
بسم الله الرحمن الرحیم

الگوریتم کوانتومی حل معادلات دیفرانسیل جزئی با استفاده از کامپیوتر کوانتومی D-Wave

محمدمهدی ماستری فراهانی

۱۴۰۳

مرکز تحقیقات فناوری‌های کوانتومی ایران

دانشگاه خوارزمی
Kharazmi University

فهرست مطالب

دانشگاه خوارزمی
Kharazmi University

یک معرفی بر معادلات دیفرانسیل

مرکز تحقیقات
فناوری‌های
کوانتومی ایران

معادلات دیفرانسیل معروف فیزیک

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$\nabla^2\phi(\boldsymbol{r}) = -4\pi\rho(\boldsymbol{r})$	Poisson's equation
$\nabla^2\phi(\boldsymbol{r}) = 0$	Laplace's equation
$\frac{\partial T}{\partial t} = a^2\nabla^2 T(\boldsymbol{r})$	Heat equation
$\nabla^2\psi - \frac{1}{c^2}\frac{\partial^2\psi}{\partial t^2} = 0$	Wave equation
$\frac{-\hbar^2}{2m}\nabla^2\psi + V(\boldsymbol{r})\psi = i\hbar\frac{\partial\psi}{\partial t}$	Schrodinger equation

Hassani, S. (2013). Mathematical Physics: A Modern Introduction to Its Foundations. Springer Science & Business Media.

معادلات دیفرانسیل معروف فیزیک

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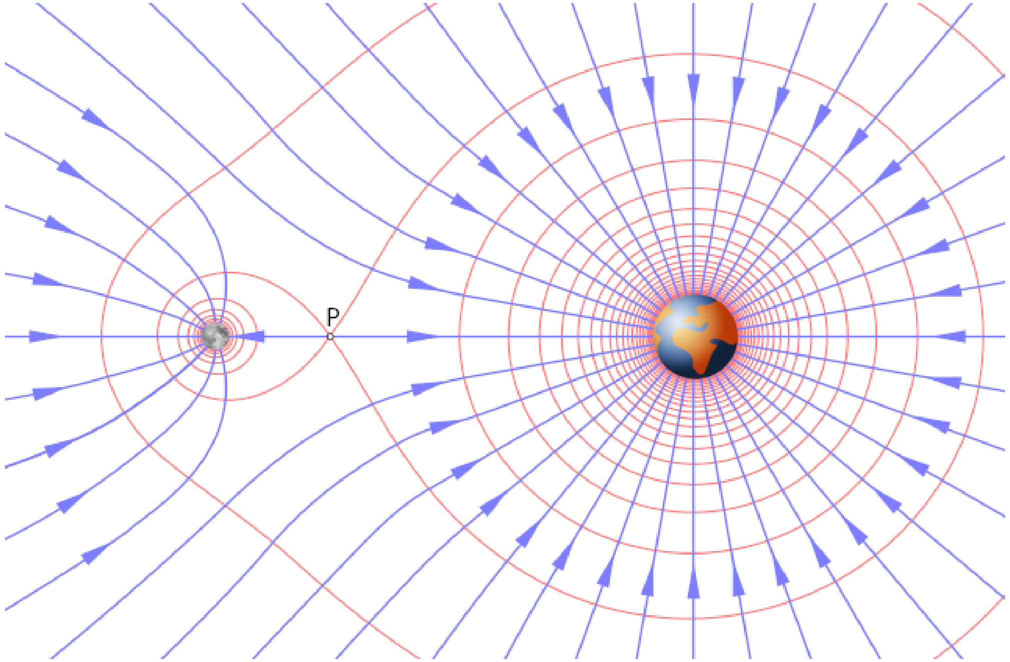

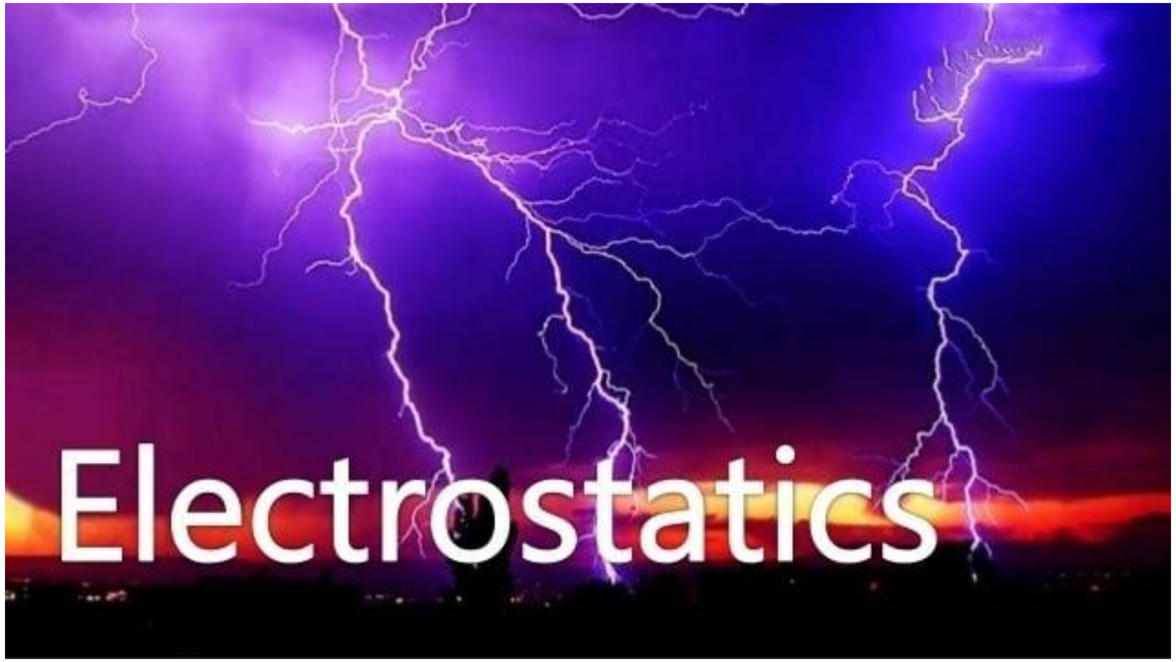

https://x-engineer.org/gravitational-potential-energy/
https://www.everythinksudiptasamanta.in/p/electrostatics.html

معادلات دیفرانسیل معروف فیزیک

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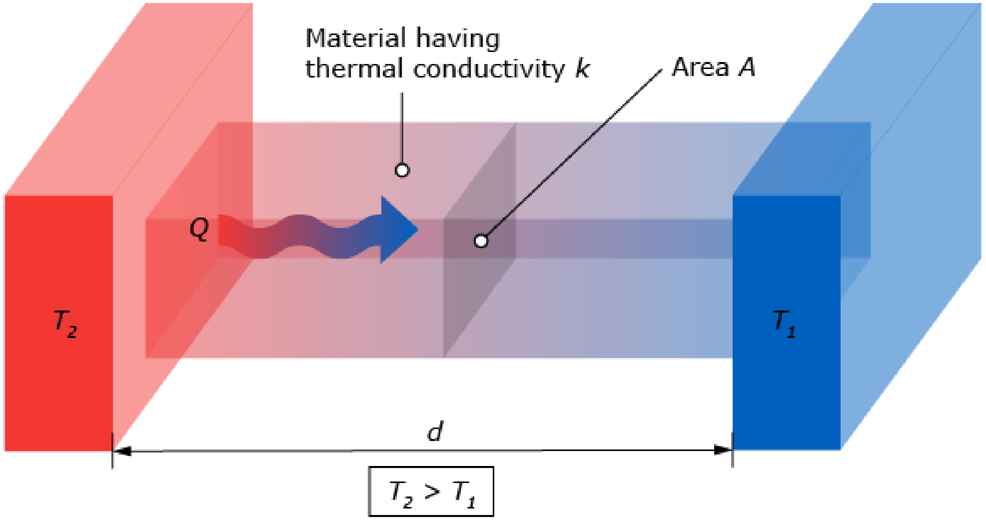
$$\frac{\partial T}{\partial t} = a^2 \nabla^2 T(\boldsymbol{r})$$



https://www.sciencedirect.com/science/article/pii/S0376042121000701

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معادلات دیفرانسیل معروف فیزیک

Kharazmi University

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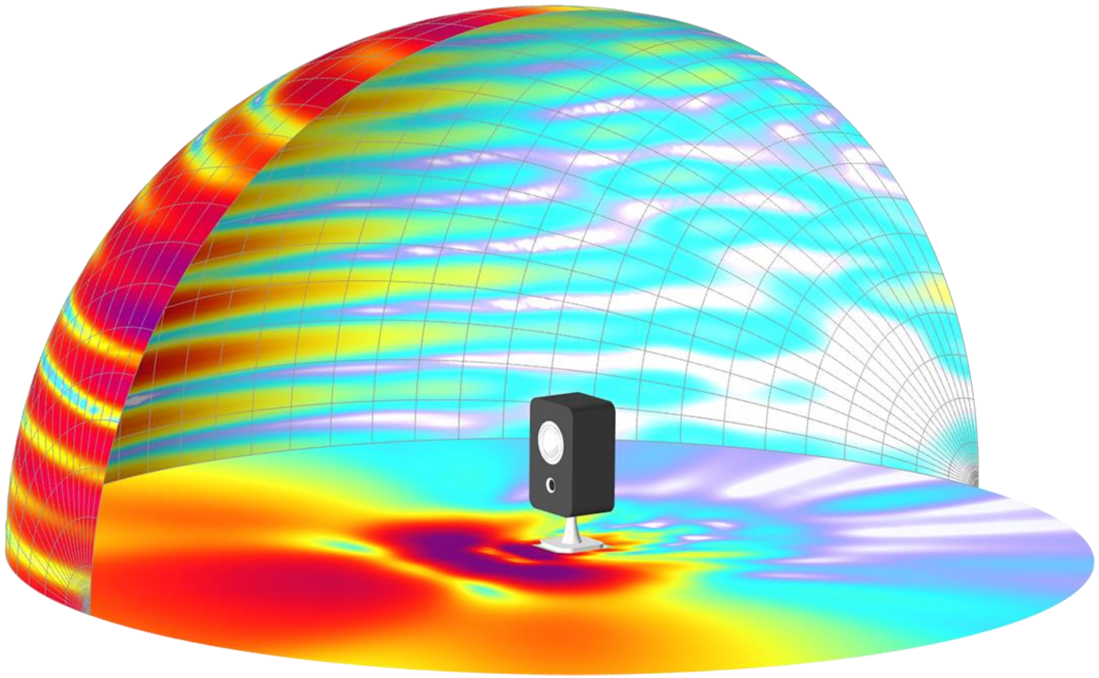

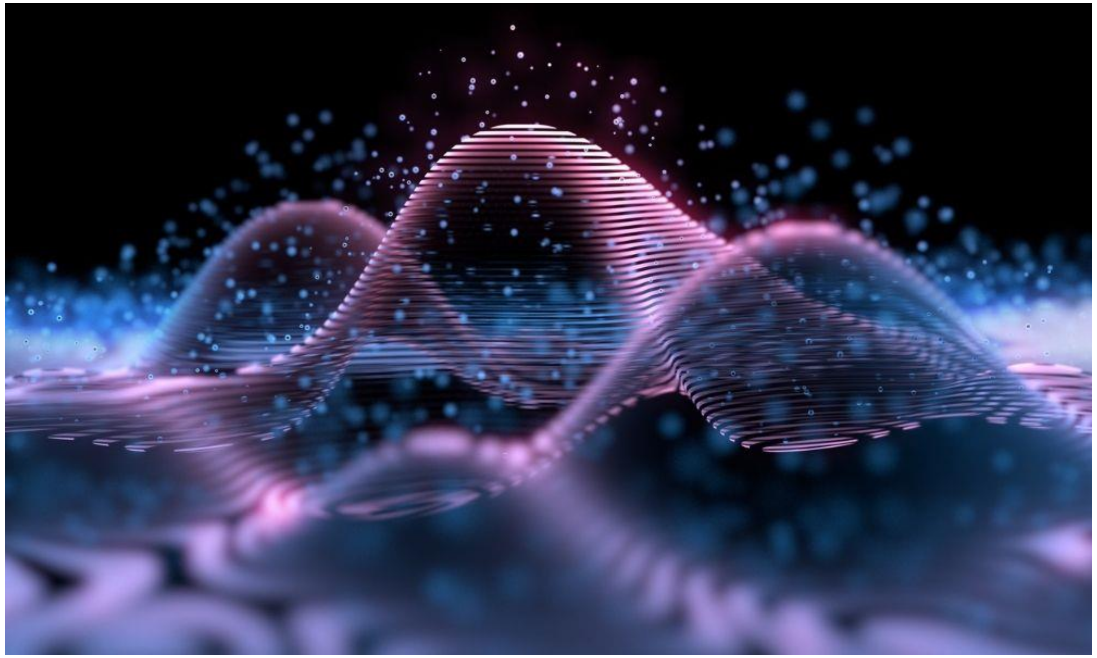

https://gamma-sci.com/2022/01/28/the-technological-applications-of-electromagnetic-waves/

https://www.comsol.com/acoustics-module

معادلات دیفرانسیل معروف فیزیک

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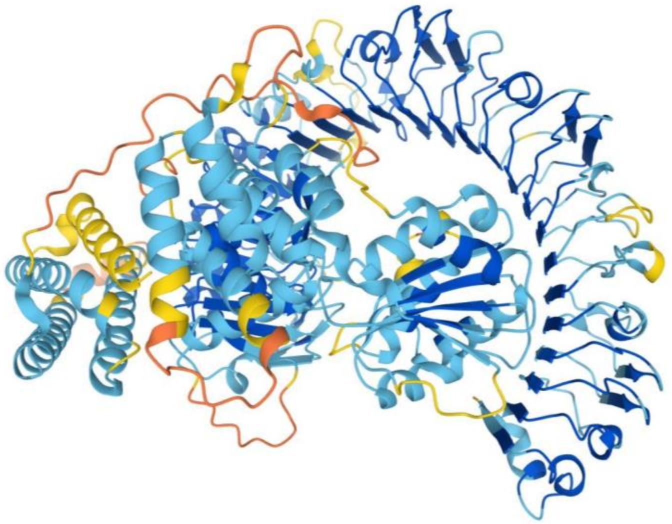

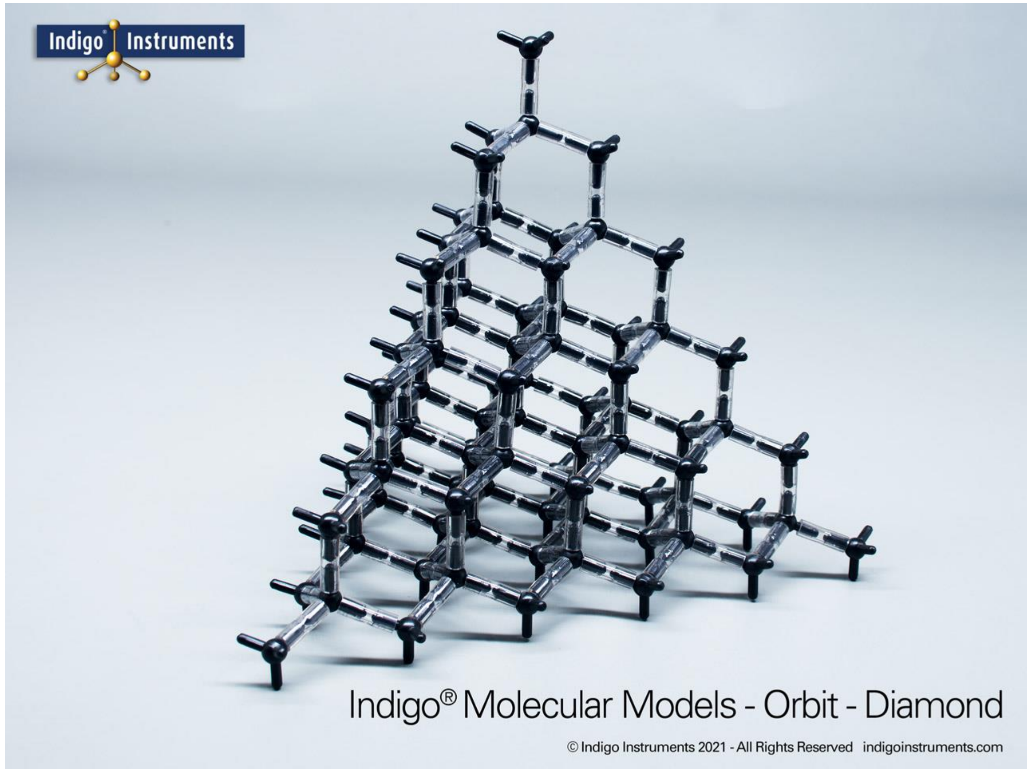

https://www.the-scientist.com/predictions-of-most-human-protein-structures-made-freely-available-69018
https://www.indigoinstruments.com/molecular_models/orbit/kits/diamond-structure-crystal-lattice-model-kit-68787w.html
https://www.labmanager.com/dna-origami-folded-into-tiny-motor-31666

ساختار یک معادله‌ی دیفرانسیل خطی

$$\mathcal{L}[u(\boldsymbol{r})] = f(\boldsymbol{r})$$

$$\alpha \frac{\partial^2 u}{\partial x^2} + \beta \frac{\partial^2 u}{\partial y^2} + \gamma \frac{\partial u}{\partial x} + \delta \frac{\partial u}{\partial y} + \eta\, u = f$$

ساختار یک معادله‌ی دیفرانسیل خطی

$$\mathcal{L}[u(\boldsymbol{r})] = f(\boldsymbol{r})$$

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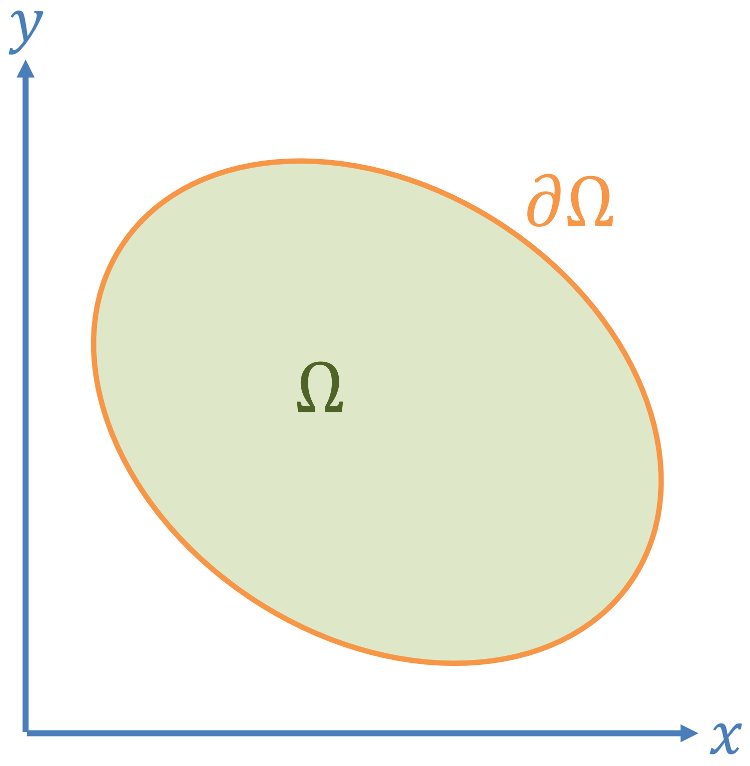
شرایط مرزی

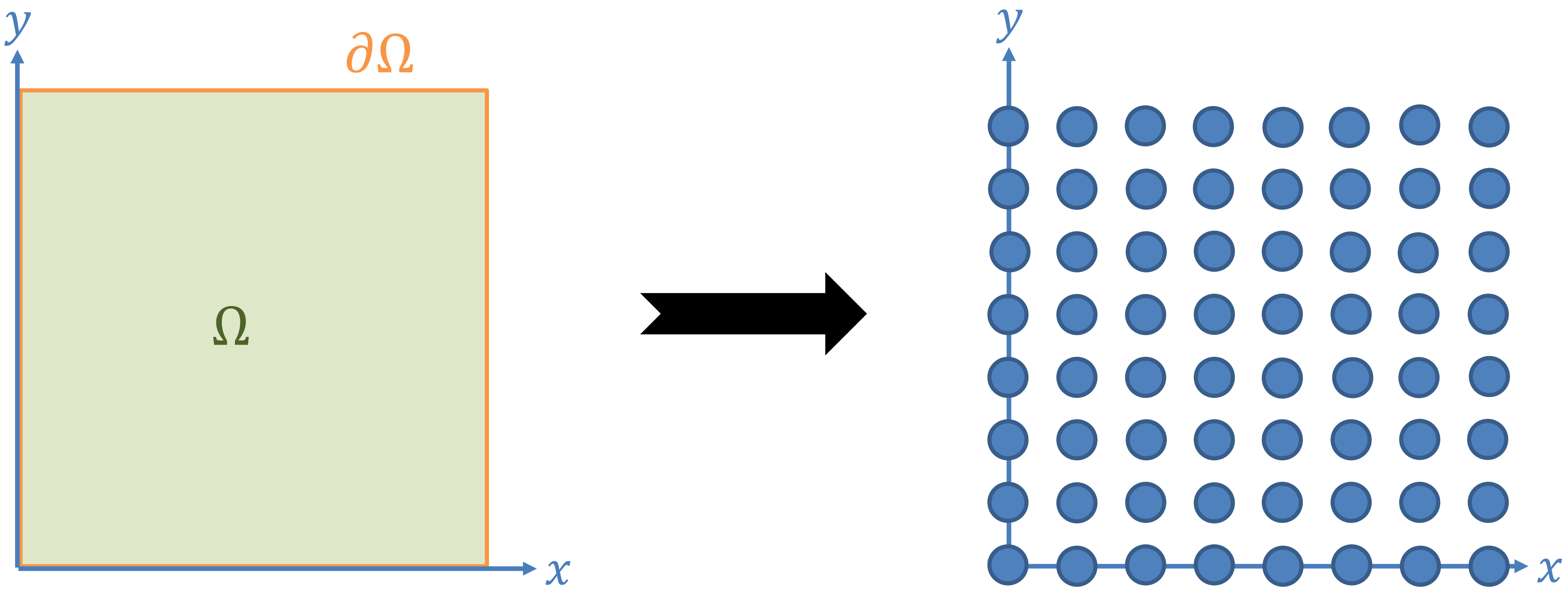


$$\mathcal{L}[u(\boldsymbol{r})] = f(\boldsymbol{r}), \qquad \boldsymbol{r} \in \Omega$$

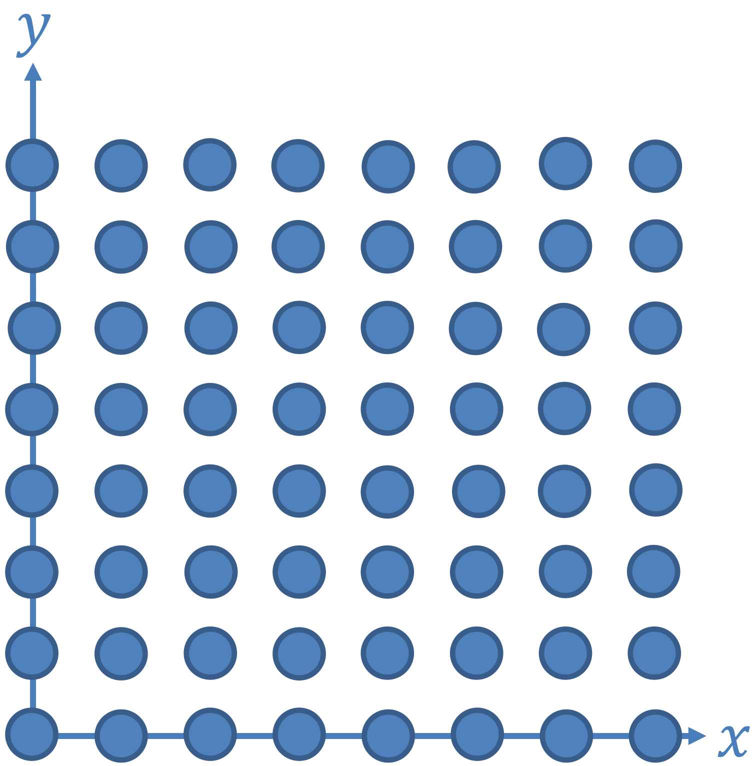
- $u(\boldsymbol{r})$ *is given*, $\quad \boldsymbol{r} \in \partial\Omega$
- $\dfrac{\partial u}{\partial r_i}$ *is given*, $\quad \boldsymbol{r} \in \partial\Omega$

گسسته‌سازی و تفاضل محدود

گسسته‌سازی



گسسته‌سازی



$$x \to x_i, \qquad i \in \{1, \cdots, n\}$$

$$y \to y_j, \qquad j \in \{1, \cdots, m\}$$

$$\Delta x = \frac{x_n - x_1}{n - 1}, \qquad \Delta y = \frac{y_m - y_1}{m - 1}$$

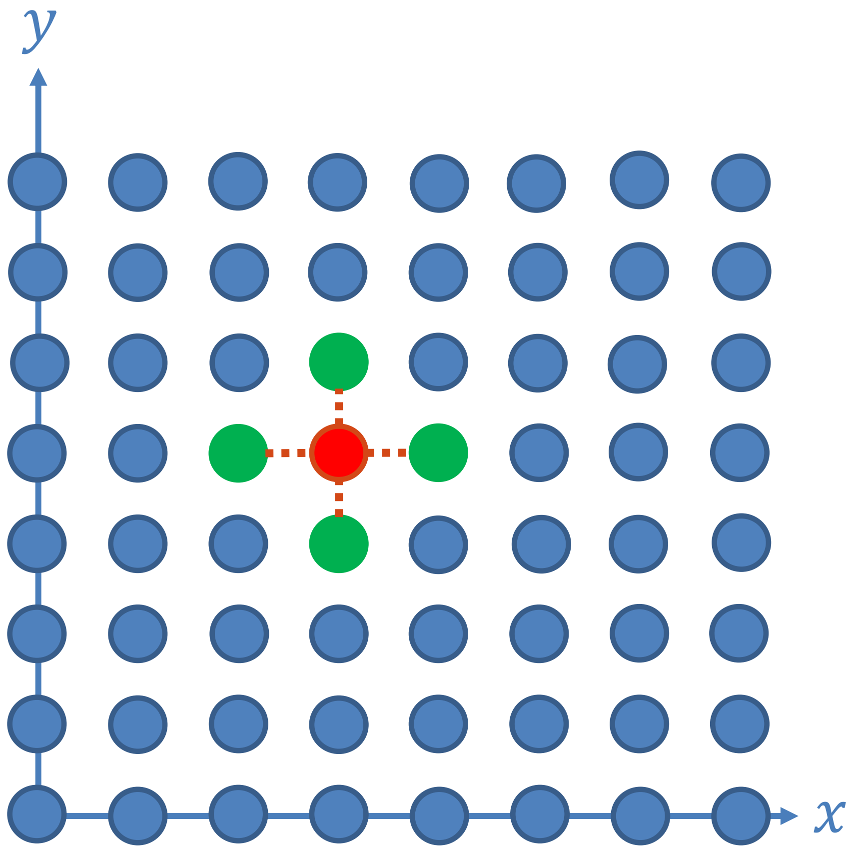
تفاضل محدود

$$\frac{df}{dx} = \frac{f(x+\Delta x) - f(x-\Delta x)}{2\Delta x} + \mathcal{O}(\Delta x^2)$$

$$\frac{d^2 f}{dx^2} = \frac{f(x+\Delta x) - 2f(x) + f(x-\Delta x)}{\Delta x^2} + \mathcal{O}(\Delta x^2)$$

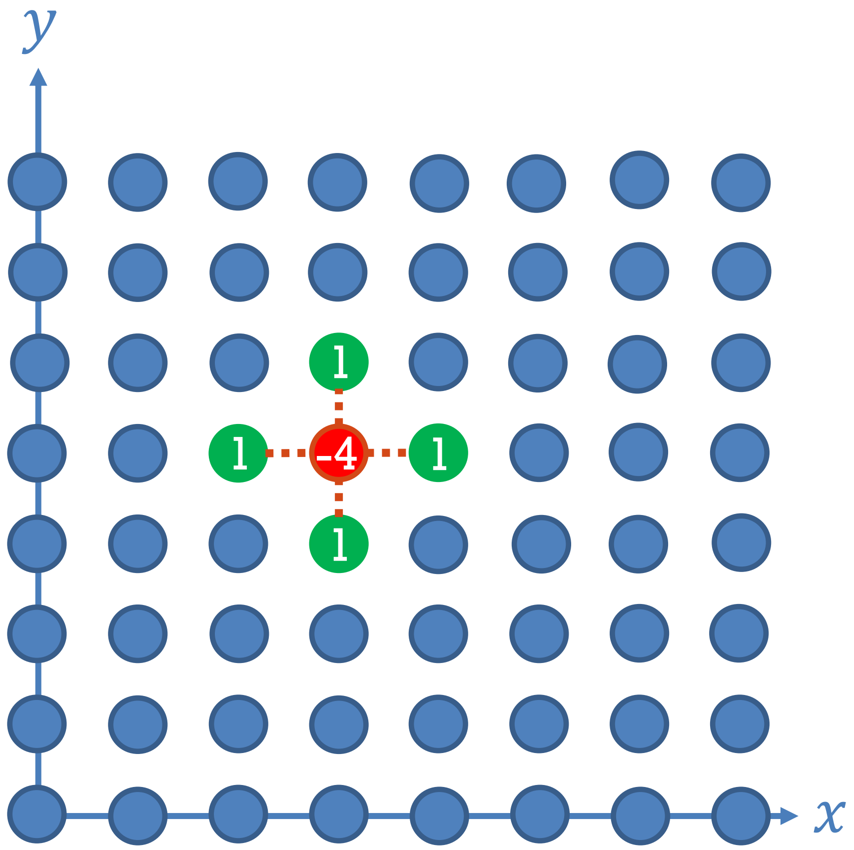
تفاضل محدود

$$\nabla^2 u = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = \frac{u(x+h,y) + u(x-h,y) + u(x,y+h) + u(x,y-h) - 4u(x,y)}{h^2}$$

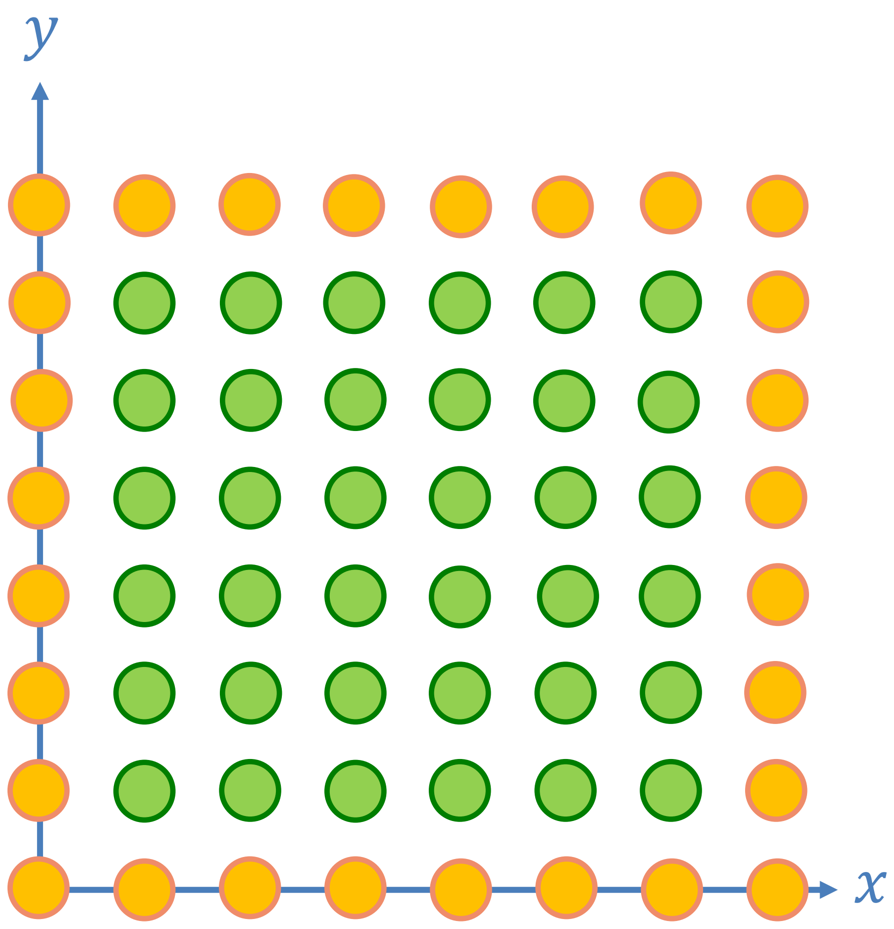


تفاضل محدود

$$\nabla^2 u = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = \frac{u(x+h,y) + u(x-h,y) + u(x,y+h) + u(x,y-h) - 4u(x,y)}{h^2}$$



تفاضل محدود



$$\mathcal{L}[u(\boldsymbol{r})] = f(\boldsymbol{r})$$

$$\downarrow$$

$$\boxed{A\,\vec{u} + \vec{b} = \vec{f}}$$

تفاضل محدود

$$\nabla^2 u = f(x,y)$$

⬇

$$A = \begin{bmatrix} C & I & 0 & 0 & 0 & 0 \\ I & C & I & 0 & 0 & 0 \\ 0 & I & C & I & 0 & 0 \\ 0 & 0 & I & C & I & 0 \\ 0 & 0 & 0 & I & C & I \\ 0 & 0 & 0 & 0 & I & C \end{bmatrix}, \qquad C = \begin{bmatrix} -4.0 & 1.0 & 0 & 0 & 0 & 0 \\ 1.0 & -4.0 & 1.0 & 0 & 0 & 0 \\ 0 & 1.0 & -4.0 & 1.0 & 0 & 0 \\ 0 & 0 & 1.0 & -4.0 & 1.0 & 0 \\ 0 & 0 & 0 & 1.0 & -4.0 & 1.0 \\ 0 & 0 & 0 & 0 & 1.0 & -4.0 \end{bmatrix}$$

الگوریتم‌های حل دستگاه معادله‌ی خطی

$$A\,\vec{x} = \vec{b}$$

$$\mathcal{O}(n^3)$$

$$\mathcal{O}(n)$$

گداخت کوانتومی
(کامپیوتر کوانتومی D-Wave)

Quantum annealing

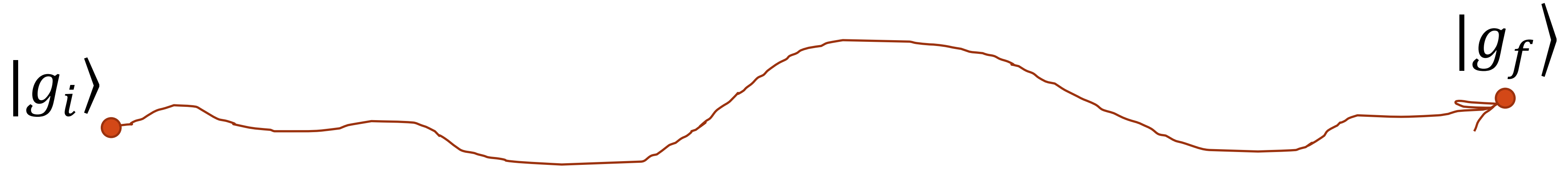
اصول گداخت کوانتومی (Quantum annealing)

$$H(t) = \left(1 - \frac{t}{T}\right) H_i + \frac{t}{T} H_f$$

$$H_i|g_i\rangle = E_i|g_i\rangle$$

$$H_f|g_f\rangle = E_f|g_f\rangle$$

به اندازه‌ی کافی کند!



S. Jansen, M. B. Ruskai, and R. Seiler, Bounds for the adiabatic approximation with applications to quantum computation, Journal of Mathematical Physics **48**, (2007)

اصول گداخت کوانتومی (Quantum annealing)

Kharazmi University

$$H(t) = \left(1 - \frac{t}{T}\right) H_i + \frac{t}{T} H_f$$

$$H_i \rightarrow |g_i\rangle$$

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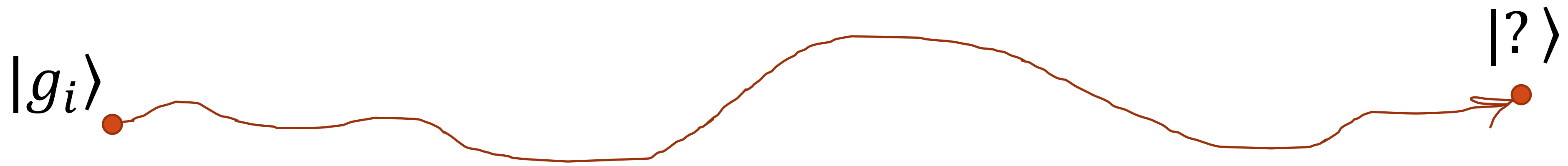
مرکز تحقیقات فناوری‌های کوانتومی ایران

اصول گداخت کوانتومی (Quantum annealing)

$$H(t) = \left(1 - \frac{t}{T}\right) H_i + \frac{t}{T} H_f$$

$H_i \downarrow |g_i\rangle$ $\quad$ $H_f \downarrow |?\rangle$



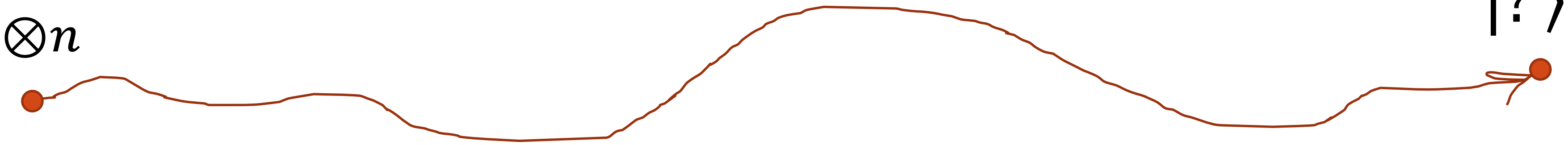
S. Jansen, M. B. Ruskai, and R. Seiler, Bounds for the adiabatic approximation with applications to quantum computation, Journal of Mathematical Physics **48**, (2007)

کامپیوتر کوانتومی D-Wave

$$H_i = \sum_i \sigma_x^{(i)} ,$$

$$H_f = \sum_i \alpha_i \sigma_z^{(i)} + \sum_{i,j} \beta_{ij} \sigma_z^{(i)} \sigma_z^{(j)}$$

$|+\rangle^{\otimes n}$



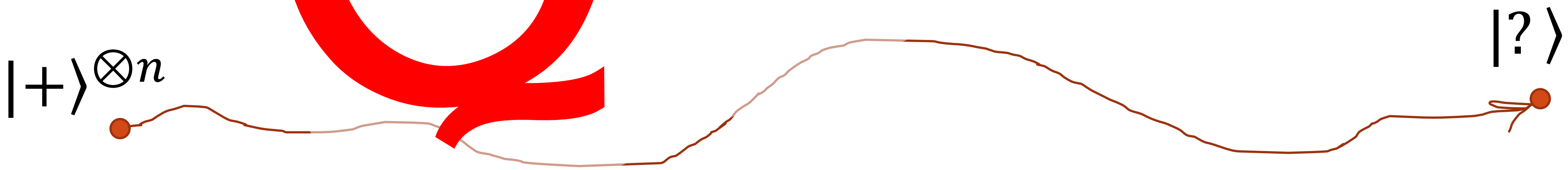
$|?\rangle$

کامپیوتر کوانتومی D-Wave

$$H_i = \sum \sigma \ldots ,$$

$$H_f = \sum_i \alpha_i \sigma_z^{(i)} + \sum_{i,j} \beta_{ij} \sigma_z^{(i)} \sigma_z^{(j)}$$

QUBO



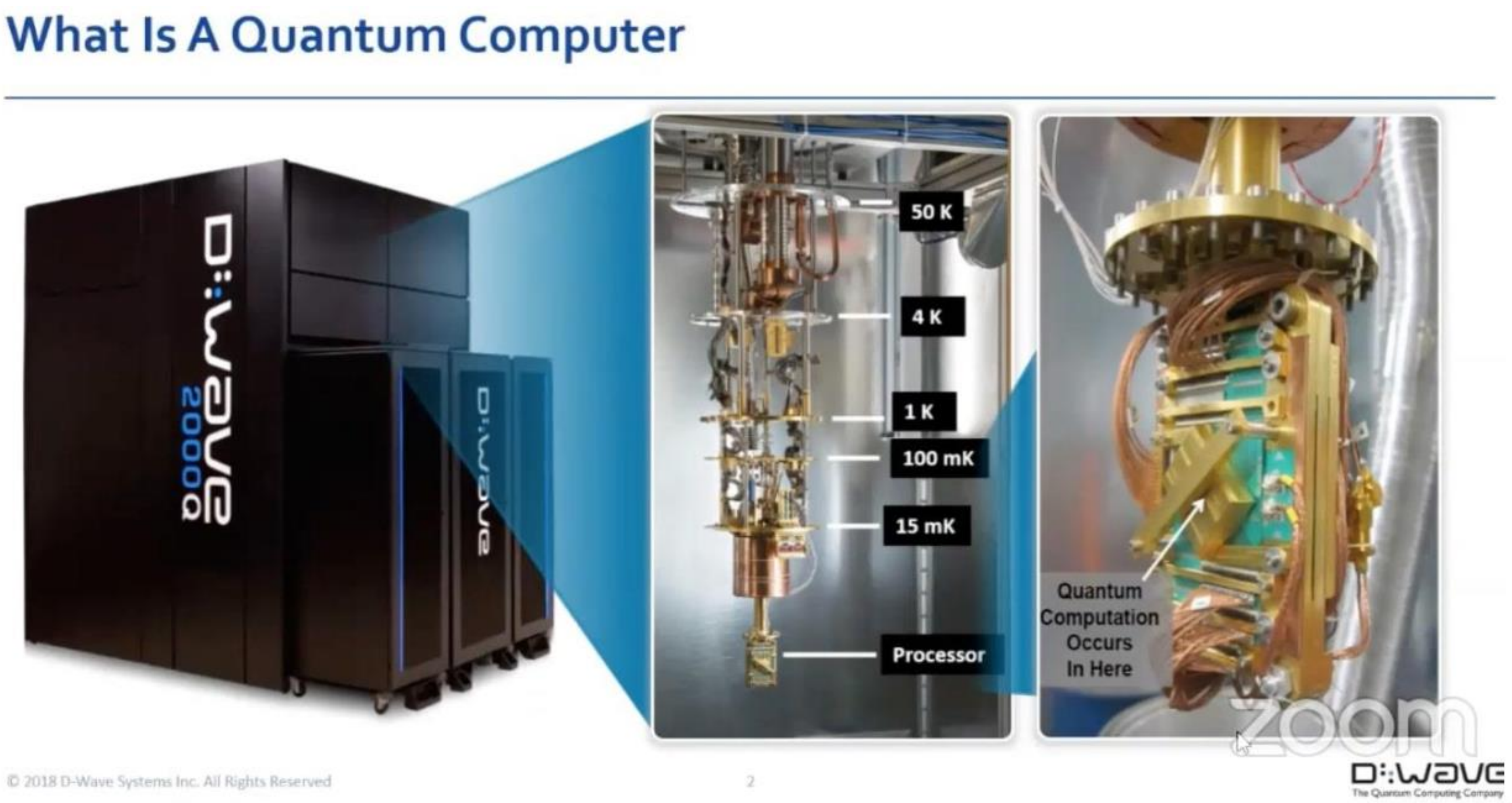
$$
\begin{aligned}
\underset{x}{\text{minimize}} \quad & f(x) \\
\text{subject to} \quad & g_i(x) \leq 0, \quad i = 1, \dots, m \\
& h_j(x) = 0, \quad j = 1, \dots, p
\end{aligned}
$$

Quadratic Unconstrained Binary Optimization

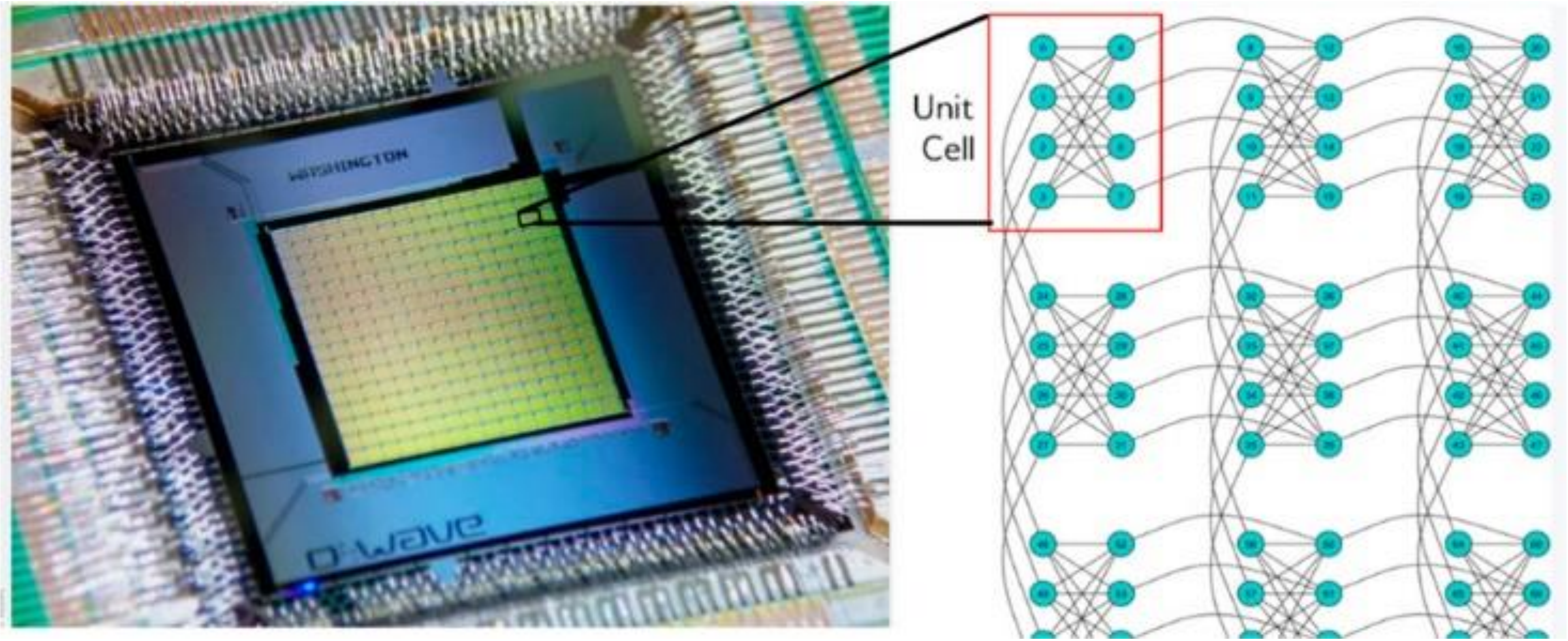
$$\min_{\boldsymbol{x}\in\{0,1\}^n} \boldsymbol{x}^T Q \boldsymbol{x}$$

$$f(\boldsymbol{x}) = \sum_{i=1}^{n} Q_{ii} x_i + \sum_{i>j} Q_{ij} x_i x_j \qquad H_f = \sum_{i} \alpha_i \sigma_z^{(i)} + \sum_{i,j} \beta_{ij} \sigma_z^{(i)} \sigma_z^{(j)}$$

کامپیوتر کوانتومی D-Wave

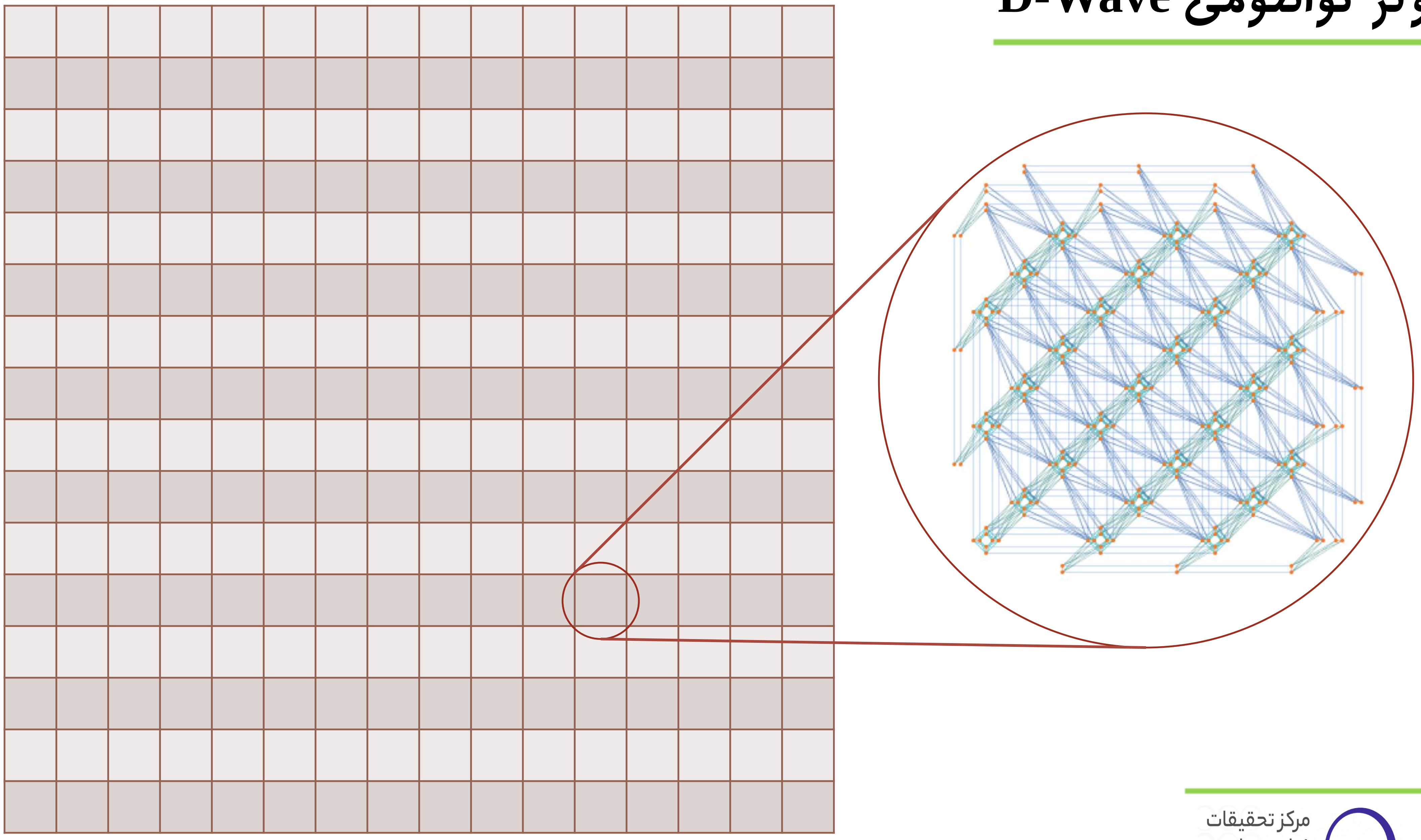


کامپیوتر کوانتومی D-Wave



Hari P. Paudel, Madhava Syamlal, Scott E. Crawford, Yueh-Lin Lee, Roman A. Shugayev, Ping Lu, Paul R. Ohodnicki, Darren Mollot, and Yuhua Duan
ACS Engineering Au **2022** *2* (3), 151-196

کامپیوتر کوانتومی D-Wave



پیاده‌سازی بر روی D-Wave

مرکز تحقیقات فناوری‌های کوانتومی ایران

تبدیل حل دستگاه معادله‌ی خطی به QUBO

$$A\vec{x} = \vec{b} \quad \rightarrow \quad \text{QUBO}$$

$$\overrightarrow{x_{sol}} = \underset{\vec{x}}{\operatorname{argmin}}\, H(x) = \underset{\vec{x}}{\operatorname{argmin}}\left(A\vec{x} - \vec{b}\right)^{\dagger}\left(A\vec{x} - \vec{b}\right)$$

F. Glover, G. Kochenberger, and Y. Du, A tutorial on formulating and using qubo models (2019).

تبدیل حل دستگاه معادله‌ی خطی به QUBO

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$$\mathbb{R} \ni x_i \rightarrow 1101 \cdots 110 \in \{0,1\}^R$$

$q_{R-1}^i \quad q_{R-2}^i \quad q_2^i \quad q_1^i \quad q_0^i$

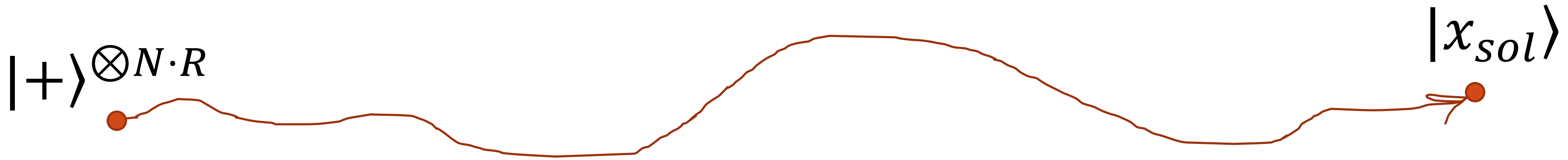
$$|x\rangle = |q_0^0, q_1^0, \cdots, q_{R-1}^0 \;\; ; \;\; q_0^1, q_1^1, \cdots, q_{R-1}^1 \;\; ; \;\; \cdots \;\; ; \;\; q_0^{N-1}, q_1^{N-1}, \cdots, q_{R-1}^{N-1}\rangle$$

$$\#qubits = N \cdot R$$

F. Glover, G. Kochenberger, and Y. Du, A tutorial on formulating and using qubo models (2019).

تبدیل حل دستگاه معادله‌ی خطی به QUBO

$$H(t) = \left(1 - \frac{t}{T}\right) H_i + \frac{t}{T} H_f$$



جواب به دست آمده از D-Wave

$$|x_{sol}\rangle = |\underbrace{q_0^0, q_1^0, \cdots, q_{R-1}^0}_{x_0} \;;\; \underbrace{q_0^1, q_1^1, \cdots, q_{R-1}^1}_{x_1} \;;\; \cdots \;;\; \underbrace{q_0^{N-1}, q_1^{N-1}, \cdots, q_{R-1}^{N-1}}_{x_{N-1}}\rangle$$

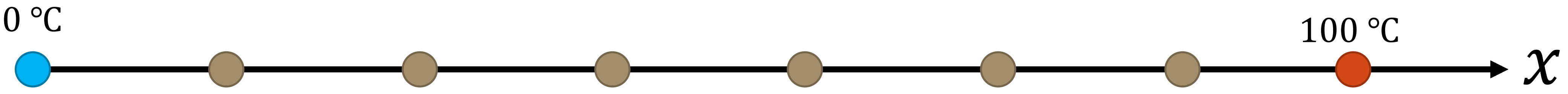
جواب به دست آمده از D-Wave

$$|x_{sol}\rangle = |q_0^0, q_1^0, \cdots, q_{R-1}^0 \quad ; \quad q_0^1, q_1^1, \cdots, q_{R-1}^1 \quad ; \quad \cdots \quad ; \quad q_0^{N-1}, q_1^{N-1}, \cdots, q_{R-1}^{N-1}\rangle$$

$$\overrightarrow{x_{sol}} = \begin{pmatrix} x_0 \\ x_1 \\ \vdots \\ x_{N-1} \end{pmatrix}$$

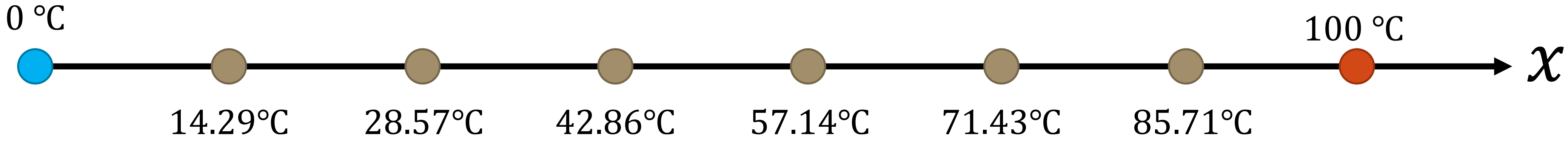
پیاده‌سازی عملی

$$\frac{\partial^2 T}{\partial x^2} = 0 \quad \rightarrow \quad \begin{pmatrix} -2 & 1 & 0 & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 & 0 \\ 0 & 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & 0 & 1 & -2 & 1 \\ 0 & 0 & 0 & 0 & 1 & -2 \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \\ u_6 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ -100 \end{pmatrix}$$



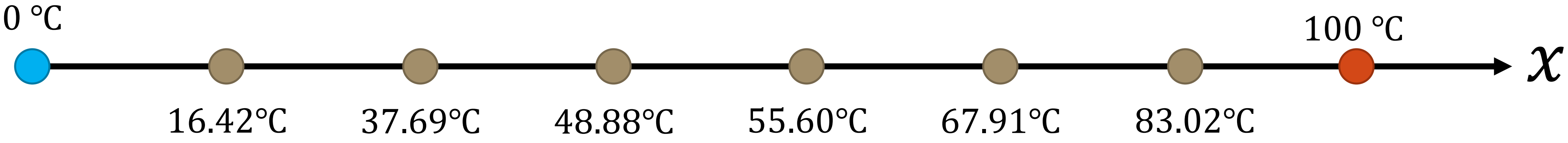
پیاده‌سازی عملی

$$\begin{pmatrix} -2 & 1 & 0 & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 & 0 \\ 0 & 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & 0 & 1 & -2 & 1 \\ 0 & 0 & 0 & 0 & 1 & -2 \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \\ u_6 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ -100 \end{pmatrix}$$



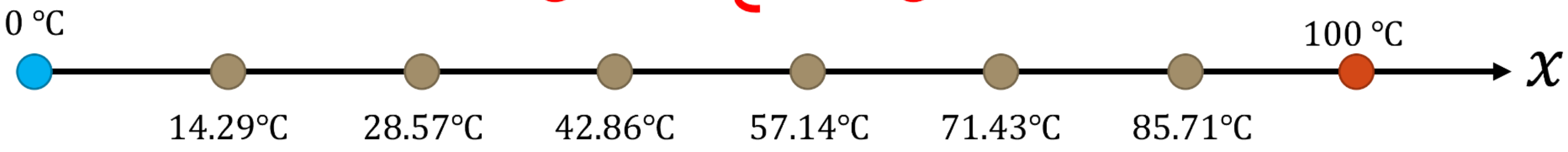
پیاده‌سازی عملی

$$\begin{pmatrix} -2 & 1 & 0 & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 & 0 \\ 0 & 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & 0 & 1 & -2 & 1 \\ 0 & 0 & 0 & 0 & 1 & -2 \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \\ u_6 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ -100 \end{pmatrix}$$

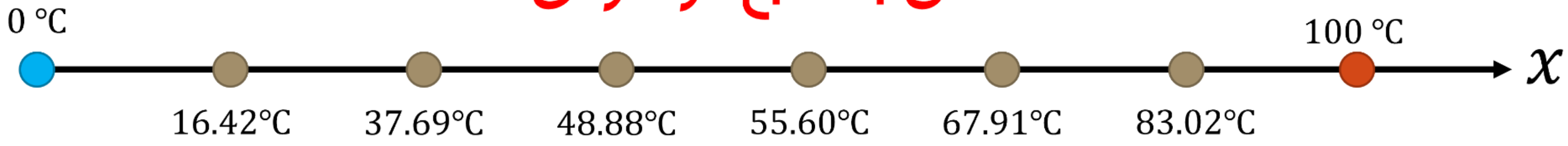


خطای محاسبه

حل با منابع کلاسیکی



حل با منابع کوانتومی



$$\epsilon = \frac{\left\| \vec{x}_{real} - \vec{x}_{annealing} \right\|}{\left\| \vec{x}_{real} \right\|} \approx 1.43$$

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سپاس از توجه شما

مرکز تحقیقات
فناوری‌های
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