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Impact of quantum and neuromorphic computing on biomolecular simulations: Current status and perspectives

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Abstract

New high-performance computing architectures are becoming operative, in addition to exascale computers. Quantum computers (QC) solve optimization problems with unprecedented efficiency and speed, while neuromorphic hardware (NMH) simulates neural network dynamics. Albeit, at the moment, both find no practical use in all atom biomolecular simulations, QC might be exploited in the not-too-far future to simulate systems for which electronic degrees of freedom play a key and intricate role for biological function, whereas NMH might accelerate molecular dynamics simulations with low energy consumption. Machine learning and artificial intelligence algorithms running on NMH and QC could assist in the analysis of data and speed up research. If these implementations are successful, modular supercomputing could further dramatically enhance the overall computing capacity by combining highly optimized software tools into workflows, linking these architectures to exascale computers.

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Introduction

The advent of exascale machines, which may dramatically speed up biomolecular simulations (BMS) [1], is accompanied by emerging high performance computing (HPC) technologies such as quantum computing and neuromorphic computing. These new architectures are becoming present in computing centers such as the Jülich Supercomputing Centre and Forschungszentrum Jülich[1] or Oak Ridge.[2] However, the biomolecular simulation (BMS) community is not exploiting these powerful platforms yet. After describing recent developments of these architectures (Sections Neuromorphic computers and Quantum computing), also assisted by artificial intelligence (AI) and machine learning (ML) (Sections Artificial intelligence-based neuromorphic hardware and Machine learning and Quantum computer), we give our opinion on whether and how these can be exploited and connected to exascale machines in the future to boost BMS (Section Modular supercomputing).

Neuromorphic computers

Neuromorphic hardware (NMH) is the collective name of a set of devices designed using principles observed in neural networks (see Figure 1). There is a vast variety of implementations, which include, among others, digital, analog, and hybrid NMH systems (see Box 1). These computers can also be used for other applications besides neural network simulations, like solving graph search problems [2**] or solving steady-state partial differential equations (PDEs) [3].

NMH is highly parallel and specialized to perform computations similar to what biological neurons (i) and their networks (ii) do. (i) In its most common and simplest form, the equation for single leaky integrate and fire (LIF) neurons [4–6] reads[3]:

$$\tau_m \frac{dv}{dt} = -[v(t) - v_{rest}] + RI(t) \quad (1)$$

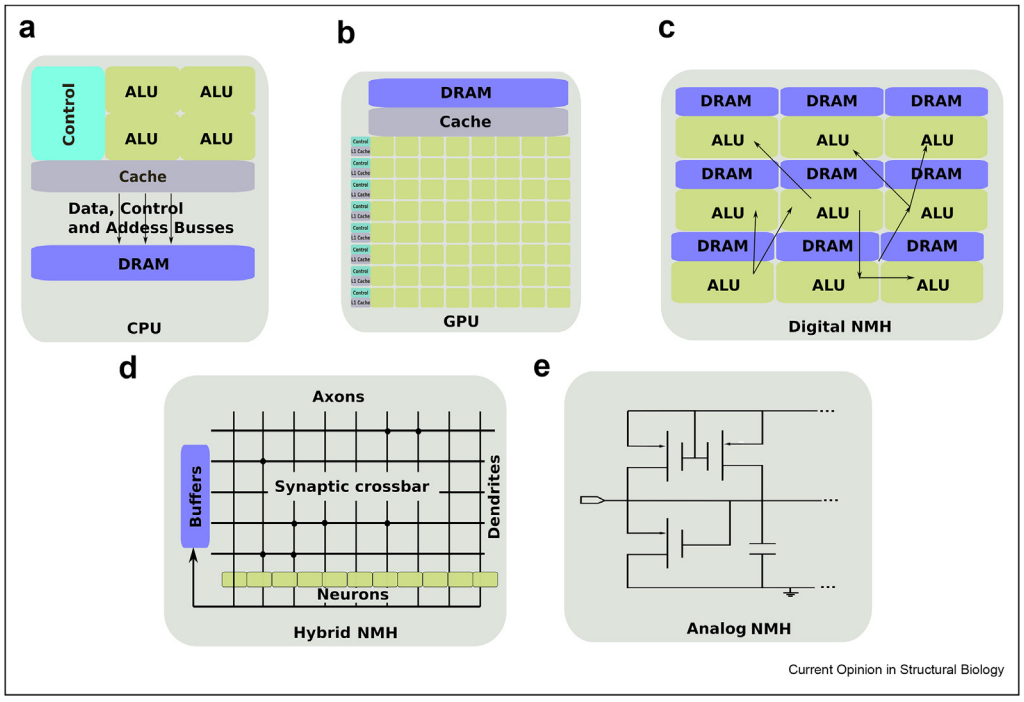
where $v(t)$ is the membrane potential at time t, τ_m is the membrane leakage time constant, R is the resistance of the

[1] https://www.fz-juelich.de/en/ias/jsc.

[2] https://www.ornl.gov/.

[3] The model of LIF neurons is the most frequently simulated or emulated model in digital and hybrid NMH.

Figure 1



Schematic of example von Neumann **(a)**, GPU **(b)**, digital NMH **(c)**, hybrid NMH **(d)**, and analog NMH **(e)** architectures (see Box 1). The arrows in **(c)** indicate connections configurable via a routing table. In (D) the processing units are the neuron units, and the synaptic crossbar implements the network connectivity. ALU represents an Arithmetic Logic Unit, and DRAM is a Dynamic Random Access Memory. The control units fetch instructions from memory and send them to the ALU to be executed. The architecture of NMH architectures like **(c)** and **(d)** differ from those in **(a)** and **(b)**, among other things, in that these components are rearranged in terms of their proximity and interconnectivity. The architecture exemplified in **(e)** is more unique in that these classic elements are not identifiable anymore. **(e)** shows a segment of analog circuitry used to emulate neural dynamics. The current flowing through the electronic circuit emulates the changes in the membrane potential of the neuron, and memory is stored by means of changing the resistance and capacitance of elements in the circuit. GPU, graphics processing unit; NMH, neuromorphic hardware.

cell membrane, and $I(t)$ is the input current to a single cell. Spiking events emerge when $v(t)$ surpasses the threshold v_{th} taking $v(t)$ to a default reset potential value v_{rest} [7].

(ii) The evolution of a stochastic network of N neurons, according to the master equation by Cowan [15] and Ohira and Cowan [16], reads:

$$\frac{\delta}{\delta t}\Phi(t) = L\Phi(t) \tag{2}$$

where $\Phi(t)$ is the neural state vector, defined as

$$\Phi(t) = \sum_{|\Omega|} P(\Omega, t)\Omega \tag{3}$$

$P(\Omega, t)$ is the probability of finding the network in the conformational state Ω of the simulated network at time t. The Liouvillian L reads:

$$L = \alpha \sum_{i=1}^{N} (\Delta_{+i} - 1)\, \Delta_{-i} + \sum_{i=1}^{N} (\Delta_{-i} - 1)\, \Delta_{+i}\, \frac{\phi}{n_i} \left(\sum_{j=1}^{N} \omega_{ij} x_j \right) \tag{4}$$

where α is the decay function after a neuron has spiked, Δ_{+i} and Δ_{-i} are the raising and lowering operators that take neuron i to and from an activation state, respectively, n_i is the number of connections to neuron i, ϕ is the activation rate function, which depends on the single neuron model (like the one described in the first equation) and ω_{ij} is the strength of the connection between neuron i and j. The fact that this hardware has been in principle designed to optimally solve equations similar to the ones above limits the use of these neuromorphic computers for BMS. However, educated mappings of mathematical equations to the operation of some hardware components [17**] could lead eventually to efficient computational solutions for completely different problems, such as those relevant for BMS.

Some digital NMH, like SpiNNaker2 [18], combine commercial multicore chips with highly optimized event communication channels between the cores. They capitalize on specialized communication technology [19–21] to mimic the way the brain sends event-based information among the components of neural networks. The word "event" in this context refers to the emergence of a neuronal spike. NMH with optimized event exchange reduces the time required to communicate

Box 1. Types of neuromorphic computers

Digital NMH, like SpiNNaker [18] or Loihi [57,59], uses components similar to those found in normal (or von Neumann) architectures based on central processing units (CPUs) and/or graphics processing units (GPUs). However, the communication protocols, the storage, the networking and the computing elements are modified to maximize the energy efficiency and the speed of information exchange.

Analog NMH, like ROLLO [8,9] or COLAMN [10], emulates the way the brain works. It uses the intrinsic characteristics of electronic devices (such as the behavior of current passing through a transistor, memristor, or an RC circuit) to emulate biological phenomena and solve differential equations describing neural activity. Some devices perform in-memory computations, namely, execute mathematical calculations as part of the normal operation of a memory unit. This may reduce the bottlenecks related to constantly moving data between memory and the central processing units in von Neumann architectures [11,12*].

Hybrid NMH, like BrainScales [13] and Truenorth [14], combines analog and digital parts to enable brain-inspired computers while keeping a flexible interface to classic digital computers. Besides addressing problems in neuroscience, it can solve machine learning tasks by emulating spiking neural networks to encode algorithms is usually implemented with artificial neural networks.

spikes in the neuronal network. However, the information that can be exchanged using these "events" can be, in principle, of an arbitrary nature.

The compute units are normal CPUs arranged in a power-efficient in a highly parallel setup that can be programmed to solve not only the equations above [22], but also for other needs [23**]. Thus, other algorithms (such as those of molecular dynamics, MD) could be translated into this kind of hardware. While the MD algorithms required to solve the differential equations describing the potential energy function could be executed in parallel using the multiple cores in the NMH chips, the updates in velocity and position could make use of the optimized networking protocols available on the chip. In a suitable mapping of an MD model, each "neuron" could be responsible for calculating the update in the position and speed of single atoms or small groups of atoms in the system. According to our proposed mapping from NMH to MD, the events could be the updates in the position and velocity of single atoms. For instance, one could replace the set of differential equations that describe the neural dynamics (Eq. (1)) with the ones describing the changes in position and velocity of an atom or group of atoms. Additionally, one could use the data, communication, and computing structures traditionally used to model synapses and exchange spikes to efficiently exchange the updates in the position of each atom relative to the rest of the system and to represent different short- and long-range interactions between them.

Most importantly, this digital NMH may provide an innovative and energy-efficient platform that can be integrated as one module in a supercomputer and enable new paradigms for accelerated MD simulations (see Section Modular supercomputing). The energy efficiency of NMH comes from (i) exchanging information between computing units (neurons) only when the "events" (defined above) take place, and doing computation only when all relevant information is available, and (ii) having a closer distance between memory and computing elements. The main side effect of (i) and (ii) is the reduction of flexibility of the algorithms used. For example, reading from external memory or defining the connectivity between neurons in a network during system configuration is usually very time-consuming. If the structure of the network does not change during the simulation, this configuration only needs to be done once, and the overhead can be compensated by the speedup in simulation time. The loading and configuration step required to deploy algorithms onto the NMH is currently one of its bottlenecks and a problem that would need to be addressed. If successful, digital and hybrid NMH could enable new paradigms for accelerated MD simulations using a much more energy efficient platform [18]. The current ideas of mapping MD simulations onto neuromorphic hardware are in their infancy. To our knowledge, no public implementation of such an approach is available, nor specific funding has been granted to projects in this direction. In summary, NMH might be useful for MD, but we don't have a proof of principle yet that it can and will actually be applied to it.

Artificial intelligence-based neuromorphic hardware

NMH implementing deep learning (DL) models has proven to provide a computational backend with high performance and low-energy consumption [24–26]. Software tools able to transform networks of artificial neural networks into their spiking neural network counterparts are available and provide an efficient mechanism to translate machine learning models on some types of digital and hybrid NMH with some limitations.

Digital NMH implementing Markov chain algorithms can perform sampling of vast parameter spaces in a tractable manner and with a low energy footprint [27,28]. Porting existing machine and deep learning algorithms for the analysis of molecular dynamics

simulation data eventually obtained by NMH is expected to be feasible with currently available software tools [29,30]. In addition, this architecture, by implementing a variety of AI and ML algorithms can provide workflows to optimize, extract features, and reduce energy consumption. This, in turn, could be exploited for BMS. As discussed by Bai et al. [31] deep learning models could be trained with simulation data produced using classical MD simulators (i) to identify parameters and additional data that is useful to optimize the simulated results; (ii) to predict the transfer of free energies using available simulated data and perform otherwise computationally intensive mapping of relevant system properties.

Some commercial neuromorphic chips have had great success in terms of performance and energy usage while solving state-of-the art problems as compared to GPUs. The area is under heavy research and might see substantial progress and new applications within the next 5 years. Current limitations of this approach include refining the training techniques to be applied to large-spiking neural models, as well as efficiently dealing with I/O and interfacing with other classical computing systems for further analysis and postprocessing. All these challenges are currently under research [32–35].

Quantum computing

Quantum computing (QC) exploits the physical properties of systems at the atomic level to perform calculations on different domains. These calculations can be of different nature and applicable to a variety of scientific fields, from chemistry to physics. It encodes problem variables using *qbits*, the quantum equivalent of a bit. In contrast to their classical counterparts, qbits can be in a state of superposition where the value they encode is both 0 and 1 at the same time. Computing on qbits means to modify the probability that, after a measurement operation on the qbit is performed, the observed value will be either a 0 or a 1. QC (along with Turing machines) might solve nondeterministic polynomial (NP) time problems. However, it might also address NP-hard problems, which classic algorithms are not able to solve within tractable time. QC can exploit a variety of different quantum principles. Here we focus on two approaches able to solve optimization problems very efficiently [36–40], gate-based and adiabatic QC (See Box 2).

Baiardi et al. [41] discuss the usage and limitations (such as those associated with data transfer and with interfacing with classic computers) of applying QC to biological processes at the molecular level. Adiabatic QC is a good candidate for future applications, particularly for optimization problems.

Box 2. Types of quantum computing paradigms

Gate-based QC uses quantum equivalents of the classical Boolean logic gates. Based on quantum circuits, they operate on a set of qbits prepared on a known state to execute a specific quantum algorithm.

Adiabatic QC maps problems onto the Hamiltonian of a quantum system, whose initial state is easy to prepare, while its final state encodes the solution to a problem. The final state Hamiltonian is reached after the system evolves according to Schrödinger's equation in an adiabatic fashion.

While QC has already been proposed to study protein folding [61], to accelerate drug discovery, [56,58], and to perform data analysis in bioinformatics [60], no application of QC to BMS has been reported.

QC implementations of Monte-Carlo algorithms [42*,43] study sampling problems and hence could be used to simulate biomolecular processes in the future, provided that the hardware can increase in the number of qbits compared to what is currently available (up to 1000 in the Atom QC).

Applying quantum chemistry approaches, such as those of Haupt et al. [44*] to QC could also lead to practical applications to highly correlated, complex metal-based enzymes such as nitrogenase [45–48]. Systems as the latter might be difficult to be treated by standard quantum mechanics/molecular mechanics (QM/MM) methods (for instance, using density functional theory), because they may be either too costly and/or not scale well and/or are not accurate enough. However, the use is limited by (i) the relatively small amount of qbits currently available in the state-of-the-art QC; (ii) the lack of a fully developed software; (iii) the complex problem mapping required to use quantum systems—algorithms in quantum computing should consider the properties of the hardware, including state superposition, entanglement, and tunneling, among others, as well as the nondeterministic nature of the observations performed at the end of the calculations. As a result, the largest QC-based quantum chemical calculations so far have been carried out on small systems (such as a diazene molecule [49]).

Mapping a problem onto quantum systems requires a reformulation of the problem components and the relationships between them. Gating QC can translate classical logic into its quantum equivalents, in contrast to adiabatic QC, which is therefore expected to be even more difficult to implement.

Tight collaborations between engineering experts in quantum computing and molecular biophysicists could enormously help to develop apt software and to find suitable problem mappings leveraging the unique features and inherent phenomena made accessible through QC. These algorithms will also have to cope with limitations, including access to required data and a suitable interface to analyze the results.

Machine learning and Quantum computer

As QC efficiently addresses optimization problems [50–52], ML-based algorithms executed using this infrastructure and targeting hybrid simulation approaches such as QM/MM could be used to improve accuracy and execution time. Combinatorial optimization of parameters for specific use cases where inputs and outputs of a simulation can be measured with discrete values can also be a target for QC systems.

Modular supercomputing

Modular supercomputing [53] is an essential concept to help NMH and QC to be adopted by the community and to help identify the specific parts of an application where each piece of hardware can provide the best computing, networking, and energy efficiency. New applications can be envisioned under the modular approach combining NMH or QC with exascale systems. Such applications could be workflows, where, e.g. simulations are carried out on the exascale system, and analysis or parallel machine learning/optimization algorithms are being executed in the NMH, or QC system. Other applications include multiscale simulations, where some specific features of a system at different scales are calculated in the QC or NMH, while the more general simulation of the system takes place on the exascale module.

Thus, exascale supercomputing, which mostly relies on GPUs to achieve high computational throughput [54*], can be complemented by QC and NMH to accelerate research, improve reliability, efficiency, and low energy consumption. Such approaches could help overcome bottlenecks related to memory access and communication between computing units, which will be critical to reach the *zettascale* (10^{21} flops/seconds), expected to be implemented in computer centers in only a few years from now [55].

Conclusions

We have presented a brief overview of emerging HPC technologies and their possible (future) implementations for BMS. We foresee that the use of NMH and QC, especially if combined with the power of AI, could dramatically enlarge the scope of BMS in a few years from now.

Editorial disclosure statement

Given the role as Guest Editor, Paolo Carloni had no involvement in the peer review of the article and has no access to information regarding its peer-review. Full responsibility for the editorial process of this article was delegated to Karissa Y. Sanbonmatsu.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

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