A QUANTUM COMPUTING ALGORITHM FOR SMOOTHED PARTICLE HYDRODYNAMICS

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ABSTRACT

This paper presents a quantum computing algorithm for the determination of function and gradient approximations in the Smoothed Particle Hydrodynamics (SPH) method. The SPH operators and domain discretisation are encoded in a quantum register using a careful normalisation procedure. The SPH summation is then performed via an inner product of quantum registers. This approach is tested in a classical sense for the kernel sum and first and second gradients of a function, using both the Gaussian and Wendland kernel functions, with comparisons for various register sizes made against analytical results. Error convergence is exponential in the number of qubits. It is hoped that this one-dimensional work will provide the foundation for a more general SPH algorithm, eventually leading to the highly efficient simulation of complex engineering problems on emerging quantum computers.

Keywords Quantum computing · Smoothed Particle Hydrodynamics

1 Introduction

Interest in quantum computing and its applications has grown dramatically in recent years. Quantum computers offer a means of performing computations of great complexity that are infeasible on classical machines. The power of quantum computation has been well documented, see Simon [11] for example, so in order to utilise this power there is a need to develop quantum numerical algorithms. The original motivation for quantum computing was based on arguments from Feynman [5] who suggested that, since the world is fundamentally quantum mechanical, it makes sense that the best way to simulate physics is by using a ‘quantum’ computer which takes advantage of the effects of quantum mechanics. The potential for quantum mechanical machines to simulate, both quantum mechanical and classical, physical systems was one of the main reasons for their early development.

The potential use of quantum computers for Smoothed Particle Hydrodynamics (SPH) simulations is of significant interest as quantum machines could drastically reduced the computational cost of SPH simulations. The SPH method is very effective in simulating problems with complex geometries and boundary interactions as it is a meshfree method. The lack of a mesh also means that parallelisation is much easier than it is for grid based methods. The accuracy of the SPH method relies upon using a large number of particles in the simulation and using a quantum machine could allow exponentially more particles to be used without significantly increasing the runtime of the computation. Alternatively simulations with a fixed number of particles could be executed in an exponentially shorter amount of time. The new
era of quantum computation offers exciting new opportunities for numerical modelling of physical systems and in particular for SPH. Although practical, large scale quantum systems are not currently available, quantum supremacy has already been achieved in specific application areas [1] and a time when machines offering commercial advantage are available is fast approaching [6].

There already exists a rich ecosystem of quantum numerical algorithms which have applications in modelling, simulation and numerical analysis. A well known example is the quantum algorithm of Harrow, Hassidim and Lloyd [7] for solving linear systems of equations to find some measure of the solution vector. Other application areas include quantum algorithms for finite differences [4], finite elements [10] and simulated annealing [12]. In this paper we will show how the SPH method of approximating functions and their derivatives can be adapted to work on a quantum computer. By encoding functions in quantum registers parts of the SPH computation can be performed using a quantum computer. Although the analysis presented here is one-dimensional, we hope to give an initial idea of how the SPH method may be employed on a quantum machine and lay the ground work for future developments. First we will give a brief introduction to a few of the key concepts required for developing quantum numerical algorithms.

## 2 Quantum computing fundamentals

The power of quantum computation comes from the way that information is represented in a quantum computer. In a classical computer the basic unit of information is the ‘bit’ which can exist in one of two distinct states 0 or 1. In a quantum computer not only can information exist as a 0 or a 1 but also as superposition of both simultaneously. In a quantum machine the basic unit of information is called a ‘qubit’. An operation acting upon a qubit effectively acts upon both 0 and 1 at the same time; by performing one operation on the qubit the operation has been performed on two different values. It follows that a two-qubit system performs the operation on four values, a three-qubit system on eight values and generally an \( m \) qubit system performs the operation on \( 2^m \) values. As the number of qubits increases the ‘quantum parallelism’ of the system increases exponentially. This ‘quantum parallelism’ is what allows certain problems to be solved significantly quicker on a quantum computer than on a classical machine since exponentially large amounts of information may be processed in polynomial time.

The qubit exists in the mathematical abstraction of a vector space. Quantum states behave in an analogous way to physical vectors and share the basic properties that vectors have. A particularly important vector space in quantum computation is the Hilbert space \( \mathbb{C}^n \), which is the vector space of \( n \)-tuples of complex numbers. A Hilbert space is essentially a vector space with an inner product and a norm defined by that inner product. The elements of \( \mathbb{C}^n \) are labelled by \(|u\rangle\), \(|v\rangle\), \(|w\rangle\) etc. An element of this vector space is written down as an \( n \)-dimensional column vector in the following way:

\[
|v\rangle = \begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{pmatrix}.
\]

(1)

The notation \(|v\rangle\) is called ‘bra-ket’ or Dirac notation. The column vector \(|v\rangle\) is referred as ‘ket-v’ and the dual vector of \(|v\rangle\), given by

\[
\langle v | = \overline{v}^T = [\overline{v_1} \ \overline{v_2} \ \ldots \ \overline{v_n}]^T
\]

(2)

is referred to as ‘bra-v’ where \(\overline{v}\) is the complex conjugate of \(v\). In general the components of the vector \(v_i\) are complex.

A qubit is represented as a two-dimensional state space in \( \mathbb{C}^2 \) with orthonormal basis vectors \(|0\rangle\) and \(|1\rangle\). The vectors in the basis set \(|0\rangle, |1\rangle\) are defined by

\[
|0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad |1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}.
\]

(3)

This is the most common basis used in quantum computing and is called the computational basis. A qubit can exist in the state \(|0\rangle\) or the state \(|1\rangle\) or a superposition state which is a linear combination of the two. The superposition state \(|\psi\rangle\) is written as

\[
|\psi\rangle = \alpha |0\rangle + \beta |1\rangle
\]

(4)

and the Hermitian conjugate (dual vector) \(\langle \psi | = (|\psi\rangle)^\dagger\) is given by

\[
\langle \psi | = \alpha^* \langle 0 | + \beta^* \langle 1 |.
\]

(5)

Here \(\alpha\) is the complex scalar amplitude of measuring \(|0\rangle\) and \(\beta\) the amplitude of measuring \(|1\rangle\). These amplitudes are essentially ‘quantum probabilities’, they represent the chance that a given quantum state will be observed when
the superposition is collapsed. Unlike traditional probabilities, described by real numbers, these amplitudes are represented by complex numbers. The probability of finding $|\psi\rangle$ in state $|0\rangle$ is $|\alpha|^2$ and in state $|1\rangle$ is $|\beta|^2$. In order to perform useful calculations on a quantum computer these qubits must be composed into registers and manipulated using quantum algorithms.

2.1 Quantum registers

Quantum computers use multiple qubits combined into registers; when the registers are measured, and the superposition is collapsed, quantum registers are just strings of bits like classical computer registers. If however each qubit in the register is in a superposition then the register of $m$ qubits is in a superposition of all $2^m$ possible bit strings that could be represented using $m$ bits. This is the great power of superposition, the number of possible bit string combinations grows exponentially with the number of qubits. A good example of the power of using quantum registers comes from algorithms for approximating the summation of a large number, $N$, of function values as occurs in the SPH method. A deterministic algorithm using $n$ function values, where $n \ll N$, has an error $e_{\text{det}}^\theta = (N - n)/N \sim 1$ as $N \to \infty$. The error in a quantum algorithm for approximating the summation is given by $e_{\text{int}}^\theta \sim n^{-1}$ as $N \to \infty$ \cite{9}. Quantum registers are very useful when operations involving a large number of values are required or when there are many possible combinations.

The state space for a quantum register of size $m$ is a linear combination of $m$ basis vectors, each of length $2^m$, such that the superposition state of length $m$ is given by

$$|\psi_m\rangle = \sum_{k=0}^{2^m-1} \alpha_k |k\rangle,$$

where $k$ is the base-10 representation of a length $m$ number in base-2. For example a three-qubit register would be represented as

$$|\psi_3\rangle = \alpha_0 |000\rangle + \alpha_1 |001\rangle + \alpha_2 |010\rangle + \alpha_3 |011\rangle + \alpha_4 |100\rangle + \alpha_5 |101\rangle + \alpha_6 |110\rangle + \alpha_7 |111\rangle,$$

where each $\alpha_k$ is a complex number. As mentioned, the probability of observing a particular bit string upon collapsing the register is the square of the absolute value of the amplitude associated with a given bit string i.e. $Pr(k) = |\alpha_k|^2$. The probabilities of observing each particular bit string sum to unity therefore so do the squares of the absolute values of the amplitudes of all $2^m$ configurations such that

$$\sum_{k=0}^{2^m-1} |\alpha_k|^2 = 1.$$

In order to produce meaningful results, the information stored in quantum registers must be able to be manipulated. Logic gates are used in classical computers to manipulate data and circuits are used to transfer data. The equivalent notions of quantum logic gates and circuits exists in quantum computing. Quantum logic gates are represented abstractly by unitary operations; these operations are reversible such that the outputs from the gate uniquely determine the inputs to the gate. A quantum gate with $m$ qubits as inputs and outputs can be represented by a matrix of degree $2^m$; a gate acting on a single qubit is represented by a $2 \times 2$ unitary matrix. Any unitary transformation is a valid elementary operation on a quantum computer because unitary matrices preserve norms of the vector they act upon and therefore the probability amplitudes of a quantum register.

Unitary transformations performed on a single qubit may be visualized as rotations and reflections about the $x$, $y$, and $z$ axes of the Bloch sphere shown in figure\cite{1}. All the possible states $|\psi\rangle = \alpha |0\rangle + \beta |1\rangle$ in $\mathbb{C}^2$ correspond to the points $(\theta, \phi)$ on the surface of the unit sphere where

$$|\psi\rangle = \alpha |0\rangle + \beta |1\rangle = \cos \left( \frac{\theta}{2} \right) |0\rangle + e^{i\phi} \sin \left( \frac{\theta}{2} \right) |1\rangle.$$

The Bloch sphere is an intuitive visual framework for understanding the effects of unitary transformations on quantum states.

An operator $\hat{A}$ transforms one quantum state $|\psi\rangle$ into another $|\phi\rangle$ such that $\hat{A} |\psi\rangle = |\phi\rangle$. The outer product of two vectors, denoted $|v\rangle \langle u|$ or $|v\rangle \otimes |u\rangle$, is the tensor product of $|v\rangle$ with the conjugate transpose of $|u\rangle$. The outer product
Figure 1: The Bloch sphere representation of a qubit

is an operator which may be represented as a matrix:

\[
|v⟩⟨u| = \begin{bmatrix}
v_1 & v_2 & \cdots & v_m \\
v_2 & v_1 & \cdots & v_{m-1} \\
\vdots & \vdots & \ddots & \vdots \\
v_n & v_{n-1} & \cdots & v_1
\end{bmatrix}
\]

\[= \frac{1}{\sqrt{2}} \left( \begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{bmatrix} \begin{bmatrix} u_1 & u_2 & \cdots & u_m \end{bmatrix} \right). \tag{10}\]

### 2.2 Inner products

Multiplying two vectors together using the inner product to produce a scalar is a useful operation in many numerical algorithms. For example matrix multiplication can be broken down into successive applications of the inner products of rows and columns to form the entries in the resultant matrix. Estimating inner products is also important especially when considering large vectors. The estimation of the inner product of two quantum states is an important operation in many quantum algorithms and has therefore been considered from a number of different perspectives. The main methods for estimating the inner product of two quantum states are the swap test \[3\] and quantum counting \[2\].

The swap test method for estimating the real part of inner product of two quantum states may be easily demonstrated. Let \(|x⟩\) and \(|y⟩\) be two complex quantum states, which can be prepared in time \(O(T)\), then consider the combination of states

\[|φ⟩ = \frac{1}{2} \left( |0⟩ (|x⟩ + |y⟩) + |1⟩ (|x⟩ - |y⟩) \right). \tag{11}\]

If we define the normalised states

\[|u⟩ = \frac{|x⟩ + |y⟩}{\sqrt{2} \sqrt{1 + |\langle x|y⟩|}} \quad \text{and} \quad |v⟩ = \frac{|x⟩ - |y⟩}{\sqrt{2} \sqrt{1 - |\langle x|y⟩|}}, \tag{12}\]

and the phase angle \(θ\) such that

\[\sin θ = \sqrt{\frac{1 + |\langle x|y⟩|}{2}} \quad \text{and} \quad \cos θ = \sqrt{\frac{1 - |\langle x|y⟩|}{2}}, \tag{13}\]

then the state \(\text{(11)}\) may be rewritten as

\[|φ⟩ = \sin θ |0⟩ |u⟩ + \cos θ |1⟩ |v⟩. \tag{14}\]
We wish to calculate the SPH approximation of the one-dimensional function \( f(x) \) at an accuracy \( \epsilon \) with a probability of success of at least \( 1 - \delta \).

Let \( G = (2 |\psi\rangle \langle \psi| - I) (Z \otimes I) \) where \( Z \) is the Pauli-Z operator and \( I \) is the identity operator. The Pauli-Z operator acts on the computational basis such that \( Z |0\rangle = |0\rangle \) and \( Z |1\rangle = -|1\rangle \). \( G \) may be represented as the rotation matrix

\[
G = \begin{pmatrix}
\cos 2\theta & \sin 2\theta \\
-\sin 2\theta & \cos 2\theta
\end{pmatrix}
\]

(15)
in the basis \( \{ |0\rangle, |1\rangle \} \). The eigenvalues of \( G \) are \( e^{\pm 2i\theta} \) with corresponding eigenvectors

\[
|w_+\rangle = \frac{1}{\sqrt{2}} (|0\rangle |u\rangle + i |1\rangle |v\rangle),
\]

\[
|w_-\rangle = \frac{1}{\sqrt{2}} (|0\rangle |u\rangle - i |1\rangle |v\rangle),
\]

(16)
such that

\[
|\phi\rangle = - \frac{i}{\sqrt{2}} (e^{i\theta} |w_+\rangle - e^{-i\theta} |w_-\rangle).
\]

(17)

Performing the quantum phase estimation algorithm on \( G \) using an initial state \( |0\rangle^{\otimes n} |\phi\rangle \) with \( n = O(1/\delta \epsilon) \) we obtain an approximation of \( \theta \) of the form \( k\pi/2^n \) where \( k \in \mathbb{Z}_2^n \) and \( |\theta - k\pi/2^n| \leq \epsilon = 1/2^{n+1} \). The estimate of \( \theta \) can be used to give an estimate of the real part of the inner product of the quantum states. The probability of obtaining \( |0\rangle \) when measuring the quantum state \( |\psi\rangle \) is \( (1 + \Re\{\langle x|y\rangle\})/2 \) and the probability of obtaining \( |1\rangle \) is \( (1 - \Re\{\langle x|y\rangle\})/2 \).

Hence by calculating the probability of obtaining either of the states, \( |0\rangle \) or \( |1\rangle \), we may calculate the real part of the inner product \( \langle x|y\rangle \) of the quantum states \( |x\rangle \) and \( |y\rangle \). The determination of the real part of the inner product of two quantum states plays an important part in our method for performing SPH approximation on a quantum computer.

3 SPH using a quantum register

We wish to calculate the SPH approximation of the one-dimensional function \( f(x) \), on the finite domain \( x \in [a, b] \) where \( a < b \) are constants, using an \( m \) qubit quantum register. Let \( \{ x_j \} \) be a partition of \( [a, b] \) such that

\[
a = x_0 < x_1 < \ldots < x_{N-1} < x_N = b,
\]

(18)

where \( N = 2^m \) is the number of subintervals. Each \( x_j \), where \( j \in \{0, \ldots, N\} \), defines the edge of a subinterval. The width of the \( k^{th} \) subinterval is given by

\[
\Delta x_k = x_{k+1} - x_k, \quad k \in \{0, \ldots, N-1\}.
\]

(19)

Each particle is located at the centre of the respective subinterval so that the particle locations are given by

\[
r_k = \frac{x_{k+1} + x_k}{2}, \quad k \in \{0, \ldots, N-1\}.
\]

(20)

The domain discretisation is shown in figure 2. The value of the function at each particle location is denoted by \( f_k = f(r_k) \).

\[
\begin{array}{cccccc}
\Delta x_0 & \Delta x_1 & \ldots & \Delta x_{N-2} & \Delta x_{N-1} \\
\hline
a = x_0 & r_0 & x_1 & r_1 & x_2 & \ldots & x_{N-2} & r_{N-2} & x_{N-1} & r_{N-1} & x_N = b
\end{array}
\]

Figure 2: The domain discretisation showing the particle locations \( r_k \) and sizes \( \Delta x_k \).

The one-dimensional SPH approximation of a function is given by

\[
f(r) \approx \sum_k f_k \Delta x_k W(r - r_k, h),
\]

(21)

where \( W(r, h) \) is a known kernel function. Derivatives of the function can then be easily estimated by replacing the kernel with the required derivative, in SPH the derivative is found by taking an exact derivative of an approximate function [9]. We wish to perform this SPH approximation using a quantum computer therefore it is necessary that we somehow encode the values in a quantum register.
Firstly we will rewrite the summation (21) as an inner product of two vectors \( f = a \cdot W \) where
\[
a = [f_0 \Delta x_0, f_1 \Delta x_1, \ldots, f_{N-1} \Delta x_{N-1}],
\]
\[
W = [W_{r,0}, W_{r,1}, \ldots, W_{r,N-1}].
\] (22)

Here the entries in the kernel vector \( W \) are calculated using the kernel function such that \( W_{r,k} = W(r - r_k, h) \). We will encode the vectors in a quantum register by calculating appropriate normalisation factors and augmenting the entries using complex values. For the vector \( a \) we may define the quantum state
\[
|a\rangle = \frac{a}{|a|},
\] (23)
where \(|\cdot|\) denotes the Euclidean norm of the vector. If we have a large number of particles then calculating this norm directly is computationally expensive and calculating it would defeat the objective of encoding the values in a quantum register. However an approximation of the form
\[
|a\rangle \approx \frac{1}{\sqrt{N}} \left( \int_a |f|^2 \mathrm{d}x \right)^{\frac{1}{2}}
\] (24)
can be readily calculated using the function \( f \) or approximated using a smaller number of its values. As \( N \) becomes large this approximation becomes increasingly accurate. So our vector \( a \) can be rewritten, using an \( m \) qubit quantum register, as \(|a\rangle |a\rangle\). The norm of \(|a\rangle\) is unity so this is a legitimate quantum state.

Encoding the kernel vector \( W \) requires a little more ingenuity since calculating the Euclidean norm of this vector would be computationally expensive. Firstly we will scale the vector using the value \( cN \)
\[
\text{Taking the inner product of } \langle a | W \rangle \text{ gives}
\]
\[
\langle a | W \rangle = \frac{1}{|a|} \left[ f_0 \Delta x_0 \left( \bar{W}_{r,0} + ib_{r,0} \right) + f_1 \Delta x_1 \left( \bar{W}_{r,1} + ib_{r,1} \right) + \ldots + f_{N-1} \Delta x_{N-1} \left( \bar{W}_{r,N-1} + ib_{r,N-1} \right) \right].
\] (29)

Therefore multiplying through by \( cN |a| \) we have
\[
cN |a| = \sum_{k=0}^{N-1} f_k \Delta x_k \left( W_{r,k} + icN b_{r,k} \right).
\] (30)
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Table 1: Values of the constant $c = \max(|W(r, h)|)$ for the Gaussian and Wendland kernels and their first and second derivatives.

| Kernel   | Derivative | c          |
|----------|------------|------------|
| Gaussian | 0          | $\frac{1}{\sqrt{\pi h}}$ |
| Wendland | 0          | $\frac{3}{4h}$ |
| Gaussian | 1          | $2e^{-1/2}/\sqrt{\pi h^2}$ |
| Wendland | 1          | $405/512h^2$ |
| Gaussian | 2          | $2/\sqrt{\pi h^3}$ |
| Wendland | 2          | $15/4h^3$ |

So retaining only the real part of the inner product we find that

$$
\sum_{k=0}^{N-1} f_k \Delta x_k W_{r,k} = c N \|a\| \Re\{\langle a|W \rangle\}.
$$

This is equivalent to the SPH approximation of a function $f(r) \approx c N \|a\| \Re\{\langle a|W \rangle\}$ but calculated using a quantum register. An $m$ qubit register, storing $N = 2^m$ values, can be used to perform SPH approximation on a quantum register. The efficiency of the computation relies upon the values $c$ and $\|a\|$ being known and there being an efficient method of encoding the quantum states $|a\rangle$ and $|W\rangle$. The kernel function and its encoding can easily be replaced by equivalent derivative kernels so that derivatives of the function may be approximated, provided that the value $c$ is altered accordingly.

In this section a method for encoding the SPH approximation of a function in a quantum register has been developed. The quantum computation required for this procedure can be simulated on a classical machine when the number of qubits is relatively small. In the next section we will show simulations of the one-dimensional SPH approximation of a function, and its derivatives, on a quantum computer for various register sizes and kernel functions.

4 Simulations

In order to test the effectiveness of the numerical scheme proposed in section 3 we shall simulate the quantum algorithm on a classical machine. For the quantum register scheme to be useful it is necessary that the scheme performs as well as the equivalent standard one-dimensional SPH method. We shall test the scheme by approximating the function

$$
f(x) = \frac{1}{1 + 25x^2},
$$

which is a scaled version of the ‘Witch of Agnesi’. The first and second derivatives of the function (32) are also approximated for a number of different register sizes and using both the Gaussian kernel,

$$
W(r, h) = e^{-q^2}/\sqrt{\pi h},
$$

and the Wendland kernel,

$$
W(r, h) = \begin{cases} 
\frac{3}{\pi} \left[ \frac{3}{10} q^2 - \frac{3}{4} q + \frac{3}{4} \right], & \text{if } 0 \leq q \leq 2, \\
0, & \text{if } q > 2,
\end{cases}
$$

where $q = |r|/h$. A key element of the quantum numerical scheme outlined above is the constant $c = \max(|W(r, h)|)$ which is used to scale the weight vector and is different for each kernel. Table 1 shows the value of $c$ for both kernels and their first and second derivatives.

Figures 3 and 4 show the quantum SPH approximation of the function (32), using various register sizes $m$, for the Gaussian and Wendland kernels respectively. For each $m$-qubit approximation the smoothing length is taken to be $h = 4/2^m$ and four additional boundary particles are used at each end of the domain. The functions are approximated at $n = 300$ uniformly distributed points $x_i$ in the domain $x \in [-1, 1]$; these points are not the domain discretisation points they are simply points in the domain where the approximation is calculated. Figures 5 and 6 show corresponding approximations of the first derivative of (32) for the Gaussian and Wendland kernels and figures 7 and 8 show the approximations of the second derivative of (32). Figure 9 shows the root-mean-square (RMS) error

$$
\text{RMS} = \sqrt{\frac{\sum_{i=1}^{n} (f(x_i) - f_i)^2}{n}},
$$

(35)
where \( f(x_i) \) is the exact value of \( f(x) \) at the point \( x_i \) and \( f_i \) is the quantum SPH approximation, as a function of the register size \( m \) for both the Gaussian and Wendland kernel approximations of the function (32).

5 Discussion

The numerical simulations shown in section 4 illustrate the potential power of using quantum computers to perform SPH calculations. A small increase in the number of qubits in the quantum register allows the computation to contain many more particles and therefore increases the accuracy significantly. This increase in accuracy can especially be seen in figures 3 to 6 when comparing the \( m = 4 \) and \( m = 8 \) approximations. For the second derivative approximation, shown in figures 7 and 8 the increase in accuracy with the size of the quantum register is still evident despite the approximation being somewhat less accurate than for the first derivative and the function itself. Figure 9 shows how the RMS error, for the approximation of (32), decreases rapidly as the size of the register is increased. The accuracy of the approximation of the function and its derivatives continues to increase as the register size becomes larger.
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Figure 7: The second derivative function \( f''(x) = \frac{50(75x^2 - 1)}{(1 + 25x^2)^3} \) and its quantum SPH approximations using the Gaussian kernel for \( m = 4, 6, 8 \) qubits.

Figure 8: The second derivative function \( f''(x) = \frac{50(75x^2 - 1)}{(1 + 25x^2)^3} \) and its quantum SPH approximations using the Wendland kernel for \( m = 4, 6, 8 \) qubits.

Figure 9: The RMS error for the Gaussian and Wendland kernel sum approximations of (32) for various \( m \) qubit registers.
The method presented in section 3 is general in that it allows for any kernel function (including derivative functions) to be used in the approximation and for arbitrary domains, functions and register sizes. By allowing the function, spatial discretisation and kernel function to be encoded in a quantum register it is possible significantly increase the number of particles that can be used in the SPH approximation. It is worth noting however that this relies upon there existing an efficient method for actually creating the encoded registers $|\alpha\rangle$ and $|\psi\rangle$. If this efficient quantum register encoding algorithm exists then this method for performing SPH approximation will have significant speed advantages over its classical counterpart.

5.1 Conclusion

This paper has shown a scheme for encoding the SPH approximation method in a quantum register. Classical simulations of the quantum scheme for both the Gaussian and Wendland kernel functions have been demonstrated for a number of different registers sizes to approximate a function and its first and second derivatives. This has demonstrated how the error in the approximation decreases exponentially with the number of qubits in the register.

At present this quantum register approach to SPH approximation has only been attempted for one-dimensional functions but it is hoped that this method can be extended to allow two and three-dimensional simulations. Also currently the quantum register approach allows the SPH approximation to be calculated for a single point at a time; it is hoped that these techniques can be modified in order to perform the calculation for multiple points, possible using a single quantum operator. The work presented here could also be extended by considering time-stepping which would allow time-varying partial differential equations to be simulated using the SPH method on a quantum machine. Quantum computing promises to revolutionise many scientific fields and none more so than numerical analysis and computational modelling. The SPH method combined with quantum computation could provide a means of performing accurate continuum mechanics simulations, involving complex geometries, which are currently intractable.

References

[1] Arute, F., Arya, K., Babbush, R., Bacon, D., Bardin, J.C., Barends, R., Biswas, R., Boixo, S., Brandao, F.G., Buell, D.A. and Burkett, B., 2019. Quantum supremacy using a programmable superconducting processor. Nature, 574(7779): pp. 505-510.
[2] Brassard, G., Høyer, P. and Tapp, A., 1998, July. Quantum counting. In International Colloquium on Automata, Languages, and Programming (pp. 820-831). Springer, Berlin, Heidelberg.
[3] Buhrman, H., Cleve, R., Watrous, J. and De Wolf, R., 2001. Quantum fingerprinting. Physical Review Letters, 87(16), p.167902.
[4] Cao, Y., Papageorgiou, A., Petras, I., Traub, J. and Kais, S., 2013. Quantum algorithm and circuit design solving the Poisson equation. New Journal of Physics, 15(1), p.013021.
[5] Feynman, R.P., 1982. Simulating physics with computers. International journal of theoretical physics, 21(6-7), pp.467-488.
[6] Gil, D., Mantas, J., Sutor, R., Kesterson-Townes, L., Flöther, F., and Schnabel, C., 2018. Coming Soon to Your Business-Quantum Computing. IBM Technical Report. 24 pages. https://www.ibm.com/thought-leadership/institute-business-value/report/quantumstrategy
[7] Harrow, A.W., Hassidim, A. and Lloyd, S., 2009. Quantum algorithm for linear systems of equations. Physical review letters, 103(15), p.150502.
[8] Heinrich, S., 2002. Quantum summation with an application to integration. Journal of Complexity, 18(1), pp.1-50.
[9] Monaghan, J.J., 2005. Smoothed particle hydrodynamics. Reports on progress in physics, 68(8), p.1703.
[10] Montanaro, A. and Pallister, S., 2016. Quantum algorithms and the finite element method. Physical Review A, 93(3), p.032324.
[11] Simon, D.R., 1997. On the power of quantum computation. SIAM journal on computing, 26(5), pp.1474-1483.
[12] Somma, R., Boixo, S. and Barnum, H., 2007. Quantum simulated annealing. arXiv preprint arXiv:0712.1008