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 Euler's totient function

$$\varphi = (p - 1) \cdot (q - 1)$$

with the constraint $n^2 \leq 2^Q < 2n^2$

- Then verify that the total probability under peaks is larger than $1/2$

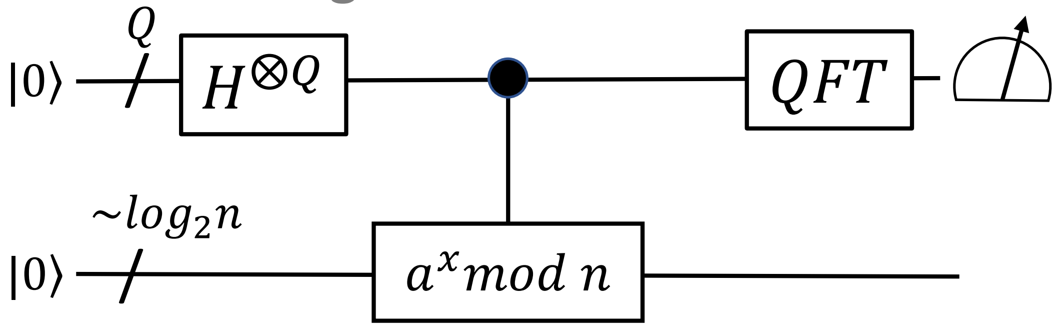
$$P = \sum_{peaks} |c_x|^2 \quad > \frac{1}{2}$$

- 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

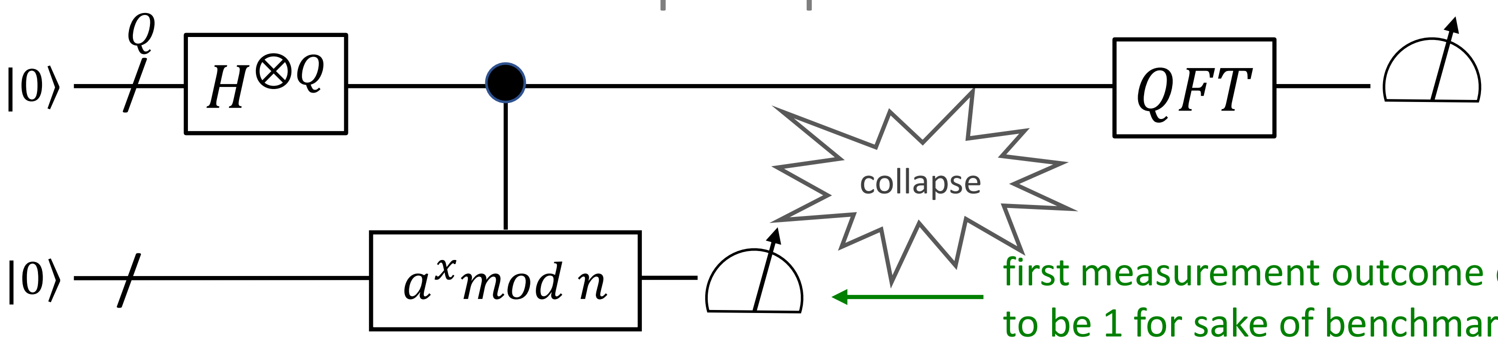
Use deferred measurement principle to save qubits

Original Shor's algorithm



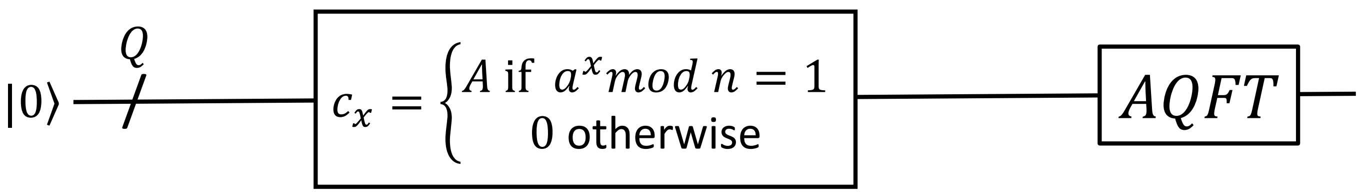
This measurement is inconvenient in a benchmark

With deferred measurement principle



first measurement outcome chosen to be 1 for sake of benchmarking

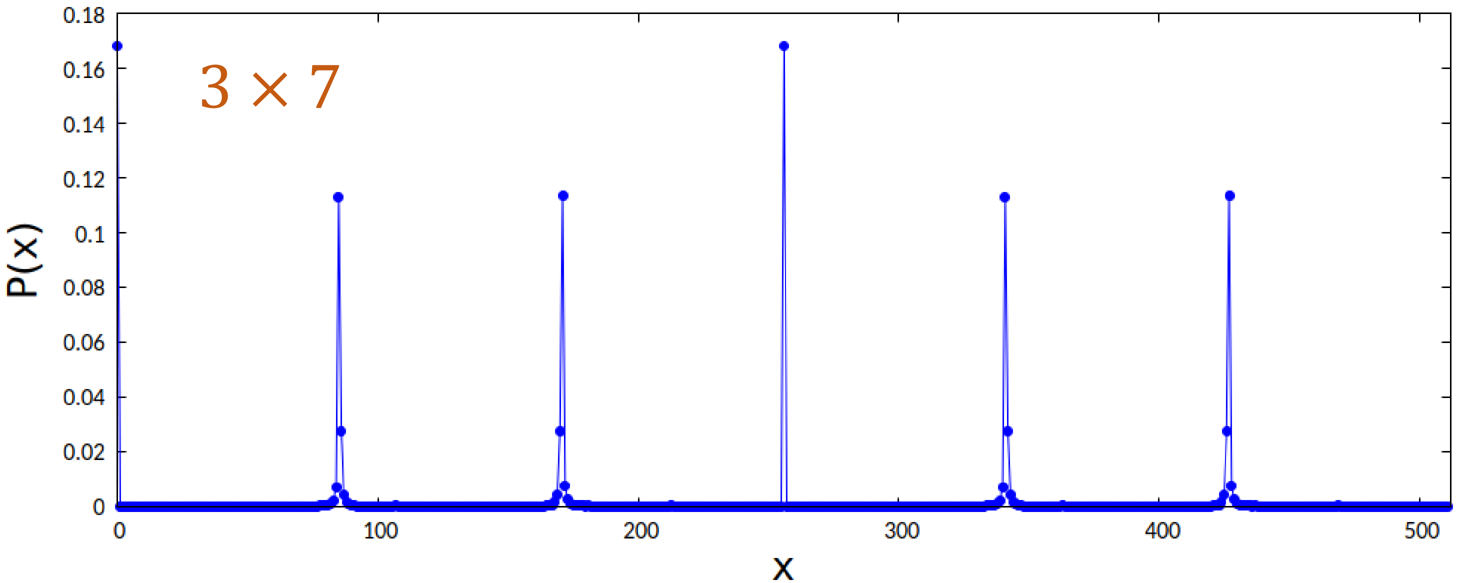
This benchmark saves $log_2 n$ qubits, only AQFT is timed

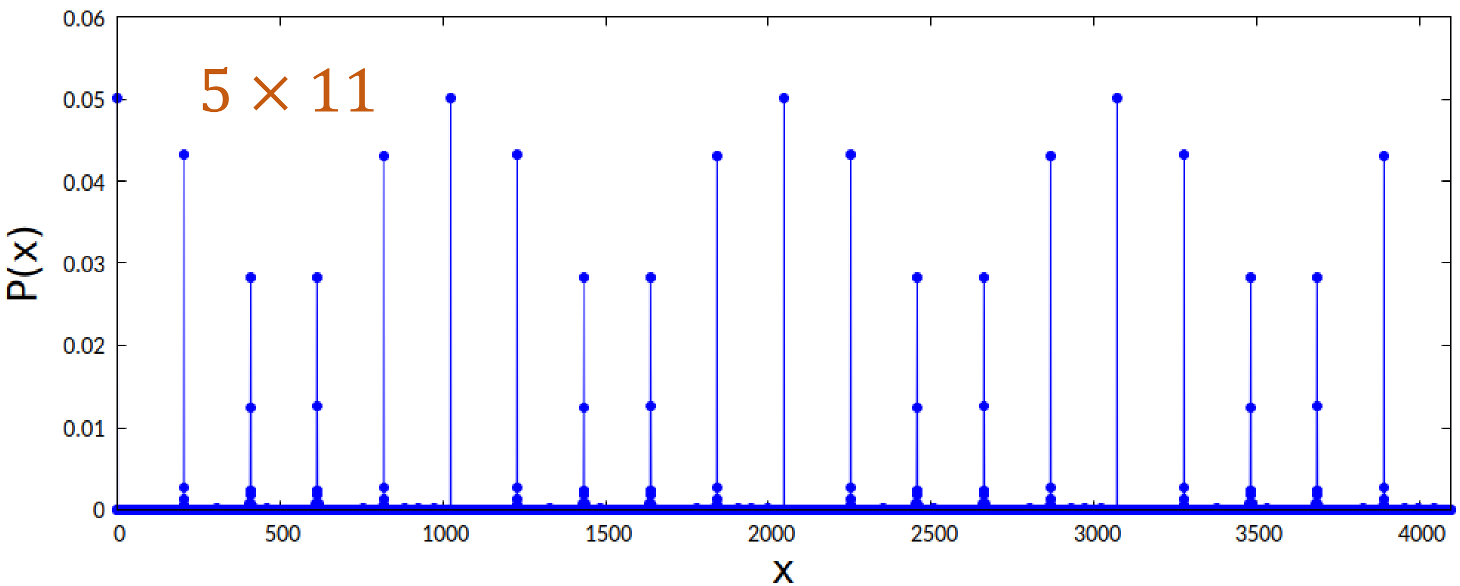


Do not measure, just check peak locations

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 $(p-1)\cdot(q-1)$, $n^2 \le 2^Q < 2n^2$

$p < q$, this way the period of $2^x \; mod \; n$ is maximized

Q	$p \times q$
9	3×7
10	3×7
11	3×13
12	5×11
13	7×11
14	7×71
15	7×23
16	11×23
17	11×31
18	17×29
19	23×31
20	19×53
21	23×61

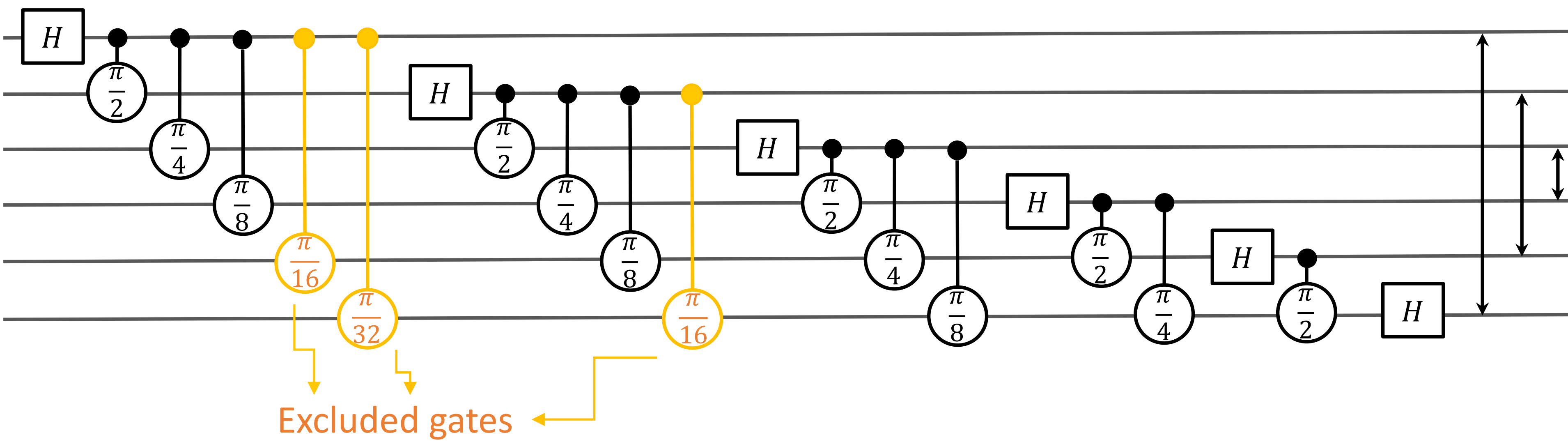
Q	$p \times q$
22	23×89
23	43×67
24	61×67
25	53×109
26	79×103
27	71×163
28	83×197
29	101×229
30	137×239
31	149×311
32	233×281
33	211×439
34	283×463

Q	$p \times q$
35	241×769
36	503×521
37	389×953
38	557×941
39	859×863
40	911×1151
41	1039×1427
42	1399×1499
43	1669×1777
44	1787×2347
45	2039×2909
46	2357×3559
47	2609×4547

Q	$p \times q$
48	4093×4099
49	3709×6397
50	5471×6133
51	5503×8623
52	8011×8377
53	8537×11117
54	11119×12071
55	12757×14879
56	12941×20743
57	17837×21283
58	22717×23633
59	24847×30557
60	28579×37571

Use AQFT* because it is faster than QFT

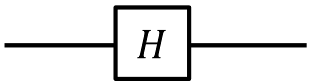
- For each H gate we compute $1 + log_2 Q$ controlled phase gates
- Phase gates computed with one memory access per state
- Complexity AQFT is O(Q log Q) versus $O(Q^2)$ for QFT



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

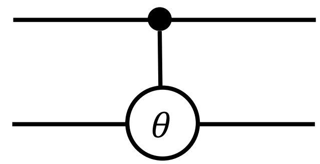
* D Coppersmith, An Approximate Fourier Transform Useful in Quantum Factoring, IBM report 1994
A Barenco et al, Approximate Quantum Fourier Transform and Decoherence, 1996

AQFT uses 3 types of gates



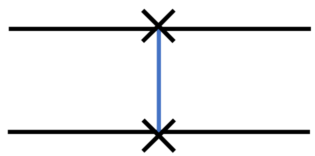
$$= \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

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

Memory exhausted
Qubits=42
States/s=1.2124e12

Main metrics

```
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
```

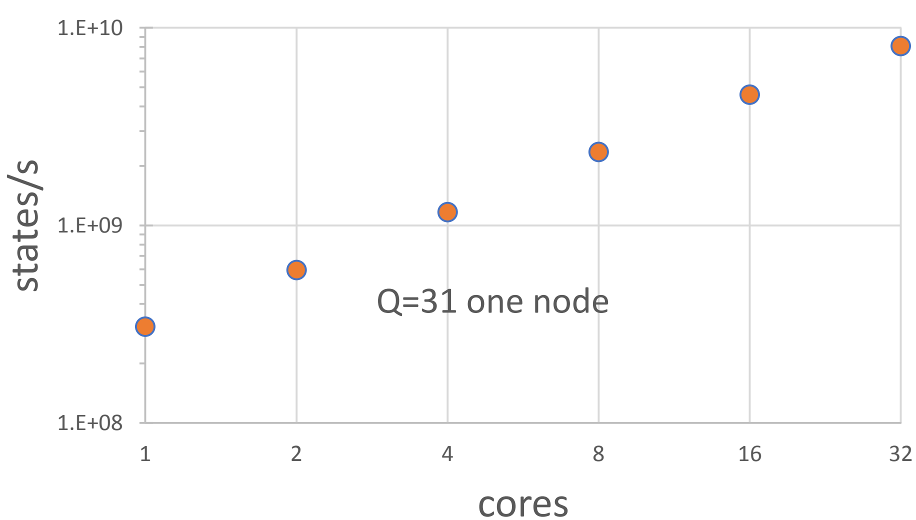
Normalized performance

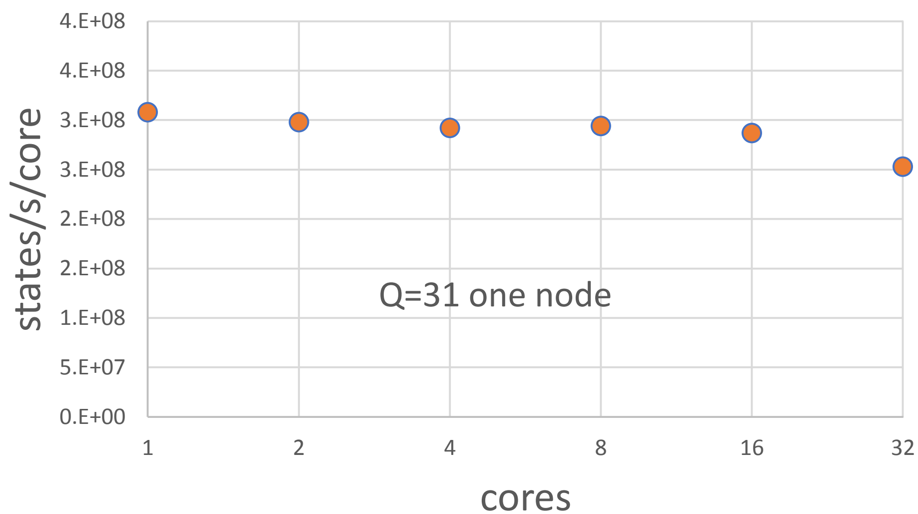
- Number of basis states each core can process in a second

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

- 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

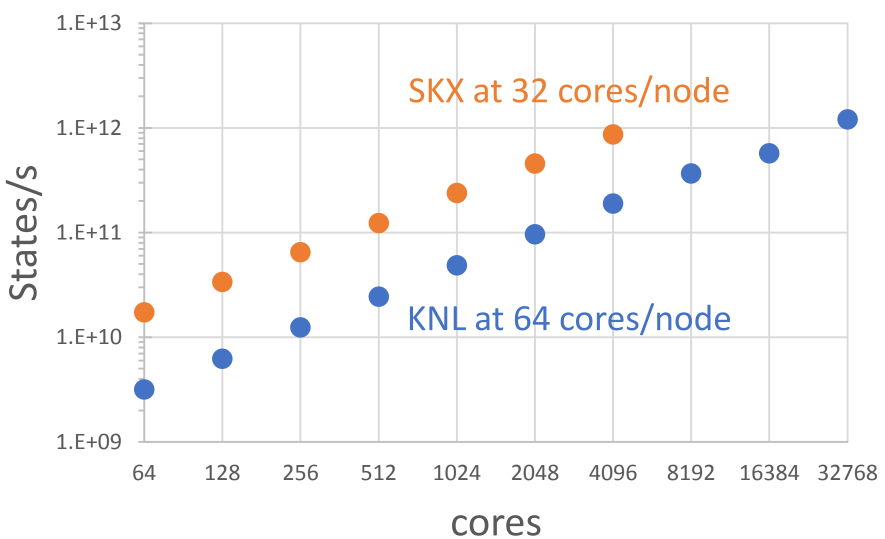
One node SKX Xeon 8160 and different core numbers, the metric is nearly constant.

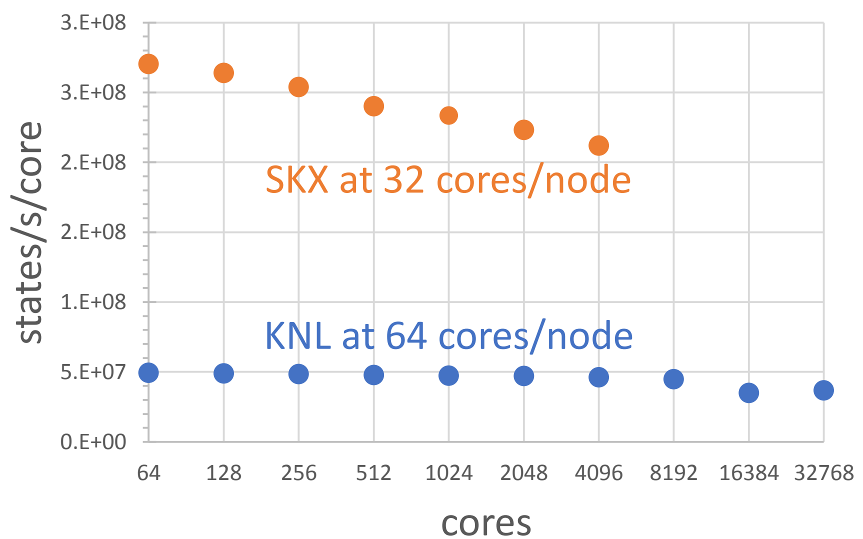




A typical comparison in TACC's Stampede 2

- 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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