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Computing for power system operation and planning: Then, now, and the future

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ABSTRACT

With the global trend of pursuing clean energy and decarbonization, power systems have been evolving in a fast pace that we have never seen in the history of electrification. This evolution makes the power system more dynamic and more distributed, with higher uncertainty. These new power system behaviors bring significant challenges in power system modeling and simulation as more data need to be analyzed for larger systems and more complex models to be solved in a shorter time period. The conventional computing approaches will not be sufficient for future power systems. This paper provides a historical review of computing for power system operation and planning, discusses technology advancements in high performance computing (HPC), and describes the drivers for employing HPC techniques. Some high performance computing application examples with different HPC techniques, including the latest quantum computing, are also presented to show how HPC techniques can help us be well prepared to meet the requirements of power system computing in a clean energy future.

KEYWORDS

Power system computing, high performance computing, quantum computing, contingency analysis, state estimation, dynamic simulation, machine learning, optimization, exascale computing.

Power systems have been relying on modeling and simulation for operation and planning since their inception over a century ago. Computing hardware and software technologies are the foundation for such modeling and simulation. Power systems used to be at the forefront of computing applications among engineering domains until the modern multi-core computing era. Given the increasing complexity and more demanding computing needs, it is time to review and recast how power system applications can and should benefit from the latest computing advancements including classical and quantum computing.

Clean energy and decarbonization has become a global target as countries across the world are committed to battling climate change. For example, in the United States, the power generated by renewable energy sources accounted for about 20% in 2021. This share is expected to increase significantly in order to achieve its clean energy goal—net-zero greenhouse gas emissions no later than 2050. Similar trends can be found in European countries which set emission targets to substantially reduce greenhouse gas emissions. In China, the installed renewable energy capacity reached 1063 GW in 2021, accounting for 44.8% of China's total power generation capacity.

With more and more renewable energy resources deployed in the power system at such a fast pace, power system computing is also evolving at an unprecedent rate. First of all, the size of power systems to be modeled is increasing, to account for the growing load demand, increasing renewable penetration and smart technology deployment, and higher reliability and better asset utilization. Secondly, the complexity of power system modeling and simulation is increasing. In addition to the size of models, the model complexity is also increased, especially when dynamic models for inverter-based resources (IBRs), electric vehicles, storage, wind/solar generators are considered. These new power system elements make the power system more dynamic and more distributed. Thirdly, the uncertainty brought by renewable energies and other active devices makes the power system more challenging to analyze: the power system is transferring from a deterministic way to a probabilistic one, significantly increasing the number of scenarios to be studied, the complexity of algorithms, and the difficulty to interpret simulation results to power system operators/planners who are used to the deterministic environment. Last, but not least, co-simulation and co-optimization are needed for energy ecosystem analysis.

All the above challenges will generate more complicated data characteristics: larger volume, higher speed, faster dynamics, and deeper heterogeneity from multiple domains. These challenges pose new requirements for faster computing techniques that can help get power application solutions much more quickly, for larger, more complicated, more dynamic problems (requiring faster responses) with higher uncertainty, in order to provide faster and better decision support for better power system reliability and resiliency. High performance computing (HPC) is one of the fundamental technologies in meeting these computational requirements. HPC involves advanced mathematical theory, parallel programming, and computational hardware to drastically improve the capability of data analytics, modeling, and computational complexity.

This paper provides a historical review of power system computing, discusses HPC technology advancements, and describes the drivers for HPC applications. Some HPC application examples with different HPC techniques, including the latest quantum computing, are also presented to show how HPC techniques can

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help us be well prepared to meet the requirements of power system computing in a clean energy future.

1 Historical review of power system computing

The power system since its inception over a century ago has been relying on computing for its design, planning, and operation, and more so as the power systems across the world are evolving to be larger and more complex in transitioning to clean energy supporting a decarbonized economy. The power system is considered the largest machine that human beings have ever made. Experiments on such a huge machine are extremely limited. Modeling and simulation powered by computing have been critical in understanding power systems. In the meantime, computing used by power systems has also evolved significantly over the past century. We divided them into five generations, enabling higher performance power system applications every 30–40 years, as shown in Figure 1.

The first generation of computing in power systems was manual calculation using sliding rules in the 1890's, when the power system was just invented and deployed in London, UK, New York, NY, and other parts of Europe and America. Sliding rules seem to be rudimentary compared with today's computing technologies, but they were important for power flow and short circuit studies—the computing tasks commensurate with the needs in power system design and deployment at the time.

The second generation of power system computing was analog computers in the 1930's, which were needed to study power system stability issues in a much larger power system, in addition to larger power flow and short circuit studies. Those analog computers are essentially miniature power systems by scaling down the voltage and current levels in an affordable lab setting with reconfigurability for studying a wide range of systems and scenarios.

In the 1970's, the arrival of digital computing significantly drove up the scale and complexity of power system computing. It was in this era of the third generation of power system computing when several major digital simulation tools for power systems were developed and still widely used today together with new tools for extensive power system simulation capabilities. Power system applications were expanded to include complex optimization and real-time capabilities for power systems and market operation. In the following 30 years or so, power system computing applications had taken the advantage of rapid advancements in the computing industry following Moore's law. For example, the clock speed of computer processor hardware was improved more than 12 times over a decade time (1997–2007) from about 300 MHz to almost 4 GHz. The computational speed of the same software codes and tools for power system applications was increasing automatically by simply upgrading the computers. Power system software developers were able to focus on power system functionality without much attention to how the computing was done in the computing hardware and the operating systems.

This free ride continued to the early 2000's, when the computing industry was undergoing an unprecedented transition from single-core processors to multi-core processors, as Moore's law reached its ceiling. This was the beginning of the fourth generation of high-performance power system computing[1]. Computer processor trending over half a century is shown in Figure 2[2]. These modern high-performance computers continue to provide increasing computational performance by using multi-core processors. However, the conventionally designed software codes and tools in a sequential computing mode including those for power system applications would still run on a single core and could no longer automatically take the advantage of such performance improvement. Power system software developers need to consider parallelizing the codes and managing data movement when writing codes to fully utilize multi-core computers. New software packages such as GridPACK™ (https://www.gridpack.org/) emerged to relieve the burden on power system engineers by encapsulating low-level parallelism and hiding the details, to enable power system engineers to continue focusing on power system functionality instead of being overwhelmed by computing details. GridPACK has extensive modules to support many applications including power flow calculation, state estimation, contingency analysis, and transient stability simulation. It provides fine-grained parallelism for multi-core computers and also offers a computational task manager for coarse-grained parallelism for distributed memory computers such as high-performance computer clusters. Today, many power system simulation tools offer parallel computing capabilities in various degrees. It should be noted that modern power systems need computing power from modern high-performance computers and thus the transition from sequential computing to parallel computing is imperative for power system applications. Narrower operating margins, growing system sizes,

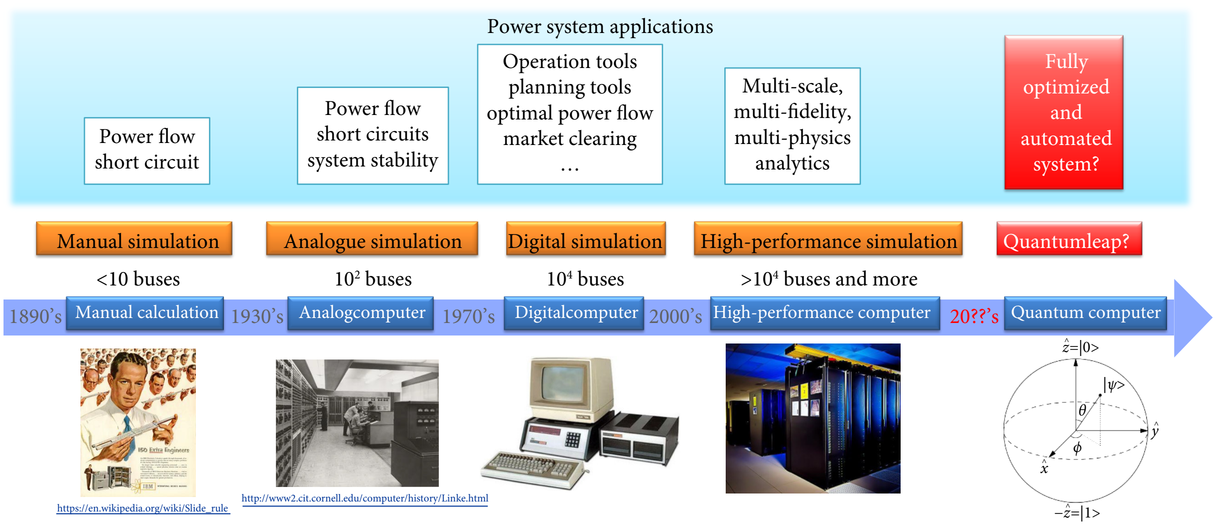

Fig. 1 Power system applications evolving with computing advancements, addressing the increasing complexity in power system planning and operation.

resilience against extreme events, new dynamics, and larger uncertainties in renewable energy and smart grids all require better and faster computation. Plus, power systems have increasing interdependency with other systems including communications systems, gas-pipeline systems, transportation systems, and building systems further require HPC to enable multi-scale, multi-fidelity, and multi-physics analytics.

Looking forward and beyond today's modern high-performance computers, quantum computing is emerging with promises to revolutionize computing and thus important for a potential fifth generation of power system computing. Though the physical principles of quantum computing have been discovered since the invention of Schrodinger equations, its implementation has taken decades of dedicated efforts from physicists and computer scientists. Quantum computing is still in its early stage, but several usable noisy quantum computers such as those offered by IBM (https://www.ibm.com/quantum) are available for domain application developers. Early trailblazers in power systems already attempted to use quantum computing to solve challenging power system optimization problems at small scales. Given the projected larger scale development of quantum computers, it holds a promise for a possible future of fully optimized and automated power systems in a decade or two if the historical power system computing cycle of 30–40 years would repeat.

In the remainder of this paper, we will further discuss computing advancements and power system computing needs and examples.

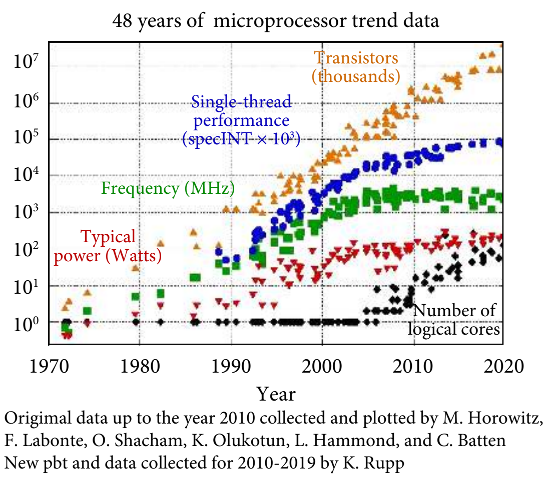

Fig. 2 Computer processor trending over half a century. Reprinted with permission from ref. [2] © Karl Rupp 2020.

2 Technology advancements in high-performance computing

High performance computing (HPC) can utilize parallel processing techniques and large computing resources to perform multiple tasks simultaneously and/or complete time-consuming tasks quickly. Through years of development, HPC technology has made significant advancements, from shared-memory computers, cluster computers, to cloud computing. And the quantum computing technique is expected to play an important role in the near future.

2.1 Shared memory computers

Shared memory computing leverages shared memory architectures to execute instructions in parallel on multi-core CPUs or many-core GPUs. A multiprocessor shared memory computer is a computer system that has more than one processing unit (PU), each sharing a global memory address space with global accessibility and visibility as shown in Figure 3.

One advantage of shared memory computing is the fast and uniform data sharing and its resultant user-friendly programming perspective to memory. The primary disadvantage lies in the lack of scalability between memory and processing units. Data synchronization between each processing units also must be explicitly managed to ensure data integrity during concurrent accesses. Common Application Programming Interfaces (APIs) that support multi-threaded programming for shared memory computing include OpenMP, Pthreads, CUDA, OpenACC in Fortran, C, C++, Java, Python, etc., with different levels of abstraction and ease of programming[3].

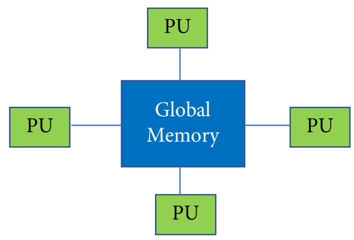

Fig. 3 Shared memory architecture.

The authors have developed a parallel power system dynamic simulation application in ref. [4] using OpenMP on shared-memory Superdome machine to enable look-ahead dynamic simulation to study pending stability problems in the power system, a novel multi-threaded application on Cray XMT system in ref. [5] to compute parallel betweenness centrality for critical power system contingency selections, and a thread group multithreading mechanism using Pthreads in ref. [6] to accelerate the computation of an agent-based power distribution system modeling and simulation tool—GridLAB-D (https://www.gridlabd.org/).

2.2 Distributed and cluster computing

Distributed and cluster computing overcomes the scalability limitation of shared memory computing by leveraging aggregated computing power with dedicated memory space together. A distributed memory computer and at its larger scale, a high-performance cluster, is a group of computing nodes that are connected through a high-speed low-latency communication network. All nodes have their own memory address space and cannot directly see another's. Explicit inter-processor communication must be defined to enable data exchange and information sharing through the communication network as shown in Figure 4.

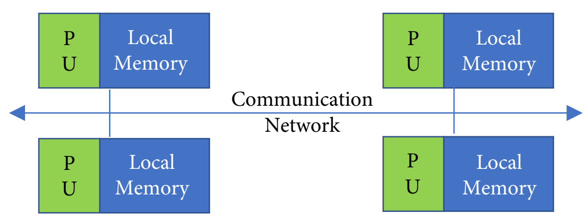

Fig. 4 Distributed memory architecture.

The significant advantages of distributed and cluster computing are scalable memory and cost effectiveness. The primary disadvantages are the non-uniform memory access times and data communication overhead. MPICH (https://www.mpich.org/) and OpenMPI (https://www.open-mpi.org/) are the two most popular implementations of the message passing interface (MPI)[7] standard to enable multiprocessing for distributed and cluster computing.

OpenSHMEM (https://www.openshmem.org/) even built a shared memory abstraction on top on a distributed memory architecture.

The authors have developed counter-based dynamic load balancing schemes using MPI in ref. [8] or massive power system contingency analysis on over 10,000 cores, a system architecture prototype in ref. [9] using low-level transmission control protocol (TCP) sockets to realize distributed power system state estimation on HPC clusters, an MPI-based real-time path rating calculation tool in ref. [10] for congestion management with high penetration of renewable energy, and performed a study in ref. [11] on comparative implementation of HPC for power system dynamic simulations on shared-memory vs. distributed-memory environments.

2.3 Hybrid distributed and shared memory computing

Hybrid parallelism blends distributed and shared memory parallel programming within one single context. It offers performance advantages common to both distributed and shared memory computing by conducting message passing between interconnected nodes and shared memory programming inside a single node as shown in Figure 5.

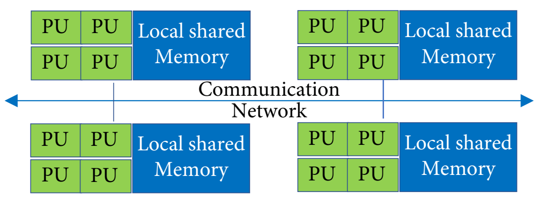

Fig. 5 Hybrid memory architecture.

Various combinations of distributed and parallel computing APIs exist (e.g., MPI+OpenMP, MPI+CUDA, OpenMP+OpenACC, etc.) as hybrid parallelism continues to prevail in HPC-based scientific and engineering application development. The authors have implemented an OpenMP+OpenACC based hybrid parallel power system dynamic simulation application on multi-core CPU and many-core GPU architecture and observed significant floating-point acceleration through CPU–GPU interoperation in ref. [12].

2.4 Cloud computing

Cloud computing is to have the on-demand availability of computer power and data center on the internet to allow users to perform work “remotely”, rather than on a local computer/server. The computing machine can be a shared-memory computer, a cluster or a hybrid one. Users can use the same configuration (files, applications, machines) from any device at any location. It becomes more and more popular in the power industry recently mainly due to its relatively easy management and maintenance, as well as configurable computing resources, which could be geographically distributed, for different types of applications with very reasonable cost. For example, the features and benefits of a cloud-hosted event-driven serverless architecture requiring low cost and maintenance effort are discussed through a use case of power grid emergency generation dispatch at ISO-New England (https://doi.org/10.1016/j.ijepes.2020.106366).

A recent IEEE Power & Energy Society task force report (https://arxiv.org/abs/2108.00303) provides a good summary of the business drivers, challenges, guidance, and best practices for cloud adoption in power systems, discusses the challenges and risks of utilizing cloud computing for power systems’ dairy needs, and provides some real-world use cases of cloud technology in the power industry.

In fact, a complex workflow that consists of cluster machines and cloud computing, and other advanced techniques, such as edge computing, can be a new solution to meet the requirement for more complicated applications. For instance, local cluster machines can be used to execute applications that need to be completed very fast while their outputs can be sent to cloud computing for further processing, leveraging the on-demand capability provided by cloud.

2.5 Quantum computing

Quantum computing is a developing computation technique based on quantum theory to utilize the various quantum states (superposition, interference, and entanglement) for computation. With these quantum states, a quantum bit (qubit), the basic information unit of quantum computing, can encode much more information than a classical two-state bit. This leads to the biggest advantage of quantum computing: exponential speedup over all classical computers and significant enhancement to artificial intelligence and machine learning (AI/ML) technologies.

Classical computers perform computation through the use of logic bits, where a bit is either 1 or 0. Quantum computers, however, leverage certain quantum mechanical phenomena for computation where a qubit can represent a mixture of 1 and 0 at the same time. By allowing particular linear-algebra operations over these mixed states, quantum computers can demonstrate exponentially increased parallelism when increasing the number of qubits. Despite being promising, quantum computing has its limitations and is believed to be only suitable for certain algorithms.

The past five years see the realm of quantum computing swiftly approaching solving practical problems. As a landmark, Google has demonstrated quantum supremacy on a 72-qubit superconducting Bristlecone testbed. IBM released its 128-qubit machine this year and announced the ambitious roadmap on building 1000-qubit hardware by 2023. Platforms based on alternative quantum technology, such as traped-ion and photonics, are also accessible through cloud service. The hardware advancements are accompanied with the rapid development of software stack (e.g., Qiskit (https://qiskit.org/), QDK (https://docs.microsoft.com/en-us/azure/quantum/overview-what-is-qsharp-and-qdk), and Cirq (https://quantumai.google/cirq)), services, and the ecosystem. These suggest the feasibility and probably urgency of examining and exploring quantum computing for power systems at this time frame.

There are several aspects quantum computing can contribute to in building the next-generation resilient, reliable, and secure power system. This includes (i) effectively solving optimization problems, which are ubiquitous in power system scheduling and planning, with polynomial or even exponential speedups; (ii) rapidly training and tuning large-scale machine learning models for power system prediction, as many of such tasks are already reliant to data-driven approaches; (iii) substantially enhancing power system cybersecurity through more secure and reliable quantum cryptography and communication.

Existing research regarding quantum computing for the power system is still in the very early stage and mostly focuses on how to adapt existing quantum algorithms for power system purposes. Given the limitations on qubit volume and fidelity of present noisy intermediate-scale quantum (NISQ) devices, quantum-classical hybrid algorithms emerge as the most promising applications for the first-generation quantum computers, this includes quantum approximated optimization algorithm (QAOA) for discrete combinatorial optimizations[13,14], the Harrow–Hassidim–Lloyd (HHL) algorithm for solving high-order sparse linear equations[15], quantum annealing for mixed-integer programming[16], variational quantum algorithms for quantum machine learning[17,18], etc.

Power systems would be a good domain to identify applications that can show the advantage of quantum computing, such as optimization, cascading failure analysis, uncertainty quantification, and AI/ML applications.

3 Drivers for high performance computing applications in power systems

With the increasing complexity of power system modeling and simulations, the main drivers for high performance computing techniques become clear: the increasing spatial scale, increasing temporal scales in power system computing, and increasing uncertainties in power systems.

3.1 Increasing spatial scales of power system computing

Power system management has progressed to the point where the boundary lines between transmission and distribution, operations and planning are becoming blurred. The widely deployed distributed energy resources (DERs), (networked) microgrids, and other devices are not only making impact on distribution systems, but also impact transmission in an aggregated way. To manage the whole power system efficiently, they would need to be considered organically, especially when there are disturbances. The dynamic behavior of inverter-based resources brings pressures of incorporating the predictive capability from planning to enhance operations as well. These needs are requiring a better integrated interplay between transmission and distribution, planning and operations[19,20].

Besides the interaction within power systems, the interactions between the power system and other systems cannot be ignored in the energy ecosystems. For example, extreme event analysis needs help from climate/weather, electric vehicle needs transportation analysis, and natural gas is tightly coupled with power system generations and load consumption, not to mention the importance of communication system in the power system, see Figure 6.

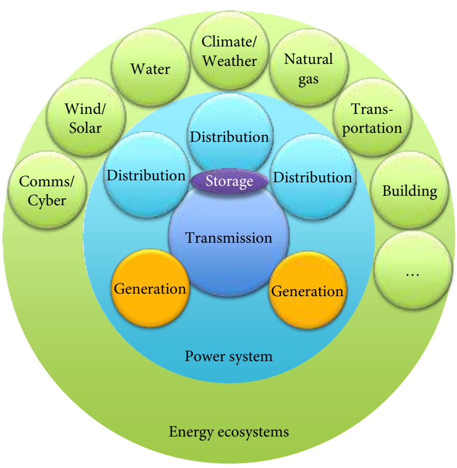

Fig. 6 Energy ecosystems require comprehensive studies on interactions among multiple energy sectors.

3.2 Increasing temporal scales of power system computing

The temporal scales of power system computing are also increasing. With inverter-dominated dynamics becoming more significant, the electromagnetic transient (EMT) study is in the time scale of microsecond, the traditional power system dynamic simulation (electromechanics) is in the time scale of millisecond, steady-state power flow type of applications is in the time scale of seconds/minutes, while the time scale for market application ranges from minutes to days. To study long-term analysis of climate change impact, the time scale will be years and decades.

The increasing temporal scales require faster computing speeds in order to help users quickly capture system behavior, analyze data, and make quick response to high dynamic grids, in addition to the computational need for fast co-simulations between different applications at different time scales.

3.3 Increasing uncertainties in power systems

With the increasing penetration of renewable energy resources, in addition to widely spread dynamic loads, the high uncertainties are aggregated from renewable, load, and even contingency. This change may make the solution that comes from deterministic approaches non-optimal, incomplete, and even worse, wrong. Therefore, advanced (collective) uncertainty quantification algorithms are required for quantitative characterization and assessment of uncertainties to help perform power system studies with renewable integration for applications such as reliability, optimization, and planning study.

In additional to the complexity brought by the uncertainty quantification algorithm, typically a much larger size of representative scenarios is required to study, in order to get better probabilistic based results. This also requires the power of HPC to accelerate the simulation process.

4 Examples of high performance computing applications in power systems

There are many researchers working on the area of HPC applications in power systems. For example, a computational platform for dynamic security assessment (DSA) of large electricity grids is presented in ref. [21] with a case study of the French grid with over 8000 scenarios and 1980 contingencies. A GPU-based massive-thread electromagnetic transient simulation was presented in ref. [22], while a cloud-based EMT simulator with an automatic code generator is presented in ref. [23]. A review paper of ref. [24] presents more HPC applications and trends for the smart grid that further shows the need of HPC technology for the future power system. This paper will focus on the applications that the authors have been working on as examples to show the power and the need of HPC techniques.

4.1 State estimation

Power state estimation (SE) is used to estimate system states (bus voltage and phase angle) based on supervisory control and data acquisition (SCADA) measurements. It is based on the assumption of quasi steady-state. The outputs of SE are used for many subsequent analyses, such as contingency analysis, optimal power flow, and dynamic security estimation. For power system operators, the faster awareness of the power system's real-time status, the more time for them to take actions to maintain system reliability for various conditions, especially when there are significant disturbances in the system.

A parallel state estimation (PSE) algorithm, based on a parallel linear solver and portioning techniques, has been developed by the authors which enables sub-second SE solution time using the real western U.S. power system model and measurements. This provides a better possibility to minimize the impact of contingencies. For example, Figure 7 shows the event intervals during the

September 8th, 2011 pacific southwest blackout. When the event interval is less than the ability to respond, there is a cascading effect, expanding the impact of disturbances. Traditionally, a SE runs every 20–30 seconds, which is not sufficient for grasping real-time condition, especially when there is a significant change. The sub-second PSE performance equips operators with the latest power system status, more opportunities to stop the cascading failure earlier [25,26].

4.2 Dynamic state estimation

Power system dynamic state estimation is to estimate the generator's dynamic states, such as rotor angle/rotor speed, to capture the synchronized wide area dynamic behaviors, i.e., state variables change with time. The application relies on phasor measurement units (PMUs) and the corresponding communication infrastructure. Considering the penetration of renewable energies and DERs, dynamic state estimation becomes critical for system transient stability and frequency stability. It is foundational for real-time stability assessment of complex power systems, as shown in Figure 8.

Various Kalman filter techniques including ensemble Kalman filter (EnKF) have been used by the authors to develop dynamic state estimation algorithms and implemented in an HPC environment[27,28].

4.3 Contingency analysis

Contingency analysis is used to assess the vulnerability of a power system. It is a what-if study: what the new system status is if one or more system elements fail. It is required by NERC operation standard. The parallelization of contingency analysis simulation is equivalent to solving multiple power flow problems with very little communication between each contingency. It is a task-level parallelization because each power flow is a sequential run due to its fast computational speed. Therefore, the challenge is the design of load balancing scheme, i.e. to achieve optimal computational time balance among all cores. A massive contingency analysis function with a dynamic load balancing scheme based on an automatic fetch counter has been developed. A near linear speedup performance on 10,240 cores has been reported in ref. [8].

Dynamic contingency analysis is to perform dynamic simulation for a set of contingencies. Unlike running a power flow, the dynamic simulation itself is a time-consuming process. Each individual dynamic simulation needs to be parallelized for fast computational speed. Thus, a two-level task manager, i.e., in addition to task-level parallelization (for contingencies), a group of cores can be assigned to each individual dynamic simulation for optimal speedup, shown in Figure 9. An example of dynamic security assessment using a two-level task manager is shown below. More detailed information can be found in ref. [29].

4.4 Transient simulation

Transient simulation (or dynamic simulation) is to study the power system's dynamic behavior and response in case of large system disturbances, e.g., a sudden change in generator or load, or a network short circuit followed by protective branch switching operations. Modeling the system dynamics (e.g., generator rotor angles and speeds) and network (e.g., bus voltage magnitudes and phase angles) relies heavily on the computationally intensive time-domain solution of numerous deferential and algebraic equations (DAEs). Speeding up dynamic simulation toward fast or faster-than-real-time simulation, through parallel and scalable solution of the DAEs, is not only to transient stability assessment itself, but also a series of subsequent applications that stem from it, e.g., dynamic contingency analysis, real-time path rating, and online security assessment, etc.

The DAEs can be solved alternatively or simultaneously with explicit or implicit integration. An alternating method with an explicit integration approach (alternating-explicit) has been implemented by the authors in ref. [30] where the first-order differential equations are discretized, allocated to, and updated in parallel on different computing processes through a customized 2nd modified-Euler (ME) integration, and the algebraic equations involving significant sparse matrix operations and linear system solutions are also accelerated through parallel implementations.

A simultaneous method with an implicit integration approach (simultaneous-implicit) has also been developed by the team in refs. [31] and [32] where the differential equations are converted to algebraic equations, lumped together with the original algebraic equations to form a single larger algebraic equation set, and solved simultaneously through implicit numerical integration and nonlinear equation solvers using Newton's method. Parallel computing and numerical tuning techniques, e.g., automatic network partitioning, variable time-stepping, accurate discontinuity handlings, etc., have been applied to achieve computational efficiency and maintain numerical robustness.

The alternating-explicit ME integration scheme is a popular choice in industry-grade software due to its simplicity and legacy implementations, but it requires a fixed small time-step to ensure numerical stability for accurate system dynamics, thus a highly efficient linear system solver such as the usage of a direct linear solver with fast lower and upper triangular decomposition as presented in our work[30] is critical to the performance improvement. The simultaneous-implicit Newton integration scheme, on the other hand, has better numerical stability and can use larger variable time-step with iterative solution, but it requires higher computational bandwidth due to the increased complexity of combined DAE model. Furthermore, convergence cannot always be guaranteed for large-scale system simulation when the initial guess is not

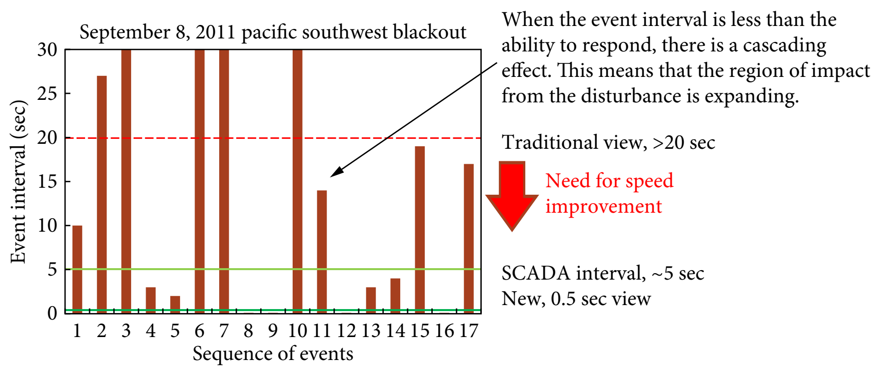

Fig. 7 Sub-second parallel state estimation performance in the Pacific Southwest Blackout in 2011.

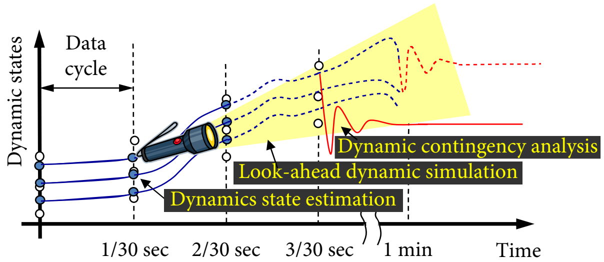

Fig. 8 Dynamic state estimation is foundational for real-time stability assessment of complex power systems.

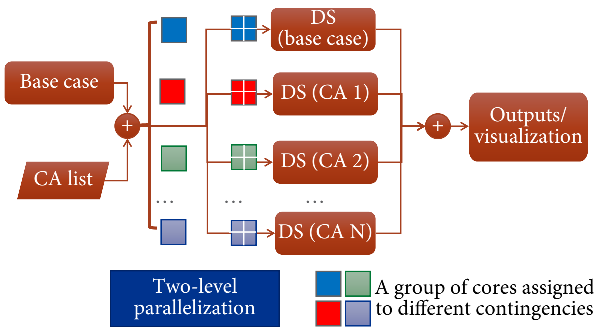

Fig. 9 A two-level task manager example for dynamic security assessment.

close enough to represent extreme cases. Hence, implementing a robust scalable nonlinear equations solver using PETSc's Time-Stepping Solvers with customized feature to enable analytical Jacobi matrix formulation and variable time-stepping is the focus of our work[31,32].

The computational performance and scalability of a 20-second dynamic simulation using these two DAE solution schemes are illustrated respectively in Table 1. In either case, faster-than-real-time dynamic simulation is achieved when running in parallel with a certain number of processes, whereas the simultaneous-implicit scheme is about 30% faster than the alternating-explicit one due to the dramatic reduction in time steps.

Table 1 Comparison of execution time (seconds) on a 20-second dynamic simulation in GridPACK[32].

# of processes	Alternating-explicit	Simultaneous-implicit
1	72.32	47.63
2	32.1	32.51
4	25.8	18.73
8	18.1	14.59
16	18.1	12.91
32	21.5	15.21

4.5 Optimal power flow

Optimization is a type of applications that requires significant support from HPC due to its extensive computational requirement. It is widely used in optimal power flow and market applications. Two examples are given below: high-performance power grid optimization (HIPPO)[33] and ExaGO/ExaSGD[34].

HIPPO is used to help power system planning for generating future electricity more efficiently. Today, next-day operations are determined by day-ahead unit commitment solutions based on available generation resources with the lowest possible cost and some reliability constraints. With the integration of renewable energy, this computation becomes more complicated with uncertainties. HIPPO solves the security constrained unit commitment (SCUC) problem faster and more accurately by leveraging knowledge of power system properties, operation requirements, and past solutions. The HIPPO will provide improved resource schedules, leading to more flexible and reliable operation in a stochastic environment. The tool was benchmarked with a MISO system[35].

For ExaSGD, security constrained AC optimal power flow analysis for the 2000-bus Texas grid model with 1000 credible contingencies was completed under 10 different weather scenarios. The entire analysis ran within 15 minutes on the Summit supercomputer using 1920 GPU devices. The whole computation used 13 PFLOPS of computing resources with estimated peak hardware utilization of ~9 PFLOPS (1 PFLOPS = 1,000,000,000,000,000 floating-point operations per second). The computation was performed using a software stack consisting of Magma linear solver and ExaGO modeling framework. This capability, when mature, will enable power system planners and operators to respond promptly to large scale events, such as hurricanes, providing optimal power dispatch under extreme conditions and significantly reducing blackout incidence.

4.6 Machine learning based remedial action scheme (RAS)

The orchestration between HPC and machine learning is a new research direction in power systems. This is natural because the large size of data generated by HPC tools could be very useful for AI/ML training. For example, the recent research work of transformative remedial action scheme tool (TRAST) has been applied and demonstrated in real-world use case analysis. In today's practice, the RAS parameters are configured through offline studies in a conservative way. The TRAST tool, whose data-driven analytical functionality can be seen in Figure 10, combines advanced statistical data analysis tools and machine learning algorithms to analyze, validate, and help create RAS plans. HPC cluster computing platform and the Microsoft cloud environment are used for steady state and dynamic simulations under massive contingencies and operating conditions. It will enhance the existing practice to determine the arming levels of RAS and finally develop use cases to demonstrate the benefits of adaptive RAS/SPS parameter settings, which can then be used to enable and validate preventive emergency controls[36].

4.7 Quantum computing based contingency analysis

As a preliminary activity, based on our previous research about quantum machine learning[37,38], simulation[17,39], and distributive quantum computing[38], we investigated the ability of quantum neural networks (QNNs), or parameterized quantum circuits in predicting the violation of contingency for an IEEE 30-bus system. Power demand, power generation, reactive demand, and reactive generation are used as the input and the probability of violation as the output. Trained by a small dataset with 20 cases, it is shown that QNN can improve the prediction accuracy for the testing set from ~49.8% (random guessing for binary classification) to ~72.2%, using only 5 qubits. Comparatively, a classical multilayer perceptron (MLP) deep-neural-networks with 4 layers and 256 neurons per layer show similar test accuracy (~72.4%) after 120 epochs. This is aligned with our previous observation that QNNs can achieve similar learning performance as compared to traditional DNNs but using 97% fewer parameters. This is achieved through encoding the classical information into (entangled) qubit states[37,40]. Nevertheless, practical power-grid problems are far more complicated, while near-term noisy intermediate-scale quantum devices are limited by the number of qubits, coherence time, and noise.

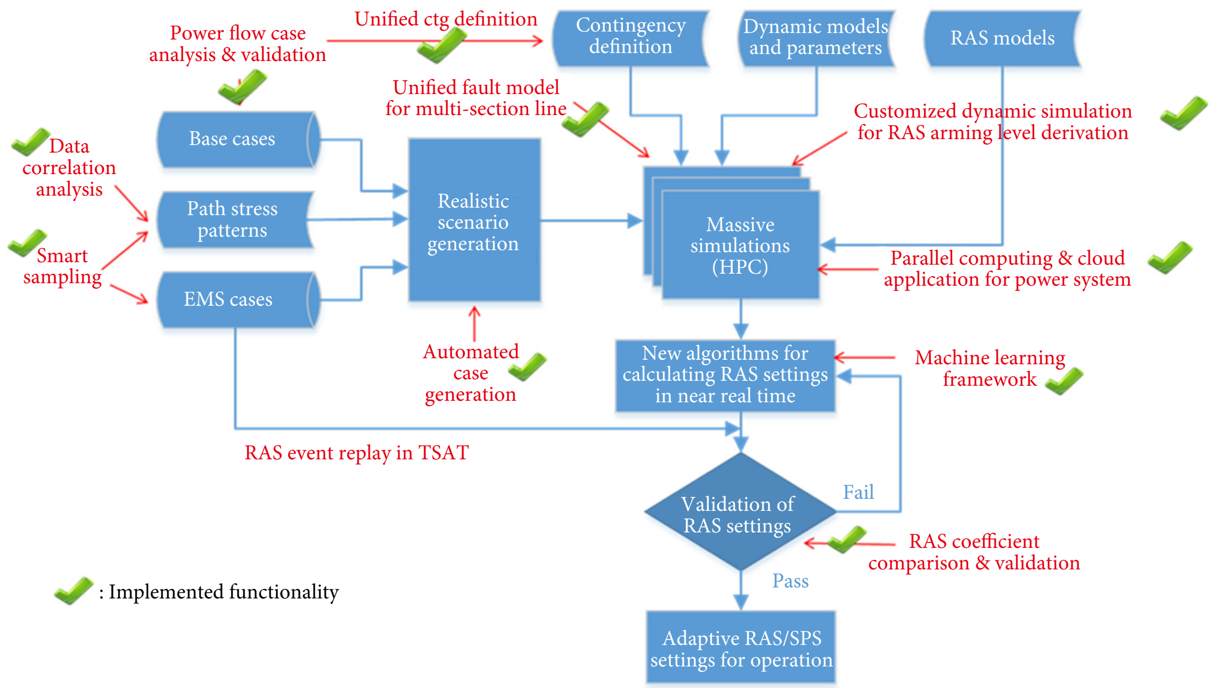

Fig. 10 **Overview of data-driven analytical functionalities in TRAST. Reprinted with permission from ref. [36] © Battelle Memorial Institute 2019.**

Despite promising, really harvesting quantum computing for electrical grid problems still have a long way to go.

5 Conclusions and future work

This paper describes the evolution of power system modeling and simulation with the growth of power systems and the advancements of computing techniques. With the increasing complexity in power system planning and operation, driven by the goal of clean energy and decarbonization, most of today's power system computing tools will not be sufficient to effectively manage future power systems. Therefore, power system computing needs to be advanced by leveraging the power of HPC techniques. Five generations of power system computing are defined along with the advancements of computing technologies. Several power system applications using various HPC techniques have been presented to show the power of advanced computing, including quantum computing.

Future work will involve (1) cross-platform HPC workflow management to orchestra and streamline HPC applications across different computing platforms at distributed locations, including edge computing, CPU, GPU, cloud computing, supercomputers, quantum computing, etc. (2) effective interaction between big data, artificial intelligence, machine learning, and HPC; and (3) re-formulation of power system applications to fit the state-of-the-art HPC techniques, advanced mathematical theories and/or advanced solvers, for complicated large-scale problems.

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Additional information

Declaration of competing interest

The authors have no competing interests to declare that are relevant to the content of this article.

References

[1] Huang, Z. Y., Nieplocha, J. (2008). Transforming power grid operations via high performance computing. In: Proceedings of the 2008 IEEE Power and Energy Society General Meeting - Conversion and Delivery of Electrical Energy in the 21st Century, Pittsburgh, PA, USA.

[2] Rupp, K. (2020). 48 Years of Microprocessor Trend Data (2020.0). Zenodo. Available at https://doi.org/10.5281/zenodo.3947824.

[3] Czarnul, P., Proficz, J., Drypczewski, K. (2020). Survey of methodologies, approaches, and challenges in parallel programming using high-performance computing systems. *Scientific Programming*, 2020: 417679.

[4] Jin, S. S., Huang, Z. Y., Diao, R. S., Wu, D., Chen, Y. S. (2013). Parallel implementation of power system dynamic simulation. In: Proceedings of the 2013 IEEE Power & Energy Society General Meeting, Vancouver, BC, Canada.

[5] Jin, S. S., Huang, Z. Y., Chen, Y. S., Chavarría-Miranda, D., Feo, J., Wong, P. C. (2010). A novel application of parallel betweenness centrality to power grid contingency analysis. In: Proceedings of the 2010 IEEE International Symposium on Parallel & Distributed Processing, Atlanta, GA, USA.

[6] Jin, S. S., Chassin, D. P. (2014). Thread group multithreading: Accelerating the computation of an agent-based power system modeling and simulation tool —C GridLAB-D. In: Proceedings of the 2014 47th Hawaii International Conference on System Sciences, Waikoloa, HI, USA.
[7] Message P Forum (1994). MPI: A message passing interface standard. Technical Report. Available at https://dl.acm.org/doi/10.5555/898758.
[8] Chen, Y. S., Huang, Z. Y., Rice, M. (2012). Evaluation of counter-based dynamic load balancing schemes for massive contingency analysis on over 10,000 cores. In: Proceedings of the 2012 SC Companion: High Performance Computing, Networking Storage and Analysis, Salt Lake City, UT, USA.
[9] Liu, Y., Jiang, W., Jin, S. S., Rice, M., Chen, Y. S. (2012). Distributing power grid state estimation on HPC clusters - A system architecture prototype. In: Proceedings of the 2012 IEEE 26th International Parallel and Distributed Processing Symposium Workshops & PhD Forum, Shanghai, China.
[10] Diao, R., Huang, Z., Makarov, Y. V., Chen, Y., Palmer, B., Jin, S., Wong, J. (2017). An HPC based real-time path rating calculation tool for congestion management with high penetration of renewable energy. *CSEE journal of power and energy systems*, 3: 431–439.
[11] Jin, S. S., Huang, Z. Y., Diao, R. S., Wu, D., Chen, Y. S. (2017). Comparative implementation of high performance computing for power system dynamic simulations. *IEEE Transactions on Smart Grid*, 8: 1387–1395.
[12] Wang, C., Jin, S. S., Chen, Y. S. (2020). Directive-based hybrid parallel power system dynamic simulation on multi-core CPU and many-core GPU architecture. In: Advances in Parallel & Distributed Processing, and Applications. Transactions on Computational Science and Computational Intelligence. Springer, Cham.
[13] Farhi, E., Goldstone, J., Gutmann, S. (2014). A quantum approximate optimization algorithm. arXiv preprint, 1411.4028.
[14] Khosravi, F., Scherer, A., Ronagh, P. (2021). Mixed-integer programming using a bosonic quantum computer. arXiv preprint, 2112.13917.
[15] Lloyd, S. (2010). Quantum algorithm for solving linear systems of equations. In: Proceedings of the 5th MLSys Conference, Santa Clara, CA, USA.
[16] Chang, C. Y., Jones, E., Yao, Y. Y., Graf, P., Jain, R. (2020). On hybrid quantum and classical computing algorithms for mixed-integer programming. arXiv preprint, 2010.07852.
[17] Stein, S. A., Baheri, B., Chen, D., Mao, Y., Guan, Q., Li, A., Fang, B., Xu, S. (2020). QuGAN: A generative adversarial network through quantum states. arXiv preprint, 2010.09036.
[18] Stein, S. A., Baheri, B., Chen, D., Mao, Y., Guan, Q., Li, A., Xu, S., Ding, C. W. (2021). QuClassi: A hybrid deep neural network architecture based on quantum state fidelity. arXiv preprint, 2103.11307.
[19] Chen, Y., Etingov, P., Fitzhenry, E., Sharma, P., Nguyen, T., Makarov, Y., Rice, M., Allwardt, C., Widergren, S. (2018). Bringing probabilistic analysis capability from planning to operation. *Control Engineering Practice*, 71: 18–25.
[20] Chen, Y., Etingov, P., Fitzhenry, E., Sharma, P., Nguyen, T., Makarov, Y., Rice, M., Allwardt, C., Widergren, S. (2015). A framework to support the fusion of operation and planning. *IFAC-PapersOnLine*, 48: 427–432.
[21] Konstantelos, I., Jamgotchian, G., Tindemans, S. H., Duchesne, P., Cole, S., Merckx, C., Strbac, G., Panciatici, P. (2016). Implementation of a massively parallel dynamic security assessment platform for large-scale grids. *IEEE Transactions on Smart Grid*, 8: 1417–1426.
[22] Zhou, Z. Y., Dinavahi, V. (2015). Parallel massive-thread electromagnetic transient simulation on GPU. In: Proceedings of the 2015 IEEE Power & Energy Society General Meeting, Denver, CO, USA.
[23] Song, Y. K., Chen, Y., Yu, Z. T., Huang, S. W., Shen, C. (2020). CloudPSS: A high-performance power system simulator based on cloud computing. *Energy Reports*, 6: 1611–1618.
[24] Green, R. C., Wang, L. F., Alam, M. (2013). Applications and trends of high performance computing for electric power systems: Focusing on smart grid. *IEEE Transactions on Smart Grid*, 4: 922–931.
[25] Chen, Y. S., Rice, M., Glaesemann, K., Huang, Z. Y. (2015). Sub-second state estimation implementation and its evaluation with real data. In: Proceedings of the 2015 IEEE Power & Energy Society General Meeting, Denver, CO, USA.
[26] Chen, Y., Rice, M., Huang, Z. (2014). SCADA-rate parallel state estimation assessed with utility data. In: proceeding of the 2014 IEEE PES General Meeting | Conference & Exposition, National Harbor, MD, USA.
[27] Huang, Z. Y., Schneider, K., Nieplocha, J., Zhou, N. (2014). Estimating power system dynamic states using extended Kalman Filter. In: Proceedings of the 2014 IEEE PES General Meeting | Conference & Exposition, National Harbor, MD, USA.
[28] Liu, Y., Singh, A. K., Zhao, J. B., Meliopoulos, A. P. S., Pal, B., Ariff, M. A. B. M., van Cutsem, T., Glavic, M., Huang, Z. Y., Kamwa, I., et al. (2021). Dynamic state estimation for power system control and protection. *IEEE Transactions on Power Systems*, 36: 5909–5921.
[29] Chen, Y. S., Palmer, B., Sharma, P., Yuan, Y., Mathew, B., Huang, Z. Y. (2018). A high performance computational framework for dynamic security assessment under uncertainty. In: Proceedings of the 2018 IEEE Electronic Power Grid (EGrid), Charleston, SC, USA.
[30] Huang, R. K., Jin, S. S., Chen, Y. S., Diao, R. S., Palmer, B., Huang, Q. H., Huang, Z. Y. (2017). Faster than real-time dynamic simulation for large-size power system with detailed dynamic models using high-performance computing platform. In: Proceedings of the 2017 IEEE Power & Energy Society General Meeting. Chicago, IL, USA.
[31] Jin, S. S., Abhyankar, S. G., Palmer, B. J., Huang, R., Perkins, W. A., Chen, Y. (2021). Toward a numerically-robust and efficient implicit integration scheme for parallel power grid dynamic simulation development in GridPACK. In: Advances in Parallel & Distributed Processing, and Applications. Transactions on Computational Science and Computational Intelligence. Springer, Cham.
[32] Abhyankar, S., Huang, R. K., Jin, S. S., Palmer, B., Perkins, W., Chen, Y. S. (2021). Implicit - integration dynamics simulation with the GridPACK framework. In: Proceedings of the 2021 IEEE Power & Energy Society General Meeting, Washington, DC, USA.
[33] Pan, F., Chen, Y., Holzer, J. Rothberg, E. (2019). HIPPO—A concurrent optimizer for solving day-ahead security constrained unit commitment problem. Available at https://www.ferc.gov/sites/default/files/2020-09/W3-A-4-Goldis.pdf.
[34] Alexander, F., Almgren, A., Bell, J., Bhattacharjee, A., Chen, J., Colella, P., Daniel, D., DeSlippe, J., Diachin, L., Draeger, E., et al. (2020). Exascale applications: Skin in the game. *Philosophical Transactions of the Royal Society A*, 378: 20190056.
[35] Chen, Y. H., Pan, F., Holzer, J., Rothberg, E., Ma, Y. M., Veeramany, A. (2021). A high performance computing based market economics driven neighborhood search and polishing algorithm for security constrained unit commitment. *IEEE Transactions on Power Systems*, 36: 292–302.
[36] Fan, X., Huang, R., Huang, Q., Li, X., Barrett, E. L., O'Brien, J. G., Hou, Z. S., Ren, H. Y., Kincic, S., Zhang, H. M. (2019). Adaptive RAS/SPS system setting for improving grid reliability and asset utilization through predictive simulation and controls: A use case for Transformative Remedial Action Scheme Tool (TRAST): Jim Bridger RAS Evaluation and Analysis. PNNL-29522. Richland, WA: Pacific Northwest National Laboratory. Available at: https://www.pnnl.gov/main/publications/external/technical_reports/PNNL-29522.pdf.
[37] Li, A., Fang, B., Granade, C., Prawiroatmodjo, G., Heim, B., Roet-

teler, M., Krishnamoorthy, S. (2021). SV-sim: Scalable PGAS-based state vector simulation of quantum circuits. In: Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis, Dallas , TX , USA.

[38] Li, A., Subasi, O., Yang, X., Krishnamoorthy, S. (2020). Density matrix quantum circuit simulation via the BSP machine on modern GPU clusters. In: Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis, Atlanta, GA, USA.

[39] Stein, S. A., Baheri, B., Chen, D., Mao, Y., Guan, Q., Xu, S., Ding, C., Li, A. (2022). QuClassi: A hybrid deep neural network architecture based on quantum state fidelity. In: Proceedings of the 5th Machine Learning and Systems Conference, Santa Clara, CA, USA.

[40] Stein, S., Ding, Y. F., Wiebe, N., Peng, B., Kowalski, K., Baker, N., Ang, J., Li, A. (2022). EQC: ensembled quantum computing for variational quantum algorithms. In: Proceedings of the 49th Annual International Symposium on Computer Architecture, New York, NY, USA.