

Generative AI for Science

Applications and Techniques

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للعلوم والتكنولوجيا

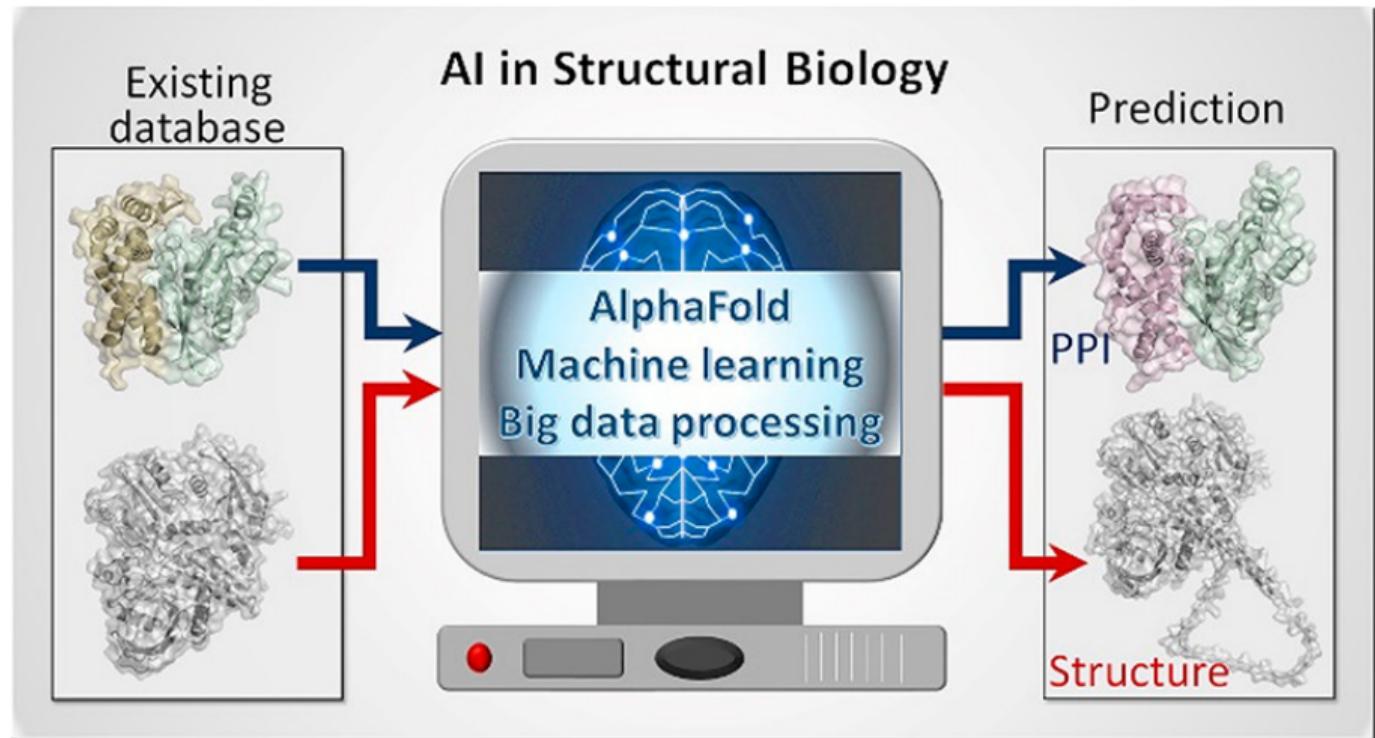
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Science and Technology

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June 23, 2025

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Where We Are

- ▶ Generative AI is helping scientists make new discoveries faster.
- ▶ We use it for things like designing proteins, finding new medicines, and predicting the weather.
- ▶ Some popular tools are AlphaFold (for proteins), Earth-2 (for climate), and SMILES (for chemicals).

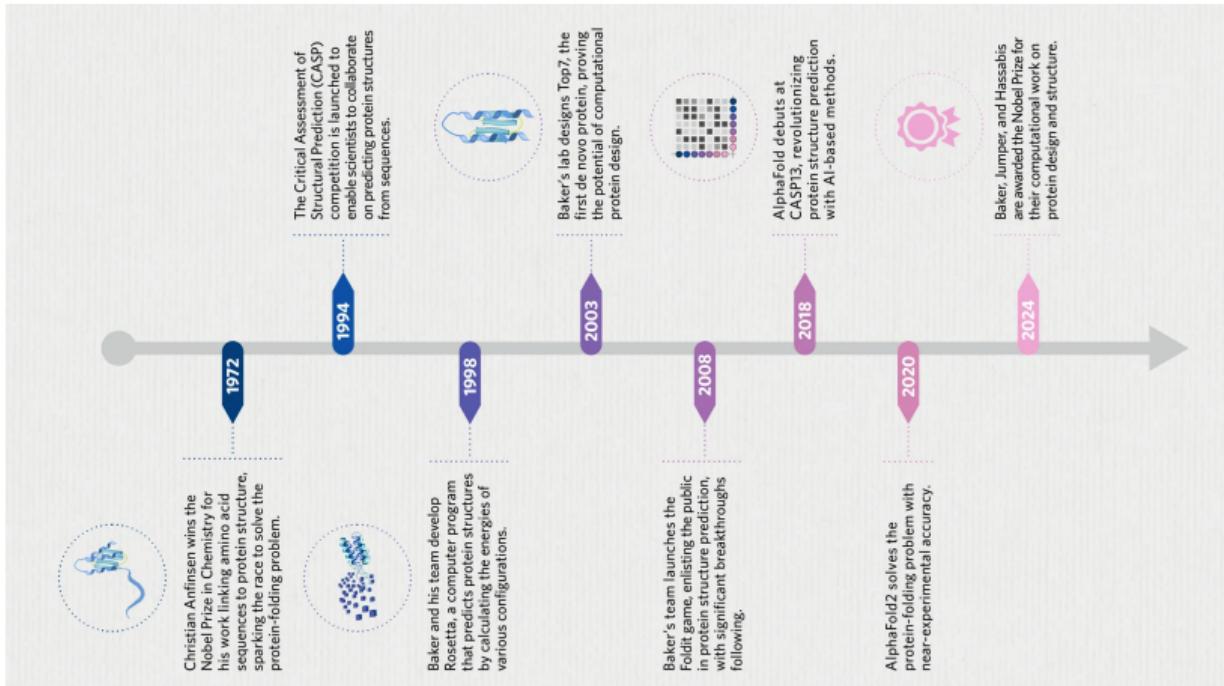
Where We Are Going

- ▶ Generative AI could help us solve big problems and understand complex systems.
- ▶ As AI gets better and computers get faster, we can do even more with these tools.
- ▶ We need to use AI responsibly and think about the impact on society.

- ▶ See how generative AI is changing scientific research.
- ▶ Find out where generative AI is used, like in protein design, drug discovery, and climate studies.
- ▶ Learn how generative AI helps solve tough science problems.
- ▶ Talk about the impact and ethics of using AI in science.
- ▶ Look at what's next for generative AI in science.

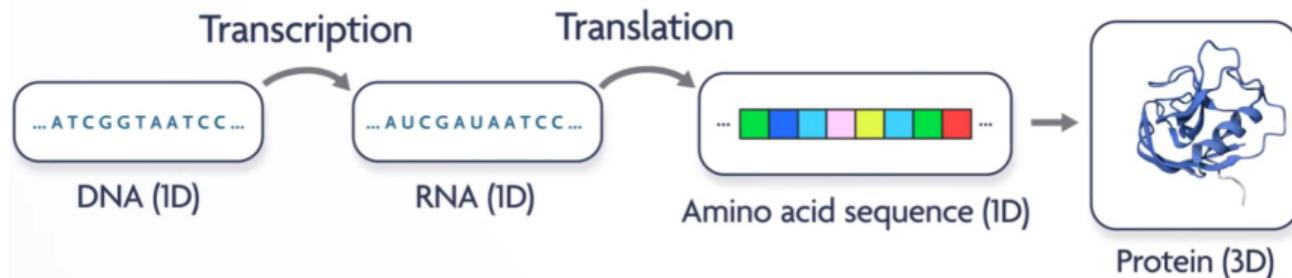
Protein Design — AlphaFold: Revolutionizing Protein Structure Prediction

AlphaFold - A Brief History



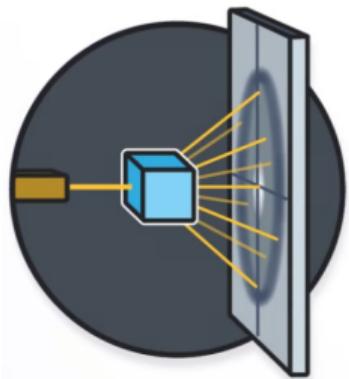
[Source: [TheScientist](#)]

Central Dogma of Molecular Biology

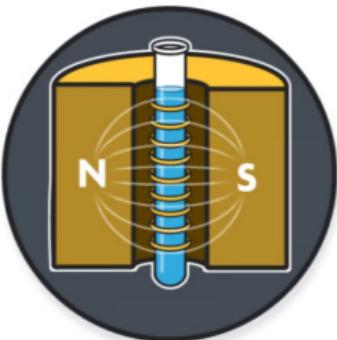


- ▶ DNA is transcribed into RNA, which is then translated into proteins.
- ▶ Proteins are made up of amino acids and fold into specific 3D structures.
- ▶ The structure of a protein determines its function in the cell.

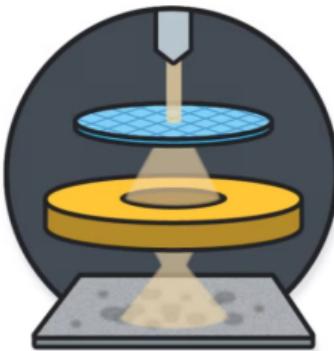
X-Ray
crystallography



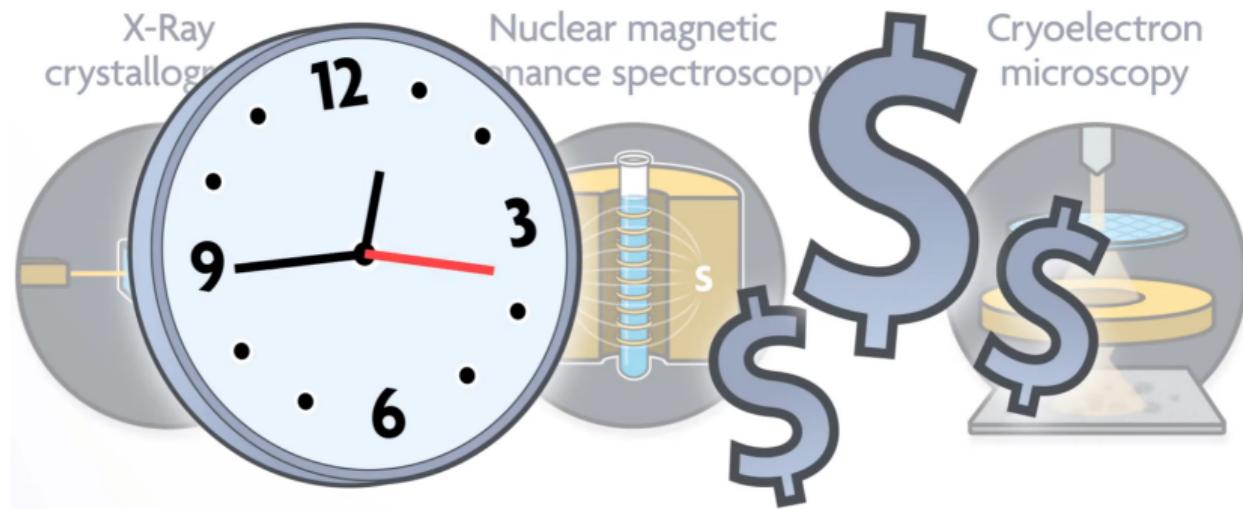
Nuclear magnetic
resonance spectroscopy



Cryoelectron
microscopy



AlphaFold - A Brief History (cont.)



Article

Highly accurate protein structure prediction with AlphaFold

<https://doi.org/10.1038/s41586-021-03819-2>

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Open access



John Jumper^{1,4}, Richard Evans^{1,4}, Alexander Pritzel^{1,4}, Tim Green^{1,4}, Michael Figurnov^{1,4}, Olaf Ronneberger^{1,4}, Kathryn Tunyasuvunakool^{1,4}, Russ Bates^{1,4}, Augustin Žídek^{1,4}, Anna Potapenko^{1,4}, Alex Bridgland^{1,4}, Clemens Meyer^{1,4}, Simon A. A. Kohl^{1,4}, Andrew J. Ballard^{1,4}, Andrew Cowie^{1,4}, Bernardino Romera-Paredes^{1,4}, Stanislav Nikolov^{1,4}, Rishabh Jain^{1,4}, Jonas Adler¹, Trevor Back¹, Stig Petersen¹, David Reiman¹, Ellen Clancy¹, Michal Zielinski¹, Martin Steinegger^{2,3}, Michalina Pacholska¹, Tamas Berghammer¹, Sebastian Bodenstein¹, David Silver¹, Oriol Vinyals¹, Andrew W. Senior¹, Koray Kavukcuoglu¹, Pushmeet Kohli¹ & Demis Hassabis^{1,4}

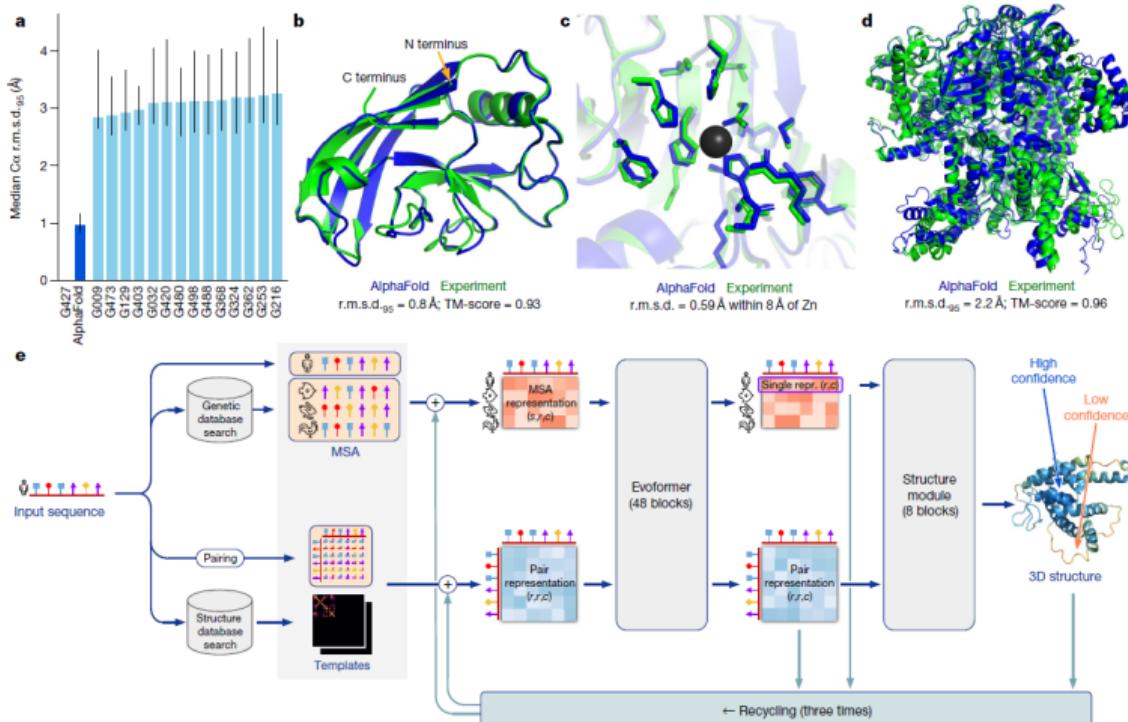
Motivation:

- ▶ Predicting a protein's 3D shape from its amino acid sequence was a huge unsolved problem for decades.
- ▶ Scientists wanted a faster, more accurate way to figure out protein structures.

Key Approach:

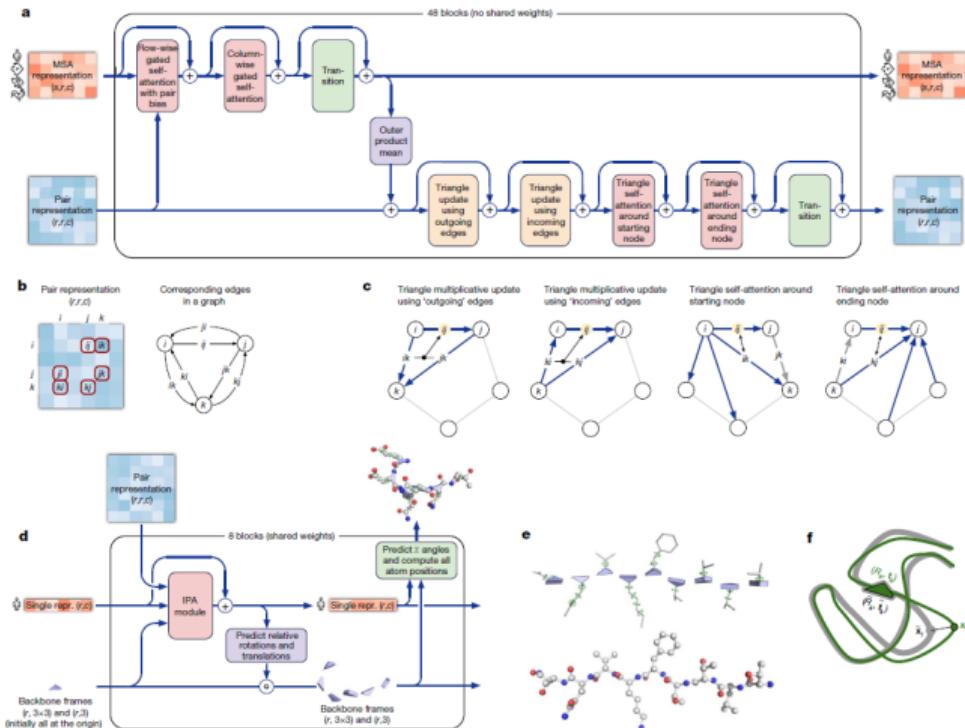
- ▶ Looked for patterns in how amino acids change together across different proteins (co-evolution).
- ▶ Used neural networks to guess which amino acids are close to each other.
- ▶ Built 3D models by connecting these predicted contacts.

AlphaFold v1 (2018) - The Early Spark (cont.)



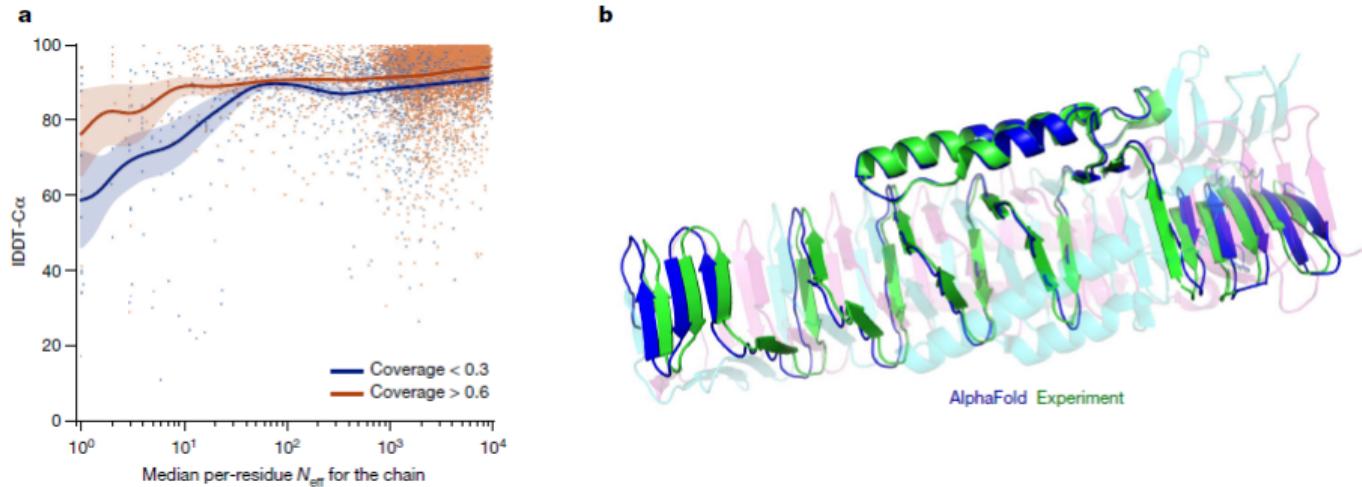
AlphaFold v1 Architecture: Neural networks predicting amino acid contacts.

AlphaFold v1 (2018) - The Early Spark (cont.)



AlphaFold v1 Architecture Details.

AlphaFold v1 (2018) - The Early Spark (cont.)



AlphaFold v1: Effect of MSA depth and cross-chain contacts.

Outcome:

- ▶ AlphaFold v1 was the best performer in the CASP13 competition.
- ▶ Proved that AI could help solve the protein folding problem.

Limitations:

- ▶ Did not predict 3D structures directly—used contact maps as a middle step.
- ▶ Needed lots of evolutionary data to work well.
- ▶ Was less accurate than later versions.

REVIEW ARTICLE**OPEN**

AlphaFold2 and its applications in the fields of biology and medicine

Zhenyu Yang¹, Xiaoxi Zeng¹✉, Yi Zhao^{1,2}✉ and Runsheng Chen^{1,3,4}✉

AlphaFold2 (AF2) is an artificial intelligence (AI) system developed by DeepMind that can predict three-dimensional (3D) structures of proteins from amino acid sequences with atomic-level accuracy. Protein structure prediction is one of the most challenging problems in computational biology and chemistry, and has puzzled scientists for 50 years. The advent of AF2 presents an unprecedented progress in protein structure prediction and has attracted much attention. Subsequent release of structures of more than 200 million proteins predicted by AF2 further aroused great enthusiasm in the science community, especially in the fields of biology and medicine. AF2 is thought to have a significant impact on structural biology and research areas that need protein structure information, such as drug discovery, protein design, prediction of protein function, et al. Though the time is not long since AF2 was developed, there are already quite a few application studies of AF2 in the fields of biology and medicine, with many of them having preliminarily proved the potential of AF2. To better understand AF2 and promote its applications, we will in this article summarize the principle and system architecture of AF2 as well as the recipe of its success, and particularly focus on reviewing its applications in the fields of biology and medicine. Limitations of current AF2 prediction will also be discussed.

Signal Transduction and Targeted Therapy (2023)8:115

; <https://doi.org/10.1038/s41392-023-01381-z>

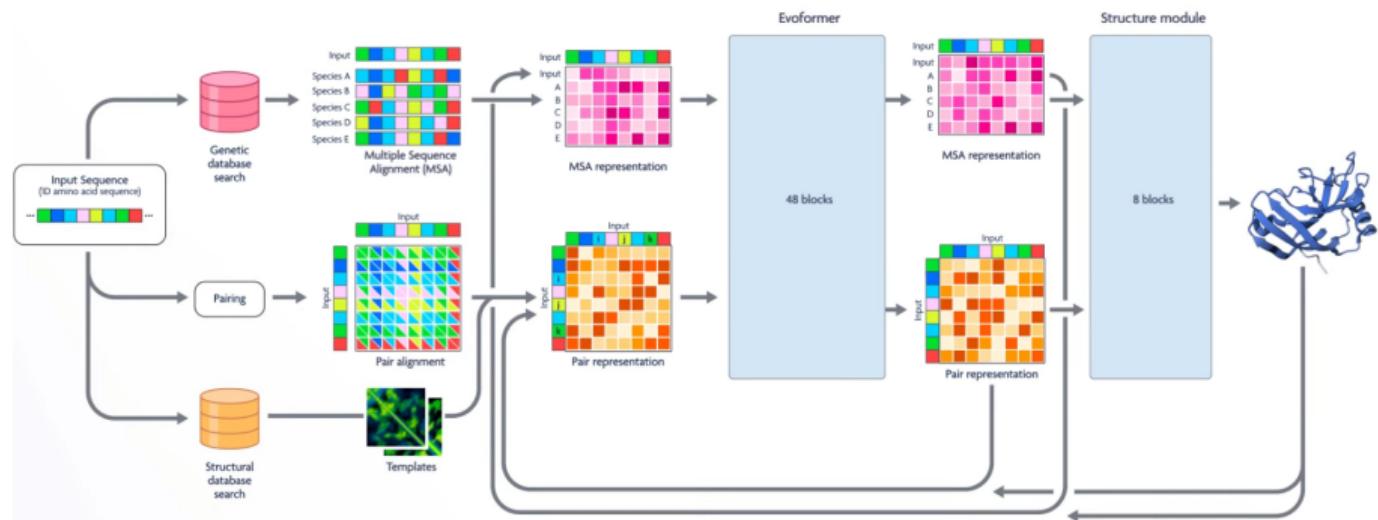
Why AlphaFold 2?

- ▶ Scientists wanted a tool that was much faster and more accurate than before.
- ▶ The goal: Predict protein shapes quickly, with very high accuracy, and less manual work.

How does it work?

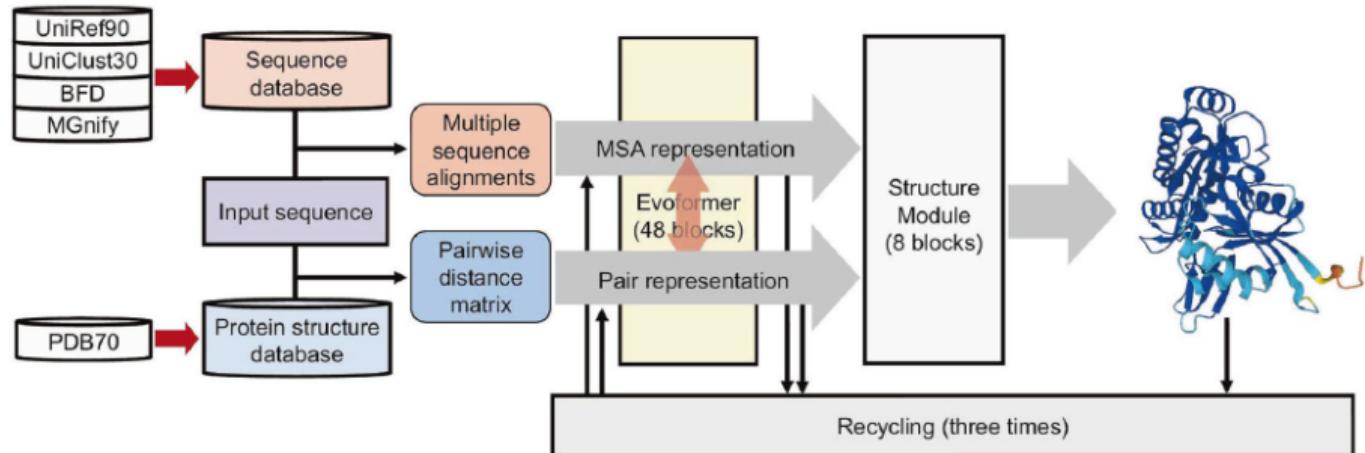
- ▶ Looks at lots of related protein sequences (MSA) and uses known structures as hints.
- ▶ Uses a special "Evoformer" module to find patterns in the data.
- ▶ Directly predicts the 3D positions of all atoms in the protein.

AlphaFold 2 Architecture

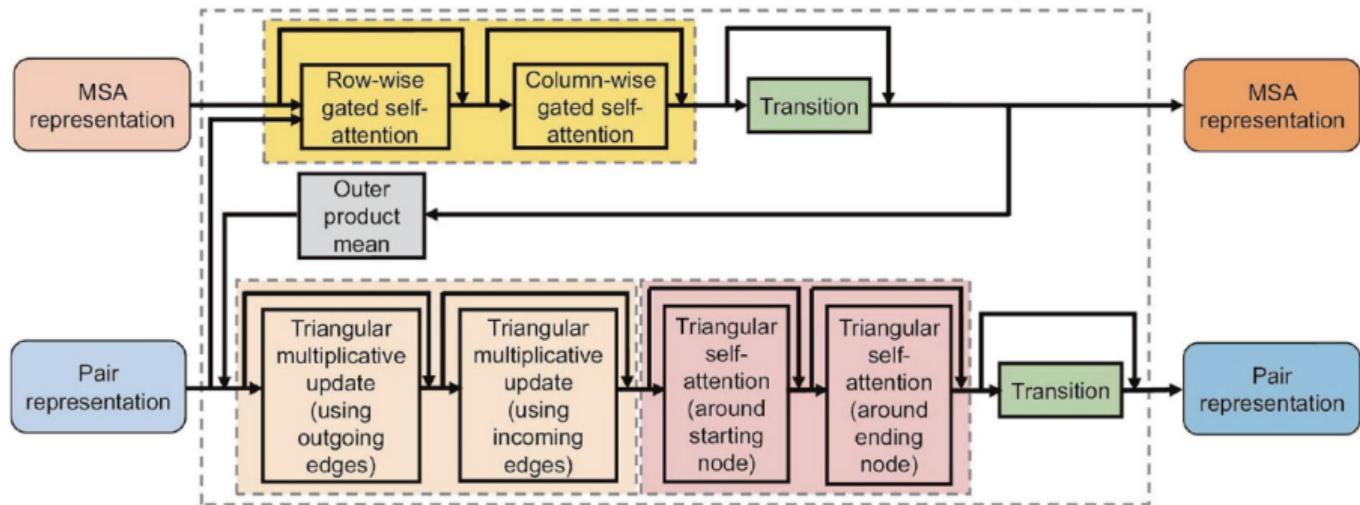


AlphaFold 2 Architecture: Directly predicts 3D coordinates from amino acid sequences.

AlphaFold 2 (2020) - A Revolution (cont.)

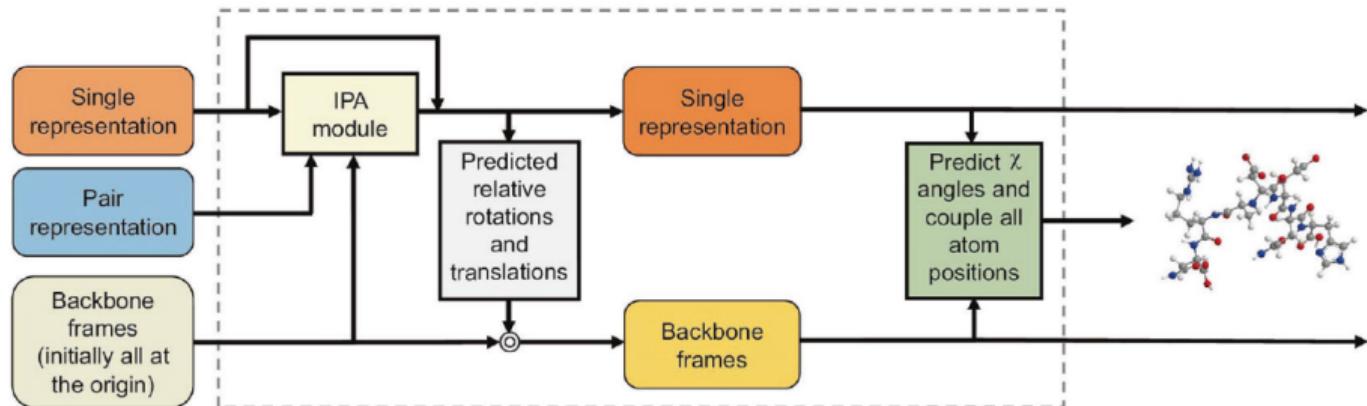


The overall architecture of AF2.

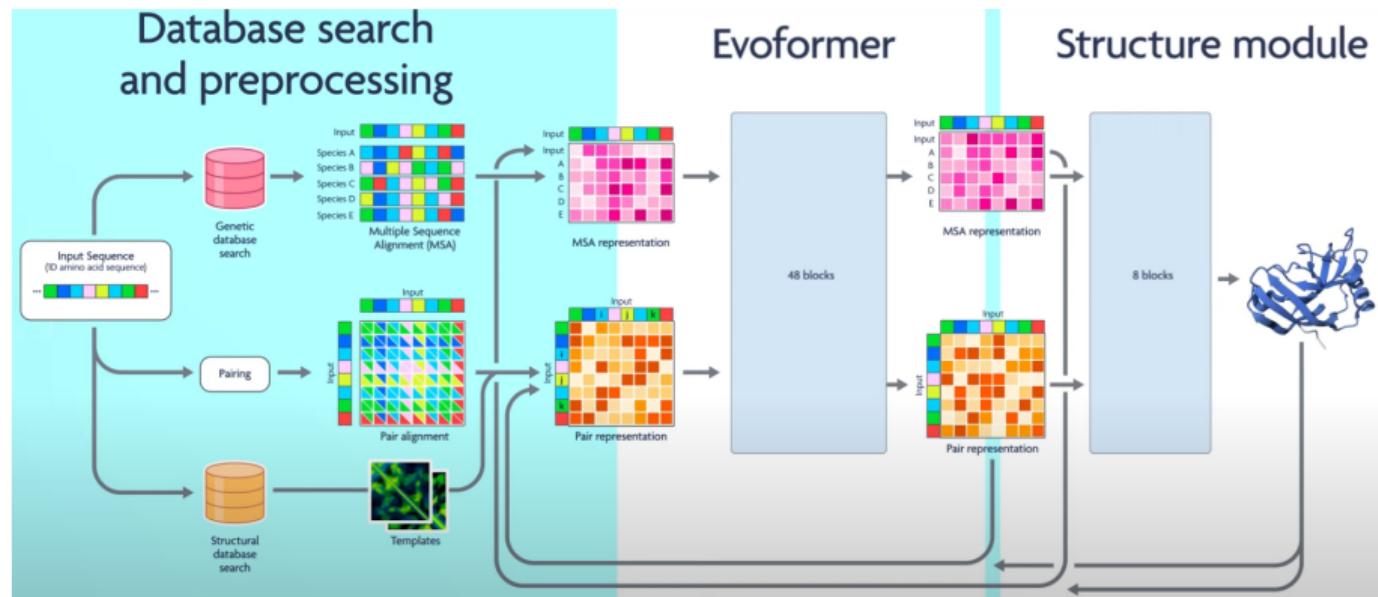


Components of a block in Evoformer.

AlphaFold 2 (2020) - A Revolution (cont.)



Components of a block in the structure module.

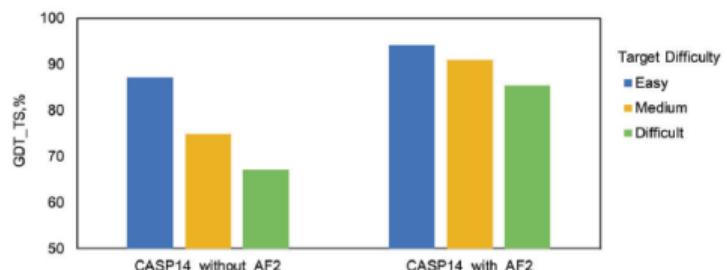
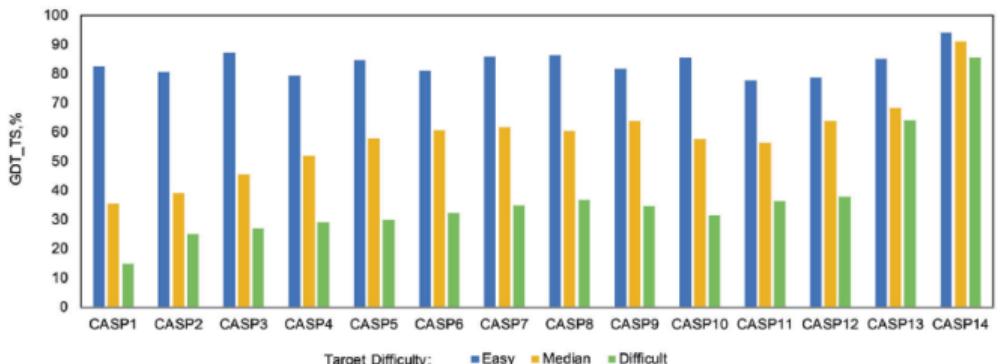


AlphaFold 2 Architecture: Directly predicts 3D coordinates from amino acid sequences.

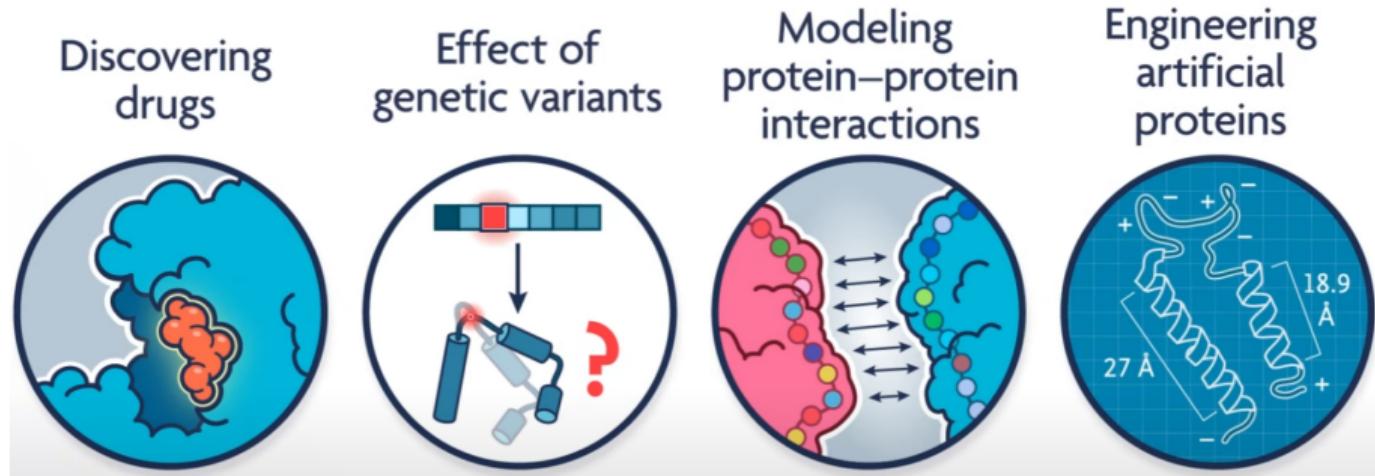
How well did it do?

- ▶ In the CASP14 competition, AlphaFold 2 was twice as accurate as any other method.
- ▶ It could predict protein shapes with errors as small as 1.5Å (that's really close!).

AlphaFold 2 (2020) - A Revolution (cont.)



Performances of protein structure prediction indicated as backbone agreement with that of structures determined by experiments for the best models in CASPs.



Applications of AlphaFold 2.

What are its limits?

- ▶ Works best for single protein chains, not big complexes.
- ▶ Has trouble with floppy or unusual protein regions.

AlphaFold 3 predicts the structure and interactions of all of life's molecules

May 08, 2024

5 min read

Introducing AlphaFold 3, a new AI model developed by Google DeepMind and Isomorphic Labs. By accurately predicting the structure of proteins, DNA, RNA, ligands and more, and how they interact, we hope it will transform our understanding of the biological world and drug discovery.



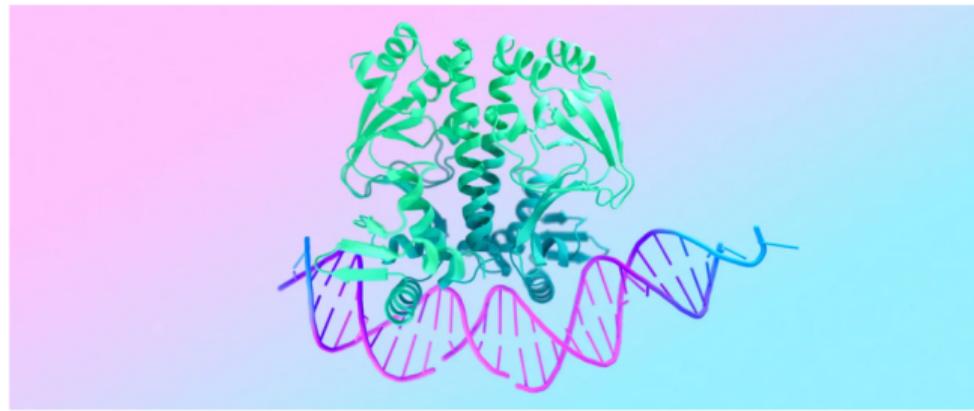
Google DeepMind
AlphaFold team



Isomorphic Labs



Share



[Source: [Google](#)]

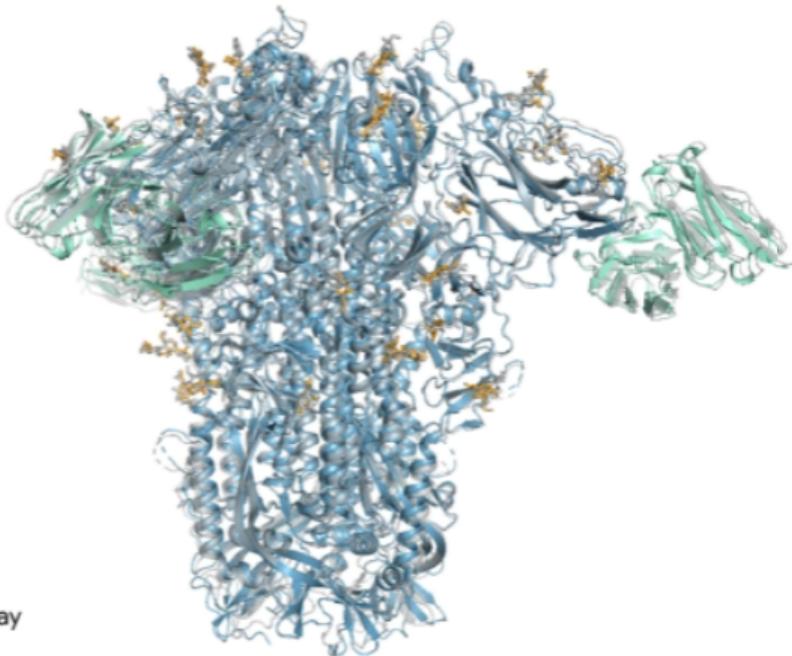
Why AlphaFold 3?

- ▶ Scientists wanted to predict not just proteins, but also DNA, RNA, and small molecules.
- ▶ Needed a tool to see how all these molecules interact together.

What's new in AlphaFold 3?

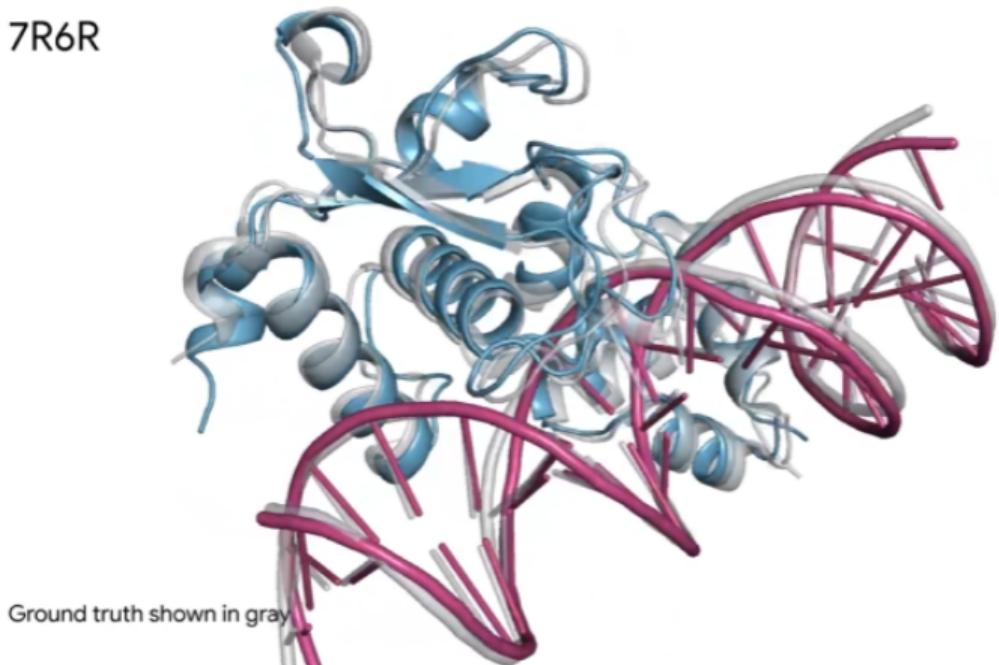
- ▶ Uses a new "Pairformer" module to better understand how pairs of molecules interact.
- ▶ Adds a diffusion-based step to build 3D shapes of molecules.
- ▶ Can handle proteins, DNA, RNA, small molecules, and ions—all in one model.

7PNM



[Source: [Google](#)]

7R6R



[Source: [Google](#)]

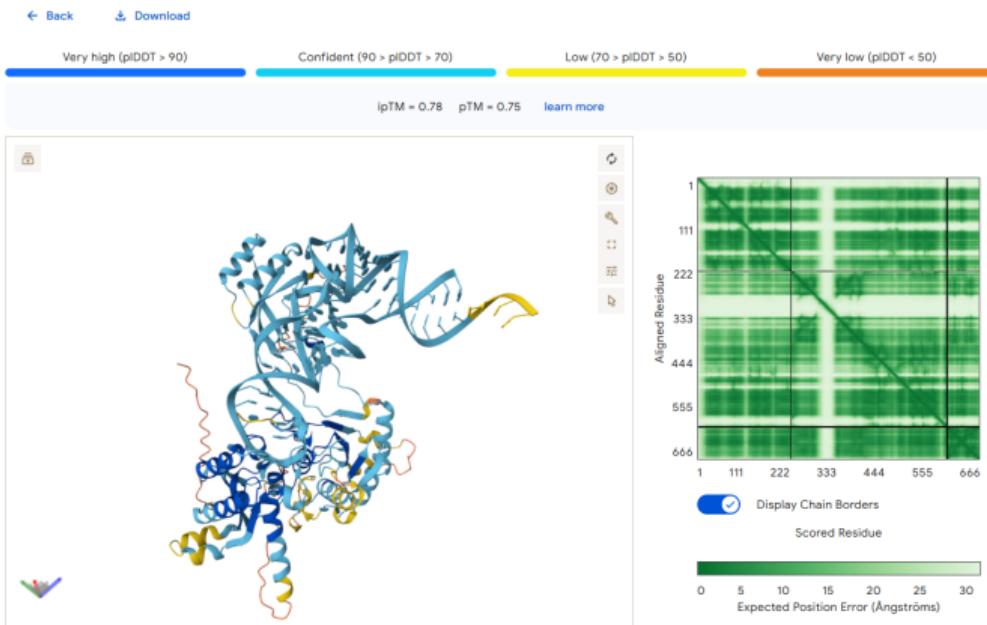
What can it do?

- ▶ Predicts how different types of molecules fit and work together.
- ▶ Helps study big molecular machines made of many parts.

How can you use it?

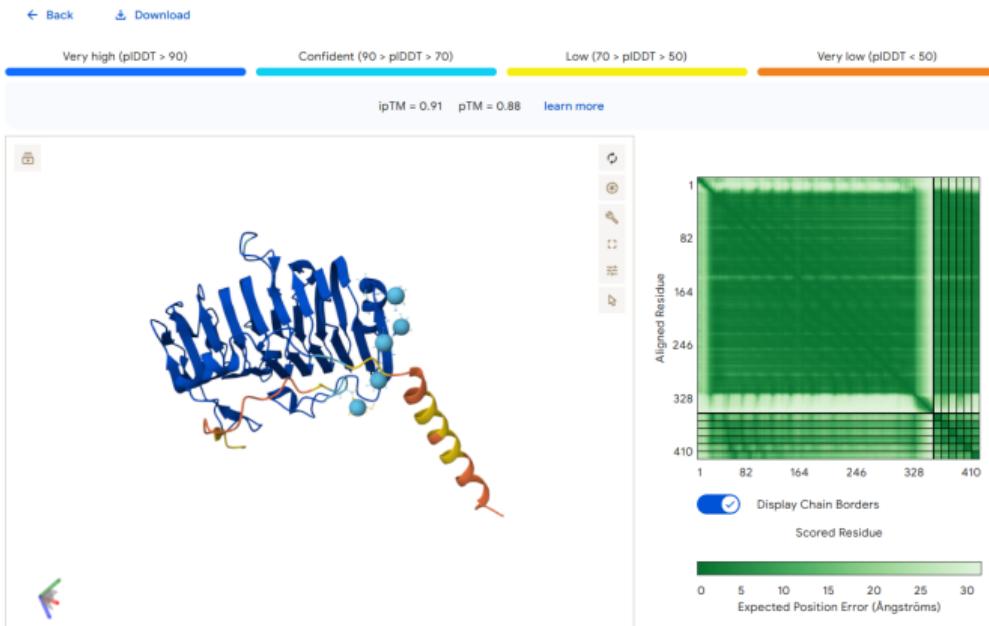
- ▶ Free public server for researchers (up to 20 predictions per day).
- ▶ Commercial access available for companies.

Protein-RNA-Ion: PDB 8AW3



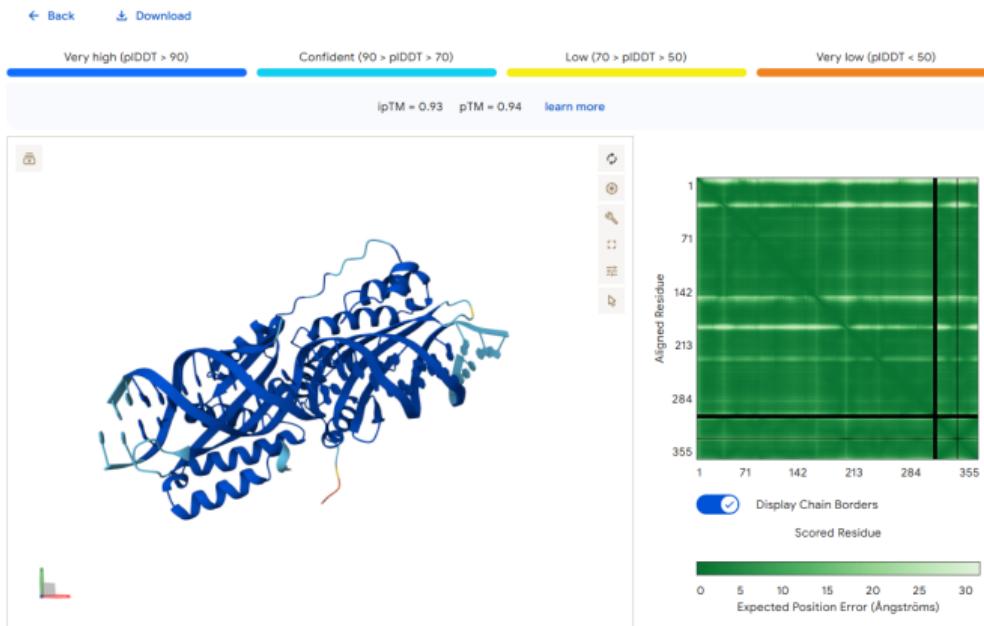
[Playground: Protein-RNA-Ion: PDB 8AW3]

Protein-Glycan-Ion: PDB 7BBV



[Playground: Protein-Glycan-Ion: PDB 7BBV]

Protein-DNA-Ion: PDB 7RCE



[Playground: Protein-DNA-Ion: PDB 7RCE]

Generative AI for Science: Drug Discovery



pubs.acs.org/jcim

Review

Generative Deep Learning for Targeted Compound Design

Tiago Sousa, João Correia, Vitor Pereira, and Miguel Rocha*



Cite This: *J. Chem. Inf. Model.* 2021, 61, 5343–5361



Read Online

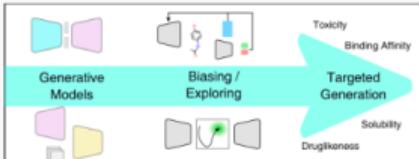
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Article Recommendations

ABSTRACT: In the past few years, *de novo* molecular design has increasingly been using generative models from the emergent field of Deep Learning, proposing novel compounds that are likely to possess desired properties or activities. *De novo* molecular design finds applications in different fields ranging from drug discovery and materials sciences to biotechnology. A panoply of deep generative models, including architectures as Recurrent Neural Networks, Autoencoders, and Generative Adversarial Networks, can be trained on existing data sets and provide for the generation of novel compounds. Typically, the new compounds follow the same underlying statistical distributions of properties exhibited on the training data set. Additionally, different optimization strategies, including transfer learning, Bayesian optimization, reinforcement learning, and conditional generation, can direct the generation process toward desired aims, regarding their biological activities, synthesis processes or chemical features. Given the recent emergence of these technologies and their relevance, this work presents a systematic and critical review on deep generative models and related optimization methods for targeted compound design, and their applications.

KEYWORDS: Deep Learning, De Novo Molecular Design, Architectures, Recurrent Neural Networks, Generative Adversarial Networks, Autoencoders, Generative Model, Optimization



[Source: JCIM]



Where We Are

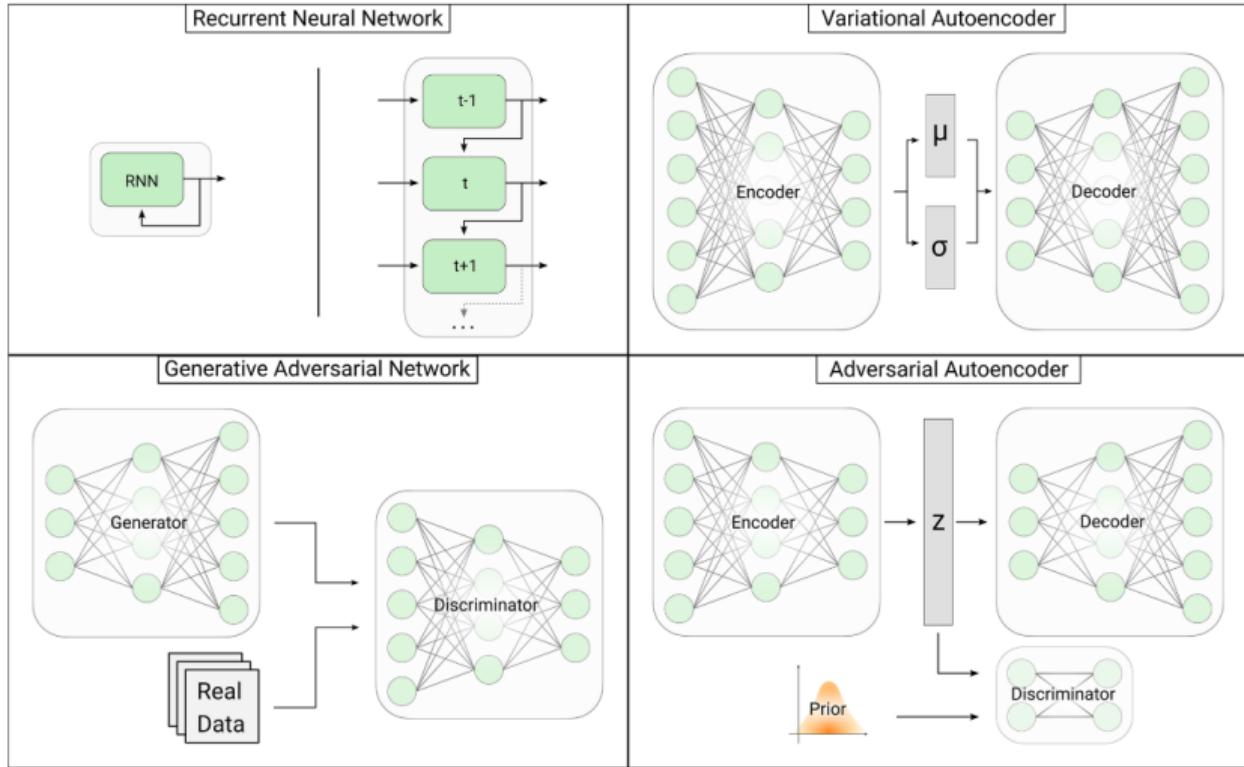
- ▶ Drug discovery is the process of finding new medicines.
- ▶ It involves identifying potential drug candidates, testing them, and bringing them to market.
- ▶ Traditional methods are slow and expensive, often taking over a decade and billions of dollars.

Where We Are Going

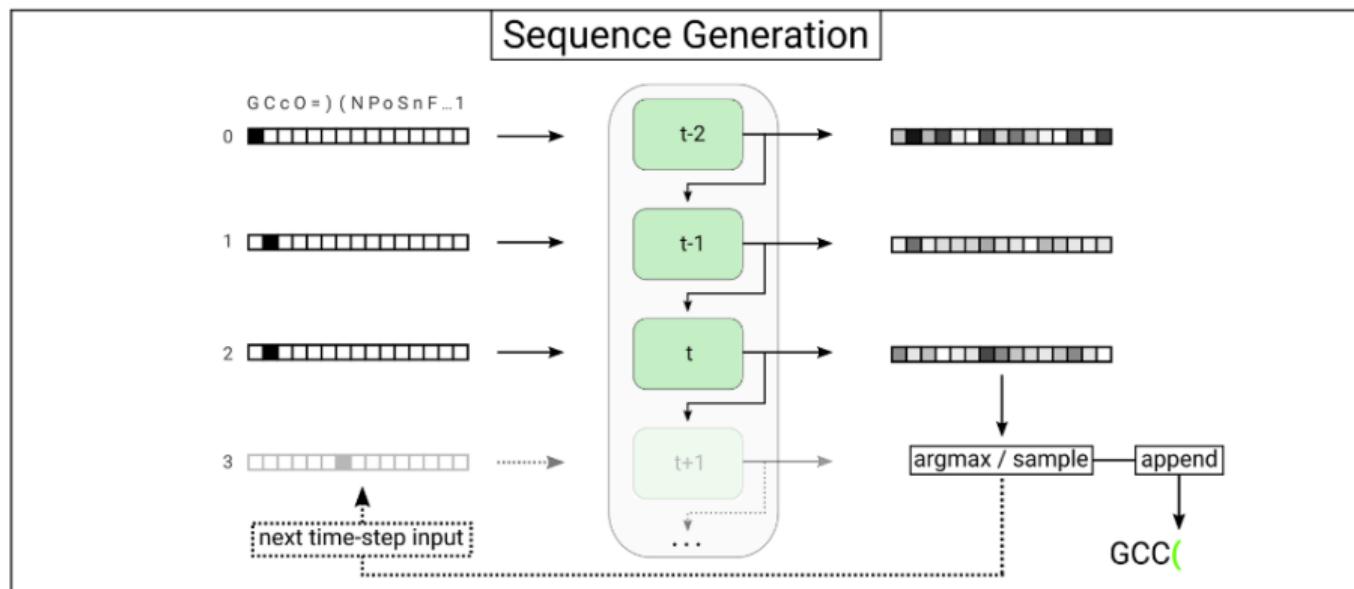
- ▶ Generative AI can speed up drug discovery by predicting how molecules will behave and interact.
- ▶ AI can analyze large datasets to find patterns and suggest new drug candidates.
- ▶ This could lead to faster development of new treatments for diseases.

- ▶ Understand how generative AI integrates into the drug discovery pipeline (e.g., SMILES → molecules → optimization).
- ▶ Recognize real-world successes of generative AI in drug discovery.
- ▶ Identify current challenges and hurdles in applying generative AI to this field.

Drug Discovery (cont.)

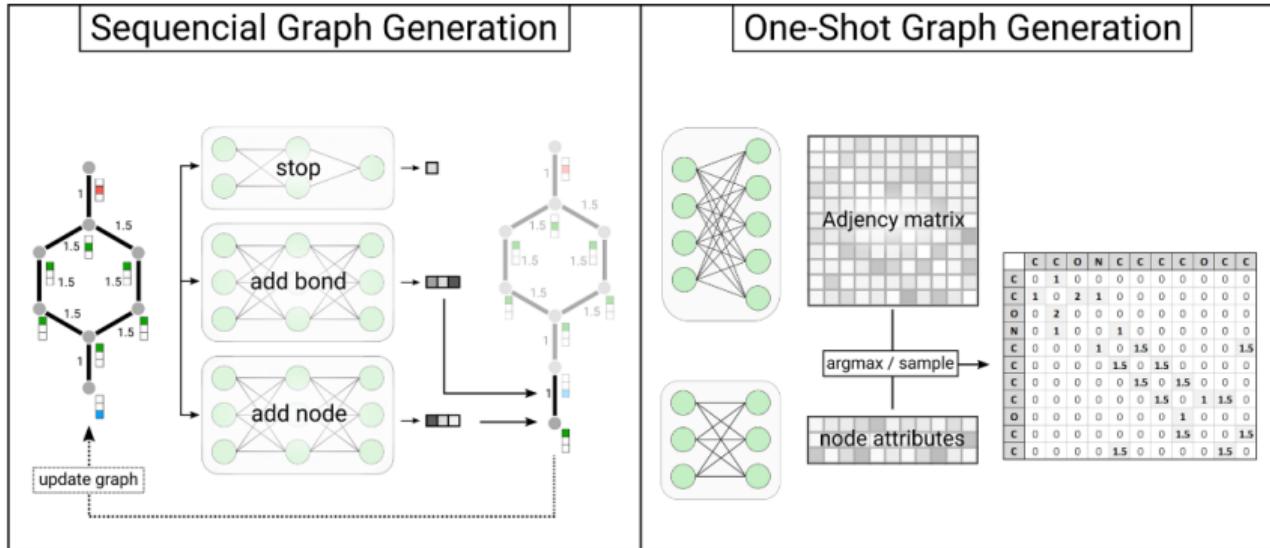


Drug Discovery (cont.)



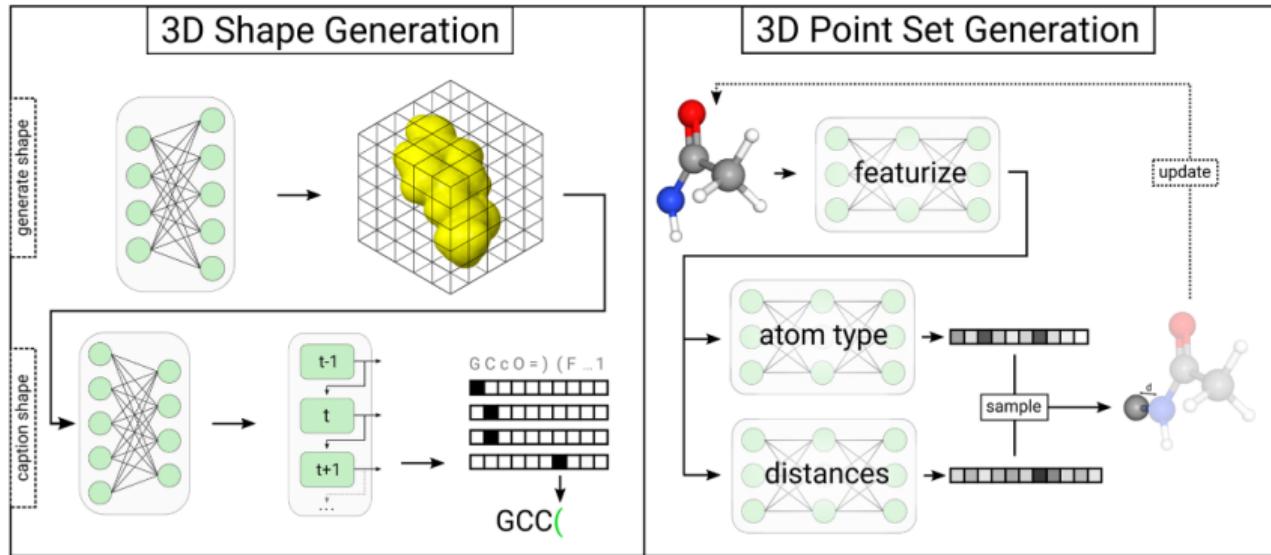
Three layer RNN, unfolded over four time-steps.

Drug Discovery (cont.)



Left: In sequential graph generation, a graph is built by evaluating a current partial graph, adding a node/edge and repeating until the network outputs a stop signal. Right: In the one-shot generation of graphs, probabilities over the full adjacency matrix and node/edge attribute tensors are reproduced.

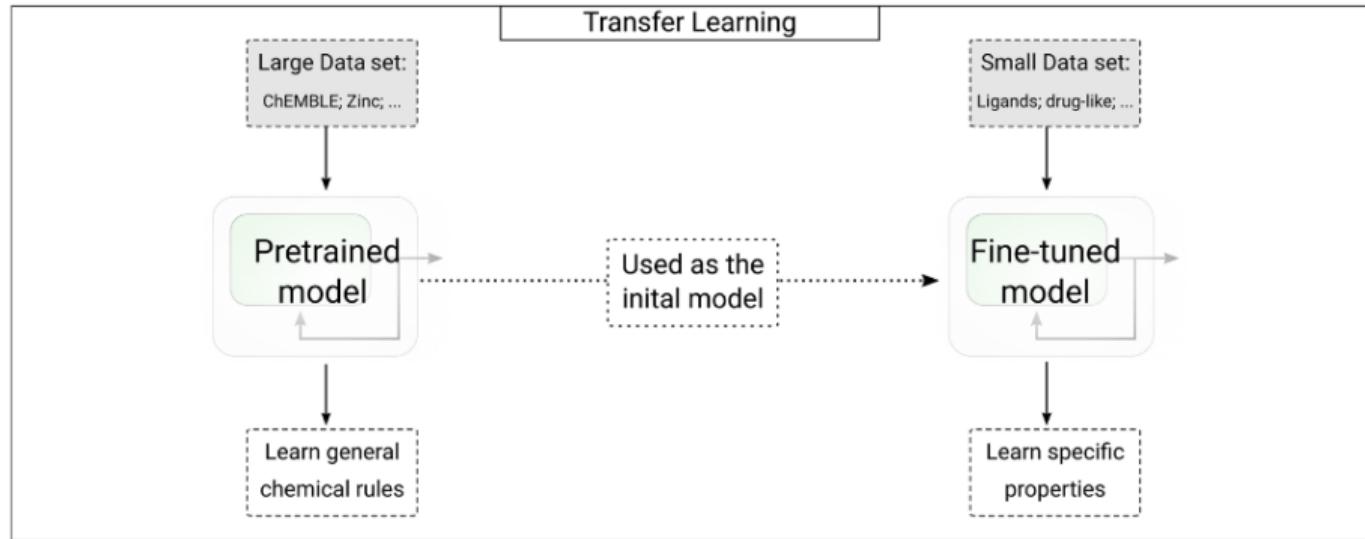
Drug Discovery (cont.)



Left: General procedure for the generation of 3D shapes as proposed by Skalic et al.

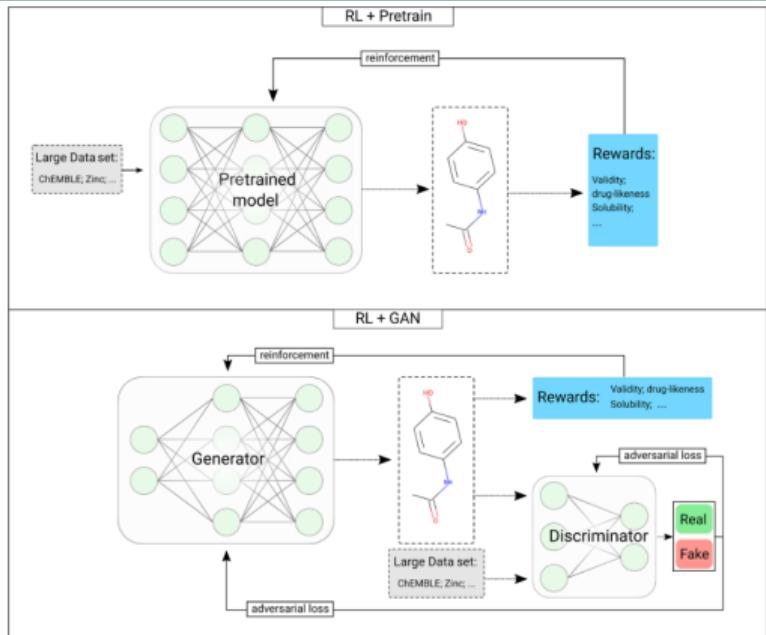
Right: General process for generating molecules as 3D point sets, proposed by Gebauer et al.

Drug Discovery (cont.)



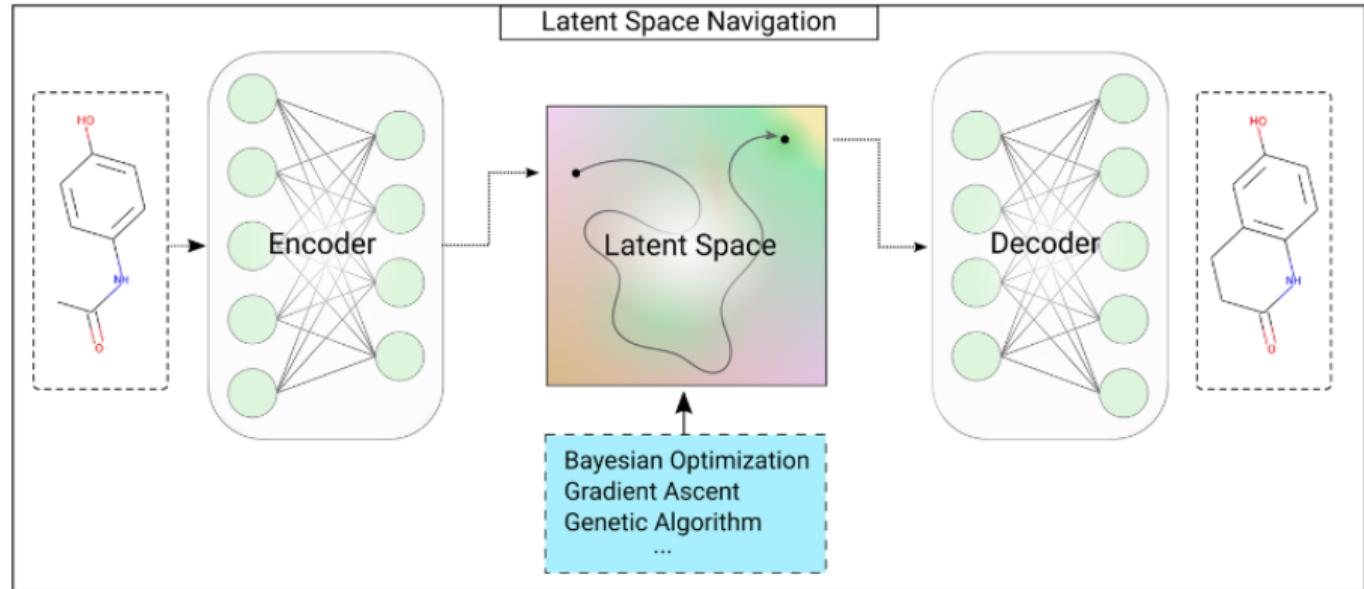
In transfer learning, a general model is first trained on a large data set and then fine-tuned toward generating the desired properties with a smaller, focused, data set.

Drug Discovery (cont.)



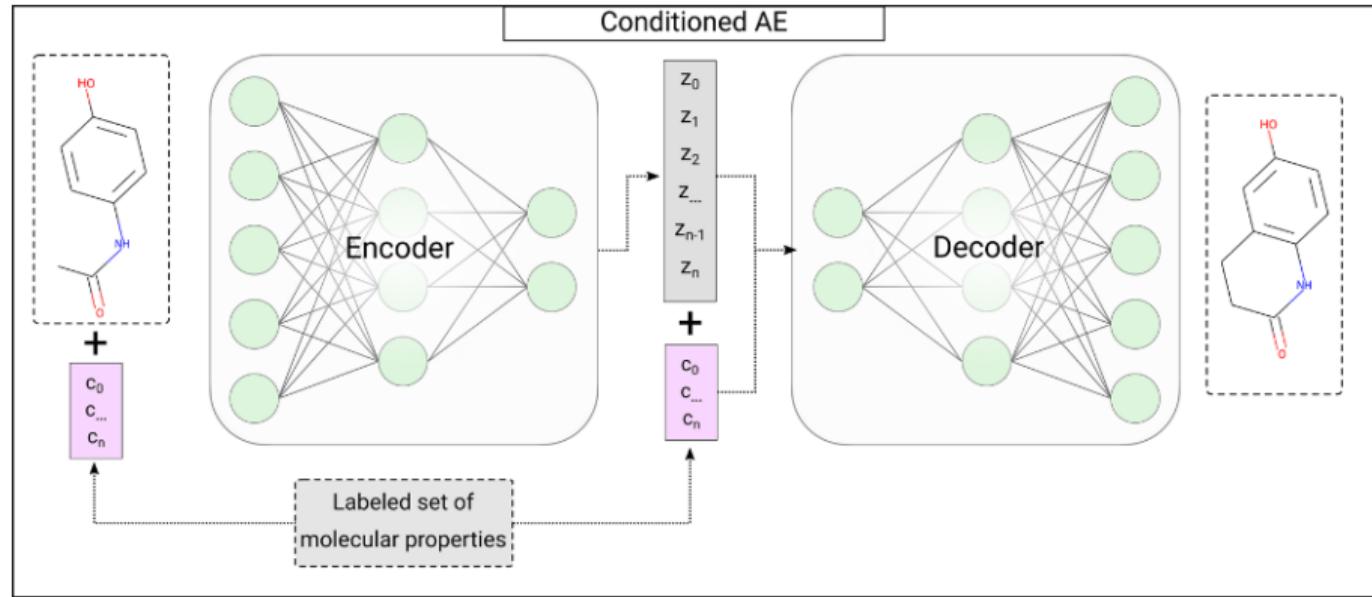
Top: Pretraining with maximum likelihood, then optimizing with RL for specific properties. Bottom: RL and GANs enable directed molecule generation toward desired objectives.

Drug Discovery (cont.)



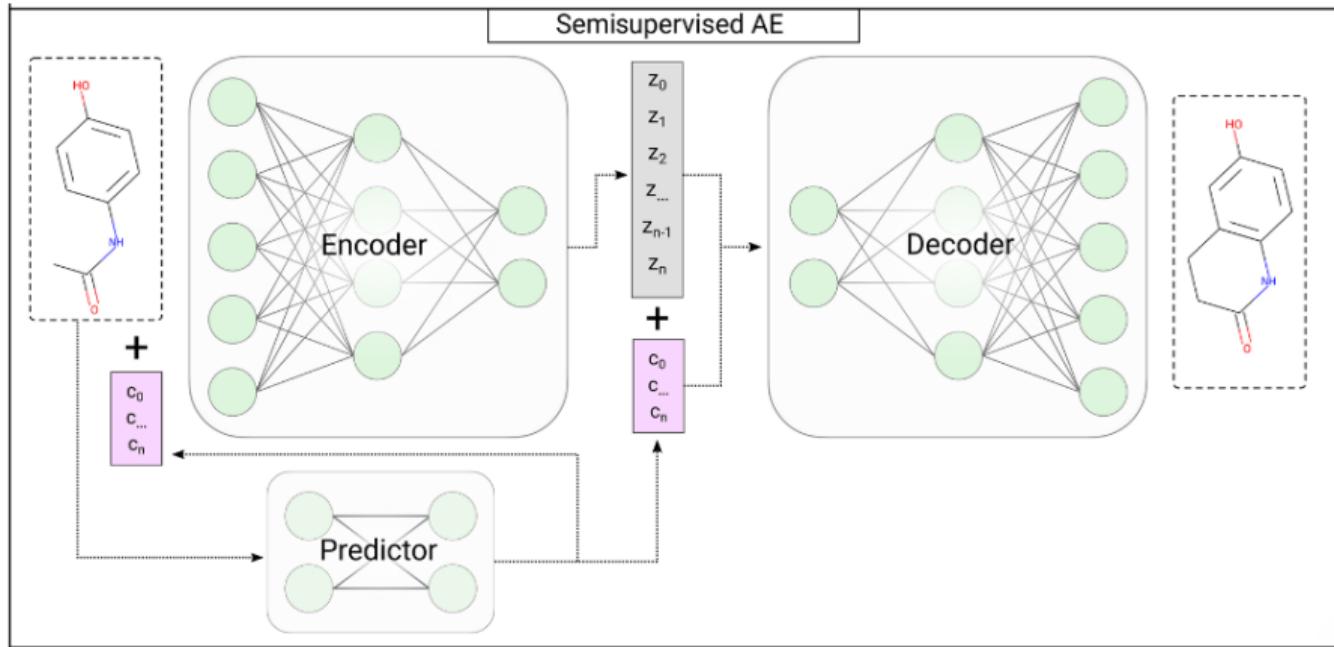
Here, the latent space of an AE is used as a reversible and continuous molecular representation allowing for the application of various optimization algorithms.

Drug Discovery (cont.)



In conditioned generation, desired properties are provided as inputs during training, enabling the model to generate molecules with targeted properties.

Drug Discovery (cont.)



In semisupervised conditioned generation, a predictor network infers missing properties for unlabeled data.

Drug Discovery (cont.)



Generative AI for Molecular Design and Synthesis

Limitations

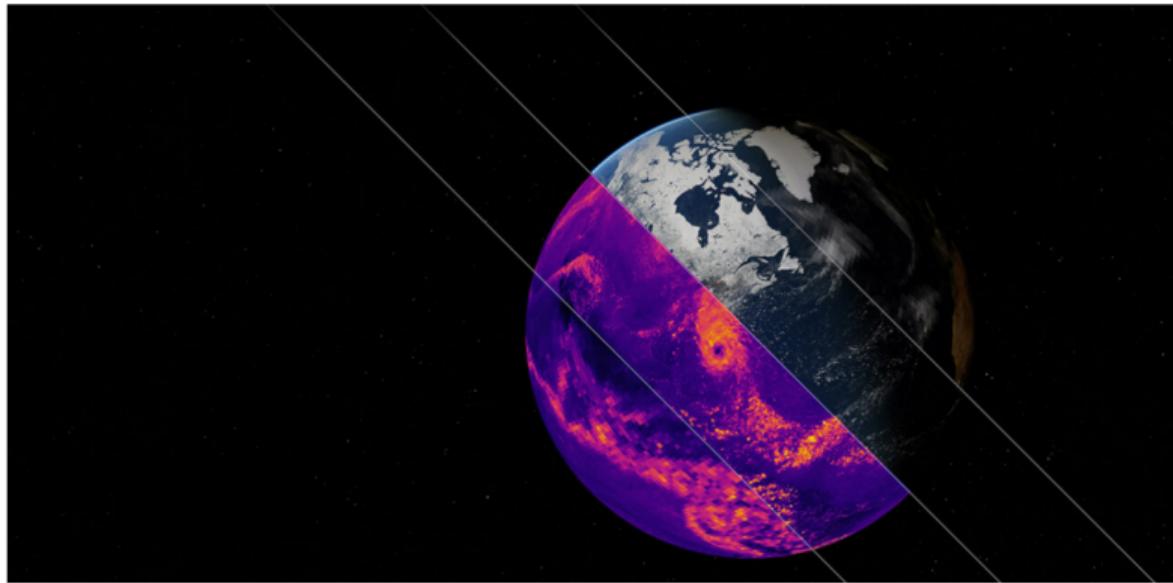
- ▶ **Synthetic feasibility:** Not all AI-generated molecules can be easily synthesized in the lab.
- ▶ **Lab validation:** Experimental validation is required to confirm predicted properties and efficacy.
- ▶ **Regulatory barriers:** Approval processes for new drugs are lengthy and complex.
- ▶ **Data bias:** Training data may not represent all relevant chemical space, leading to biased predictions.
- ▶ **Model collapse:** Generative models can produce limited diversity or converge to trivial solutions.

Generative AI for Science: Climate Simulation

Clear Skies Ahead: New NVIDIA Earth-2 Generative AI Foundation Model Simulates Global Climate at Kilometer-Scale Resolution

First-of-its-kind AI model to transform climate modeling and analytics for better prediction, understanding and response to climate change.

June 10, 2025 by [Timothy Costa](#)

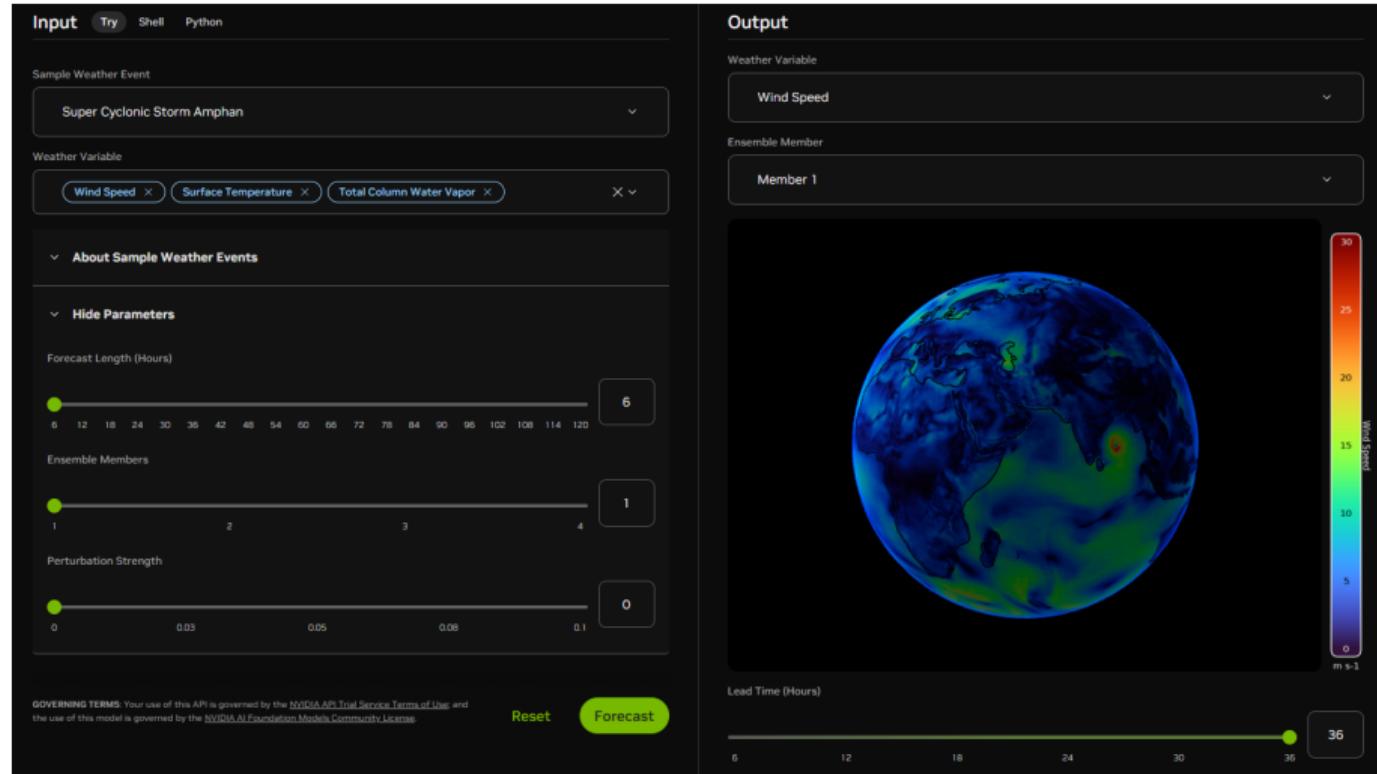


Applications of Generative AI in Climate Simulation

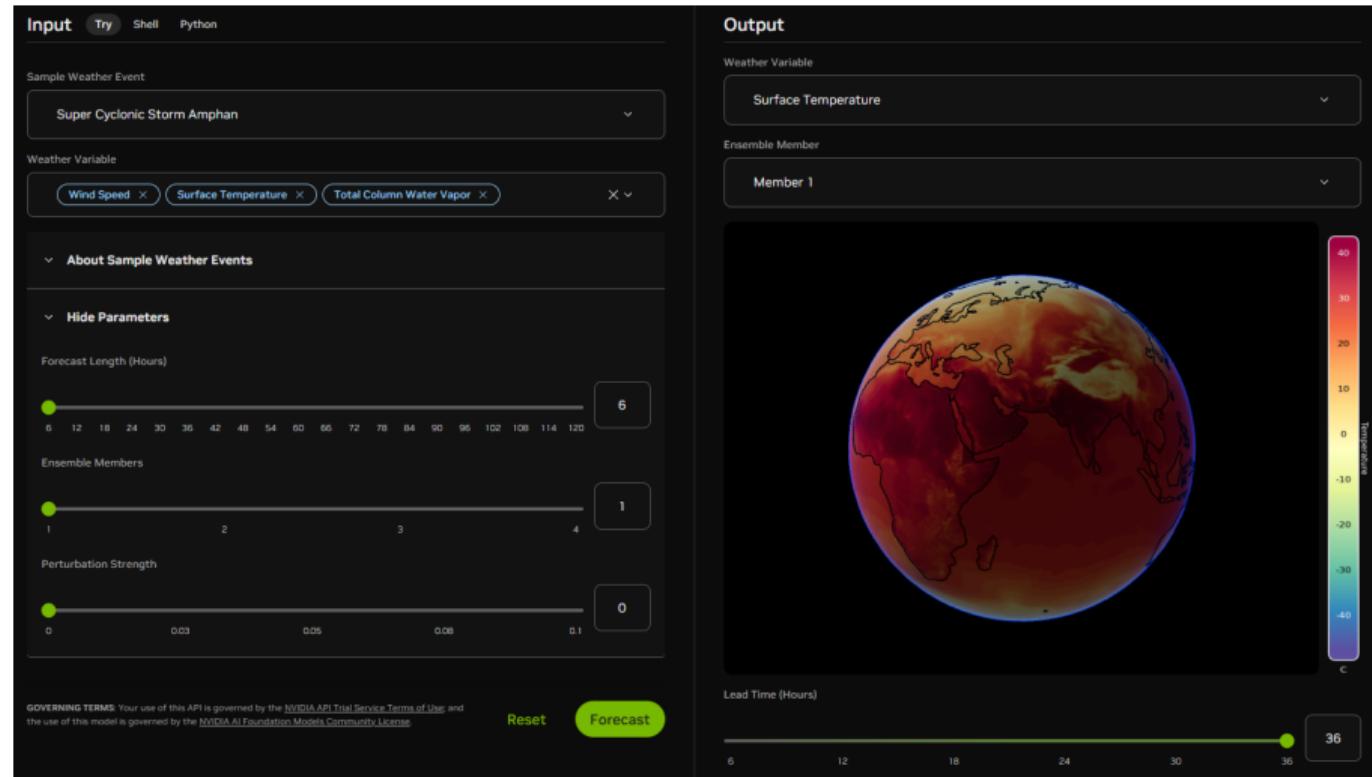
- ▶ **High-Resolution Climate Modeling:** Generative AI enables kilometer-scale global climate simulations, providing much finer detail than traditional models.
- ▶ **Faster Simulations:** AI-driven models can generate climate predictions much faster, supporting rapid scenario analysis and decision-making.
- ▶ **Extreme Weather Prediction:** Enhanced resolution and speed help in forecasting extreme weather events, such as hurricanes and floods, with greater accuracy.
- ▶ **Data Gap Filling:** AI models can fill in missing observational data, improving the completeness and reliability of climate datasets.
- ▶ **Scenario Exploration:** Researchers can quickly test the impact of different interventions or policy decisions on future climate outcomes.

- ▶ **Support for Climate Research and Policy:** These advances empower scientists and policymakers with better tools for understanding climate risks and planning mitigation strategies.

Climate Simulation (cont.)



Climate Simulation (cont.)



Climate Simulation (cont.)

Input Try Shell Python

Sample Weather Event
Super Cyclonic Storm Amphan

Weather Variable
Wind Speed × Surface Temperature × Total Column Water Vapor ×

>About Sample Weather Events

Hide Parameters

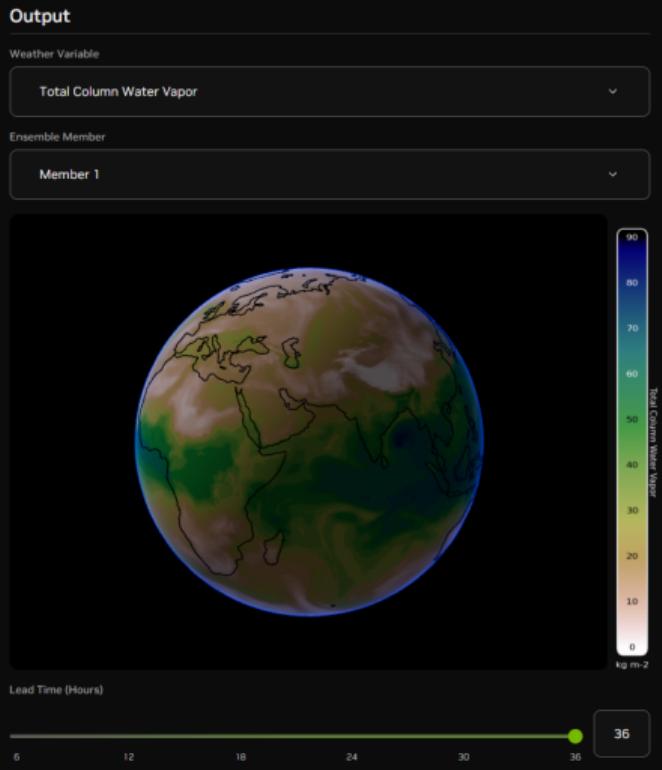
Forecast Length (Hours)
6

Ensemble Members
1

Perturbation Strength
0

GOVERNING TERMS: Your use of this API is governed by the [NVIDIA API Trial Service Terms of Use](#) and the use of this model is governed by the [NVIDIA AI Foundation Models Community License](#).

Reset **Forecast**



Climate Simulation (cont.)



nvidia/fourcastnet

Climate Digital Twin Cloud Platform

NVIDIA Earth-2 combines the power of AI, GPU acceleration, physical simulations, and computer graphics to develop applications that can simulate and visualize weather and climate predictions at a global scale with unprecedented accuracy and speed. The platform consists of development tools, microservices, and reference implementations for AI, visualization, and simulation. NVIDIA NIM™ microservices for Earth-2 allow users to leverage AI-accelerated models to optimize and simulate real-world outcomes for climate and weather.

NVIDIA Earth-2 Platform

- ▶ **Overview:** Earth-2 is NVIDIA's platform for kilometer-resolution global climate simulations, leveraging GPU acceleration and scalable microservices architecture.
- ▶ **Key Features:**
 - High-performance, real-time climate modeling.
 - Modular microservices for flexible deployment.
 - Integration with advanced generative AI models.
- ▶ **Use Cases:**
 - **NOAA Adoption:** Used by the National Oceanic and Atmospheric Administration for advanced weather and climate forecasting.
 - **Digital Twin Demonstrations:** Enables creation of digital twins of the Earth for scenario analysis and visualization.

Latest Advances: cBottle & CorrDiff

► Climate in a Bottle (cBottle):

- 5km resolution global climate model designed to provide actionable insights for policymakers.
- Enables rapid scenario analysis and supports climate-related decision-making.
- See: climatesciencefair.emersoncollective.com

► CorrDiff:

- Ultra-high-resolution local weather forecasting using generative AI.
- Delivers detailed, accurate predictions for specific regions and extreme events.

[youtube.com: Climate in a Bottle](https://www.youtube.com/watch?v=KJyfjwvXWUo)

[youtube.com: CorrDiff](https://www.youtube.com/watch?v=KJyfjwvXWUo)

Limitations and Challenges

- ▶ **Uncertainty Propagation:** Generative AI models may not fully capture or propagate uncertainties inherent in climate systems, which is critical for robust scientific predictions.
- ▶ **Data Assimilation:** Integrating real-time observational data into AI-driven simulations remains a significant challenge, limiting model adaptability and accuracy.
- ▶ **Cost and Trust:** High computational costs and the need for rigorous validation can hinder adoption. For example, models like CorrDiff are still under testing and not yet fully trusted for operational use.
- ▶ **Interpretability:** Understanding the decision-making process of complex AI models is difficult, which can impact scientific transparency and acceptance.

Generative AI for Science: **Chemical Pathways** **with SMILES**

nature machine intelligence



Article

<https://doi.org/10.1038/s42256-023-00788-1>

Leveraging large language models for predictive chemistry

Received: 16 May 2023

Accepted: 22 December 2023

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Infusing Linguistic Knowledge of SMILES into Chemical Language Models

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Abstract

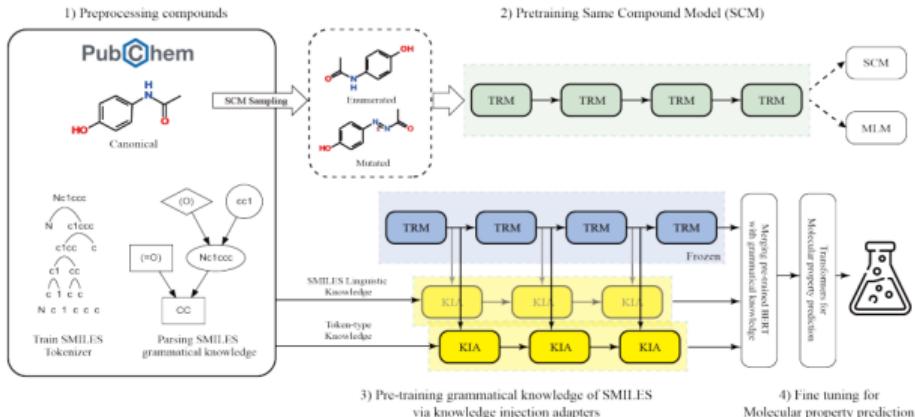
The simplified molecular-input line-entry system (SMILES) is the most popular representation of chemical compounds. Therefore, many SMILES-based molecular property prediction models have been developed. In particular, transformer-based models show promising performance because the model utilizes a massive chemical dataset for self-supervised learning. However, there is no transformer-based model to overcome the inherent limitations of SMILES, which result from the generation process of SMILES. In this study, we grammatically parsed SMILES to obtain connectivity between substructures and their type, which is called the grammatical knowledge of SMILES. First, we pretrained the transformers with substructural tokens, which were parsed from SMILES. Then, we used the training strategy “same compound model” to better understand SMILES grammar. In addition, we injected knowledge of connectivity and type into the transformer with knowledge adapters. As a result, our representation model outperformed previous compound representations for the prediction of molecular properties. Finally, we analyzed the attention of the transformer model and adapters, demonstrating that the proposed model understands the grammar of SMILES.

Motivation:

- ▶ Automate synthesis planning to reduce manual effort and errors.
- ▶ Accelerate chemistry research and development by rapidly exploring chemical pathways.
- ▶ Enable discovery of novel compounds and efficient reaction routes using generative models.
- ▶ Leverage SMILES representations for scalable and machine-readable chemistry workflows.

Chemical Pathways with SMILES (cont.)

(a) Model overview



(b) Tokenization

CC(=O)CC(C1=C(O)c2ccccc2OC1=O)c3cccc3

1) Pre-tokenization

CC [=O] CC [(C1)=C(O)c2ccccc2Oc1=O] c3cccc3

2) Byte-pair encoding

CC [=O] CC [(C1) =C(O) c2ccccc2 Oc1 =O] c3cccc3

(c) Grammatical parsing

1) Linear connectivity

CC [=O] CC [(C1)=C(O)c2ccccc2] Oc1 [=O] c3cccc3

2) Ring connectivity

CC [=O] CC [(C1)=C(O)c2ccccc2] Oc1 [=O] c3cccc3

3) Parentheses skipping

CC [=O] CC [(C1)=C(O)c2ccccc2] Oc1 [=O] c3cccc3

4) Token typing

CC [=O] CC [(C1)=C(O)c2ccccc2] Oc1 [=O] c3cccc3

Key Components:

- ▶ **SMILES Representation:** A text-based format for encoding chemical structures, enabling easy manipulation and analysis.
- ▶ **Generative Models:** AI models that learn from existing chemical data to generate new SMILES strings representing valid chemical compounds.
- ▶ **Reaction Prediction:** Models that predict possible reactions and their outcomes based on input SMILES strings.
- ▶ **Synthesis Planning:** Algorithms that suggest synthetic routes for target molecules by analyzing reaction networks.

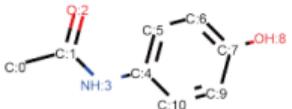
Chemical Pathways with SMILES (cont.)

Attention Analysis

Attention analysis on SCM

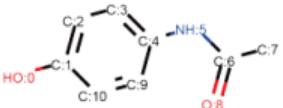
(a)

CC(=O)Nc1ccc(O)cc1
(Canonical SMILES)



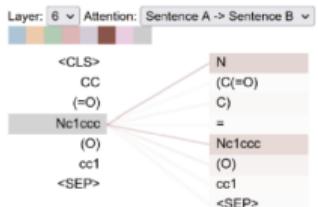
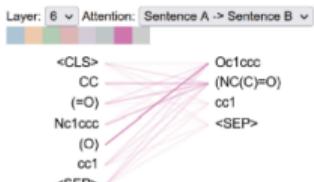
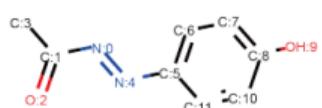
(b)

Oc1ccc(NC(C)=O)cc1
(Enumerated SMILES)



(c)

N(C(=O)C)=Nc1ccc(O)cc1
(Mutated SMILES)



Recent Breakthroughs:

- ▶ **Leveraging Negative Reactions:**

Science Advances paper demonstrates that incorporating negative reaction data significantly improves reactivity predictions.

- ▶ **Emerging Foundation Model: ChemDFM**

Introduction of ChemDFM, a large-scale foundation model for chemistry, enabling broad generalization across chemical tasks.

[cell.com](https://www.cell.com)

Chemical Pathways with SMILES (cont.)



LMH
Lady Margaret Hall

[github/sanjaradylov/smiles-gpt](https://github.com/sanjaradylov/smiles-gpt)

Limitations:

- ▶ **Long SMILES Strings (LLD):** Generative models may struggle with very long or complex SMILES representations, leading to invalid or incomplete outputs.
- ▶ **Coverage Gaps:** Rare or less-studied chemical reactions and compounds may be underrepresented, limiting the model's ability to generalize.
- ▶ **Experimental Validation:** AI-generated pathways and compounds require laboratory validation to confirm feasibility and safety.

Generative AI for Science: **Generative Models in Physical Simulations**

A Generative Approach to Control Complex Physical Systems

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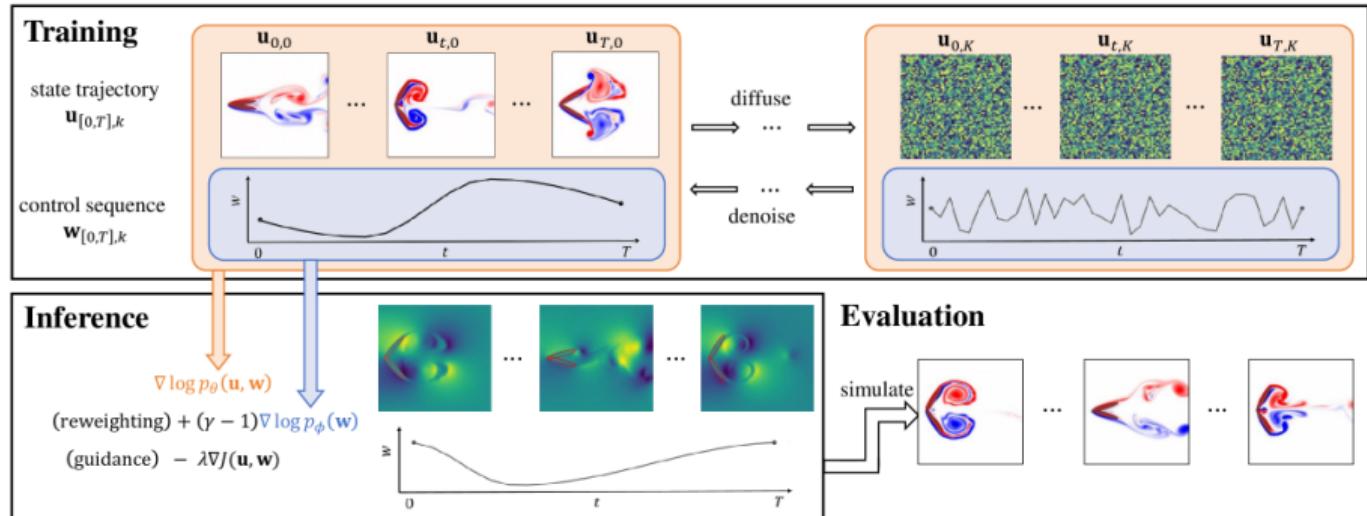
Why use Generative Models for Physical Simulations?

- ▶ Simulating things like fluids or materials is slow and needs a lot of computer power.
- ▶ Traditional methods solve tough math equations (PDEs) step by step, which takes time.
- ▶ Generative models can learn how these systems behave, so we can get results much faster.
- ▶ This means scientists can try out more ideas and make discoveries quicker.

What can Generative AI do in Simulations?

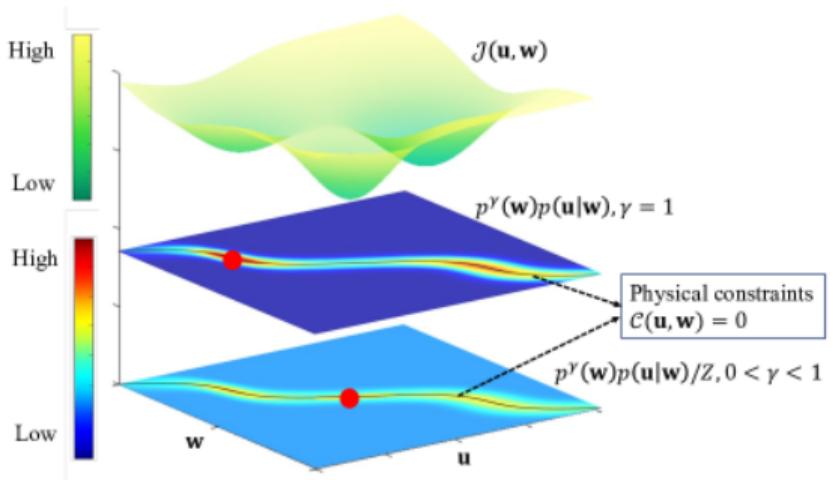
- ▶ **Faster Simulations:** Quickly create realistic simulations without heavy calculations.
- ▶ **Learn from Data:** Use real data to make new, believable scenarios.
- ▶ **Work at Different Scales:** Model things from tiny atoms to big objects.
- ▶ **Predict the Future:** Guess what might happen next in a system.
- ▶ **Mix with Experiments:** Combine with real-world data to make better predictions.
- ▶ **Help Scientists and Engineers:** Make it easier to test new ideas and designs.

Generative Models in Physical Simulations (cont.)



DiffPhyCon: A tool that uses generative models to simulate physical systems.

Generative Models in Physical Simulations (cont.)



How prior reweighting helps: By adjusting how we sample, we can find better solutions in our simulations.

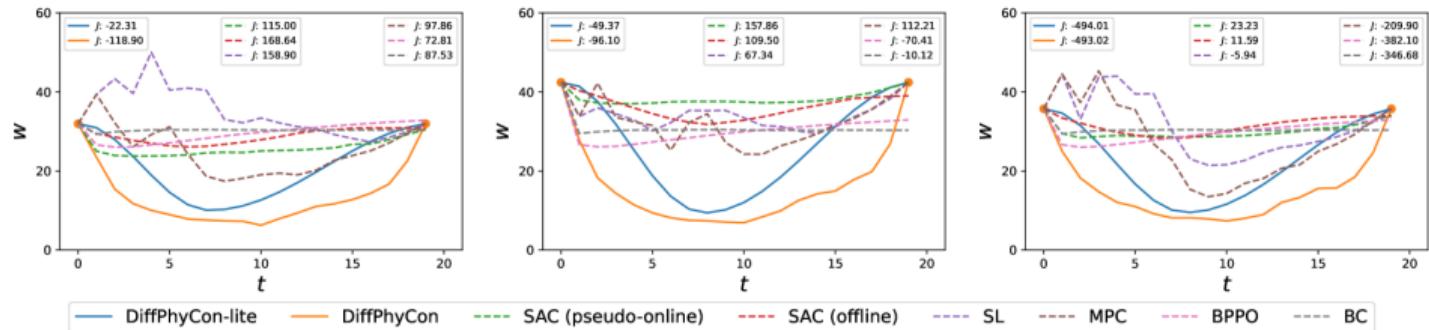
Algorithm 1 Inference for DiffPhyCon

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1: Require Diffusion models  $\epsilon_\theta(\mathbf{z}_k, \mathbf{c}, k)$  and  $\epsilon_\phi(\mathbf{w}_k, \mathbf{c}, k)$ , control objective  $\mathcal{J}(\cdot)$ , covariance matrix  $\sigma_k^2 I$ , control conditions  $\mathbf{c}$ , schedule  $\alpha_k$ , hyperparameters  $\lambda, \gamma, K$ 
2: Initialize optimization variables  $\mathbf{z}_K = [\mathbf{u}_K, \mathbf{w}_K] \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ 
3: for  $k = K, \dots, 1$  do
4:    $\hat{\mathbf{z}}_k = (\mathbf{z}_k - \sqrt{1-\alpha_k} \epsilon_\theta(\mathbf{z}_k, \mathbf{c}, k)) / \sqrt{\alpha_k}$ 
5:    $\mathbf{z}_{k-1} = \mathbf{z}_k - \eta(\epsilon_\theta(\mathbf{z}_k, \mathbf{c}, k) + \lambda \nabla_{\mathbf{z}} \mathcal{J}(\hat{\mathbf{z}}_k)) + \xi_1, \xi_1 \sim \mathcal{N}(0, \sigma_k^2 \mathbf{I})$  // transition to next diffusion step
6:    $\mathbf{w}_{k-1} = \mathbf{w}_{k-1} - \eta(\gamma - 1) \epsilon_\phi(\mathbf{w}_k, \mathbf{c}, k) + \xi_2, \xi_2 \sim \mathcal{N}(0, \sigma_k^2 \mathbf{I})$  // prior reweighting
7: end for
8: return  $\mathbf{u}^*, \mathbf{w}^* = \mathbf{z}_0$ 

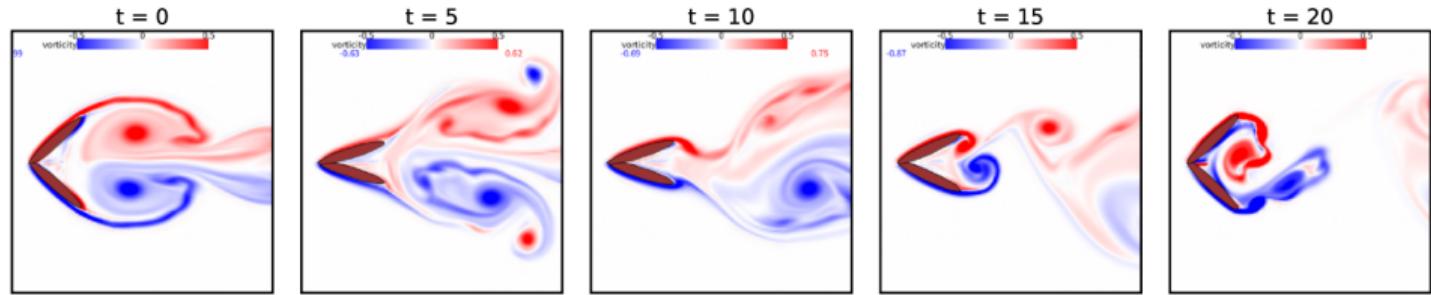
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Generative Models in Physical Simulations (cont.)



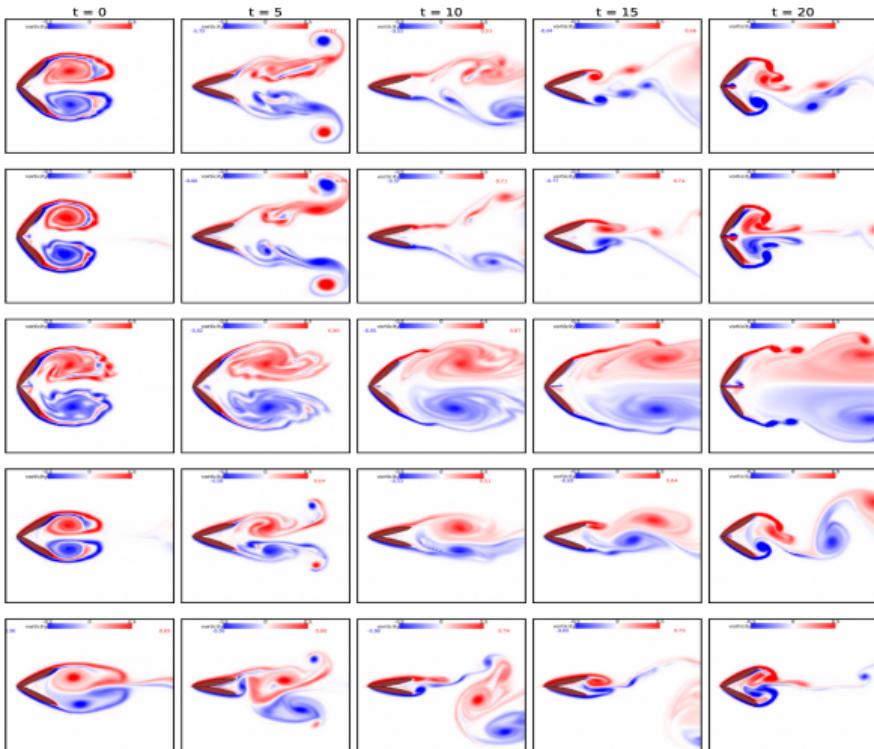
Comparing control curves for three jellyfish. Each curve shows how well the control works.

Generative Models in Physical Simulations (cont.)



See how the jellyfish moves and how the water flows around it, using DiffPhyCon.

Generative Models in Physical Simulations (cont.)



Challenges and Things to Watch Out For

- ▶ **Needs Lots of Data:** Training these models often needs a lot of good data.
- ▶ **Complex Systems:** Some systems are so complicated that models struggle to learn them.
- ▶ **Hard to Understand:** It can be tricky to see why the model makes certain choices.
- ▶ **Still Needs Computers:** Even though it's faster, training and running these models can still use a lot of computer power.
- ▶ **Checking Results:** We must always check if the model's results match real experiments.
- ▶ **Follow the Laws of Physics:** The model should respect things like energy conservation to be realistic.

Generative AI for Science: **Summary and Future Directions**

Key Takeaways

- ▶ Generative AI is transforming scientific research across various domains.
- ▶ It enhances the speed and accuracy of simulations, predictions, and data analysis.
- ▶ Applications range from protein design to climate modeling and drug discovery.

Future Directions

- ▶ Continued advancements in AI models will lead to even more sophisticated simulations and predictions.
- ▶ Integration of AI with experimental data will enhance the reliability of scientific findings.
- ▶ Ethical considerations and responsible AI use will be crucial as these technologies evolve.

Conclusion

- ▶ Generative AI holds immense potential to accelerate scientific discovery and innovation.
- ▶ Ongoing research and development will unlock new possibilities in understanding complex systems.
- ▶ Collaboration between AI experts and domain scientists is essential for maximizing impact.

Generative AI for Science: **References**

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- ▶ Science Advances: Chen, H., Zhang, Y. (2023). Leveraging negative reactions for improved reactivity predictions. *Science Advances*, 9(12), eadk1426.

Additional Resources:

- ▶ NVIDIA Earth-2:
https://build.nvidia.com/nvidia/fourcastnet?snippet_tab=Try
- ▶ SMILES: <https://www.daylight.com/dayhtml/doc/theory/theory.smiles.html>
- ▶ AlphaFold: <https://alphafold.ebi.ac.uk/>
- ▶ Earth-2: <https://www.nvidia.com/en-us/research/earth-2/>

Credits

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