計算科学・量子計算における情報圧縮

Data Compression in Computational Science and Quantum Computing

2022.10.6

#1:計算科学・量子計算と情報圧縮

Computational science, quantum computing, and data compression

---

理学系研究科　大久保　毅

Graduate School of Science, **Tsuyoshi Okubo**

*This lecture will be given by

Tsuyoshi Okubo and Prof. Synge Todo

Outline

- Background
    - Background of the lectures
    - Tentative lecture schedule
    - Evaluation
- Introduction
    - Huge data in physics
        - Why do we need data compression?
    - Examples of data compression
    - Quantum many-body problems and quantum computation

Background of lecturer

大久保　毅 (OKUBO Tsuyoshi)

Project Associate Professor,
(**Quantum software endowed chair**)
Institute for Physics of Intelligence
Sci. Bldg. #1 950

Research:

Statistical Physics, Condensed matter physics, Magnetism,
(Computational Physics)

- Random packing of disks
- Sciophysics (analysis of hierarchical society...)
- Ordering of (classical) frustrated spin system
  - Topological excitations, Skyrmion, ...
- **Tensor network methods**
  - Quantum spin systems
  - Quantum computer applications
  - Data science applications
- ….

TeNeS

https://www.pasums.issp.u-tokyo.ac.jp/tenes/en

量子ソフトウェア寄付講座 (Quantum software endowed chair)

https://qsw.phys.s.u-tokyo.ac.jp

東京大学

大学院理学系研究科

(知の物理学研究センターと連携)

「量子ソフトウェア」寄付講座

- 産業界の動向の把握
- 本学の量子関連研究領域の教育強化
- 協賛・協力企業との更なる産学連携の可能性

運営への協賛

協賛企業・協力企業

SCSK株式会社
株式会社NTTデータ
株式会社電通国際情報サービス
日鉄ソリューションズ株式会社
株式会社三井住友フィナンシャルグループ・株式会社日本総合研究所
日本電気株式会社
BIPROGY株式会社
富士通株式会社
blueqat株式会社
凸版印刷株式会社

- 量子コンピュータ人材育成への貢献
- 自社のR&D、ビジネス応用に向けた人材育成やスキル向上
- 東京大学および協賛・協力企業間の共創、連携の強化

量子ネイティブ育成
(専門講座等)

受講生（学部生・大学院生／社会人）

- 量子機械学習や量子アプリケーションの最先端知見・スキルの獲得と社会実装における課題の解決
- 量子ネイティブの育成と研究成果の社会への還元

Computational Science Alliance, The University of Tokyo

Computational Science Alliance

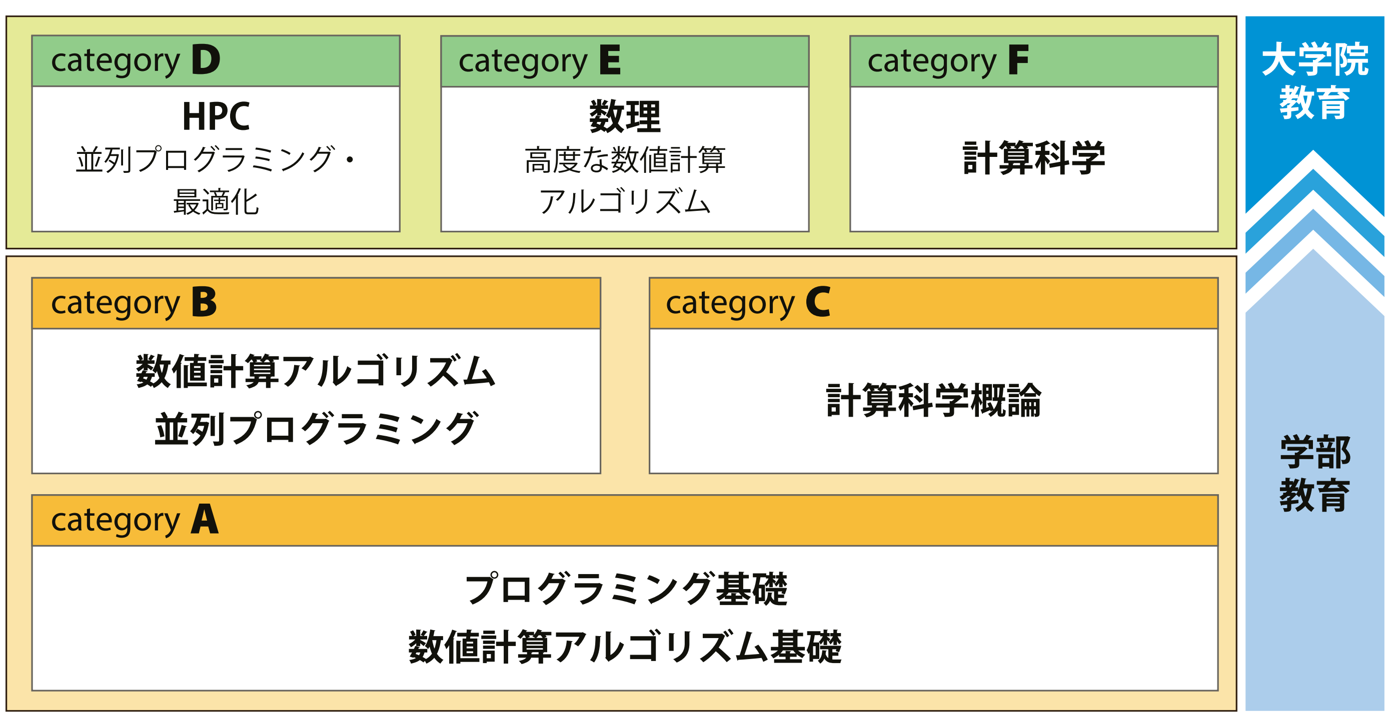
The University of Tokyo

https://www.compsci-alliance.jp

Train experts for computational and computer sciences.

計算科学アライアンス認定講義

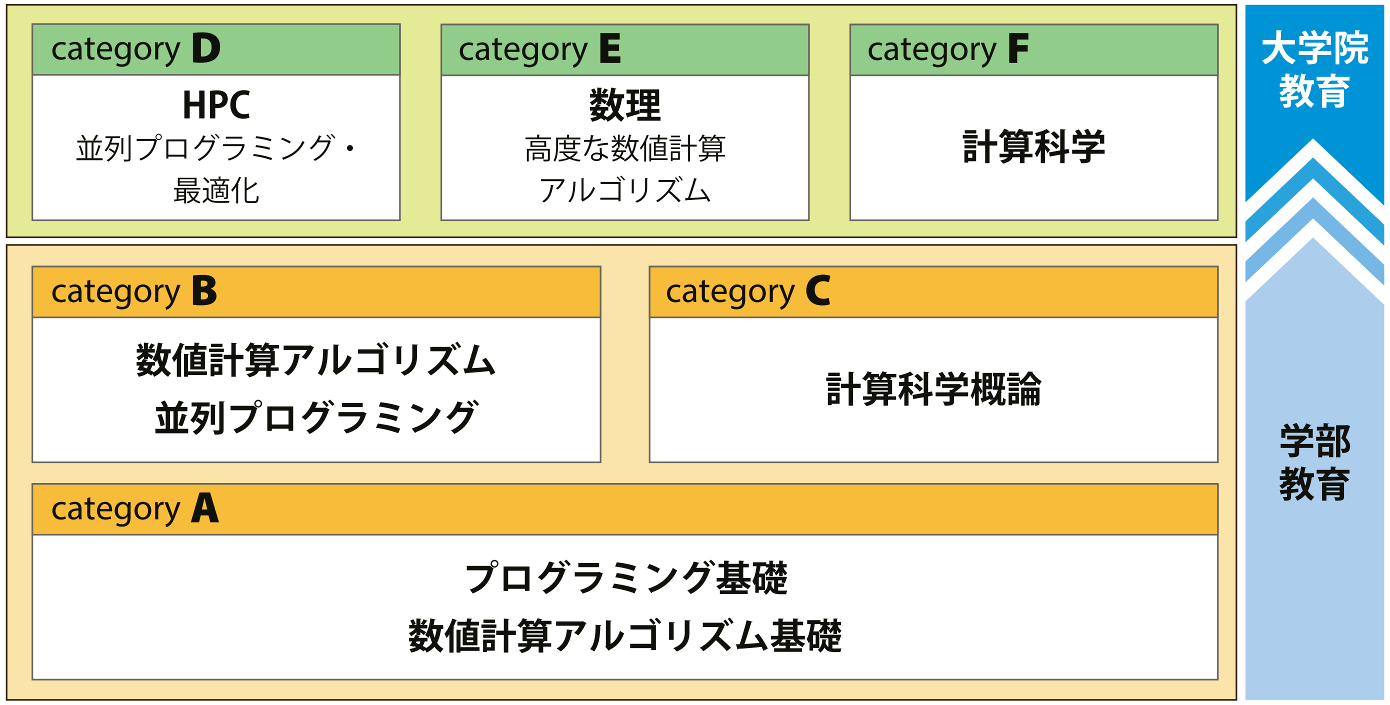
- 平成２９年度から実習にも力点をおいた新しい講義を立ち上げ
- 計算科学・計算機科学に関する80以上の学部・大学院講義とあわせ、「計算科学アライアンス認定講義」として体系化
- 認定講義を内容に応じて6つのカテゴリに分類
- 所定の単位を取得した学生には「修了認定証」を発行
- この講義はカテゴリE



- 学部
  - カテゴリA,B,Cからそれぞれ1.5単位以上
- 大学院
  - カテゴリD,E,Fのうち2つのカテゴリを選択しそれぞれから2単位以上

計算科学アライアンス認定講義：大学院

- カテゴリD - 最先端のスーパーコンピュータを駆使するのに必要とされる技術。種々の並列アルゴリズム、MPI並列やOpenMP並列などの並列プログラミング、メモリアクセス最適化などのチューニング
  - 例：**計算科学アライアンス特別講義I、II**
- カテゴリE - 最先端の数値計算アルゴリズムとその数理的基礎付け。差分法・有限要素法・有限体積法、特異値分解、最適化問題などの手法とその応用
  - 例：**計算科学・量子計算における情報圧縮**
- カテゴリF - 各分野におけるシミュレーション手法とその研究成果。電子状態計算、分子動力学、量子多体計算、数値流体力学、構造計算、ゲノム解析など
  - 例：**多体問題の計算科学**



(Tentative)

Lecture schedule

Notice

- No classes on Nov. 3, Nov. 17, and Nov. 22
- Classes will be also held on Jan. 5 and Jan. 19

Okubo

1. Computational science, quantum computing, and data compression (Today)
2. Review of linear algebra
3. Singular value decomposition
4. Application of SVD and generalization to tensors
5. Entanglement of information and matrix product states

Todo

6. Application of MPS to eigenvalue problems

Okubo

7. Tensor network representation
8. Data compression in tensor network
9. Tensor network renormalization

Todo

10. Quantum mechanics and quantum computation
11. Simulation of quantum computers
12. Quantum-classical hybrid algorithms and tensor network
13. Quantum error correction and tensor network

Important infomations

Style: This course will be a hybrid of face-to-face and online.

(Zoom information is on UTAS and ITC-LMS.)

It is from 13:00 to 14:45 (105 min. lecture).

Evaluation: Based on 2 reports:

Exercises include algorithms and computer simulations.

(I will probably provide python codes (jupyter notebooks).)

Notice!

> The grade will be evaluated based on
> the sum of scores of two reports.
> (So, if you will miss one of them, it will be big disadvantage.)

Slides: The lecture slides will be uploaded to

- ITC-LMS (Information Technology Center Learning Management System)
- https://github.com/utokyo-qsw/data-compression

Introduction: Huge data in physics

Computer science and data science

1. Experimental Science
2. Theoretical Science
3. Computational Science
4. Data Science
5. AI?

“Data compression in computational science and quantum computing " is related to the 3rd and 4th sciences.

Huge data in physics

Many-body problems in physics

- Celestial movement（天体運動）
- Gases, Liquids
- Molecules, Polymers (eg. Proteins), ...
- Electrons in molecules and solids
- Elemental particles (Quantum Chromo Dynamics)
（量子色力学）

In these problems, "systems" contain huge degrees of freedom:

$6N$-dimensional phase space for classical mechanics

$O(e^N)$-dimensional Hilbert space for quantum system

Complex particle system

Eg. Poliovirus capsid in electrolyte solution

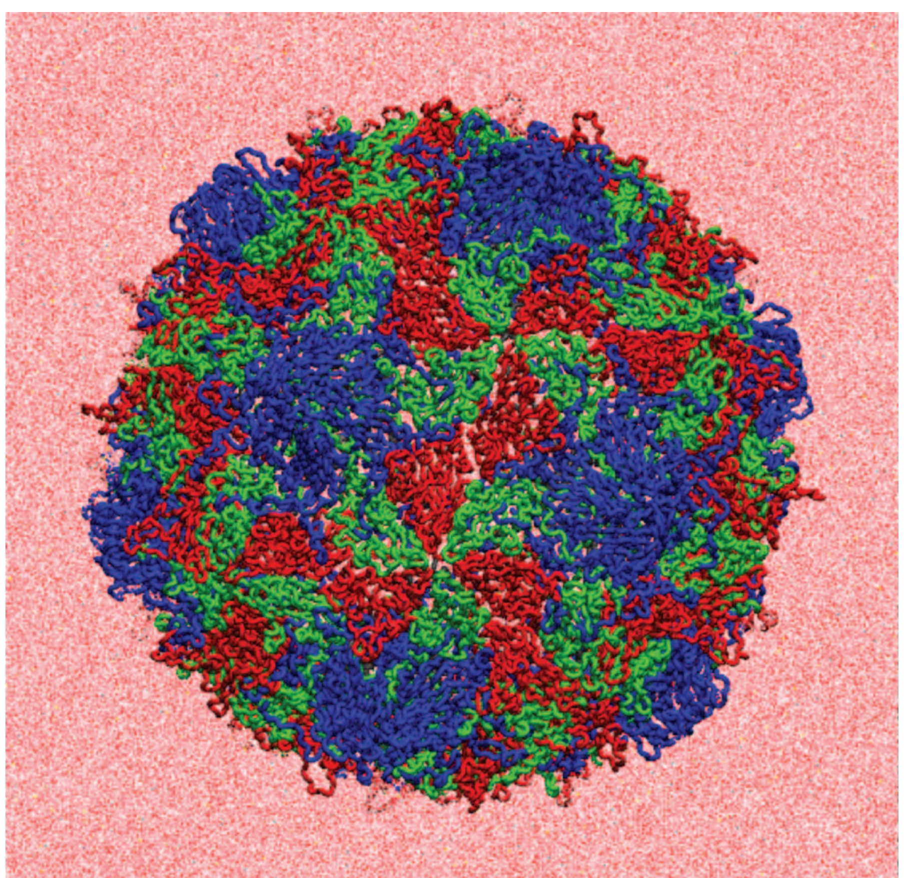
（ポリオウイルス　カプシド）　　　　**（電解質溶液）**

Y. Ando et al, J. Chem. Phys. **141**, 165101(2014).

Long-range coulomb interaction

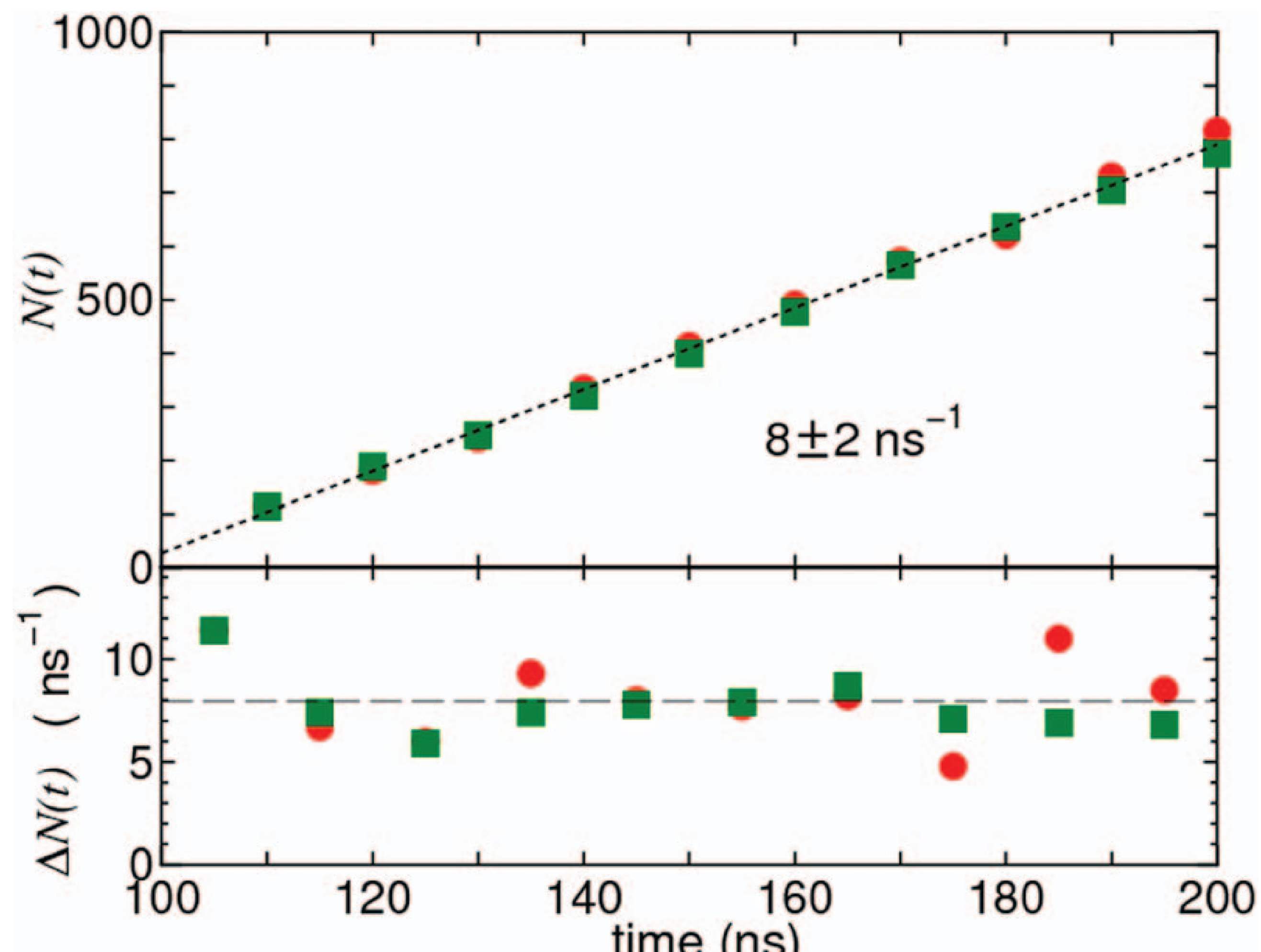
（クーロン相互作用）

Poliovirus capsid



6.5 million atoms

Dynamics of water molecules

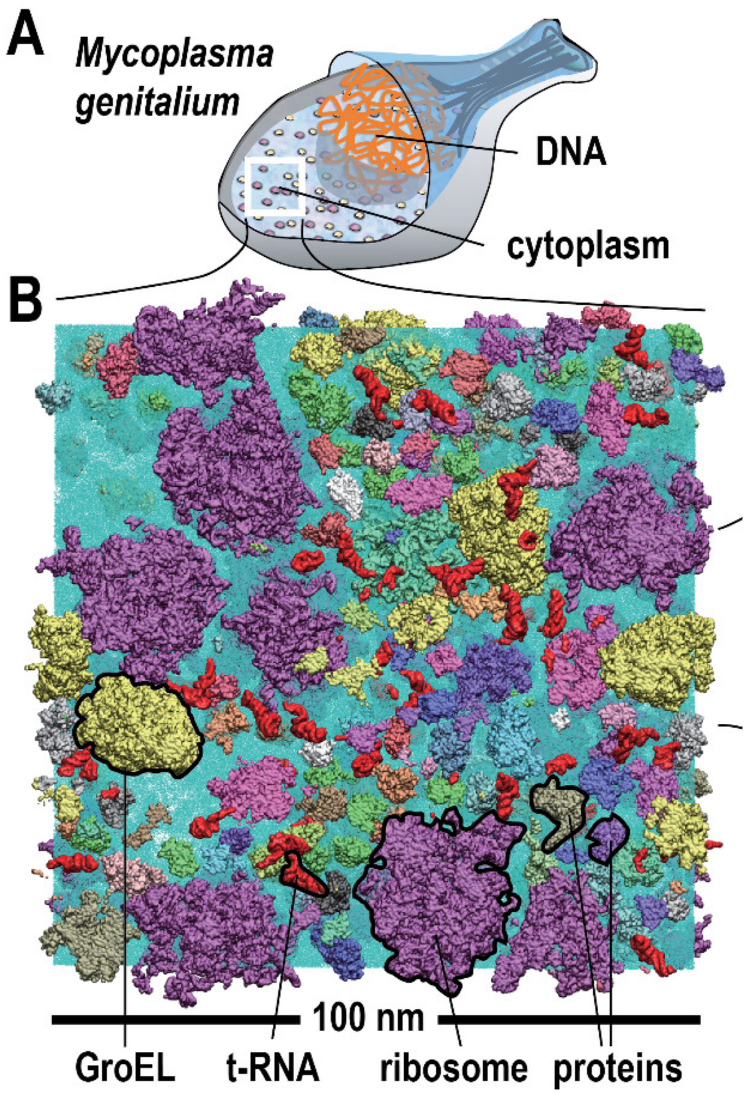


Biological system

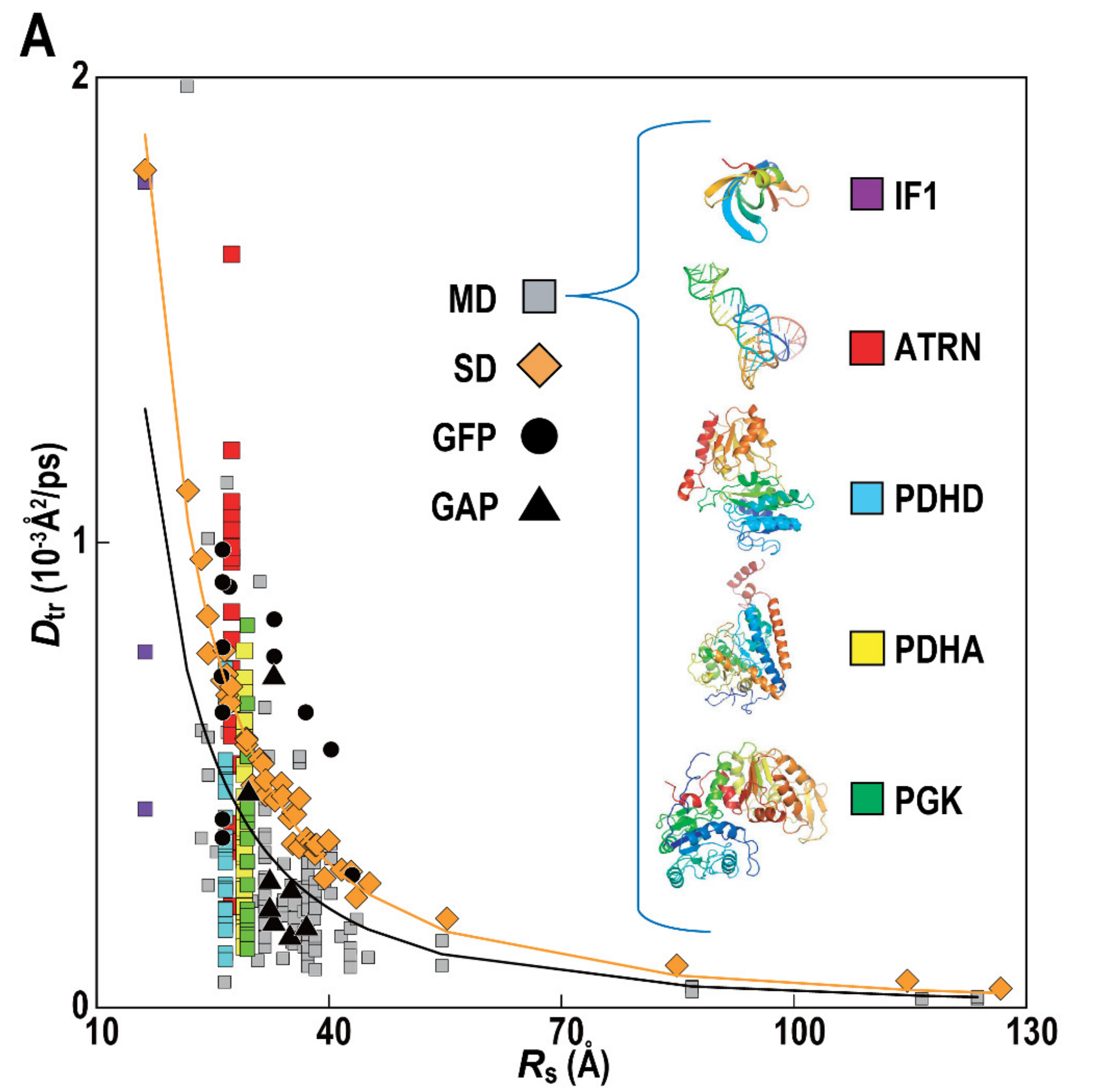
Atomistic model of bacterial cytoplasm (バクテリアの細胞質)

→ **100 million atoms**

I. Yu, et al., elife **5**, e19274 (2016).



Diffusion constant of various molecules



Diffusion constant of various molecules

Localized electrons as quantum spin systems

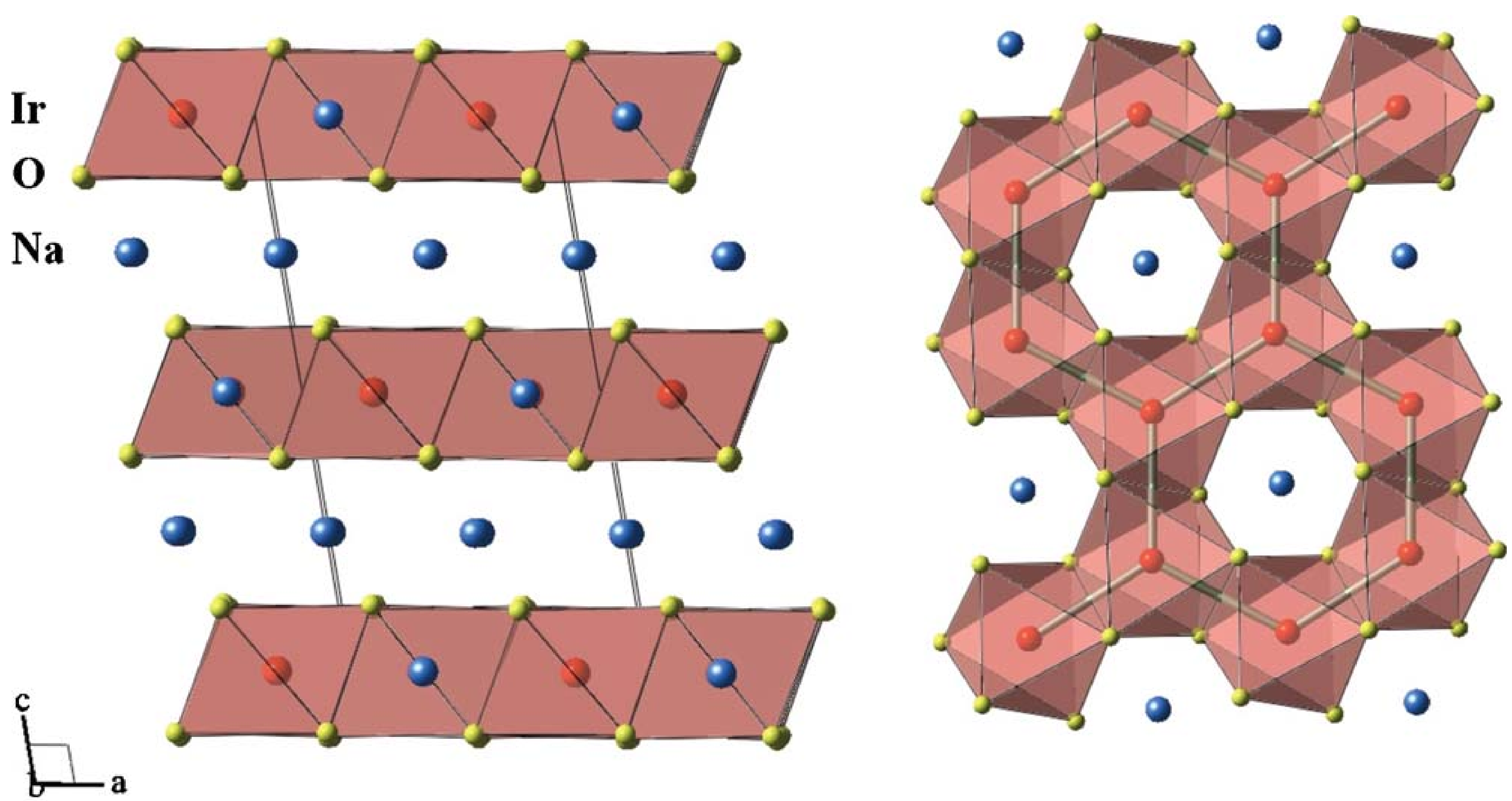
Eg. Antiferromagnetic Mott insulator Na_2IrO_3

（反強磁性）　　　　　（モット絶縁体）

Y. Singh and P. Gegenwart, Physical Review B **82**, 064412 (2010)

$$\mathcal{H} = \sum_{i,j} J_{ij} S_i S_j$$

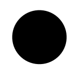
S_i : spin operator



(a)　　　　(b)

Quantum systems

Example of quantum system: Array of quantum bits

1 bit  A quantum bit is represented by two basis vectors.

$$|0\rangle, |1\rangle \quad \text{or} \quad (|\uparrow\rangle, |\downarrow\rangle)$$

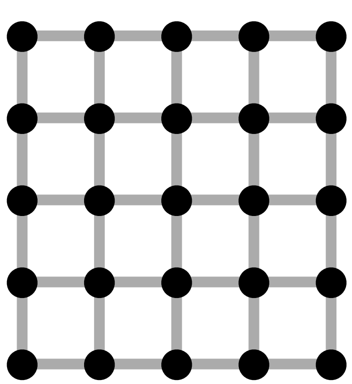
2 bits  The vector space is spanned by four basis vectors.

$$|0\rangle \otimes |0\rangle, |0\rangle \otimes |1\rangle, |1\rangle \otimes |0\rangle, |1\rangle \otimes |1\rangle$$

Simple notation: $|00\rangle, |01\rangle, |10\rangle, |11\rangle$

$$|\Psi\rangle = \sum_{\alpha,\beta=0,1} C_{\alpha,\beta}|\alpha\beta\rangle$$

$C_{\alpha,\beta}$:complex number

N bits 

Dimension of the vector space $\underline{= 2^N}$

Exponentially large!

$$|\Psi\rangle = \sum_{\{i_1,i_2,\ldots i_N\}} \Psi_{i_1 i_2 \ldots i_N} |i_1 i_2 \ldots i_N\rangle$$

Introduction: Why do we need data compression?

Why do we need data compression?

1. We cannot understand huge information directly.

⇒ We try to characterize "systems" thorough a few parameters.

Examples:

Thermodynamics:

Systems are characterized by thermodynamic quantities,

Internal energy, Entropy, Pressure, Volume, Particle number,...

Critical phenomena and renormalization group:

（臨界現象）　　　　（繰り込み群）

Critical systems are characterized by a few critical exponents.

Along the renormalization flow, irrelevant information is removed.

Why do we need data compression?

2. We cannot treat entire data in the present computers.

Available memories in the present computers:

		Double precision real number = 8 Bite
Personal computers:	~10 GB	$\sim 10^{9}$
Supercomputers:	~100 GB / node	$\sim 10^{10}$
Fugaku@RIKEN, **Oakbridge-CX**@UTokyo, **Ohtaka**@ISSP, UTokyo ...	~1 PB (whole system)	$\sim 10^{14}$

Notice: In quantum system, the size of Hilbert space is $O(e^N)$

Why do we need data compression?

2. We can not treat entire data in the present computers.

→ Try to reduce the "effective" dimension of a (vector) space.

By taking a proper basis set,
we can represent a (quantum) state efficiently.

- Krylov subspace
- Low-rank approximation (#3 and #4)
- Tensor network states (#5 - #8, #11-#13)
- ...

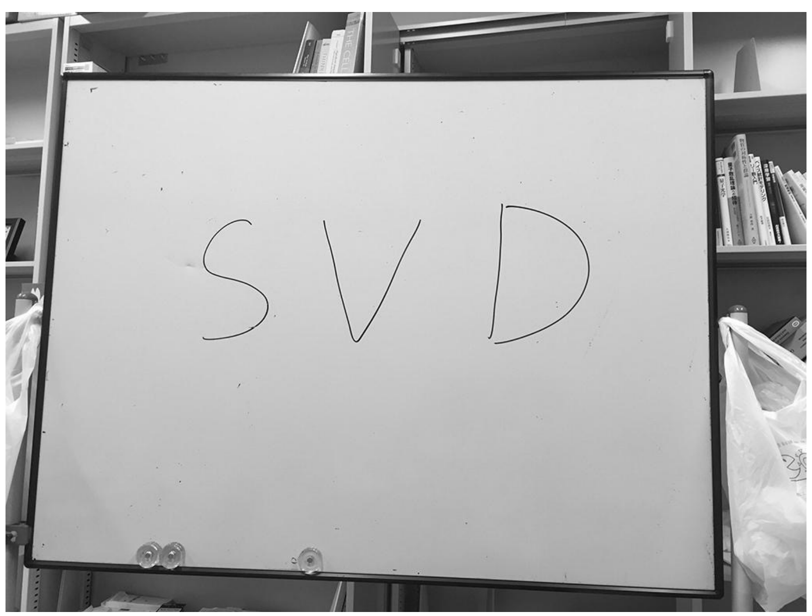
Introduction: Examples of data compressions

Examples of data compression 1

Compression of an image

$\boxed{\text{image} = \text{matrix}}$

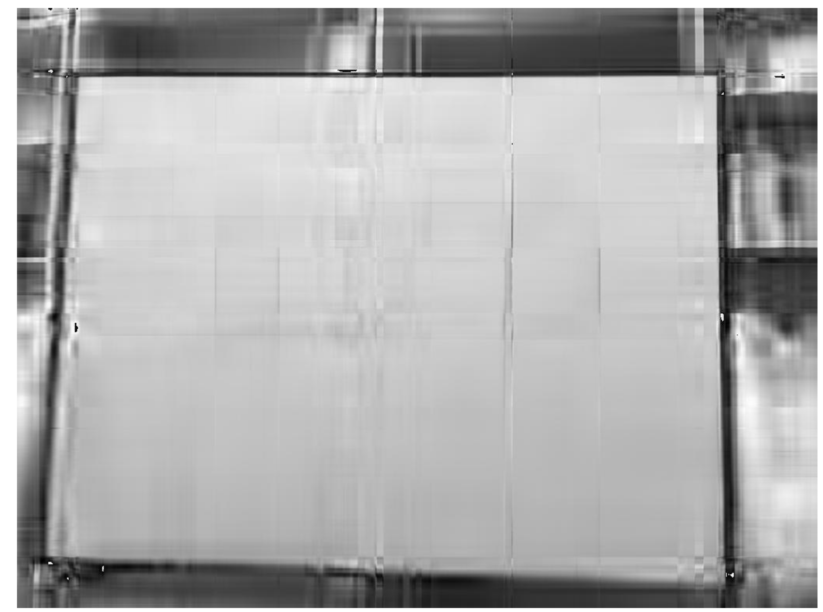
Original



$\chi = 768$

of "singular values"

Compressed



$\chi = 10$

$\chi = 100$

Examples of data compression 1

Compression of a color image

$\boxed{\text{image} = \text{tensor}}$

Original

$\chi = 768$

About 10% compressed

SVD

HOSVD

Singular value decomposition （特異値分解）

Singular value decomposition (SVD):

For a K × L matrix M,

$$M = U \Lambda V^\dagger$$

$U, V^\dagger$: (half) unitary

Λ : Diagonal

$$\Lambda = \begin{pmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_N \end{pmatrix}$$

$$M_{i,j} = \sum_m U_{i,m} \lambda_m V^\dagger_{m,j}$$

Singular values: $\lambda_m \geq 0$

Singular vectors: $\sum_i U_{i,m} U^\dagger_{m,j} = \delta_i, j$

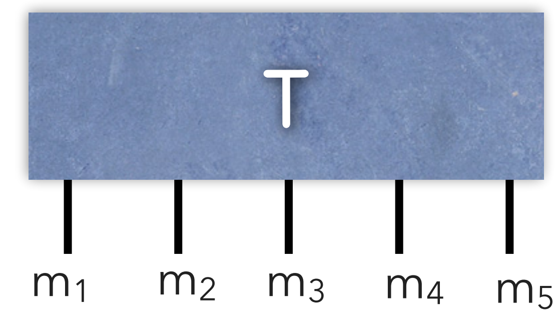
$\sum_i V_{i,m} V^\dagger_{m,j} = \delta_i, j$

By taking only several larger singular values,
we can approximate M as **a lower rank matrix**.

(low-rank approximation)

Examples of data compression 2

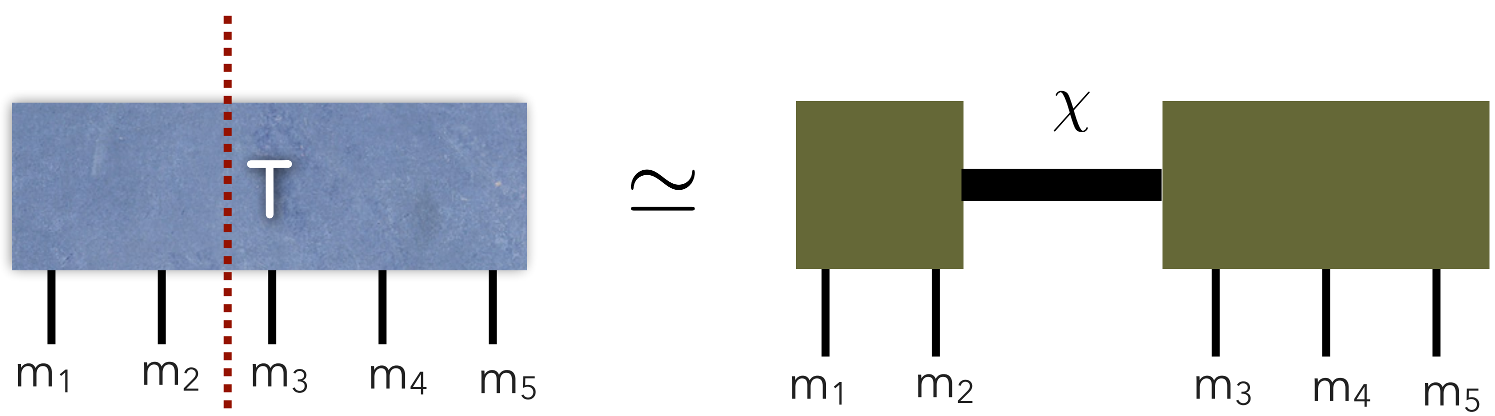
$T_{m_1,m_2,\cdots,m_N}$:N-leg tensor (or Vector)



We can consider it as a matrix by making two groups:

$$T_{\{m_1,m_2,\cdots,m_M\},\{m_{M+1},\cdots,m_N\}}$$

We can perform the low rank approximation of T.



We may consider similar approximation for each block.

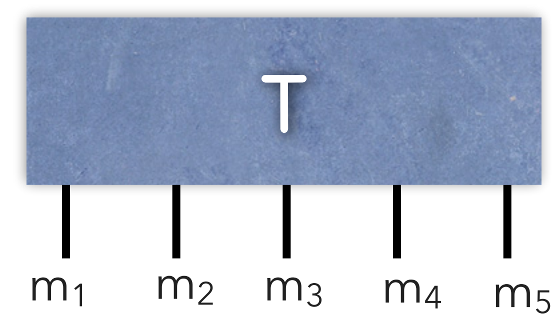
Tensor network decomposition

Examples of data compression 2

Wave function: $$|\Psi\rangle = \sum_{\{m_i=\uparrow\downarrow\} \text{ or } \{m_i=0,1\}} T_{m_1,m_2,\cdots,m_N} |m_1, m_2, \cdots, m_N\rangle$$

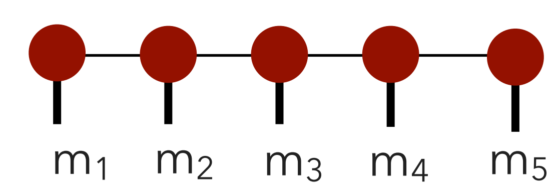
(波動関数)

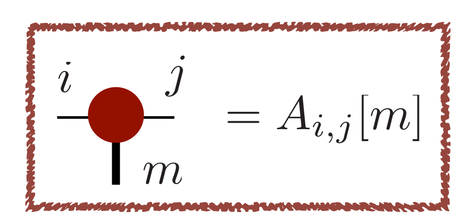
$T_{m_1,m_2,\cdots,m_N}$ N-rank tensor (or Vector)



$\boxed{\text{\# of Elements} = 2^N}$

Approximation as
a product of "matrices"





Matrix Product States **(行列積状態)**

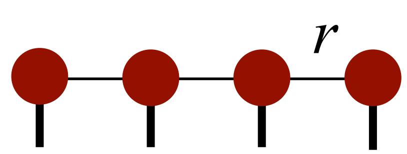
(Tensor train decomposition)

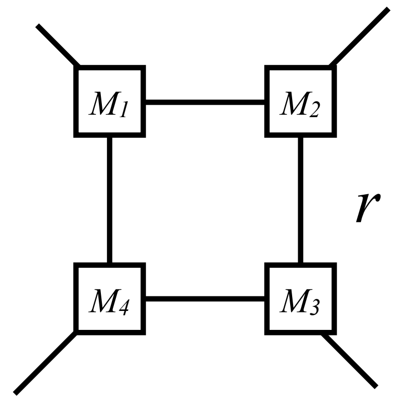
$$T_{m_1,m_2,\cdots,m_N} \simeq A_1[m_1]A_2[m_2]\cdots A_N[m_N]$$

$A[m]$: Matrix for state m

Application of MPS to data science

Tensor train (TT) and tensor ring (TR) decompositions for real data.





COIL-100 dataset = 32 x 32 x 3 x 7200 tensor

Pixel color # of pictures

Compression by tensor ring decomposition.

(Q. Zhao, et al arXiv:1606.05535)

error Rank

	ϵ	r_{max}	$\bar{r}$	Acc. (%) ($\rho = 50\%$)	Acc. (%) ($\rho = 10\%$)
CP-ALS	0.20	70	70	97.46	80.03
	0.30	17	17	97.56	83.38
	0.39	5	5	90.40	77.70
	0.47	2	2	45.05	39.10
TT-SVD	0.19	67	47.3	99.05	89.11
	0.28	23	16.3	98.99	88.45
	0.37	8	6.3	96.29	86.02
	0.46	3	2.7	47.78	44.00
TR-SVD	0.19	23	12.0	99.14	89.29
	0.28	10	6.0	99.19	89.89
	0.36	5	3.5	98.51	88.10
	0.43	3	2.3	83.43	73.20

Compressing deep neural network

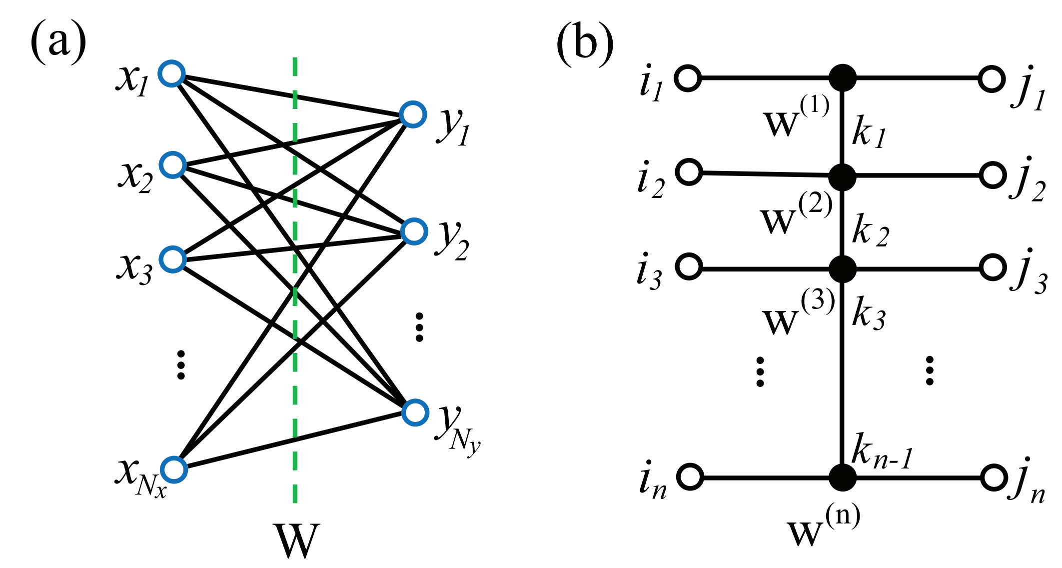
Z.-F. Gao et al, Phys. Rev. Research **2**, 023300 (2020).

MPO approximation of the weight matrix

x_i: input neuron (pixel)
y_i: output neuron

W_{ij}: weight matrix connecting x and y

MPO approximation of W



Example: application to classification problems

TABLE I. Test accuracy a and compression ratios ρ obtained in the original and MPO representations of LeNet-5 on MNIST and VGG on CIFAR-10.

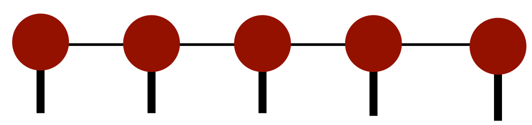
Data set	Network	Original Rep a (%)	MPO-Net a (%)	MPO-Net ρ
MNIST	LeNet-5	99.17 ± 0.04	99.17 ± 0.08	0.05
CIFAR-10	VGG-16	93.13 ± 0.39	93.76 ± 0.16	$\sim$0.0005
	VGG-19	93.36 ± 0.26	93.80 ± 0.09	$\sim$0.0005

a:**accuracy (%)**

ρ:**compression ratio**

Examples of tensor network decompositions

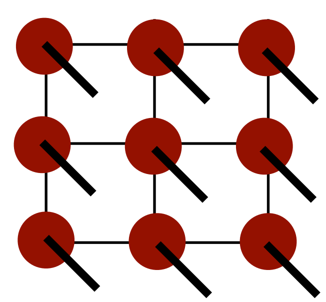
MPS:



Good for 1d gapped systems

(1d correlation in data)

PEPS, TPS:

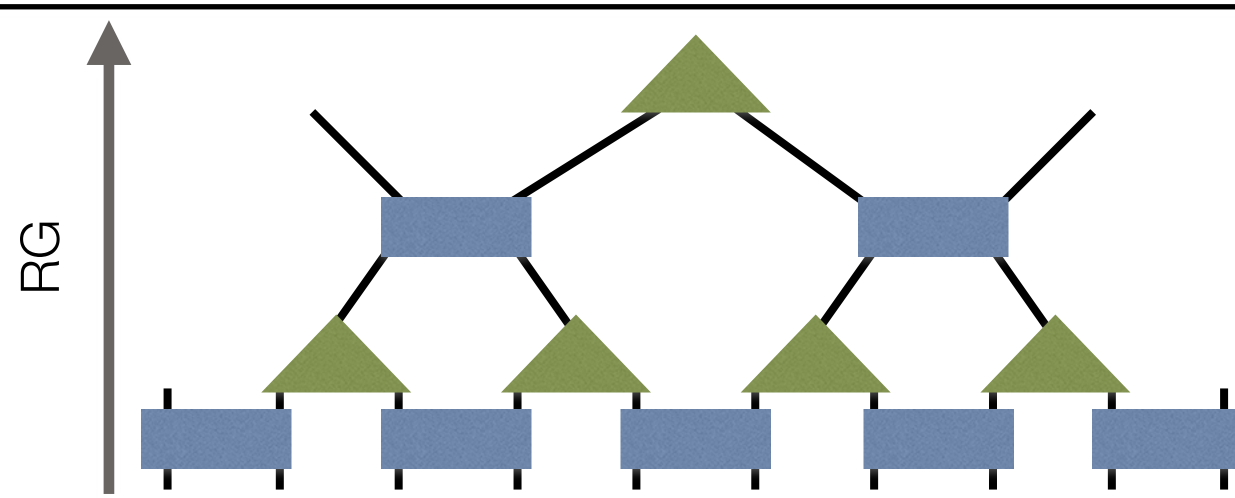


For higher dimensional systems

Extension of MPS

(higher correlation in data)

MERA:

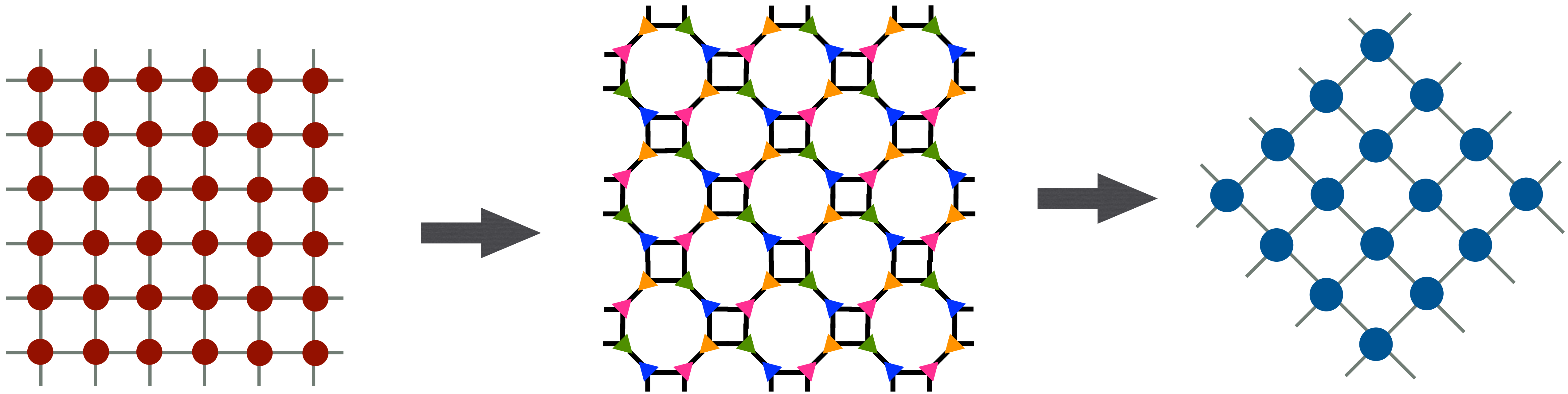


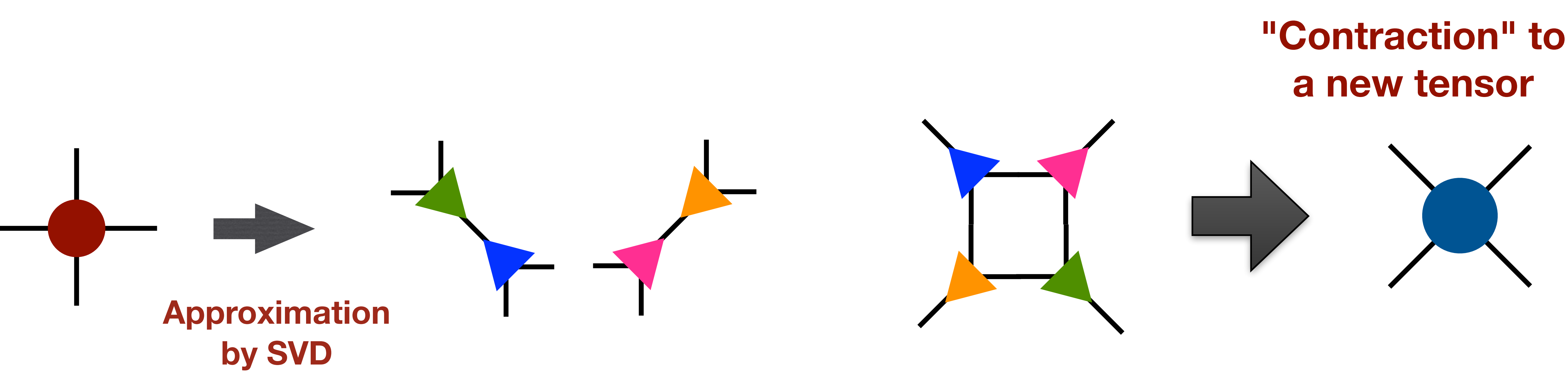
Scale invariant systems

（スケール不変）

Real space renormalization（実空間繰り込み）

Corse graining of a tensor network representing a **scaler.**





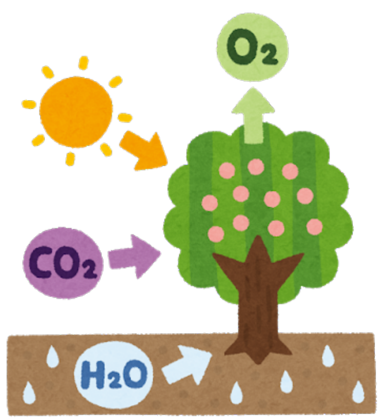
Introduction: Quantum many-body problems and quantum computing

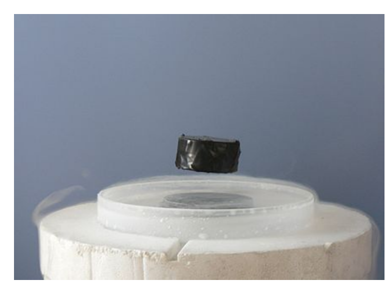
Motivation: Quantum many-body problems

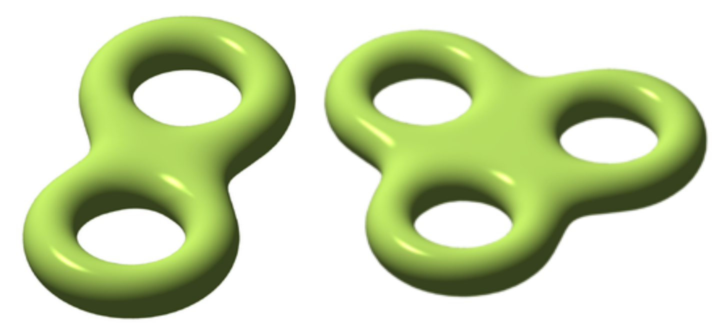
A variety of phenomena

- Chemical reaction
- Superconductivity
- Topological states
- ...

Quantum many-body problems







Cited from wikipedia: "Meisner effect", "Torus"

Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}|\Psi\rangle = \mathcal{H}|\Psi\rangle$$

$$\mathcal{H}|\Psi\rangle = E|\Psi\rangle$$

$\mathcal{H}$:Hamiltonian

$|\Psi\rangle$:Wave function (state vector)

E :Energy

To solve the problem numerically by (classical) computer,
we need huge memory and huge computation time.

Quantum systems

Example of quantum system: Array of quantum bits

1 qubit — A quantum bit is represented by two basis vectors.

$$|0\rangle, |1\rangle \quad \text{or} \quad (|\uparrow\rangle, |\downarrow\rangle)$$

2 qubits — The Hilbert space is spanned by four basis vectors.

ヒルベルト空間

$$|0\rangle \otimes |0\rangle, |0\rangle \otimes |1\rangle, |1\rangle \otimes |0\rangle, |1\rangle \otimes |1\rangle$$

Simple notation: $|00\rangle, |01\rangle, |10\rangle, |11\rangle$

$$|\Psi\rangle = \sum_{\alpha,\beta=0,1} C_{\alpha,\beta}|\alpha\beta\rangle$$

$C_{\alpha,\beta}$:complex number

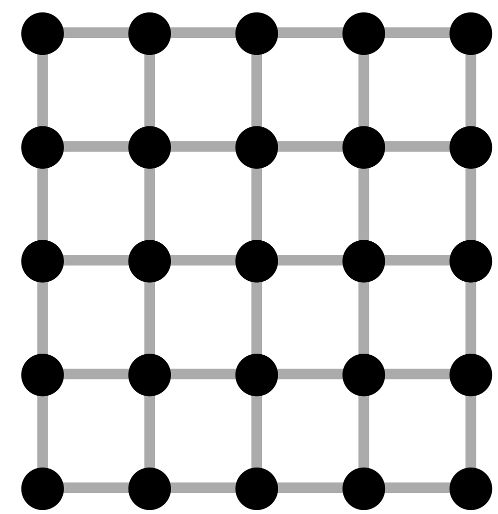
The Hamiltonian for 2-qubit system can be represented on these bases.

$$\mathcal{H} \to \begin{pmatrix} H_{0,0;0,0} & H_{0,0;0,1} & H_{0,0;1,0} & H_{0,0;1,1} \\ H_{0,1;0,0} & H_{0,1;0,1} & H_{0,1;1,0} & H_{0,1;1,1} \\ H_{1,0;0,0} & H_{1,0;0,1} & H_{1,0;1,0} & H_{1,0;1,1} \\ H_{1,1;0,0} & H_{1,1;0,1} & H_{1,1;1,0} & H_{1,1;1,1} \end{pmatrix}$$

Matrix element: $H_{\alpha,\beta;\alpha',\beta'} \equiv \langle\alpha\beta|\mathcal{H}|\alpha'\beta'\rangle$

Quantum systems

Example of quantum system: Array of quantum bits



N bits: Dimension of the Hilbert space $= 2^N$

Hamiltonian is $2^N \times 2^N$ matrix

Need to solve eigenvalue problem of huge matrix!

In physics,

- We often interested in the "ground state" (smallest eigenvalue)

基底状態

We can concentrate to a special state.

- Typical system only has "short range" interactions

Hamiltonian matrix becomes sparse.

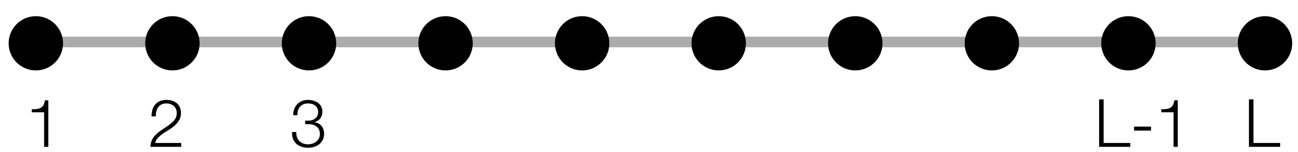
Quantum spin: S=1/2

Matrix representation of the spin operators: $S=\frac{1}{2}$

$$S_x=\frac{1}{2}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix},\ S_y=\frac{1}{2}\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix},\ S_z=\frac{1}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$$

We can consider S=1/2 spin as a quantum bit : $|0\rangle=\begin{pmatrix}1\\0\end{pmatrix},\ |1\rangle=\begin{pmatrix}0\\1\end{pmatrix}$

Spins on a chain:



"Transverse field Ising model" （横磁場イジング模型）

$$\mathcal{H}=-\sum_{i=1}^{L-1}S_{i,z}S_{i+1,z}-\Gamma\sum_{i=1}^{L}S_{i,x}$$

L=2

$$\mathcal{H}=\begin{pmatrix}-1/4 & -\Gamma/2 & -\Gamma/2 & 0\\ -\Gamma/2 & 1/4 & 0 & -\Gamma/2\\ -\Gamma/2 & 0 & 1/4 & -\Gamma/2\\ 0 & -\Gamma/2 & -\Gamma/2 & -1/4\end{pmatrix}$$

Difficulty in quantum many-body problems

Schrödinger equation: $i\hbar \frac{\partial}{\partial t}|\Psi\rangle = \mathcal{H}|\Psi\rangle$

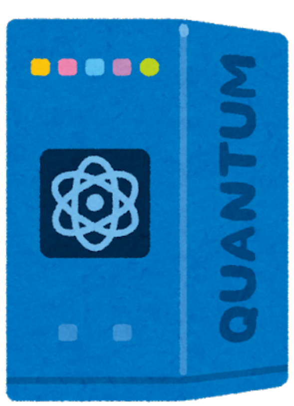
- Dimension of the vector space is exponentially large

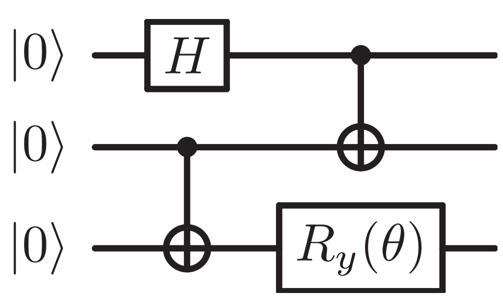
To solve the problem exactly by (classical) computer, we need huge memory and huge computation time.

e.g., We can simulate only ~50 qubits in classical supercomputer.

Quantum computer

It can treat quantum state directly, and then (ideally) there is no problems originated form the exponentially large vector space.





Classical computer?

- There are several techniques to treat quantum many-body problems.
  - One of them is data compression based on tensor networks.
- We may use them to simulate quantum computers.

Quantum circuit

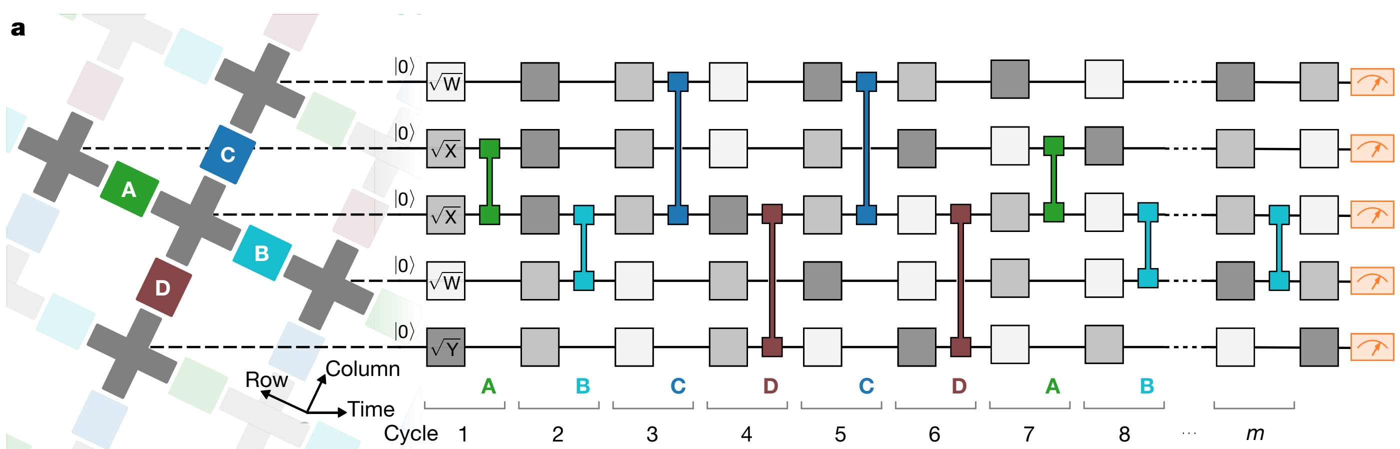
Quantum circuit:

Circuit based on gate operations on quantum bits

Unitary matrices (tensors)

2-dim complex vectors

Google's "quantum supremacy" circuit

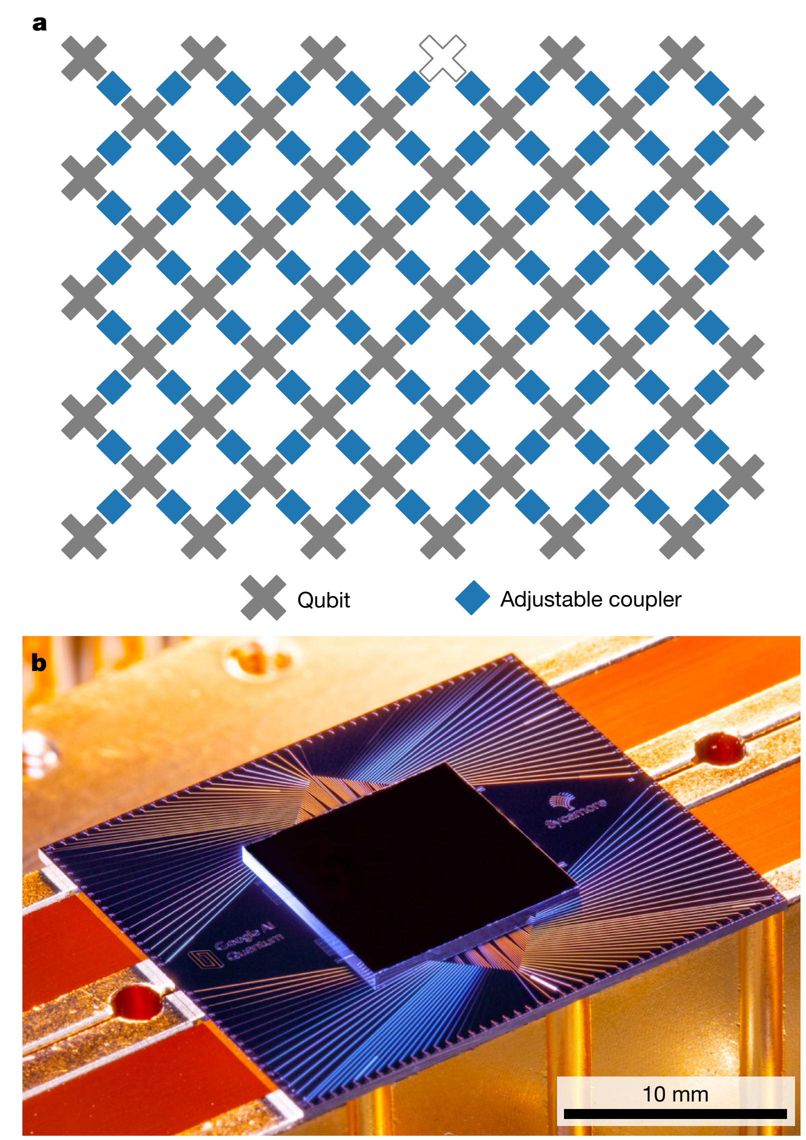


Quantum circuit = tensor network

Classical simulation of quantum circuits
= contraction of tensor networks

"quantum supremacy" circuit

F. Arute, *et al.*, Nature 574, 505 (2019)



Original estimation
10,000 years

TN based simulation
304 second !

Y. A. Liu, *et al.*, Gordon bell Prize in SC21 (2021),
(cf. quantum computer =200s)

Next week (Oct. 13)

Notice

- No classes on Nov. 3, Nov. 17, and Nov. 22
- Classes will be also held on Jan. 5 and Jan. 19

1. Computational science, quantum computing, and data compression
2. Review of linear algebra
3. Singular value decomposition
4. Application of SVD and generalization to tensors
5. Entanglement of information and matrix product states
6. Application of MPS to eigenvalue problems
7. Tensor network representation
8. Data compression in tensor network
9. Tensor network renormalization
10. Quantum mechanics and quantum computation
11. Simulation of quantum computers
12. Quantum-classical hybrid algorithms and tensor network
13. Quantum error correction and tensor network