Quantum factorization simulation as a benchmark for HPC

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Why quantum factorization as a benchmark

- Quantum factorization a widely known & relevant problem, it is known to be hard to simulate
- Good to quantify the ability of a computer to simulate ideal quantum circuits
- The output is reproducible, easy to validate and understand
- Each additional qubit doubles RAM usage, CPU power and internode communication: excellent to test large machines
- Runs in a reasonable time: 1/2-3 hours
- Minimal portable code with ~300 lines of C and MPI
- It just runs: no input or special knowledge from user

Summary of the benchmark

- Simulates a quantum computer with state $|\psi\rangle = \sum_{x=0}^{(2^Q-1)} c_x \, |x\rangle$
- The test consists on running a simplified Shor's algorithm* with increasing number of Q qubits until resources are exhausted.
- Only timing of Fourier Transform AQFT, not the modular exponentiation
- For each Q run the simplified Shor's algorithm to factorize an integer n

$$n = p \cdot q$$

- p and q are chosen to maximize the period r of $2^x \, mod \, n$

  with the constraints $n^2 \leq 2^Q < 2n^2$ with r even and $2^{r/2} \neq -1 \, mod \, n$
- Then verify that the total probability under peaks is larger than $1/2$

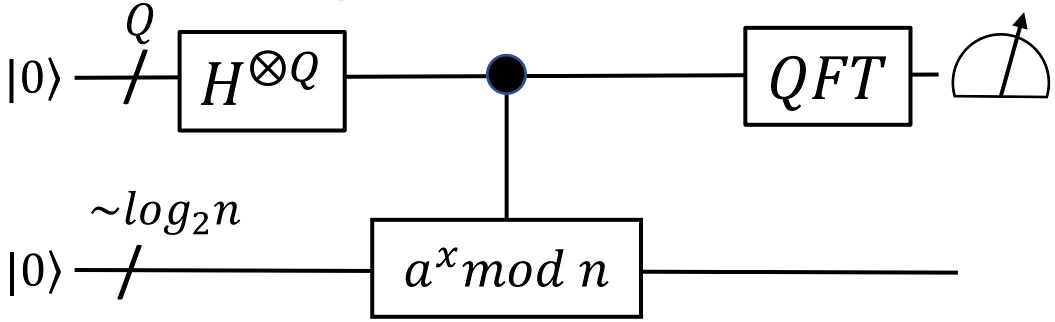
$$P = \sum_{peaks} |c_x|^2 \quad > \frac{1}{2}$$

- Peaks located at $x = \frac{2^Q}{(p-1)(q-1)} \times \text{integer}$

* PW Shor, "Polynomial-Time algorithms for prime Factorization and Discrete Logarithms on a Quantum Computer", SIAM J. Comp 1997

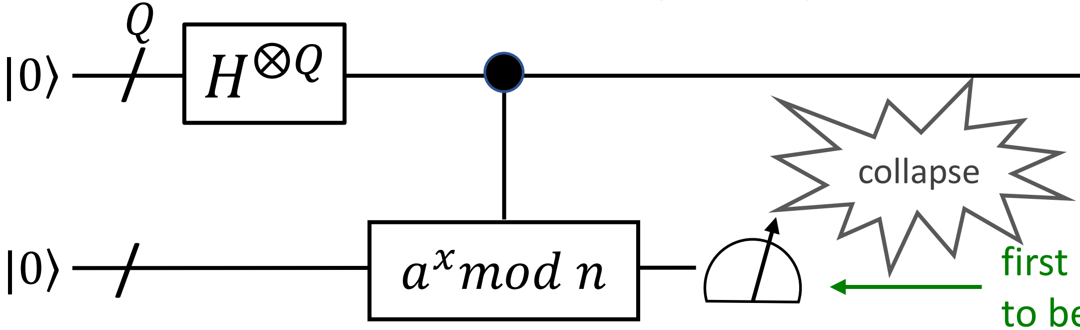
Use deferred measurement principle to save qubits

Original Shor’s algorithm



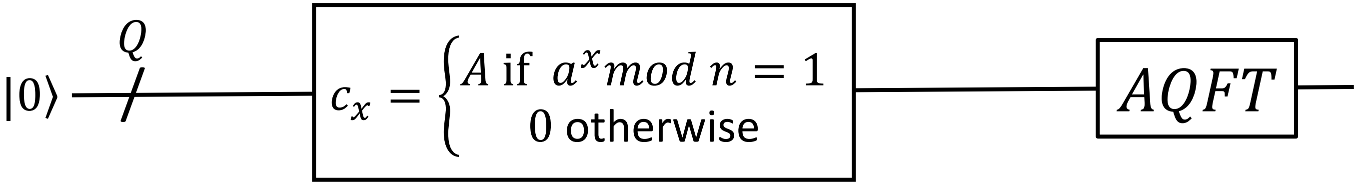
This measurement is inconvenient in a benchmark

With deferred measurement principle



first measurement outcome chosen to be 1 for sake of benchmarking

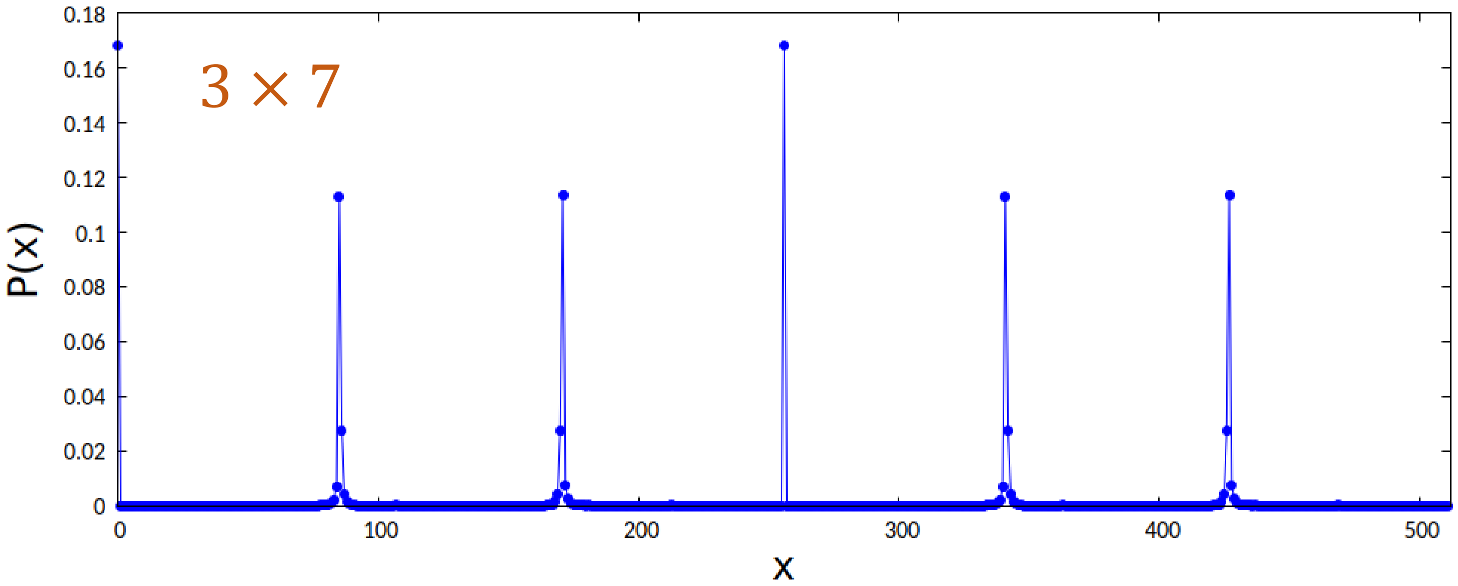
This benchmark saves $log_2 n$ qubits, only AQFT is timed

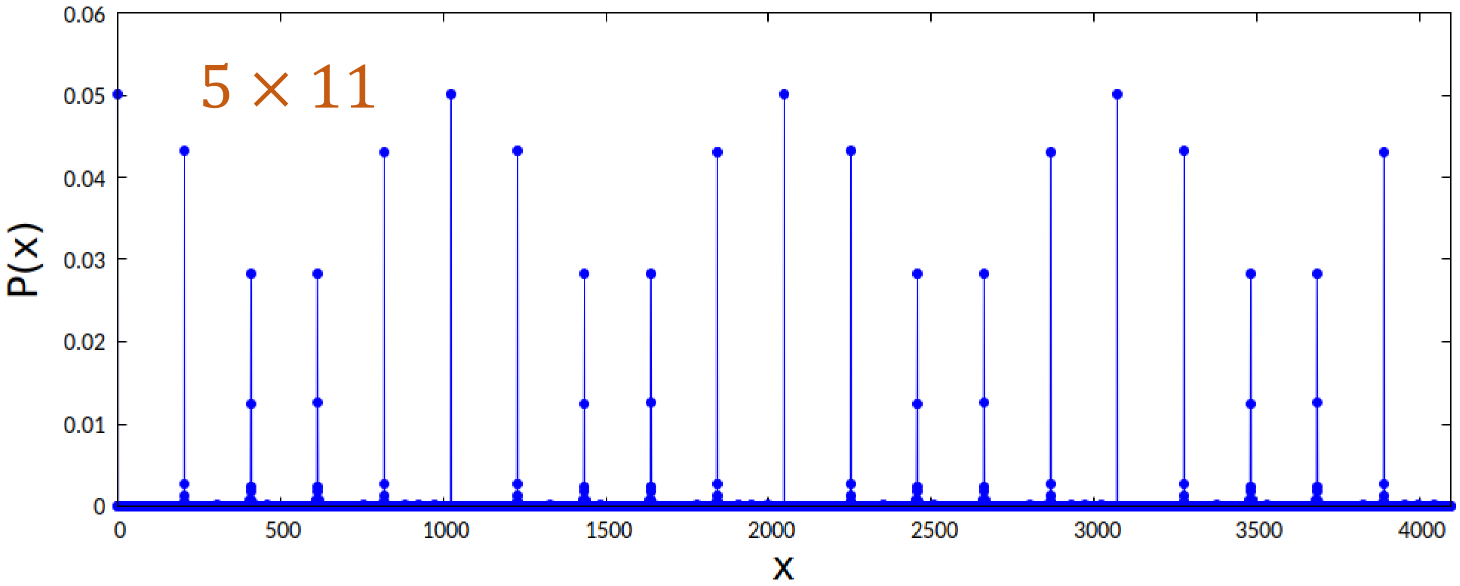


Do not measure, just check peak locations

A is a normalization const.

Verify location of peaks for each $n = p \cdot q$





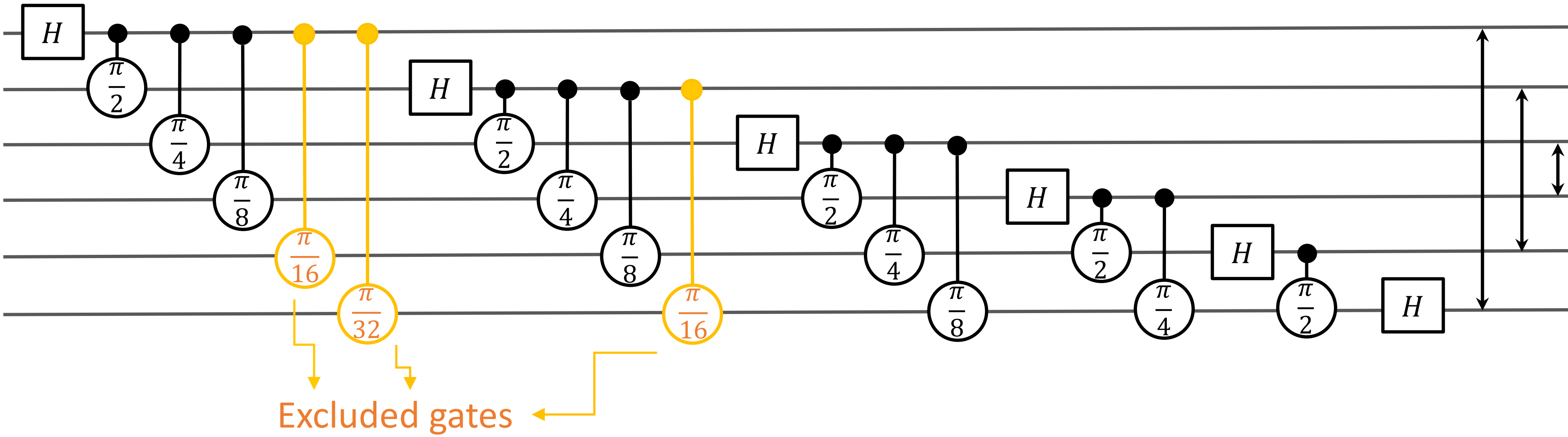
List of factorizations used in the test

$n = p \cdot q$ chosen to maximize period r of $2^x\ mod\ n,\ n^2 \leq 2^Q < 2n^2$
with r even and $2^{r/2} \neq \pm 1\ mod\ n$

Q	$p \times q$
9	3×7
10	3×7
11	3×13
12	5×11
13	7×11
14	5×23
15	11×13
16	11×23
17	5×71
18	19×23
19	23×29
20	19×53
21	23×61
22	29×67
23	47×61
24	29×139
25	29×199
26	47×173
27	71×163
28	83×197
29	79×293
30	103×317
31	149×311
32	101×647
33	149×619
34	269×487
35	167×1109
36	479×547
37	479×773
38	367×1427
39	859×863
40	563×1861
41	1039×1427
42	947×2213
43	1307×2269
44	2027×2069
45	2039×2909
46	2357×3559
47	2237×5303
48	3917×4283
49	4127×5749
50	4813×6971
51	6173×7687
52	6029×11131
53	7243×13103
54	10357×12959
55	12757×14879
56	11399×23549
57	19427×19541
58	20771×25847
59	24847×30557
60	27779×38653

Use AQFT* because it is faster than QFT

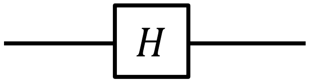
- For each H gate we compute $1 + log_2 Q$ controlled phase gates
- Phase gates computed with one memory access per state
- Complexity AQFT is $\mathrm{O}(\mathrm{Q}\log\mathrm{Q})$ versus $\mathrm{O}(Q^2)$ for QFT



Results in the approximation $f_y \cong \frac{1}{\sqrt{N}} \sum_{x=0}^{N-1} c_x e^{2\pi i x y/N}$

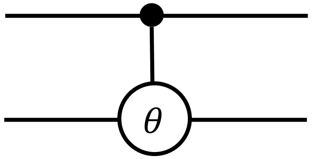
* D Coppersmith, An Approximate Fourier Transform Useful in Quantum Factoring, IBM report 1994
A Barenco et al, Approximate Quantum Fourier Transform and Decoherence, 1996

AQFT uses 3 types of gates



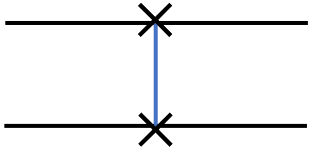
$$= \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

Hadamard



$$= \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & e^{i\theta} \end{bmatrix}$$

Controlled phase



$$= \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

Swap qubits

- The essentially heavy part of computation is the Approximate Fourier Transform, computed simulating gates
- Modular exponentiation $a^x \bmod n$ is not implemented gate-by-gate and it is not timed. We compute directly in C, and the computation time is negligible.
- Exponentiation could be implemented with stabilizer-group gates, thus simulated efficiently, not in this benchmark

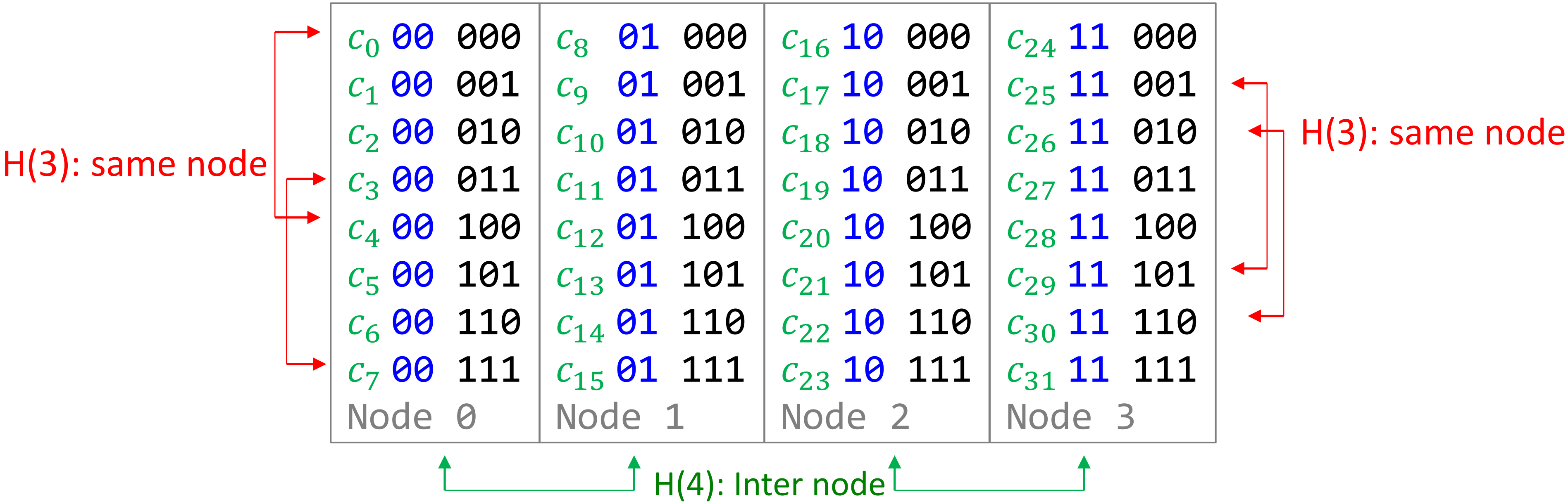
How are the coefficients distributed between nodes

- The state of the quantum registers $|\psi\rangle = \sum_{x=0}^{(2^Q-1)} c_x\,|x\rangle$ is distributed among nodes
- A basis state is described in binary as

$$|x\rangle = |b_Q b_{Q-1} \ldots b_{Q-M+1}\rangle \otimes |b_L b_{L-1} \ldots\, b_2\, b_1\rangle$$

- The black digits denote indices of amplitudes within each node.
- The blue digits denote node index.
- The number of nodes is $p = 2^M \quad Q = L + M$
- For example the Hadamard gate at qubit q combines the amplitudes c_x and c_y where x and y differ only in bit q.
- Depending on the value of q, we may be combining data between nodes or within node

Example H gate with *Q=5, L=3, M=2*



c_0 00 000	c_8 01 000	c_{16} 10 000	c_{24} 11 000
c_1 00 001	c_9 01 001	c_{17} 10 001	c_{25} 11 001
c_2 00 010	c_{10} 01 010	c_{18} 10 010	c_{26} 11 010
c_3 00 011	c_{11} 01 011	c_{19} 10 011	c_{27} 11 011
c_4 00 100	c_{12} 01 100	c_{20} 10 100	c_{28} 11 100
c_5 00 101	c_{13} 01 101	c_{21} 10 101	c_{29} 11 101
c_6 00 110	c_{14} 01 110	c_{22} 10 110	c_{30} 11 110
c_7 00 111	c_{15} 01 111	c_{23} 10 111	c_{31} 11 111
Node 0	Node 1	Node 2	Node 3

H(3): same node

H(3): same node

H(4): Inter node

How to use the benchmark (MPI version)

This is system dependent. In computers with mpicc and slurm, first prepare a batch file with number of nodes and number of tasks equal to a power of 2 and then launch

```
#SBATCH –o output-8nodesx64cores
#SBATCH --nodes=8     # 8 nodes
#SBATCH –n 256        # 64 cores per node
#SBATCH –p normal     # for KNL processors
#SBATCH –t 02:00:00   # usually less than 2 hours
ibrun ./quansimbench
```

```
> mpicc -Ofast quansimbench.c -o quansimbench -lm -Wall
> sbatch quansimbench.batch
```

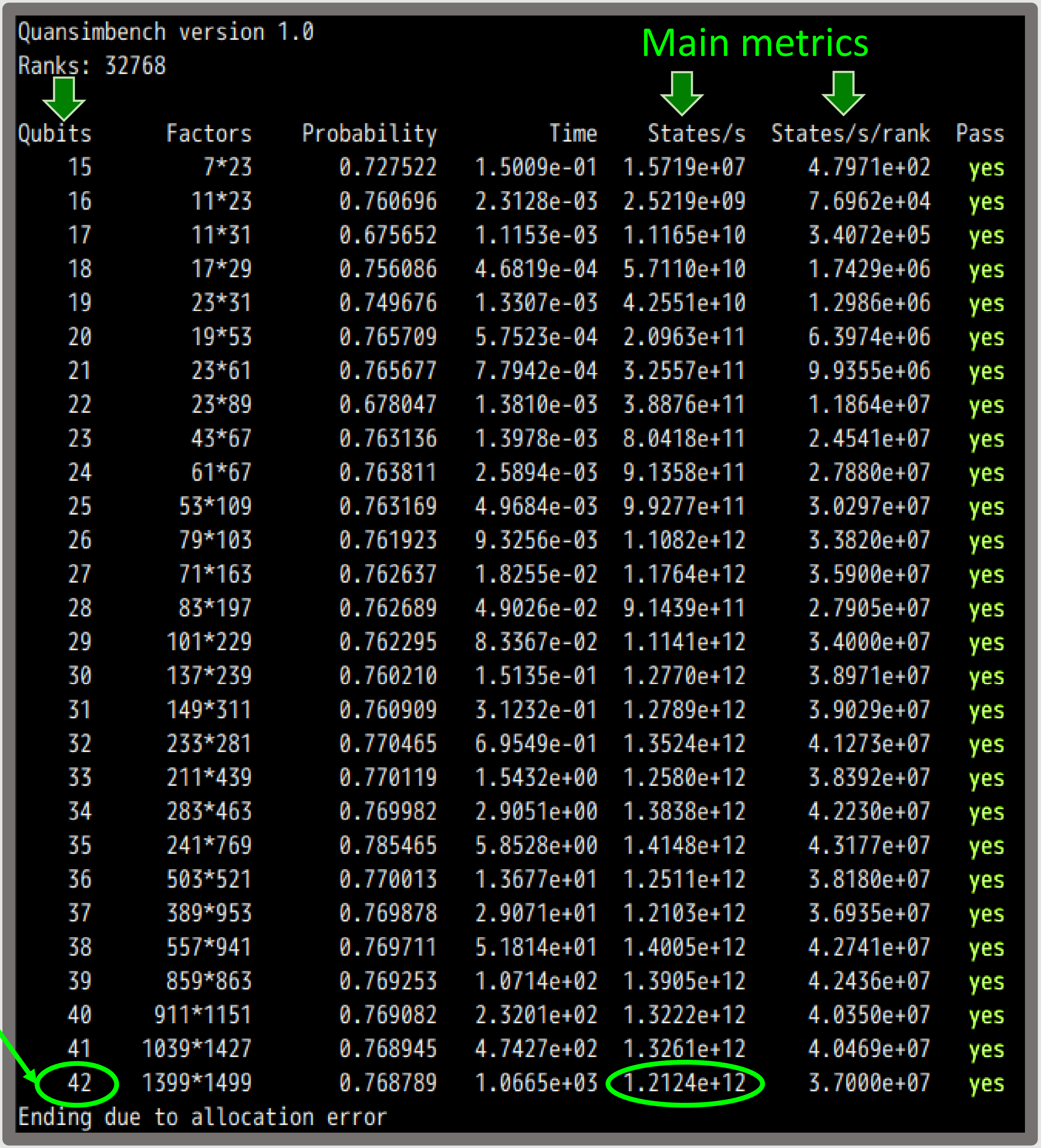
May need to add processor specific options such as

–xCORE-AVX512 for SKX
–xMIC-AVX512   for KNL

and may use OpenMP as well.

Typical output

- 32768 KNL cores
- 512 nodes
- memory limited
- less than 1h run



```
Quansimbench version 1.0
Ranks: 32768

Qubits      Factors   Probability       Time    States/s  States/s/rank  Pass
    15         7*23      0.727522 1.5009e-01  1.5719e+07     4.7971e+02   yes
    16        11*23      0.760696 2.3128e-03  2.5219e+09     7.6962e+04   yes
    17        11*31      0.675652 1.1153e-03  1.1165e+10     3.4072e+05   yes
    18        17*29      0.756086 4.6819e-04  5.7110e+10     1.7429e+06   yes
    19        23*31      0.749676 1.3307e-03  4.2551e+10     1.2986e+06   yes
    20        19*53      0.765709 5.7523e-04  2.0963e+11     6.3974e+06   yes
    21        23*61      0.765677 7.7942e-04  3.2557e+11     9.9355e+06   yes
    22        23*89      0.678047 1.3810e-03  3.8876e+11     1.1864e+07   yes
    23        43*67      0.763136 1.3978e-03  8.0418e+11     2.4541e+07   yes
    24        61*67      0.763811 2.5894e-03  9.1358e+11     2.7880e+07   yes
    25       53*109      0.763169 4.9684e-03  9.9277e+11     3.0297e+07   yes
    26       79*103      0.761923 9.3256e-03  1.1082e+12     3.3820e+07   yes
    27       71*163      0.762637 1.8255e-02  1.1764e+12     3.5900e+07   yes
    28       83*197      0.762689 4.9026e-02  9.1439e+11     2.7905e+07   yes
    29      101*229      0.762295 8.3367e-02  1.1141e+12     3.4000e+07   yes
    30      137*239      0.760210 1.5135e-01  1.2770e+12     3.8971e+07   yes
    31      149*311      0.760909 3.1232e-01  1.2789e+12     3.9029e+07   yes
    32      233*281      0.770465 6.9549e-01  1.3524e+12     4.1273e+07   yes
    33      211*439      0.770119 1.5432e+00  1.2580e+12     3.8392e+07   yes
    34      283*463      0.769982 2.9051e+00  1.3838e+12     4.2230e+07   yes
    35      241*769      0.785465 5.8528e+00  1.4148e+12     4.3177e+07   yes
    36      503*521      0.770013 1.3677e+01  1.2511e+12     3.8180e+07   yes
    37      389*953      0.769878 2.9071e+01  1.2103e+12     3.6935e+07   yes
    38      557*941      0.769711 5.1814e+01  1.4005e+12     4.2741e+07   yes
    39      859*863      0.769253 1.0714e+02  1.3905e+12     4.2436e+07   yes
    40     911*1151      0.769082 2.3201e+02  1.3222e+12     4.0350e+07   yes
    41    1039*1427      0.768945 4.7427e+02  1.3261e+12     4.0469e+07   yes
    42    1399*1499      0.768789 1.0665e+03  1.2124e+12     3.7000e+07   yes
Ending due to allocation error
```

Memory exhausted
Qubits=42
States/s=1.2124e12

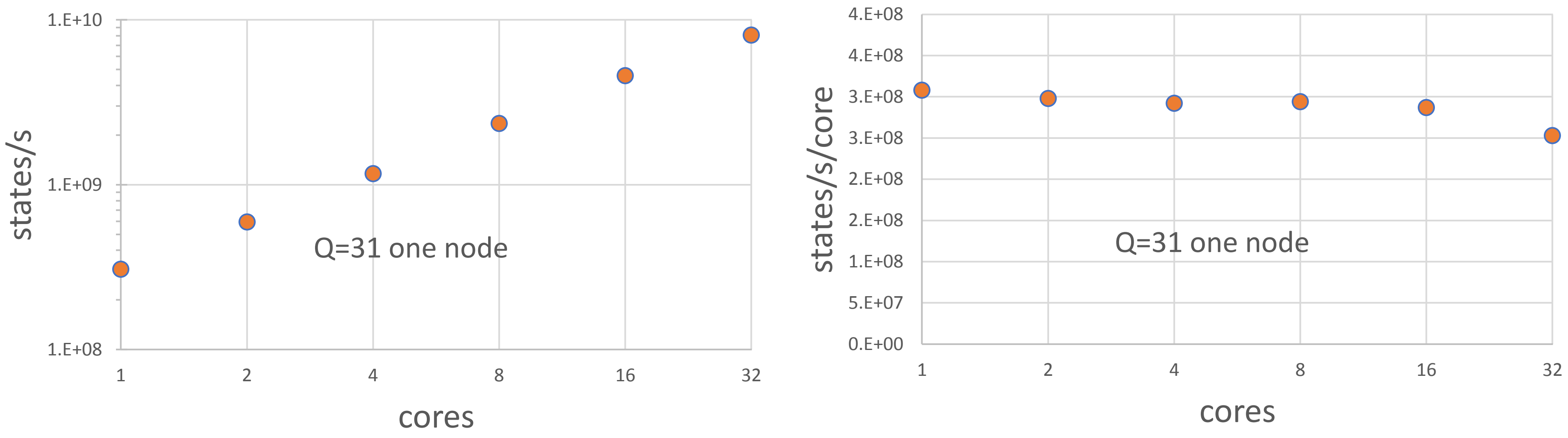
Normalized performance

- Number of basis states each core can process in a second

$$States/(s\ core) = \frac{gates \times 2^{Q}}{Rawtime \times cores}$$

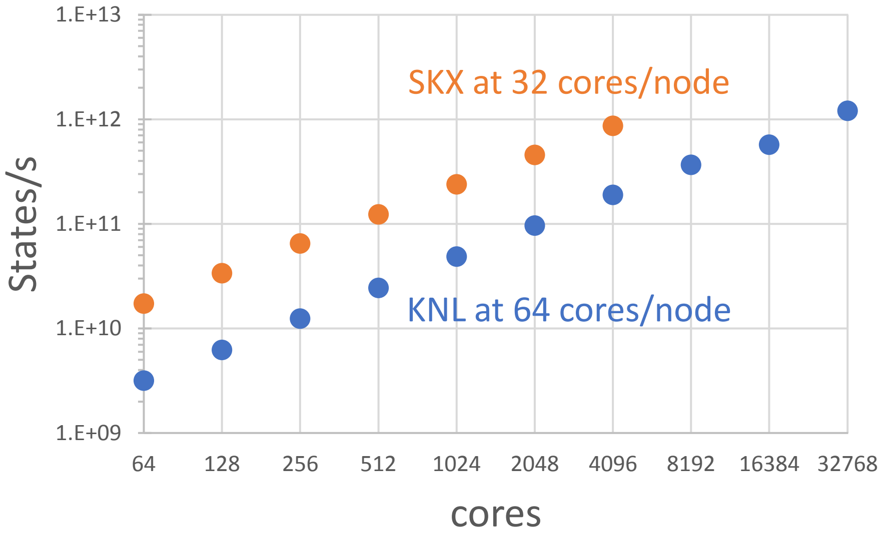
- In an ideal computer that should be a constant
- In reality it will vary due to the network and memory access
- Useful to compare cores
- Raw time useful to compare whole systems

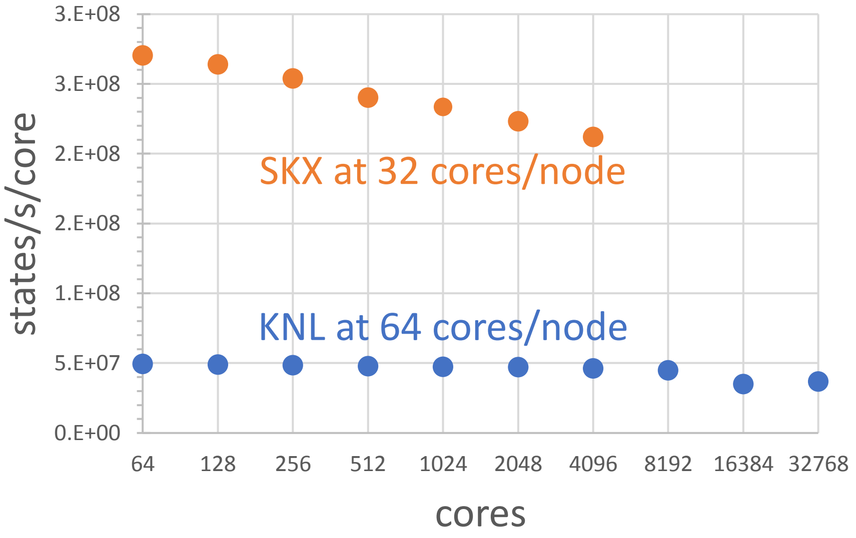
One node SKX Xeon 8160 and different core numbers, the metric is nearly constant.



A typical comparison in TACC’s Stampede 2

- Compare KNL Xeon Phi 7250 vs. SKX Xeon 8160 nodes
- From 1 to 512 nodes
- Left graph shows overall performance
- Right graph shows memory/switch slowdown in per core basis





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