A Hybrid Classical-Quantum framework for solving Free Boundary Value Problems and Applications in Modeling Electric Contact Phenomena

Merey M. Sarsengeldin\textsuperscript{a,b,*}

\textsuperscript{a}Department of Mathematics, University of Central Florida, Orlando, Fl, US
\textsuperscript{b}National Academy of Sciences, Institute of Mathematics and Mathematical Modeling, Almaty, Kazakhstan

Abstract

In this paper we elaborate a hybrid classical-quantum framework which allows one to model and solve heat and mass transfer problems occurring in electric contacts. We utilize special functions and Harrow-Hassidim-Lloyd (HHL) quantum algorithm for finding temperature and arc flux functions exactly and approximately for the Stefan type problems. The Stefan type problems we are considering are based on Generalized Heat Equation with free boundaries. As examples we consider exact and approximate solutions of inverse one-phase and two-phase Stefan problems. An Inverse Generalized One-Phase Stefan Problem is considered as a model problem. Computational experiments were conducted and demonstrated on IBM Quantum Machine.

Keywords: Stefan Problem, Free Boundary Value Problems, Quantum Computing, HHL quantum algorithm, Electric Contacts, Arc Heating.

1. Introduction

In this study we develop a hybrid classical-quantum framework which allows one model heat and mass transfer problems occurring in electric contact phenomena. Along with the agreement with the experimental data this framework allows one efficiently find temperature function, arc flux, and unknown moving phase transformation boundary functions using quantum algorithms. In this particular study we utilize Harrow Hassidim Lloyd (HHL) \[1\] algorithm for finding coefficients of heat temperature functions represented in the form of heat polynomials \[2-5\] and arc flux function.

*Corresponding author
Email address: dr.sarsengeldin@gmail.com (Merey M. Sarsengeldin)
Pioneering investigations in 1980s brought a new computing paradigm known as quantum computing, in which information is encoded in a quantum system. In the 1990s, a series of works dedicated to quantum algorithms showed that they could do tasks faster than the best-known classical algorithms. Consistent advances in theory and experiments have resulted in a plethora of powerful quantum algorithms that outperform their classical counterparts in terms of computational power; however, due to the challenges associated with their physical realization, their applications are limited to a few use cases. Careful physical realization of algorithms on near-term quantum computers might lead to profound results in computational speed-up.

In this paper, we will study Free Boundary Value Problems (FBVPs) using one of the powerful quantum algorithms proposed by Harrow-Hassidim-Lloyd. The HHL algorithm is widely used in quantum machine learning, for solving PDEs, ODEs and was physically realized on different quantum architectures. It consists of three steps: phase estimation, controlled rotation, and uncomputation. The FBVPs are reduced to following equation where we apply HHL algorithm

\[ M |x\rangle = |b\rangle, \]  

In this study we assume that \( M \) is Hermitian and sparse matrix, and \( b \) is a vector column. This condition can be relaxed and it can be shown that \( \tilde{M} = \begin{bmatrix} 0 & M \\ M^T & 0 \end{bmatrix} \) can be brought to Hermitian matrix. Since \( \tilde{M} \) is Hermitian, we can solve the equation \( \tilde{M} \tilde{y} = \begin{bmatrix} \tilde{b} \\ 0 \end{bmatrix} \) to obtain \( \tilde{y} = \begin{bmatrix} 0 \\ \tilde{x} \end{bmatrix} \).

As a result, we’ll assume \( M \) is Hermitian for the rest of the article. We will assume an ideal case in this study and refer the reader to related literature for other approaches of Hamiltonian simulation and quantum phase estimation.

Stefan type Free Boundary Value Problems (FBVPs) that take phase transformations into account can be used for modeling processes stated in and agree with experimental data. These problems are among the most difficult in the theory of non-linear parabolic equations where along with the temperature function they require determination of an unknown moving boundary function (Direct Stefan Problem) or a flux function (Inverse Stefan Problem). In some specific cases Heat Potentials can be constructed which allow boundary value problems to be reduced to integral equations. However, there are additional challenges in the case of domains that degenerate at the initial time due to the singularity of integral equations, which belong to the family of pseudo-Volterra equations and which are difficult to solve in the general case. The reader
can refer to the extensive list of papers and literature on the FBVPs in [35]. Despite the importance and comprehensiveness of all of these studies, developing exact and approximate methods for solving FBVPs capable adequately model electric contact phenomena still remains a challenge in the theory of partial differential equations and mathematical physics.

In this paper we consider a class of PDEs with free boundaries

$$\frac{\partial \theta}{\partial t} = a^2 \left( \frac{\partial^2 \theta}{\partial x^2} + \frac{\nu}{x} \frac{\partial \theta}{\partial x} \right), \quad \alpha(t) < x < \beta(t), \quad -\infty < \nu < \infty, \quad t > 0,$$

(2)

which can be solved by the series of linear combinations of special functions which a priori satisfy the equation [2]

$$S^1_{\gamma,\nu}(x,t) = \left(2a\sqrt{t}\right)^{\gamma} \Phi \left( \frac{\gamma}{2}, \frac{\nu+1}{2}; -\frac{x^2}{4a^2 t} \right), \quad -\infty < \gamma, \nu < \infty,$$

(3)

$$S^2_{\gamma,\nu}(x,t) = \left(2a\sqrt{t}\right)^{\gamma} \left( \frac{x^2}{4a^2 t} \right)^{\frac{1-\nu}{2}} \Phi \left( \frac{1-\nu}{2}, \frac{3-\nu}{2}; -\frac{x^2}{4a^2 t} \right),$$

(4)
and gain exponential speed up when quantum HHL algorithm applied.

**Algorithm 1: Quantum HHL Algorithm in Qiskit**

**Data:** Load the data \( |b \rangle \in \mathbb{C}^N \)

**Result:** Apply an observable \( M \) to calculate \( F(x) = \langle x | M | x \rangle \).

initialization;

while outcome is not 1 do
  • Apply Quantum Phase Estimation (QPE) with \( U = e^{iMt} := \sum_{j=0}^{N-1} e^{i\lambda_j t} |u_j \rangle \langle u_j| \). Which implies \( \sum_{j=0}^{N-1} b_j |\lambda_j\rangle_{n_l} \langle u_j|_{n_b} \) in the eigenbasis of \( M \)
    where \( |\lambda_j\rangle_{n_l} \) is the \( n_l \)-bit binary representation of \( \lambda_j \).
  • Add an ancilla qubit and apply a rotation conditioned on \( |\lambda_j\rangle \),
    \( \sum_{j=0}^{N-1} b_j |\lambda_j\rangle_{n_l} \langle u_j|_{n_b} \left( \sqrt{1 - \frac{C^2}{\lambda_j^2}} |0\rangle + \frac{C}{\lambda_j} |1\rangle \right) \), \( C \) - normalization constant.
  • Apply \( QPE^\dagger \). This results in
    \( \sum_{j=0}^{N-1} b_j |0\rangle_{n_l} \langle u_j|_{n_b} \left( \sqrt{1 - \frac{C^2}{\lambda_j^2}} |0\rangle + \frac{C}{\lambda_j} |1\rangle \right) \);

if If the outcome is 1, the register is in the post-measurement state

\( \left( \frac{1}{\sqrt{\sum_{j=1}^{N-1} |b_j|^2/|\lambda_j|^2}} \right) \sum_{j=0}^{N-1} b_j |0\rangle_{n_l} |u_j|_{n_b} \) then
  Apply an observable \( M \) to calculate \( F(x) = \langle x | M | x \rangle \);
else
  repeat the loop;
end
end

2. Main results

Equation 2 with arbitrary \( \nu \) is a generalized heat equation which can serve as a model for bridging processes in electrical contacts with variable cross section. For special cases \( \nu = 0, 1, 2 \) equation 2 is transformed to the heat equation in linear, spherical and cylindrical coordinates respectively.

Following formulas will ease our further calculations
\[
\lim_{x \to \sqrt{t}} \frac{1}{4a_1^2 t} \Phi \left( -\frac{\beta}{2}, \mu, -\frac{z^2}{4a_1^2 t} \right) = \frac{\Gamma(\mu)}{\Gamma(\mu + \frac{\alpha^2}{2a_1^2})},
\]

(5)

\[
\frac{\partial \theta}{\partial x} = \sum_{n=0}^{\infty} \left( 4a_1^2 t \right)^n \left[ A_n \left( \frac{-x}{4a_1^2 t} \right) L_{n-1}^\mu \left( \frac{-x^2}{4a_1^2 t} \right)^{\mu} + B_n \left( \frac{x^2}{4a_1^2 t} \right)^{-\mu} \left( \frac{2x}{4a_1^2 t} \right) \left( 1 - \mu \right) \right.
\]

(6)

\[
\left. \Phi \left( 1 - \mu - n, 2 - \mu, -\frac{x^2}{4a_1^2 t} \right) - \left( \frac{-x^2}{4a_1^2 t} \right)^{-\mu} \left( \frac{x^2}{4a_1^2 t} \right)^{-\mu} \Phi \left( 2 - \mu - n, 3 - \mu, -\frac{x^2}{4a_1^2 t} \right) \right]\]

\[
\frac{\partial \theta}{\partial x} \bigg|_{x = \sqrt{t}} = \sum_{n=0}^{\infty} \left( 4a_1^2 t \right)^n \left( \frac{2a_1 \sqrt{t}}{4a_1^2 t} \right)^{2n-1} \left( \frac{-\alpha}{a_1} \right)^n \left[ A_n \left( L_{n-1}^\mu \left( \frac{-\alpha}{2a_1} \right) \right) + B_n \left( \mu - 1 \right) \right.
\]

(7)

\[
\left( \frac{\alpha^2}{4a_1^2} \right)^{-\mu} \Phi \left( 1 - \mu - n, 2 - \mu, -\frac{\alpha^2}{4a_1^2} \right) + (\mu - 1) \left( \frac{\alpha^2}{4a_1^2} \right)^{-\mu} \Phi \left( 1 - \mu - n, 2 - \mu, -\frac{\alpha^2}{4a_1^2} \right) \right].
\]
2.1. HHL algorithm for exact solution of one phase Inverse Stefan Problem with variable cross section domain

Let’s consider following one phase inverse Stefan Problem with variable cross section which is used for modeling arcing and bridging processes in electrical contacts.

\[
\frac{\partial \theta}{\partial t} = a^2 \left( \frac{\partial^2 \theta}{\partial x^2} + \nu \frac{\partial \theta}{\partial x} \right), \quad 0 < x < \alpha(t), \quad 0 < \nu, t < 1, \tag{8}
\]

\[
\theta(0, 0) = T_m, \quad \alpha(0) = 0, \tag{9}
\]

\[
\left( \beta \theta + \gamma \frac{\partial \theta}{\partial x} \right) \bigg|_{x=0} = P(t), \tag{10}
\]

\[
\theta(\alpha(t), t) = T_m, \tag{11}
\]

\[
\lambda \frac{\partial \theta}{\partial x} \bigg|_{x=\alpha \sqrt{t}} = L_\gamma \frac{\partial \alpha(t)}{\partial t}. \tag{12}
\]

the solution can be represented in the following form

\[
\theta(x, t) = \sum_{n=0}^{\infty} (4a^2 t)^n \left[ A_n L_n^{\mu-1} \left( -\frac{x^2}{4a^2 t} \right) + B_n \left( \frac{x^2}{4a^2 t} \right)^{1-\mu} \Phi \left( 1 - \mu - n, 2 - \mu, -\frac{x^2}{4a^2 t} \right) \right], \tag{13}
\]

where \( k \) is defined from boundary conditions.

From conditions 10, 11 and 12 we get following expressions

\[
\beta \sum_{n=0}^{\infty} (4a^2 t)^n A_n L_n^{\mu-1}(0) + \sum_{n=0}^{\infty} P^n(0) \frac{t^n}{n!} = 0, \tag{14a}
\]

\[
\sum_{n=0}^{\infty} (4a^2 t)^n \left[ A_n L_n^{\mu-1} \left( -\frac{\alpha^2}{4a_1^2} \right) + B_n \left( \frac{\alpha^2}{4a_1^2} \right)^{1-\mu} \Phi \left( 1 - \mu - n, 2 - \mu, -\frac{\alpha^2}{4a_1^2} \right) \right] = T_m, \tag{14b}
\]

\[
\sum_{n=0}^{\infty} (4a_1^2 t)^n \left( \sqrt{t} \right)^{2n-1} \left[ -\frac{\alpha}{a_1} \right] \left[ A_n \left( L_n^{\mu} \left( -\frac{\alpha}{2a_1} \right) \right) + B_n \left( \mu - 1 \right) \left( \frac{\alpha^2}{4a_1^2} \right)^{-\mu} \Phi \left( 1 - \mu - n, 2 - \mu, -\frac{\alpha^2}{4a_1^2} \right) \right] = L_\gamma \frac{1}{2\sqrt{t}}. \tag{14c}
\]

After multiplying both sides of 14c by \( \sqrt{t} \) and comparing coefficients at same powers of \( t \) in 14a, 14b and 14c problem 8-13 is reduced to the equation1.
2.1.1. Application for the calculation of the arc heat flux for melting of a micro-asperity at electrical contact closure in vacuum circuit breakers

On the Figure 2, problem 15-18 models temperature and contact dynamics in region $D_0$ at the initial stage before mechanical bounce where $D_0 [-l \leq z \leq 0]$ and $D_1 [0 \leq z \leq \sigma_b(r,t)]$ are the zones of temperature dynamics and pressure of metal vapours in contact gap, including the zone of evaporated micro-asperity with adjoining evaporated area inside contact, $D_2 [\sigma_b(r,t) \leq z \leq \sigma_m(r,t)]$ melted zone and $D_3 [\sigma_m(r,t) \leq z < \infty]$ is the solid zone.

The initial stage of heating and melting of a micro-asperity up to boiling temperature can be described by the bridge model, which is presented and discussed in details in [36]. This liquid bridge can be considered as a bar with variable cross-section $S(z)$. The shape of the cross-section $S(z)$ is chosen from the analysis of a Talyrond trace (profilogram) of the contact surface and in this case it’s identified with a paraboloid having the altitude $l$ and the radius of the base $h$.

Let us consider a model problem which is responsible for modeling initial stage of heating and melting of micro asperity in region $D_0$.

$$\frac{\partial \theta}{\partial t} = a^2 \left( \frac{\partial^2 \theta}{\partial r^2} + \frac{v}{r} \frac{\partial \theta}{\partial r} \right),$$

the domain

$$D_0 : \quad 0 \leq r < \alpha(t), \quad 0 < t < T,$$
boundary condition at $r = \alpha(t)$

$$\theta(\alpha(t), t) = f(t), \quad (16)$$

and the Stefan condition

$$-\lambda \frac{\partial \theta(\alpha(t), t)}{\partial r} = P(t) - L\gamma \frac{d\alpha}{dt}. \quad (17)$$

At the initial time the domain $D_0$ collapses into zero, thus the initial and concordance conditions are

$$\alpha(0) = \theta(0, 0) = f(0) = 0. \quad (18)$$

It is required to find the functions $\theta(r, t)$ and $P(t)$, where $\alpha(t)$ and $f(t)$ are given.

We represent the Heat Temperature function of problem 15-18 in the form

$$\theta(r, t) = \sum_{n=0}^{\infty} A_n (4a^2 t)^n L_n^{(\beta)} \left( -\frac{r^2}{4a^2 t} \right) \quad (19)$$

where $\beta = \frac{\nu-1}{2}$ and can be found like it’s demonstrated in [36], $L_n(x)$ are associated Laguerre polynomials. The function 19 satisfies the heat equation 15 for arbitrary constants $A_n$. Satisfying the boundary condition 16 we get

$$f(t) = \sum_{n=0}^{\infty} A_n (4a^2)^n L_n^{(\beta)} \left( -\frac{\alpha^2}{4a^2} \right) t^n, \quad (20)$$

$$\sum_{n=0}^{\infty} \frac{f^{(n)}(0)}{n!} t^n = \sum_{n=0}^{\infty} A_n (4a^2)^n L_n \left( -\frac{\alpha^2}{4a^2} \right) t^n, \quad (21)$$

where

$$L_n^{(\beta)} \left( -\frac{\alpha^2}{4a^2} \right) = \frac{(\beta + 1)n}{n!} {}_1F_1(-n; \beta + 1; t)$$

$$\Gamma(\beta + n) \frac{\Gamma(\beta)}{\Gamma(\beta + n)} = \frac{\int_0^\infty x^{\beta-n-1}e^{-x}dx}{\int_0^\infty x^{\beta-1}e^{-x}dx}$$

where $(\beta)_n$ — Pochhammer symbol Equation 21 can be reduced to the equation $A_n$ coefficients of Heat temperature function 15 can be determined.
The unknown heat flux $P(t)$ can be found now from the expression \[ P(t) = \lambda \frac{\partial \theta(\alpha(t), t)}{\partial r} - L \frac{d\alpha}{dt} \] which can be written in the form

\[ P(t) = \lambda \frac{\partial \theta(\alpha(t), t)}{\partial r} - L \frac{d\alpha}{dt} \] (22)

where the right side is already found.

2.2. HHL algorithm for exact solution of two phase Inverse Stefan Problems with variable cross section domain

Let’s consider an inverse two phase Stefan problem. An inverse two phase Stefan problem with variable cross section is used for modeling bridging and arcing phenomena with phase transition predominantly from solid to liquid or vice-versa.

\[
\frac{\partial \theta_1}{\partial t} = a_1 \left( \frac{\partial^2 \theta_1^2}{\partial x^2} + \frac{\nu}{x} \frac{\partial \theta_1}{\partial x} \right), \quad 0 < x < \beta(t), \quad 0 < \nu, t < 1 \quad (23)
\]

\[
\frac{\partial \theta_2}{\partial t} = a_2 \left( \frac{\partial^2 \theta_2^2}{\partial x^2} + \frac{\nu}{x} \frac{\partial \theta_2}{\partial x} \right), \quad \beta(t) < x < \infty \quad (24)
\]

\[
\theta_1(0, 0) = T_m, \quad (25)
\]

\[
\theta_2(x, 0) = f(x), \quad (26)
\]

\[
f(0) = T_m, \quad \alpha(0) = 0, \quad \lim_{x \to \infty} f(x) \approx f(X) = 0, \quad \lim_{x \to \infty} \theta(x, t) \approx \theta(X, t) = 0, \quad (27)
\]

\[
\left( \beta \theta + \gamma \frac{\partial \theta}{\partial x} \right) \bigg|_{x=\infty} = P(t), \quad (28)
\]

\[
\theta_1(\alpha(t), t) = \theta_2(\alpha(t), t) = T_m \quad (29)
\]

\[
-\lambda_1 \frac{\partial \theta_1}{\partial t} \bigg|_{x=\alpha(t)} = -\lambda_2 \frac{\partial \theta_2}{\partial x} \bigg|_{x=\alpha(t)} + L \gamma \frac{\partial \alpha(t)}{\partial x} \quad (30)
\]

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The solution of above problem [31] can be represented in the following form

$$\theta_1(x, t) = \sum_{n=0}^{\infty} (4a_1^2)^n \left[ A_n L_n^{\mu-1} \left( \frac{-x^2}{4a_1^2 t} \right) + B_n \left( \frac{x^2}{4a_1^2 t} \right)^{1-\mu} \Phi \left( 1 - \mu - n, 2 - \mu, \frac{-x^2}{4a_1^2 t} \right) \right]$$

$$\theta_2(x, t) = \sum_{n=0}^{\infty} (4a_2^2)^n \left[ C_n L_n^{\mu-1} \left( \frac{-x^2}{4a_2^2 t} \right) + D_n \left( \frac{x^2}{4a_2^2 t} \right)^{1-\mu} \Phi \left( 1 - \mu - n, 2 - \mu, \frac{-x^2}{4a_2^2 t} \right) \right]$$

(31)

(32)

From conditions [10] [11] and [12] we get following expressions

$$\frac{(-1)^n}{n!} C_n + D_n = \frac{f^{2n}(0)}{(2n)!},$$

(33a)

$$\beta \sum_{n=0}^{\infty} (4a_1^2)^n A_n L_n^{\mu-1}(0) + \sum_{n=0}^{\infty} P^n(0) \frac{t^n}{n!} = 0,$$

(33b)

$$\sum_{n=0}^{\infty} (4a_1^2)^n \left[ A_n L_n^{\mu-1} \left( \frac{-a_1^2(t)}{4a_1^2 t} \right) + B_n \left( \frac{a_1^2(t)}{4a_1^2 t} \right)^{1-\mu} \Phi \left( 1 - \mu - n, 2 - \mu, \frac{-a_1^2(t)}{4a_1^2 t} \right) \right] = T_m,$$

(33c)

$$\sum_{n=0}^{\infty} (4a_2^2)^n \left[ C_n L_n^{\mu-1} \left( \frac{-a_2^2(t)}{4a_2^2 t} \right) + D_n \left( \frac{a_2^2(t)}{4a_2^2 t} \right)^{1-\mu} \Phi \left( 1 - \mu - n, 2 - \mu, \frac{-a_2^2(t)}{4a_2^2 t} \right) \right] = T_m,$$

(33d)

$$\sum_{n=0}^{\infty} (4a_1^2)^n \left[ A_n \left( \frac{2a_1^2(t)}{4a_1^2 t} \right) L_n^{\mu-1} \left( \frac{-a_1^2(t)}{4a_1^2 t} \right) + B_n \left( \frac{a_1^2(t)}{4a_1^2 t} \right)^{1-\mu} \left( \frac{2a_1^2(t)}{4a_1^2 t} \right) \right] \Phi \left( 1 - \mu - n, 2 - \mu, \frac{-a_1^2(t)}{4a_1^2 t} \right) = L \gamma \frac{d \alpha(t)}{d t}$$

(33e)

The idea of the collocation method applied in this problem is to subdivide $0 < t < T_n$ into $k$ intervals and after substituting solution functions [31] [32] into the boundary conditions [28] [29] [30] at points $t_1, t_2, ..., t_k$, reduce the problem to the problem [1] where we apply HHL algorithm to determine coefficients $A_n, B_n, C_n, P_n$. For computational purposes we use Qiskit and IBM’s quantum device.
3. Experimental Results, Discussion and Conclusion

We used IBM Q\cite{37} and Qiskit for experiments and programming purposes. Inverse One and Two Phase Stefan Problems were solved demonstrating fidelity of 0.94. We refer reader to [38] for details of experiments. Proposed method in combination with Fa Di Bruno’s Formula and Quantum HHL algorithm can be used for exact solutions for direct/inverse Stefan type problems and MBVPs in general for arbitrary $\nu$ in [2] and arbitrary $\alpha(t)$. Special functions method in combination with HHL algorithm can be also used for approximate solutions of boundary value problems with fixed boundaries as well. Variational Quantum Linear Solver \cite{39} can be applied alternatively even though it’s weaker in terms of computational power than HHL algorithm, it can be implemented on NISQ computers whereas HHL requires more robust computers.

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