CERFACS

CENTRE EUROPÉEN DE RECHERCHE ET DE FORMATION AVANCÉE EN CALCUL SCIENTIFIQUE

Journée TQCI – 14 Novembre

Presented by

Adrien Suau
adrien.suau@cerfacs.fr
CERFACS, LIRMM

In collaboration with

Gabriel Staffelbach
gabriel.staffelbach@cerfacs.fr
CERFACS

Henri Calandra
henri.calandra@total.com
Total

Aida Todri-Sanial
aida.todri@lirmm.fr
LIRMM, CNRS

Eric Bourreau
eric.bourreau@lirmm.fr
LIRMM

Hamiltonian Simulation

Or solving the 1-D wave equation using quantum computing

Time-dependent Schrödinger equation

The solution of

$$\frac{d}{dt}\left|\Psi\left(t\right)\right\rangle = -iH\left|\Psi\left(t\right)\right\rangle$$

is given by

$$\left|\Psi\left(t\right)\right\rangle = e^{-iHt}\left|\Psi\left(0\right)\right\rangle.$$

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Remark:

If we are able to implement e^{-iHt} as a quantum gate, we can solve the time-dependent Schrödinger equation.

Problem formalisation:

Given an Hamiltonian matrix H, a time t, a precision ϵ and a basis of several quantum gates, find a sequence of quantum gates $U = U_1 \dots U_n$ picked from the given basis that approximates the unitary matrix e^{-iHt} such that

$$\left|\left|e^{-iHt} - U\right|\right|_{\mathsf{sp}} \leqslant \epsilon.$$

According to Costa, Jordan, and Ostrander[1], the wave equation

$$\frac{d^2}{dt^2}\phi = \frac{d^2}{dx^2}\phi$$

- + boundary conditions
- + initial conditions
- + fixed propagation speed $c = 1$.

can be solved by simulating the action of a specific Hamiltonian to a quantum state encoding the initial state.

[1] Pedro C. S. Costa, Stephen Jordan, and Aaron Ostrander. "Quantum algorithm for simulating the wave equation". In: *Physical Review A* 99 (1 Jan. 2019). Phys. Rev. A 99, 012323 (2019). DOI: 10.1103/PhysRevA.99.012323. eprint: 1711.05394v1. URL: http://arxiv.org/abs/1711.05394v1.

Implementing Hamiltonian simulation

Simulation of the Hamiltonian by decomposing H into a sum of 1-sparse Hamiltonians

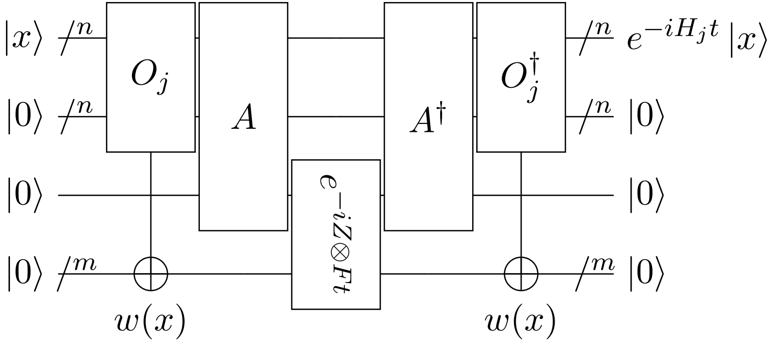
$$H = H_1 + H_2$$

Encode each H_i with an oracle

Required procedures:

- Quantum adder
- Quantum constant comparator
- Quantum logic gates (AND, OR, ...)

Simulate each H_j separately



```python
def simulate_unsigned_integer_weighted_hamiltonian(
    O: Oracle, n: int, int_size: int, time: float
) -> NamedRoutine:
    r""" [Documentation...] """
    oracle_ancilla_size = O.arity - (n + n + int_size)
    # Aliases to make the code more readable.
    x = list(range(0, n))
    m = list(range(n, 2 * n))
    v = list(range(2 * n, 2 * n + int_size))
    p = 2 * n + int_size
    a = list(range(2 * n + int_size + 1, 2 * n + int_size + 1 + oracle_ancilla_size))

    routine = NamedRoutine(
        "simulate_unsigned_integer_weighted_hamiltonian",
        arity=2 * n + int_size + 1 + oracle_ancilla_size,
    )

    routine.protected_apply(O, x, m, v, a)
    routine.protected_apply(A(n), x, m, p)

    routine.apply(exp_ZFt(int_size, time), p, v)

    routine.protected_apply(A(n).dag(), x, m, p)
    routine.protected_apply(O.dag(), x, m, v, a)

    return routine
```

Approximate e^{-iHt} with e^{-iH_1t} and e^{-iH_2t}

First-order approximation formula:

$$\begin{aligned} e^{-iHt} &= S_2(t) + \mathcal{O}\left(|t|^3\right) \\ &= e^{-i\frac{t}{2}H_1}e^{-itH_2}e^{-i\frac{t}{2}H_1} + \mathcal{O}\left(|t|^3\right) \end{aligned}$$

Approximate e^{-iHt} with e^{-iH_1t} and e^{-iH_2t}

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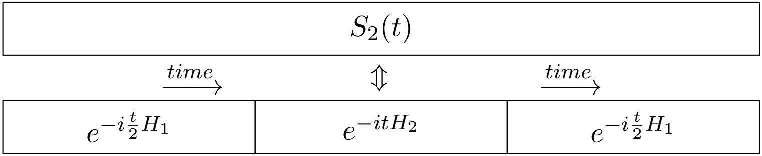
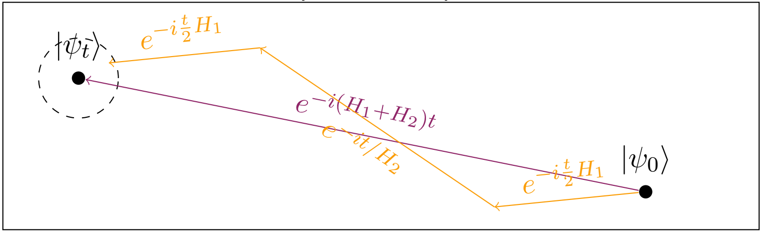


Approximate e^{-iHt} with $e^{-iH_1 t}$ and $e^{-iH_2 t}$

First-order approximation formula:

$$\begin{aligned} e^{-iHt} &= S_2(t) + \mathcal{O}\left(|t|^3\right) \\ &= e^{-i\frac{t}{2}H_1} e^{-itH_2} e^{-i\frac{t}{2}H_1} + \mathcal{O}\left(|t|^3\right) \end{aligned}$$

n-qubit state space



Approximate e^{-iHt} with e^{-iH_1t} and e^{-iH_2t}

k^{th} order approximation formula:

$$\begin{aligned} S_{2k}(t) &= \left[S_{2k-2}(p_k t)\right]^2 S_{2k-2}([1-4p_k]t) \left[S_{2k-2}(p_k t)\right]^2 \\ &= e^{-iHt} + \mathcal{O}\left(|t|^{2k+1}\right) \end{aligned}$$

Approximate e^{-iHt} with e^{-iH_1t} and e^{-iH_2t}

k^{th} order approximation formula:

$$
\begin{aligned}
S_{2k}(t) &= \left[S_{2k-2}(p_k t)\right]^2 S_{2k-2}([1-4p_k]t) \left[S_{2k-2}(p_k t)\right]^2 \\
&= e^{-iHt} + \mathcal{O}\left(|t|^{2k+1}\right)
\end{aligned}
$$

$S_{2k}(t)$				
	$\xrightarrow{\textit{time}}$	$\Updownarrow$	$\xrightarrow{\textit{time}}$	
$S_{2k-2}(p_k t)$	$S_{2k-2}(p_k t)$	$S_{2k-2}([1-4p_k]t)$	$S_{2k-2}(p_k t)$	$S_{2k-2}(p_k t)$

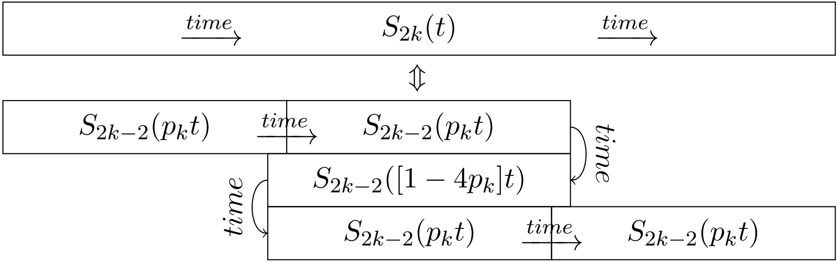
Implementing Hamiltonian simulation

Step 4

Approximate e^{-iHt} with $e^{-iH_1 t}$ and $e^{-iH_2 t}$

k^{th} order approximation formula:

$$
\begin{aligned}
S_{2k}(t) &= \left[S_{2k-2}(p_k t)\right]^2 S_{2k-2}([1-4p_k]t) \left[S_{2k-2}(p_k t)\right]^2 \\
&= e^{-iHt} + \mathcal{O}\left(|t|^{2k+1}\right)
\end{aligned}
$$

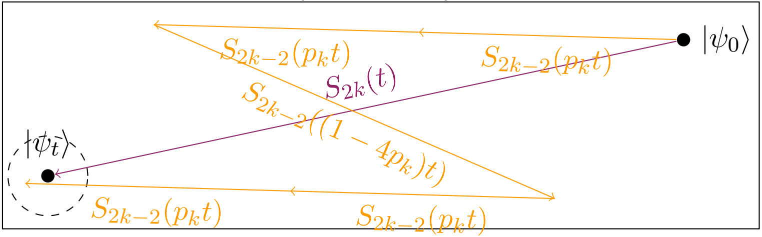


Approximate e^{-iHt} with e^{-iH_1t} and e^{-iH_2t}

k^{th} order approximation formula:

$$S_{2k}(t) = [S_{2k-2}(p_k t)]^2 \, S_{2k-2}([1-4p_k]t) \, [S_{2k-2}(p_k t)]^2$$
$$= e^{-iHt} + \mathcal{O}\left(|t|^{2k+1}\right)$$

n-qubit state space



Improve the previous approximation by scaling t

$$\left|\left|e^{-iHt} - S_{2k}(t)\right|\right| \in \mathcal{O}\left(\left|t\right|^{2k+1}\right)$$

implies

$$\left|\left|e^{-iHt} - \left[S_{2k}\left(\frac{t}{r}\right)\right]^r\right|\right| \in \mathcal{O}\left(\frac{\left|t\right|^{2k+1}}{r^{2k}}\right)$$

Improve the previous approximation by scaling t

$$\left|\left|e^{-iHt} - S_{2k}(t)\right|\right| \in \mathcal{O}\left(|t|^{2k+1}\right)$$

implies

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$S_{2k}(t)$

$\xrightarrow{time}$ $\Updownarrow$ $\xrightarrow{time}$

$S_{2k-2}(\frac{t}{r})$ | $S_{2k-2}(\frac{t}{r})$ | ……… $\times(r-4)$ ……… | $S_{2k-2}(\frac{t}{r})$ | $S_{2k-2}(\frac{t}{r})$

Improve the previous approximation by scaling t

$$\left|\left|e^{-iHt} - S_{2k}(t)\right|\right| \in \mathcal{O}\left(|t|^{2k+1}\right)$$

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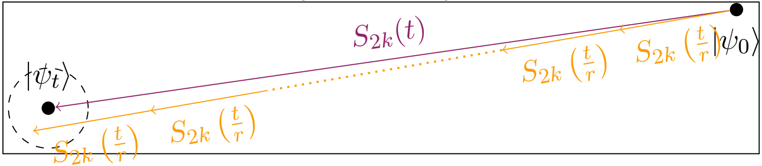
n-qubit state space



Quantum wave equation solver

Hamiltonian matrix to simulate:

$$H = \begin{pmatrix} 0 & \cdots & \cdots & 0 & 1 & 1 & 0 & \cdots & 0 \\ \vdots & & & \vdots & 0 & -1 & 1 & \ddots & \vdots \\ \vdots & & & \vdots & \vdots & \ddots & \ddots & \ddots & 0 \\ 0 & \cdots & \cdots & 0 & 0 & \cdots & 0 & -1 & 1 \\ 1 & 0 & \cdots & 0 & 0 & \cdots & \cdots & \cdots & 0 \\ 1 & -1 & \ddots & \vdots & \vdots & & & & \vdots \\ 0 & 1 & \ddots & \ddots & \vdots & & & & \vdots \\ \vdots & \ddots & \ddots & -1 & \vdots & & & & \vdots \\ 0 & \cdots & 0 & 1 & 0 & \cdots & \cdots & \cdots & 0 \end{pmatrix}$$

Hamiltonian matrix to simulate:

$$H = \begin{pmatrix} 0 & \cdots & \cdots & 0 & 1 & 1 & 0 & \cdots & 0 \\ \vdots & & & \vdots & 0 & -1 & 1 & \ddots & \vdots \\ \vdots & & & \vdots & \vdots & \ddots & \ddots & \ddots & 0 \\ 0 & \cdots & \cdots & 0 & 0 & \cdots & 0 & -1 & 1 \\ 1 & 0 & \cdots & 0 & 0 & \cdots & \cdots & \cdots & 0 \\ 1 & -1 & \ddots & \vdots & \vdots & & & & \vdots \\ 0 & 1 & \ddots & \ddots & \vdots & & & & \vdots \\ \vdots & \ddots & \ddots & -1 & \vdots & & & & \vdots \\ 0 & \cdots & 0 & 1 & 0 & \cdots & \cdots & \cdots & 0 \end{pmatrix} = H_1 + H_2$$

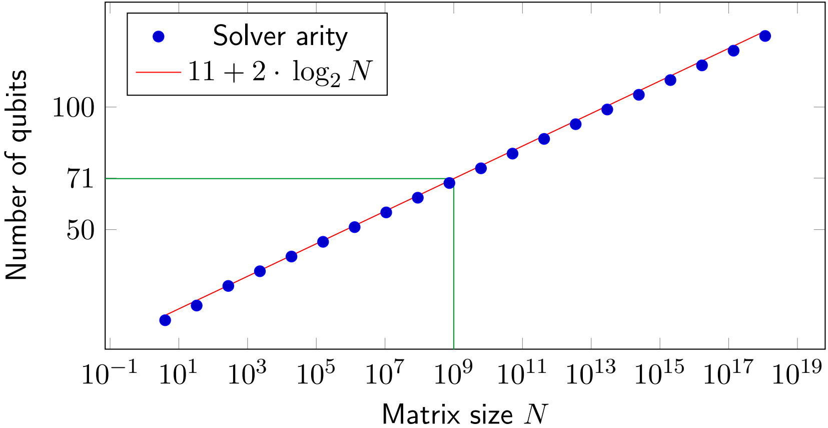
Implementation results

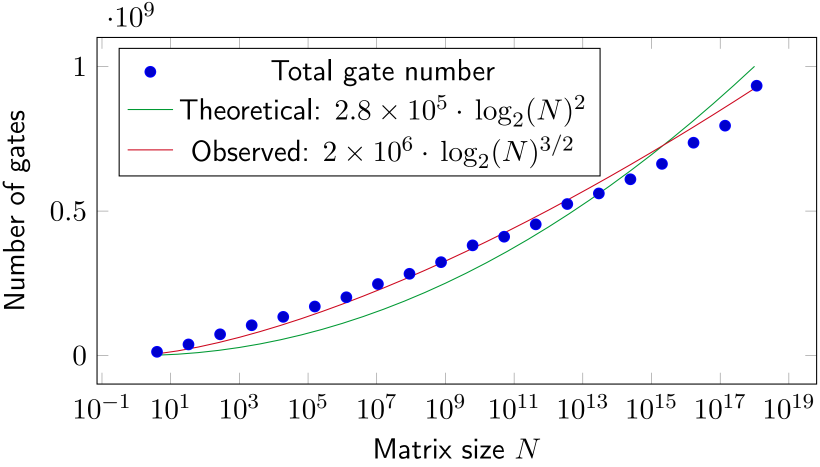
Hamiltonian Simulation

Default values

The default values used for each graph are:

- Precision $\left|\left|e^{-iHt} - U\right|\right|_{\text{sp}} \leqslant \epsilon = 10^{-5}$
- Order of the product-formula used $PF_{\text{order}} = 1$
- Simulation physical time $t = 1$


Solver arity
$11 + 2 \cdot \log_2 N$
Number of qubits
100
71
50
10^{-1} 10^{1} 10^{3} 10^{5} 10^{7} 10^{9} 10^{11} 10^{13} 10^{15} 10^{17} 10^{19}
Matrix size N



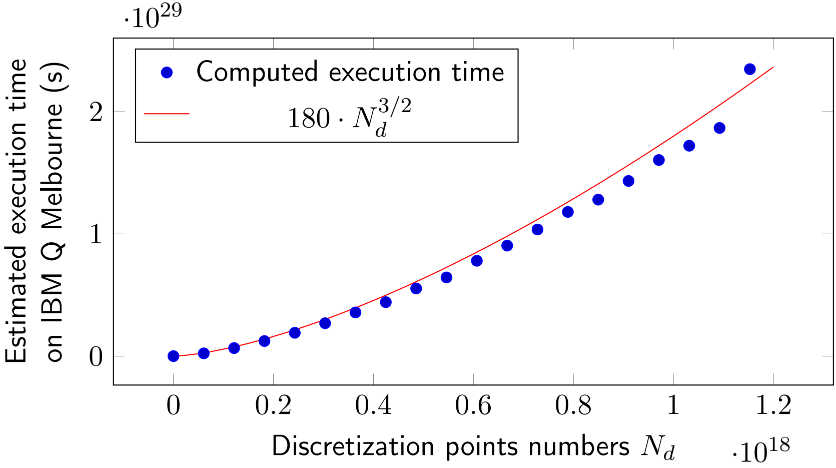
$\cdot 10^9$
1
0.5
0
Number of gates
Total gate number
Theoretical: $2.8 \times 10^5 \cdot \log_2(N)^2$
Observed: $2 \times 10^6 \cdot \log_2(N)^{3/2}$
10^{-1} 10^1 10^3 10^5 10^7 10^9 10^{11} 10^{13} 10^{15} 10^{17} 10^{19}
Matrix size N

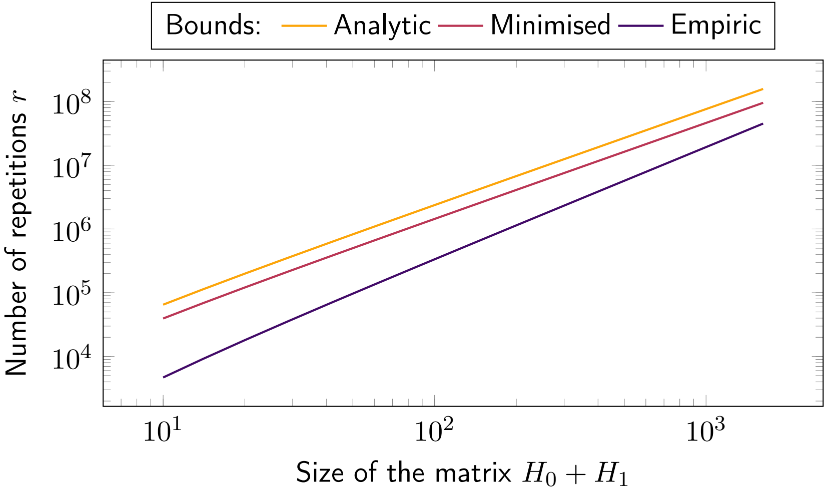
Implementation results

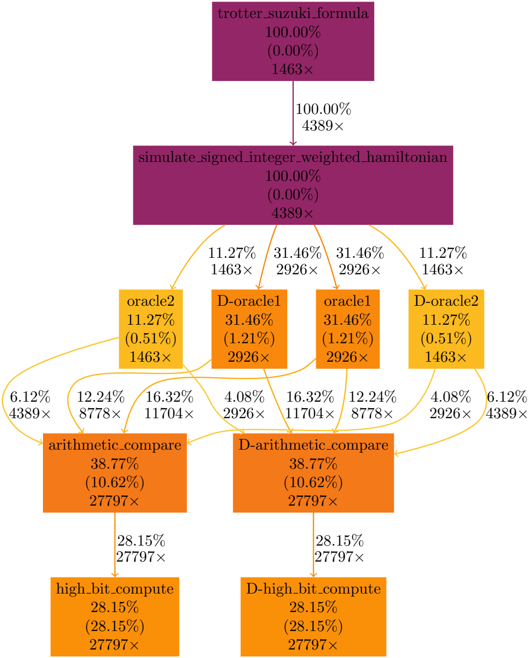
Quantum wave equation solver

Execution time estimation

- Hardware gate time are available online (at least for IBM chips).
- We averaged `CNOT` execution time over all the circuit.
- We ignored topology and number of qubits issues.


$\cdot 10^{29}$
Computed execution time
$180 \cdot N_d^{3/2}$
Estimated execution time
on IBM Q Melbourne (s)
0
1
2
0
0.2
0.4
0.6
0.8
1
1.2
Discretization points numbers N_d
$\cdot 10^{18}$


Bounds: Analytic Minimised Empiric
Number of repetitions r
10^4
10^5
10^6
10^7
10^8
10^1
10^2
10^3
Size of the matrix $H_0 + H_1$


trotter_suzuki_formula
100.00%
(0.00%)
1463×
100.00%
4389×
simulate_signed_integer_weighted_hamiltonian
100.00%
(0.00%)
4389×
11.27%
1463×
31.46%
2926×
31.46%
2926×
11.27%
1463×
oracle2
11.27%
(0.51%)
1463×
D-oracle1
31.46%
(1.21%)
2926×
oracle1
31.46%
(1.21%)
2926×
D-oracle2
11.27%
(0.51%)
1463×
6.12%
4389×
12.24%
8778×
16.32%
11704×
4.08%
2926×
16.32%
11704×
12.24%
8778×
4.08%
2926×
6.12%
4389×
arithmetic_compare
38.77%
(10.62%)
27797×
D-arithmetic_compare
38.77%
(10.62%)
27797×
28.15%
27797×
28.15%
27797×
high_bit_compute
28.15%
(28.15%)
27797×
D-high_bit_compute
28.15%
(28.15%)
27797×

Conclusion

- Hamiltonian simulation algorithm implemented
- Quantum wave equation solver implemented
- QLM is an ideal tool to test algorithms without all the hardware-related issues (noise, reliability, submition queues, ...)

- Towards a "Q-BLAS" library (PhD started in November 2019)
- Focus on linear algebra and partial differential equation solving (with a quantum computer)

Thank you for your attention!

Any question?

Contact information:

- Mail: adrien.suau@cerfacs.fr
- Phone: +33(0)5 61 19 31 19