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# A Hybrid Classical-Quantum HPC Workload

Aniello Esposito\*, Jessica R. Jones<sup>†</sup>, Sebastien Cabaniols<sup>‡</sup> and David Brayford<sup>§</sup>

HPC/AI EMEA Research Lab

Hewlett Packard Labs

Location: \*Basel Switzerland, <sup>†</sup>Bristol UK, <sup>‡</sup>Grenoble France, <sup>§</sup>Munich Germany

Email: \*aniello.esposito@hpe.com, <sup>†</sup>j.r.jones@hpe.com, <sup>‡</sup>sebastien.cabaniols@hpe.com, <sup>§</sup>david.kenneth.brayford@hpe.com

Abstract—A strategy for the orchestration of hybrid classicalquantum workloads on supercomputers featuring quantum devices is proposed. The method makes use of heterogeneous job launches with Slurm to interleave classical and quantum computation, thereby reducing idle time of the quantum components. To better understand the possible shortcomings and bottlenecks of such a workload, an example application is investigated that offloads parts of the computation to a quantum device. It executes on a classical high performance computing (HPC) system, with a server mimicking the quantum device, within the multiple program, multiple data (MPMD) paradigm in Slurm. Quantum circuits are synthesized by means of the Classiq software suite according to the needs of the scientific application, and the Qiskit Aer circuit simulator computes the state vectors. The Harrow-Hassidim-Lloyd (HHL) quantum algorithm for linear systems of equations is used to solve the algebraic problem from the discretization of a linear differential equation. Communication takes place over the message passing interface (MPI), which is broadly employed in the HPC community. Extraction of state vectors and circuit synthesis are the most time consuming, while communication is negligible in this setup. The present test bed serves as a basis for more advanced hybrid workloads eventually involving a real quantum device.

Index Terms—quantum, hybrid, simulation, supercomputing, hpc

## I. INTRODUCTION

Quantum computers hold the potential to solve certain very difficult problems with moderate input sizes efficiently but accessibility and usability lag behind. On the other hand, supercomputers and their data-intensive applications are large but operate with proven tools developed over decades. Several promising algorithms for quantum architectures have been developed over the past decades [1]. However, as was explained in [2, Sec. 1.1], parallelism is not as easy to realise in quantum algorithms. A more suitable approach therefore, given the small size of early noisy, intermediate-scale quantum (NISQ) devices, is to offload portions of a classical code that would most benefit from quantum speed-up. Many HPC applications could profit from this approach in a hybrid workload, but how that might happen in a practical sense has not been standardized yet. It is therefore crucial that today's computational scientists are able to adapt early on to make use of these machines as they become available, while ideally keeping as much as possible from the proven HPC ecosystem, in order to shape hybrid workflows to their needs. In [2] some of the challenges that will need to be addressed to make a hybrid classical-quantum supercomputer truly useful to the wider scientific community are explained. Assuming

that those challenges can be addressed, a hybrid classicalquantum system can be thought of as broadly similar to any other HPC system with more than a single node architecture, e.g. with a mixture of accelerators such as GPUs and FPGAs. That means that most of the tools at our disposal today, such as Slurm [3] and MPI [4], can be repurposed. Slurm already supports heterogeneous jobs and can be configured to schedule hybrid classical-quantum jobs on a suitable hybrid machine.

The first part of this work presents an example hybrid workload as described above. It makes use of the HHL quantum algorithm to solve a system of linear equations repeatedly, where a quantum device is mimicked by a circuit simulator within the MPMD paradigm. This testbed allows the investigation of possible shortcomings and bottlenecks of the workload design, which is the main purpose and contribution of this part. A solid understanding of this preliminary stage is crucial before including a real quantum device, which would then allow investigation of the performance of both the hardware and software. In the second part, a general and more sophisticated strategy for hybrid classical-quantum workloads is proposed that employs heterogeneous Slurm jobs. This approach allows the idle time of a quantum device to be further reduced, thereby increasing the efficiency of hybrid workloads. This is an improvement over MPMD from the first part, where the quantum device is not released during a Slurm job and can be left idle.

### II. THE HYBRID WORKFLOW

## A. General Considerations

A realistic architecture of a hybrid classical-quantum system in the near future could consist of a large number of classical compute nodes, as found in today's supercomputers, and at least one or two orders of magnitude fewer nodes with quantum hardware, likely NISQ devices with 10-100 qubits each, sharing a common high-speed interconnect as shown in Fig. 1. The quantum devices are exposed as regular compute nodes to a workload manager (WLM) using a hardware interface that is assumed to be compatible with the possibly very different cooling requirements of the various architectures. From an algorithmic point of view, offloading portions of a classical code to quantum devices presents another challenge, namely that of data transfer speed, which will affect how those portions are selected. Hoefler et.al. [5] demonstrated, with some fairly pessimistic, if realistic, assumptions about I/O speed, that it is necessary to minimise the amount of data



Figure 1. Schematic representation of a tightly coupled hybrid system, where quantum devices access via an interface the same high-speed network as the classical compute nodes and service nodes.



Figure 2. Schematic representation of the interaction between a classical application running on the HPC system and an interface server for a quantum device. A WLM spans a single job that includes both components running in a MPMD model. The subroutine  $qsolve_Axb(\ldots)$  handles the synthesis of the quantum circuit depending on A and b on the HPC system, as well as the communication with the quantum device. For the present case, a quantum circuit simulator mimics the quantum device.

being transferred to benefit from the advantages conferred by quantum computation. Algorithm selection is therefore key in realising quantum advantage. The problem of quantum error correction (QEC) is ignored for the moment. However, it is important to note that this must be addressed before widespread adoption of systems of this type in the HPC community. See [2, Sec. 1.2] for further discussion on this issue.

# B. Example Application

The discretization of linear differential equations is a standard numerical method for solving problems in engineering. The resulting algebraic problem in the form of a system of linear equations Ax = b can be solved in principle on a quantum device by the HHL [6] algorithm. Fig 2 shows a classical application calling a subroutine qsolve\_Axb(...) that passes the the matrix A and right-hand-side b and returns the solution x. The routine synthesizes the HHL quantum circuits based on A and b by means of the Classiq [7] software suite. The circuits are represented by strings of quantum circuit intermediate representation code (quantum



Figure 3. Iterative solution of a linear system of equations Ax = b as it is used for the time evolution of a discretized partial differential equation. At each time step the circuit for the HHL algorithm is synthesized for a different right hand side and the solution is computed on a quantum device (quantum circuit simulator in the present case). Note that the matrix A is synthesised only once as long as the discretization grid does not change.

assembly language (QASM)) [8], and these are transferred via MPI\_Send/Recv calls using mpi4py [9]. MPI has been chosen for communicating data because of its established role in supercomputing, but other mechanisms are also imaginable, such as the Maestro middleware [10]. The quantum device that is supposed to process the quantum circuit is accessed through an interface running in another application. Though, in the present case, the quantum device is mimicked by the Qiskit Aer [11] circuit simulator, which computes the final state vector and sends the solution back to the classical application. In the simplest scenario, both applications are executed within a single job using the MPMD model, where the job is allocated and started by Slurm (see appendix A). The classical application and the quantum circuit simulator share a single MPI\_COMM\_WORLD, which required minor changes in Qiskit Aer. Alternatively, dynamic process management in MPI could be used to create an inter-communicator from the individual communicators of the two applications in order to send and receive information. In the case of a linear timedependent differential equation, a system of linear equations needs to be repeatedly solved, as illustrated in Fig 3. When a discretization grid does not change over time, the matrix Aremains the same. The Classiq software allows the righthand-side b to be synthesized separately, and then combined the final circuit without having to synthesize A again. In the present use case, the circuit for every time step is sent to the quantum device, which then computes the solution and sends it back to the classical application where the bvector is assembled for the next time step. Experiments have been conducted on a HPE Cray EX system featuring two AMD EPYC 7763 (Milan) CPUs per node, giving a total of 128 cores and 512GB memory connected via the Slingshot interconnect. The NumPy [12] and mpi4py packages made use of the highly tuned math and MPI libraries from the HPE Cray programming environment. Only moderate matrices and right-hand-sides of sizes up to N = 64 have been considered and the number of qubits needed for the quantum algorithm is  $O(\log(N))$ . The present implementation uses Python and

### Table I

Complexity of the various phases of solving a linear system of equations in the hybrid workflow and a comparison to the classical counterpart. The synthesis of the circuit for the matrix A has to be done only once, depending on the change in discretization, and  $\kappa$  is the condition number of A.

| operation                               | quantum             | classical |
|---|---------------------|-----------|
| Solving $Ax = b$                        | $O(\kappa \log(N))$ | O(N)      |
| Synthesis of circuit for b              | $O(\log(N))$        | N/A       |
| Synthesis of circuit for A              | $O(\log(N))$        | N/A       |
| Readout information from quantum device | O(1) - O(N)         | N/A       |

data is represented by NumPy arrays, but an implementation in C/C++ that passes pointers or references to arrays of floating point numbers is straightforward. This workload has been demonstrated during the International Supercomputing Conference (ISC) 2023.

### C. Results and Discussion

The most time consuming portion of the workload in Fig. 3 is the synthesis of A and b into quantum circuits, followed by the extraction of the state vector from the circuit simulator. The former is most probably due to the connection of the Classig software to an external server, which could be highly improved by using an on-premise solution, and further optimizations of the synthesis can be considered once this bottleneck has been removed. The matrix A is usually sparse in terms of non-zero entries depending on the discretization scheme, but for the circuit generation an efficient decomposition in tensor products of Pauli matrices is more important. The full extraction of the state vector is not necessary as long as only a portion of the simulation domain in real-space is of interest, although this could be insufficient in a timedependent problem. The precision of the solution is another peculiarity of the quantum algorithm that deviates by several percent from the classical solution. As long as precision can be traded for efficiency this is not an issue, but otherwise one has to include more qubits for precision and error correction. Another approach would be use the approximate solution as an input to an iterative refinement procedure. Finally, the complexities of the individual portions of the quantum algorithm are summarized in Table I. Assuming that only part of the state vector is needed and that the injection of the circuit in the quantum device, as well as the circuit transfer time, remain negligible, the conditions under which this hybrid workload can eventually outperform its purely classical counterpart are given.

### D. Anatomy of an Improved Hybrid Workload

The MPMD model used in Sec. II-B is simple, but it blocks a quantum device for the whole duration of the classical application and so potentially wastes precious resources. A reduction of this idle time can be achieved by using the Slurm support for heterogeneous jobs (hetjobs) to split a job across differing hardware. A simple scenario consists of two heterogeneous jobs {job1, job2}, each requiring classical and quantum computing resources. As is typical in HPC, the



Figure 4. Schematic representation of two Slurm heterogeneous jobs requiring a quantum device that is exposed as a compute node. As soon as the quantum device is no longer needed by the first heterogeneous job it can be released while the classical part continues to run. The second heterogeneous job can start using the quantum device.

two jobs are submitted to a queue. Once resources are available to start, both the classical and quantum parts of job1 begin. At a crucial point in the execution, there is a synchronisation to allow the classical part to wait on results from its quantum counterpart. The classical part polls the quantum resource for completion. Once the quantum computation is finished, the resource is freed and then immediately consumed by the guantum part of job2, which has been waiting in the queue for the resource to become available. This is illustrated in Fig 4, where it is assumed that the quantum device is the bottleneck, since their availability will initially be limited compared to that of traditional hardware. Sources for the job scripts can be found in the appendix A. Usually, the consumption of classical and quantum resources does not start at the same time, however this can be achieved by splitting, checkpointing, and restarting the classical part appropriately. Here follow screen captures of the output of squeue at critical moments during the execution of the two hetjobs. The various states of a job can be "pending" (PD), "completing" (CG), or "running" (R).

| JOBID PA | RTITION | NAME | USER ST | TIME | NODES | NODELIST (REASON) |
|----------|---------|------|---------|------|-------|-------------------|
| 105756+1 | Q       | job2 | seb PD  | 0:00 | 1     | (Resources)       |
| 105754+1 | Q       | job1 | seb R   | 0:21 | 1     | qnode1            |
| 105756+0 | HPC     | job2 | seb PD  | 0:00 | 2     | (Resources)       |
| 105754+0 | HPC     | job1 | seb R   | 0:21 | 2     | hpcn[136-137]     |

Listing 1. job2 waits while job1 uses the quantum resource

In Listing 1, job1 has been allocated the quantum resource, qnode1 and, the two HPC machines are waiting for the end of the quantum computation. job2 is waiting on resources because the quantum machine, qnode1 is busy.

| JOBID PART | ITION | NAME | USEF | R ST | TIME | NODES | NODELIST (REASON) |
|------------|-------|------|------|------|------|-------|-------------------|
| 105754+1   | Q     | job1 | seb  | CG   | 0:31 | 1     | qnode1            |
| 105756+1   | Q     | job2 | seb  | PD   | 0:00 | 1     | (Resources)       |
| 105756+0   | HPC   | job2 | seb  | PD   | 0:00 | 2     | (Resources)       |
| 105754+0   | HPC   | job1 | seb  | R    | 0:33 | 2     | hpcn[136-137]     |

Listing 2. The quantum part of job1 is completing.

In Listing 2, the quantum part of job1 is done; the quantum resource is being liberated, while the classical part of job1

is still running. Meanwhile, job2 is still pending as it waits for the resources it needs to become available.

| JOBID PARTITIC | N NAME US | ER ST  | TIME  | NODES | NODELIST (REASON) |
|----------------|-----------|--------|-------|-------|-------------------|
| 105756+1 Q     | job2 sel  | D D O  | 00:00 | 1     | (Resources)       |
| 105756+0 HPC   | job2 sel  | D PD ( | 00:00 | 2     | (Resources)       |
| 105754+0 HPC   | jobl sel  | DR (   | 0:45  | 2     | hpcn[136-137]     |

Listing 3. Classical part of job1 is still computing, while job2 is still pending, but the Q resource is almost ready again now.

In Listing 3 job1's classical part is still computing, while job2 is still pending, but the quantum resource is almost ready again now.

| JOBID PAR | TITION | NAME | USER | ST | TIME | NODES | NODELIST (REASON) |
|-----------|--------|------|------|----|------|-------|-------------------|
| 105756+1  | Q      | job2 | seb  | R  | 0:01 | 1     | qnode1            |
| 105754+0  | HPC    | job1 | seb  | R  | 1:01 | 2     | hpcn[136-137]     |
| 105756+0  | HPC    | job2 | seb  | R  | 0:01 | 2     | hpcn[138-139]     |

Listing 4. Classical part of job1 is still computing, while job2 is running

Listing 4 shows job1 is continuing its classical computation. job2 is now running, with the quantum computation in progress and the classical computation eventually waiting for the results (blocking MPI call).

### **III.** CONCLUSION

A hybrid classical-quantum workload for the repeated solution of a system of linear equations has been executed on a single HPE Cray EX system within the MPMD model of Slurm. The circuits are generated by a classical scientific application and then evaluated by a simulator imitating a quantum device. Synthesis of a circuit is ideally done locally and not remotely, which is really an administrative or legal (licensing) issue, rather than a technical one. The lower precision of the results from a quantum device needs to be taken into account and improved by either using more qubits and an improved algorithm, or by classical techniques such as iterative refinement for this particular use case. Extraction of the full state vector has to be avoided if possible. For the more flexible case, where a quantum resource does not have to be bound to a classical application until its termination in an MPMD job, a strategy using heterogeneous jobs in Slurm has been presented, where the quantum device can be freed up during the job runtime, and used by the next heterogeneous job. In the next step the use case will be executed as a heterogeneous job to profile the framework and eventually, the circuit simulator will be replaced by an actual quantum device.

### APPENDIX

Listing 5 shows the MPMD Slurm job script for the example in Sec. II-B

#!/bin/bash
#SBATCH -N 1
#SBATCH -t 10
#SBATCH --exclusive
srun -n 2 -c 1 -u -l --multi-prog multi.conf

Listing 5. Slurm MPMD job script

with the configuration file

0 python hhl\_demo.py 1 python circuit\_simulator.py

| Listing 6. | multi.com | f Slurm | MPMD | configuration | file |
|------------|-----------|---------|------|---------------|------|
|------------|-----------|---------|------|---------------|------|

The heterogeneous Slurm jobs shown in Sec. II-D are based on a script like the following

| #!/bin/bash  |   |
|--|---|
| #  |   |
| <pre># The first allocation is the classic HPC allocation and<br/>will survive</pre>       |   |
| <pre># the computational tasks even when the quantum part of th     job is finished.</pre> | e |
| #  |   |
| # The -C quantum is our quantic resource selector and we                                   |   |
| only have one (mimicked by   |   |
| <pre># requiring qnode1, a unique, particular system).</pre>                               |   |
|  |   |
| #SBATCH -N2  |   |
| #SBATCH -C classic   |   |
| #SBATCH -p HPC   |   |
| #SBATCHexclusive   |   |
| #SBATCH het job  |   |
| #SBATCH -N1  |   |
| #SBATCH -C quantum   |   |
| #SBATCH -p Q   |   |
| #SBATCH -w gnode1  |   |
| #SBATCHexclusive   |   |
|  |   |
| srun -n2ntasks-per-node=1 python hhl_demo.py : -n1   |   |
| ntasks-per-node=1 python circuit simulator.py  |   |

Listing 7. hetjob.sh, the main job script

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