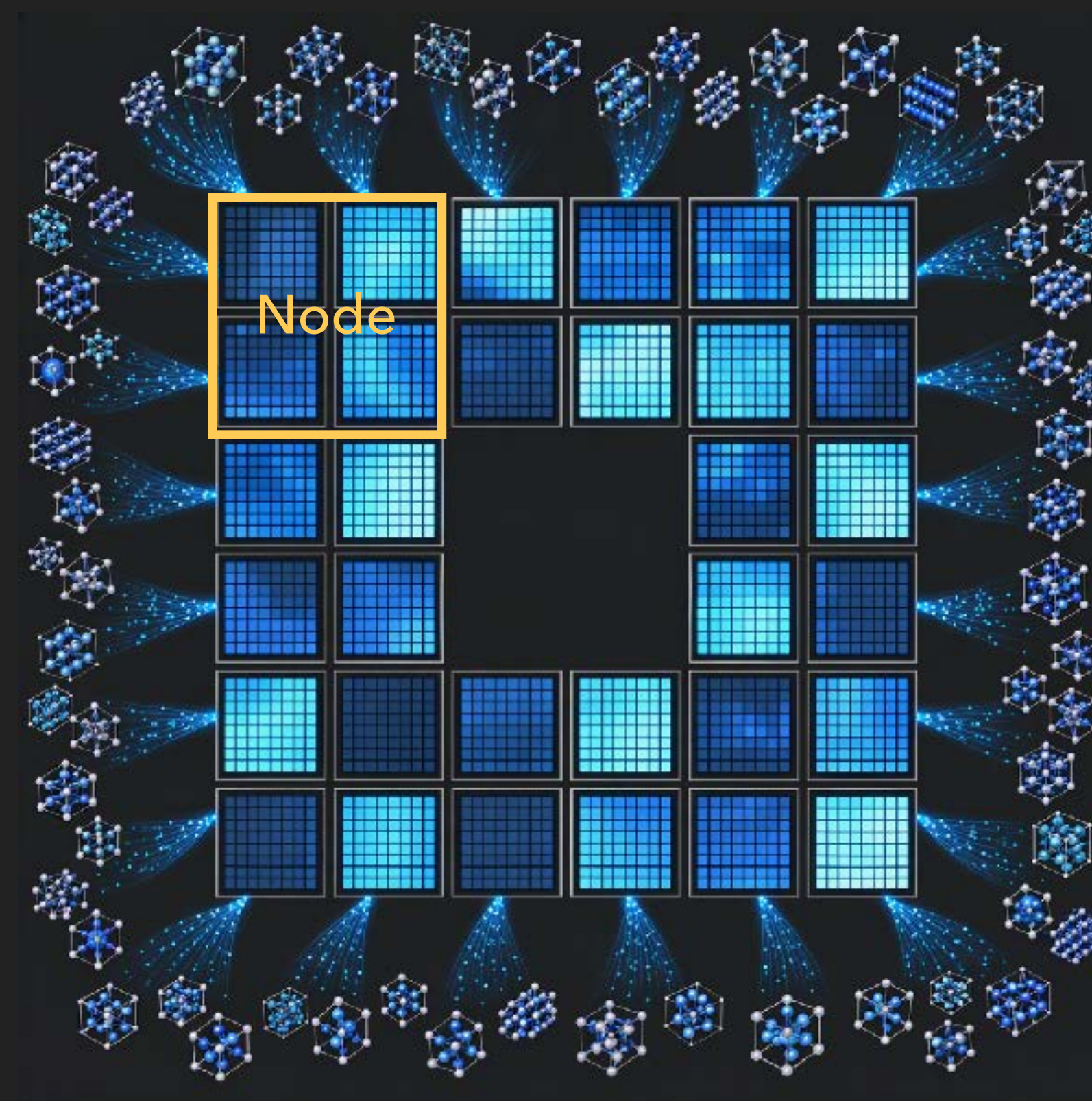
Batches of Chemical Systems



BATCHES OF CHEMICAL SYSTEMS



DISTRIBUTED BATCHES OF CHEMICAL SYSTEMS

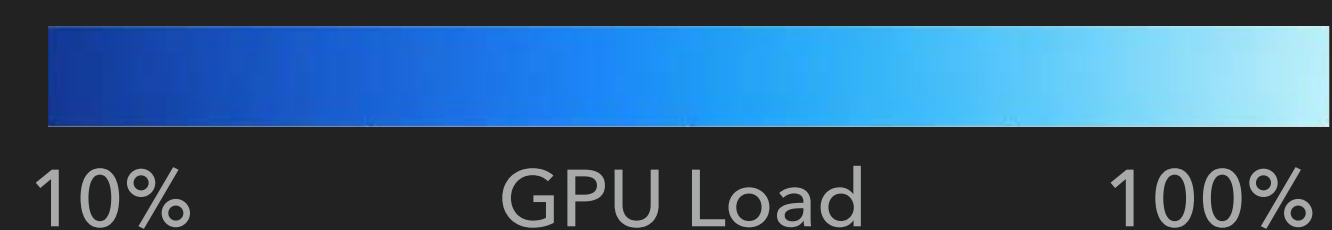


Managed multi-GPU
workers

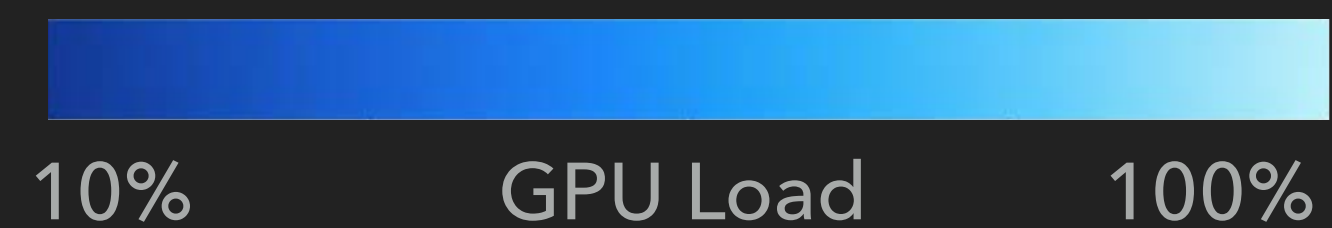
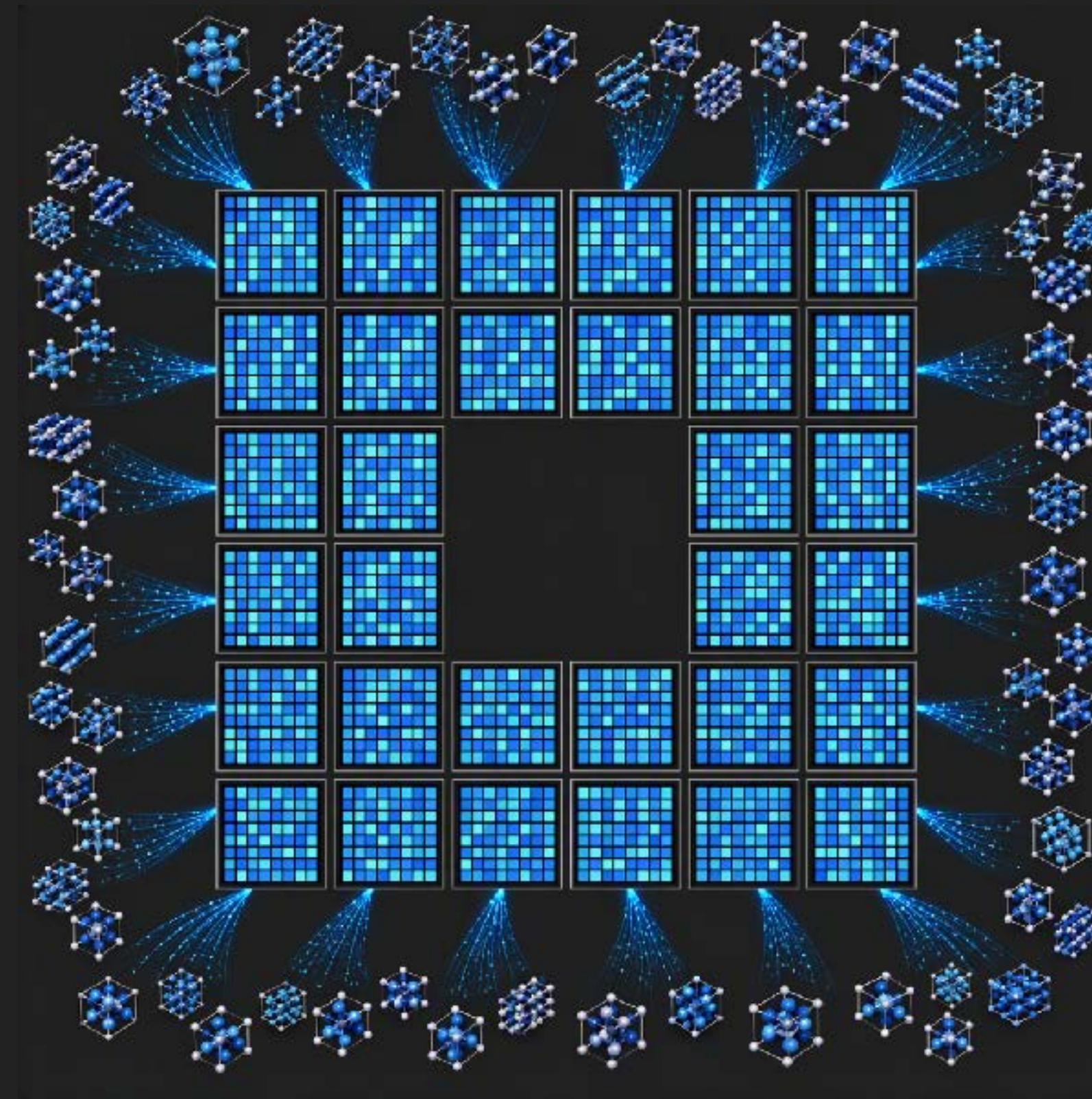
No CPU calls

Communication
between tasks in GPU
memory

Better Load Balancing
Less Padding



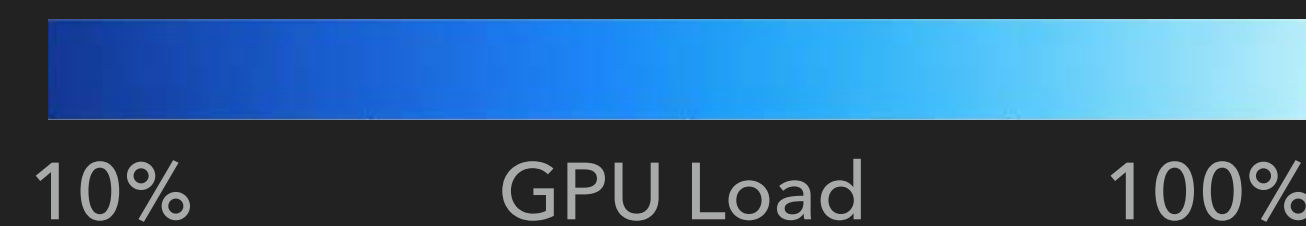
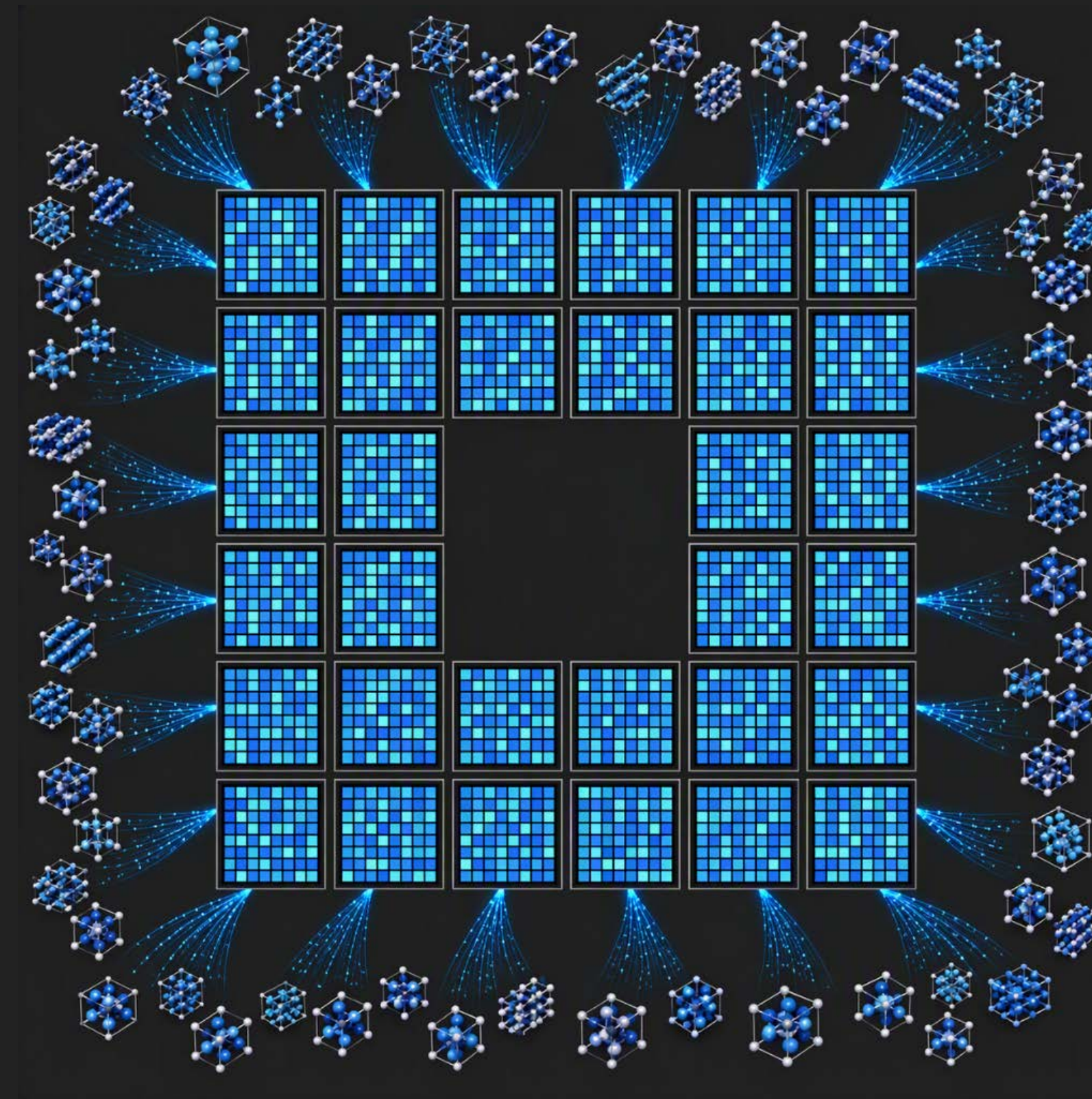
PADDED & BALANCED BATCHES OF CHEMICAL SYSTEMS



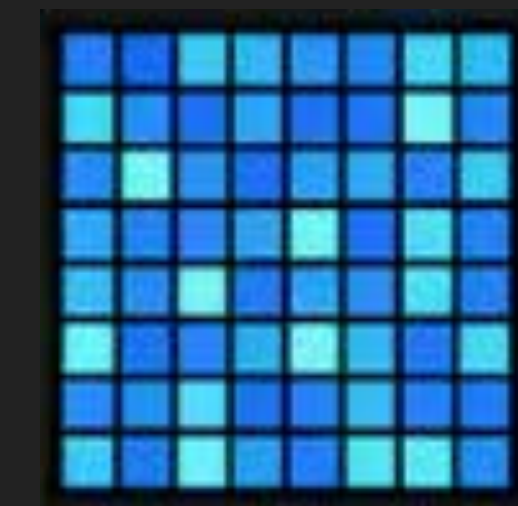
Balanced
multi-GPU
workers

Asynchronous
early dropout

PADDED & BALANCED BATCHES OF CHEMICAL SYSTEMS

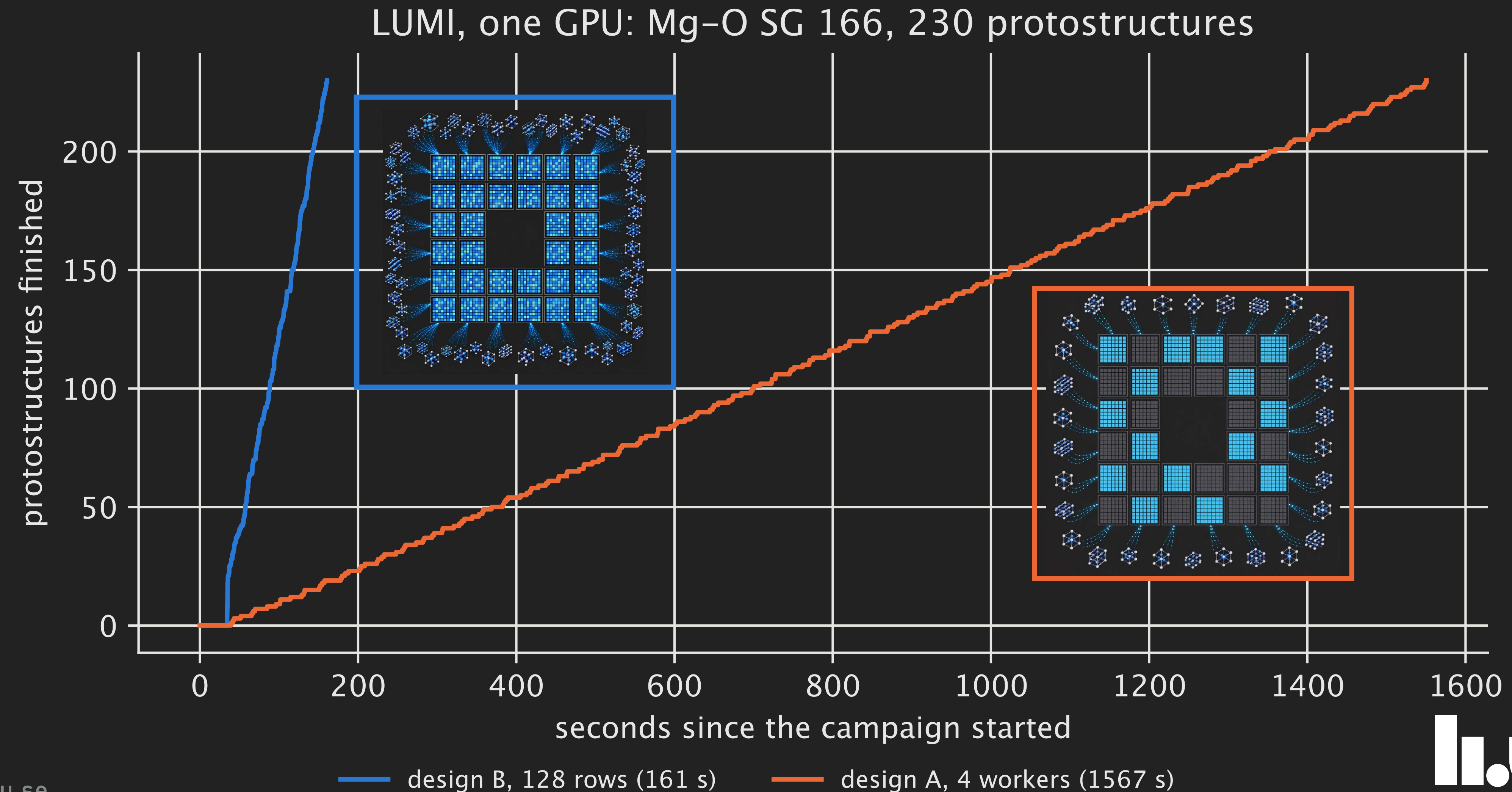


100% balancing cannot
be achieved

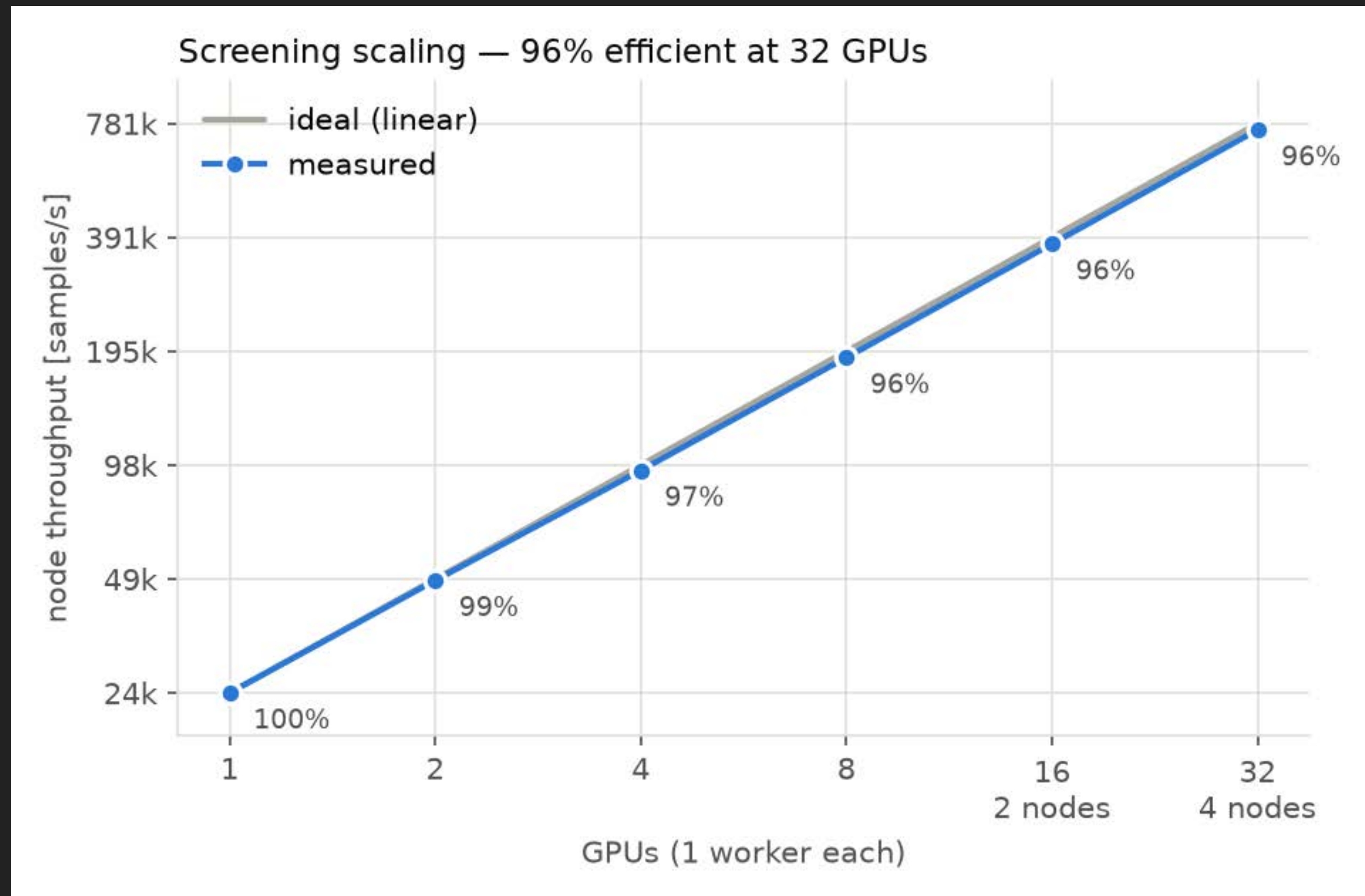
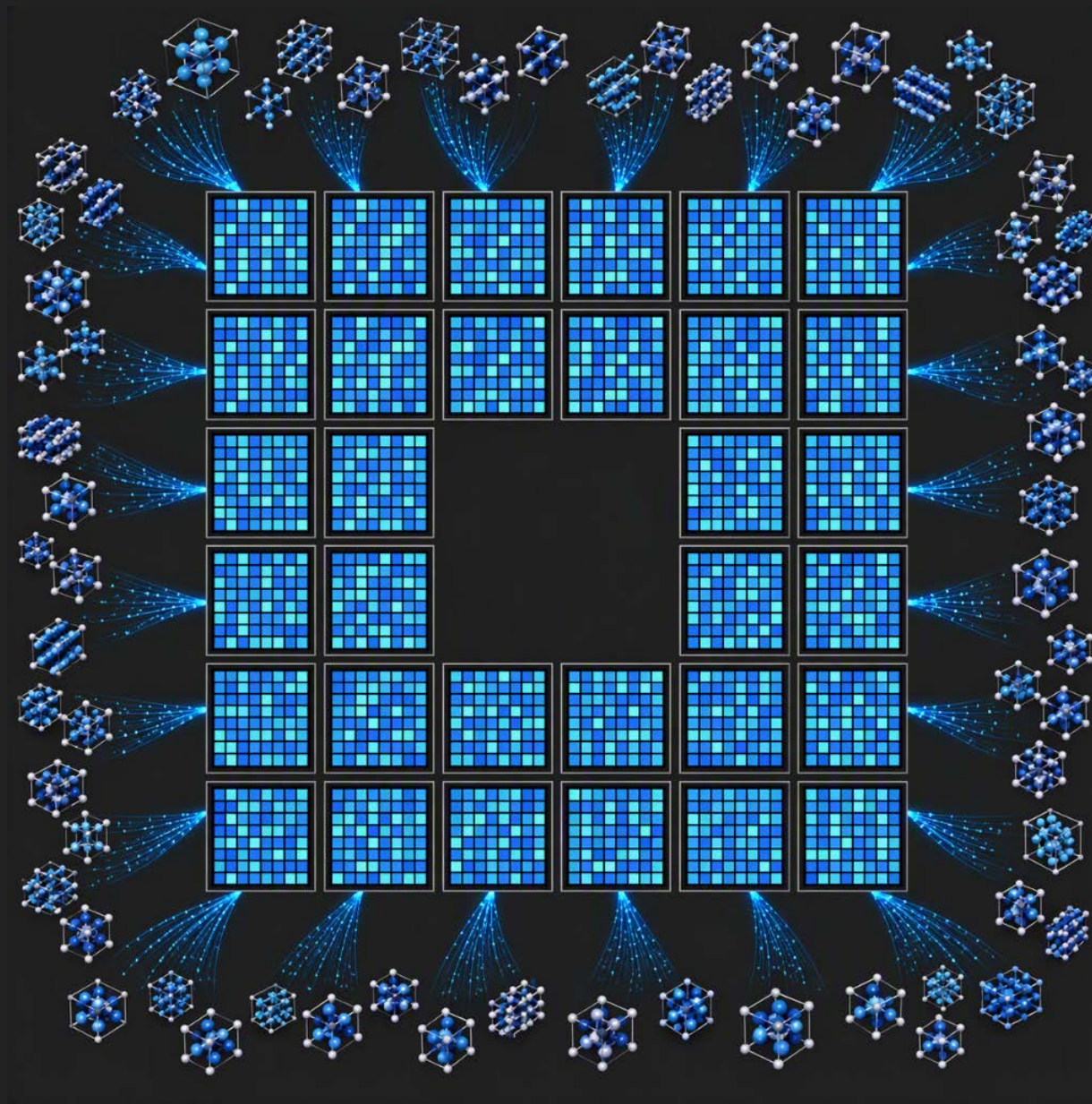


Unavoidable size
difference between
structures

HOW DOES THIS TRANSLATE TO PERFORMANCE?



ORCHESTRATION!? COMMUNICATION OVERHEAD?



We are fast!

Roughly one
million relaxations
per GPU per day!

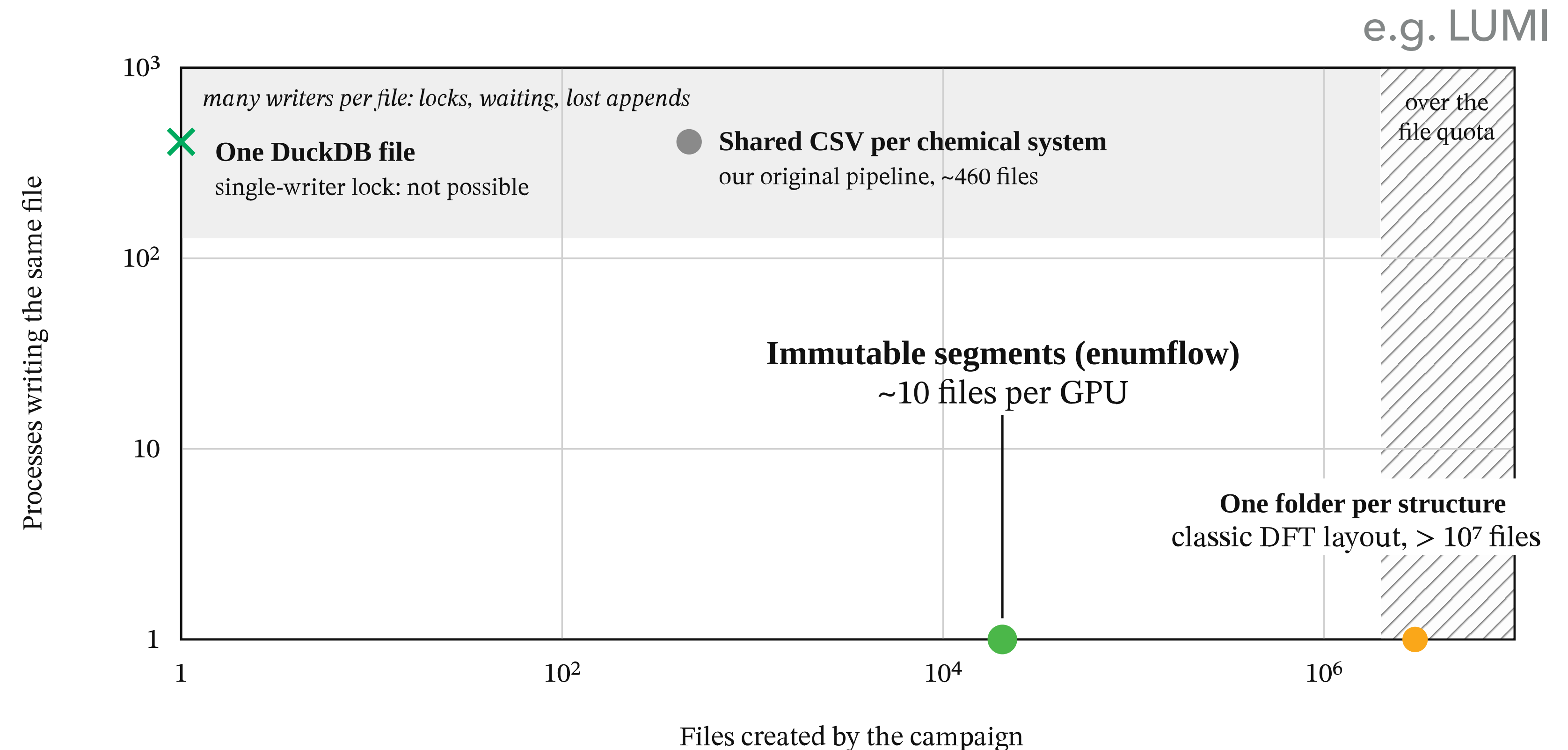
We can not store it!

One million files
per GPU per day!

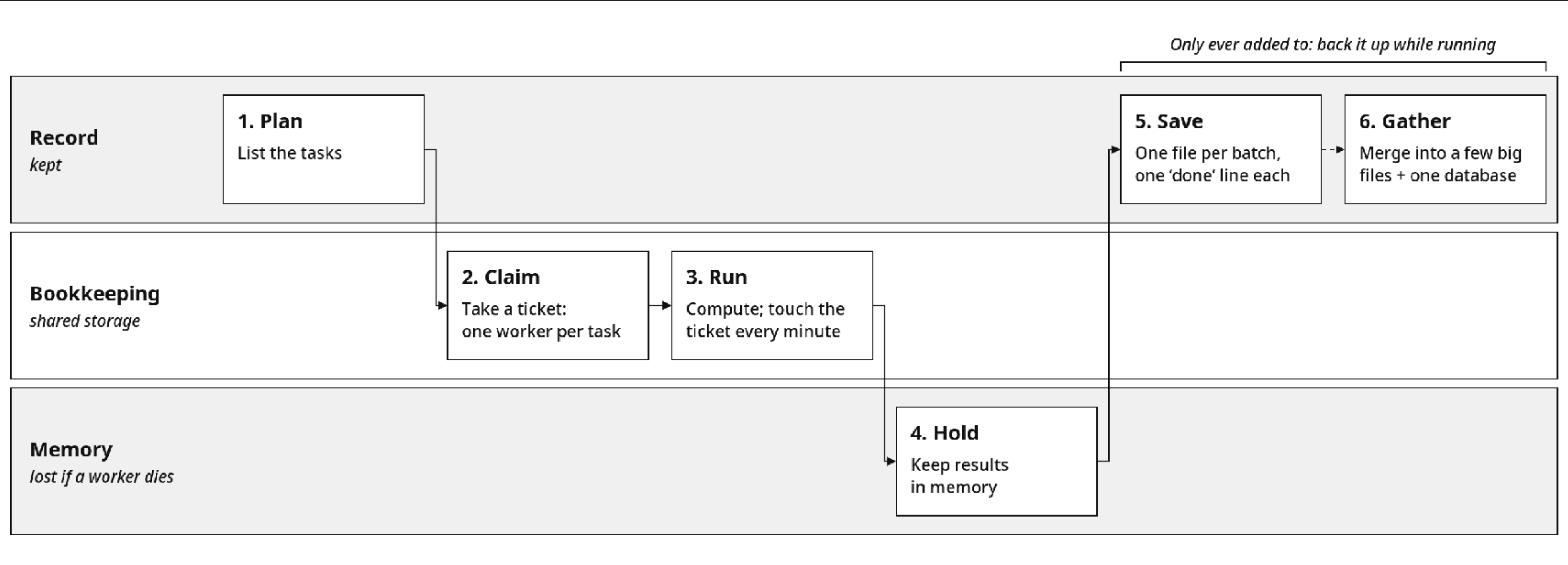
STORING MILLIONS OF STRUCTURAL RELAXATION?!

Screening a protostructure requires initializing at least 50 crystal structures per composition

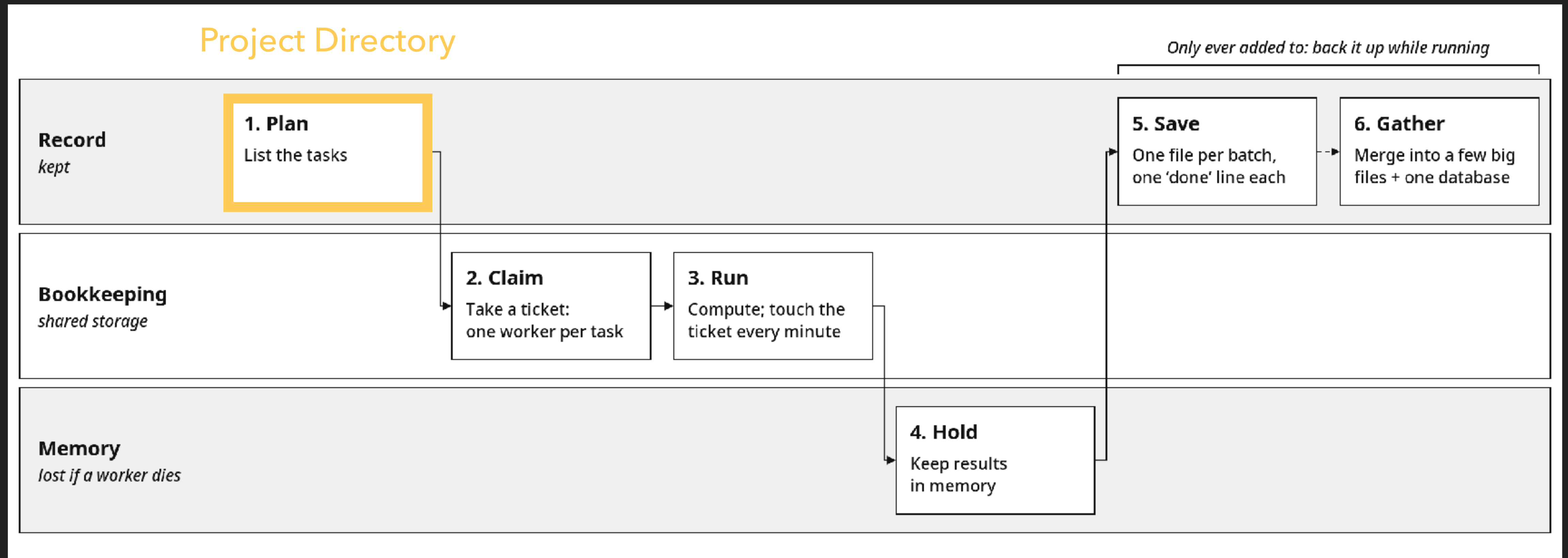
➔ Millions of structures need to be initialized, relaxed, and tracked



STORING MILLIONS OF STRUCTURAL RELAXATION?!

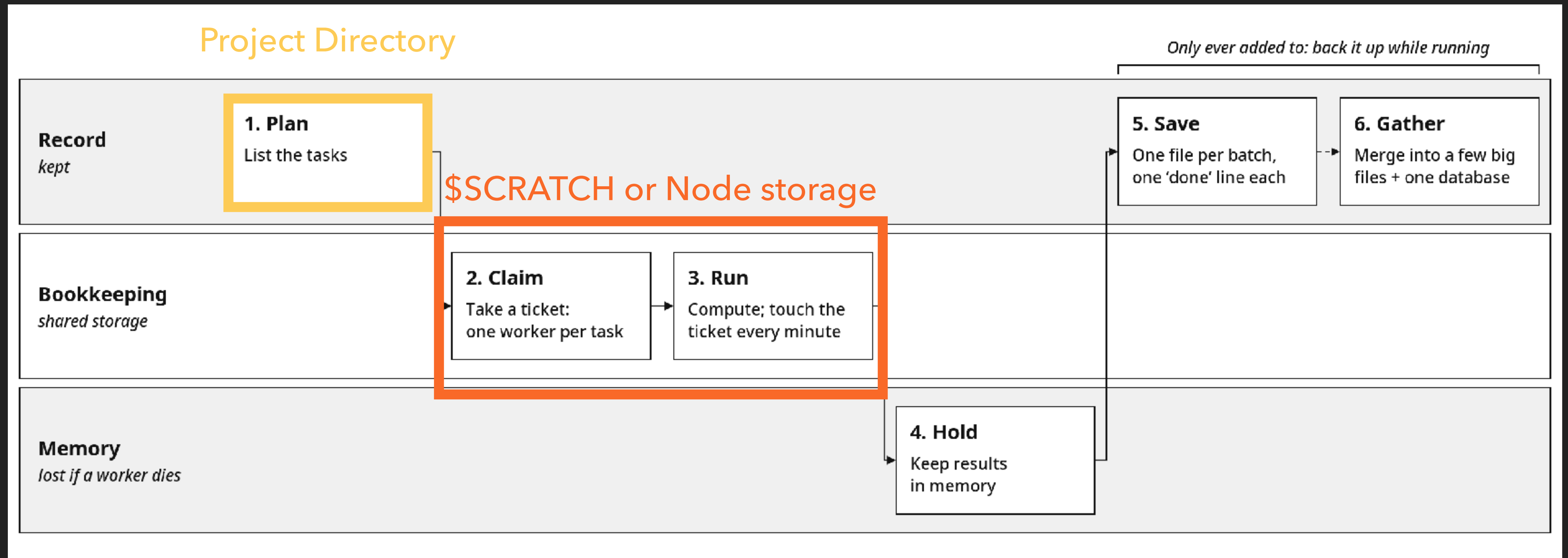


STORING MILLIONS OF STRUCTURAL RELAXATION?!



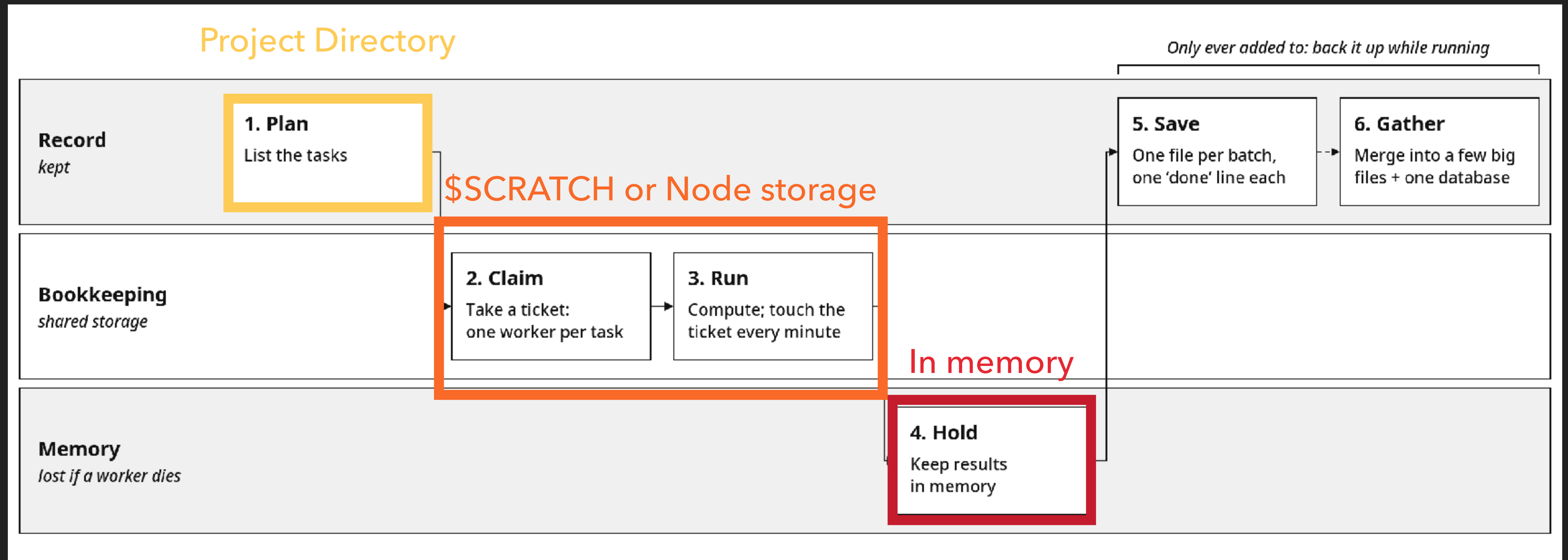
Minimal storage, minimal I/O, trackable, easy on-the-fly backup

STORING MILLIONS OF STRUCTURAL RELAXATION?!



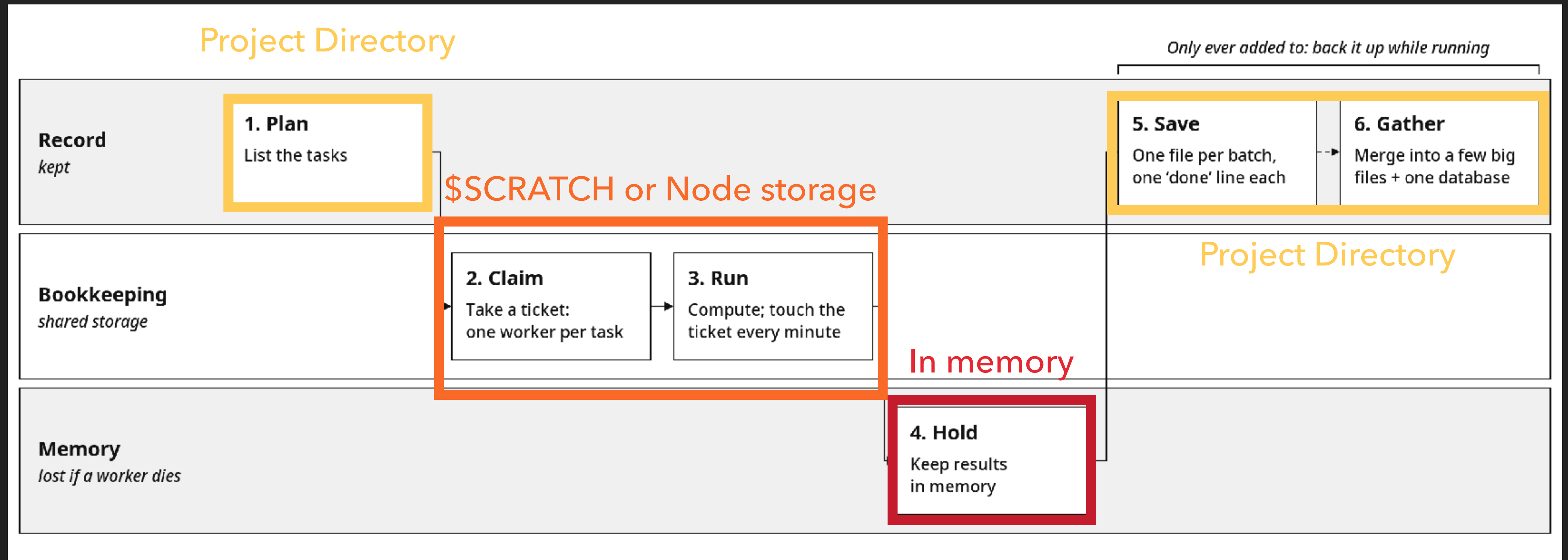
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STORING MILLIONS OF STRUCTURAL RELAXATION?!



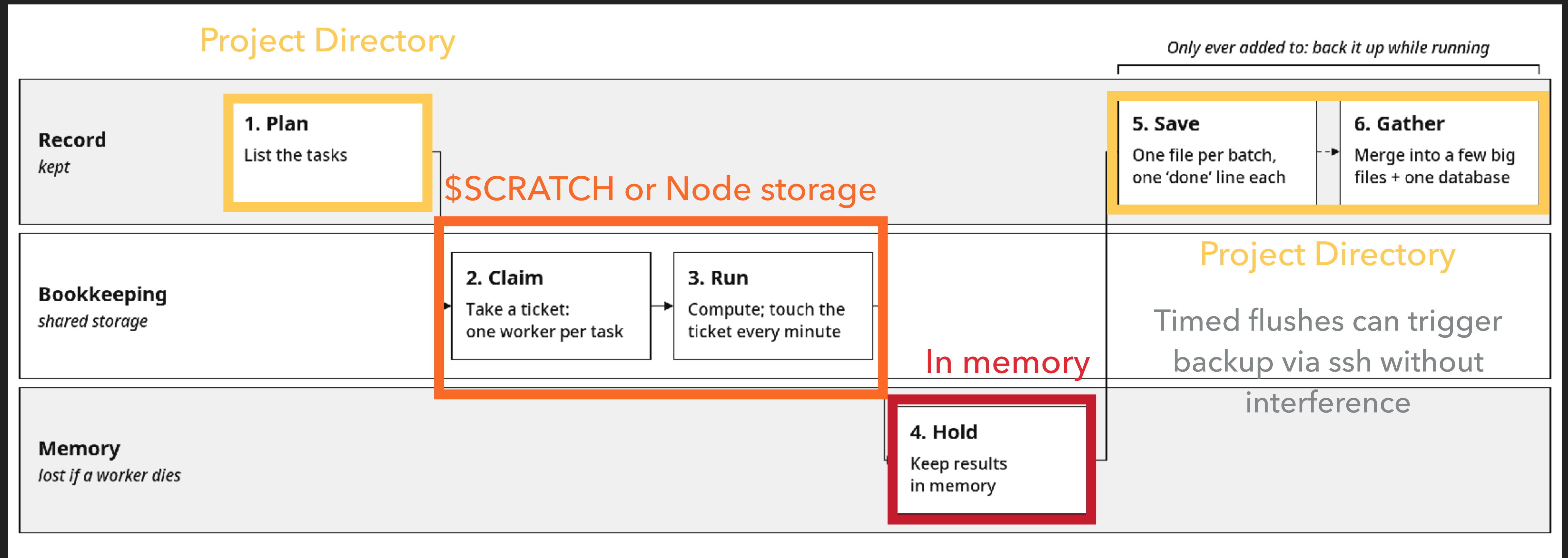
Minimal storage, minimal I/O, trackable, easy on-the-fly backup

STORING MILLIONS OF STRUCTURAL RELAXATION?!



Minimal storage, minimal I/O, trackable, easy on-the-fly backup

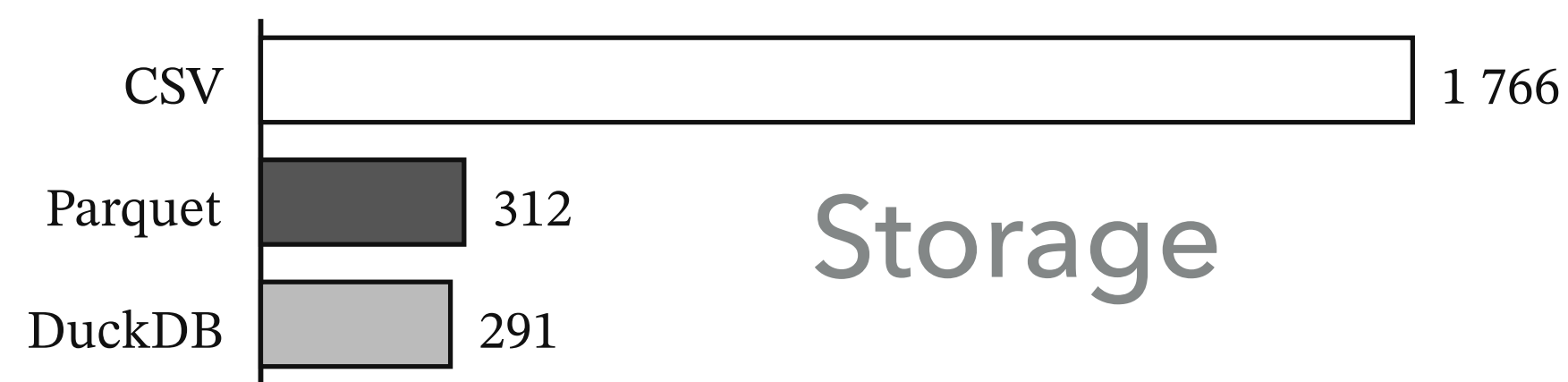
STORING MILLIONS OF STRUCTURAL RELAXATION?!



Minimal storage, minimal I/O, trackable, easy on-the-fly backup

STORING MILLIONS OF STRUCTURAL RELAXATION?!

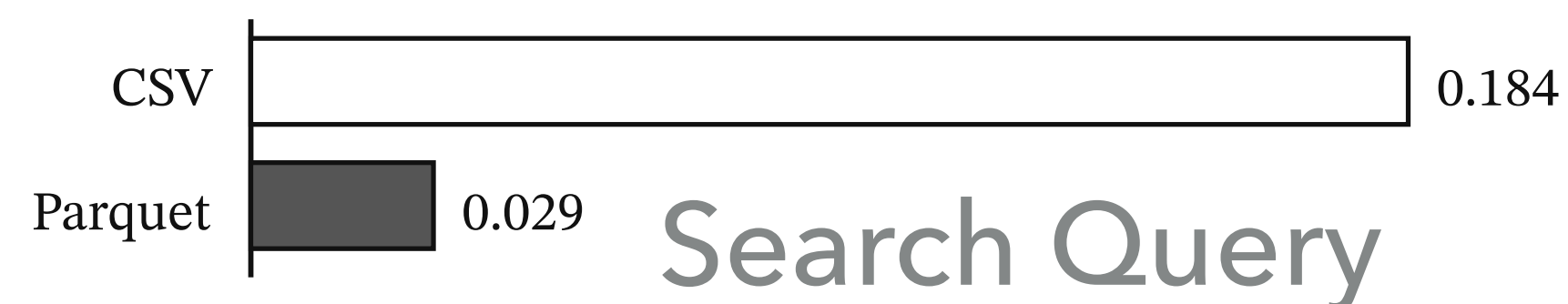
(a) Size on disk (bytes per structure)



(b) Read every structure back as numbers (s)



(c) Lowest energy per protostructure (s)

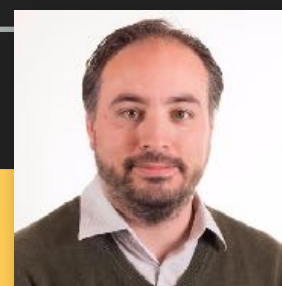
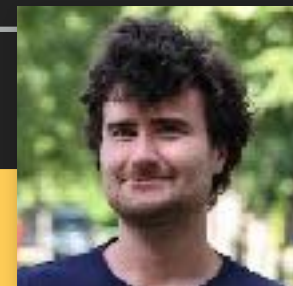
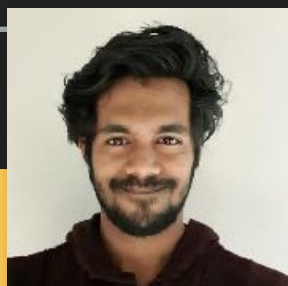


(d) Write 100 000 structures (s)



Benchmark: 100 000 synthetic relaxed structures (4 to 40 atoms, five elements, six numerical properties)

Less I/O cost means the GPUs do not idle

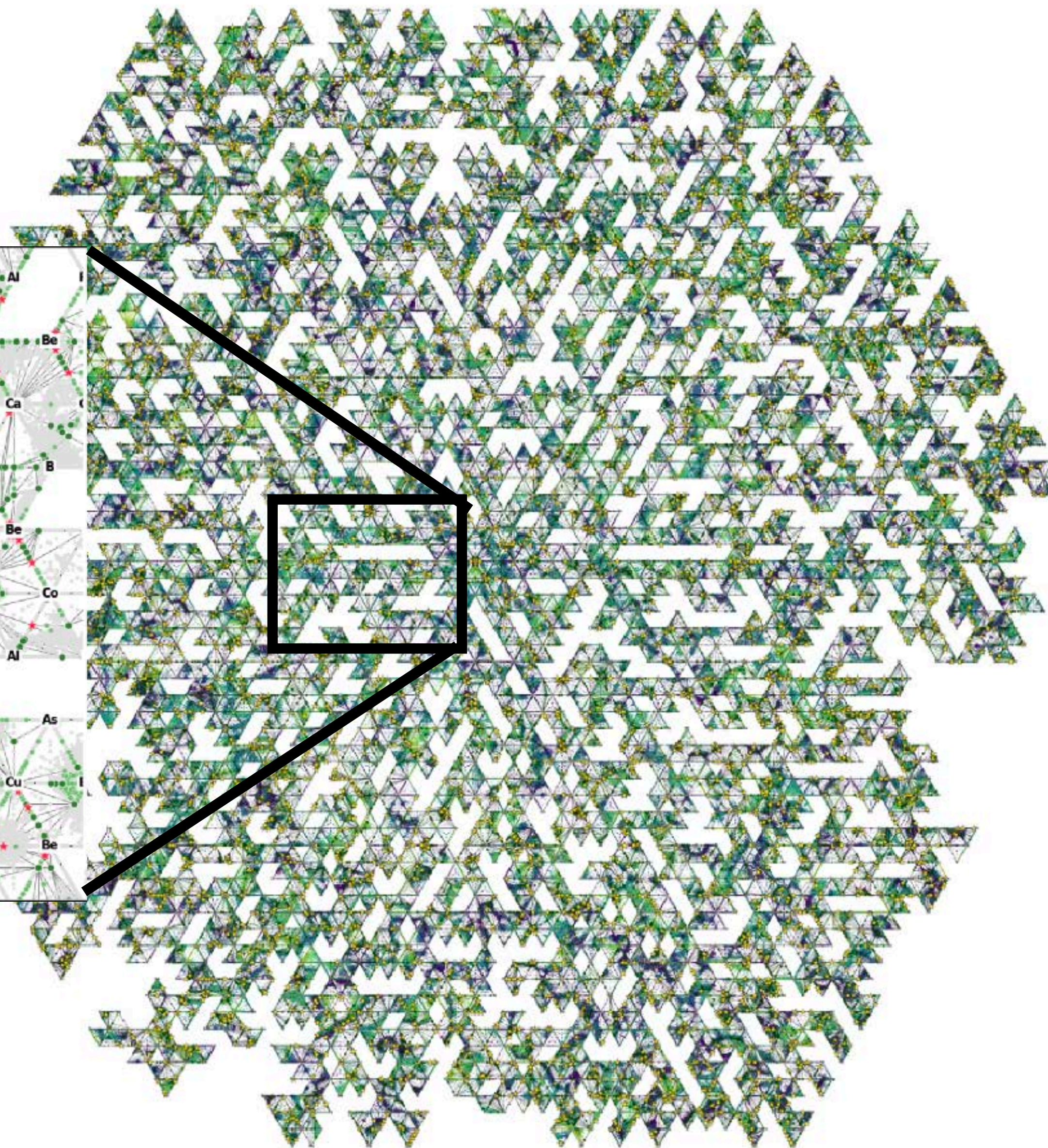
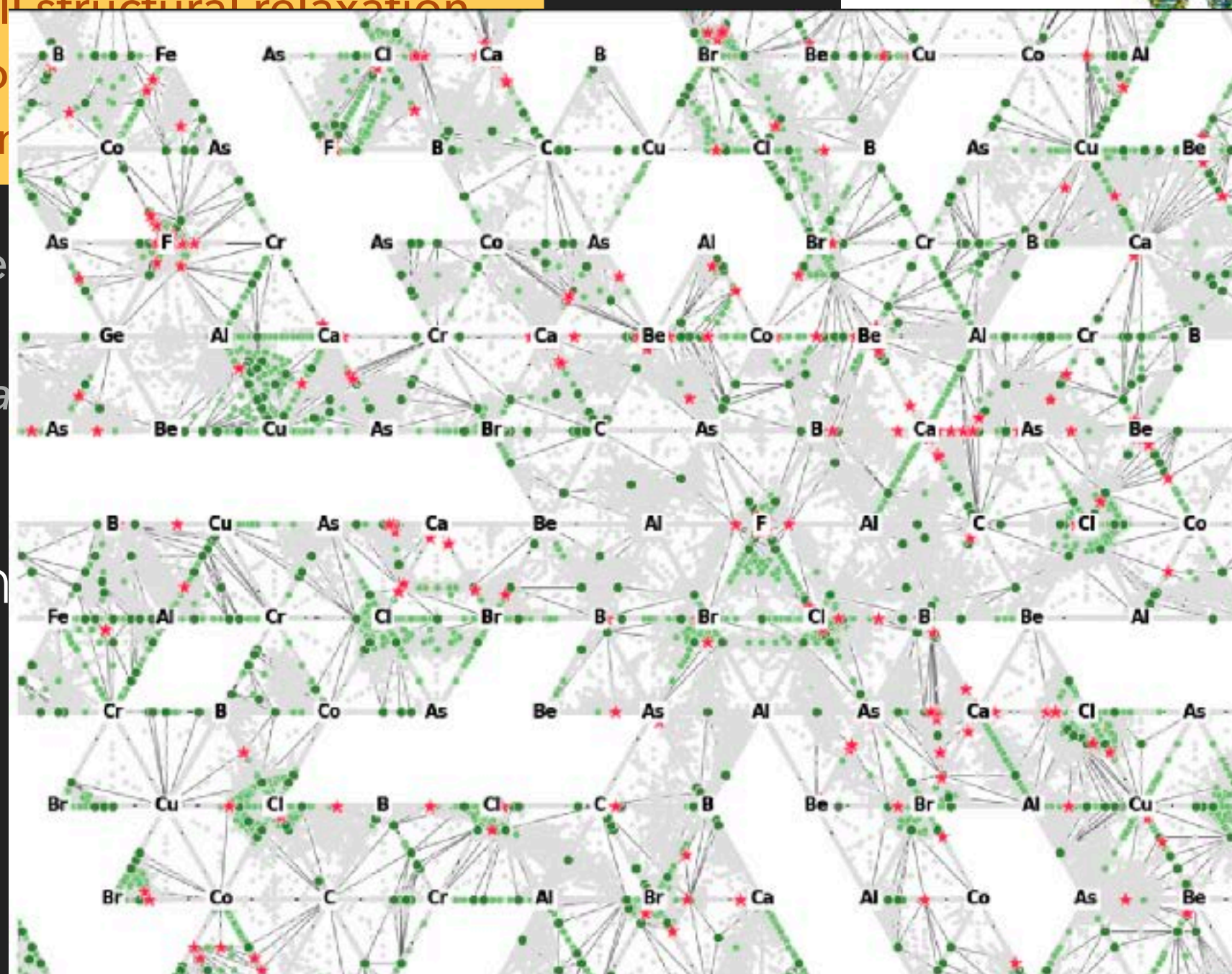


httk-symgen

> 1.2 Million full structural relaxation
> 100 Million
per day per r

Parackal, A. S., Trybel
(2026). Screening
materials discovery. a

About 40 Billion
39,357,581,710



SUMMARY

- Pressure is a powerful thermodynamic variable allowing us to find new chemistry and new (multi-) functional materials
- New (HP) materials can be extremely complex and their prediction requires new methods and strong synergy between computations and experiment
- Predictions can be strongly accelerated by performing “simple math” first on new GPU architectures
- Accelerating calculations is not the only challenge
 - Utilizing large memory GPUs efficiently for small structures is only possible via efficient batching and vectorization
 - Storage and file numbers become quickly a problem!
 - Extreme scale throughout needs to be managed

Trial and error



Efficient Exploration



Next Test: MIG (Multi-Instance GPU) orchestration