偏微分方程式制約付き最適化問題のための量子アルゴリズム

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株式会社豊田中央研究所
佐藤勇気

Outline

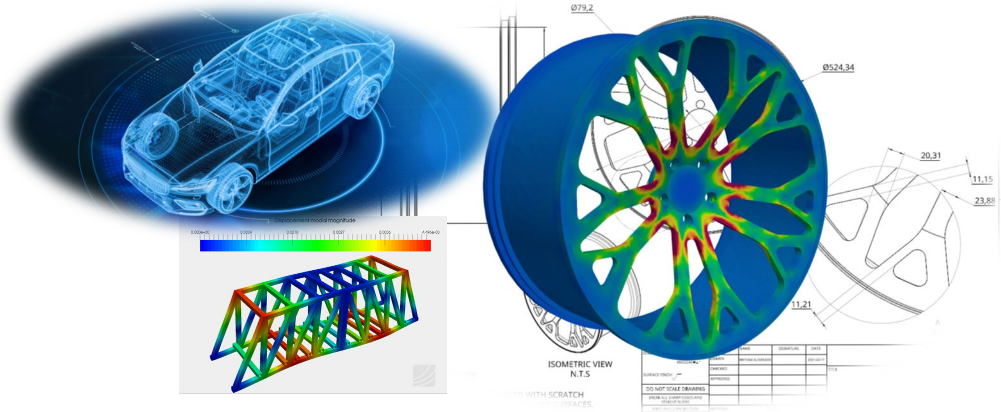
- Introduction
- Preliminary
- Proposed method
- Numerical example
- Conclusion

Introduction

Computer-aided Engineering; CAE

Simulation model

Simulation result



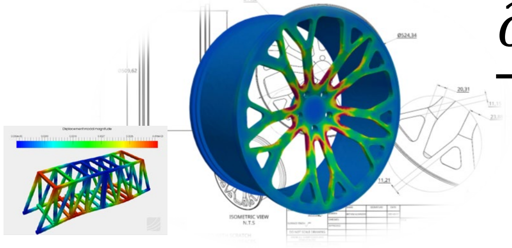
Design optimization

Numerical analysis
(Solid mechanics, heat transport, fluid dynamics, etc.)

Capability of large-scale CAE depends on that of solving partial differential equations (PDEs) of large-scale systems

Can a quantum computer accelerate CAE?

Conventional approach



Forward simulation: PDE solver

$$\frac{\partial u(t,x)}{\partial t} = \kappa \nabla^2 u(t,x) \xrightarrow{\text{Discretization}} \boldsymbol{u}^{s+1} = A\boldsymbol{u}^s$$

Explicit or implicit time integration

For spatial DOFs N, one needs to handle $N \times N$ sparse matrix, which requires $\mathcal{O}(N) \sim \mathcal{O}(N^3)$ complexity ($N \sim 10^6 - 10^{10}$)

Design optimization: PDE-constrained optimization

$$\min_{\xi} \; F(u(\xi))$$

$$\text{subject to: } \frac{\partial u(t,x;\xi)}{\partial t} = \kappa(\xi)\nabla^2 u(t,x;\xi)$$

Iteratively solve PDEs, updating design parameters ξ to an optimum

Solving PDEs as fast as possible is quite important!

Classification of forward problems

	Steady state	Time evolution
Linear	・Steady-state heat eq. $-\nabla \cdot (k\nabla T) = Q$ ・Linear elastic eq. $-\nabla \cdot \boldsymbol{\sigma} = \boldsymbol{f}$ ・Wave eq. in freq. domain $(\nabla^2 + k^2)u = 0$	・Heat eq. $\frac{\partial T}{\partial t} = \nabla \cdot (k\nabla T) + Q$ ・Linear elastic wave eq. $\frac{\partial^2 u}{\partial^2 t} = \nabla \cdot \boldsymbol{\sigma} + \boldsymbol{f}$ ・Wave eq. in time domain $\frac{\partial^2 u}{\partial t^2} = c^2\nabla^2 u$
Non linear	・Steady-state Navier-Stokes eq. $(\boldsymbol{u} \cdot \nabla)\boldsymbol{u} = -\nabla p + \mu\nabla^2\boldsymbol{u}$	・Navier-stokes eq. $\frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u} \cdot \nabla)\boldsymbol{u} = -\nabla p + \mu\nabla^2\boldsymbol{u}$

Hamiltonian simulation

Schrödinger equation

$$\frac{\partial \psi(t)}{\partial t} = -iH\psi(t) \quad \Rightarrow \quad \psi(t) = e^{-iH(t-t_0)}\psi(t_0)$$

Hamiltonian simulation

$$|\psi(t)\rangle = e^{-iH(t-t_0)}|\psi(t_0)\rangle$$

$|\psi(t_0)\rangle$: quantum state on a quantum computer

We need to
- transform PDEs of interest into the Schrödinger equation
- implement $e^{-iH(t-t_0)}$ on quantum computers

The first one is required for simulating classical physics!

Summary of our method

Hamiltonian simulation for hyperbolic partial differential equations by scalable quantum circuits (Sato et al., published in Physical Review Research, 2024)

Hyperbolic PDE

$$\frac{\partial^2 u(t,\boldsymbol{x})}{\partial t^2} = c^2 \nabla^2 u(t,\boldsymbol{x})$$

$$\psi(t,\boldsymbol{x}) = \begin{pmatrix} \frac{\partial u(t,\boldsymbol{x})}{\partial t} \\ ic\nabla^\top u(t,\boldsymbol{x}) \end{pmatrix}$$

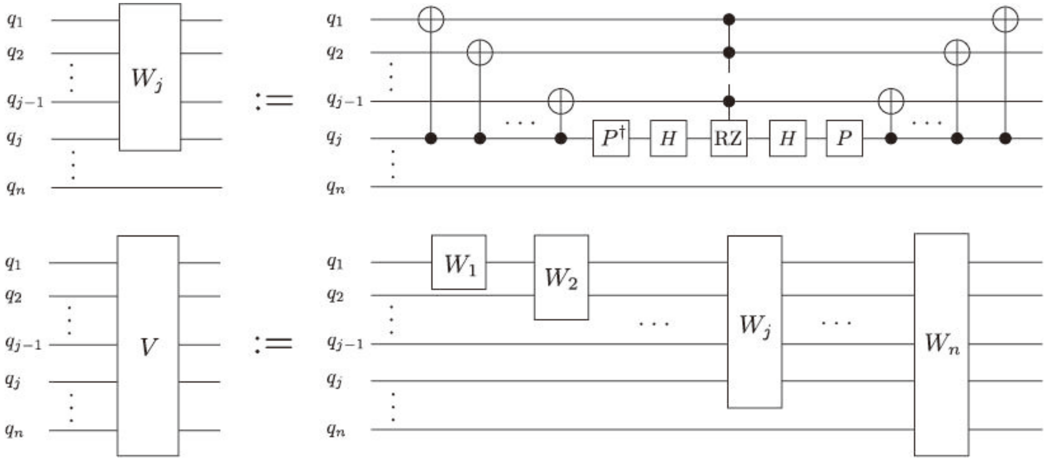
$$\mathcal{H} = c\begin{pmatrix} 0 & \nabla \\ -\nabla^\top & 0 \end{pmatrix}$$

Schrödinger equation

$$\frac{\partial \psi(t,\boldsymbol{x})}{\partial t} = -i\mathcal{H}\psi(t,\boldsymbol{x})$$

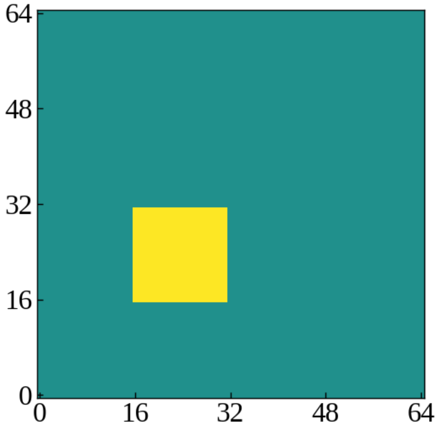
$\exp(-i\mathcal{H}\tau)$

Quantum circuit for Hamiltonian simulation



$\frac{\partial u(t,\boldsymbol{x})}{\partial t}$

Simulation result



Provided quantum circuits explicitly

Only be applied to conservative and homogeneous system

Extension to non-conservative systems

Linear Combination of Hamiltonian Simulation for Nonunitary Dynamics with Optimal State Preparation Cost (An et al., published in Physical Review Letters, 2023)

Extension of Hamiltonian simulation that is useful to solve ODEs

$$\frac{\partial \boldsymbol{u}(t)}{\partial t} = -(\boldsymbol{L}(t) + i\boldsymbol{H}(t))\boldsymbol{u}(t), \quad L^\dagger = L, H^\dagger = H$$

$$\longrightarrow \quad \boldsymbol{u}(t) = \int_{\mathbb{R}} \frac{1}{\pi(1+k^2)} \mathcal{T} e^{-i\int_0^t (H(s)+kL(s))ds} dk \, \boldsymbol{u}(0)$$

We proposed a quantum algorithm for linear PDE (Sato et al.,PRApplied, 2025)

$$\varrho(\boldsymbol{x})\frac{\partial^2 u(t,\boldsymbol{x})}{\partial t^2} + \zeta(\boldsymbol{x})\frac{\partial u(t,\boldsymbol{x})}{\partial t} - \nabla\cdot\kappa(\boldsymbol{x})\nabla u(t,\boldsymbol{x}) + \alpha(\boldsymbol{x})u(t,\boldsymbol{x}) = 0$$

Solution is embedded in the amplitude of a quantum state, so we cannot access full solution efficiently

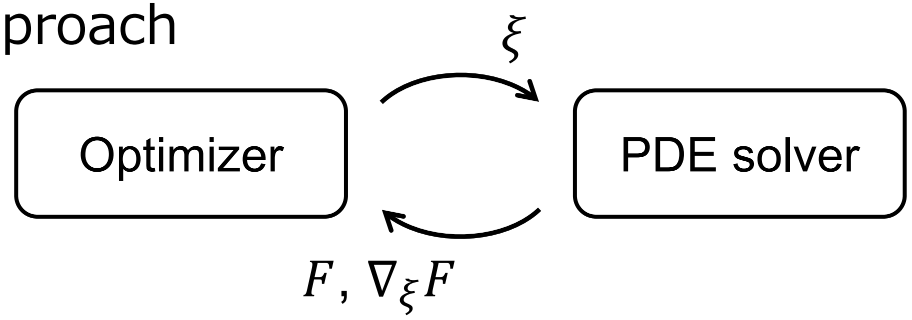
Classical-quantum hybrid approach

PDE-constrained optimization

$$\min_{\xi} \; F(u(\xi))$$

$$\text{subject to: } \frac{\partial u(t,x;\xi)}{\partial t} = \kappa(\xi)\nabla^2 u(t,x;\xi)$$

Conventional approach



Can a quantum PDE solver efficiently compute the objective function value?

Classical-quantum hybrid approach might require substantial overhead because of the accumulation of measurement error at each optimization step.

(Catli, et al., arXiv:2502.04285v1, 2025.)

Is it possible to perform forward simulation and optimization in a fully-coherent manner?

Contributions

We propose a fully quantum algorithm for PDE-constrained optimization incorporating a quantum PDE solver and quantum optimization

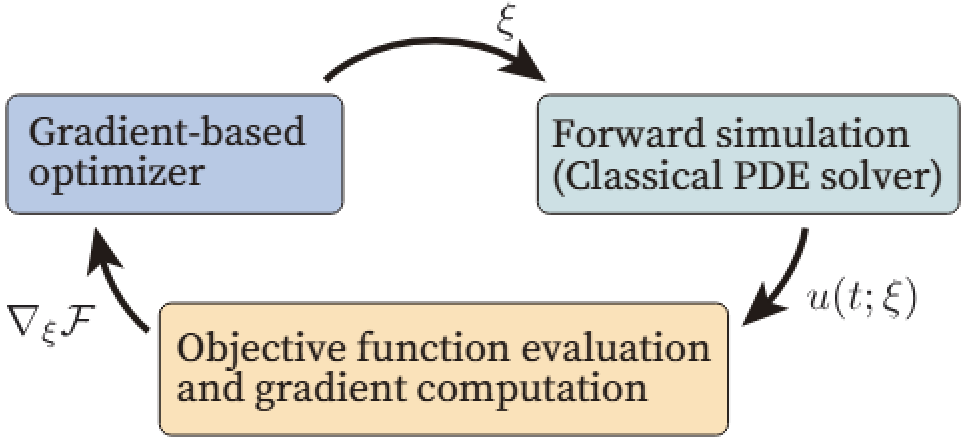
1. We construct explicit block-encoding of the objective function using a quantum PDE solver as its subroutine.
2. We provide the complexity analysis of the proposed method and discuss whether quantum computers can accelerate design optimization.

Concept of the proposed method

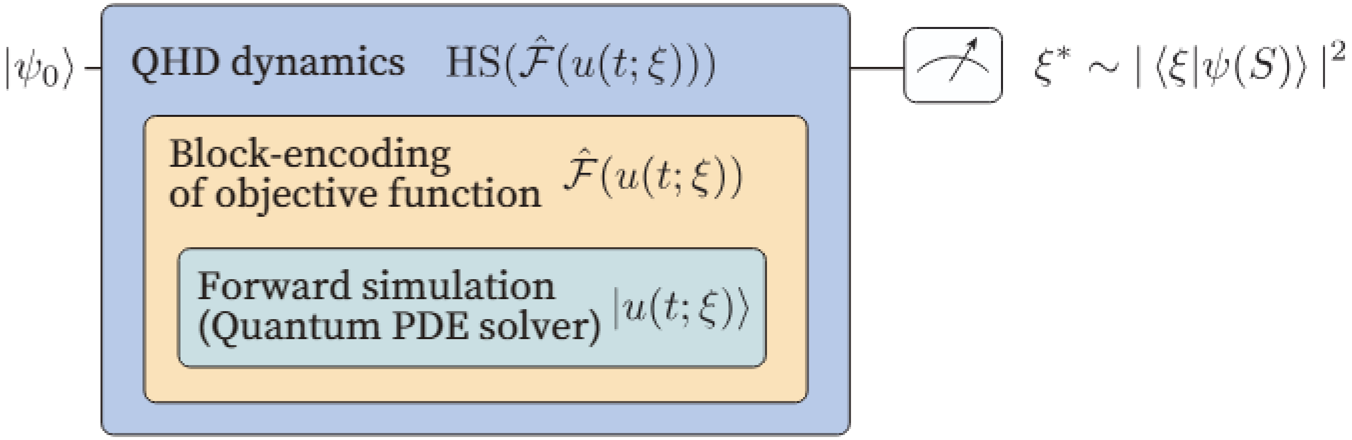
PDE-constrained optimization

$$\min_{\xi} \; F(u(\xi))$$

$$\text{subject to: } \frac{\partial u(t,x;\xi)}{\partial t} = \kappa(\xi)\nabla^2 u(t,x;\xi)$$



Classical approach



Quantum approach (this work)

Quantum Hamiltonian Descent

Quantum algorithm for continuous optimization based on quantum dynamics

$$\min_{\xi \in [0,1]^M} F(u(\xi))$$

subject to: $\dfrac{\partial u(t,x;\xi)}{\partial t} = \kappa(\xi)\nabla^2 u(t,x;\xi)$

$$H = \frac{1}{2} e^{-\nu s} \sum_{\mu=1}^{M} \frac{\partial^2}{\partial \xi_\mu^2} + e^{\nu s} \hat{F}$$

$\hat{F}$: Objective function as a potential term of Hamiltonian

$$\frac{\partial \psi(s)}{\partial s} = -iH\psi(s) \longrightarrow \xi^* \sim \langle \xi | \psi(s) \rangle$$

Measurement outcome is solution candidate

We need to implement time-dependent Hamiltonian simulation with the objective function as a potential term

Time-dependent Hamiltonian simulation

Time-dependent Hamiltonian

$$H = \frac{1}{2} e^{-\nu s} \underbrace{\sum_{\mu=1}^{M} \frac{\partial^2}{\partial \xi_\mu^2}}_{=\Lambda} + e^{\nu s} \hat{F}$$

Interaction picture simulation with truncated Dyson series (Better complexity)

$$H_I = e^{i\frac{1}{\nu}(e^{\nu s}-1)\hat{F}} \frac{e^{-\nu s}}{2} \Lambda e^{-i\frac{1}{\nu}(e^{\nu s}-1)\hat{F}} \longrightarrow |\psi(s)\rangle = e^{-i\frac{1}{\nu}(e^{\nu s}-1)\hat{F}} \underbrace{\mathcal{T} e^{-i\int_0^s H_I(s')ds'}}_{\text{Truncated Dyson series}} |\psi(0)\rangle$$

Product formula (simplest implementation)

$$U(s_{j+1}, s_j) = e^{-i\frac{1}{2}e^{-\nu s_j}\Lambda \Delta s} e^{-ie^{\nu s_j}\hat{F}\Delta s} \longrightarrow |\psi(s)\rangle = U(s, s-\Delta s) \cdots U(\Delta s, 0)|\psi(0)\rangle$$

We need access to the objective function as a time evolution operator
→We realize it by constructing block-encoding

Block-encoding (BE)

Embed arbitrary matrix into a unitary matrix as a block matrix,
which enables us to access arbitrary matrix on a quantum computer

Block-encoding a matrix A into a unitary U_A

$$U_A = \begin{pmatrix} \frac{A}{\alpha} & * \\ * & * \end{pmatrix}$$

α:normalization constant

Another description (quantum computing convention)

$$(\langle 0| \otimes I) U_A (|0\rangle \otimes I) = \frac{A}{\alpha} \longrightarrow U_A |0\rangle \otimes |\psi\rangle = \frac{1}{\alpha} \underline{|0\rangle} \otimes A|\psi\rangle + |\perp\rangle$$

Postselection by auxiliary qubits

Extended forward simulation

PDE constraint (ODE by spatial discretization)

$$\frac{\partial u(t;\xi)}{\partial t} = -A(\xi)u(t;\xi)$$

Forward simulation of all parameters in superposition

$$\frac{\partial \tilde{u}(t)}{\partial t} = -\tilde{A}\tilde{u}(t) \qquad \tilde{A} = \sum_{\xi} |\xi\rangle\langle\xi| \otimes A(\xi)$$

$$\tilde{u}(0) = \sum_{\xi} \psi_{\xi} |\xi\rangle \otimes |u(0)\rangle \longrightarrow \tilde{u}(t) = \sum_{\xi} \psi_{\xi} |\xi\rangle \otimes \|u(t;\xi)\| |u(t;\xi)\rangle$$

ODE solver gives forward simulation results of all parameters in superposition

Extended forward simulation

m bit representation of ξ

$$\xi = \frac{1}{2^m - 1} \sum_{b=1}^{m} \xi^{(b)} 2^{b-1}$$

Parameterization of $A(\xi)$

$$A(\xi) = A_0 + A_1 \xi$$

Representation of $\tilde{A}$

$$\tilde{A} = \sum_{\xi} |\xi\rangle\langle\xi| \otimes A(\xi) = I^{\otimes m} \otimes A_0 + \frac{1}{2^m - 1} \sum_{b=1}^{m} 2^{b-1} |1\rangle\langle 1|_b \otimes A_1$$

With the BE of A_μ, we can construct BE of $\tilde{A}$ by linear combination of block encoded matrices

Block-encoding of the objective function

$$F\big(u(\xi)\big) = \sum_{j\in\mathcal{J}} \big(u_j(T;\xi)\big)^2$$

Assume that the objective function is a quadratic form

BE of the objective function

Forward sim.

$$|\xi\rangle|u_0\rangle|0\rangle \to \frac{\|u(t;\xi)\|}{\alpha}|\xi\rangle|u(T;\xi)\rangle|0\rangle + \sqrt{1-\frac{\|u(t;\xi)\|^2}{\alpha^2}}|\xi\rangle|\chi\rangle$$

Reflection

$$\to \frac{\|u(t;\xi)\|}{\alpha}|\xi\rangle(2P-I)|u(T;\xi)\rangle|0\rangle - \sqrt{1-\frac{\|u(t;\xi)\|^2}{\alpha^2}}|\xi\rangle|\chi\rangle$$

Inv. of forward sim. and state prep.

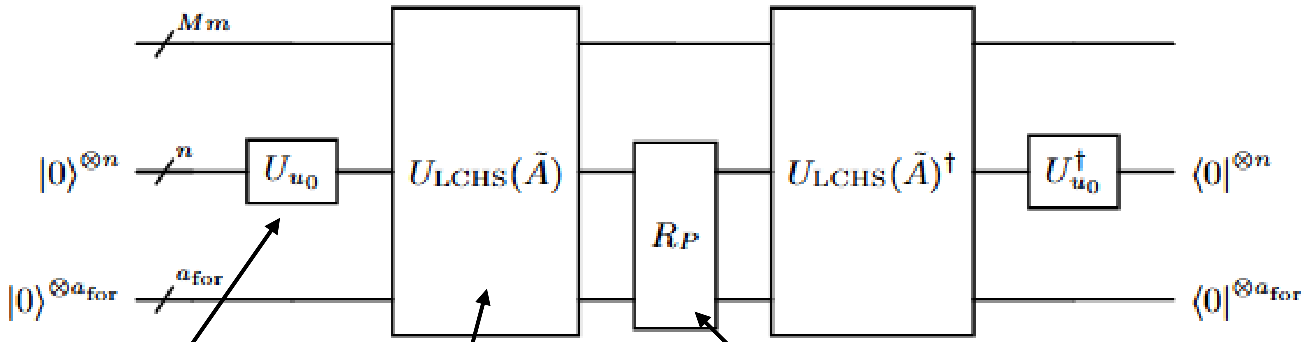
$$P|j\rangle|k\rangle = \begin{cases} |j\rangle|k\rangle & j\in\mathcal{J} \text{ and } k=0 \\ 0 & \text{otherwise} \end{cases}$$

$$\to \left(\frac{2F\big(u(\xi)\big)}{\alpha^2} - 1\right)|\xi\rangle|0\rangle|0\rangle + |\xi\rangle|\perp\rangle$$

Diagonal block encoding of the objective function

Block-encoding of the objective function

Quantum circuit for block-encoding $\hat{\mathcal{F}} = \sum_{\xi} F\big(u(\xi)\big)|\xi\rangle\langle\xi|$



Initial state for PDE

Forward simulation

Reflection for 0 state
(marking domain of integration)

$$\mathcal{F}_{\mathrm{quad}} = \sum_{j\in\mathcal{J}} \|u_j(T;\xi)\|^2,$$

$$\mathcal{F}_{\mathrm{err}} = \sum_{j\in\mathcal{J}} \|u_j(T;\xi) - u_{\mathrm{ref},j}\|^2,$$

Gate complexity (under the assumption of strongly convexity)

Proposed method

$$\tilde{O}\left(\frac{dN^{\frac{1}{d}}M^3T}{\epsilon}\right)$$

Conventional method

$$\tilde{O}\left(\frac{d^{1+\frac{1}{p}}N^{\frac{1}{d}\left(1+\frac{1}{p}+d\right)}T^{1+\frac{1}{p}}}{\epsilon^{1/p}}\right)$$

N: DOF of discretized PDE
T: Simulation time of PDE
M: # of design parameters
d: Spatial dim. of PDE

Our quantum approach is effective when $N \gg M$

Numerical experiment A

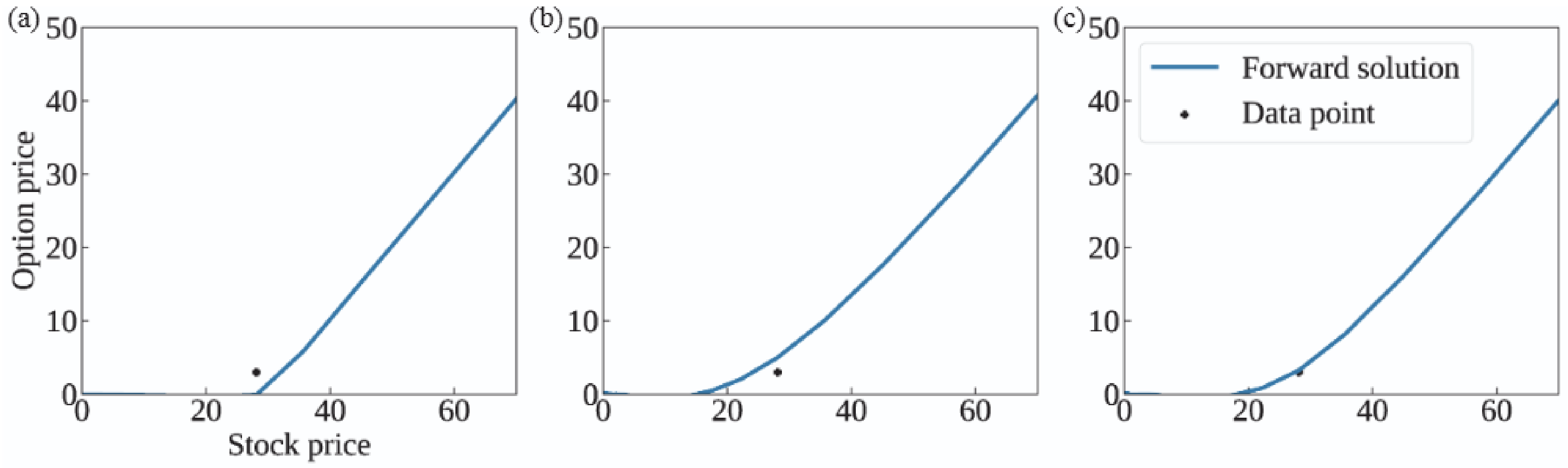
Parameter calibration problem of Black-Scholes equation

$$\frac{\partial V}{\partial \tau} + rs\frac{\partial V}{\partial s} + \frac{\sigma^2 s^2}{2}\frac{\partial^2 V}{\partial s^2} = rV$$

V: Option
s: Stock price
r: risk-free rate
σ: Volatility

$$F\left(V(\sigma)\right) = (V(\sigma) - V_{\mathrm{data}})^2$$

Estimate volatility σ from data of call option price V



Reference solution A
$\sigma = \sigma_{\min}$

Reference solution B
$\sigma = \sigma_{\max}$

Optimum solution
$\sigma = \sigma_{\mathrm{opt}}$

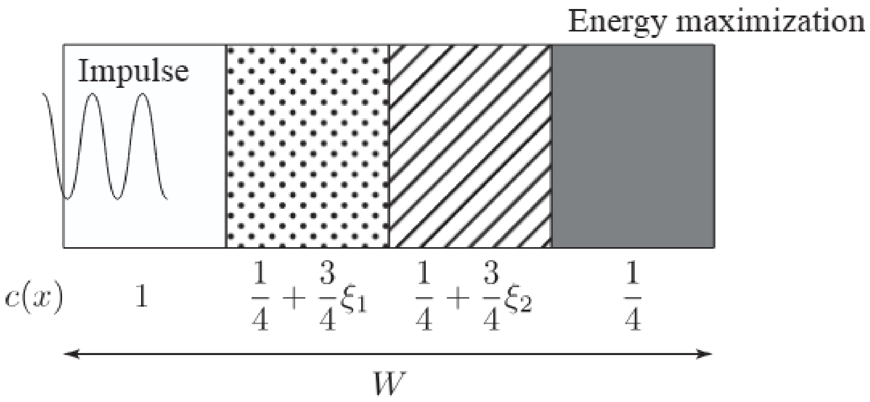
Numerical Experiment B

Material parameter optimization for acoustic system

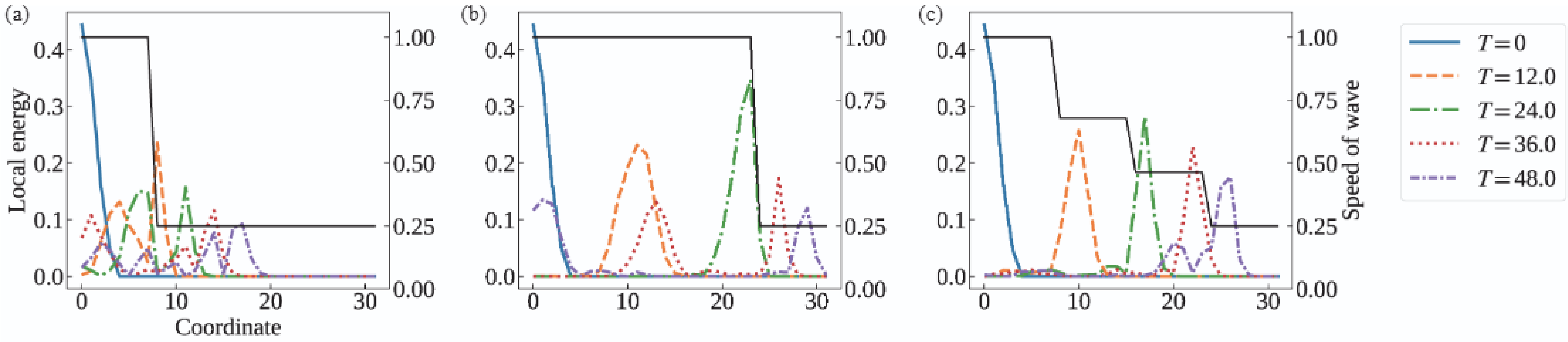
$$\frac{\partial^2 w}{\partial t^2} = c(x)^2 \frac{\partial^2 w}{\partial x^2}$$

w: Pressure
c: speed of sound

$$F\big(w(c)\big) = -w(c)^2$$



Optimize the material's refractive index to maximize transmission of a left-incident wave into the gray region on the right, with minimal loss.



Reference solution A   Reference solution B   Optimum solution

Conclusions

We proposed a fully quantum algorithm for PDE-constrained optimization incorporating a quantum PDE solver and quantum optimization

1. We constructed explicit block-encoding of the objective function using a quantum PDE solver as its subroutine.
2. We provided the complexity analysis of the proposed method, which suggests that our quantum approach is effective when design optimization involves large-scale PDE with modest design parameters.

Future work

- Forward simulation: Extension to nonlinear PDE
- Optimization: Extension to discrete optimization