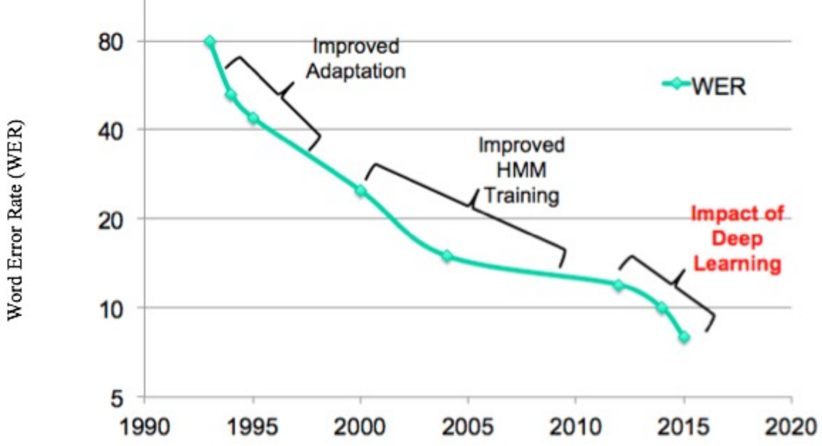
Microsoft

Deep learning for scientific computation

Max Welling
Distinguished Scientist, Microsoft Research

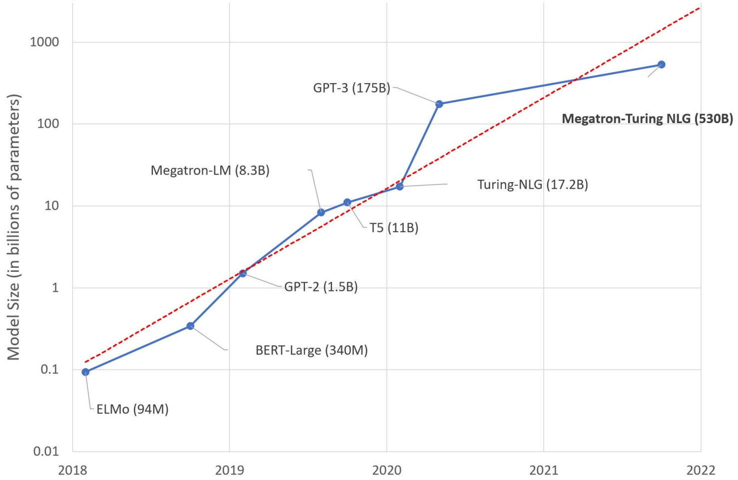
The deep learning disruption

Speech Recognition

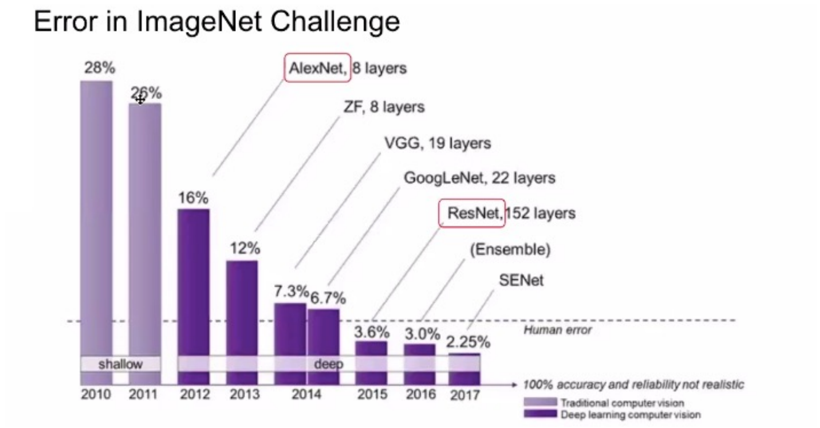


Source: Kartik Audhkhasi blog; https://minghsiehece.usc.edu/2017/04/the-machines-are-coming/

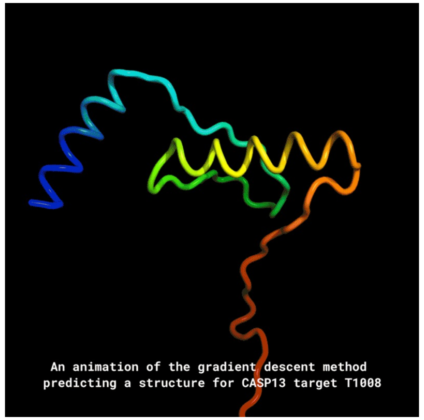
Natural Language Models



Source: https://www.microsoft.com/en-us/research/blog/using-deepspeed-and-megatron-to-train-megatron-turing-nlg-530b-the-worlds-largest-and-most-powerful-generative-language-model/



(Source: Angshuman Gosh | DLDC 2021)



Protein Folding

https://deepmind.com/blog/article/AlphaFold-Using-AI-for-scientific-discovery

Molecules

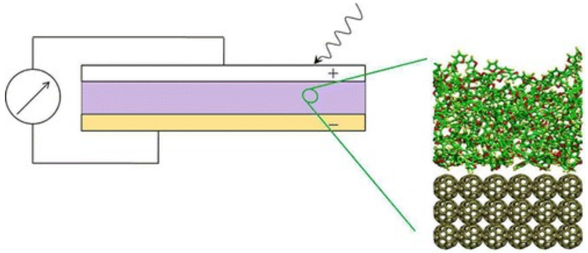
Everything material is made of molecules*

* Except 4 fundamental forces (electromagnetic force, gravity and strong & weak nuclear forces), and unless you break them up (plasma, quarks/leptons)

Molecules are at the root of solving many of the health, environmental and climate challenges we are facing today.

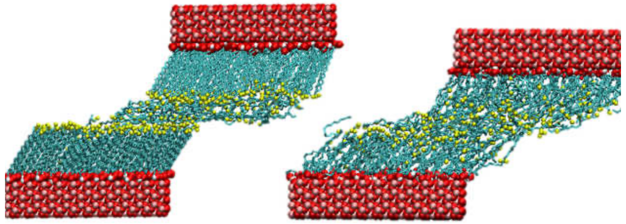
Drug discovery

Markus Reiher et al. PNAS 2017;114:29:7555-7560



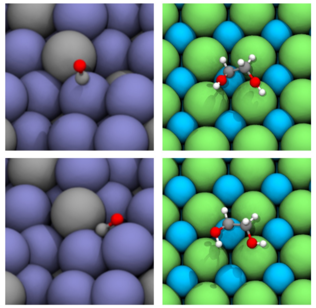
Photovoltaics

S.Y Reddy et al. Synthetic Metals 162, 23, 2012, 2117-2124



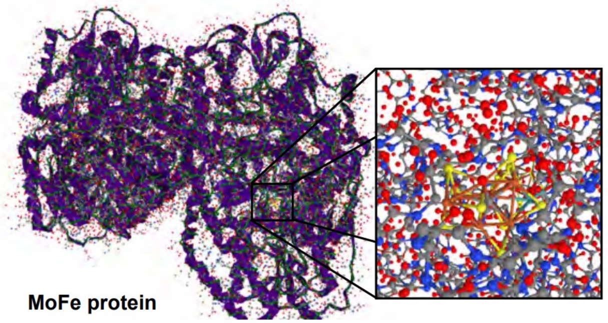
Tribology and lubricants

James Ewen, Tribology Group, Imperial College London



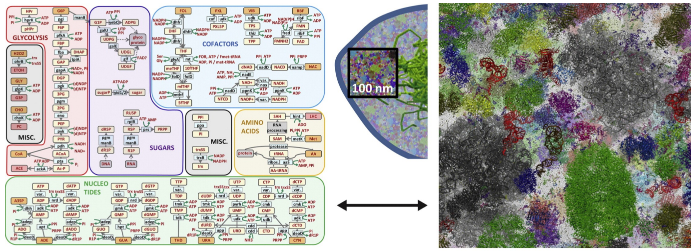
Catalyst design (e.g., fuel cells)

Lowik Chanussot et al. ACS Catal. 2021, 11, 10, 6059–6072



Nitrogen fixation

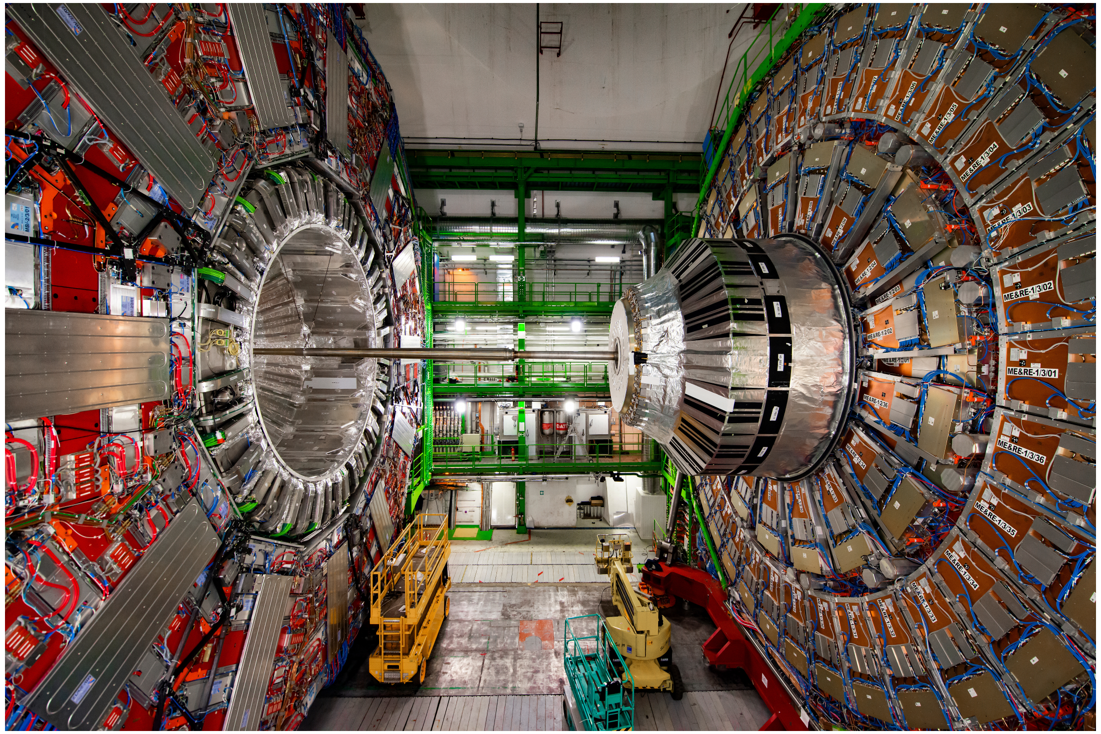
Shaher Bano Mirza et al. Journal of Molecular Graphics and Modelling 2016



Whole cell modelling

Michael Feig et al. Mol Graph Model. 2015 May ; 58: 1–9

We need a new microscope



LHC: The microscope of the particle physicists

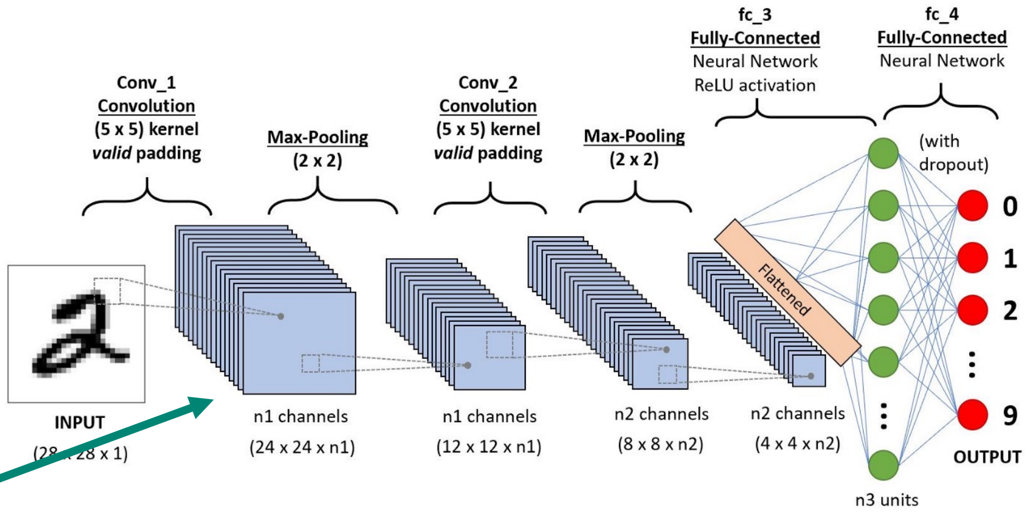
SKA: The telescope of the astronomers

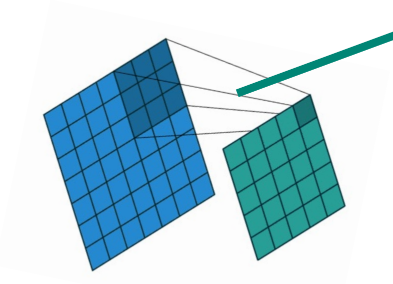
The new microscope is computational

Large scale, self-learning simulations on modern supercomputers

Deep learning and GNNs

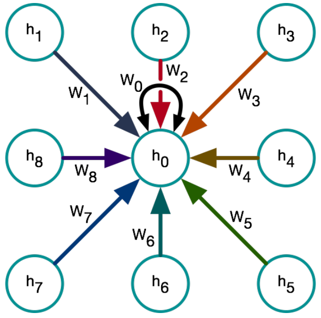
Convolutional Neural Network



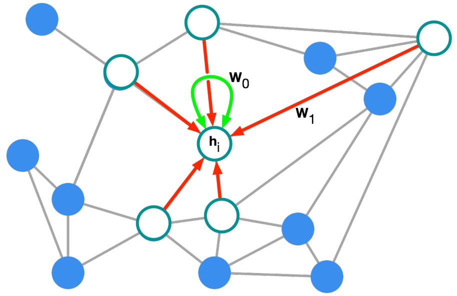


Convolution

Convolution as message passing

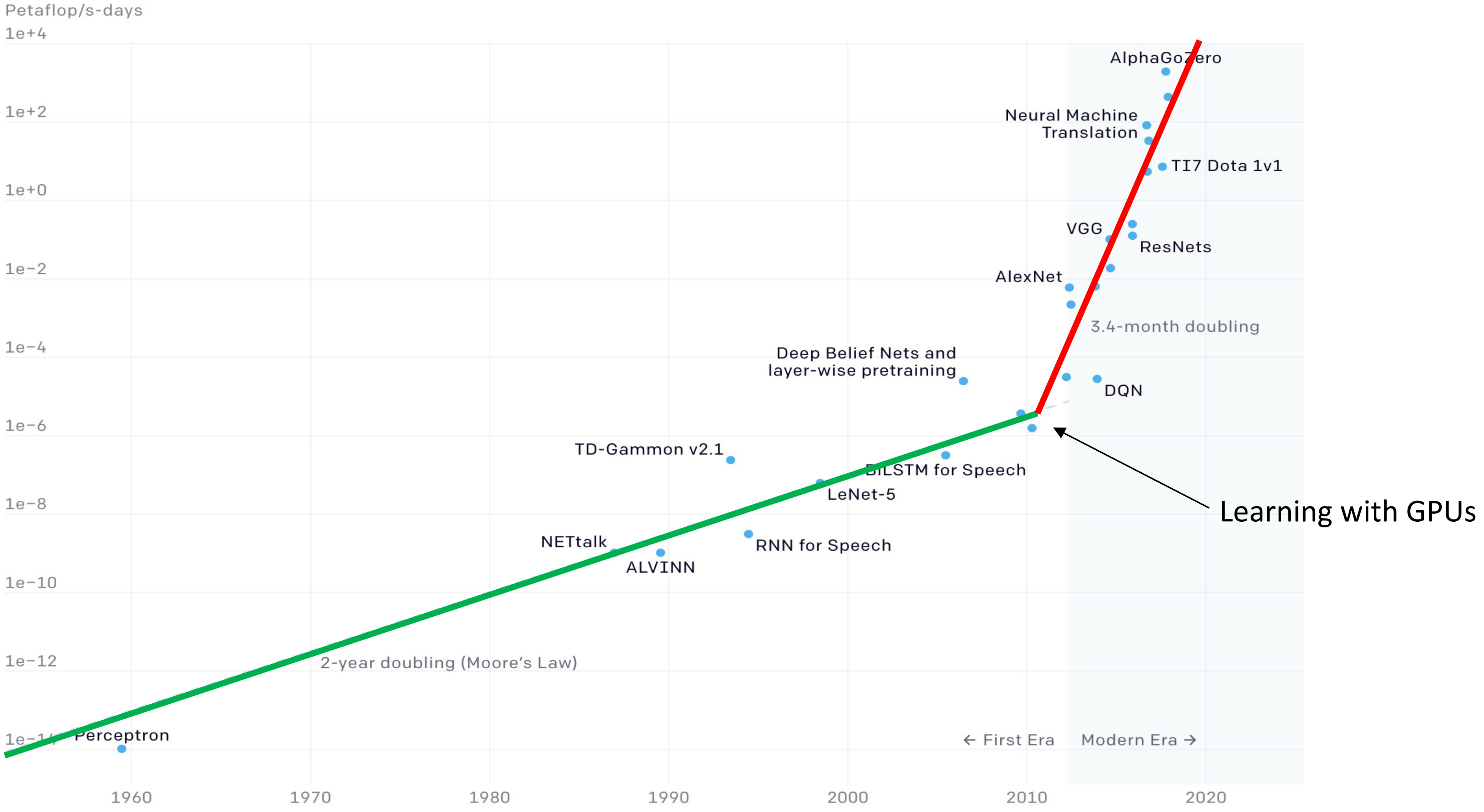


Graph convolution



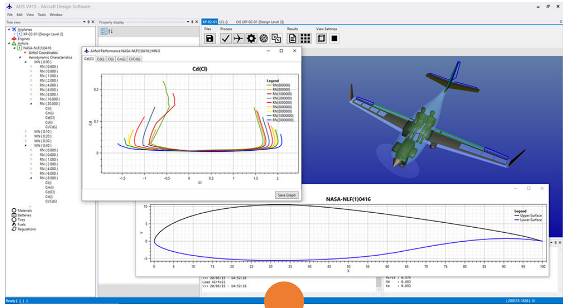
Convolution on a set

Moore's Law for Deep Learning



A new paradigm?

COMPUTATIONAL COMPLEXITY



OAD ADS

NASA

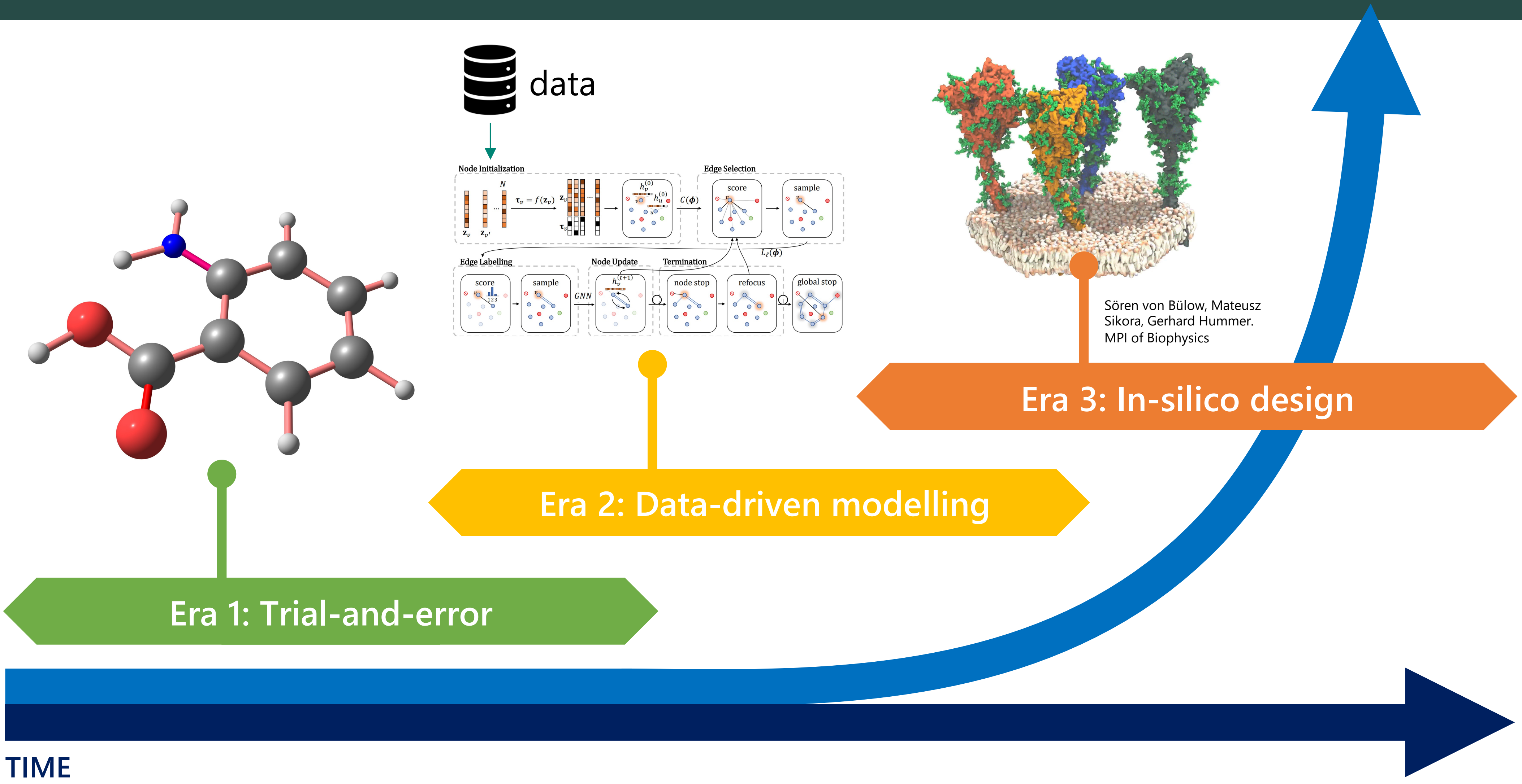
Era 3: In-silico design

Era 2: Data-driven modelling

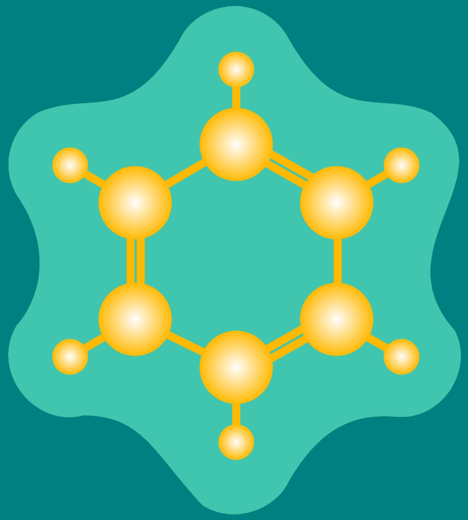
Era 1: Trial-and-error

TIME

Molecules and materials design

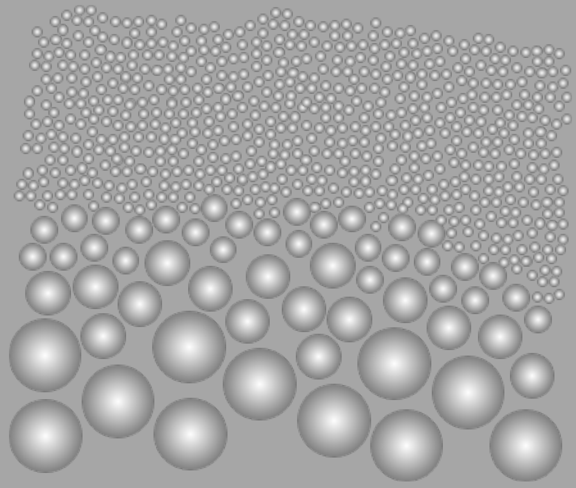


Three key challenges



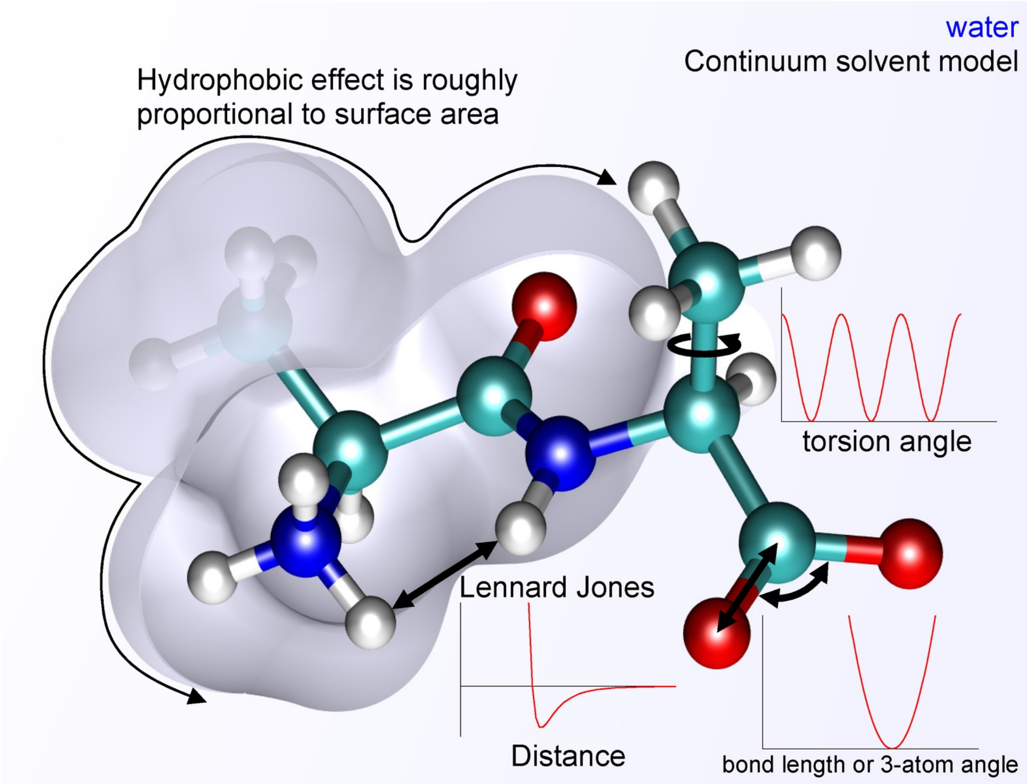
More accurate simulations (simulating quantum mechanics)

Faster simulations (from femtoseconds to microseconds)

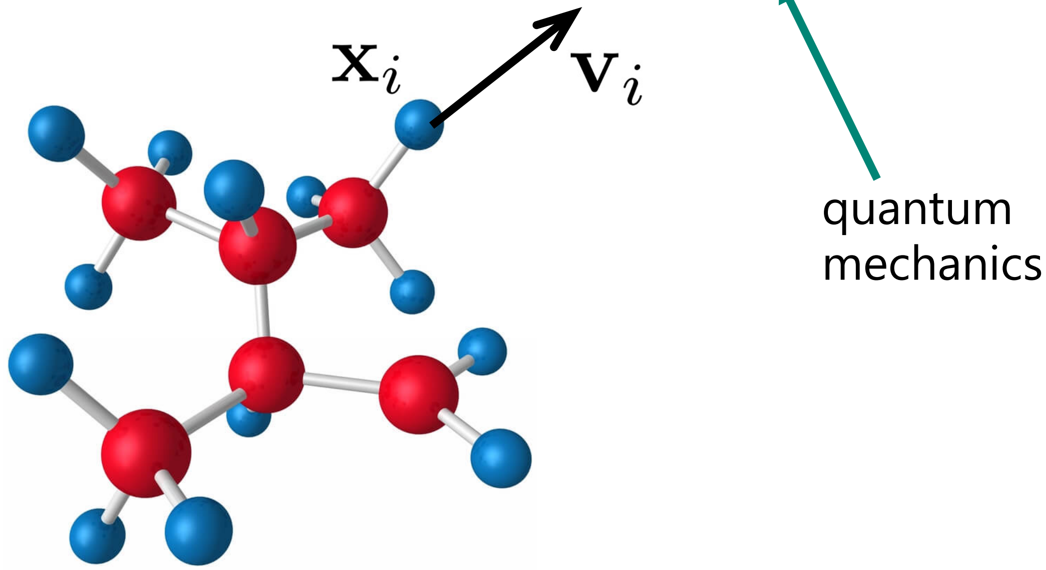


Scaling to large system sizes: billions of atoms (bacteria)

Simulating molecules



$$\frac{d\mathbf{x}_i}{dt} = \mathbf{v}_i$$
$$m_i \frac{d\mathbf{v}_i}{dt} = -\nabla_i U(\mathbf{x}_1, \ldots, \mathbf{x}_N)$$

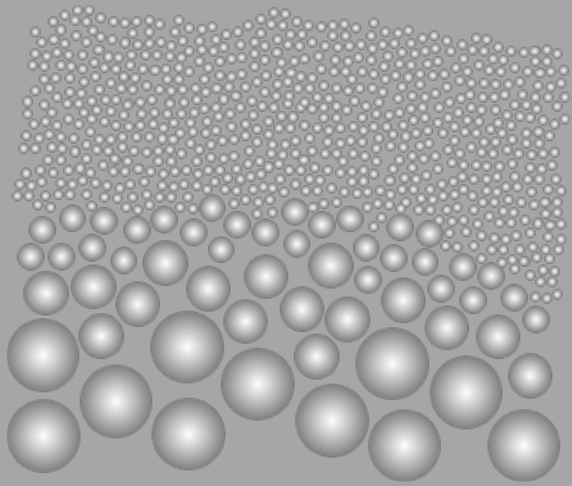


Opportunity: Use ML to learn forces on atoms due to electronic structure (usually computed though DFT)

Three key challenges

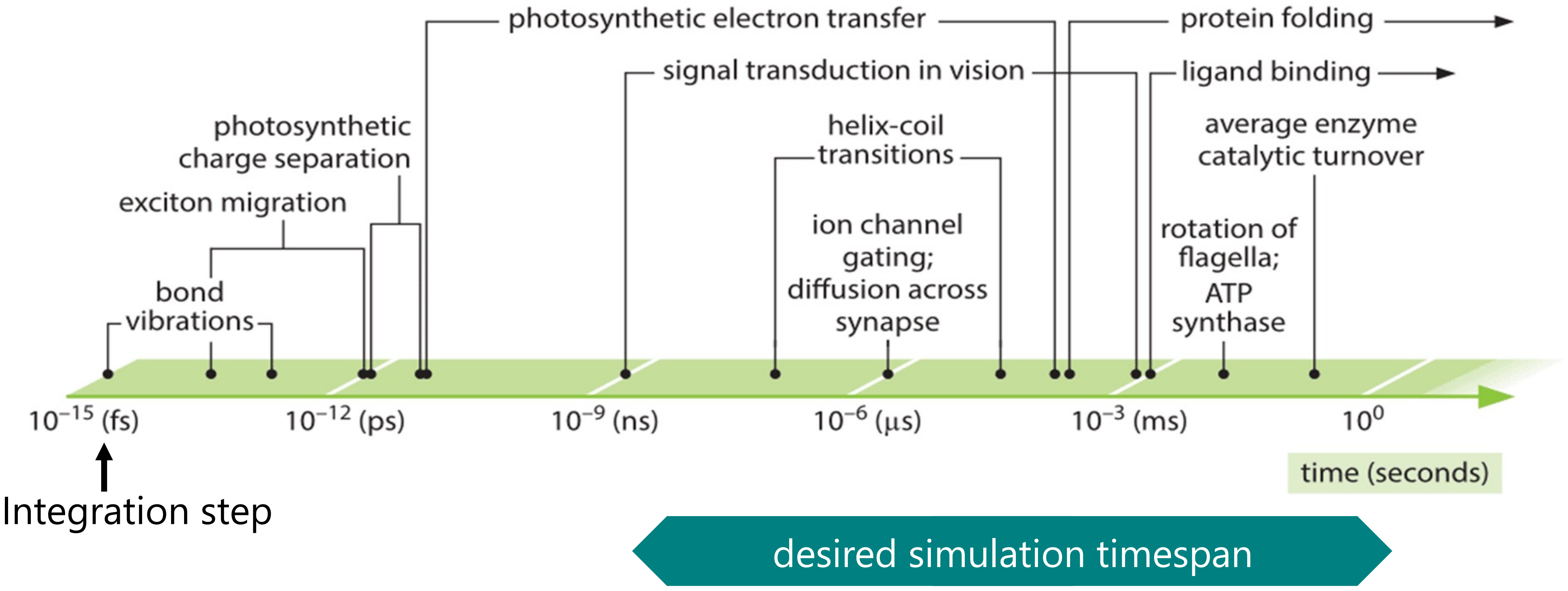
More accurate simulations (simulating quantum mechanics)

Faster simulations (from femtoseconds to microseconds)



Scaling to large system sizes: billions of atoms (bacteria)

Curse of sequentiality



Simulations with current MD technology require 10^6 to 10^{15} sequential steps.
But: chips no longer become faster for sequential computation.

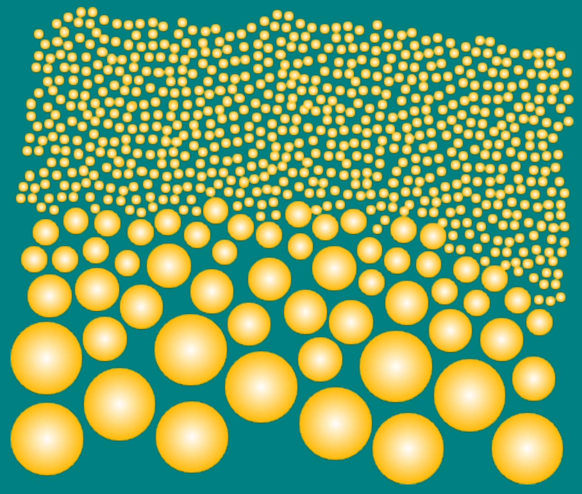
Figure from "Cell Biology by the numbers"

Opportunity: Use ML to increase the integration steps in molecular dynamics simulations.

Three key challenges

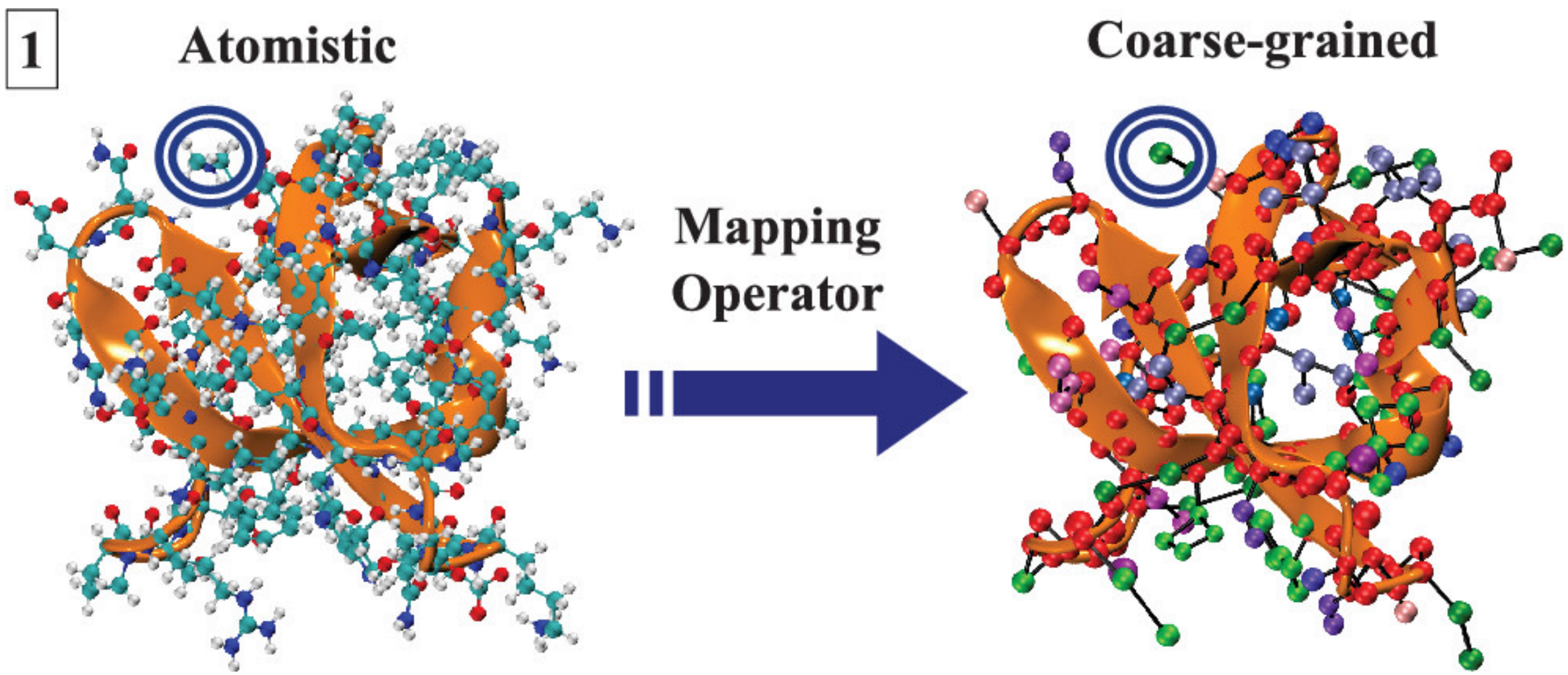
More accurate simulations
(simulating quantum mechanics)

Faster simulations
(from femtoseconds to microseconds)



Larger simulations
(from a dozen atoms to billions of atoms)

Coarse graining methods



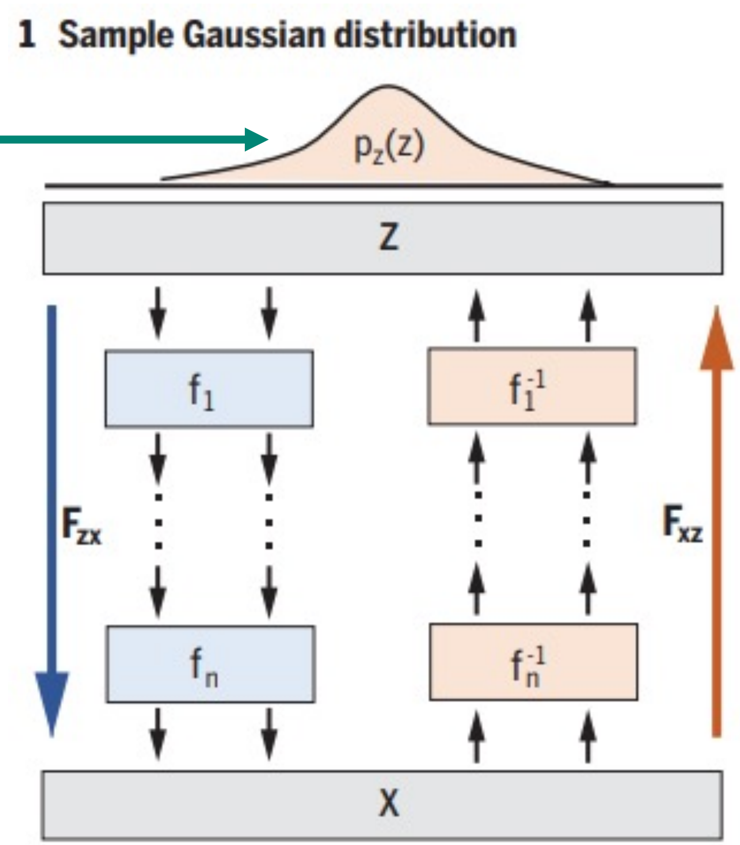
W.G. Noid, **Perspective: Coarse-grained models for biomolecular systems**

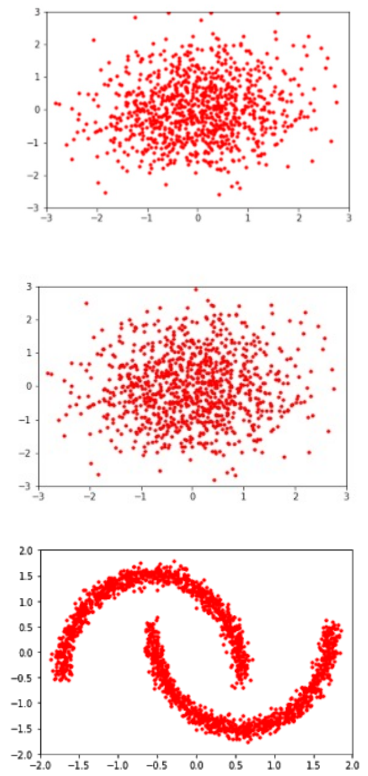
J. Chem. Phys. **139**, 090901 (2013); https://doi.org/10.1063/1.4818908

Opportunity: Use ML to learn to coarse grain

In silico molecule synthesis

Condition on desired properties





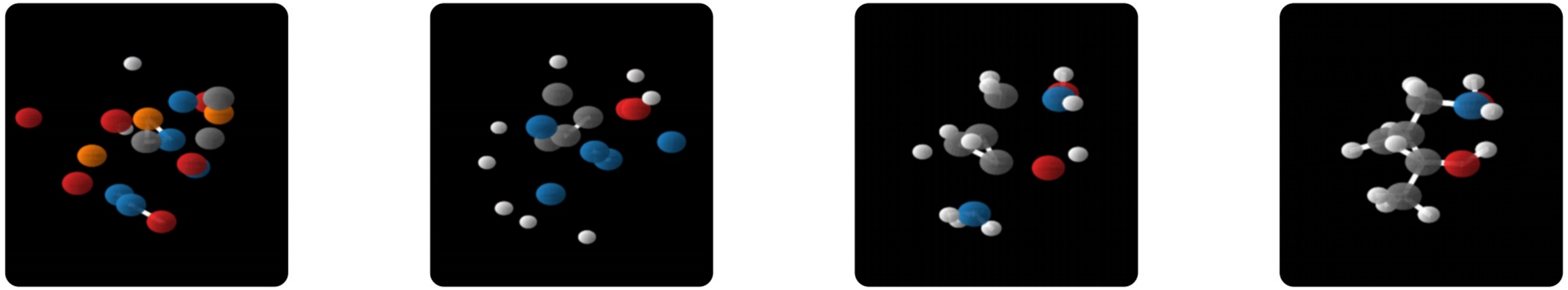
Opportunity: Use ML to learn to generate molecules with prescribed properties

Molecule generation with equivariant GNNs

E(n) Equivariant Normalizing Flows

NeurIPS 2021 · Victor Garcia Satorras, Emiel Hoogeboom, Fabian B. Fuchs, Ingmar Posner, Max Welling

$\mathcal{N}(0, \mathrm{I})$ $\quad\quad$ $p_V(\mathbf{x}, \mathbf{h})$



$g_\theta : \mathbf{z}_x, \mathbf{z}_h \mapsto \mathbf{x}, \mathbf{h}$

Molecule generation

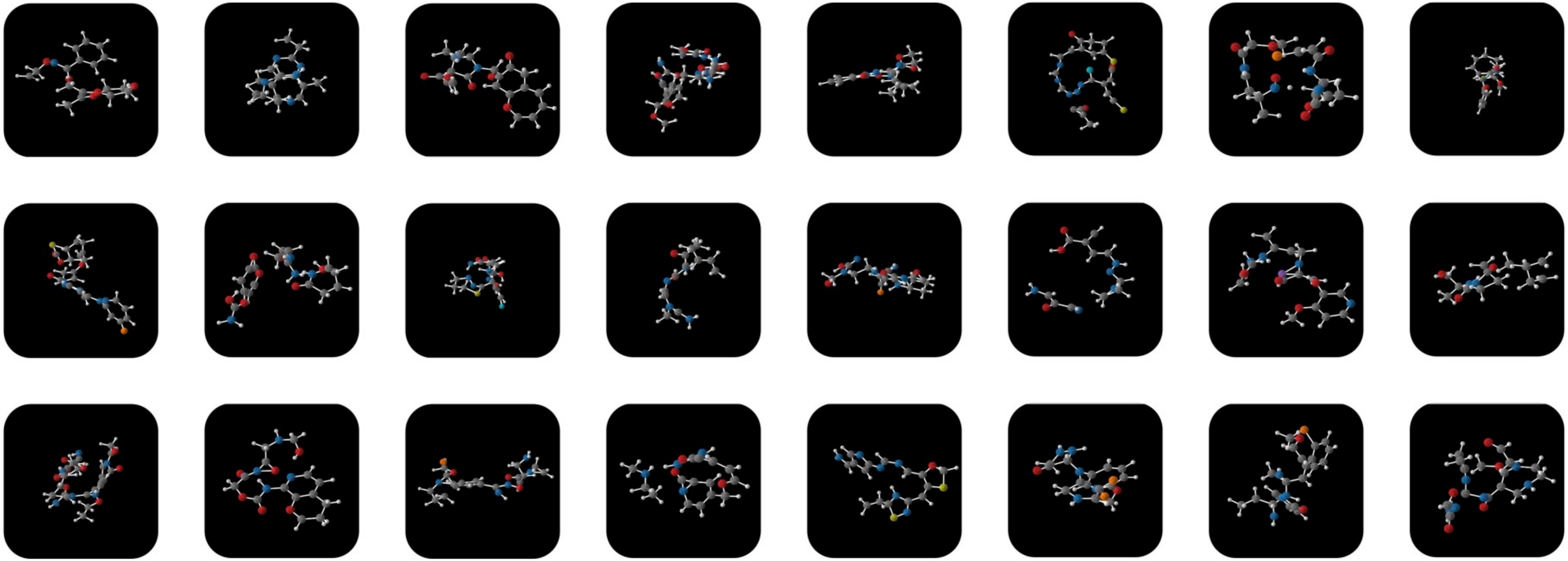


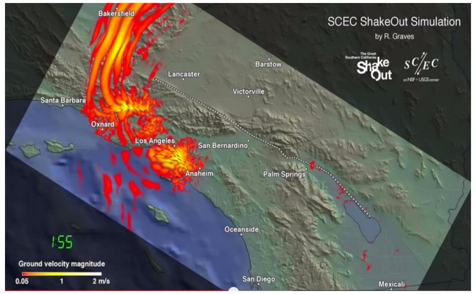
Figure 7. Random samples taken from the EDM trained on geom drugs.

Equivariant Diffusion for Molecule Generation in 3D

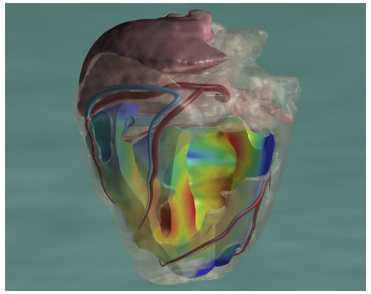
Emiel Hoogeboom [*1] Victor Garcia Satorras [*1] Clément Vignac [*2] Max Welling [1]

Partial differential equations

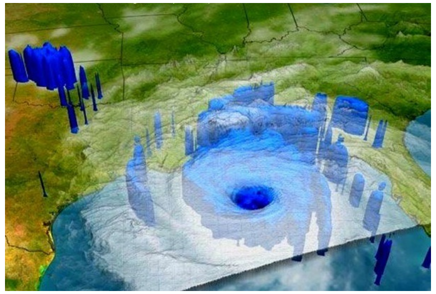
PDEs and ODEs are used throughout the sciences to describe the evolution of systems of interest.



Earthquakes

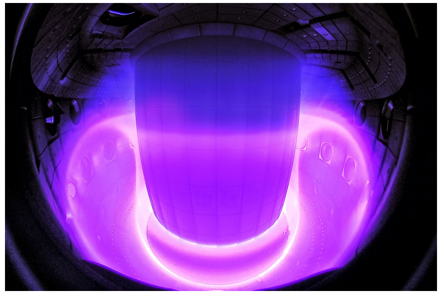


Heart dynamics

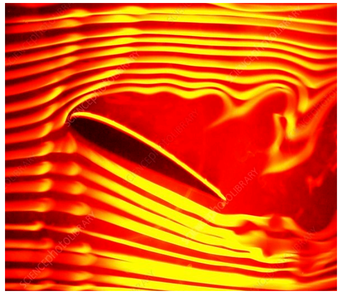


Weather prediction

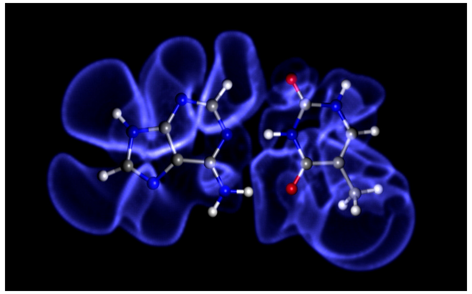
Galaxy collisions



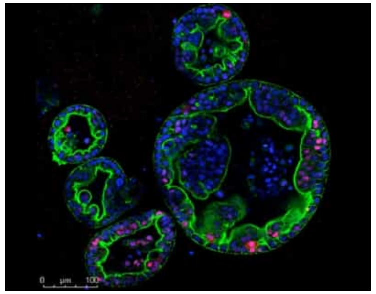
Plasma physics



Airplane design



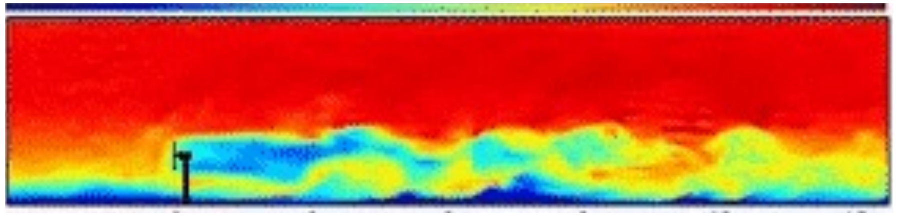
Electronic structure

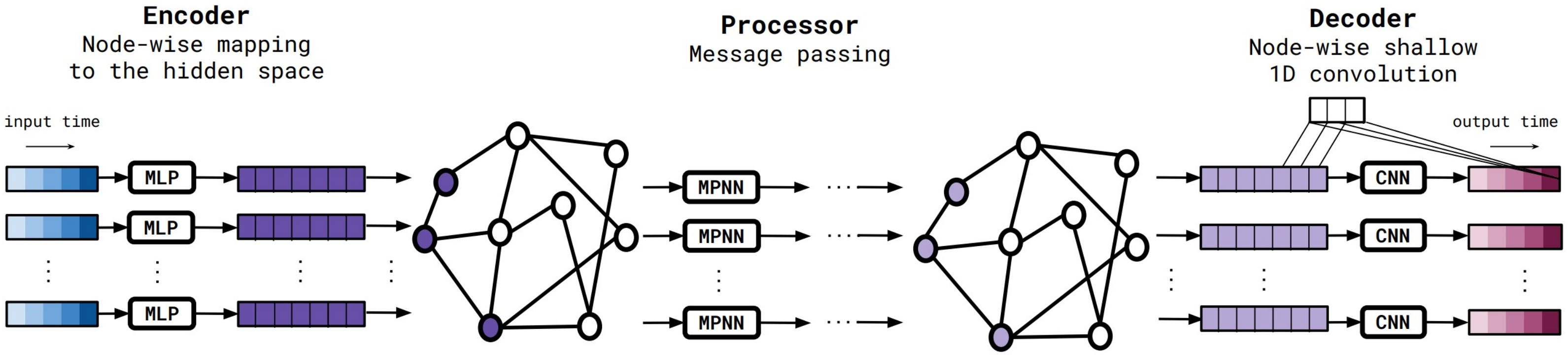


Tumor development

Solving PDEs with GNNs

- Accurate numerical integration is slow and tedious.
- Deep learning shows great promise for solving PDEs.





MESSAGE PASSING NEURAL PDE SOLVERS

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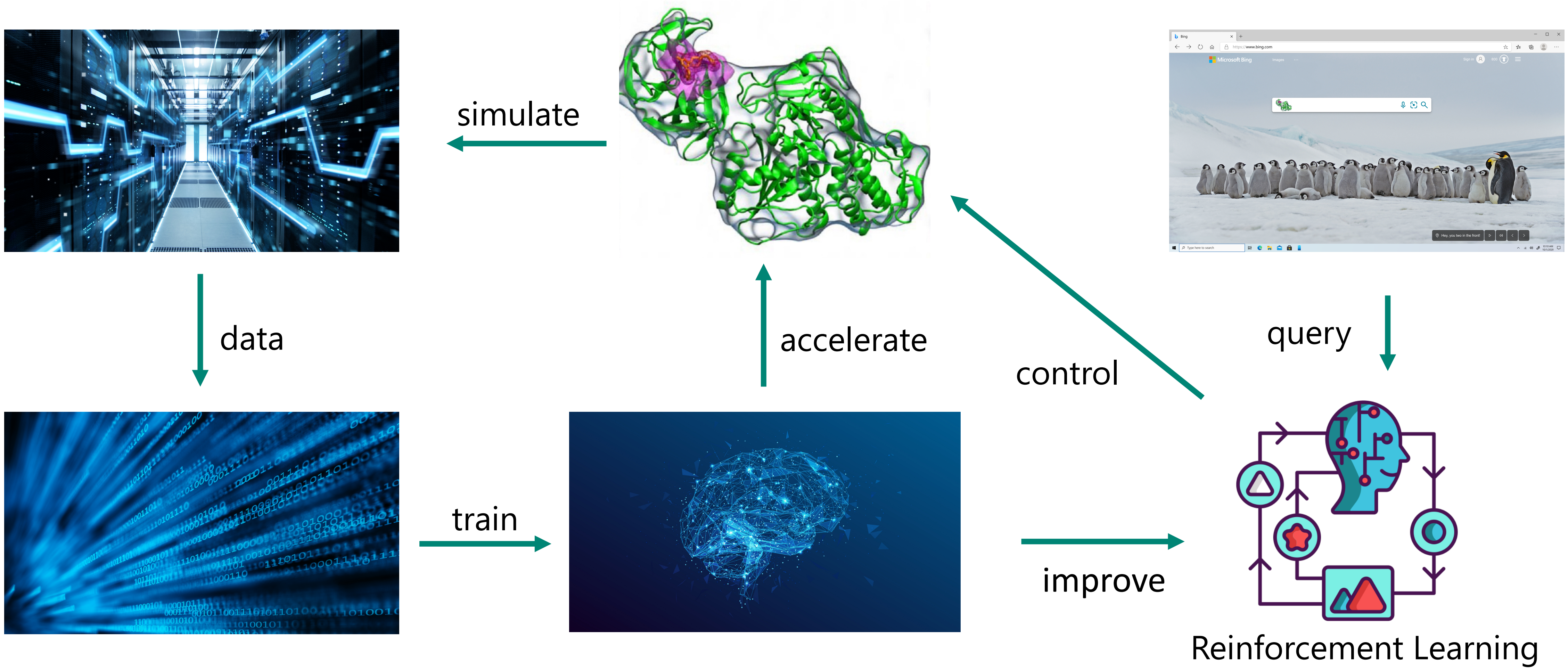
Opportunity: Use ML to learn to numerically solve PDEs.

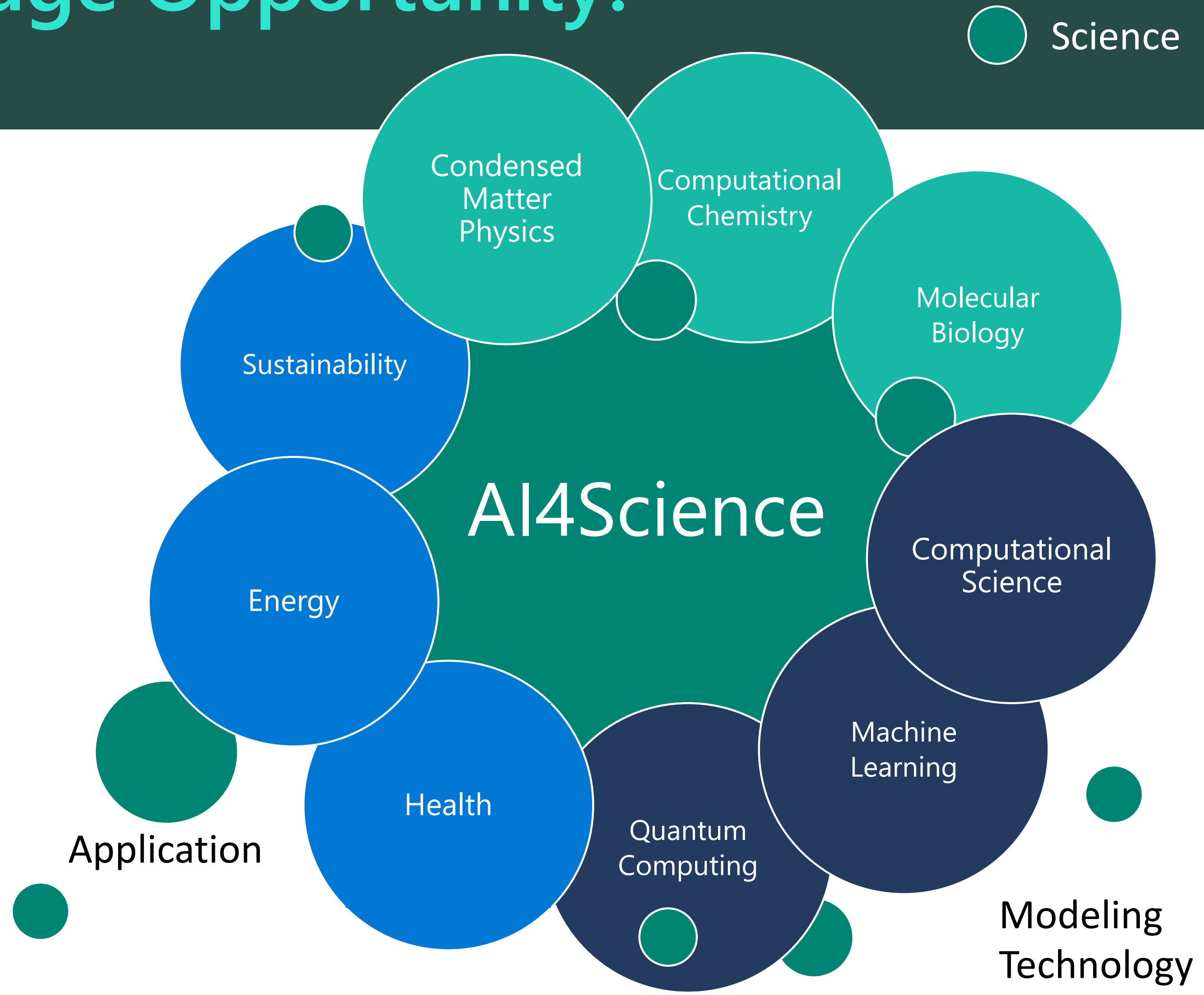
A search engine for molecules?



Opportunity: Build a search engine for chemical space

Why AI4Science? A Huge Opportunity!

- A convergence of science, modelling technology and applications!
- A "golden age" of designing new materials/chemicals/catalysts/drugs?
- A Cambrian explosion of new materials?



Microsoft Research Amsterdam

Thank you for your attention. Questions?