Exploiting Quantum Power Flow in Smart Grid Co-Simulation

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***Abstract*—Our electricity infrastructure is getting more complex and heterogeneous. Holistically analyzing grids is therefore increasingly challenging. Co-simulation, i.e. the coordinated execution of independent subsystem simulators, is inherently well suited to handling these challenges. However, the computational needs of calculating power flows within the simulated grid may limit the scalability for large-scale co-simulations. Recent advances in quantum computing offer a potential solution to these concerns: The computing paradigm‘s potential for exponentially speeding up power flow has been shown. To utilize these capabilities for smart grid simulations, we propose quantum–classical co-simulation: integrating simulators running on quantum hardware with an otherwise classical co-simulation. Specifically, we focus on exploiting quantum power flow in smart grid co-simulations. This concept is promising for applications that require comprehensive grid simulation and whose scalability is impeded by the computational properties of power flow. This paper highlights the concept of quantum–classical co-simulation, and advocates for its criticality and applications in supporting smart grid analytics. We encourage and facilitate research by recommending a five-item research roadmap. We also provide a detailed discussion on the potential obstacles in implementing this concept, to help bring its theoretical value to practice.**

***Index Terms*—quantum–classical co-simulation, power-system simulation, quantum computing, distributed simulation**

I. Introduction

Major global trends are affecting power grids. Driven by the need for reduced emissions and changing consumer expectations, we are seeing an increase of intermittent renewables, the rising proliferation of distributed energy resources, and the growing electrification of transport, just to name a few. In order not to compromise their resilience and reliability, grids are becoming more interwoven with information and communications technology (ICT) for pervasive monitoring and automated control, transforming them to smart grids [1].

The heightened complexity of grids makes comprehensive simulation necessary for the in-depth analysis, dependable operation, and strategic planning of our electricity infrastructure. As Palensky *et al.* put it: ‘Simulation is fundamental in power engineering‘ [2, p. 34]. However, simulating smart grids holistically is challenging due to their nature as systems of systems. A simulation paradigm that deals inherently well with these challenges is co-simulation [3], where a coupled system is simulated by coordinating stand-alone simulations of its subsystems [4]. For example, a power-system co-simulation may contain independently developed simulation models for the power grid, electric-vehicle charging, and household consumption (see Figure 1b)).

As grid simulations become more comprehensive and the need for repeated simulation runs increases (e.g. for different contingency scenarios [5]), so does the required computational capacity. One way to tackle this challenge is distributed and parallelized co-simulation; however, further research is needed to realize this potential fully [2], [6]. Particularly, the computational demand of calculating the flow of power in the simulated grid—i.e. power-flow analysis—makes frequent simulation runs of large grids expensive [7]. Therefore, accelerating power-flow analysis by improving its computational scalability could have a significant impact on making complex and comprehensive smart grid simulation tasks tractable.

Quantum computing may provide the solution. It is a novel computing paradigm that exploits quantum-mechanical effects for information processing. In theory, quantum computers promise exponential speed-up for many fundamental computational problems [8]. Studies indicate great promise in utilizing this new way of computing to tackle challenges in various application domains [9]; among them is power-systems

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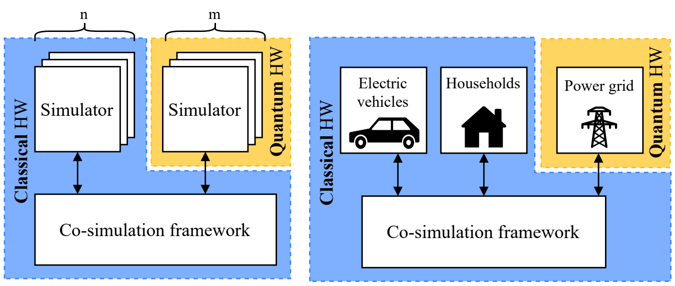

(a) Architectural concept

(b) Example of co-simulation with quantum power-flow simulator

Fig. 1: Quantum–classical co-simulation

engineering, as surveyed by Ullah *et al.* [10] and Golestan *et al.* [11]. Importantly, the feasibility of quantum DC [12] and AC [13] power flow has been demonstrated—with the potential for substantially enhanced scalability.

We propose combining the strengths of quantum computing and co-simulation for power-systems applications. We encourage interdisciplinary research to realize this potential. This paper's contributions towards that goal are:

1) Introducing *quantum–classical co-simulation*: one or more simulators of an otherwise classical co-simulation are executed on quantum hardware (see Figure 1a).
2) Highlighting the option of using quantum power flow in smart grid co-simulations for improved scalability.
3) Laying out five essential research items composing a near- to mid-term research roadmap.
4) Identifying and analyzing obstacles for the feasibility and utility of quantum–classical co-simulation.

Although quantum computing has great potential in various areas, it is likely not suitable for all simulators. Consider the example in Figure 1b: Only the expensive power-flow simulator is run on quantum hardware, whereas the less demanding simulators are executed on classical computers. Quantum–classical co-simulation allows using the appropriate computing paradigm for each subsystem. Consequently, no simulators must be unnecessarily adapted for quantum hardware, and no simulators, for which efficient quantum implementations are available, are constrained to classical hardware. This approach is attractive for application scenarios that:

1) require (or significantly profit from) co-simulation due to the complexity and heterogeneity of the involved subsystem simulators, and
2) suffer from the particularly high computational demand of one or a few simulators that could be sped up on quantum hardware (e.g. large-scale power flow).

Examples that meet these criteria are electric-vehicle grid integration, contingency analysis, and distribution-grid management. They require considering heterogeneous aspects, such as renewable generation, driver behavior, and weather events. Therefore, various research projects have applied co-simulation to such tasks (see [14] for an overview). Often, many simulation runs are required to assess different scenarios adequately. For large-scale grids, the computational cost of power-flow analysis may become prohibitive. Hence, superior scalability would facilitate conducting more comprehensive and detailed simulation studies.

II. Background

This chapter provides basic background in three areas and presents the respective state of the art: First, we give a high-level insight into quantum computing. Second, we briefly introduce power-flow analysis and discuss how it can be performed with quantum computers. Third, we explain co-simulation and highlight the simulation paradigm's significance for smart grid analysis and validation.

A. Quantum Computing

A quantum computer is 'a device that leverages specific properties described by quantum mechanics to perform computation' [15, p. 3]. Quantum computers work in a fundamentally different way than classical—i.e. non-quantum—computers. In classical computers, the basic unit of information is the bit, while quantum computers use the quantum bit, or *qubit*, in short. Whereas a bit is in exactly one of two states, a qubit can be in a *superposition* of two basis states:

$$|\psi\rangle = \alpha\,|0\rangle + \beta\,|1\rangle\,, \tag{1}$$

$$\text{where} \quad |0\rangle = \begin{pmatrix}1\\0\end{pmatrix} \quad \text{and} \quad |1\rangle = \begin{pmatrix}0\\1\end{pmatrix}. \tag{2}$$

One of the fundamental interpretations of the coefficients, $\alpha,\ \beta \in \mathbb{C}$, is that their square corresponds to the probability of a measurement resulting in the corresponding basis states. The sum of all probabilities must therefore yield 1—see Born's rule in (3).

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

The surface of a complex unit 2-sphere, a so-called Bloch sphere (see Figure 2), represents all possible states of one qubit; the two antipodes represent the basis states $|0\rangle$ and $|1\rangle$, respectively.

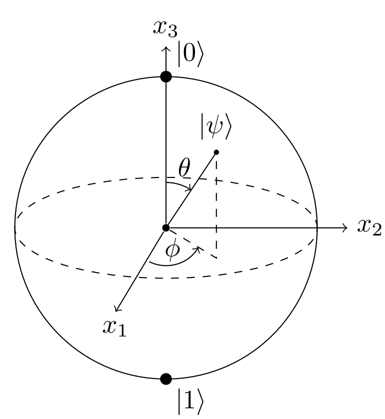

Fig. 2: Representation of quantum state $|\psi\rangle$ in the Bloch sphere.

Superposition, together with the non-classical phenomena of *entanglement* and *tunneling*, allows for computation that exceeds classical capabilities. These properties are exploited in either general-purpose gate-based quantum computation, or optimization-focused quantum annealing. Furthermore, there are hybrid quantum–classical algorithms that leverage the respective strengths of quantum and classical computing resources [16]. Quantum computers can potentially improve the scalability of various fundamental computational problems exponentially [8]: for example, integer factorization, database search, and solving linear systems of equations. The latter was achieved using the HHL algorithm [17] and is particularly important for our work.

B. Quantum Power Flow

As one of the fundamental power-systems problems, power-flow analysis is critical for the operation, control, and planning of grids [12]. In a power-flow study, the goal is to determine the voltage angle and magnitude for each bus and the flow of real and reactive power in each line [18]. To achieve this, the active (4) and reactive (5) power balance equations for each node must be solved:

$$P_i = \sum_{k=1}^{N} |V_i||V_k|(G_{ik}\cos\theta_{ik} + B_{ik}\sin\theta_{ik}), \tag{4}$$

$$Q_i = \sum_{k=1}^{N} |V_i||V_k|(G_{ik}\cos\theta_{ik} - B_{ik}\sin\theta_{ik}), \tag{5}$$

where P_i and Q_i are the net injection at bus i of active and reactive power respectively, N is the number of buses, $|V|$ is the voltage magnitude, $\theta_{ik} = \theta_i - \theta_k$ is the voltage-angle difference between bus i and k, and G and B are the real and imaginary parts of the bus admittance matrix. Since the AC power-flow equations are non-linear, approximative numerical methods are employed, such as the Newton–Raphson method which is widely used for power flow. One starts with an initial estimation that is iteratively refined using linear approximations. Alternatively, the non-linear AC power flow can be simplified to linear DC power flow if three asumptions are made [19]:

- small differences between voltage angles,
- negligible line resistance, and
- flat voltage profile.

Applying these simplifying assumption to (4) and (5) yields the DC power-flow equation:

$$P_i = \sum_{k=1}^{N} B_{ik}\theta_{ik} \tag{6}$$

which results in a system of equations to determine the vector of voltage angles $\boldsymbol{\theta}$ based on the vector of active-power injections $\mathbf{P}$. Just as in (4) and (5), the matrix $\mathbf{B}$ describes node-to-node susceptances; keep in mind that since line resistances are negleted, each susceptance b becomes $b = -1/x$, where x is the reactance between two nodes. Assuming $\mathbf{B}$ is invertible, the system of linear equations can be written as:

$$\mathbf{P} = \mathbf{B}\boldsymbol{\theta} \iff \mathbf{B}^{-1}\mathbf{P} = \boldsymbol{\theta}. \tag{7}$$

The voltage angles are then used to compute the line flows. In contrast to AC power flow, DC power flow is linear and can therefore be solved directly and much faster.

Solving both, AC and DC power flow, boils down to solving systems of linear equations—either for iterative approximations (AC) or directly (DC). Therefore, the aforementioned HHL algorithm can be used to solve power flow on quantum computers. To be more precise, we can use it to approximately prepare a quantum state $|\theta\rangle$ that we can query for information on $\boldsymbol{\theta}$. The fastest classical algorithm for this task—the conjugate gradient method—has a time complexity of $\mathcal{O}(N)$, whereas HHL theoretically achieves $\mathcal{O}(\log N)$. Eskandarpour *et al.* [12] have demonstrated the feasibility of using the HHL algorithm to solve DC power flow. This approach was later expanded by a hybrid quantum–classical approach by Gao *et al.* that promises comparable precision with a reduced number of qubits [20]. Moreover, Feng *et al.* [13] use a variant of the Newton–Raphson method together with an augmented version of the HHL algorithm for a quantum solution method to general AC power flow; their approach was experimentally analyzed by Sævarsson *et al.* [21]. Even though the HHL algorithm provides exponential speed-up in theory [22], there are major caveats that limit its practical utility and impede scalability [23].

C. Smart Grid Co-Simulation

In a co-simulation, multiple models with different representations and runtime environments are jointly executed [24]. Therefore, modeling can be done on the subsystem level 'without having the coupled problem in mind' [24, p. 516]. Simulators can either be coupled to each other bilaterally, or to a central orchestrating framework that synchronizes the simulators and handles the data exchange between them [25]. We are focusing on the latter—orchestrated co-simulation—as it simplifies the simulation architecture when dealing with a larger number of simulators [26].

Recent years have seen a surge in research on co-simulation. Hafner and Popper [27] give an overview of the state of the art, and Gomes *et al.* [4] provide a survey focused on technical aspects. Even though co-simulation itself is not limited to an application domain, a lot of research centers on power systems [28]. An empirical analysis of smart grid co-simulation can be found in [29] and a comprehensive literature review in [14]. Moreover, Palensky *et al.* [2] provide an extensive primer on co-simulation with a focus on its application for ICT-heavy power grids. Due to the need for sophisticated synchronization and data-exchange capabilities, co-simulation is often done with the help of frameworks. One important aspect of such frameworks is their compatibility with established standards, two of the most important are the High-Level Architecture (HLA) that facilitates the reuse and interoperation of simulations [30], and the Functional Mock-Up Interface (FMI) which focuses on the interchange of dynamic models for co-simulation [31].

Finally, we must differentiate the proposed concept of quantum–classical co-simulation from what is sometimes called *quantum co-simulation* in literature. The term refers to the co-simulation of a quantum processor together with its controlling classical hardware [32]. Whereas these projects focus on simulating quantum computers, we focus on using quantum computers as a platform to execute simulation models.

III. Proposed Research

So far, we have argued for the value of quantum–classical co-simulation and the potential of quantum power flow for making some smart grid co-simulation tasks computationally tractable. However, much research—at the intersection of power-systems engineering, co-simulation, and quantum computing—is needed to realize the latent value for academic and industrial applications. We propose five near- to mid-term research items. In Figure 3, they are assigned a relative position to eachother on a timeline.

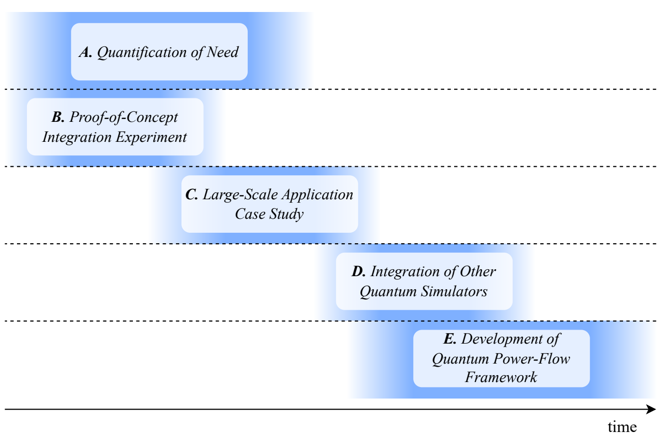

Fig. 3: Proposed near- to mid-term research.

A. Quantification of Need

So far, we have discussed the need for quantum–classical co-simulation in qualitative terms. However, this need is rooted in computational performance, making it inherently quantifiable. Therefore, it should be thoroughly quantified to what degree certain applications are limited by the scalability properties of classical power-flow computation. Specifically, the focus ought to be on applications that take advantage of the co-simulation paradigm. The research should reveal which applications need quantum–classical co-simulation and to what extent. Additionally, research should assess at what scale the improved scalabiltiy of quantum algorithms is needed.

B. Proof-of-Concept Integration Experiment

The feasibility of integrating a quantum-based simulator with an orchestrated co-simulation needs to be tested. First, a small-scale experiment is sufficient to assess the concept. A small exemplary grid with only a few interacting systems may be used—for example, the 3-bus or 5-bus systems used in [21] or the WSCC 9-bus system used in [12]. Besides being a proof of concept for the proposed approach, such experiments should a) assess the impact of the obstacles discussed later in Section IV, and b) serve as an explorative basis to uncover further issues. At this stage, performance evaluation is not a priority. The performance advantage of most quantum algorithms lies in their scalability; therefore, we do not expect speed-up in small-scale test scenarios.

C. Large-Scale Application Case Study

After an initial proof-of-concept demonstration, one can move on to larger and more realistic scenarios. The study of technical integration aspects should be extended by a thorough examination of application scenarios. For example, a simulation environment with a quantum power-flow simulator could be exploited to conduct a contingency analysis of the simulated grid. At this stage, performance comparison is appropriate: A co-simulation using classical power flow is to be compared with one using quantum power flow. The focus of the performance assessment must be primarily on scalability. The absolute performance heavily depends on the quantum hardware available (and accessible) at that time and is therefore secondary to scalability analysis. This implies that experiments must be conducted at multiple scales (e.g. grid sizes) to adequately judge scalability.

D. Integration of Other Quantum Simulators

Thus far, we have focused on one application of quantum–classical co-simulation: using quantum power flow in smart grid co-simulations. However, other subsystems could also be simulated on quantum computers, either using gate-based approaches or quantum annealing. As hardware and platforms improve, the classical-to-quantum transition is likely becoming easier and less time-consuming. There are various subsystems that could take advantage of better scalability: Numerous power grid applications need computationally expensive optimization, such as unit commitment. Also, advances in quantum machine learning are highly promising, such as quantum reinforcement learning [33]. The latter approach could be combined with the concept proposed in [3] to train reinforcement-learning agents in smart grid co-simulations.

E. Development of Quantum Power-Flow Framework

Current implementations of quantum power flow are at an early, experimental stage. However, complex real-world projects require an easy-to-use refined implementation of power-flow analysis. The emerging fields of quantum software engineering [34] and quantum software architecture [35] provide guidelines, principles, and best practices—among them the Talaverna principles [36]—for crafting robust high-quality quantum software. The simulator must be usable as a configurable black box. One should be able to integrate the quantum simulator into a smart grid co-simulation without in-depth knowledge on quantum computing. This would enable transitioning various smart grid co-simulation projects from classical to quantum power flow. Therefore, a dependable and interoperable quantum power-flow framework should be developed, analogous to classical frameworks such as open-source software MATPOWER [37]. The development will likely hinge on the experiences and results of the feasibility study (Section III-B) and the large-scale case study (Section III-C).

IV. Obstacles

Exploiting the potential benefits of quantum–classical co-simulation, specifically using quantum power flow for smart grid simulation, comes with difficulties. We have compiled a non-exhaustive list of obstacles for the feasibility and utility of the concept.

A. Cloud-Based, Distributed Co-Simulation

The distributed execution of an orchestrated co-simulation itself is challenging, particularly when dealing with cloud resources [2], regardless whether quantum computing is involved. The technical realization itself is not problematic; many co-simulation frameworks offer suitable programming interfaces. However, the overhead and latency introduced by networking is challenging. For frequent communication between distant simulators, these factors may prove detrimental to performance, thus negating the advantage of parallelized execution. Hence, simulators with frequent and comprehensive data exchange should be executed on the same machine [2].

Furthermore, using cloud-based quantum computing introduces problems similar to other high-demand shared computing resources. There may be significant wait times associated with a computing job. Since every time step creates a computing job, the compounded idling time would be unacceptable for co-simulation. It is therefore necessary to find platforms that allow queuing up only once before the simulation starts, with little to no idling afterwards.

B. Quantum Encoding and Information Extraction

Alongside the execution of a quantum algorithm, there are two other key aspects of quantum computing: encoding the classical data before the computation, and extracting information afterwards [38]. These operations pose a threat to performance and can negate the positive effects of an efficient quantum algorithm. Consider a power-flow simulator running on quantum hardware and communicating with other simulators: Frequent data exchange requires a proportional number of quantum-encoding and information-retrieval steps. This overhead may destroy the quantum advantage. Consequently, this could induce constraints on how frequently a quantum simulator communicates with other simulators.

In addition to the number of encoding and retrieval steps, there is the challenge of their respective complexity. Particularly, when dealing with an algorithm that promises sublinear complexity, even operations that scale linearly with the problem size compromise any quantum advantage. With HHL, for example, retrieving all components of the solution vector would take at least $\mathcal{O}(N)$ steps [17]. Therefore, an efficient method for extracting a subset of information is required.

C. Hardware Limitations

Various challenges and obstacles surrounding quantum computing relate to hardware. For quantum–classical co-simulation—specifically for quantum power flow—we deem two to be especially noteworthy: First, the effect of noise, caused by various external influences [39], can be detrimental to a quantum power flow computation [21]. If it runs as part of a co-simulation, it could consequently threaten the validity and stability of the entire coupled simulation. As of now, we are in the era of noisy intermediate-scale quantum computers [40] and therefore have to find ways to address this noise. However, we want to note that Bertels *et al.* [41] suggest that some research should be based on assuming perfect, noise-free qubits to prepare the appropriate algorithms and methods for once hardware is sufficiently advanced. The second hardware-related challenge we need to highlight is the lack of quantum random access memory (QRAM) (as described in [42]). Some algorithms rely on efficiently storing and accessing intermediate result: Golestan *et al.* [11] point out that the AC quantum power flow approach by Feng *et al.* [13] cannot provide a quantum advantage without QRAM. A hardware aspect that likely has a comparatively small impact on quantum power flow is the number of available qubits, since the number of required qubits scales logarithmically with system size [21].

D. Tool Interoperability

Co-simulation is usually performed with frameworks for synchronization and data exchange; they provide interfaces for coupling various simulators (for an overview, see [43]). Similarly, applied quantum computing also strongly hinges on tools: platforms from major software vendors—such as IBM, Google, and Microsoft—allow for higher-level programming using libraries for well-established languages. A comparison of available quantum-computing platforms can be found in [10].

Since both, co-simulation and quantum computing, rely on tools in practice, integrating a quantum-based simulator with a co-simulation requires the respective tools be interoperable. Interoperability benefits significantly if the chosen quantum platform is compatible with the widely-established co-simulation standards HLA and FMI.

V. Conclusion

We introduce the novel concept of quantum–classical co-simulation to tackle smart grid simulation challenges. With quantum–classical co-simulation, only the constituent subsystems that need quantum speed-up and for which an efficient quantum solution exists are run on quantum computers; the remaining simulators are executed on classical hardware. We highlight the potential of exploiting quantum power flow to improve the computational scalability of large-scale power-systems co-simulations.

In this paper, we encourage and facilitate research at the intersection of power-systems engineering, co-simulation, and quantum computing to realize the potential value of quantum–classical co-simulation in practice. We propose five short- to mid-term research items, from preliminary proof-of-concept experimentation to reusable software solutions. Furthermore, we identify and analyze four likely obstacles to the efficient realization of the proposed concept: networking overhead, quantum encoding and information extraction, hardware limitations, and tool interoperability. The next step in our research endeavor will be conducting an experimental study to determine the feasibility of the concept; we will verify the conjectured list of obstacles and potentially expand it.

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