TOWARDS QUANTUM SIMULATIONS OF NUCLEAR REACTIONS

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OUTLINE

- Real time propagation with a quantum computer
- Simulation of nuclear dynamics
- Approximate time evolution of two interacting neutrons: simulations and actual quantum calculations on the LLNL and AQT testbeds
- Control-centric quantum computing

UNITARY TRANSFORMATIONS

The standard operations performed by a quantum computer on qubits is a **UNITARY TRANSFORMATION.** An example are rotations from one point to another of the Bloch sphere.

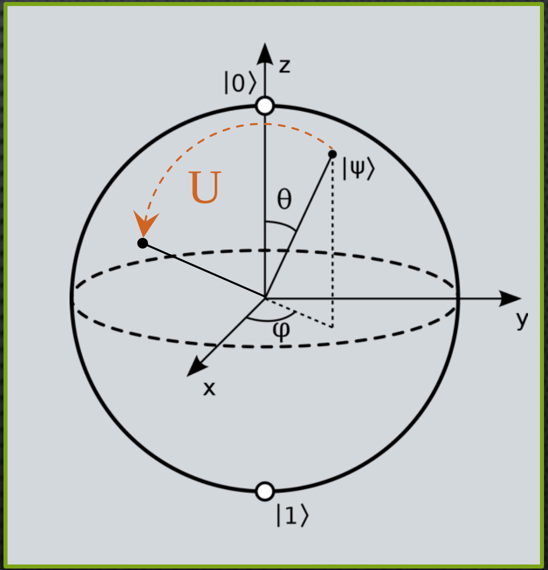
$$R_x(\theta) \equiv e^{-i\frac{\theta}{2}\sigma_x} = \cos\frac{\theta}{2}I - i\sin\frac{\theta}{2}\sigma_x = \begin{bmatrix} \cos(\theta/2) & -i\sin(\theta/2) \\ -i\sin(\theta/2) & \cos(\theta/2) \end{bmatrix}$$

However, the most relevant example for our problem is a time propagator:

$$U(t) = \exp(i\frac{H}{\hbar}t)$$

These operations can be performed on *N* qubits spanning a Hilbert space of needed dimensionality. And in principle the cost might just be polynomial in the number of degrees of freedom….

Bloch Sphere



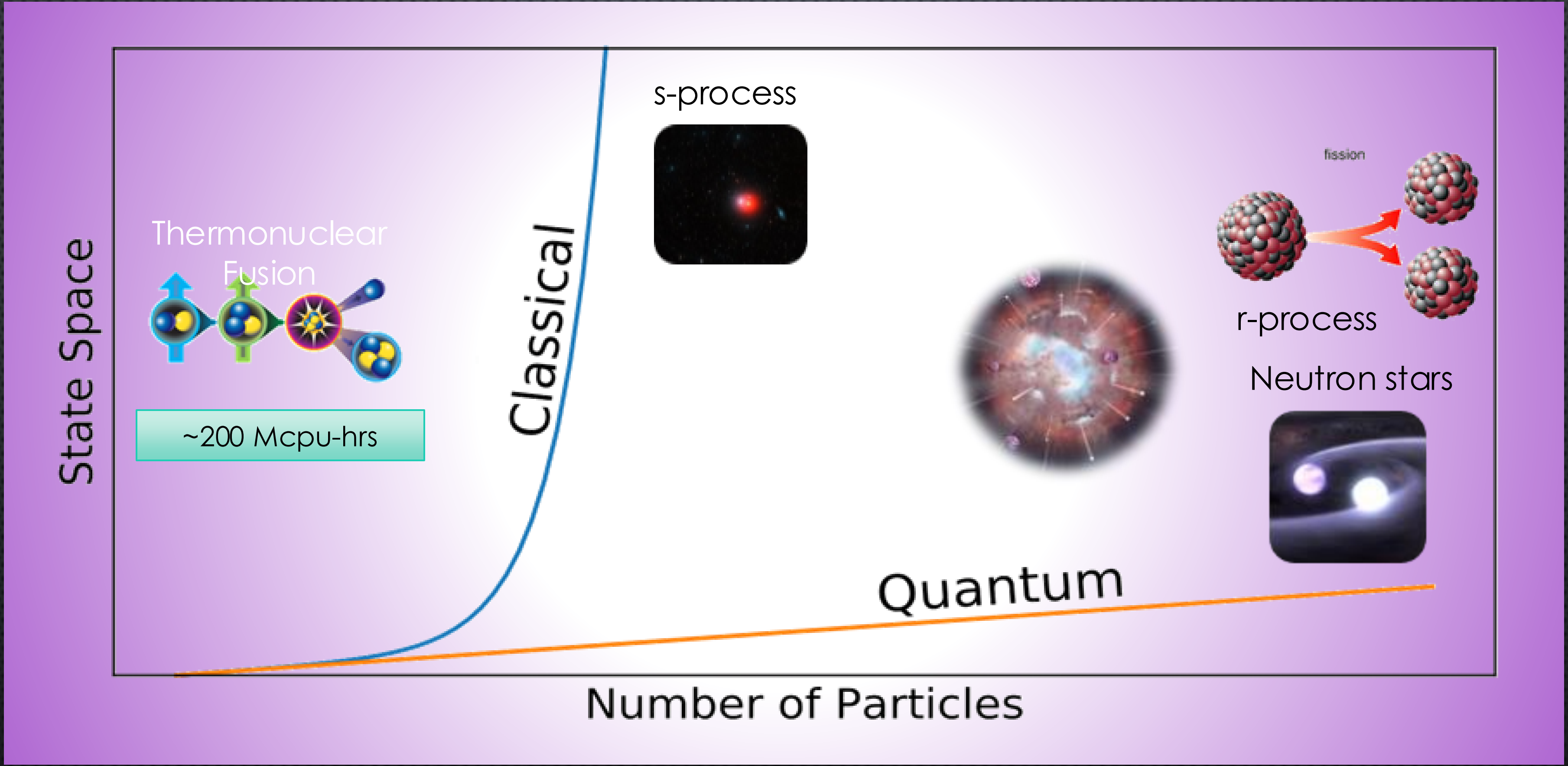
SIMULATING REACTIONS

The concept is somewhat simple. A reaction is just a time dependent process. A quantum computer is a tool that implements the time evolution of a quantum system so It should be relatively "easy" to describe a process just as it occurs, without approximations, provided that:

1) We actually know the Hamiltonian of the system (and for nuclear physics this is already not trivial, unless you do full fledged QCD…)
2) We can implement computations:
   a) In a reasonably large model Hilbert space (we don't really need it to be infinite, right?)
   b) Such that noise doesn't kill the signal over the time scale relevant for the process
3) We know how to tame dissipation (since nature gave us quasi elastic and inelastic processes…)

And yes, at this point a reasonable person should just turn around and give up, but if it is not difficult, it is not fun!

THE DREAM…..



State Space
Thermonuclear Fusion
~200 Mcpu-hrs
Classical
s-process
fission
r-process
Neutron stars
Quantum
Number of Particles

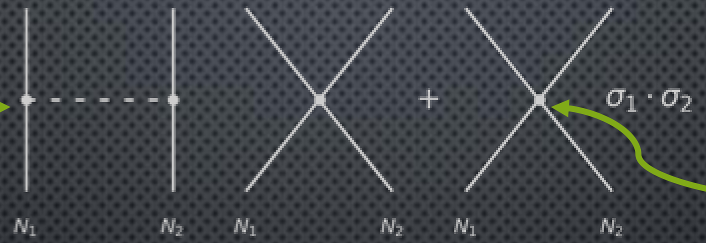
REALITY: A SIMPLE, YET NON-TRIVIAL, NUCLEAR PHYSICS PROBLEM…

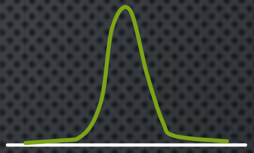
Describe how two neutrons evolve in time under the effect of their mutual interaction

- Interaction at leading-order (LO) of chiral effective field theory (spin tensor!)
- Implementation of real-time evolution of the system of 2 neutrons
- Realistic device-level simulations gauged on LLNL's QPU without/with measured noise
- Measurements/calculations on the LLNL testbed
- A simple extension on a digital machine (AQT testbed @ LBL) including some kind of evolution of the coordinates

NUCLEON NUCLEON INTERACTION (LO)

One-pion exchange (OPE)





Regularized contact (cutoff in momentum)

$$H_{\text{int}}^{\text{LO}} = V_{\text{OPE}}\,[1 - \delta_{R_0}(\vec{r})] + [C_0 + C_1\,\vec{\sigma}^1 \cdot \vec{\sigma}^2]\,\delta_{R_0}(\vec{r})$$

regulator function

$$V_{\text{OPE}} = \frac{f_\pi^2 m_\pi}{12\pi}\left[T_\pi(r)\,S_{12} - \left(Y_\pi(r) - \frac{4\pi}{m_\pi^3}\,\delta(\vec{r})\right)\vec{\sigma}^1 \cdot \vec{\sigma}^2\right]\vec{\tau}^1 \cdot \vec{\tau}^2$$

Spin independent

Spin dependent

TIME PROPAGATION

Formal solution of the time-dependent Schroedinger equation:

$$\exp\left(-\frac{i}{\hbar}\hat{H}t\right) = \exp\left[-\frac{i}{\hbar}\left(\hat{T}+\hat{V}_{SI}+\hat{V}_{SD}\right)t\right]$$

- V_{SI}: **SPIN-INDEPENDENT** part of the interaction
- V_{SD}: **SPIN-DEPENDENT** part of the interaction

In the short-time limit, we can separate the terms depending on V_{SI} and V_{SD}:

$$\exp\left[-\frac{i}{\hbar}\left(\hat{T}+\hat{V}_{SI}\right)\delta t\right]\exp\left[-\frac{i}{\hbar}\hat{V}_{SD}\delta t\right]+o(\delta t^2)$$

TIME PROPAGATION

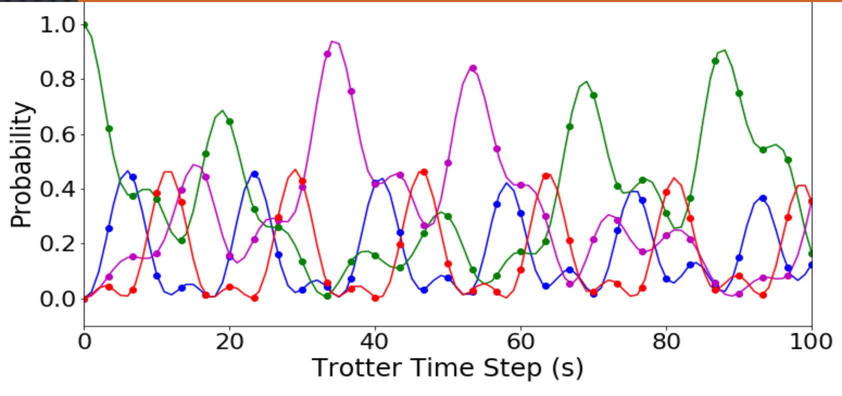
First application: "frozen" nucleons → Spin/isospin Hamiltonian only

$$\exp\left[-\frac{i}{\hbar}\hat{V}_{SD}\delta t\right] = \exp\left[-\frac{i}{\hbar}\left(\sum_{i,j=1}^{A}\sum_{\alpha,\beta=x,y,z}\sigma_{i\alpha}A(r_{ij})_{ij;\alpha\beta}\sigma_{j\beta}\right)\delta t\right]$$

coordinates appear as "parameters"

Computer simulation of the actual device

Occupation probability



Lines: analytic results

Circles: synthetic data: probability of measuring state $|\alpha\rangle$ after a time t (obtained by repeating the process over and over)

The time evolution with a tensor Hamiltonian introduces spin-parallel components

$|0\rangle = |\uparrow\uparrow\rangle$ $|1\rangle = |\uparrow\downarrow\rangle$ $|2\rangle = |\downarrow\uparrow\rangle$ $|3\rangle = |\downarrow\downarrow\rangle$

"COPROCESSING" SCHEME FOR FULL TIME EVOLUTION

$$\exp\left(-\frac{i}{\hbar}\hat{H}t\right) = \exp\left[-\frac{i}{\hbar}\left(\hat{T}+\hat{V}_{SI}+\hat{V}_{SD}\right)t\right]$$

As a first step in the direction of simulating the full dynamical evolution of a scattering process, we employed a mixed scheme in which the coordinates are evolved classically.

Remind that:

$$\exp\left[-\frac{i}{\hbar}\left(\hat{T}+\hat{V}_{SI}\right)\delta t\right]\exp\left[-\frac{i}{\hbar}\hat{V}_{SD}\delta t\right]+o(\delta t^2)$$

With T. Chistolini, A. Hashim, Y. Kim, W. Livingston, D. Santiago, I. Siddiq @LBLi, Phys. Rev. A 108, 032417 (2023)

We can make the (very crude) approximation of evolving the coordinates of the nucleons classically (using V_{SI}), and evolving the spin of the nucleons with the second factor in the propagator. Since the coordinates are evolved on a classical computer, we call this "coprocessing" scheme.

"COPROCESSING" SCHEME FOR FULL TIME EVOLUTION

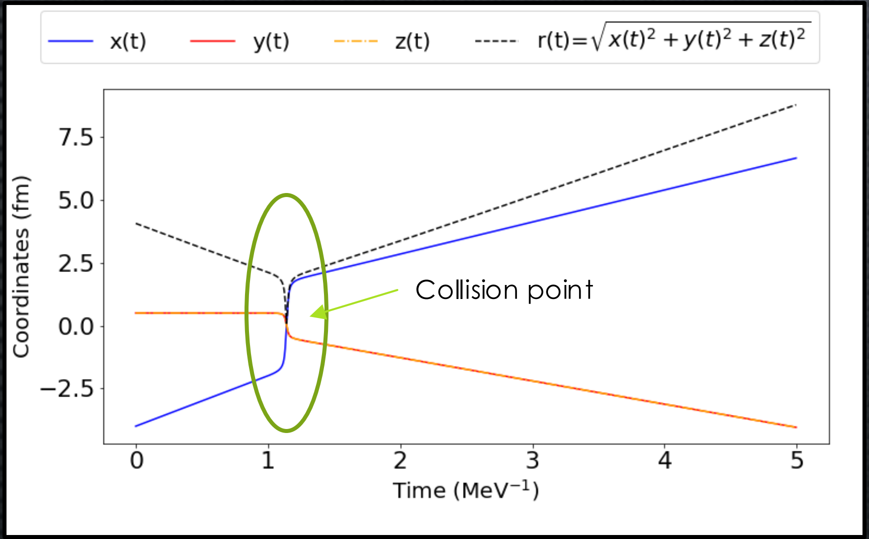
This approach has severe limits. In particular:

- The true space evolution is obviously not classical
- while there is feedback of the special evolution on the spin evolution, the opposite does not happen. This could be fixed in several ways.

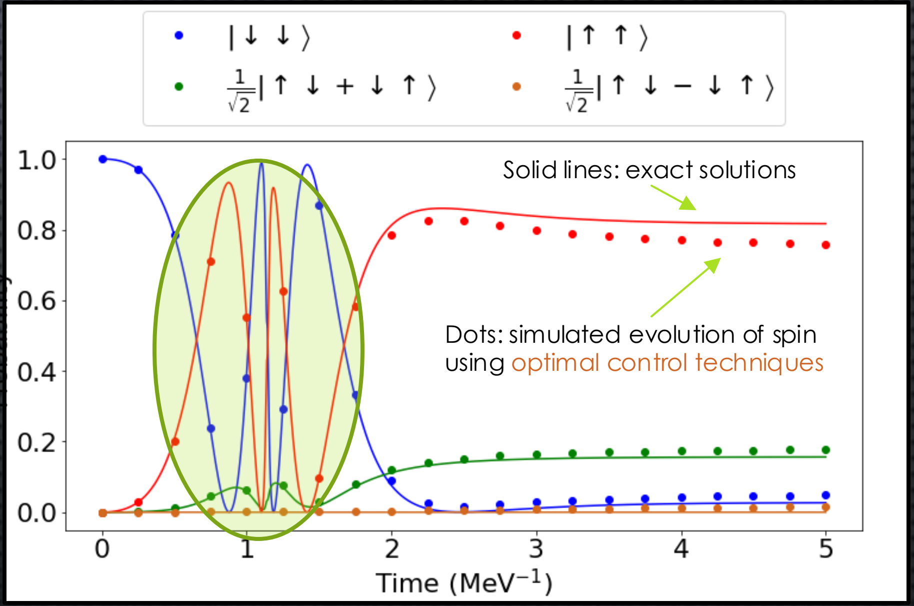
For the moment the aim is essentially to study the stability of a quantum computation in which the Hamiltonian has a heavy parametric dependence on time dependent quantities.

Essentially, one is studying the evolution of a state of a time-dependent Hamiltonian (which is one of the important features of the propagator when we use the Trotter decomposition)

TIME EVOLUTION OF SPIN (IDEAL CASE)

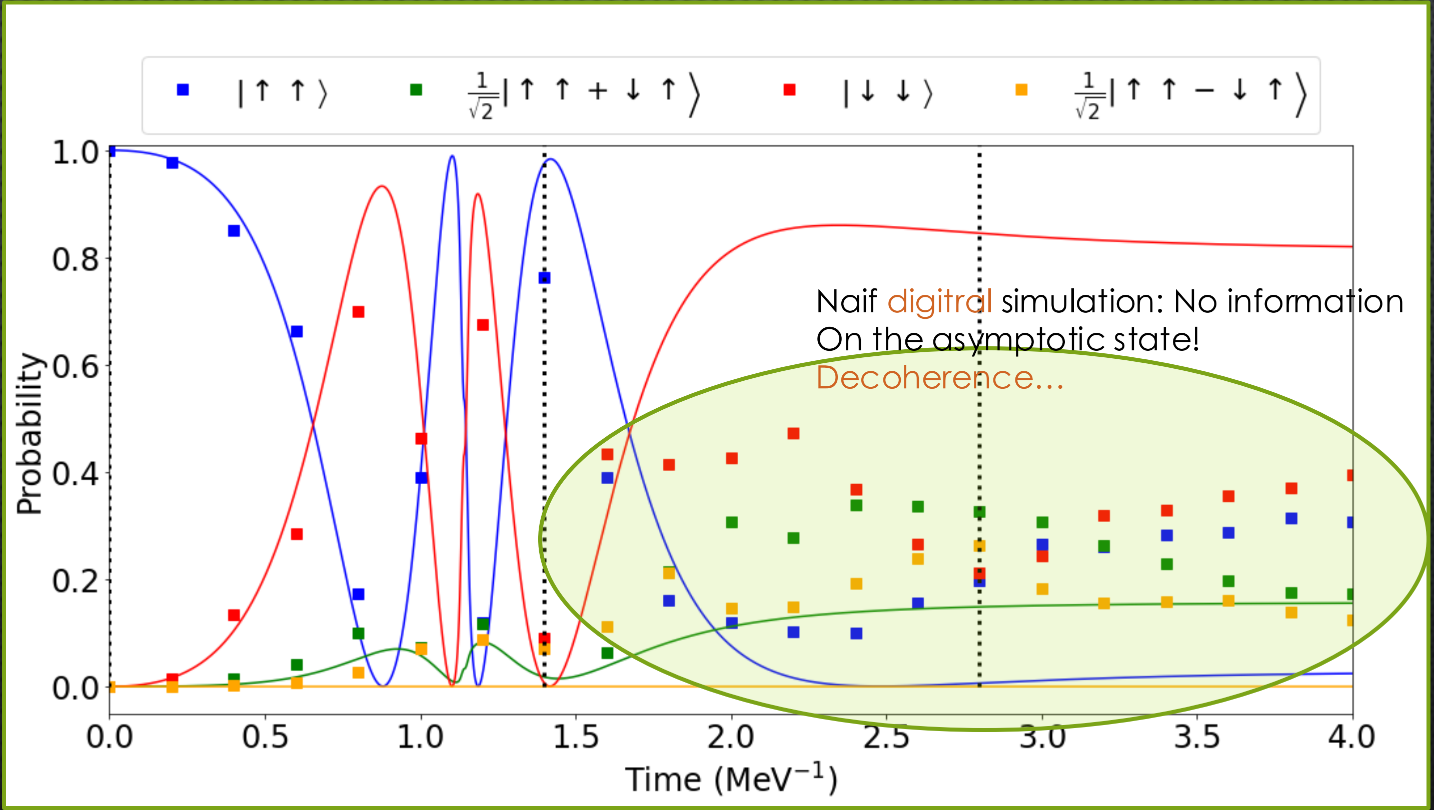


Evolution of the relative coordinate

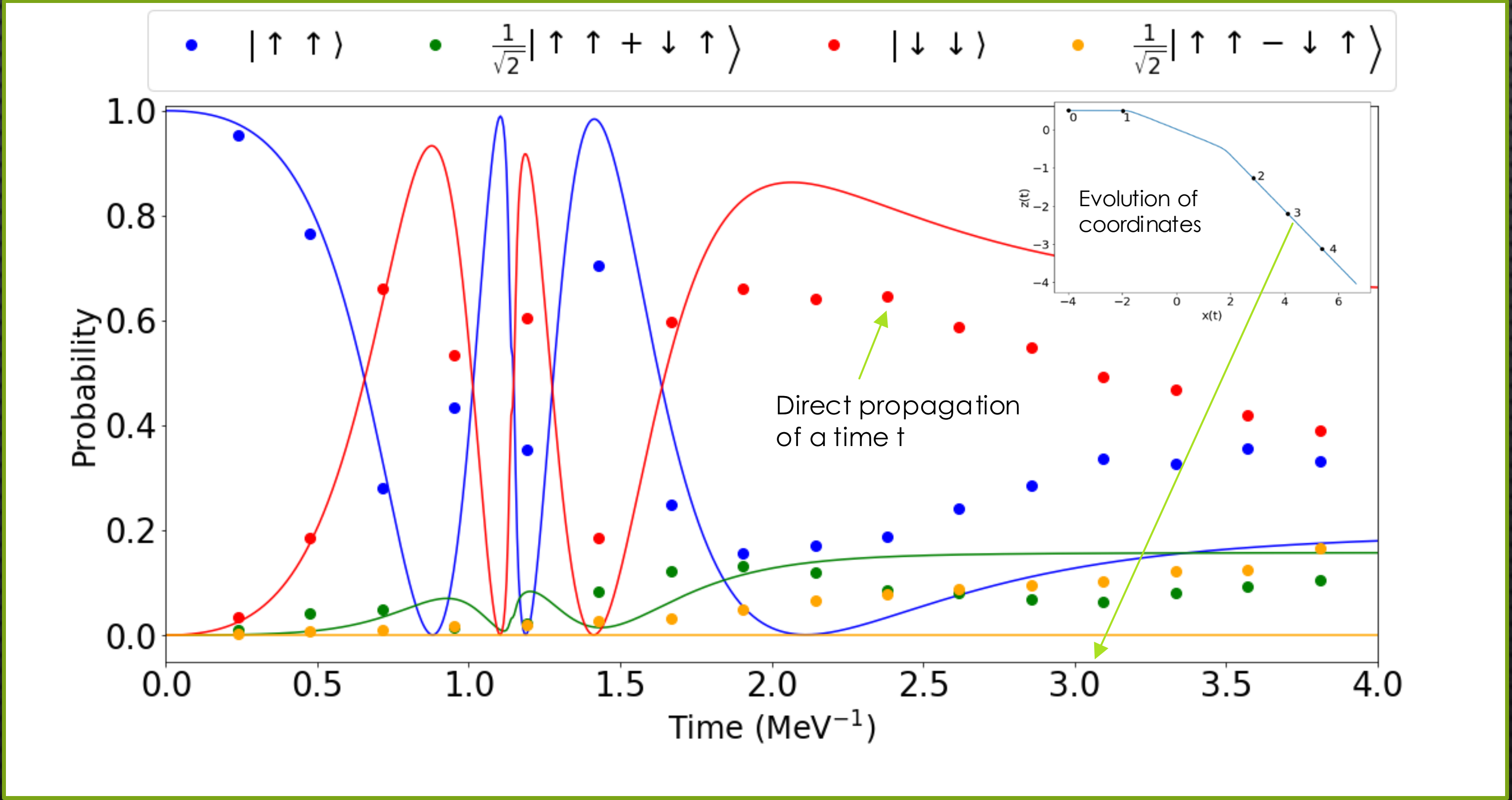


Evolution of the spin state (simulated, Optimal control)

TIME EVOLUTION OF SPIN (AQT@LBL)

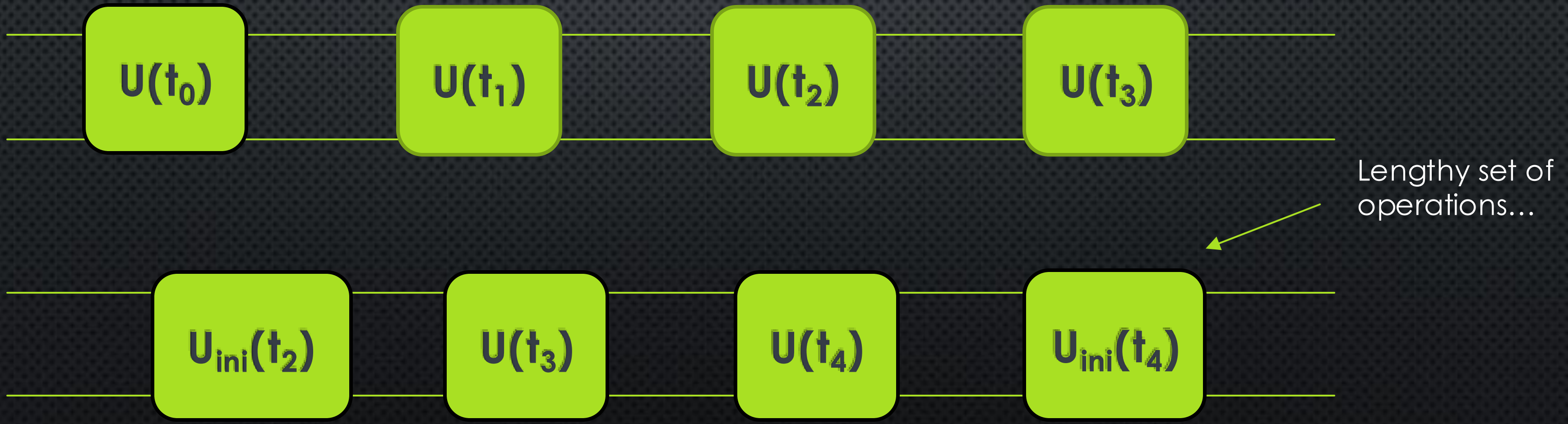


“LONG TIME” PROPAGATOR



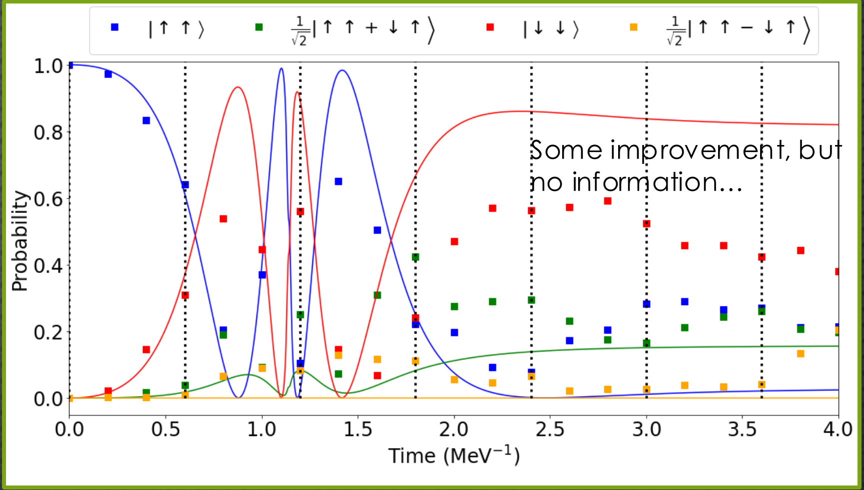
REINIZIALIZATION

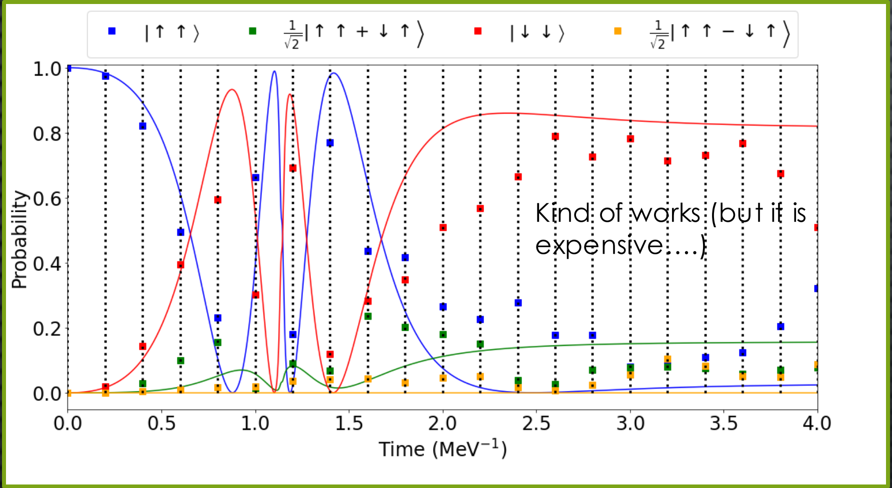
A possible, non scalable, approach consists of re-initializing the state at each time-step. Of course this requires STATE TOMOGRAPHY, followed by a circuit (set of (controlled) rotations) giving back the required state.



REINIZIALIZATION

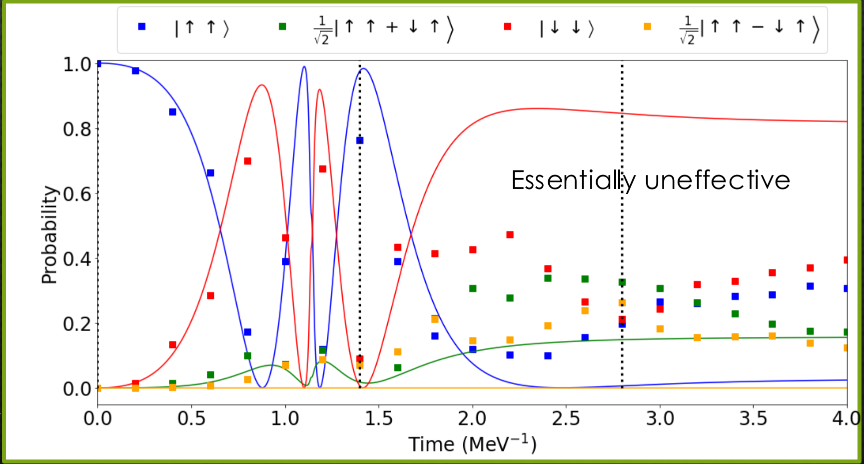
Every 3 time steps



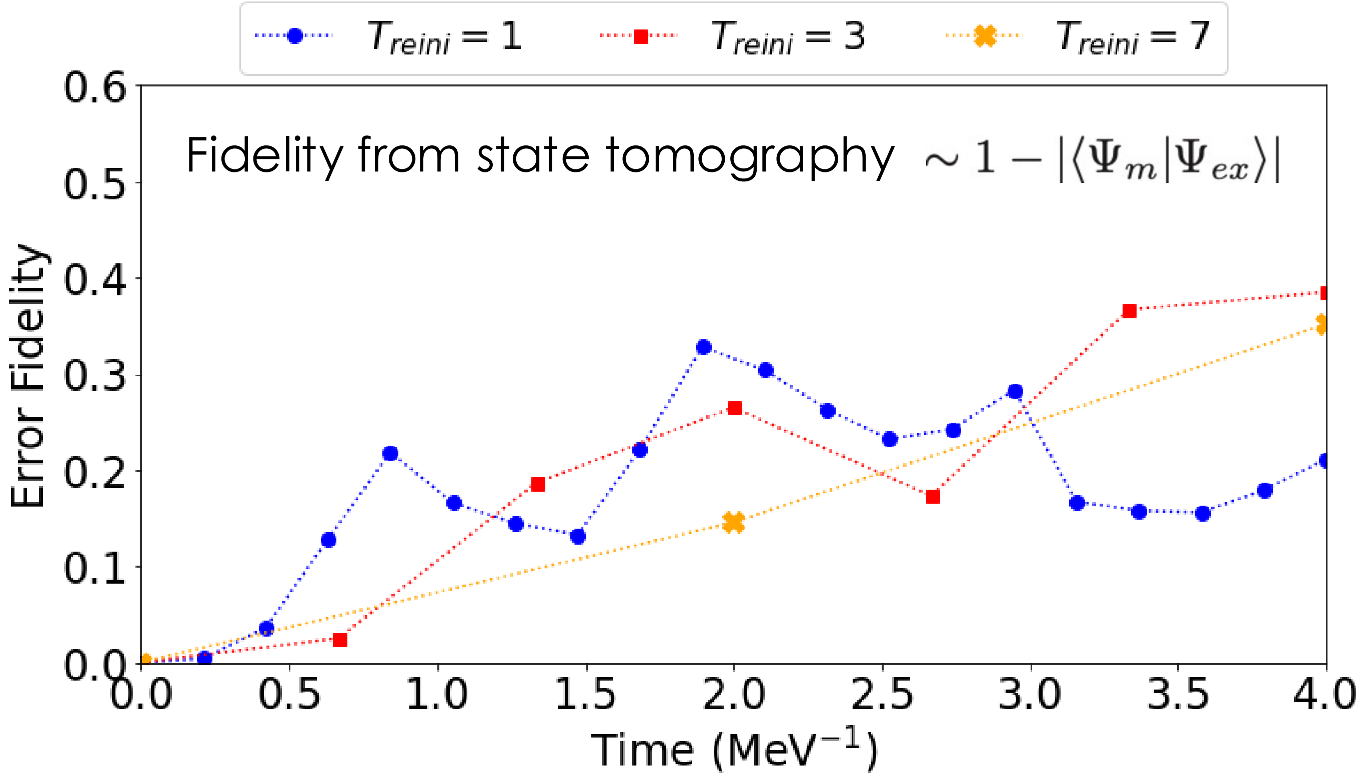


Every time step

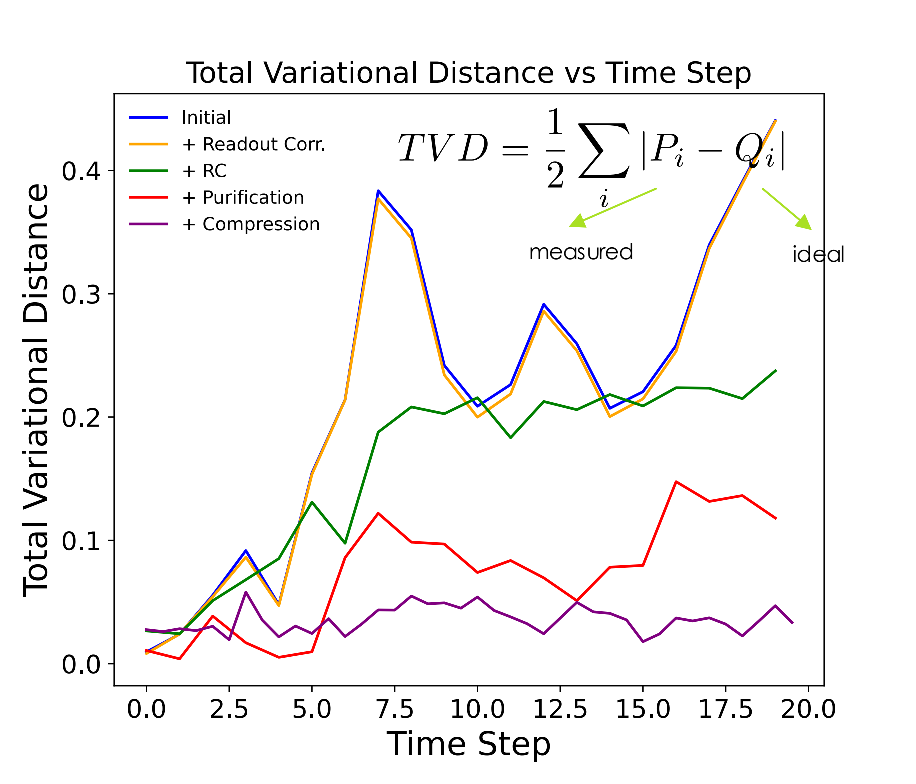
Every 7 time steps



FIDELITY IN THE REINIZIALIZATION PROCEDURE



FURTHER IMPROVEMENTS



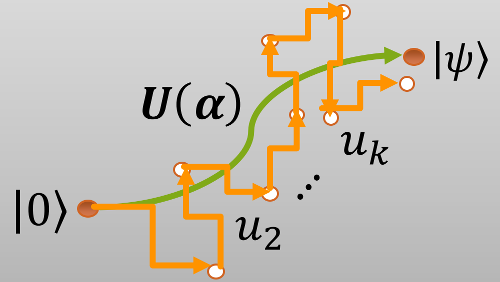
The results shown for the reinizialization strategy were obtained without implementing any error correction procedures. These might help to increase the time interval between successive reinizializations.

“DIGITAL” QUANTUM COMPUTING

Useful theorem (Solovay-Kitaev)

Given an Hilbert space $\mathscr{H}$, any unitary transformation $U \in U(\mathscr{H})$ can be approximated with arbitrary precision δ by a circuit of size *poly(1/ δ)* over the standard gates basis, possibly using ancillary qubits (i.e there exists a

This guarantees that we can approximate for instance an arbitrary time evolution under a Hamiltonian H with a circuit depth that will increase at most a polinomially with the required accuracy.



$$U(\alpha, t) = u_1(\alpha, \Delta t) u_2(\alpha, \Delta_t) \ldots$$

THIS THEOREM IS AT THE BASIS OF UNIVERSAL QC SCHEME

WARNING: other problems like decoherence (thermal effects) and dissipation

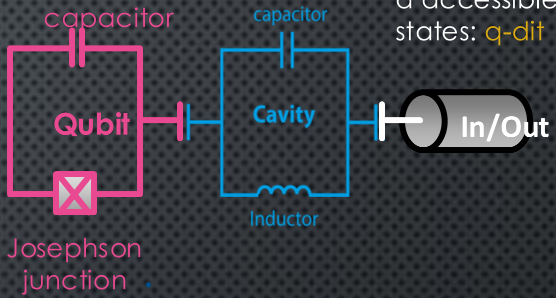
"CONTROL-CENTRIC" APPROACH TO QUANTUM COMPUTATION

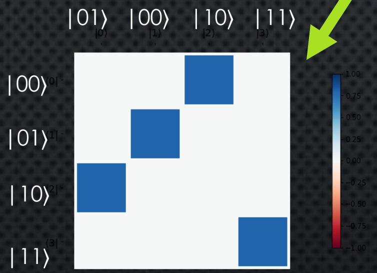
Given some control parameterization $f(t,\alpha) = \sum_k \alpha_k \phi_k(t)$

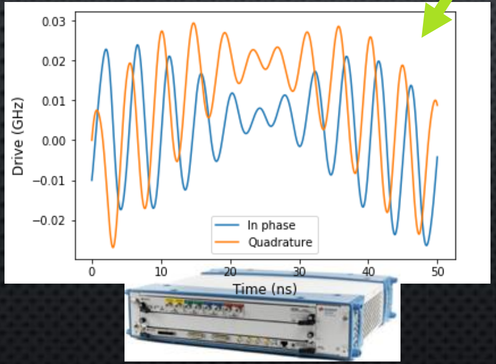
all unitary transformations in time T can be expressed as

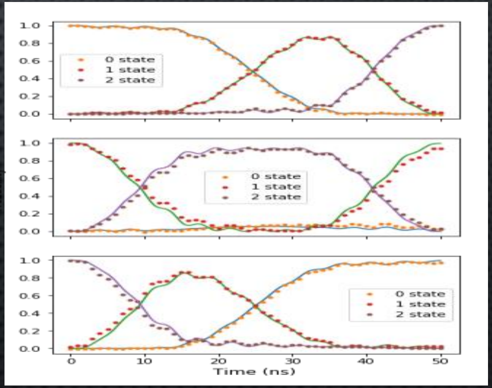
$$U(t,\alpha) = Te^{-i\int_0^t dt'[\hat{H}_0 + f(t',\alpha)\hat{H}_c]}$$

Device with d accessible states: q-dit





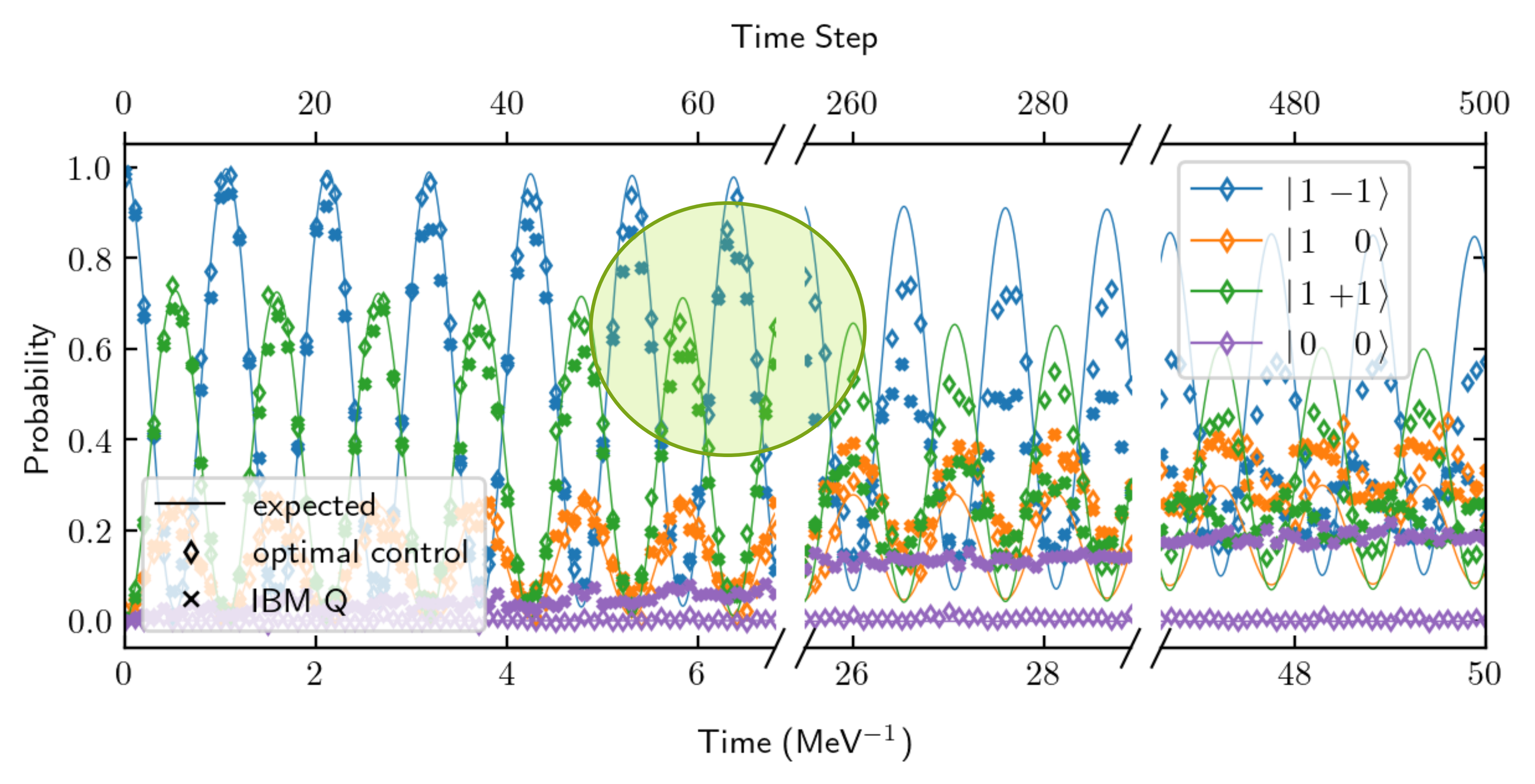




See e.g. S. Schirmer, "Hamiltonian Engineering for Quantum Systems." , Proceedings of the 7th International Conference on Cooperative Control and Optimization (2007)

Optimization methods, machine learning (Q@Tn ML-QFORGE project (Jonathan Dubois, Kyle Wendt (LLNL), Simone Taioli, Paolo Trevisanutto (ECT*-LISC), FP, Piero Luchi, (UNITN)) – PRA 101, 062307 (2020) – INFN Quart&T Project (UNIMIB, FBK, TIFPA, INFN-LNF and others, 2024)

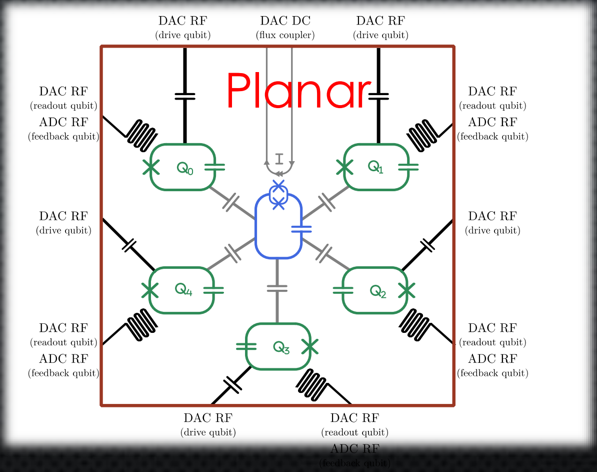
RESULTS ON LLNL TEST BED SIMULATION

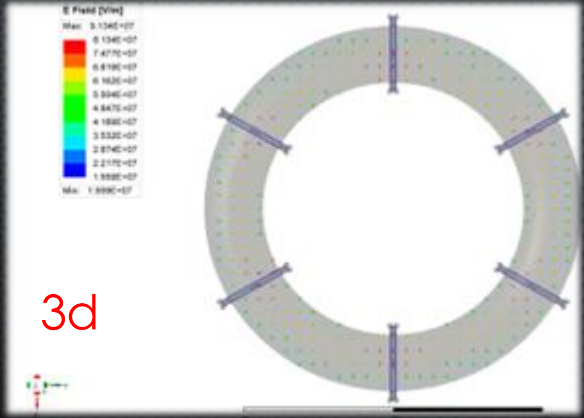


QUART&T @INFN

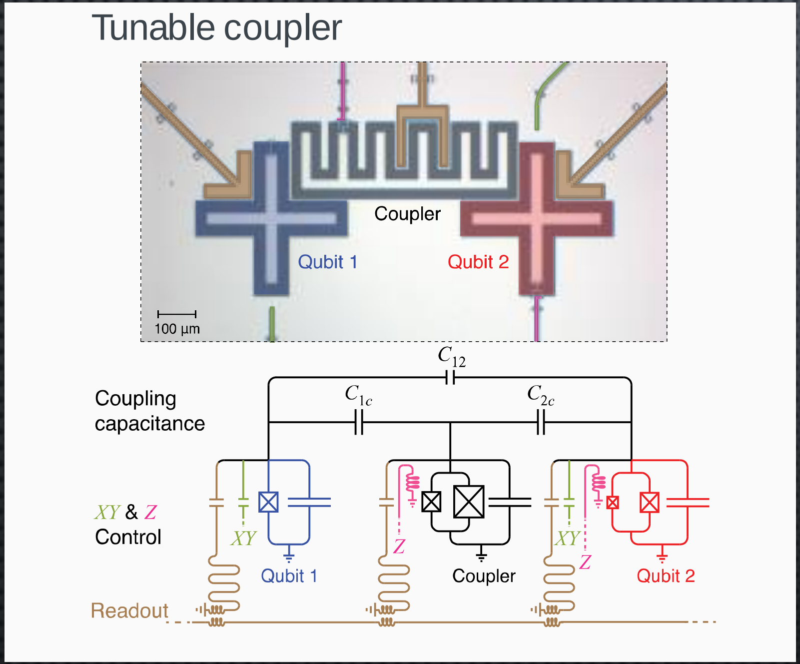
The National Committee for Technolgy Transfer and Applications of INFN has recently decided to fund a project that wants to devise devices designed for simulations of systems of interest in nuclear physics and field theory (QUantum ARchitecture for Theory & Technology).

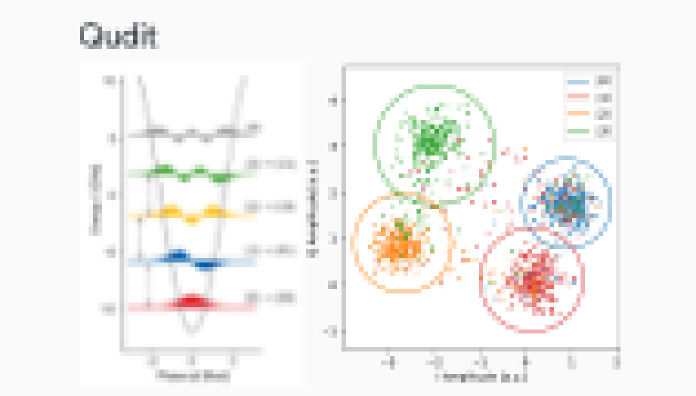
The project lead by Andrea Giachero in Milano Bicocca involves the Trento group with the leadership of the theory work package (A. Roggero) and FBK with the group of F. Mantegazzini for the construction of planar quantum chips.





QUART&T @INFN





Implementation of qudits with all-to-all connectivity.

Tunable coupling: possibility of controlling The coupling between qubits (change the machine Hamiltonian)

CO-DESIGN

CONCLUSIONS

- Optimal control techniques can definitely help to realize proofs of concept for quantum algorithms that need to be robust over time (as for the case of scattering studies)

- A path for the study of nuclear reactions with realistic interactions is visible. However, there are still many open problems (like a more accurate implementation of space propagators with a reasonable scaling) which still need to be addressed.

- Digital QC requires a more elaborated circuit optimization, but some interesting demonstration might not be too far.

- In both cases, it is very important to have access to low level optimization -> work in strict cooperation with the experimental groups!

THANK YOU!