Report: Week 6

Quantum Information and Computing (2021/22)

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Quantum N-body system

We denote each subsystem wavefunction with $|\psi_i\rangle \in \mathcal{H}^D$.

The wavefunction $|\Psi\rangle \in \mathcal{H}^{D^N}$ of a **pure state** of the whole system is

$$|\Psi\rangle = \sum_{\alpha_1,\ldots,\alpha_N} C_{\alpha_1,\ldots,\alpha_N} |\alpha_1\rangle \otimes \cdots \otimes |\alpha_N\rangle, \qquad |\alpha_i\rangle \in \{|0\rangle, \ldots, |D-1\rangle\}, \tag{1}$$

with ($C_{\alpha_1,\ldots,\alpha_N} \in \mathbb{C}$), while for the special case of a **separable pure state**,

$$|\Psi\rangle = \left(\sum_{\alpha_1} C_{\alpha_1} |\alpha_1\rangle\right) \otimes \cdots \otimes \left(\sum_{\alpha_N} C_{\alpha_N} |\alpha_N\rangle\right). \tag{2}$$

The non-separable case is defined by $\mathbf{D^N}$ complex coefficients, while the separable wavefunction requires $\mathbf{D \cdot N}$ complex coefficients.

We expect a **significantly smaller initialisation time** for a separable wave function.

Density matrix

For a pure state of an N-body wavefunction $|\Psi\rangle$, its **density matrix** is defined as

$$\rho = |\Psi\rangle\langle\Psi| = \sum_{i,j=0}^{d^N-1} C_j^* C_i |i\rangle\langle j| . \tag{3}$$

It is **positive semi-definite**, **hermitian**, with $\mathrm{Tr}(\rho) = 1$; for a pure state it holds $\rho^2 = \rho$ (the state is **idempotent**).

A **reduced density matrix** on the k^{th} subsystem is computed by tracing over all remaining subsystems:

$$\rho_k = \mathrm{Tr}_1 \cdots \mathrm{Tr}_{k-1} \mathrm{Tr}_{k+1} \cdots \mathrm{Tr}_N \rho, \qquad \mathrm{Tr}_i \rho = \sum_{j=0}^{d-1} \langle j|\rho|j\rangle . \tag{4}$$

In general: $\dim(\rho_k) = D^{N-1} \times D^{N-1}$.

We concentrate on **two-spin one-half** (qubits) states, $|\Psi\rangle \in \mathcal{H}^{D^2}$.

Listing 1: Implementation of the initialisation of a random (non-)separable state.

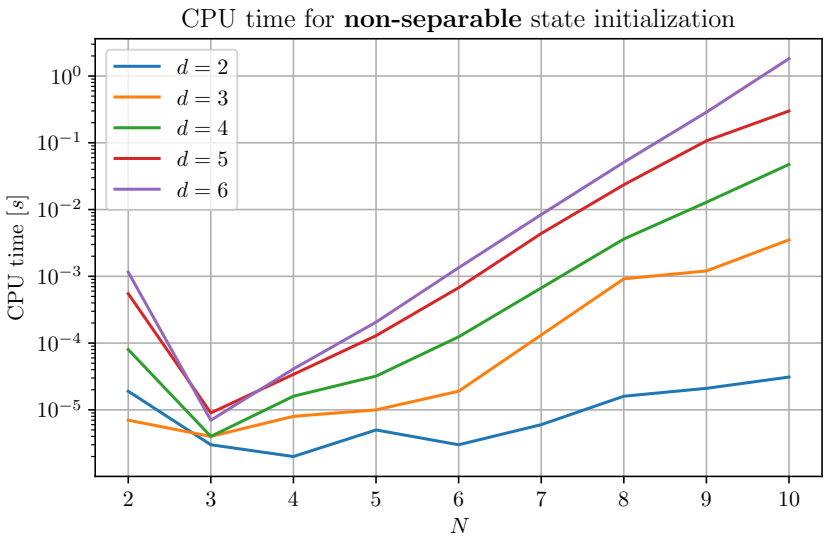
```
if (isSep) then
    dim = N * D
else
    dim = D**N
end if
```

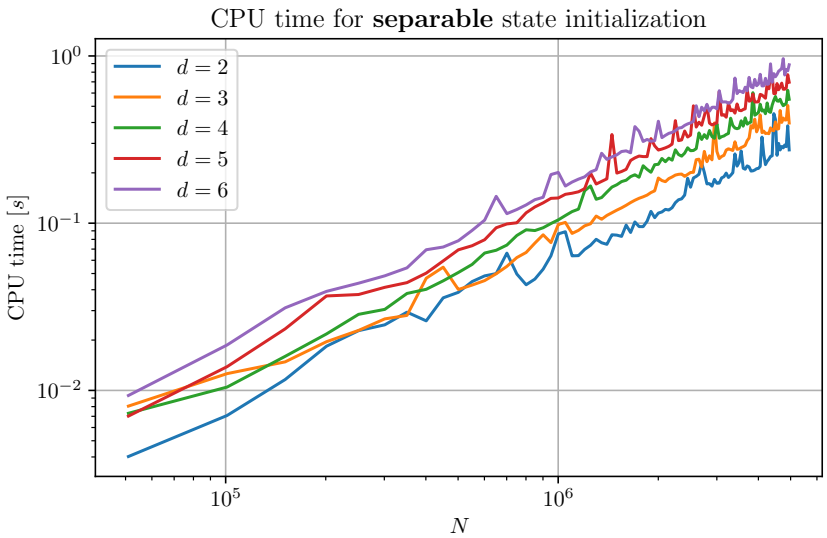
Listing 2: Implementation of the right partial trace for a bipartite system.

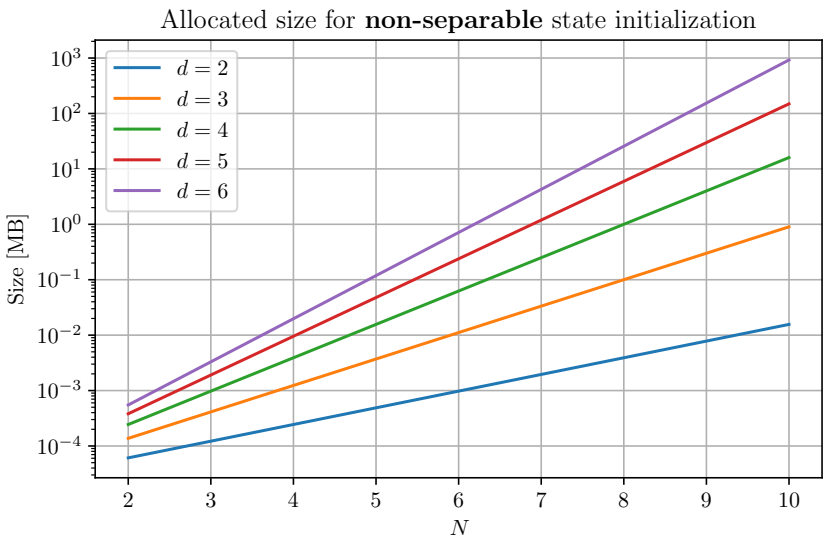
```
if (IAND(dim, dim-1).EQ.0) then ! Check if dimension is a power of 2
    rho_a = (0.d0,0.d0)
    do ii = 1,D
        do jj = 1,D
            do kk = 1,D
                rho_a(ii,jj) = rho_a(ii,jj) + &
                rho( (ii-1) * D + kk, (jj-1) * D + kk)
            end do
        end do
    end do
else
    call check(debug=.TRUE.,
               msg="System is not bipartite, aborting.", &
               msg_type="Error", stop_exec=.TRUE.)
end if
```

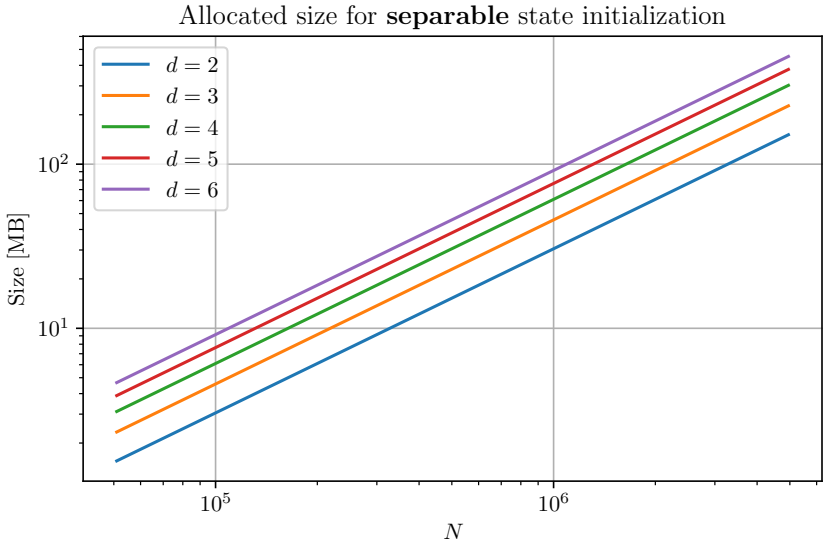
- We measure the **CPU time** needed to initialise a fully defined N-body **pure** state for both the separable and non-separable cases.
- We exploit the native functions `CPU_TIME()` and `SIZEOF()`.

Performance graphs









Listing 3: Implementation of the density matrix initialisation and reduction.

```
- State coefficients:
(-0.2201 -0.0005i)
(-0.5162 +0.6659i)
( 0.1632 +0.1195i)
( 0.4051 -0.1914i)

- Density matrix (rho):
( 0.0485 +0.0000i) ( 0.1133 +0.1468i) (-0.0360 +0.0262i) (-0.0891 -0.0423i)
( 0.1133 -0.1468i) ( 0.7099 -0.0000i) (-0.0047 +0.1704i) (-0.3366 +0.1709i)
(-0.0360 -0.0262i) (-0.0047 -0.1704i) ( 0.0409 +0.0000i) ( 0.0432 +0.0797i)
(-0.0891 +0.0423i) (-0.3366 -0.1709i) ( 0.0432 -0.0797i) ( 0.2007 -0.0000i)
Tr(rho):
( 1.0000 -0.0000i)
Tr(rho^2):
( 1.0000 -0.0000i)

- Reduced density matrix, right system (rho_a):
( 0.7584 -0.0000i) (-0.3725 +0.1972i)
(-0.3725 -0.1972i) ( 0.2416 -0.0000i)
Tr(rho_a):
( 1.0000 -0.0000i)

- Reduced density matrix, left system (rho_b):
( 0.0894 +0.0000i) ( 0.1566 +0.2265i)
( 0.1566 -0.2265i) ( 0.9106 -0.0000i)
Tr(rho_b):
( 1.0000 -0.0000i)
```