

Machine learning for physicists

<https://github.com/wangleiphy/ml4p>

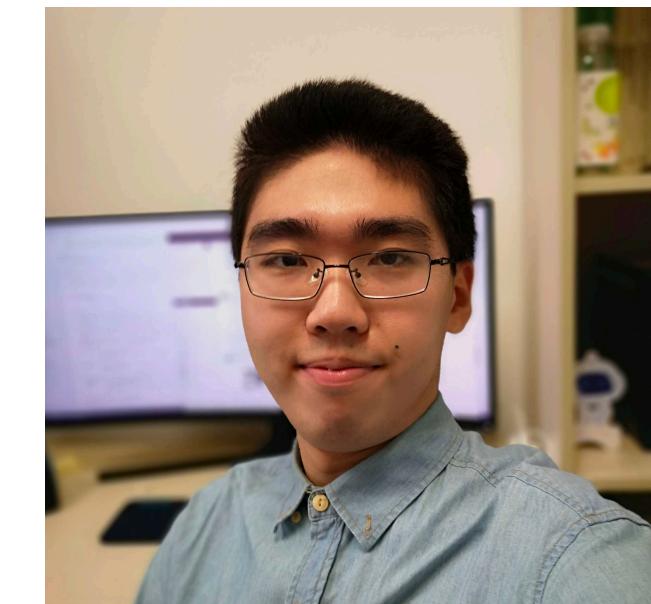
每周四上午10点

课程微信群

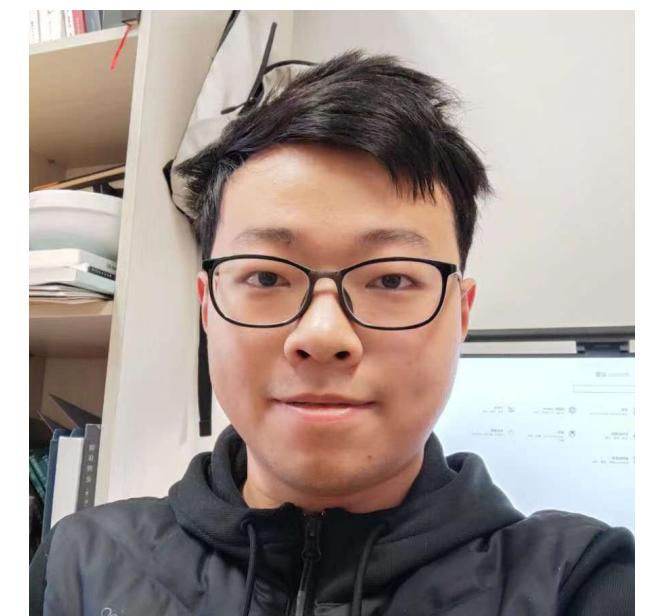
2.23	Overview
3.2	Machine learning practices
3.9	A hitchhiker's guide to deep learning
3.16	Research projects hands-on
3.23	Symmetries in machine learning
3.30	Differentiable programming
4.6	Generative models-I
4.13	Generative models-II
4.20	Research projects presentation
4.27	AI for science: why now ?



助教



李子航

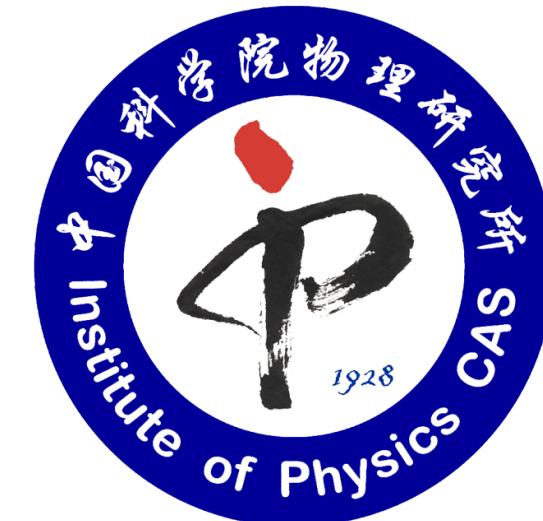


李扬帆

考核方式: project + presentation (1学分)

AI for science: why now ?

Lei Wang (王磊)
Institute of Physics, CAS
<https://wangleiphy.github.io>

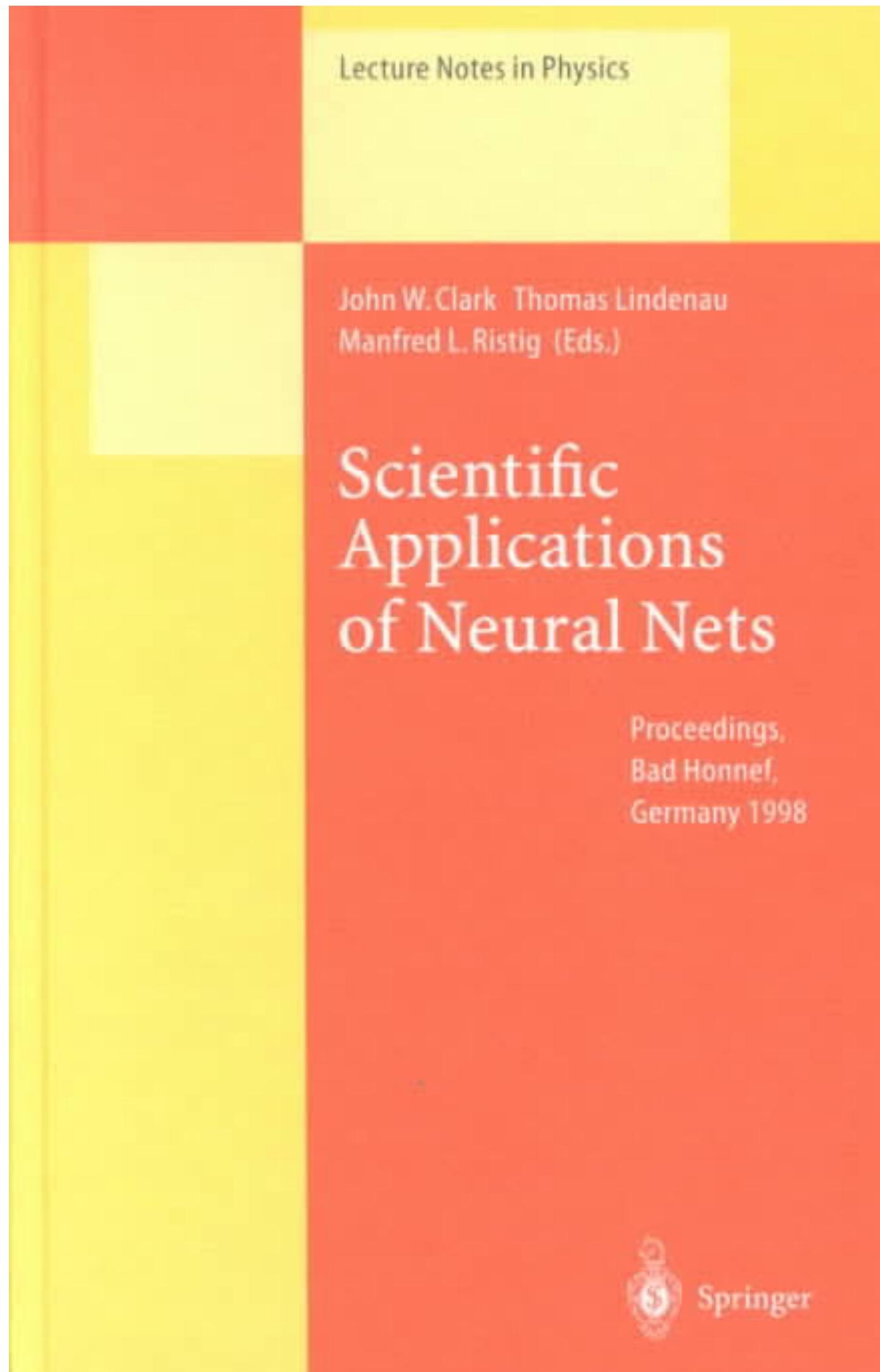




EPFL
AI4Science
initiative



AI for science: 25 years ago



8 Doing Science With Neural Nets: Pride and Prejudice

When neural networks re-emerged on the scene in the mid-80s as a new and glamorous computational paradigm, the initial reaction in some sectors of the scientific community was perhaps too enthusiastic and not sufficiently critical. There was a tendency on the part of practitioners to oversell the

:

In conclusion, as a methodology for classification or function approximation in scientific problems, computational analysis based on neural networks is expected to prove most valuable in applications for which (i) the data set is large and complex, (ii) there is as yet no coherent theory of the underlying phenomenon, or quantitative theoretical explication is impractical,

Why now, again ?
What has changed ?
What has not ?

Science is more than fitting, so is machine learning

Discriminative learning



Generative learning



$$y = f(x)$$

or $p(y | x)$

$$p(x, y)$$

The swing of deep learning

generative representation learning



2010

ReLU, Batchnorm,
ResNet ...

2006 deep belief net

2020 **G**enerative **P**re-**T**raining

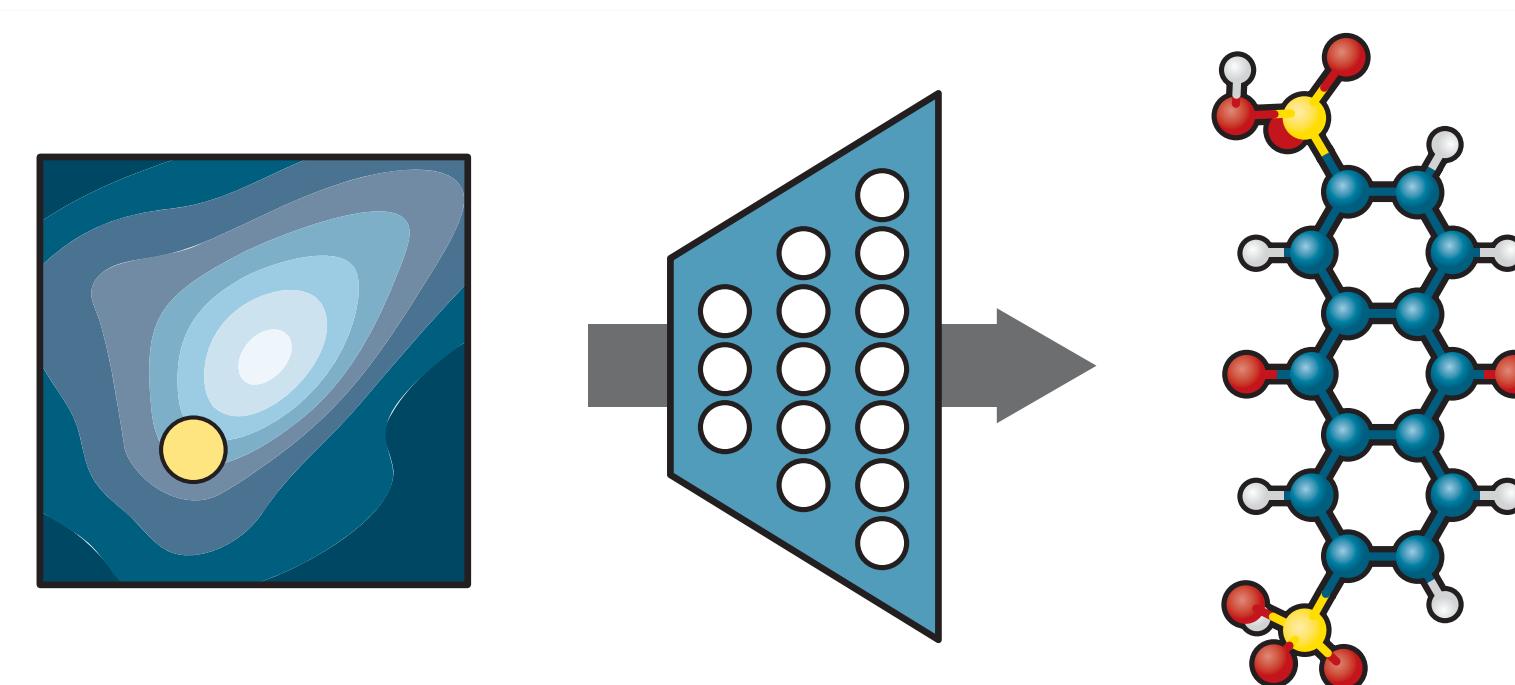
Generative AI for Science

1

How to Build a GPT-3 for
Science

Scientific language model

2



Matter inverse design

3

$$F = E - TS$$

Nature's cost function

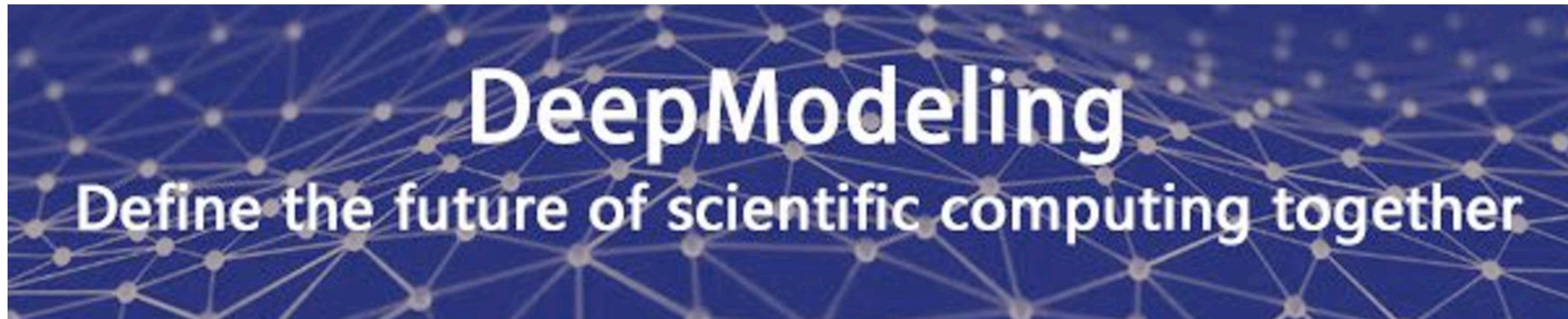
The Universe as a generative model

$$S = \int d^4x \sqrt{-g} \left[\frac{m_p^2}{2} R - \frac{1}{4} F_{\mu\nu}^a F_a^{\mu\nu} + i \bar{\psi}^i D_\mu \psi^i + \left(\bar{\psi}_L^i V_{ij} \not{D} \psi_R^j + h.c. \right) - |D_\mu \not{\Phi}|^2 - V(\not{\Phi}) \right]$$



Discovering physical laws: **learning** the action
Solving physical problems: **optimizing** the action

Open source/model facilities



A screenshot of a GitHub repository card for **CompVis/stable-diffusion-v1-4**. The card includes the repository name, a 'like' button with 3.09k likes, and several tags: Text-to-Image, Diffusers, arxiv:2207.12598, arxiv:2112.10752, arxiv:2103.00020, arxiv:2205.11487, arxiv:1910.09700, stable-diffusion, stable-diffusion-diffusers, and License: creativeml-openrail-m. A smiling emoji with hands clasped is on the right.

Open benchmarks

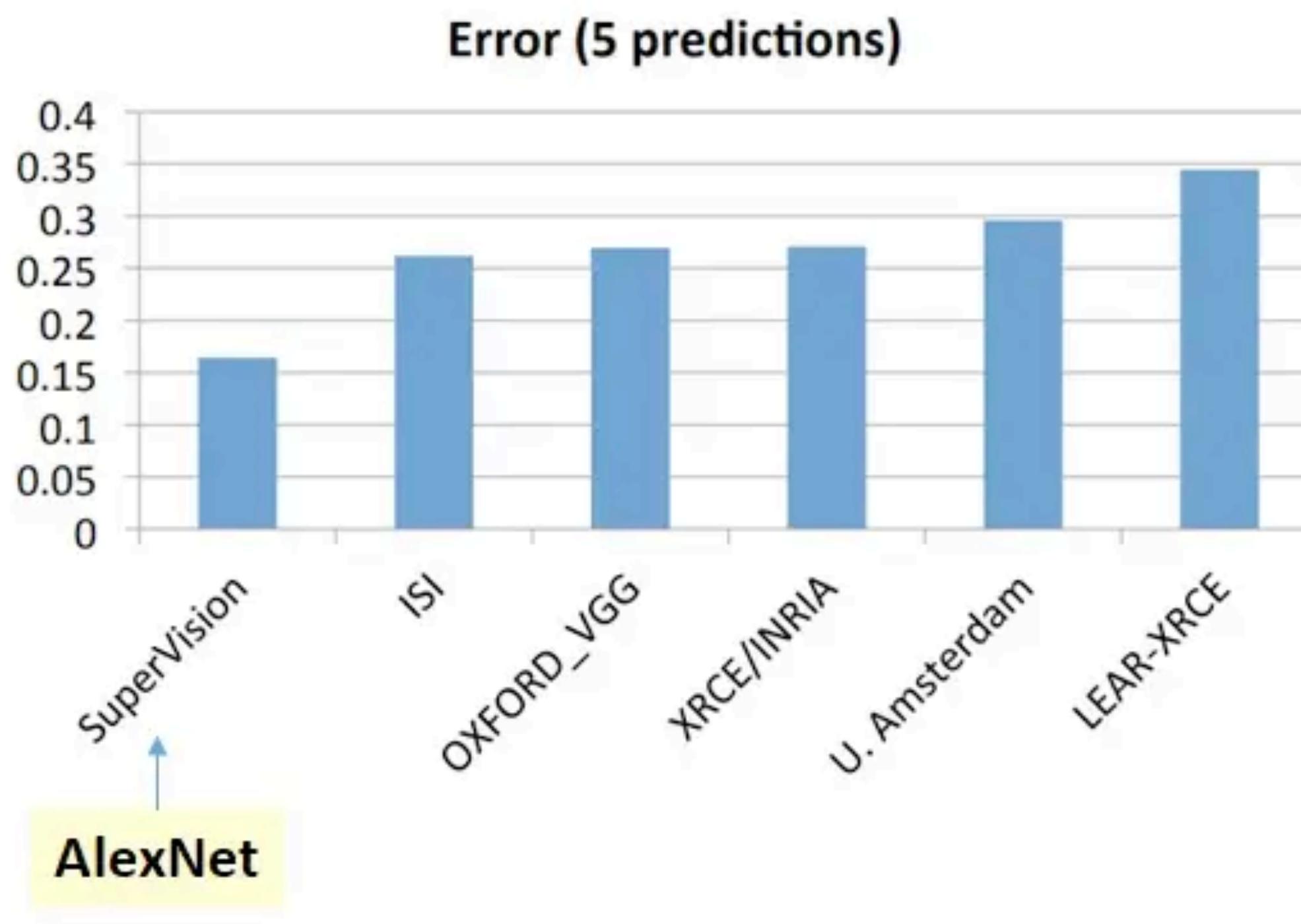
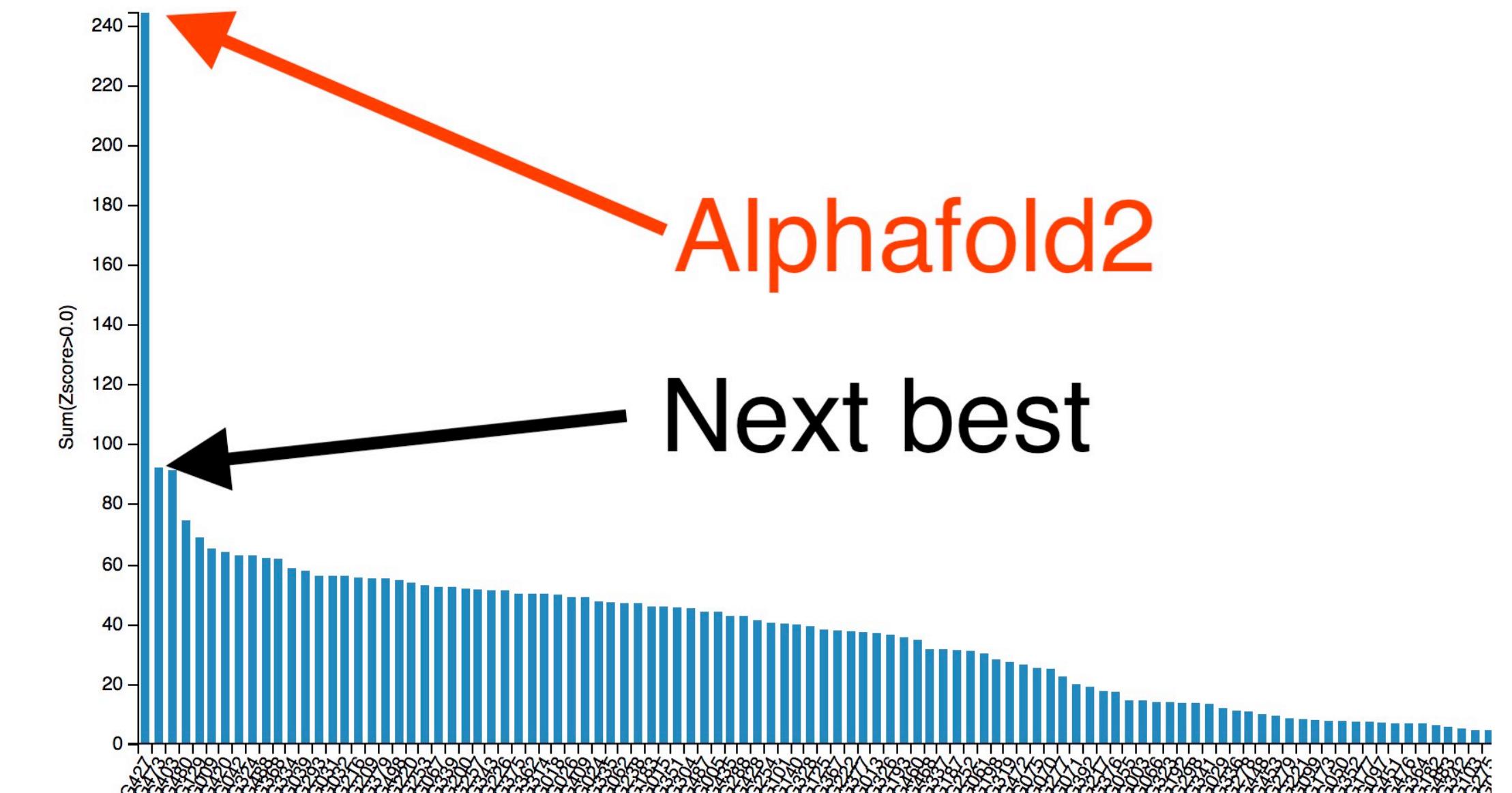


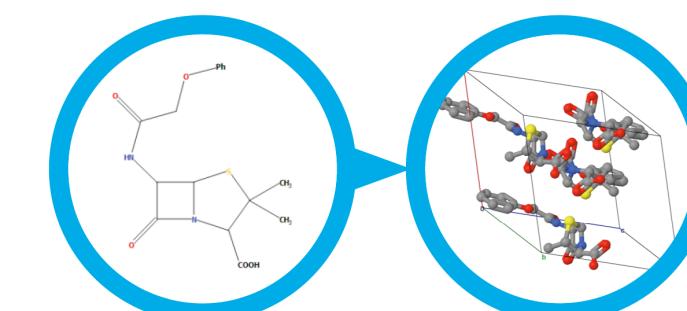
Image recognition: ILSVRC 2012

“The imagenet moment”



Protein structure prediction: CASP14

kaggle



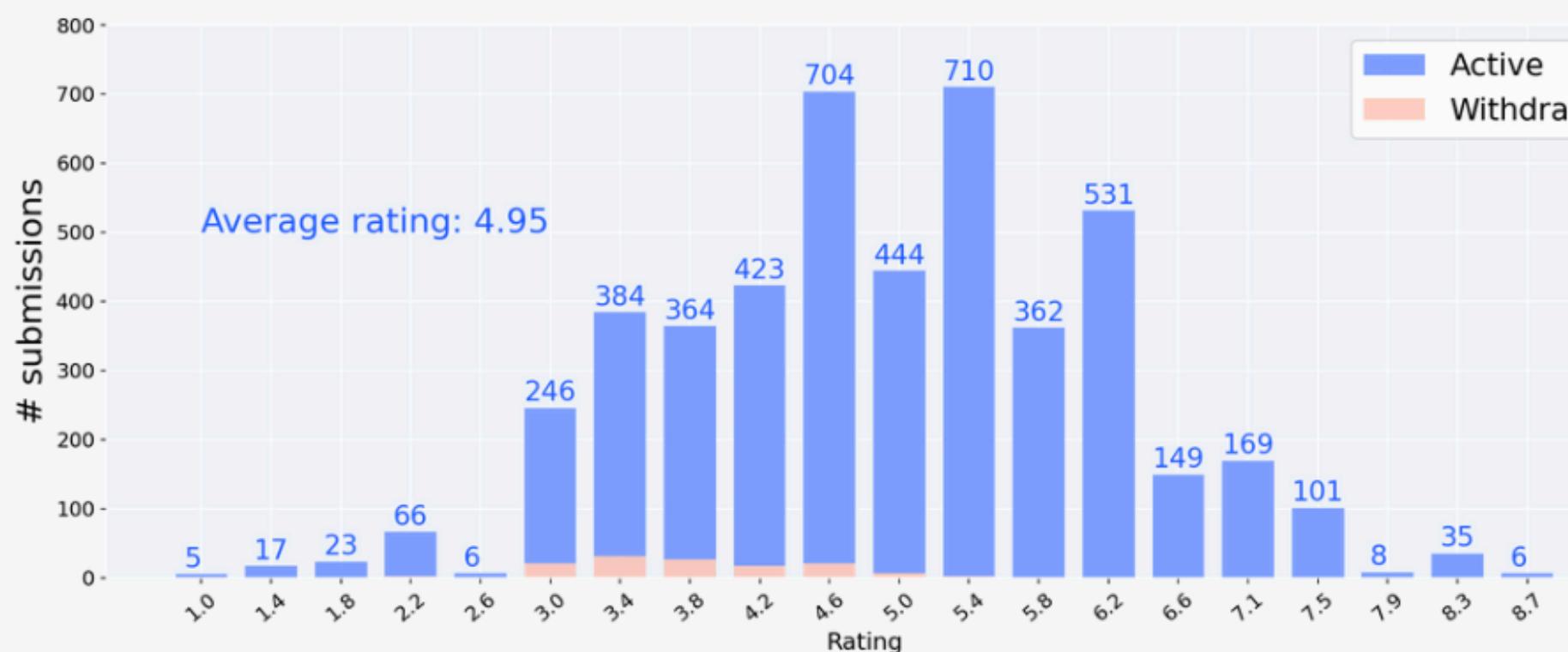
CSP
blind test

Open review

ICLR 2023 Statistics

Github

👉 Rating distribution.



Open
Review
.net

Add Public Comment

Reply Type: all Author: everybody Visible To: all readers Hidden From: nobody

👉 R1 : ratings @2022-11-05-18:22-UTC.

👉 ICLR 2022 statistics.

All Accepted

Oral

Spotlight

Poster

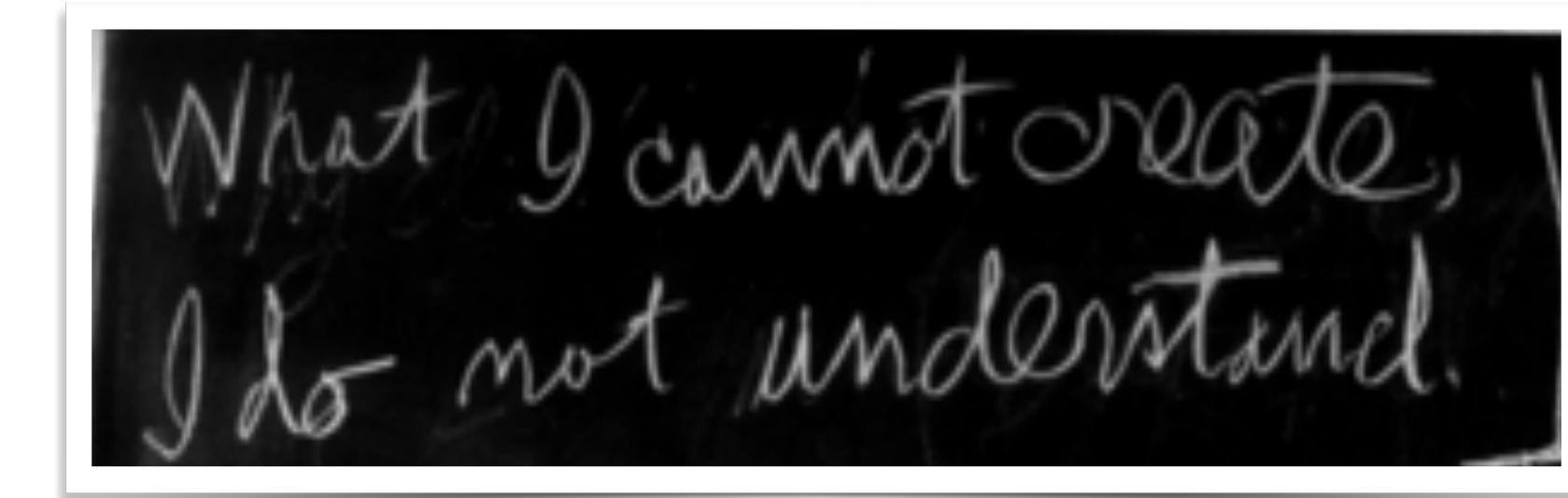
Rejected

Statistics

# (4753)	Title	R1	std	Ratings
1	Git Re-Basin: Merging Models modulo Permutation Symmetries	8.67	0.94	10, 8, 8
2	Rethinking the Expressive Power of GNNs via Graph Biconnectivity	8.67	0.94	10, 8, 8
3	Emergence of Maps in the Memories of Blind Navigation Agents	8.50	0.87	8, 8, 8, 10

AI for science: why now?

① Generative AI

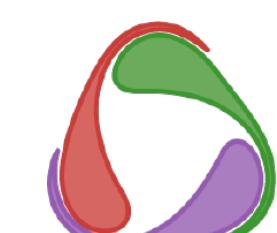
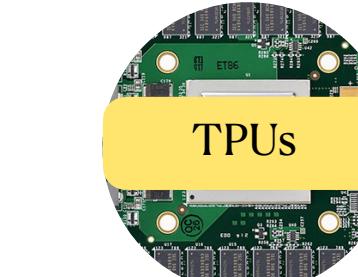


② Open source/model/data/
benchmark/review/...



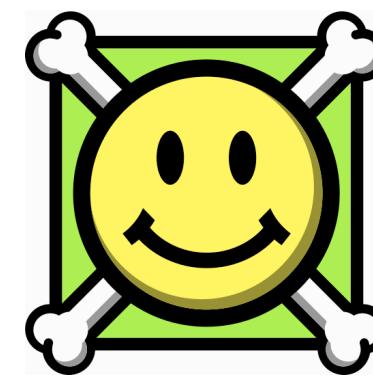
...

data/hardware/software/...



...

Data: we live in a digital age



Hardware

Tensor Processing Units as Quantum Chemistry Supercomputers

Ryan Pederson,^{1, 2, 3} John Kozlowski,^{4, 2, 3} Ruyi Song,^{5, 2, 3} Jackson Beall,³ Martin Ganahl,³ Markus Hauru,³ Adam G.M. Lewis,³ Shrestha Basu Mallick,^{2, 3} Volker Blum,^{5, 6} and Guifre Vidal^{2, 3, 7}

¹*Department of Physics and Astronomy, University of California, Irvine, CA 92617, USA*

²*X, the Moonshot Factory, Mountain View, CA 94043, USA*

³*Sandbox@Alphabet, Mountain View, CA 94043, USA*

⁴*Department of Chemistry, University of California, Irvine, CA 92617, USA*

⁵*Department of Chemistry, Duke University, Durham, NC 27708, USA*

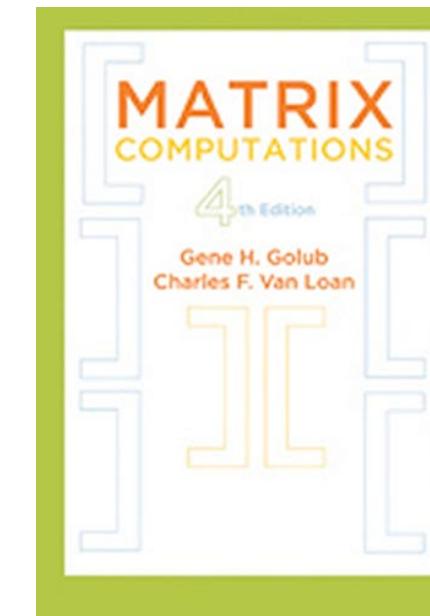
⁶*Thomas Lord Department of Mechanical Engineering and Materials Science, Duke University, Durham, NC 27708, USA*

⁷*Google Quantum AI, Mountain View, CA 94043, USA*

(Dated: February 4, 2022)

We demonstrate the use of Google’s Tensor Processing Units (TPUs) to both accelerate and scale up density functional theory (DFT) calculations of electronic structure. Utilizing 512 TPU v3 cores, we perform the largest $O(N^3)$ DFT computation to date, with $N = 247\,848$ orbitals, corresponding to a cluster of over 10 000 water molecules with more than 100 000 electrons. A full TPU v3 pod (2048 TPU v3 cores) and a TPU v4 pod (8192 TPU v4 cores) are projected to handle up to $N \approx 500\,000$ and $N \approx 1\,000\,000$ orbitals respectively. Lower-scaling (e.g. linear-scaling) variants of DFT can consider even larger numbers of orbitals, although they often only work for restricted classes of systems, such as insulating systems, require additional approximations and incur increased code complexity. As a result, when computationally affordable, cubic-scaling DFT as considered here is preferable due to its algorithmic simplicity and more general applicability. Our work thus paves the way towards systematic use of conventional –and more broadly and straightforwardly applicable– $O(N^3)$ DFT at unprecedented scales, with potential impact in areas such as quantum chemistry, drug discovery, materials science, and nanotechnology.

Pederson et al, 2202.01255



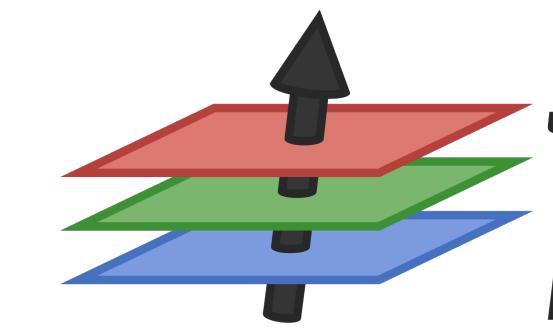
- [35] Martin Ganahl et al., “Tensor Processing Units for Simulating Quantum Circuits,” *in preparation*.
- [36] Ross Shillito, Alexandru Petrescu, Joachim Cohen, Jackson Beall, Markus Hauru, Martin Ganahl, Adam G. M. Lewis, Alexandre Blais, and Guifre Vidal, “Classical simulation of superconducting quantum hardware using Tensor Processing Units,” *in preparation*.
- [37] Martin Ganahl et al., “Density Matrix Renormalization Group using Tensor Processing Units,” *in preparation*.
- [62] John Kozlowski et al., “Full protein density functional theory with Tensor Processing Units,” *in preparation*.
- [63] Ruyi Song et al., “Accelerated quantum chemistry calculations with Tensor Processing units: from Biology to Materials Science,” *in preparation*.

Differentiable programming tools

HIPS/autograd



TensorFlow



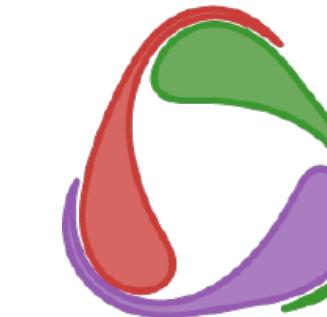
flux

PyTorch



[M]^s

MindSpore



SciML



NiLang

Differentiation tensor operations on hardware accelerators

Differentiable Programming Tensor Networks

Hai-Jun Liao,^{1,2} Jin-Guo Liu,¹ Lei Wang,^{1,2,3,*} and Tao Xiang^{1,4,5,†}

PennyLane: Automatic differentiation of hybrid quantum-classical computations

Ville Bergholm,¹ Josh Izaac,¹ Maria Schuld,¹ Christian Gogolin,¹ Shahnawaz Ahmed,² Vishnu Ajith,³ M. Sohaib Alam,^{4,5} Guillermo Alonso-Linaje,¹ B. Akash Narayanan, Ali Asadi,¹ Juan Miguel Arrazola,¹ Utkarsh Azad,¹ Sam Banning,¹ Carsten Blank,⁶ Thomas R Bromley,¹ Benjamin A. Cordier,⁷ Jack Ceroni,¹ Alain Delgado,¹ Olivia Di Matteo,^{1,8} Amintor Dusko,¹ Tanya Garg,⁹ Diego Guala,¹ Anthony Hayes,¹ Ryan Hill,¹⁰ Aroosa Ijaz,¹ Theodor Isacsson,¹ David Ittah,¹ Soran Jahangiri,¹ Prateek Jain,¹¹ Edward Jiang,¹ Ankit Khandelwal,¹² Korbinian Kottmann,¹³ Robert A. Lang,¹⁴ Christina Lee,¹ Thomas Loke,¹⁵ Angus Lowe,¹ Keri McKiernan,¹⁶ Johannes Jakob Meyer,¹⁷ J. A. Montañez-Barrera,¹⁸ Romain Moyard,¹ Zeyue Niu,¹ Lee James O'Riordan,¹ Steven Oud,¹⁹ Ashish Panigrahi,²⁰ Chae-Yeun Park,¹ Daniel Polatajko,²¹ Nicolás Quesada,¹ Chase Roberts,¹ Nahum Sá,²² Isidor Schoch,²³ Borun Shi,²⁴ Shuli Shu,¹ Sukin Sim,²⁵ Arshpreet Singh,²⁶ Ingrid Strandberg,²⁷ Jay Soni,¹ Antal Száva,¹ Slimane Thabet,^{28,29} Rodrigo A. Vargas-Hernández,^{14,30} Trevor Vincent,¹ Nicola Vitucci, Maurice Weber,³¹ David Wierichs,³² Roeland Wiersema,^{30,33} Moritz Willmann, Vincent Wong,³⁴ Shaoming Zhang,^{35,36} and Nathan Killoran¹

Differentiable quantum chemistry with PySCF for molecules and materials at the mean-field level and beyond

Xing Zhang and Garnet Kin-Lic Chan

Differentiate through domain-specific computational processes to solve modeling, control, optimization, and inverse problems

JAX, M.D. A framework for differentiable physics*

Samuel S Schoenholz** and Ekin D Cubuk

nature|methods

PERSPECTIVE

<https://doi.org/10.1038/s41592-021-01283-4>



Differentiable biology: using deep learning for biophysics-based and data-driven modeling of molecular mechanisms

Mohammed AlQuraishi^{1,2} and Peter K. Sorger^{1,2}

微分万物：深度学习的启示*

王磊^{1,2,†} 刘金国³

(1) 中国科学院物理研究所 北京 100190

(2) 松山湖材料实验室 东莞 523808

(3) 哈佛大学物理系 剑桥 02138

《物理》

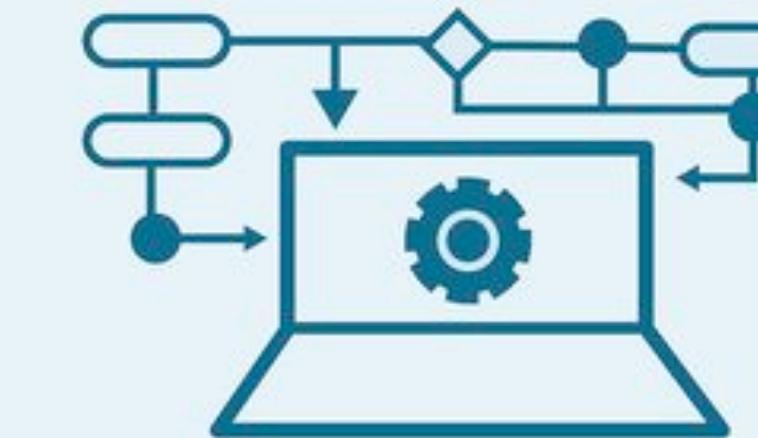
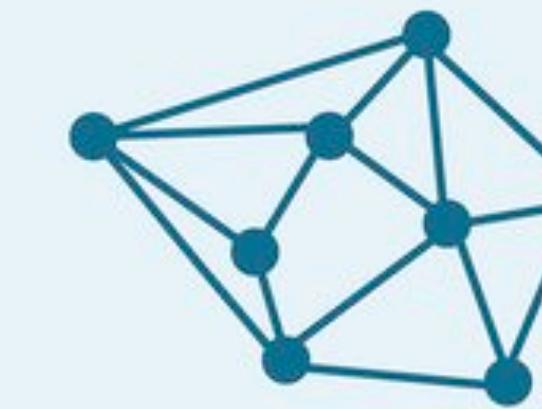
2021年2月

There's plenty of room at the Top Science 2020

The Top

Technology

01010011 01100011
01101001 01100101
01101110 01100011
01100101 00000000



Software

Opportunity

Software performance engineering

Algorithms

New algorithms

Hardware architecture

Hardware streamlining

Examples

Removing software bloat

New problem domains

Processor simplification

Tailoring software to hardware features

New machine models

Domain specialization

The Bottom
for example, semiconductor technology

