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Evolutionary optimization for Variational Quantum Algorithms

Daniel Faílde Balea (dfailde@cesga.es)

ICE-8 Quantum Information in Spain

Santiago de Compostela May 29^{th} to June 1^{st}

Variational Quantum Algorithms (VQAs)

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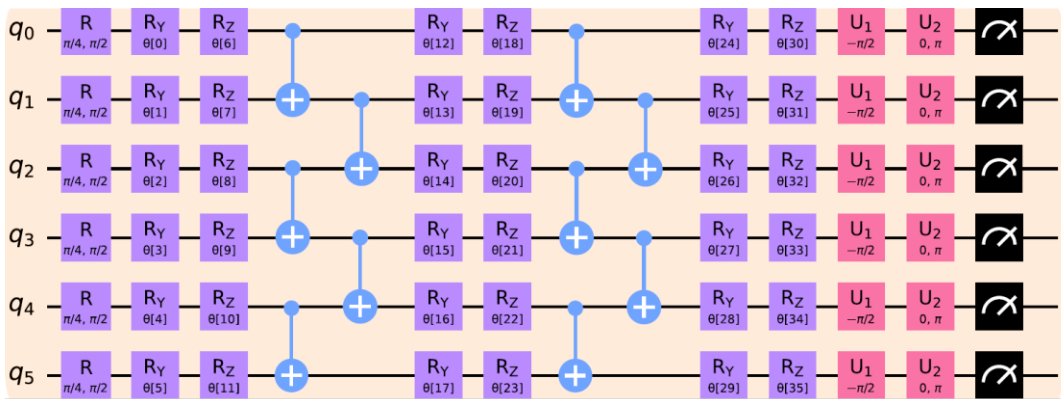
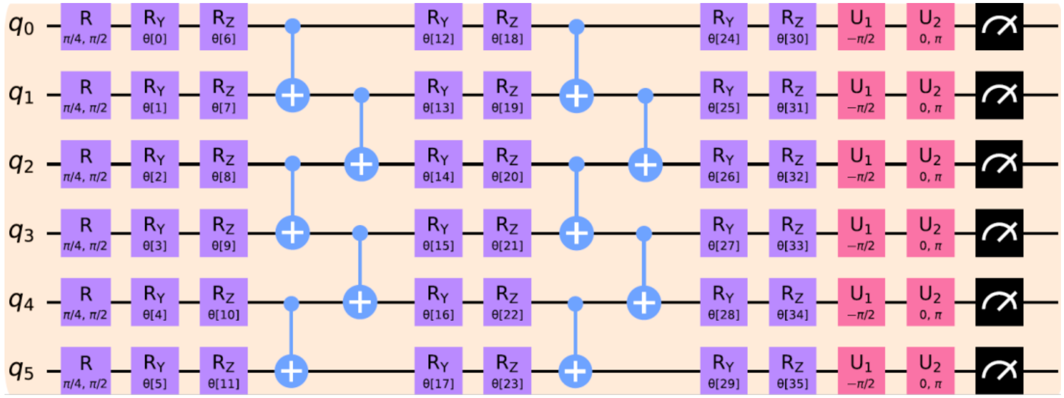


Low-depth parameterized circuit

VQAs Applications

- Combinatorial Optimization
- Ground State calculation (VQE)
- Quantum Machine Learning
- Dynamical Simulations
- Factoring
- Systems of equations
- Error correction
- …

Variational Quantum Algorithms (VQAs)



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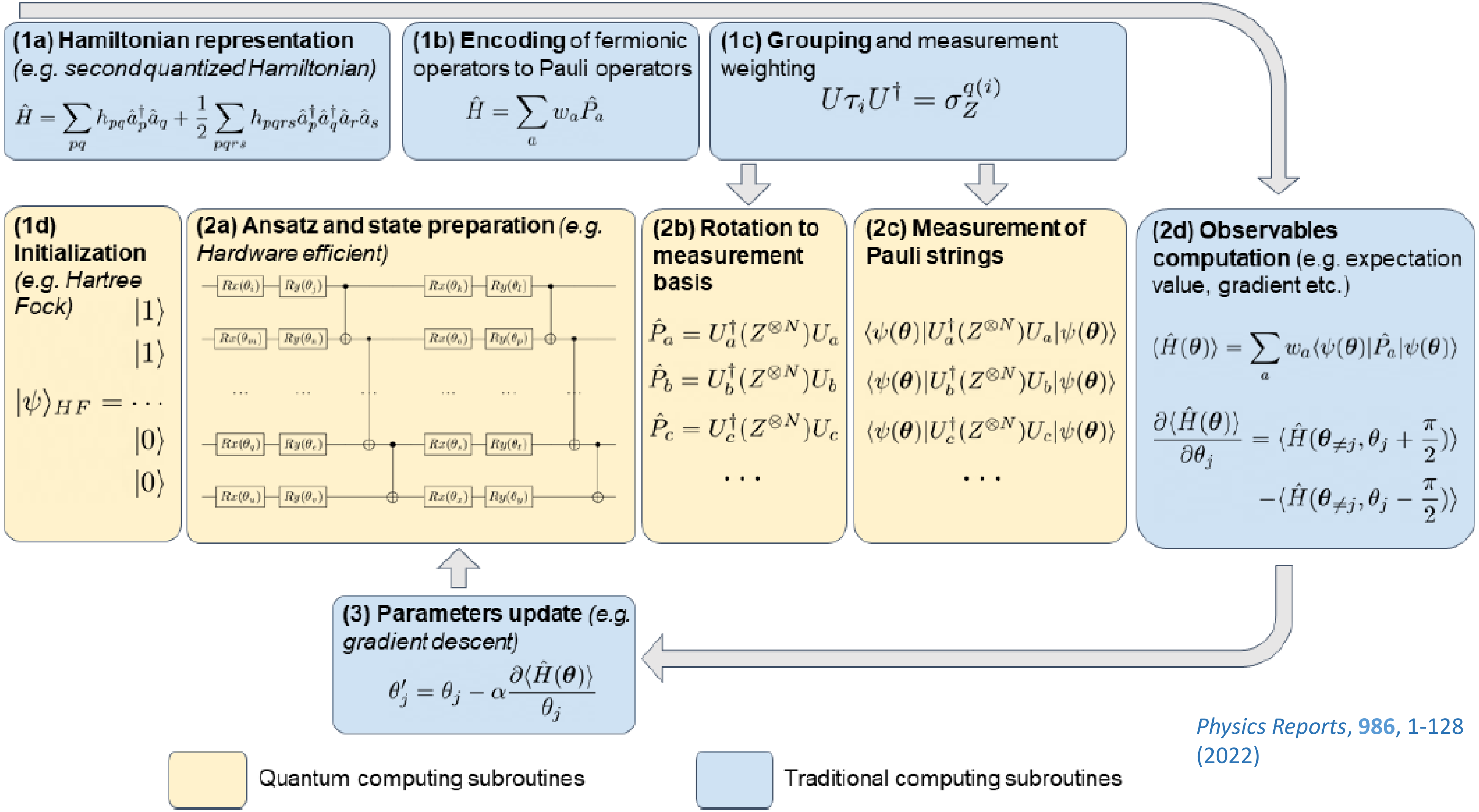
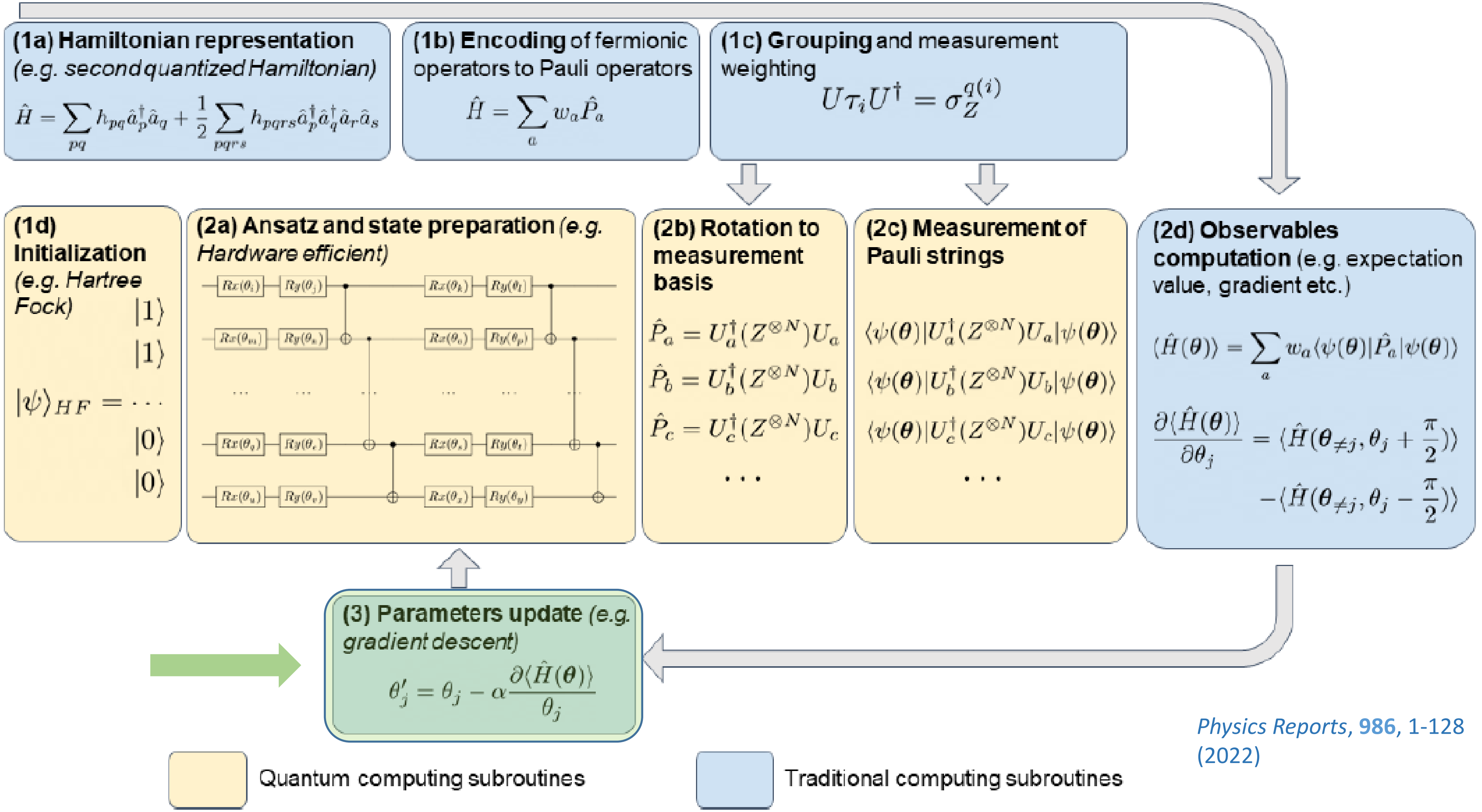
VQE structure



Physics Reports, **986**, 1-128 (2022)

VQE structure



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Crucial issues towards efficient scalable VQE

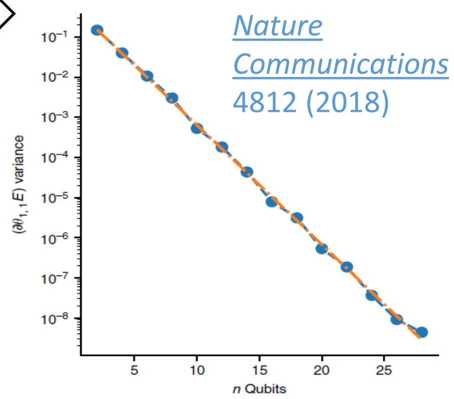
Ansatz selection

- **Expressibility**. The degree of information that your quantum circuit has to reproduce the ground state (or another) of the system.

- **Trainability**. Easiness of fitting the parameters. Reducing the number of parameters taking, for instance, some Information from your Hamiltonian (UCC, HVA, QAOA ansatz…)

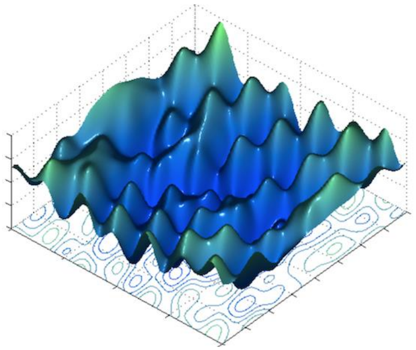
Problems in the optimization landscape

- **Barren Plateaus.** Exponentially vanishing gradients.



Nature Communications **9**, 4812 (2018)

- **Local minima.**



Mitigating problems in the optimization landscape

Smart circuit construction and adaptative ansatzs (HVA, ADAPT-VQE, random gate activation…)

Resilient optimization methods (Quantum Natural Gradient, ¿…?)

Quantum **4**, 269 (2020)

⇨ ***Scalable VQAs***

- Depends on gradients
- Complexity
- Number of circuit executions

Mitigating problems in the optimization landscape

Smart circuit construction and adaptative ansatzs (HVA, ADAPT-VQE, random gate activation…)

Resilient optimization methods (Quantum Natural Gradient, Differential Evolution?)

Scalable VQAs

- Gradient free
- Easy to paralelize

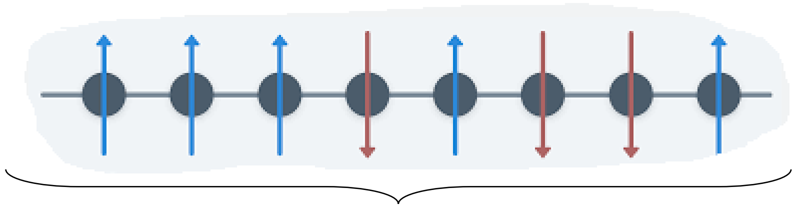
arXiv:2303.12186

Using Differential Evolution to Avoid Local Minima in Variational Quantum Algorithms

D. Faílde,* J.D. Viqueira, M. M. Juane, and A. Gómez
Centro de Supercomputación de Galicia (CESGA), Santiago de Compostela, Spain
(Dated: March 23, 2023)

Local minima problem

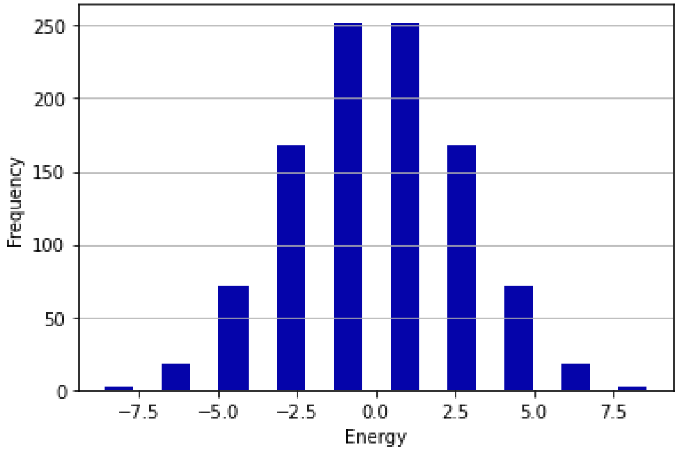
Ising chain without magnetic field



n qubits/atomic spins

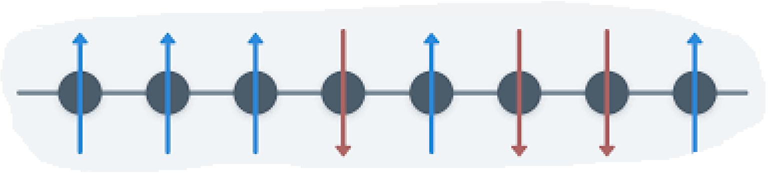
$$H = -\sum_{\langle i,j \rangle} J_{ij}\sigma_i\sigma_j - \sum_i h_i\sigma_i$$

$$J = 1$$
$$h_i = 0$$



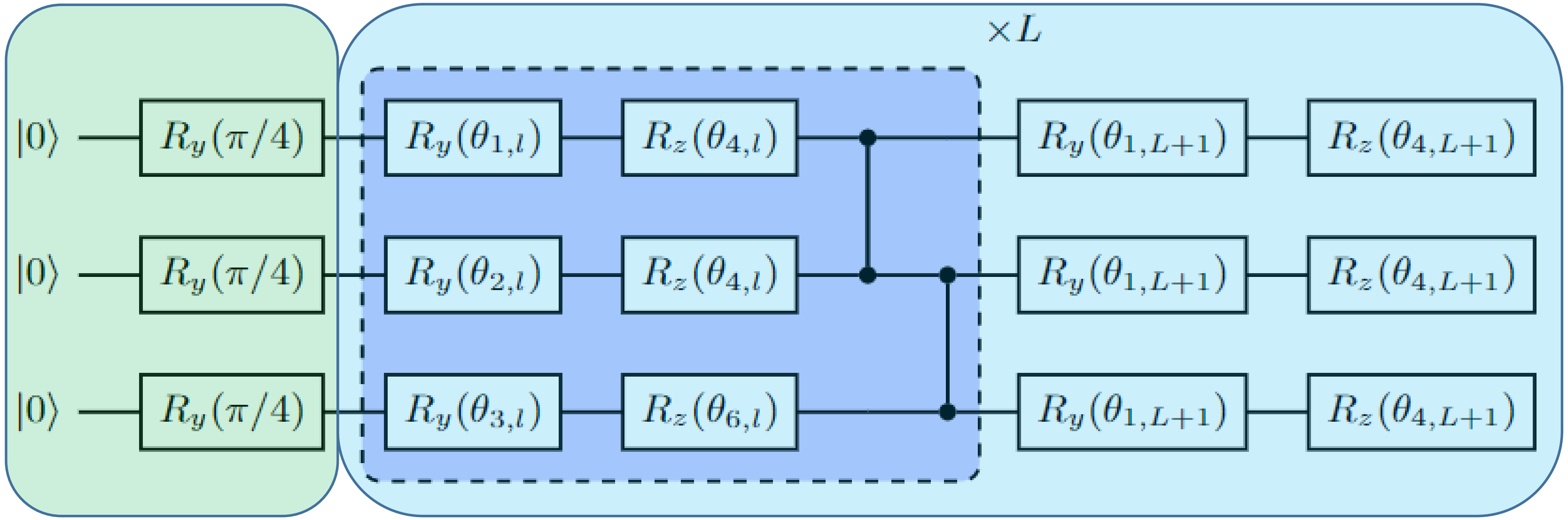
	Energy (a.u.)	*Degeneracy*
• Ground state:	n-1	2
• First excited level:	n-3	2(n-1)
• Second excited level:	n-5	(n-1)(n-2)

Ising chain without magnetic field



$$H = -\sum_{i=1}^{N-1} \sigma_i^y \sigma_{i+1}^y \qquad GS \rightarrow |\pm i\rangle^{\otimes n}$$

Variational quantum circuit:



Initialization *Ansatz*

High expressibility and relative low trainability

Total number of parameters
$$\boldsymbol{N_\theta = 2n(L+1)}$$

Local optimizers

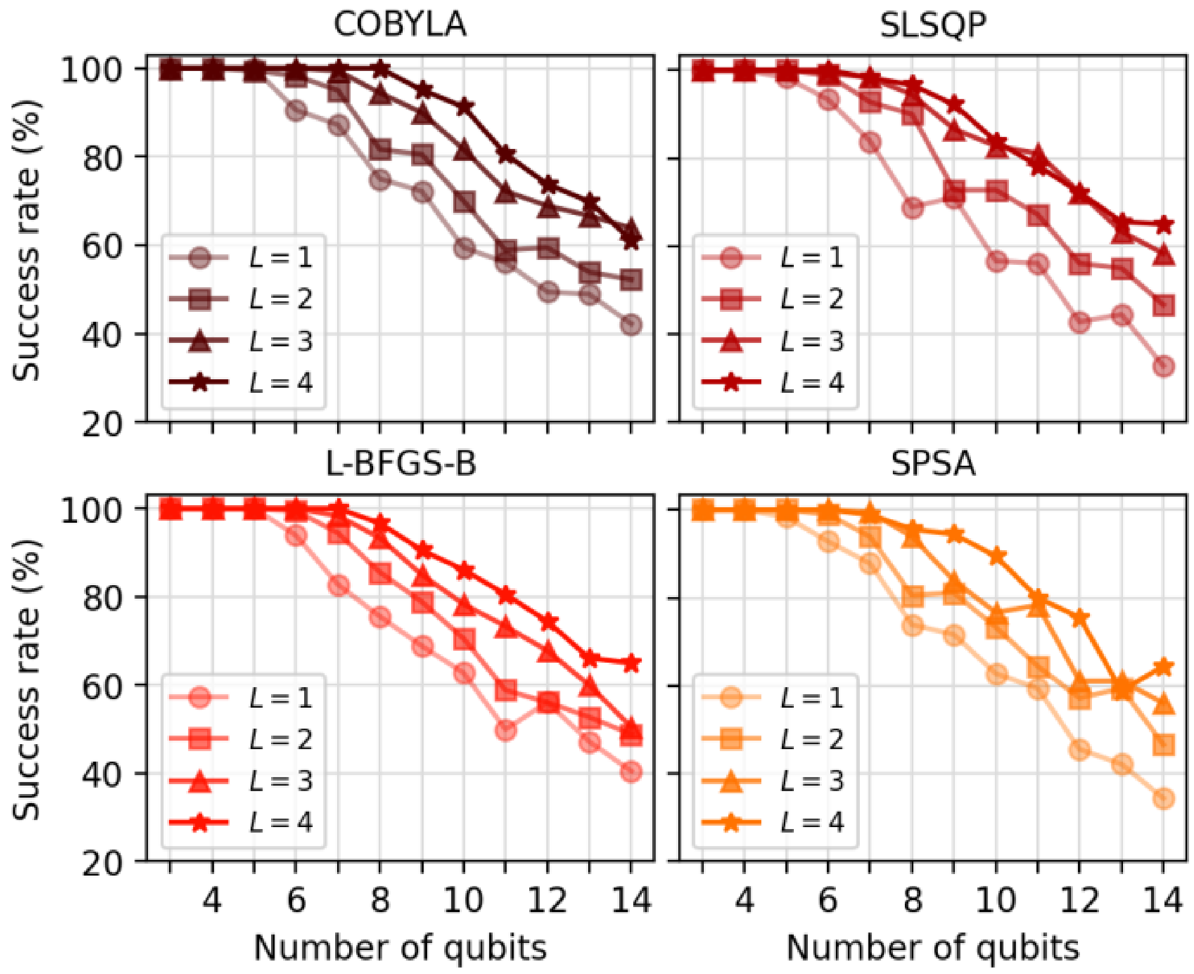
Simulation Details

- Each point correspond to 180 different optimizations (statevector simulations).
- The maximun number of iterations and function evaluations are the unique adjusted parameters.
- Relative tolerance $\delta = 1 - |E_\theta / E_{GS}|$ of 10^{-2} to declare optimization as sucessfull.

Results

- $L = 1$. We observe a significant reduction in the success rate (SR) when increasing the number of qubits.
- SR improves when increasing L, but the tendency remains unalterable.
- Optimization always ends in the ground state of the system or in one excited state.

Local minima problem!



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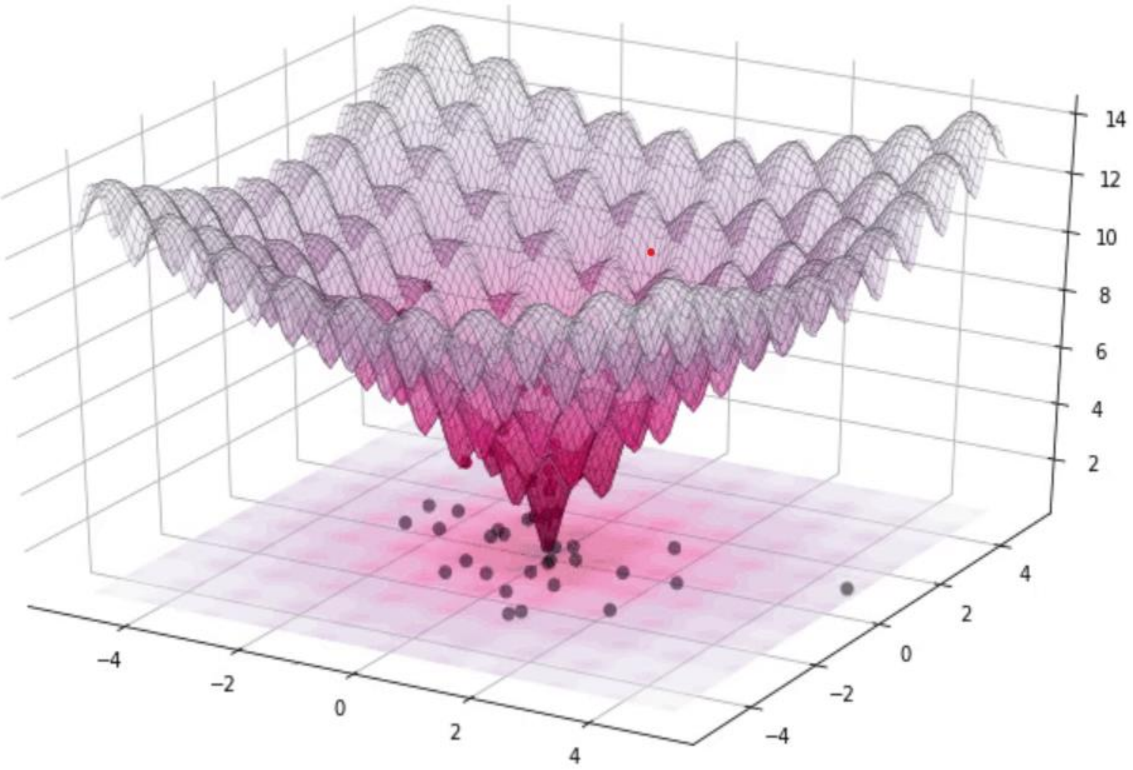
Evolutionary optimization using Differential Evolution (DE)

Differential Evolution (DE)



https://pablormier.github.io/2017/09/05/a-tutorial-on-differential-evolution-with-python/

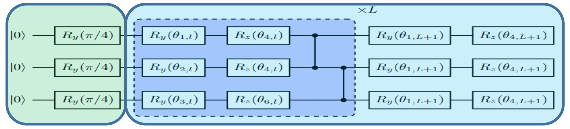
Possible solution: Use an evolutionary algorithm that can update the position of the *particles* with the remaining members of the population **even if they get trapped in a local minimum or barren plateau.**

Differential Evolution structure

Initialization

Create a population of $S = p\,N_\theta$ individuals, i,e., $S = \{\vec{x}_1, \ldots, \vec{x}_P\}$. Individuals are vectors $x_i = (\theta_{1i}, \ldots, \theta_{N_\theta i})$ of length N_θ.

I) Energy Evaluation / II) Replacement*



Converge?

No → III) Mutation

For each individual $\vec{x}_i$ generate a new one $\vec{x}_i^m$ (mutant)

$$\vec{x}_i^m = \vec{x}_{best} + F(\vec{x}_j - \vec{x}_k)$$

IV) Recombination

Some parameters of $\vec{x}_i' s$ are replaced by $\vec{x}_i^m$ following a crossbreeding strategy (binomial or exponential) → **Generates a modified vector $\vec{x}_i^*$**

Yes → End

* $\vec{x}_i^*$ replaces $\vec{x}_i$ if its energy is lower. Otherwise, it is discarded. (Not in the first iteration)

Recombination strategies

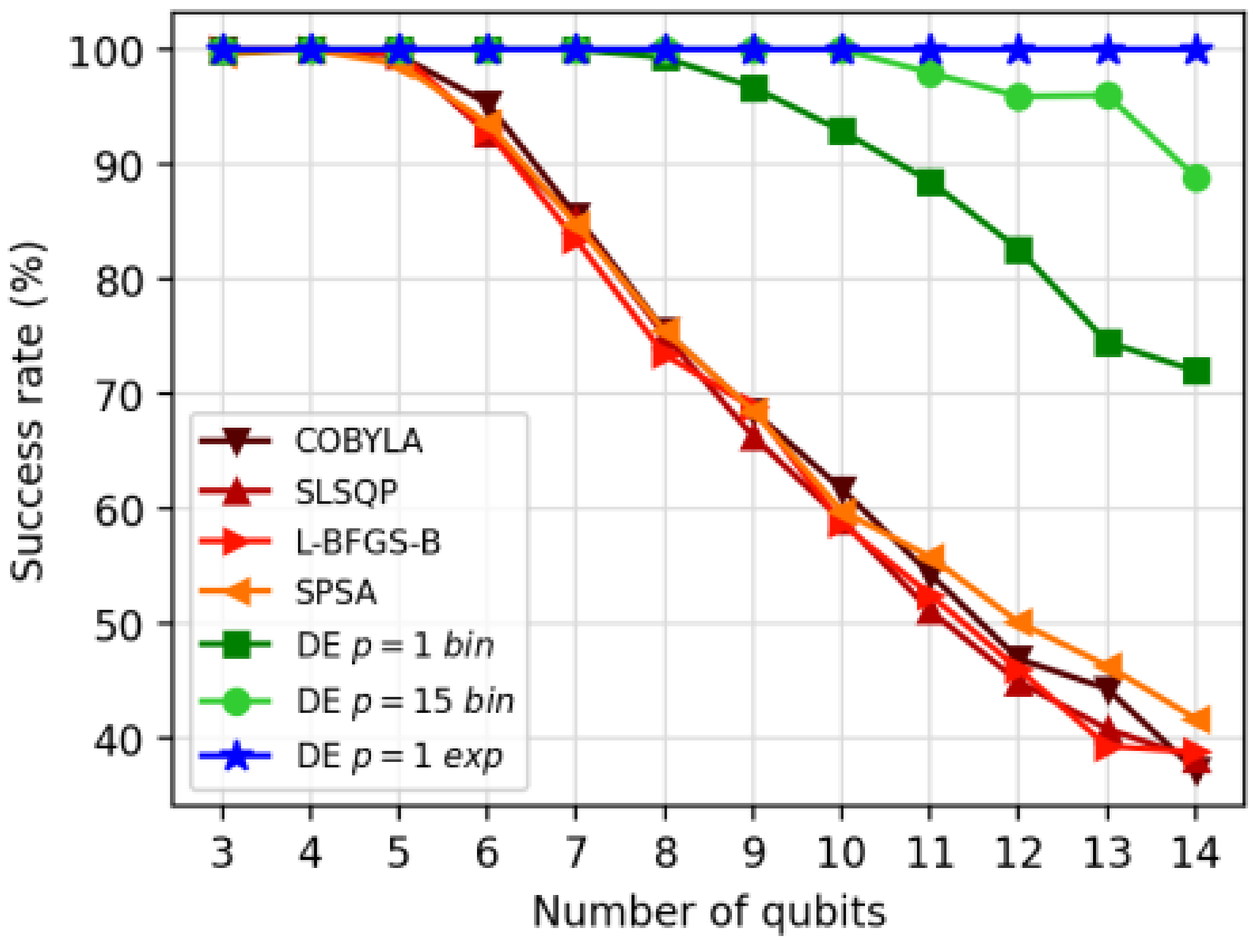
Binomial Every element in the vector $\vec{x}_i$ has a probability C of being substituted by the one in $\vec{x}_i^m$

$$\left.\begin{aligned} \vec{x}_i &= (\theta_{1,i}, \theta_{2,i}, \dots, \theta_{N_\theta,i}) \\ \vec{x}_i^m &= (\theta_{1i}^m, \theta_{2,i}^m, \dots, \theta_{N_\theta,i}^m) \end{aligned}\right\} \quad \vec{x}_i^* = (\theta_{1,i}, \theta_{2,i}^m, \theta_{3,i}, \dots, \theta_{N_\theta,i})$$

Exponential All elements between two randomly chosen in the vector $\vec{x}_i$ are taken from $\vec{x}_i^m$

$$\vec{x}_i^* = (\theta_{1,i}, \underbrace{\theta_{2,i}^m, \theta_{3,i}^m, \dots, \theta_{N_\theta-1,i}^m}_{\text{Taken from } \vec{x}_i^m}, \theta_{N_\theta,i})$$

Local optimizers vs DE



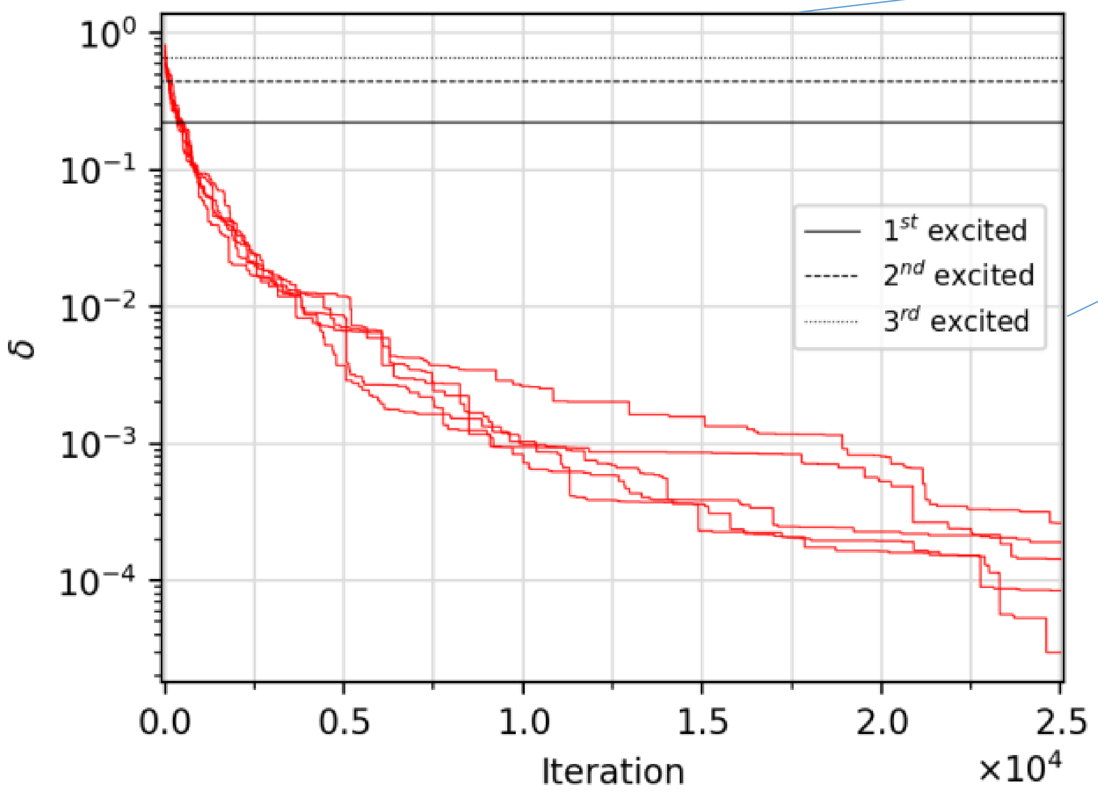
Simulation Details

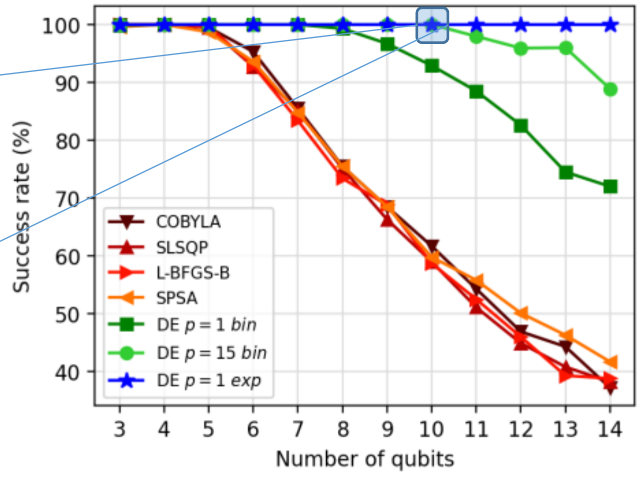
- Each point corresponds to 1000 (100 ps=15, 100 DE ps=1 exp) different optimizations. For each optimization, parameters initialize randomly in the interval $[-\pi, \pi)$.
- DE optimization run in parallel processors using *Multiprocessing.*

Results

- DE default configuration (binomial crossover) with $p = 1$, i.e., same conditions as local optimizers, clearly outperforms the previous methods.
- Increasing the population improves the SR altough it does not seem to compensate.
- DE with exponential crossover gets a 100% SR in the range studied.

Exponential crossover

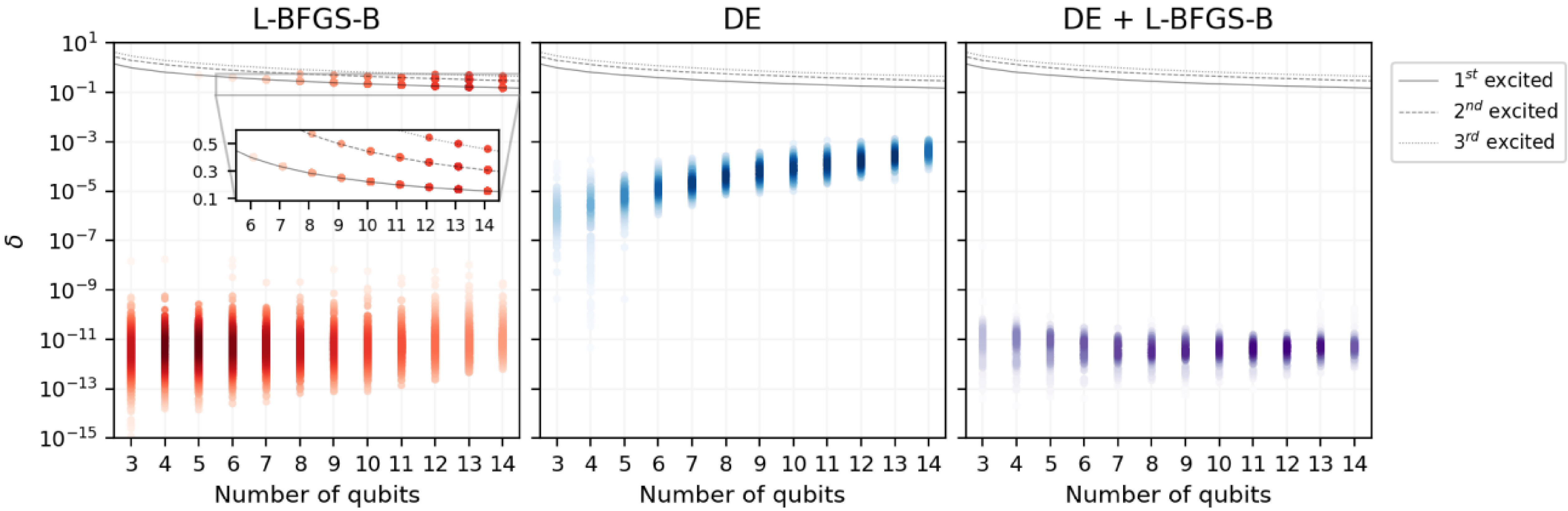




Features

- Maximizes parameter space exploration
- Losses convergence when approaching to the global minimum

Hybrid optimization strategy



* These data correspond to DE p=1 and exponential crossover.

Conclusions and outlook

- DE outperfoms regular local optimization methods in this **local minima problem**.

- SR can be enhanced by just increasing the population size, modifying the recombination criteria or using hybrid strategies.

- Classical **computational time** for DE is **higher** compared with local optimizers. However, the algorithm is **easy to parallelize** and run in multiple processors.

- Same performance in other problems, such as the **TFIM** and **Hubbard model** (preliminary results).

- Already implemented on scipy. https://gitlab.com/proyectos-cesga/quantum/react-eu/vqe_ising_chain_de.git

REACT-EU

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Andrés Gómez Tato, PhD
Administrador aplicaciones y proyectos

G. Díaz-Camacho M. Mussa J. D. Viqueira D. Faílde C. Rodríguez-Ramos

¡Thanks!

dfailde@cesga.es

Gonzalo Ferro Costas, PhD
Técnico superior de proyecto NEASQC

AXENCIA GALEGA DE INNOVACIÓN

UNIÓN EUROPEA

Xacobeo 21-22

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DESPREGAMENTO DUNHA INFRAESTRUTURA BASEADA EN TECNOLOXÍAS CUÁNTICAS DA INFORMACIÓN QUE PERMITA IMPULSAR A I+D+i en GALICIA

Apoiar a transición cara a unha economía dixital

Operación financiada pola Unión Europea, a través do FONDO EUROPEO DE DESENVOLVEMENTO REXIONAL (FEDER), como parte da resposta da Unión á pandemia da COVID-19

PROGRAMA OPERATIVO
FEDER GALICIA
2014-2020

Unha maneira de facer Europa

Irais Bautista Guzmán
Técnica superior de proxecto Quantum Spain