Collaboration:

Key to Scaling and Accelerating Quantum Research in Healthcare and Life Sciences

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IBM Research

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IBM

Cleveland Clinic – IBM Research *Discovery Accelerator*

TEN YEAR MISSION Deploy the next frontier of computing technologies including ***AI, hybrid cloud*** and ***quantum computing*** to revolutionize the practice of healthcare and discovery in life sciences and foster the development of the next generation workforce.

Clinical and biomedical research resources and expertise.

Next frontier of computing technologies and expertise

IBM Quantum System one at Cleveland Clinic

First on-premises IBM Quantum System One (127 qubits) unveiled in March 2023

First Quantum System **dedicated to healthcare and life sciences** with the mission to create a HCLS innovation ecosystem in America's heartland with outreach and impact around the world

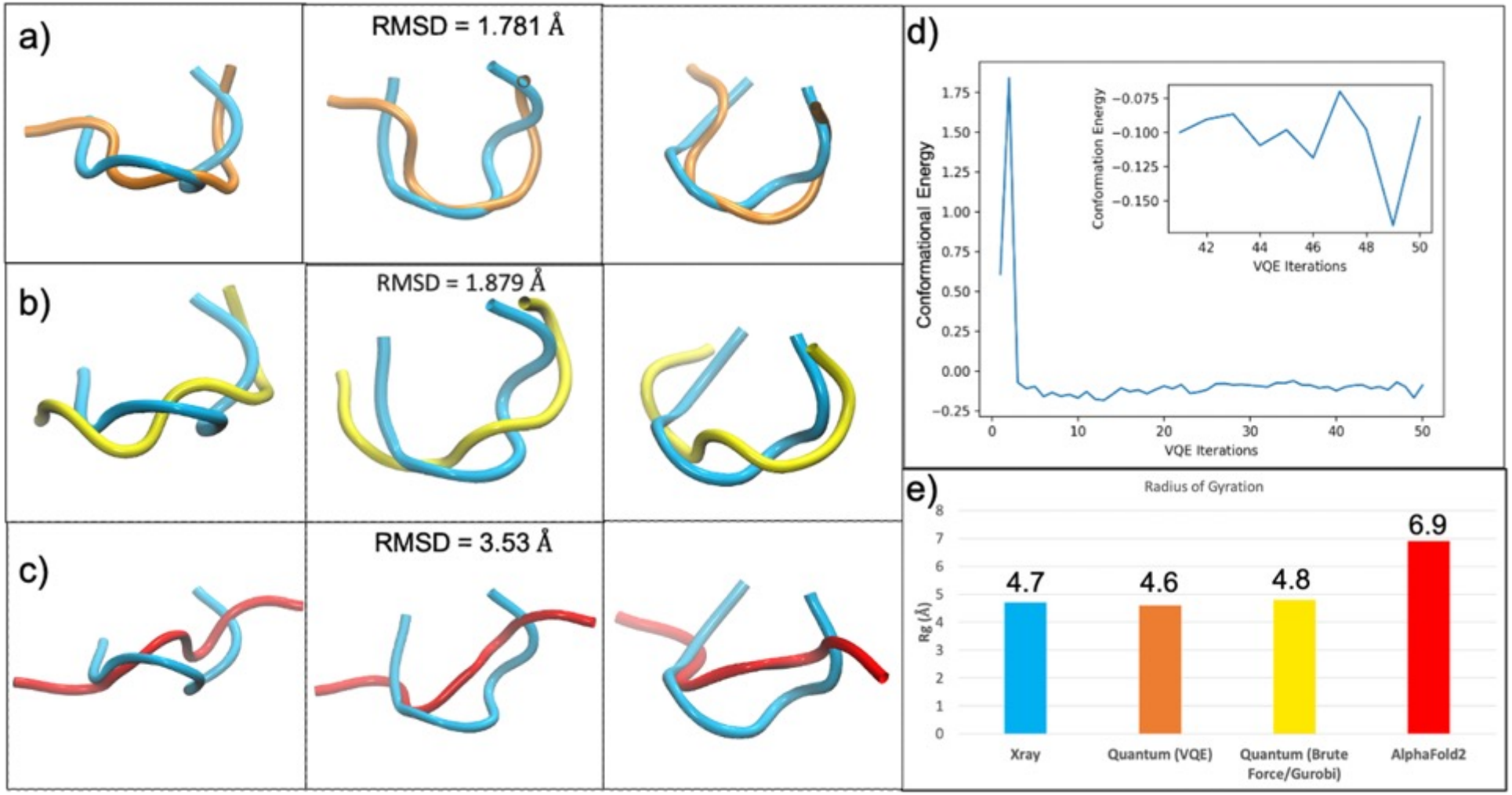
A Perspective on Protein Structure Prediction Using Quantum Computers

Hakan Doga,* Bryan Raubenolt,* Fabio Cumbo, Jayadev Joshi, Frank P. DiFilippo, Jun Qin,
Daniel Blankenberg, and Omar Shehab

J. Chem. Theory Comput. 2024, 20, 3359–3378

Test case: The Zika, Dengue, and West Nile Virus Helicase "P-loop"

- Experimental structure
- IBM_Cleveland (RMSD=1.781)
- Classical solver (RMSD= 1.879)
- AlphaFold2 (RMSD = 3.53)



Courtesy of Dr. Daniel Blankenberg and Dr. Hakan Doga

Quantum Working Groups

IBM Quantum working groups bring together the best scientists in our field to accelerate our path to achieving Quantum Advantage by 2025, across domain areas:

Optimization

Quantum Optimization: Potential, Challenges, and the Path Forward

arXiv:2312.02279

Materials & HPC

Quantum-centric Supercomputing for Materials Science: A Perspective on Challenges and Future Directions

arXiv:2312.09733

High-Energy Physics

Quantum Computing for High-Energy Physics: State of the Art and Challenges. Summary of the QC4HEP Working Group

arXiv:2307.03236

Healthcare & Life Sciences

Towards quantum-enabled cell-centric therapeutics

arXiv:2307.05734

Sustainability

Collaborative projects in the fields of Materials and Energy leveraging quantum computers.

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HCLS Working Group: Purpose and Mission

<u>Purpose:</u> To bring useful quantum computing to the world for the healthcare and life sciences industry

Our working group will pave the way towards useful quantum computing by *empowering* research on quantum computers and on our platform, and by promoting the growth of the quantum industry.

<u>Workomg Group Mission:</u>

Find the way, *Go the way*, *Show the way* to useful quantum computing for healthcare and life sciences through **collaboration**

HCLS Working Group Institutions

Algorithmiq	MIT
Amgen	Moderna
Athos	My Next Health
Broad Institute	NTU
Capgemini	Oak Ridge National Lab (ORNL)
Carelon	Poznan Supercomputing and Network Center (PSNC)
Cleveland Clinic	QC Ware Corp
Deloitte	STFC
DESY	University of Chicago
Harvard Medical School	University of Melbourne
IBM	University of Queensland
Capgemini	University of Toronto
Keio University	UptownBasel
Leiden University	Virginia Tech
LLNL	Washington University in St. Louis
Purdue University	Yonsei University

- ~70 members from ~30 institutions (increased from ~45 members at kickoff meeting)
- Academia, industry, national labs, government, startups represented

Perspective article:
Towards quantum-enabled cell-centric therapeutics

Towards quantum-enabled cell-centric therapeutics

Saugata Basu[1], Jannis Born[2], Aritra Bose[3], Sara Capponi[4,5], Dimitra Chalkia[6], Timothy A Chan[7,8], Hakan Doga[9], Frederik F. Flöther[10], Gad Getz[11,12,13,14], Mark Goldsmith[15], Tanvi Gujarati[9], Aldo Guzmán-Sáenz[3], Dimitrios Iliopoulos[6], Gavin O. Jones[9], Stefan Knecht[15], Dhiraj Madan[16], Sabrina Maniscalco[15], Nicola Mariella[17], Joseph A. Morrone[3], Khadijeh Najafi[18], Pushpak Pati[2], Daniel Platt[3], Maria Anna Rapsomaniki[2], Anupama Ray[16], Kahn Rhrissorrakrai[3], Omar Shehab[18], Ivano Tavernelli[19], Meltem Tolunay[9], Filippo Utro[3], Stefan Woerner[19], Sergiy Zhuk[17], Jeannette M. Garcia [†‡9], and Laxmi Parida[†‡3]

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[5]Center for Cellular Construction, San Francisco, CA, USA
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[7]Center for Immunotherapy and Precision-Immuno-Oncology, Cleveland Clinic, Cleveland, OH, USA
[8]National Center for Regenerative Medicine, Cleveland Clinic, Cleveland, OH, USA
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[19]IBM Quantum, IBM Research Europe, Zurich, Switzerland

August 1, 2023
https://arxiv.org/abs/2307.05734

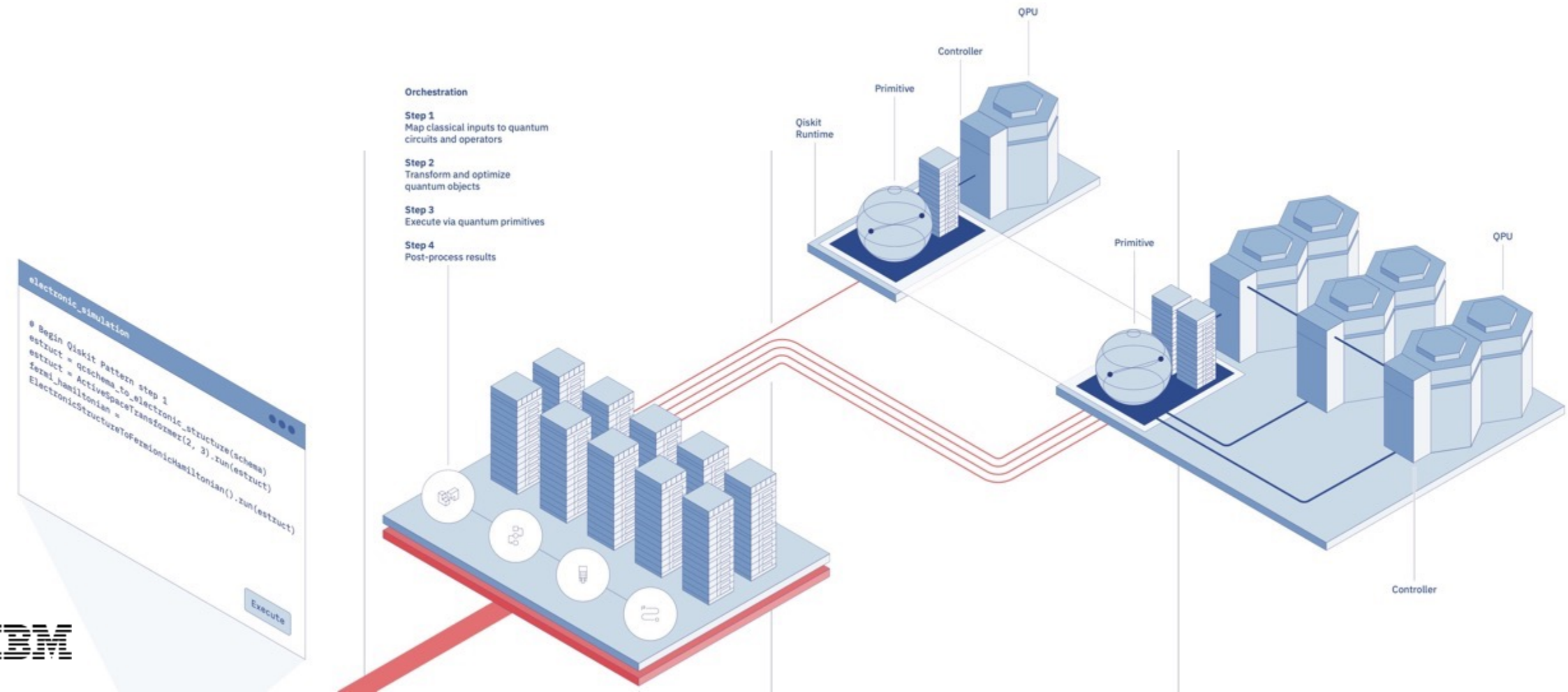
Quantum Enabled Cell-Centric Therapeutics covers four key areas:

- First is the use of quantum neural networks (QNNs) to learn about how immune cells send and receive signals from limited data.
- The second is using hybrid classical-quantum generative neural networks to model the environment around tumors.
- The third is using a novel hybrid quantum optimization algorithm to model an individual cells' response to a therapeutic intervention.
- And the fourth is using quantum to perform topological data analysis to better capture the interactions between cells.

Quantum Computing for Healthcare and Life Sciences*: Working Group Themes and Subgroups*

Topic Area	Subgroup
Biomarkers	
Clinical trial optimization and design	Clinical Trial simulation
	Clinical Trial Design (including site selection and cohort selection)
QML for Omics	Bayesian classification (model averaging)
	Topological analysis on omics data
	Q-Cell Engineering
	Perturbation modeling with Optimal Transport
	Network medicine with quantum walks
Quantum Simulation for Drug and Molecule Discovery	Protein/mRNA folding
	Drug discovery: Alchemical Hamiltonians
	Drug discovery: Electronic Structure

Thank you


Orchestration
Step 1
Map classical inputs to quantum circuits and operators
Step 2
Transform and optimize quantum objects
Step 3
Execute via quantum primitives
Step 4
Post-process results
Qiskit Runtime
Primitive
Controller
QPU
Primitive
QPU
Controller
electronic_simulation
Execute