Bachelor thesis

To obtain the degree Bachelor of Science (B. Sc.)

Exploring the potential of quantum computing for multi-scale material modelling

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Date: 10.04.2026

Abstract (deutsch)

Die Simulation von Experimenten anstelle ihrer physikalischen Durchführung senkt die Kosten für die Entwicklung neuer Produkte oder Bauverfahren. Unternehmen und akademische Einrichtungen verlassen sich auf diese Methoden der Materialmodellierung und -simulation, um genaue Vorhersagen zum Materialverhalten zu erhalten, die für die Optimierung von Konstruktionsentwürfen, additiven Fertigungsprozessen, Sicherheitsaspekten und vielem mehr unerlässlich sind. Diese Simulationen sind jedoch rechnerisch sehr aufwendig und bringen moderne Supercomputer oft an ihre Grenzen. Quantencomputer sind dafür bekannt, Komplexitätsbarrieren zu überwinden, und könnten die Leistungssteigerung liefern, die für die Materialsimulation und -modellierung erforderlich ist, um den aktuellen Anforderungen gerecht zu werden. Diese Arbeit gibt einen Überblick über die relevante Literatur und analysiert das Potenzial des Quantencomputings in der Materialsimulation mit dem Ziel, ein Verständnis für kurzfristige und zukünftige Anwendungen zu vermitteln. Die Analyse kommt zu dem Schluss, dass die Optionen kurzfristig nicht in der Lage sind, mit klassischen Simulationen in Bezug auf den Umfang mitzuhalten, aber theoretische Leistungssteigerungen mit Hardware der Post-NISQ-Ära möglich sind.

Schlagwörter: Materialsimulation, Quantencomputing, Multi-skalige Materialmodellierung, Quantenalgorithmen

Abstract (english)

Simulating experiments instead of performing them physically reduces the cost of developing new products or construction methods. Companies and academic institutions rely on these material modelling and simulation methods to provide accurate predictions of material behaviour, which are essential for optimising structure designs, additive manufacturing processes, safety aspects, and more. However, these simulations are computationally expensive and often push modern supercomputing to its limits. Quantum computers are renowned for overcoming complexity barriers, and could deliver the performance enhancement required for material simulation and modelling to meet current demands. This thesis will review the relevant literature and analyse the potential of quantum computing in material simulation, with the aim of providing an understanding of near-term and future applications. The analysis concludes that, in the near term, options are not capable of matching classical simulations in scale, but theoretical performance improvements with post-NISQ-era hardware are possible.

Keywords: material simulation, quantum computing, multi-scale material modelling, quantum algorithms

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1 Introduction

Material simulation is a tool used to calculate the optimal state and behaviour of materials under custom-defined conditions. Companies utilise material simulation to achieve a more cost-efficient design process. Modern supercomputing plays a major role in this, as the calculations performed by material simulation algorithms require a large amount of computing power. However, the exponential scaling of classical algorithms limits the size of simulations without assumptions drastically. Quantum computing's ability to provide better scaling algorithms has already been demonstrated in areas such as cybersecurity. This thesis assesses the improvements that quantum computation could bring to material simulation.

1.1 Initial situation

From a material simulation perspective, quantum computing represents a revolutionary change. It offers new hope as supercomputers currently need massive performance improvements for modest increases in simulation size, due to simulation algorithms that often scale exponentially with system size [San23]. The rate at which classical supercomputing hardware has been improving has not kept pace with the desired computation power of companies relying on material simulation. A change in hardware can open up a new era of highly accurate and efficient simulations.

On the other hand, quantum computing is still trying to establish itself in the field of computation. Quantum advantage, an area in which quantum computers offer significant performance improvements, has been demonstrated on abstract problems and is waiting to be applied to commercial and industrial applications [Chu25]. One such application is material simulation, which could introduce quantum computing to academia, companies, and the general public in the long term, thereby improving its image beyond a sole threat to cybersecurity with which it is often associated.

Both the material simulation and quantum computing communities are interested in expanding the research in material simulation on quantum computers. The aim of this thesis is to evaluate the potential of quantum computers in this field.

1.2 Objective of the work

This thesis explores the potential of near-term quantum hardware for material simulation, focusing primarily on the Noisy Intermediate-Scale Quantum (NISQ) era. Different hardware and architectures are examined individually, together with the implementation of new and existing material simulation methods for quantum computing, in order to gain an overview of the current state of affairs. Acknowledging the limitations of modern classical supercomputing, the thesis explores how quantum computing could enhance scalability and performance

to address current issues in material simulation and evaluate the ability of quantum computers to solve these problems.

1.3 Research approach

To achieve the objective of this study, a comprehensive literature review is conducted using the Preferred Reporting Items for Systematic reviews and Meta-Analyses (PRISMA) method. The information gained from this review is then used to evaluate the current state of software and hardware in the field of quantum computing and to provide an outlook on the potential and limitations of quantum computers for use in material simulation. This is achieved by assessing the results of current research and the improvements to quantum hardware promised by quantum chip manufacturers in the near future, in order to gain an understanding of the value of quantum computers for material simulation.

1.4 Structure of the work

The following Sec. (2) provides the necessary information on material simulation and quantum computing to understand this thesis. It introduces the various material simulation algorithms, their properties, and the scales at which they are commonly used. Subsequently, Sec. (3) elaborates on the research question of this thesis. Sec. (4) outlines the methodology applied to gather the necessary information to answer the research question. Sec. (5) focuses on bringing an understanding of the literature review towards the needs of each scale and presents different approaches and their principles. In order to provide a representative evaluation of the potential of quantum computers in material simulation, the different scales are separated due to the wide variety of computations required to achieve results at each scale. Afterwards, Sec. (6) divides the research question into subcategories according to Sec. (3) and discusses them in the context of the current scale.

2 Fundamentals

Material simulation and quantum computing are not commonly associated with each other. Literature research and subsequent evaluation require specific knowledge of both fields. This section provides readers with the necessary information and offers a basic understanding of material simulation and quantum computing. Sec. (2.1) provides a general overview of the subject, along with a description of the material simulation methods referred to in later parts of this thesis. Sec. (2.2) elaborates on the basic principles of quantum computers, limited to the knowledge required to understand the features of the material simulation methods referred to in the literature review of this thesis.

2.1 Material simulation

Experiments and prototypes of new product designs often present challenges in terms of equipment availability and development cost [LeS13]. Companies have long relied on computer simulation to substitute those at the cost of modelling/simulating real-world behaviour incompletely [LeS13]. A correctly performed experiment will always behave according to the physical environment in which it is performed. Digital computers are given the same problem, but without the natively present physical environment. Material simulation, i.e. the process of calculating the physical behaviour and properties of materials on a digital computer, is a computationally expensive task that is often run on supercomputers to produce results that closely resemble real-world behaviour within a feasible timeframe [LeS13]. The equations and material properties simulated vary greatly depending on the methods used [Suk25; Nie24]. The material simulation methods referred to in this thesis are grouped by the physical scale on which their calculations are based, ranging from solving sub-atomic equations of electron interactions to the simulation of the behaviour of objects implemented by a continuum mesh representation at macroscale [Suk25; Nie24]. To put this into a perspective, it is computationally infeasible to simulate a water droplet with a radius of 1μm using the commonly used sub-atomic material simulation method, Density Functional Theory (DFT) [Sho22]. Nevertheless, research to improve the safety of aeroplanes, for example, is conducted using material simulation [Dan06]. Such algorithms used in the simulation of larger scale include assumptions and approximations of physical properties, which allow for more deviation in the results when compared to real-world experiments [Sho22].

To minimise the assumptions that have to be made on a larger scale, an incremental approach is often chosen [Ell11]. The multi-scale approach, visualised in Fig. (1) makes use of multiple different material simulation methods at different scales [Ell11]. It iteratively increases the size of the simulation, taking the results of the smaller-scale simulations as input for the current step [Jam25]. This way, more accurate results on a higher level can be achieved due to the

fundamental physics equations being part of the input [Sho22; Ell11]. This approach has found success and is widely used in classical computing today to mediate the limits of modern supercomputing [Ell11].

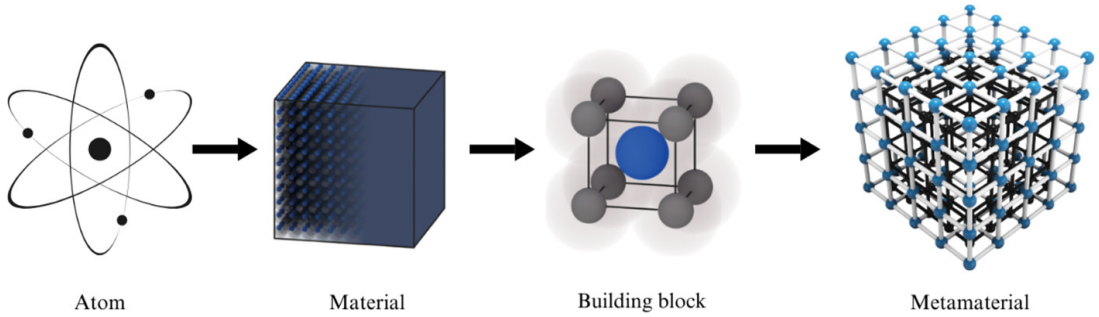


Figure 1: Visualisation of the multi-scale modelling approach. Multi-scale material modelling/simulation calculates properties on a smaller scale to use as input for larger scales. Adapted from [Jam25].

In this thesis, representative material simulation algorithms on different scales are assessed. In the following part, a basic explanation for the relevant classical algorithms is provided. The algorithms on quantum computers will be explained along the paper they appear in under Sec. (5). The algorithms are sorted by ascending scale.

Density Functional Theory (DFT) computes ground-state properties by solving approximations of the Schrödinger equation [Sho22]. Rather than describing electrons by their wavefunction, DFT uses the electron density to reduce complexity [Sho22]. Due to the sub-atomic scale of DFT and the exponential complexity involved, simulations can only be performed on a few hundred atoms, with supercomputers barely able to exceed a thousand atoms [Sho22].

Dynamic Mean Field Theory (DMFT) also operates on a sub-atomic scale [Kot04]. In contrast to DFT, DMFT provides more precise information about electron behaviour [Kot04]. Often used to model metals due to their high electronic correlation, DMFT abstracts starting from a lattice of atoms or electrons and creates an impurity and a bath [Kot04]. The impurity consists of one lattice site and is computed to the full extent of the current quantum mechanical knowledge [Kot04]. The bath is an initially estimated representation of the remaining lattice structure, reducing the properties of the environment to a passive state[Kot04]. The atoms or electrons can only interact with the impurity but not with each other inside the bath [Kot04]. The properties of the impurity are then compared to those of the bath, with the behaviour of the bath being iteratively optimised to match that of a lattice consisting of impurities [Kot04].

Molecular Dynamics (MD) is a method that operates on the atomic scale [Ald59]. MD numerically solves Newtonian equations for interacting atoms [Ald59]. To do this, interatomic forces, known as potentials, are required to represent the properties of the atoms [Ald59]. These are typically determined by

lower-scale simulations such as DFT [Sho22]. Starting with a self-constructed state, the simulation computes the neighbouring forces acting on each atom and updates their trajectory at each time step [Ald59]. MD enables simulations involving millions of atoms to be performed on modern supercomputers [Hed99].

The Monte Carlo (MC) method is not limited to material simulation, it is a general statistical approach applicable on multiple material simulation scales [Sun85]. MC involves sampling randomly from a set of possibilities, allowing an accurate representation of the entire set to be obtained using a limited subset, based on the law of large numbers [Sun85]. However, MC is unable to calculate the evolution of a system over time, focusing instead on computing optimal system configurations for specific cases (e.g. ground state) [Sun85]. This is achieved by randomly selecting configurations and repeatedly calculating the desired criteria until the entire set of possible configurations is sufficiently approximated to determine the optimal result [Sun85]. The scale of MC simulations is variable, thus having a wide range of possible computational limits [Sun85].

The Finite Element Method (FEM) is a highly abstracting material simulation algorithm [Fis07]. It simulates continuum structures instead of individual particles [Fis07]. FEM requires the properties of the material as input, as it is unable to derive them from fundamental physical equations itself [Fis07]. Based on these properties, the FEM solves partial differential equations to simulate an object's behaviour over time [Fis07]. The method outputs the evolution of stresses, strains, and other physical phenomena within the object over time [Fis07]. Due to its high level of abstraction compared to other material simulation methods discussed in this thesis, FEM can simulate large objects and is also used in the aerospace industry [Dan06].

2.2 Quantum computing

Quantum computers are a new type of computer that aims to extend the capabilities of classical computers [Rie22]. They use a different way of computing to achieve significantly more efficient algorithms than their classical counterpart [Rie22]. However, quantum computers are not necessarily faster than classical computers in every respect [Rie22]. The area of algorithms in which quantum computers excel is known as the ”quantum advantage” or ”quantum supremacy” and its scale is still subject to further research [Rie22].

Instead of classical binary bits, quantum computers use quantum bits (qubits) to store information [Pee24]. The advantage of qubits over classical bits is their ability to be in a state between the two classical states [Hug21]. This state makes use of the superposition that atoms and photons can achieve under the right circumstances [Rie22]. It represents the probability of being either a 1 or a 0 [Pee24]. A new notation is required to properly represent the state of a quantum computer. A classical 1 on a quantum computer will thus be referred to as

$|1\rangle$ and a classical 0 as $|0\rangle$ [Pee24]. Superposition now allows for notations in the form of:

$$H|0\rangle = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}} (|0\rangle + |1\rangle) \tag{1}$$

Where the qubit is not currently a $|1\rangle$ or a $|0\rangle$ and only reading its value will flip the qubit to one of the two, with some probability described by:

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle, \alpha, \beta \in \mathbb{C} \tag{2}$$

with

$$|\alpha|^2 + |\beta|^2 = 1 \tag{3}$$

Eq. (1) describes the application of the Hadamard gate to a qubit [She06]. Similar to how classical computers use logical operators such as XOR to manipulate bits, gates manipulate qubits [She06]. The Hadamard gate in particular is used to change a qubit's state into superposition, with a 50% probability of being either a $|1\rangle$ and $|0\rangle$ respectively [She06]. Gates are represented by matrices on the spectrum of complex numbers [She06]. Basic gates include the Pauli-X, Pauli-Y, Pauli-Z and the Hadamard gate:

$$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \tag{4}$$

The Bloch Sphere (Fig. (2)) is commonly used to visualise qubits, as well as the effect of gates on them [Gle05]. The Pauli gates each allow for rotation by 180° around the x-, y- or z-axis, while the Hadamard gate (assuming the gate is used on a definite state of $|1\rangle$ or $|0\rangle$) maps the z-axis to the x-axis [Gle05]. This results in a 50% chance for either state, as depicted through the same distance from the resulting vector to the states $|1\rangle$ and $|0\rangle$ on the Bloch sphere.

This qubit behaviour is currently compromised to an extent by noise and other imperfections. Because of this and the ongoing process of scaling quantum computers to considerable size, the current era of quantum computers is referred to as the NISQ-era [Abu25]. In addition to the noisy environment and the inability to perform large-scale computations, insufficiently long decoherence times are a problem that has to be addressed [Abu25]. similar to volatile memory in classical storage (e.g. random-access memory), qubits lose their state if certain conditions are met [Rie22]. In classical computers, volatile memory periodically refreshes (reads out the value and then sets it again) the charges of the states in the memory, thus losing the stored data if power is lost [Ham24]. The decoherence time of a qubit indicates the loss of information stored on the qubit over time [Rie22]. As the information in qubits is more complex than its classical counterpart, reading and setting the same state again is not possible

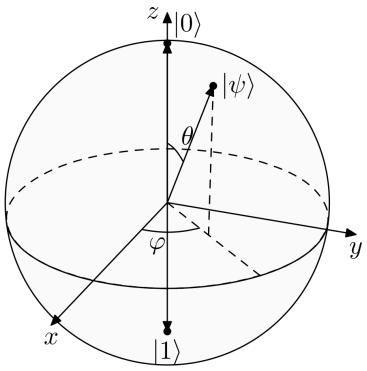


Figure 2: Bloch Sphere representation of a qubit. Vectors originating from the origin of the coordinate system, pointing to one point on the surface of the sphere represent the states of a qubit. $|1\rangle$ and $|0\rangle$ lie on opposite sides of the z axis [Gle05].

[Rie22]. In qubits, the loss of contained information (decoherence) occurs over time, in fractions of a second [Bla02]. The decoherence time varies depending on the physical implementation of the qubits [Bla02]. IBM, a leading producer of quantum computer architectures, relies on superconducting qubits [Bra22]. Other ways to physically implement a qubit include trapped-ion qubits, quantum dot qubits and photonic qubits [Lor21]. While the physical particles they operate can vary drastically, only the similarities are required for understanding the rest of this thesis.

All kinds of qubits can be described with the time-dependent Schrödingers wave equation:

$$\hat{H}\Psi(x,t) = \hat{E}\Psi(x,t) \tag{5}$$

Where $\hat{H}$ is a so-called Hamiltonian that describes the change of the wave function $\Psi(x,t)$ and $\hat{E}$ is the kinetic energy [Dav18]. The Hamiltonian can be described either as a matrix or as an equation [Vov21]. Through manipulation of this Hamiltonian, qubits can mimic quantum systems, a process used by several material simulation algorithms on quantum scale [Yos24]. However, this behaviour cannot easily be observed, as the measuring the qubit(s) results in the state flipping to one of the two observable states. Therefore, the behaviour is approximated by measuring the same process multiple times and then calculating the probabilities of the state [Gha23]. To accurately reproduce the behaviour of the quantum system, multiple thousands of values are measured for the algorithms covered by this thesis [Hag24; Gha23]. The measurement process of these individual values is referred to as a 'shot' in the rest of this thesis.

A major advantage of qubits over binary bits is entanglement [Sho97]. The

state of n entangled qubits can be expressed as a state vector in $[0,1]^n$, where there are 2^n possible states [Sho97]. This exponentially growing state space, which is the result of entanglement, can be used to describe more complex systems with a significantly reduced qubit count compared to the number of binary bits required for the same application [Sho97]. This property originates from the fact that entanglement allows for additional descriptors of the general state with notation $|00\rangle$ denoting the probability of the two entangled qubits flipping to a 0 [Sho97].

Entanglement is achieved by applying the CNOT-gate onto two qubits [Rie22]. The basis gate operations of quantum computers are limited to one- and two-qubit gates, which can construct higher order gates [Pow23].

$$CNOT = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \tag{6}$$

To visualise an algorithm for a quantum computer, the model of a quantum circuit is used [Nam20]. Each qubit is represented by a line, interrupted with boxes with the name of the applied gate inside and connected to other qubits in case of entanglement as seen in an example circuit in Fig. (3) [Fig17].

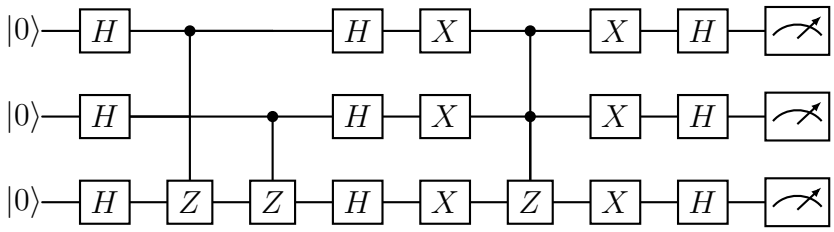


Figure 3: A small scale quantum circuit representing the Grover's algorithm, a popular quantum search algorithm [Fig17]. The three horizontal lines each represent a qubit. These qubits initially start in the state depicted at the start of the line. Each gate applied to a qubit is represented by a box with the variable defining the gate inside. Vertical lines between qubits indicate entanglement operations. The last symbol on each line indicates the qubit being measured.

In addition to gate-based quantum computers, quantum annealers are systems that use quantum mechanics to find a global minimum of an energy function [Falde11]. The relation between quantum computers and quantum annealers can be compared to that between digital classical computers and analog classical computers. However, quantum annealers are only well suited for combinatorial problems and do not operate based on aforementioned gates [Falde11].

Combinatorial problems that are equivalent to the NP-hard task of finding a solution to the Ising model can be converted into a cost function, which is then encoded into the Hamiltonian that acts on the qubits [Falde11]. The Ising model consists of a graph with a binary variable assigned to each vertex, representing the spin of atoms [Mis12]. The model allows vertices to be influenced by neighbouring vertices, making it useful for analysing energy distribution in molecular systems [Mis12].

This efficiency in combinatorial problems arises from quantum tunnelling [Falde11]. Quantum tunnelling describes the ability to pass through energy fluctuations without needing to follow the local maximum of a function [Falde11]. This leads to a more efficient exploration of the energy landscape, while simultaneously solving problems (e.g. freezing at local minimums) associated with classical computing [Falde11].

3 Problem statement

The question of what quantum computing's potential and limitations are in the field of material simulation is the focus of this thesis. The current way of performing high-end simulations is based on the multi-scale approach. While this approach appears promising in general, its performance and transferability in the context of quantum computing still need to be addressed. Specifically, this thesis evaluates the challenges of adopting known methods into the quantum computer environment, of creating new methods based on an understanding of the quantum advantage and the possible performance gains, are evaluated. This evaluation needs to take place across several dimensions to provide an accurate overall picture. The dimensions elaborated on in the following and discussed in Sec. (6) are:

- Understanding the Quantum Advantage
- Framework
- Accuracy
- Efficiency
- Scalability
- Reliability

Understanding the quantum advantage provides the major picture, allowing for assessment about possible performance gains about algorithms yet to be implemented. The difference in hardware properties compared to their classical counterparts brings along new possibilities, but also limitations. In particular, the design of the individual qubit itself is of interest, with different types of qubits and the newly introduced superposition state. The quantum computing field in isolation has made significant advancements in understanding the quantum advantage in other areas, which may be useful for material simulation as well. The field of material simulation on the other hand has found success with quantum algorithms on multiple different scales. This brings the need for evaluation of whether some scales are better suited to be implemented on quantum computers than others.

To incentivise more research in this area, researchers have been working on abstraction layers above the fundamental operations on quantum computers to closer resemble modern programming. Those frameworks potentially help in making quantum computing more approachable and easier to understand, to a level thats still enabling the quantum advantage to show. In continuation, generic problem handling and embedding are prospect to be implemented generically with researchers coming from material simulation as well as other

areas in mind. These possibilities and their cost in terms of performance need to be addressed.

Sec. (2.2) has described the results of quantum computing as being of probabilistic nature. This raises the question whether the accuracy achieved from classical simulations is possible to match or even beat. Standalone material simulation algorithms acting on high level meshes lack the accuracy to provide realistic predictions and thus rely on the multi-scale approach classically. Quantum advantage is most often only talked about regarding speed of computation, yet the accuracy of these algorithms are crucial to their potential real-world use.

The efficiency of quantum computers in the crucial parts of the algorithms needs to be significant enough to account for the amount of shots needed for an accurate result. With computation time improving in several orders of magnitude in other areas, it is the most attractive aspect that leads many to look into this area of research [Mav18]. Still, the origin of this performance improvement is to be addressed in order to make decisions of circuit design and algorithm adaptation from methods performing well on classical computers. In the context of hybrid computation, communication overhead is a new factor that needs to be accounted for.

The limitations of classical supercomputing towards material simulation is the scalability of classical algorithms. The runtimes of those scale exponentially, making it infeasible to perform simulations on high quantities of atoms with subatomic scale algorithms, as seen in Sec. (2.1). Increased performance on small scale demonstrations might not be enough, if the runtimes can not be reduced to polynomial or even linear. With research in the area of quantum computing increasing drastically over the last decade, near-term applications surpassing demonstrative simulations may be in reach.

Lastly, the reliability of NISQ devices is one of the two defining parts of their era. Error mediation and prevention through software is currently impeding the observation of the actual quantum advantage. Progress on the hardware side to provide fault-tolerant devices can impact the view on quantum computing as a whole.

Assessing those topics is the foundation of judging the potential quantum computers have to improve the material simulation landscape and what it takes to get there.

4 Methodology

As discussed in Sec. (1), the research field of material simulation is highly active. In order to efficiently find relevant papers for this thesis, a structured approach is required. The PRISMA statement provides such an approach, and is therefore used in this thesis to identify the current limitations of material simulation. The PRISMA statement is chosen because of its flexibility and reproducibility. It provides a generic systematic review framework that can be adapted to each specific use case.

After sufficient papers have been found and assessed, the potentials and limitations of quantum computers for use in the field of material simulation are identified and studied as the primary scope of this thesis.

4.1 PRISMA review

The PRISMA method is a widely used research tool for systematic reviews and literature research [Pag21c; Pag21b]. The standardised approach of PRISMA leads to usability in vastly different areas as well as reproducability for future work to build upon the current. The statement provides a two-step plan to i) identify possibly relevant papers and ii) then filter out duplicate, inaccessible and non-relevant papers. These steps are kept generic and the specific search and filter parameters are left open for the individual use cases.

In this thesis, the review part of the papers is only the first step. To eliminate papers outside the scope of interest, multiple, more specific queries branching from a single general root are used. This effectively applies the PRISMA method multiple times to the more specific queries. This method enables problems to be identified in each branch individually, providing the system required for this thesis.

This thesis uses the Scopus search engine, which queries multiple databases, to search for papers. Furthermore, the queries consist of a concatenation of words connected by logical operators, which simplifies the query writing process. These words are searched for in the title, abstract or keywords of a paper. The root query included in all branches searches for quantum computing related keywords as well as material simulation of some kind. For each branch, common names of the corresponding scale and the most well-known material simulation algorithms in each respective scale were used to find suitable papers. The specified branch contains a more restrictive version of the root query to identify any relevant papers that do not explicitly state a simulation scale. Fig. (4) provides an overview of the branches, whose queries are then elaborated on in Sec. (5) and the specific queries are found in appendix A.

The results obtained from the database queries are collectively assessed using the PRISMA methodology. First, duplicate papers are identified and removed.

Next, the remaining papers are screened based on their titles and abstracts.

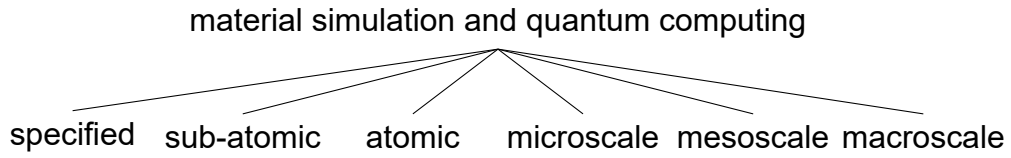


Figure 4: Visualization of the branched PRISMA literature research. Each branch is referred to by the term used in this figure.

During this stage, the papers found are classified as relevant or irrelevant to the research question defined in Sec. (3). Those that do not address the research focus or lack sufficient relevance are excluded from further consideration.

The remaining studies are then evaluated for accessibility, and all retrievable papers are included in the next stage. In the final step, the full texts of these papers are reviewed in detail to extract the necessary information for the systematic analysis.

4.2 Analysis

After identifying the relevant papers in the literature review, a structured evaluation of their results is conducted. The selected works offer different perspectives on the research topic and reveal recurring patterns across the field. Sec. (3) outlines the key aspects of interest that guided this analysis.

The central research question, introduced in Sec. (3), covers multiple dimensions, including the general concept of quantum advantage, quantum computing frameworks, as well as accuracy, efficiency, scalability, and reliability. Based on these dimensions, relevant information from each paper is systematically extracted and grouped according to these thematic areas.

The collected data is quantified based on the findings of the evaluated papers to enable a comparative analysis of the literature and identify a common consensus among researchers. Specifically, data for the used architecture (gate-based quantum computing or quantum annealing) and the findings of an improvement in either accuracy or efficiency is accumulated. Accuracy is categorised as better than classical computing when researchers explicitly mention improvement, similar to classical computing when the results of both quantum and classical calculations align, and worse than classical computing when the results are unreliable with noticeable deviations from reality and classical calculations. An improvement in efficiency is considered significant, when either the time or memory space scaling is improves sufficiently for the Bachmann-Landau notation to change. To evaluate and visualise this, the open-source statistical software jamovi is used to generate the visualisations presented in Sec. (6) [Lov26].

5 Results

The following subsections present the results of the literature review conducted according to the PRISMA method, as outlined in Sec. (4.1). For each branch, papers representing the general consensus of the relevant literature are presented in the associated subsection. The combined literature research includes 85 papers. The process of elimination is further visualised by Fig. (5).

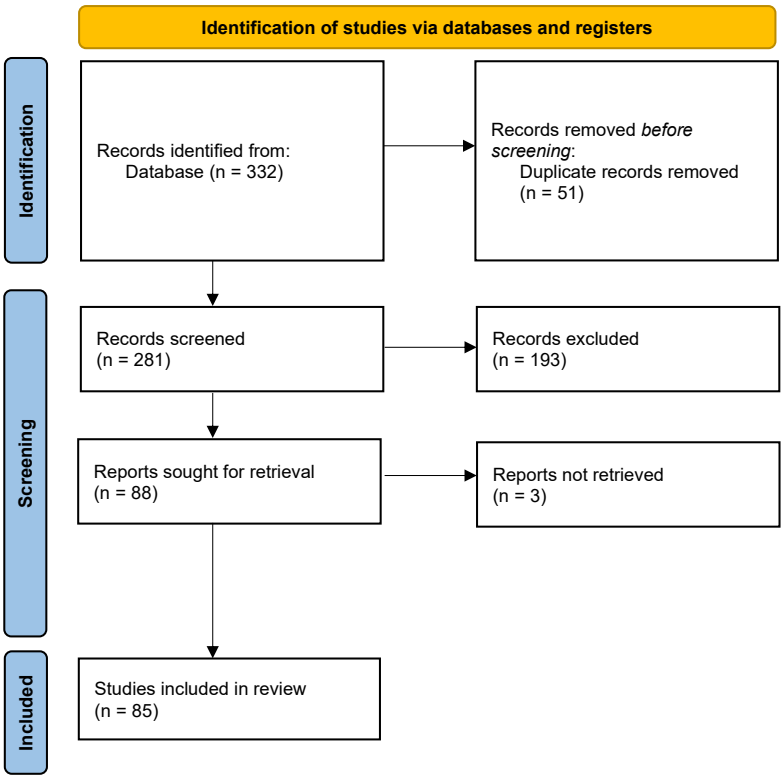


Figure 5: visualization of the literature research conducted. Official PRISMA flowchart template adapted from [Pag21a].

The specified branch is a more constrained version of the root for the other branches. It queries for papers on material simulation/modelling and quantum computing/annealing from the year 2000 onwards. The root query differs only in its description of material simulation, allowing the concatenated words to also appear separately. In addition to the root, the scale-based branches query for scale-related descriptors and associated methods. The exact queries are presented in appendix (A).

The count of relevant papers for each scale are:

- specified branch: 15
- sub-atomic branch: 21
- atomic branch: 19
- microscale branch: 22
- mesoscale branch: 3
- macroscale branch: 8

The following subsections aim to provide an overview of the current state of research in material modelling, while also presenting the information processed in Sec. (6).

5.1 Specified branch

The specified branch includes papers that fail to mention a specific scale in its title, keywords or abstract. It focuses on the general area of material simulation not tied to a specific scale for an initial overview.

With the most optimistic vision out of all of the papers in this review, the editorial by E. Osaba et al. emphasises the amount of progress already made in industrialising quantum computers [Osa25]. It is a review of five papers including a general overview from IBM and a paper attempting to solve classical simulation issues with quantum machine learning (QML) [Abu25; Eid25]. The focus of the five papers is mostly on QML in different applications [Osa25]. While E. Osaba et al. acknowledge the current NISQ era to need improvements before being able to be deployed at large scale, they argue quantum computers will soon enhance industries and scientific research [Osa25]. The three main aspects mentioned in this paper are:

- companies achieving higher qubit counts and laying groundwork for research about scalability
- frameworks that implement abstraction layers to enable code for quantum computers to be written in modern programming languages (e.g. python).
- existing approaches to mediate (part of the) current problems of the NISQ era (e.g. quantum-classical).

Higher qubit counts are deemed necessary by many other research papers and, together with noise, pose one of the greatest challenges of the NISQ era [Sel25; Cli24]. J. Selisko et al. present an approach for DFT together with DMFT simulations with a quantum-classical system [Sel25]. For this, up to 14

qubits from the quantum computers at IBM were used to simulate their proof of concept simulation of $Ca_2Cu_2Cl_2$. The classical computer handles most of the computations, forwarding only the impurity calculations of DMFT to the quantum computer. This impurity calculation is from the Anderson impurity model (AIM) DMFT works with and which is the major source of complexity in this simulation. The conclusion from this proof of concept simulation is the quantum computers accuracy being on par with classical approaches, but the scalability still remains a task for future work [Sel25].

The specialised framework ArQTiC presented by L. Bassman et al. is an open source software package for material simulation on quantum computers [Bas22]. The Architecture for Time-dependent Circuits (ArQTiC) library provides an interface to define the simulation parameters and essentially does not need prior knowledge about quantum computers to be used. It can handle the actual circuit generation by itself, but also offers manual construction of those. To adhere to the current diversity of backend implementations, ArQTiC can convert its programs to Qiskit, PyQuil and Cirq. These allow execution of the programs on the IBM (Qiskit), Rigetti (PyQuil) and Google (Cirq) quantum computers [Abu25; LaR19; Kar25]. The main features of ArQTiC's specialization are the two implemented algorithms used for many material simulation approaches:

- real-time Hamiltonian evolution
- imaginary-time evolution

As described in Sec. (2.2) calculating Hamiltonians are a major part of material simulation on quantum computers. Imaginary-time evolution is a way to find the ground state energy of a quantum system [Yi25]. This way of calculating the ground state energy of a quantum system is complex to implement on a low level [Bas22]. This originates from imaginary-time evolution not using unitary gates and thus needing an approximative approach on quantum computers [Bas22]. In summary, ArQTiC implements two common algorithms used in material simulation as well as providing a basis framework to work with quantum computers.

The work of J. Liu et al. optimizes a Variational Quantum Eigensolver (VQE) algorithm to reduce circuit depth to mediate the problem of short decoherence times in qubits [Liu24]. Across different scales, VQE has gained the most attention and was extensively used [Gha25; Lee22; Win23]. VQE is well suited for approximating the energy state of a quantum system [Har25]. The VQE method calculates the ground-state energy $\hat{E}_g$ by parametrizing the wave function Ψ from Schrödinger's equation (5) to solve:

$$\hat{E}(a^*) = \langle \Psi(a^*) | \hat{H} | \Psi(a^*) \rangle = \min_{a \in A} \langle \Psi(a) | \hat{H} | \Psi(a) \rangle, a \in A \tag{7}$$

With A being a subset of the Hilbert space [Guo25]. In this case, the Hilbert space describes the set of all possible states the quantum system can be in [You88]. The VQE can also be adapted to solve for energy states other than the ground-state energy [Guo25].

J. Liu et al. show that more accurate simulations can be achieved with higher parameter count [Liu24]. J. Liu et al. use perturbation theory to reduce the amount of parameters needed for calculating correlations of periodic materials [Liu24]. Perturbation theory is one option to approximate Schrödinger's equation [Liu24]. It works by incrementally applying a small change (perturbation) to a known starting state [Meh76]. In this case, a starting wave function $|\Psi_0\rangle$ which then converges toward the resulting state until the error falls below the maximum threshold [Liu24]. With their VQE-based algorithm that is optimized by multireference perturbation theory (MRPT), the convergence to an accurate result when using an increasing amount of parameters is greatly accelerated as seen in Fig. 6.

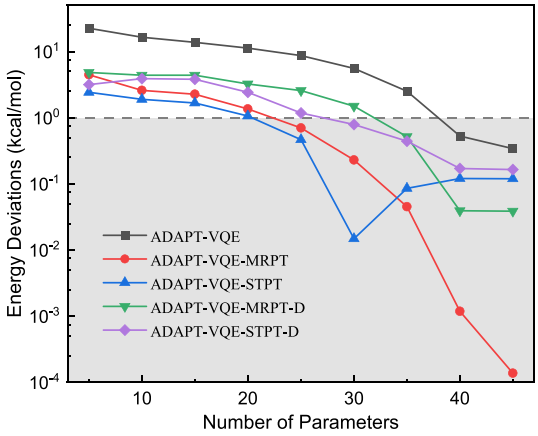


Figure 6: Energy deviations (ΔE = |E - E_{exact}| in kcal mol^{-1}) as a function of the number of variational parameters in the ADAPT-VQE and ADAPT-VQE-PT approaches for one-dimensional hydrogen chain. Figure and caption from [Liu24].

As access to quantum computers is restricted and costly, researchers rely on simulations of quantum computers instead of reserving computing time at providers [Alv25; Dev24; Cla23]. Simulators for quantum computers also allow for calculations with a manually defined amount of noise, helping the understanding of quantum advantage in the post-NISQ era [Dev24]. S. Devendrababu et al. use the VQE to simulate 1D and 2D lattices of the Fermi Hubbard Model on the Qiskit Aer estimator [Dev24]. The Hubbard model is a simplification of solids at atomic scale, representing the atoms in lattice like structures with limited movement options compared to the real world [Cel23]. This model is described by a Hamiltonian, making it a candidate for quantum material sim-

ulation of solids [Alv25]. While S. Devendrababu found their current implementation to need improvements, A. Alvertis et al. used a simulator to evaluate their approach with the extended Hubbard model with more promising results [Dev24; Alv25]. The latter emphasises the importance of further research and progress in the fault tolerance of quantum computers for reaching a state where quantum computing can compete with classical computing in some areas of commercial material simulation [Alv25].

5.2 Sub-atomic branch

DFT is the go-to method for sub-atomic material simulation [Ma20; Yao21]. It encompasses the most fundamental physical properties while keeping a feasible runtime [Sho22]. Researchers agree with that and compare their propositions to DFT, aiming for similar accuracy with significant speed up [Gha25; Har25]. S. Hariharan et al. present a wide variety of sub-atomic scale quantum algorithms applicable in the field of quantum chemistry [Har25]. The algorithms are grouped by suitability for NISQ-devices.

Algorithms that can only be deployed on fault-tolerant quantum computers are still waiting for those to exist in order to use their advantage proven by S. Hariharan et al. [Har25]. For now, the algorithms working on current quantum computers are prospect to elaborate research [Gha25; Aro25]. Not just VQE, but also the Variational Quantum Linear Solver (VQLS) and Quantum Space Estimation (QSE) are addressed by S. Hariharan et al. [Har25]. While QSE is the extension of VQE to handle more diverse energy states, VQLS works similar to VQE but performs approximations on linear systems instead [Har25]. S. Hariharan et al. argue that, in contrast to algorithms requiring fault-tolerant hardware, the near-term applicable algorithms offer no proven performance improvement [Har25].

In contrast to quantum algorithm research using DFT as their benchmark, other researchers decided to enhance DFT with quantum computing [Nie24; Ma20]. X. Nie et al. applies embedded DMFT to extend the accuracy of the more general DFT calculations [Nie24]. The results show that the limitations classical devices set on DMFT are possibly mediated by near-term quantum computing [Nie24]. H. Ma et al. directly substitutes the classical calculations of Schrödinger's equation with a quantum algorithm using quantum phase estimation algorithm and VQE [Ma20]. In agreement with S. Hariharan et al., H. Ma et al. did not find a speed up when using VQE [Har25; Ma20]. However, their approach promises scalability and applicability on near-term hardware [Ma20].

The general consensus of the quantum research towards DFT and sub-atomic modelling in general is a similar performance to classical computing on NISQ devices with some post NISQ-era algorithms proving to offer a significant speed up. Although the potential of increased performance is apparent in algorithms suited for fault-tolerant quantum computers, these are yet to be available [Ma20; Har25].

5.3 Atomic branch

Continuing with variations of DFT, N. Pollard et al. simulate small amounts of aluminium atoms for optimal structure with quantum embedded DFT [Pol25]. With the help of VQE, the hybrid DFT calculations by N. Pollard et al. found the optimum structure of aluminium clusters consisting of a range from three to eight aluminium atoms as well as gold clusters with four and 13 atoms respectively. The 13 gold atoms were not possible to compute on the IBM cloud service due to insufficient memory. With achieving accuracy in agreement with other studies with no significant speed up, N. Pollard et al. provide an important proof of concept method for metal analysis. The main takeaway is the limitation of the hardware regarding scalability of the algorithm [Pol25].

S. Rajasekaran makes use of the general understanding of quantum advantage by proposing an algorithm based on Grover's algorithm [Dho25]. The Grover's algorithm is one of the earliest examples of quantum advantage and is widely known in the quantum computing community [Gro96]. It is an efficient search algorithm, searching a binary array for ones in $O(\sqrt{N})$ iterations, offering a quadratic speed up over classical search algorithms [Gro96]. S. Rajasekaran et al. create an array which stores whether a pair of particles is close enough to interact with each other, tackling a classically computational large task of solving the close neighbour problem [Dho25]. With optimisations to the general algorithm around Grover's algorithm, S. Rajasekaran et al. found significant performance improvement compared not just to classical, but also already existing material simulation propositions to use Grover's algorithm in this way [Dho25].

A quantum annealing approach with a claimed million-fold speed up is presented by A. King et al. [Kin21b]. The paper compares classical Path-Integral Monte Carlo (PIMC) with Quantum Monte Carlo (QMC) and achieves significant speed up while matching accuracy. With mappings to the Ising model, the researchers extract the combinatorial quantum advantage from the D-Wave quantum annealers with up to 1440 qubits [Kin21b].

In general, researchers found improved performance while attaining accuracy compared to classical algorithms, including DFT and PIMC [Pol25; Kin21b]. In both gate-based quantum computing and quantum annealing, promising results with extensive speed up are demonstrated, which demonstrate the possibilities coming with improved hardware [Pol25; Kin21b].

5.4 Microscale branch

At microscopic scale, the simulations abstract to a mesh or lattice of atoms, allowing the Ising model to efficiently abstract at this scale [Kai20]. Due to the Ising model, introduced in Sec. (2.2), being solved efficiently by quantum annealers, research at this scale is predominantly on quantum annealers [Kin21a; End22]. The Ising model combines the advantage of the quantum annealer with

an efficient model of the microscale structure which can result in computation times of 0.8 to 2.5 seconds for a simulation that takes a state of the art classical algorithm more than 4000 seconds [End22]. As further backed by Fig. (7), quantum annealing shows great potential in this specific field of material simulation [San23]. Overall, this demonstrates that quantum annealing may become a powerful approach for microscale material simulations, where problems can be naturally expressed in an Ising framework [San23].

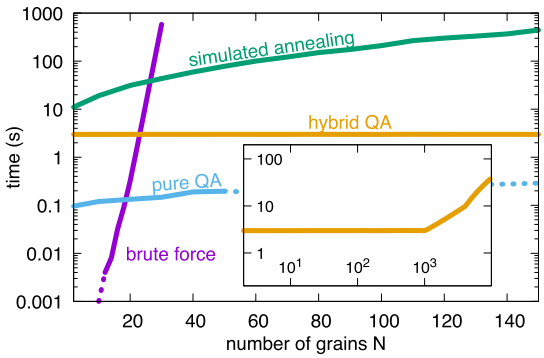


Figure 7: Elapsed computation time as a function of the number of grains. Different methods and algorithms are compared. Dashed parts of the QA curve belong to the regime of chain breaks. For large system sizes, only the hybrid quantum annealing approach remains feasible, showing an almost constant computing time need for less than 1000 spin variables (inset). Figure and caption from [San23].

Furthermore, the microscale branch offers insight into the effort that is put into quantum computing getting more accessible with the introduction of abstraction layers and material property databases to encourage more research towards quantum material simulation [Ser25; Win23]. V. Serhieiev et al. present a design for a higher level programming environment, to bring quantum computing closer to the current state of classical computing in terms of programming environments [Ser25]. In classical computing, the individual bit operations are long lost in the abstraction layers modern programming languages introduce. In contrast, the current leading programming environments provided by the manufacturers of quantum computers are heavily based on gate-based operations [Abu25]. The proposed architecture provided by V. Serhieiev et al. additionally encompasses a result visualization and a MC-based simulation engine [Ser25]. While talks with other researchers revealed interest in this kind of architecture, implementation of these is left for future work [Ser25]. In contrast, the Joint Automated Repository for Various Integrated Simulations (JARVIS) infrastructure is already being expanded to host information towards quantum computing algorithms [Win23]. JARVIS now includes the AtomQC package, consisting of VQE and Variational Quantum Deflation (VQD) algorithms for simulating solid

state materials [Win23; Cho21]. Both advances show interest in enabling a wider range of people to access and advance in quantum computing supported material simulation, which possibly results in an influx in research in this area [Ser25].

At the same time, research for microscopic scale material simulation also keeps getting limited by NISQ-era hardware [Lor21]. V. Lordi et al. also incentivise the use of material simulation for the modelling of novel qubit designs, which hints at an inter-dependency between the two areas [Lor21]. With more research in either area, the other can progress and open new research opportunities for cascading progress [Lor21].

5.5 Mesoscale branch

The area of mesoscale material simulation on quantum computers is lacking extensive research. The paper of R. Zheng et al. sees potential in the near-term [Zhe23]. Yet, the literature research did not provide any other relevant papers. R. Zheng et al. focus on the development of qubits instead of software. The paper specialises in increasing decoherence times by combatting dephasing. Dephasing is one way for the qubits to lose their information [Zhe23]. Phase changes happen through interactions with the environment and result in the change of values from α and β in Eq. (2) [Zhe23]. These interactions with the environment are amplified with excited states of qubits [Zhe23]. At the same time, R. Zheng et al. found enhanced many-body simulation capabilities from atoms in excited states. The states they address are called Rydberg states [Zhe23]. Rydberg atoms are highly susceptible to environmental changes, making them unfitting as qubits [Zhe23]. The solution proposed by R. Zheng et al. points a laser at the qubit, creating a Rydberg dressed state instead. A Rydberg dressed state is more resilient and still contains the beneficial properties towards entanglement for many-body quantum simulation [Zhe23].

5.6 Macroscale branch

The macroscale is dominated by research on quantum annealers and focuses on the finite element method [Suk25; Ngu24; Rai22]. As described in Sec. (2.2), quantum annealers are well suited for combinatorial problems. The topology optimization of structures, for example to minimize the needed material for a certain load on supporting beams, is one such problem. N. Sukulthanasorn et al. developed a framework on the quantum annealers from D-Wave for topology optimization problems [Suk25]. This method makes use of the Quadratic Unconstrained Binary Optimization (QUBO) model [Suk25]. The QUBO model is a diverse tool commonly used in the quantum annealing space [Glo19]. It is a NP-hard problem and can be adapted to solve many other NP-hard problems [Glo19]. The problem consists of a collection of binary variables $x_i \in [0, 1]$ that

construct a cost function with individual weights $a_{i,j} \in \mathbb{R}$:

$$y = x^t Q x \tag{8}$$

With x being the vector including all x_i and the values of cost function Q at line i and column j are $a_{i,j}$ [Glo19]. This cost function is then iteratively improved towards either minimizing or maximizing the output [Suk25]. The quantum-classical approach from N. Sukulthanasorn et al. performs the structural analysis on a classical computer, then lets QUBO handle the optimization and updates the topology to repeat this process until specified convergence criteria is satisfied [Suk25]. This proposition yields results with similar accuracy to the classical counterpart and is more efficient in terms of the raw problem [Suk25]. While classical computers currently outperform quantum annealers due to sheer size and no hybrid communication overhead, N. Sukulthanasorn et al. see near-term applications for topology optimization on quantum annealers.

QUBO is mathematically equivalent to the Ising model [Hus20; Ngu24]. Thus, it is logical to assume improved performance of modelling those on quantum annealers based on the research of N. Sukulthanasorn et al.. The work of V. Nguyen et al. and O. Raisuddin et al. confirms this by implementing FEM on quantum annealers using the properties of the Ising Hamiltonian [Ngu24; Rai22]. An Ising Hamiltonian is a Hamiltonian that describes a spin system, i.e. the Ising model [Ngu24].

While V. Nguyen et al. convert the Ising Hamiltonian directly to QUBO, O. Raisuddin et al. propose a more structured formulation of the finite element problem, embedding the governing equations into the QUBO framework through an energy minimization approach [Ngu24; Rai22]. Both methods enable the representation of FEM problems on quantum annealers by exploiting the binary nature of the Ising model, although they differ in how the physical constraints are incorporated into the optimization problem. The results of both works demonstrate that finite element formulations can be successfully mapped onto quantum annealing architectures. However, the scalability of these approaches remains limited by current hardware constraints, particularly in terms of qubit count and connectivity [Ngu24; Rai22; Suk25]. Additionally, the level of discretization achievable in practice is still below that of classical FEM implementations [Ngu24; Rai22; Suk25].

6 Discussion

The results of the literature research conducted using the PRISMA method now are evaluated in terms of the research question and its implications mentioned in Sec. (3). The Sec. (5) sorts the papers according to the scale of the aforementioned material simulation methods to group algorithms with similar approaches and provide an understanding of the requirements of each scale. This thesis mainly focuses on understanding the potential that quantum computers offer in the general area of material simulation. Consequently, the subsequent subsections are categorised according to the various potential improvements that quantum computers could offer. The possibilities and limitations described in these subsections rely on the information presented in Sec. (5) to provide an understanding of the intricacies of each scale separately, so that the potential of quantum computing can be evaluated as a whole. Nevertheless, properties tied to specific scales are mentioned as such.

6.1 Understanding the Quantum Advantage

As elaborated in Sec. (2.2), the properties of entanglement enable the exponential scaling of the state space with linear scaling qubit count. Along with the ability to encode material states in quantum states, which can represent quantum systems more naturally than classical representations, provides promising groundwork for material simulation as part of the quantum advantage. On the other side, the observation of the material state has become more challenging, as the observed states always collapse to the classical basis states, creating the need for several thousand shots to approximate the resulting behaviour of the simulated material [Hag24].

This aspect of quantum computing substitutes memory space with computational iterations. Algorithms such as Grover's or Shor's algorithm, two major examples for the demonstration of the quantum advantage, have been proven to provide quadratic or even exponential speedups compared to classical calculations [Gro96]. Assuming the algorithm takes advantage of compact material state implementation, this trade-off could improve both storage requirements and computation time. This is enabled by the fact that both the simulated system and the quantum computer are governed by quantum mechanical Hamiltonians between the simulated material properties and the qubit properties. Both are quantum systems with a Hamiltonian acting on them as explained in Sec.(2.2). The qubit Hamiltonian is influenced by gates, which allow tuning towards the quantum system to be simulated. Most researchers assessing quantum computing for material simulations on a low scale make use of this property with promising results [Yao21; Nie24].

The paper from J. Dhoriyani et al. also demonstrates that general research into the quantum advantage can be of great use for material simulation as well [Dho25]. In this paper, the quantum advantage of Grover's algorithm is suc-

cessfully adapted for use in material simulation. The proposition of J. Dhoriyani et al. has outperformed existing material simulation algorithms on a quantum computer, implying further possibilities beyond the initial wave of improvements involving the transfer of current knowledge of efficient classical computing into the quantum space.

Quantum annealing offers a fresh perspective on quantum advantage, as combinatorial problems are a part of quantum advantage exclusively for quantum annealing due to quantum tunnelling. While this mediates the advantage of implementing the Hamiltonians directly onto the qubits, the efficiency of solving equivalent problems to the Ising model is another source of quantum advantage that can provide decreased runtimes with advantageous scaling.

Still, researchers predominantly use gate-based quantum computing in the field of material simulation because it is more versatile and provides a clearer connection to material simulation than quantum annealing. Fig. (8) shows the type of quantum device used in the papers of the PRISMA research. With a clear difference in quantity, gate-based quantum computers provide more possibilities to display quantum advantage in the material simulation landscape.

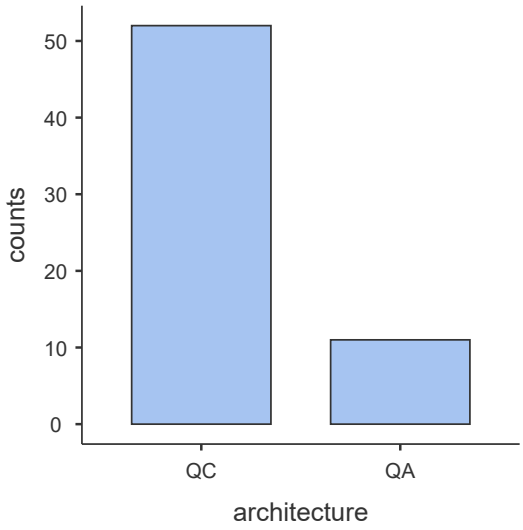


Figure 8: gate-based Quantum Computer (QC) and Quantum Annealer (QA) usage in the papers from the PRISMA literature research according to criteria mentioned in Sec. (4.2). Created with jamovi [Lov26].

6.2 Framework

Just like at the start of classical computers being commercialised, quantum computers from different companies are currently addressed differently and have distinct architectures. IBM, Google, Rigetti and many others have their own programming language to address their quantum computers [Ser25]. V.

Serhieiev et al. are creating another layer above those to enable individuals to work with all quantum computers while only learning one language as elaborated in Sec. (5.4) [Ser25]. However, frameworks like the project of V. Serhieiev are not yet widely available, nor do they provide the level of abstraction and convenience found in classical programming languages. Circuit creation is comparable to the low-level computer language Assembly, requiring detailed knowledge of the underlying hardware and its constraints. This creates a significant barrier to entry, particularly for researchers from application domains such as material science, who are primarily interested in modelling physical systems rather than the specifics of quantum hardware.

As is apparent in classical computing, frameworks that introduce higher levels of abstraction help immensely in lowering the barrier of entry, allowing researchers originating from other areas to adapt performant systems without needing to understand the full intricacies of highly complicated devices. In quantum computing, higher levels of abstraction specifically mean automatic circuit generation, hardware-independent code and consistent interfaces for creating programming languages comparable to modern classical ones.

In the near-term, many frameworks focus on hybrid quantum-classical algorithms, such as the VQE, which are specifically designed to combat the noise in current-era NISQ devices [Yos24; Fan21; Yao21]. While these approaches improve the feasibility of practical near-term applications, they often introduce additional computational overhead and do not fully realise the theoretical quantum advantage.

Consequently, frameworks play a crucial role in making quantum computing more accessible and enabling greater participation in research. While researchers are already beginning to implement higher levels of abstraction, further research is required to develop these into mature, widely adopted programming frameworks. For material simulation in particular, however, the ability to implement the quantum system's Hamiltonian directly must be preserved. This, however, does not increase the barrier of entry, as researchers who benefit from using these frameworks are also required to understand the concept of Hamiltonians in general when implementing material simulation algorithms on classical computers.

6.3 Accuracy

Researchers looking to exploit quantum advantage in material simulation have a wide range of established classical methods as a point of comparison. As a result, classical simulations currently serve as the primary benchmark for evaluating the performance and accuracy of quantum approaches, particularly since most industrial applications still rely on those.

A central challenge for accuracy in quantum computing lies in the indirect estimation of physical observables, as already discussed in Sec. (6.1). When assuming fault-tolerant quantum computers, the physical process on the qubits

themselves in principle provides an exact representation of the quantum system that is simulated to the accuracy of our current fundamental physical understanding of the behaviour of particles, through e.g. Schrödinger's equation. The approximation of this representation through shots is the main point of lost accuracy. While increasing the number of shots improves statistical accuracy, it also introduces additional computational overhead. With polynomial scaling of shots in relation to the simulated system's size to retain the same accuracy, even a polynomially scaling algorithm that will then be executed $O(N^x)$ times with a fixed x for statistical accuracy still is significantly more efficient than an exponentially scaling algorithm.

The assumption of fault-tolerant devices is not a near-term perspective. However, near-term possibilities with accuracies competing with a classical benchmark are provided by researchers [Sel25; Sch22]. The inaccuracies NISQ devices introduce can be mediated by the use of frameworks, like the VQE. This shows sufficient accuracy on NISQ devices is possible with the computational trade offs regarding time and circuit size efficiency.

Fig. (9) illustrates that quantum annealers currently do not provide a noticeable improvement in accuracy compared to classical approaches. Their advantage primarily lies in computational speed and in more reliably finding optimal or near-optimal solutions through quantum tunnelling, as discussed in Sec. (5.6).

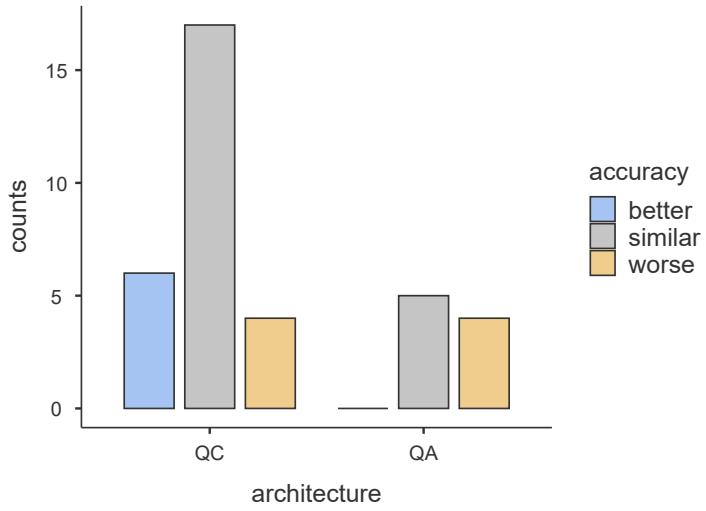


Figure 9: Accuracy of an algorithm based on the architecture (gate-based Quantum Computer (QC) and Quantum Annealer (QA)) used in the papers from the PRISMA literature research according to criteria mentioned in Sec. (4.2). Created with jamovi [Lov26].

For the combinatorial problems considered, the solutions themselves are exact within the given formulation. Therefore, the overall accuracy is not limited

by the optimization process, but by the underlying models used to represent the material system. In other words, the quality of the results depends on how well the physical system is approximated, rather than on the solver used to compute the solution.

Consequently, while quantum computing holds promise for achieving desired accuracy, retaining similar results as classical simulations, significant hardware improvements are needed to be a candidate for real world applications.

6.4 Efficiency

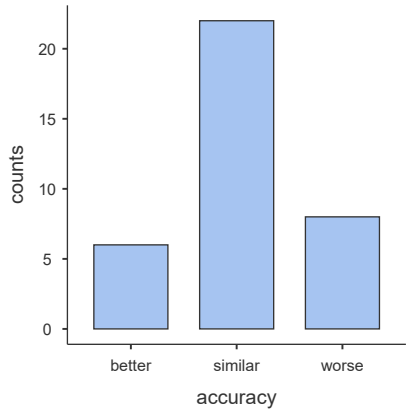
Regarding speed of computation, the quantum annealers seem to offer the most drastic improvement in the near-term. One reason for this is the specialization of quantum annealers towards combinatorial problems. This property not only simplifies research by testing whether the problem at hand can be adapted to be of advantageous structure for quantum annealing, but also allows the devices to be improved towards one specific case. The advantage of quantum tunnelling drastically reduces computation time, as demonstrated by existing research [Suk25; San23]. The million-fold speed up mentioned in Sec. (5.3) should still be considered with a degree of scepticism. The statement of the annealer performing the task three million times faster at a specific configuration is backed by empirical evidence, but only shows a part of the whole picture. The majority authors of the paper claiming this speed up are or have been employed by the currently leading quantum annealer manufacturer, D-Wave, leading to an interest in presenting the annealer as advantageous as possible [Kin21b]. Still, other researchers have also found computation times decreasing by multiple orders of magnitude, which still leads to the conclusion of quantum annealers being a promising contender to host material simulation algorithms in the future [Ngu24; End22].

On gate-based quantum computers, the story is less apparent. Many algorithms optimize the design of the Hamiltonian and trade accuracy for a decrease in computation time, but the performance boost is mainly considered to be the reduced memory overhead when storing material properties. Widely adapted algorithms for performing material simulation calculations are designed to run on noisy hardware and thus focus on error correction and maintaining the desired state. VQE and other algorithms of that class have not provided a performance boost, instead solely allowing the calculations to reliably work on quantum hardware. In comparison, algorithms like the Harrow-Hassidim Lloyd (HHL) algorithm, that are designed for fault-tolerant quantum computers, offer exponential speed up over classical counterparts [Har25].

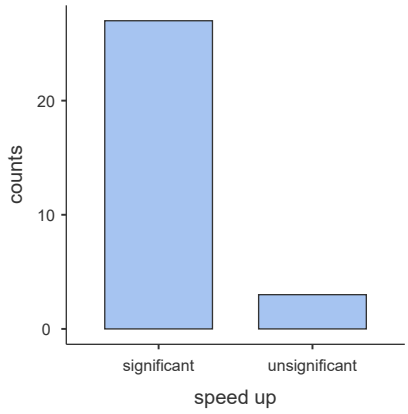
Another increase in computation efforts emerges from the hybrid approach. Currently, quantum computers can not handle independent execution of full simulations as they rely on classical computers for error mitigation as well as pre- and post-processing. Although the communication overhead has not been

a major concern in current research, it is a property that should be considered when choosing an approach for a novel algorithm, in the era post NISQ-devices, this property could play part in the decision of the architecture.

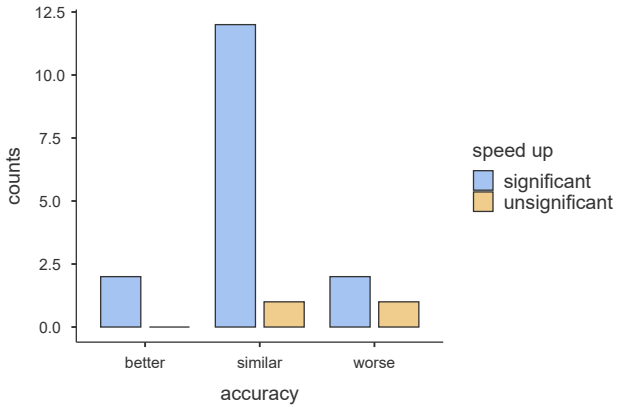
With the data acquired from the literature research (Fig. 10), algorithms that offer performance boosts as well as an increase in accuracy in comparison to classical state of the art implementations already exist. From a software point of view, the quantum computing space provides some near-term methods matching classical counterparts in performance and accuracy, but lacking in scale due to hardware constraints.



(a) Accuracy of the evaluated algorithms



(b) Speed up of the evaluated algorithms



(c) Speed up of the algorithms sorted by the accuracy

Figure 10: The speed up and accuracy of the simulation algorithms used in the papers from the PRISMA literature research compared to classical counterparts according to criteria mentioned in Sec. (4.2). Graphs created with jamovi [Lov26].

6.5 Scalability

The most prominent problem with quantum computing is the lack of fault-tolerant hardware. As seen throughout earlier sections in this Discussion, the software backed with many proof of concept implementations is ready to be deployed at scale. The computation power of modern NISQ devices is lacking scalability, as proof of concept simulations often bring the quantum hardware accessible to the researchers to its limits [Pol25]. IBM is working on delivering its first fault-tolerant quantum computer with 200 qubits in 2029, according to their current roadmap [IBM26]. This will be a major step towards near-term applications, but likely not enough to justify real world applications.

A much more promising progress is being made in the area of quantum annealing. The current largest quantum annealer consists of 5616 qubits from the manufacturer D-Wave [Osa25]. Researchers have already simulated several hundred grains on smaller annealers and stated the current possibility to simulate several thousands [San23]. For small projects and simulations, renting computation time on a quantum annealer may be a near-term perspective with real world applications.

In general, the fact that quantum hardware will not be available to buy commercially in the near future is to be taken into account, leading to a high demand on limited hardware. While both gate-based quantum computing as well as quantum annealing have promising near-term capabilities, these will not be available to the needed extent to process simulations at scale.

6.6 Reliability

Even though the takeaway from the majority of papers over the different scales is an improvement in efficiency while atleast retaining classical accuracy, improvements in time constraints, which are often tailored for quantum advantage, are lacking due to the need for error correction and other imperfections in NISQ-era hardware. Although these error ranges do not hinder accuracy to the extent of large deviations in results, the achieved results are noticeably off compared to quantum hardware simulations with zero errors.

Towards consistency and reproducibility, quantum computers approximate simulation results in a different way than classical computers, as elaborated on in Sec. (2.2). Still, classical simulations also work with approximations and across the literature research, papers have consistently shown to atleast match the classical results of algorithms deemed sufficient for replacing real world experiments.

With IBM promising fault-tolerant hardware in the near future, the era of noisy and faulty quantum computers slowly comes to a close [IBM26]. The possibilities emerging from post NISQ-era devices are widely regarded as the first quantum devices with potential for real-world applications [Har25; Abu25]. Still, as mentioned in the preceding Sec. (6.5), this hardware will not be avail-

able for widely adapted use in the near future. Instead, this development is a good foundation for further research to achieve long term results.

Gate-based quantum computing is not yet ready to handle programs, especially multi-scale simulations, on its own. Quantum annealers, on the other hand, are generally not suited for independent use, but already show significant performance improvements in the area of combinatorial problems. The first step of quantum advantage appearing in commercial use will likely be an embedded quantum-classical algorithm that only forwards the critical sections to the quantum computer and processes the majority of the program still on classical computers. This prediction is based on the current state of research towards efficient software, together with the apparent lack of scalable and reliable hardware and its availability.

7 Conclusion

This thesis conducts a literature review after the PRISMA method towards quantum computing in the material simulation field. The goal of which is to assess near-term possibilities of adopting quantum computers for real world applications. The work concluded that limited access to quantum computers, especially fault-tolerant versions is the leading limitation regarding progress in this area, as researchers have shown promising software implementations already.

On most separate scales, real possibilities of the quantum advantage showing have been identified. Smaller scales profit more off of the quantum computing characteristics, making use of the similarities of the qubit structure being similar to the quantum systems to be modelled. Several algorithms on both the quantum annealers and the gate-based quantum computers have proven to provide an exponential speed up compared to state-of-the-art classical methods. The application of quantum computing in mesoscale material simulation has yet to be studied sufficiently to make a concluding remark, yet the lack of research in this area can also indicate the absence of quantum advantage possibilities on that scale. On the macroscale, existing combinatorial problems are optimal for a quantum annealer, which already showed a significant improvement on the microscale as well.

In terms of multi-scale simulations, quantum computers are not currently able to handle these themselves due to resource constraints regarding both memory and computation power. The lack of hardware currently leads to focusing the existing performance on the most critical parts, letting classical computers handle the management and coordination around the major computation tasks. Now and for the foreseeable future, quantum computers are embedded into classical computers and act only as a computation instance instead of complete systems due to heavy resource constraints. Thus, the performance of quantum computers may be used in separate methods of a multi-scale approach supervised and managed by the classical embedding system.

As IBM has plans on launching their first fault-tolerant quantum computer this decade, the research on post-NISQ algorithms gains in importance in finding and testing more simulation methods to use the quantum advantage to the full extent. For quantum computing to reach the first companies and be accessible on a wider scale, however, the amount of hardware needs to increase significantly. This will most likely not happen in the near-term, as big challenges in development remain, making the quantum advantage a promising prospect for material simulation, but remaining theoretical until solutions to these hardware problems are found.

List of Symbols and Abbreviations

Abbreviation	Term
ArQTiC	The Architecture for Time-dependent Circuits
DFT	Density Functional Theory
DMFT	Dynamic Mean Field Theory
FEM	Finite Element Method
HHL	Harrow-Hassidim Lloyd
JARVIS	Joint Automated Repository for Various Integrated Simulations
MC	Monte Carlo
MD	Molecular Dynamics
MRPT	Multireference Pertubation Theory
NISQ	Noisy Intermediate Scale Quantum
PIMC	Path-Integral Monte Carlo
PRISMA	Preferred Reporting Items for Systematic reviews and Meta-Analyses
QMC	Quantum Monte Carlo
QSE	Quantum Space Estimation
qubit	quantum bit
QUBO	Quadratic Unconstrained Binary Optimization
VQD	Variational Quantum Deflation
VQE	Variational Quantum Eigensolver
VQLS	Variational Quantum Linear Solver

Symbol	Description
$CNOT$	CNOT-gate
$\hat{E}$	Energy of the system
H	Hadamard gate
$\hat{H}$	Hamiltonian
X	Pauli-X gate
Y	Pauli-Y gate
Z	Pauli-Z gate
$\Psi(x,t)$	wave function of a quantum system

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Appendices

A PRISMA Queries

The relevant Scopus operators are to interpret as:

- AND/OR: analouge to the logic operators.
- TITLE-ABS-KEY: the following term is to appear in the title, abstract or as a keyword in the paper.
- <word>*: this word is to appear as a prefix to any continuation.
- PRE/<number>: the following term is to appear up to <number> words after the preceeding term.
- PUBYEAR < 1999: the paper is released after 1999.

The queries have a joined branch:

```
(
 (
  TITLE-ABS-KEY(material) AND
  (
   TITLE-ABS-KEY( modelling ) OR
   TITLE-ABS-KEY( simulat* )
  )
 )
AND
```

```
 (
   TITLE-ABS-KEY ( NISQ ) OR
   (
    TITLE-ABS-KEY ( quantum PRE/0 ( computer* OR
                      algorithm OR annealing ) )
   )
  )
) AND PUBYEAR > 1999
```

where each branch specific query is inserted with an ”AND” into the outtermost brackets.The branching subqueries are:

```
(
 TITLE-ABS-KEY ( density functional theory ) OR
 TITLE-ABS-KEY ( DFT ) OR
 TITLE-ABS-KEY ( first principle ) OR
 TITLE-ABS-KEY ( first-principle ) OR
 TITLE-ABS-KEY ( sub-atomic )
)
```

for the sub-atomic scale,

```
(
 TITLE-ABS-KEY ( atomic-scale ) OR
 TITLE-ABS-KEY ( nano-scale ) OR
 TITLE-ABS-KEY ( molecular dynamics )
)
```

for the atomic scale,

```
(
 TITLE-ABS-KEY ( micro* ) OR
 TITLE-ABS-KEY ( DDD ) OR
 TITLE-ABS-KEY ( discrete dislocation dynamics ) OR
 TITLE-ABS-KEY ( phase-field ) OR
 TITLE-ABS-KEY ( monte carlo )
)
```

for the microscale,

```
(
 TITLE-ABS-KEY ( meso* ) OR
 TITLE-ABS-KEY ( continuum dislocation dynamics ) OR
 TITLE-ABS-KEY ( CDD ) OR
 TITLE-ABS-KEY ( crystal plasticity ) OR
```

```
 TITLE-AbS-KEY ( cellular automata ) OR
 TITLE-ABS-KEY ( grain-scale ) OR
 TITLE-ABS-KEY ( polycrystalline )
)
```

for the mesoscale,

```
(
 TITLE-ABS-KEY ( macroscale ) OR
 TITLE-ABS-KEY ( FEM ) OR
 TITLE-ABS-KEY ( finite element method ) OR
 TITLE-ABS-KEY ( finite element ) OR
 TITLE-ABS-KEY ( finite method ) OR
 TITLE-ABS-KEY ( continuum )
)
```

and for the macroscale. The last branch is a more specified version of the root. The aim of this query is to incorporate those papers that did not include any scales in the title, abstract or keywords, yet still match the scope of this thesis. This branch is not inserted into the root, but serves as a whole query itself.

```
(
 TITLE-ABS-KEY
 (
  material PRE/0 ( modelling OR simulat* )
 )
 AND
 (
   TITLE-ABS-KEY ( NISQ ) OR
   (
    TITLE-ABS-KEY ( quantum PRE/0 ( computer* OR
                      algorithm OR annealing ) )
   )
  )
) AND PUBYEAR > 1999
```

B Use of Artificial Intelligence for this thesis

This thesis limits the use of artificial intelligence to the following aspects:

- ChatGPT assisting in:
  - finding LaTeX commands and notation.
  - understanding of different topics.

  - structuring of the text.

- DeepL Write assisting in:
  - fixing spelling and grammar mistakes.
  - translation.
  - extending vocabular and formal speech.

ChatGPT is used in Sec. (4.2) and Sec. (6) to provide recommendations for improving of the structure of the written text. DeepL Write is used throughout the whole thesis to prevent spelling and grammatical errors and ensure formal language.

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