Antonio Macaluso

Senior Researcher at German Research Center for Artificial Intelligence (DFKI)

() antoniomacaluso.com

PERSONAL INFORMATION

Family name, First name: Macaluso, Antonio

Nationality: Italian

PROFILE SUMMARY

I currently hold the position of Senior Researcher at the German Research Center for Artificial Intelligence (DFKI), where I lead the Quantum Artificial Intelligence unit within the Intelligent Information Systems research team at the Department for Agents and Simulated Reality. My primary research interests lie in exploring the feasibility and potential advantages of quantum algorithms in various areas of Artificial Intelligence, including supervised learning, reinforcement learning, multi-agent systems, planning, and scheduling.

In addition to my research responsibilities, I am actively involved in teaching, particularly in delivering quantumrelated topics to students at Saarland University who may not have a background in physics. Furthermore, I contribute to editorial reviews for several journals and peer-reviewed conferences. Prior to my current role, I also gained valuable experience working in industry.

Education

PhD in Computer Science and Engineering Dept. of Computer Science and Engineering, University of Bologna

Thesis: A Novel Framework for Quantum Machine Learning [6, 12] Supervisors: Prof. Claudio Sartori, Prof. Stefano Lodi (University of Bologna) Reviewers: Prof. Martin Kliesch (TU Hamburg), Prof. Claudio Moraga (TU Dortmund)

Master's Degree in Statistical Sciences - 110/110 L

Dept. of Statistical Sciences "Paolo Fortunati", University of Bologna

Title: Evaluating the efficacy of drugs in tumor cells through Machine Learning Supervisor: Prof. Stefano Lodi Main subjects: Statistics, Statistical Learning, Probability, Maths

Master in Data Science - 28/30

Bologna Business School, University of Bologna

Main subjects: Machine Learning, Big Data, Business Intelligence, Statistics Additional info: Full-tuition scholarship granted by Cineca for attendance to the Master

Bachelor's Degree in Statistical Sciences - 110/110 L

Dept. of Statistical Sciences "Paolo Fortunati", University of Bologna

Thesis: Data Mining for Pattern Analysis of University Students Supervisors: Prof. Claudio Sartori Main subjects: Statistics, Probability, Maths November 2017- December 2020

October 2014 - September 2017

October 2015 - October 2016

October 2011 - July 2014

CURRENT POSITIONS

Senior Researcher

German Research Center for Artificial Intelligence (DFKI), Saarbruecken

I am the leader of the Quantum Artificial Intelligence unit within the Intelligent Information Systems (I2S) research group at DFKI. This unit was established upon my arrival at DFKI, under the guidance of PD Dr. Matthias Klusch, who leads the I2S team. Our research unit is dedicated to exploring the feasibility and potential advantages of quantum algorithms across various domains of Artificial Intelligence. As a Senior Researcher, my responsibilities extend beyond conducting research. I oversee complex research projects, coordinate workshops and conferences, and actively participate in securing new projects through efforts to acquire funding.

TEACHING

Lecturer - Quantum Artificial Intelligence [Cod. 146584] Saarland Informatics Campus, Saarland University, Germany

Info: 3 Credit Points, 26 hours, A.Y. 2023-24, Course evaluation

Course synopsis: This course adopts a computer science perspective on Quantum Artificial Intelligence and consists of two parts. The first part briefly introduces the fundamentals of quantum computation, including gate-based and adiabatic quantum computational models. The second part explores the feasibility and potential advantages of using quantum computational methods to address specific AI problems, emphasizing machine learning and optimization.

Lecturer - Quantum Computing for NP-hard Problems and AI

Dept. of Computer Science and Engineering, University of Bologna, Italy

Info: 3 Credit Points, 15 hours, A.Y. 2023-24, Syllabus

Course synopsis: This course is designed for Ph.D. students with no prior knowledge of quantum computing. It provides a computer science perspective on the quantum algorithms for solving traditional NP-hard problems with a particular focus on AI applications. The course is divided into three parts. Part I introduces the fundamental concepts of gate-based and adiabatic quantum computational models. Part II describes hybrid quantum-classical algorithms, with a focus on machine learning and combinatorial optimization. In part III, the course explores the advantages of utilizing quantum computational methods to address computationally hard AI problems.

Lecturer - Quantum Artificial Intelligence [Cod. 139530] October 2022 - February 2023 Saarland Informatics Campus, Saarland University, Germany

Info: 3 Credit Points, 26 hours, A.Y. 2022-23, Course evaluation

Course synopsis: This course adopts a computer science perspective on Quantum Artificial Intelligence and consists of two parts. The first part briefly introduces the fundamentals of quantum computation, including gate-based and adiabatic quantum computational models. The second part explores the feasibility and potential advantages of using quantum computational methods to address specific AI problems, emphasizing machine learning and optimization.

Lecturer - Quantum Machine Learning Seminar [Cod. 136315] Saarland Informatics Campus, Saarland University, Germany

Info: 7 Credit Points, 16 hours, A.Y. 2023-24

Course synopsis: This course on Quantum Machine Learning aims to show what benefits quantum technologies can provide to the area of machine learning. While machine learning algorithms are used to compute massive amounts of data, quantum machine learning employs qubits and quantum operations to improve computational speed and data storage. A closer look at selected methods in the context of quantum machine learning will be taken with a particular focus on hybrid quantum-classical algorithms for supervised learning and reinforcement learning.

March 2022 - present

October 2023 - February 2024

October 3-11, 2023

April 2022 - July 2022

Lecturer - Quantum Computing

Deep Learning Italia, Italy (e-learning platform)

Course synopsis: This course offers a comprehensive introduction to the fundamentals of quantum computation, structured into three main segments. The initial part explores basic mathematical concepts and highlights the distinctions between classical and quantum computing. The second segment delves into the core principles of quantum computing, commencing with the foundational postulates of quantum mechanics and progressing to the formal and technical definition of algorithms. The third section is dedicated to describing and implementing quantum algorithms. It introduces two influential quantum algorithms utilizing IBM's giskit framework.

Platform information: e-learning platform for academic and industrial training programs ~ 3000 users, 70+ instructors from academy and industry recognized by Fondazione Bruno Kessler and University of Macerata.

Teaching activities from over 5 years ago

Teaching Assistant - Systems and Algorithms for Data Science Dept. of Statistical Sciences "Paolo Fortunati", University of Bologna, Italy

Activities: lectures, tutorials, exam assistance for courses with 30 to 80 students

Courses (Master's Degree in Statistical Sciences):

Systems and algorithms for Data Science [cod. 85189] (15 hours) - A.Y. 2017-18 Machine Learning Systems for Data Science [cod. 90477] (15 hours) - A.Y. 2019-20

Tutor - Statistics

Dept. of Statistical Sciences "Paolo Fortunati", University of Bologna, Italy

Info: 20 hours

Project Statistics and Sport: Tutoring activities aim to help high school students gain a deeper understanding of statistics. Following a series of lectures introducing fundamental statistical concepts, the students conducted an in-depth data analysis project on the performance of NBA basketball teams. They presented their project at the University of Bologna. This project was conducted at *Liceo Scientifico Copernico*, Bologna.

Lecturer - Machine Learning

Cineca, School on Scientific Data Analytics and Visualization, Italy

Course synopsis: The course aims to introduce supervised and unsupervised machine learning algorithms within a distributed computing environment, utilizing the R programming language. Additionally, it will cover various libraries for parallel computing. Furthermore, the course will provide insights into libraries for data analysis and visualization.

PREVIOUS POSITIONS

Researcher

German Research Center for Artificial Intelligence (DFKI), Saarbruecken

My research activities focused on designing and implementing quantum algorithms for complex artificial intelligence problems with a particular focus on improving supervised learning classical methods by means of quantum computation. Moreover, a plethora of novel quantum solutions for selected AI problems with applications in the automotive industry have been developed. These include reinforcement learning for collision-free navigation of autonomous vehicles, coordination of multi-agent systems for cooperative services, and optimizing flexible production processes in Industry 4.0.

April 2017 - May 2017

Oct. 2017 - Dec. 2019

June 2016

August 2021 - February 2022

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Ph.D. Student - Computer Science and Engineering

Dept. of Computer Science and Engineering, University of Bologna

The main focus of my Ph.D. was the designing and implementation of novel quantum machine learning algorithms. In particular, the contribution of my dissertation was twofold:(i) the proposal of a general framework for supervised learning [6, 12] whose special cases are a new quantum neural network architecture [14, 7] and the quantum counterpart of ensemble algorithms in machine learning [3, 16]; (ii) the proposal of a quantum algorithm for approximating non-linear activation function in quantum neural networks [15].

Research Assistant

Dept. of Statistical Sciences "Paolo Fortunati", University of Bologna

As a research assistant, I worked to support a research project aiming at investigating the socio-economic and health conditions of the elderly in Egypt, with a particular focus on public and private solidarity. My tasks were the management and analysis of demographic data from the Labor Market Panel Survey: Egypt (1998, 2006, 2012), Jordan (2010), Tunisia (2014) - Economic Research Forum (Conference paper).

Work Experience (Industry)

R&D Machine Learning Engineer

Menarini Silicon Biosystems, Via G. Di Vittorio, 21b/3, 40013 Castel Maggiore BO, Italia

Menarini Silicon Biosystems offers unique rare cell technologies in the study of cells and their molecular characterization. As a machine learning software engineer I worked on designing and testing advanced deep learning algorithms for in vitro diagnostic (IVD) medical devices.

Data Scientist

Cineca, via Magnanelli 6/3, 40033 Casalecchio di Reno, Bologna, Italy

Cineca is the largest HPC centre in Italy. As Data Scientist, I worked on developing and deploying machine learning solutions based on real-world data. I followed projects regarding three areas: *i*) prediction of dropout university students (Dissemination article); *ii*) monitor and predict the fault of trains using HPC infrastructure; *iii*) application of unsupervised techniques in text mining problems for the transport industry.

Scholarship and Awards

 $\left(2021\right)$ IBM Quantum Researchers Program Award for accessing high-quality quantum hardware

(2015) Cineca: full-tuition scholarship (14k \in) for attendance to the Master in Data Science (BBS)

CO-SUPERVISION OF GRADUATE STUDENTS

I report the list of students (past and present) under my supervision who have worked on a thesis on quantum artificial intelligence. In all the cases, the student did not have prior knowledge of quantum computing.

Alessandro Rizzo (MSc)

Master's Degree in Artificial Intelligence, University of Bologna, Italy

Supervisors: Prof. Claudio Sartori, Dr. Antonio Macaluso, Dr. Andrea Bulgarelli

Title: Quantum Convolutional Neural Networks for Particle Identification in High Energy Physics

Abstract: This master's thesis explores the application of Quantum Convolutional Neural Networks (QCNNs) to the task of particle identification in the field of High Energy Physics (HEP). The study investigates the potential advantages offered by QCNNs in handling complex particle identification challenges, leveraging both quantum computing principles and convolutional neural network architectures. Through experimentation and analysis, the thesis aims to shed light on the efficacy and feasibility of integrating quantum computing into particle identification processes, with implications for advancing the capabilities of HEP experiments and detectors.

December 2014 - December 2015

January 2021 - June 2021

May 2016 - June 2019

March 2023 - February 2024

Akash Sinha (MSc)

Master of Science, Saarland Informatics Campus, Saarland University, Germany

Supervisors: PD Dr. Matthias Klusch, Dr. Antonio Macaluso

Title: On Quantum Deep Reinforcement Learning for Collision-Free Navigation in Self-Driving Cars

Abstract: Collision-free navigation (CFN) for self-driving cars poses a challenging optimization problem, with notable advancements in approximate solutions using deep reinforcement learning. Quantum computing has gained renewed attention, including within the automotive industry. Quantum reinforcement learning (QRL) techniques show promise for faster training, especially in simplified domains. However, these methods have not yet been applied to real-world CFN scenarios and would typically demand an onboard quantum device for testing. This study explores the feasibility and potential advantages of QRL techniques for CFN in the current NISQ era without necessitating an onboard quantum device. This thesis introduces Nav-Q as the first QRL approach for CFN, outlining its functionality without onboard quantum hardware, and presenting a comparative assessment against classical alternatives.

Francesco Aldo Venturelli (MSc)

Master's Degree in Physics, University of Bologna, Italy

Supervisors: Prof. Stefano Lodi, Dr. Riccardo Mengoni, Dr. Antonio Macaluso

Title: Quantum Convolutional Neural Networks for Data-Efficient Image Classification

Abstract: This master's thesis delves into the realm of Quantum Convolutional Neural Networks (QCNNs) and their application to data-efficient image classification tasks. The research explores the potential of QCNNs to significantly enhance the efficiency of image classification models, capitalizing on the synergy between quantum computing principles and convolutional neural network architectures. Through rigorous experimentation and analysis, the thesis aims to demonstrate the advantages of integrating quantum computing techniques into image classification processes, offering promising insights for data-efficient and accurate image recognition systems.

Lorenzo Cellini (MSc)

Master's Degree in Artificial Intelligence, University of Bologna, Italy

Supervisors: Prof. Michele Lombardi, Dr. Antonio Macaluso

Title: QAL-BP: Quantum Augmented Lagrangian Approach to the Bin Packing

Abstract: This thesis introduces QAL-BP, a novel Quadratic Unconstrained Binary Optimization (QUBO) framework tailored for bin packing, suitable for quantum computation. QAL-BP merges augmented Lagrangian methodology, embedding bin packing constraints in the objective function while analytically estimating penalty multipliers. This yields a versatile model that eliminates instance-dependent Lagrangian coefficients, often needed in other QUBO formulations. We evaluate our method on bin-packing instances using a real Quantum Annealing device and compare it with simulated annealing and Gurobi classical solvers. Results validate our formulation's accuracy and showcase quantum computing's potential for the bin-packing problem, as more robust quantum technology emerges. As a result of the thesis, a journal paper has been published to *Scientific Reports* [1].

Supreeth Mysore Venkatesh (MSc)

Saarland Informatics Campus, Saarland University, Germany

Supervisors: PD Dr. Matthias Klusch, Dr. Antonio Macaluso

Title: On Quantum Coalition Structure Generation

Abstract: This thesis develops and assesses hybrid quantum-classical algorithms for solving the NP-hard coalition structure generation (CSG) problem in cooperative game theory. The first algorithm, BILP-Q [11], offers solutions for general coalitional games and is compatible with gate-based quantum computing and quantum annealing. It surpasses state-of-the-art classical solutions in time/gate complexity. The second proposed method, GCS-Q [9], addresses CSG in Induced Subgraph Games using quantum annealing. GCS-Q excels over current classical and quantum alternatives in runtime. Lastly, the third approach, QuACS [10], follows GCS-Q's strategy but employs gate-based quantum computation.

August 2021 - October 2022

February 2023 - Dec. 2023

September 2022 - March 2023

Matteo Antonio Inajetovic (MSc)

Master's Degree in Artificial Intelligence, University of Bologna, Italy

Supervisors: Prof. Claudio Sartori, Dr. Antonio Macaluso

Title: Variational Quantum Splines: Moving Beyond Linearity for Quantum Activation Functions

Abstract: Activation functions play a crucial role in neural networks since they allow the learning of complex and non-trivial patterns in the data. However, the unitarity constraint of quantum operators forbids non-linearity and poses a considerable obstacle to developing powerful quantum machine learning models. Recently, the idea of the QSplines [15] has been proposed to approximate a non-linear activation function by implementing the quantum version of the spline functions using a fault-tolerant quantum algorithm. This thesis proposes the Variational Quantum Splines, which use hybrid quantum-classical optimization to approximate non-linear activation functions using near-term quantum computing.

The idea of Variational QSplines proposed in the thesis has been published as a conference paper [5].

Filippo Orazi (MSc)

September 2021 - March 2022

Master's Degree in Artificial Intelligence, University of Bologna, Italy

Supervisors: Prof. Claudio Sartori, Prof. Stefano Lodi, Dr. Antonio Macaluso

Title: Development and evaluation of the Multiple Aggregator Quantum Algorithm

Abstract: This thesis extends and implements the generalized version of the quantum Single Layer Perceptron (qSLP) [14] using the Multiple Aggregator Quantum Algorithm [6, 12]. In particular, this work proposes the generalized qSLP to generate an exponentially large number of parametrized linear combinations in superposition that can be learned using quantum-classical optimization. As a consequence, the number of hidden neurons scales exponentially with the number of qubits and, thanks to the universal approximation theorem, our algorithm opens the possibility of approximating any function on quantum computers. Experiments show that the proposed generalized qSLP outperforms the existing full quantum machine learning model already implemented in the IBM Qiskit framework on standard benchmark datasets.

The generalized qSLP has been recently published as a conference paper [7].

Nicolò Cangini (MSc)

Master's Degree in Computer Engineering, University of Bologna, Italy

Supervisors: Prof. Claudio Sartori, Prof. Stefano Lodi, Dr. Antonio Macaluso

Title: Quantum Supervised Learning: Algorithms and Implementation

Abstract: This thesis introduces the fundamentals of quantum computing, with an emphasis on utilizing quantum algorithms for supervised learning. It encompasses both theoretical exploration and practical experimentation, conducted within the IBM Qiskit environment, enabling simulations of actual quantum computers. Additionally, the study provides an overview of quantum machine learning and examines the application of the HHL algorithm for supervised learning tasks.

Organization of Scientific Meetings

First DFKI-Workshop on Quantum Computing

German Research Center for Artificial Intelligence (DFKI), Saarbruecken, Germany

The objective of the workshop was to convene all the quantum computing projects at DFKI, fostering the development of an internal community dedicated to this topic. This collaborative community aims to facilitate joint research efforts and enhance project acquisition endeavors.

Reviewer Activity

I am a reviewer for the journals Neural Networks (Elsevier), Annalen der Physik (Wiley), and Quantum Machine Intelligence (Springer).

November 24, 2021

January 2019 - July 2019

$\mathbf{Q}(\mathbf{AI})^2$ - Quantum Artificial Intelligence for Automotive Industry

Funded by *BMBF* (4M) - Project webpage

The project's objective is to establish a comprehensive foundation of quantum algorithms for AI applications, with a strong emphasis on industrially relevant scenarios that can benefit from the accelerated capabilities of quantum AI. I am currently spearheading the research efforts for this project at DFKI. Specifically, our attention is directed towards three distinct NP-hard problems within the field of AI. The primary aim is to assess the feasibility and advantages of devising quantum algorithms for their solutions. Each problem corresponds to a dedicated work package, and for two of these challenges, we are collaborating with project partners who provide real-world industrial use cases.

Partners: Forschungszentrum Jülich GmbH, Peter Grünberg Institut (Jülich), Mercedes-Benz AG (Böblingen), BMW AG (München), Robert Bosch GmbH (Renningen), Volkswaagen AG (München).

Research Collaborations

University of Bologna, Bologna, Italy

Continuing from my dissertation work, I am engaged in collaboration with my former research group, focusing on the application of quantum computing to classical machine learning. Specifically, I lead thesis projects, involving student co-supervision, aimed at further developing the algorithms proposed in my Ph.D. thesis. This work builds upon the formulation of the quantum Single Layer Perceptron [14] and the Multiple Aggregator Quantum Algorithm [6, 12]. Recently, a paper that extends the qSLP to accommodate an arbitrary number of neurons has been published, demonstrating its superiority over existing Quantum Machine Learning (QML) models implemented in qiskit [7]. Additionally, a hybrid quantum-classical version of the original Quantum Splines proposed in my thesis [15] has also been published [5]. Furthermore, leveraging my foundational knowledge in machine learning, I am collaborating with the Department of Physics and the National Italian Institute for Nuclear Physics (INFN) on the application of conventional deep learning algorithms for fluorescence microscopy image segmentation [4, 2].

National Institute for Astrophysics (INAF), Bologna, Italy

I collaborate with the Agile Team at the Italian National Institute for Astrophysics (INAF) to advance deep learning algorithms for γ -ray burst analysis. My primary role involves providing support and addressing methodological challenges, starting with specific issues related to space observation and satellite data. This collaboration has yielded two journal publications [13, 8]. Additionally, in recent times, we have begun exploring the use of Quantum Convolutional Neural Networks for particle identification in High Energy Physics, guided by joint supervision of Master's students from the University of Bologna.

INVITED TALKS

International Winter School on Quantum Machine Learning

Technische Universität Kaiserslautern-Landau (RPTU), Kaiserslautern, Germany

 ${\bf Title:}$ Introduction to Quantum Machine Learning

Absract: Quantum Machine Learning (QML) is an emerging field aiming to harness the unique properties of quantum computation to enhance the performance of models beyond traditional machine learning algorithms. This lecture on QML discusses the advantages that quantum technologies can bring to the field of machine learning. This involves employing fault-tolerant end-to-end quantum algorithms or hybrid quantum-classical methods. This QML lecture adopts a computer science perspective and is organized into two parts. In the first part, we present two distinct approaches to QML, differentiating between fault-tolerant algorithms designed for an ideal quantum computer and hybrid quantum-classical algorithms, which are tailored for near-term quantum computers, taking into account a limited number of noisy qubits. In the second part, we explore the specific applications of QML algorithms, with a particular emphasis on supervised learning and reinforcement learning in various real-world scenarios.

February 2024

April 2021 - March 2024

2021 - present

2020 - present

QuCoLiMa - Quantum Computers: from Basics to Compilers

Saarland University, Saarbruecken, Germany

Title: Quantum Computing: A Classical Perspective

Absract: In this talk, we approach the intriguing field of quantum computing from a classical standpoint. While quantum computing is often discussed within the realm of quantum mechanics and complex mathematical frameworks, this presentation takes a novel approach by examining its principles and potential impact through the lens of classical computing paradigms. We delve into the fundamental concepts of quantum computing, exploring how they contrast with classical computing principles and algorithms. By highlighting key differences and similarities, we aim to demystify quantum computing for audiences familiar with classical computing, providing insights into its promise, challenges, and real-world applications. Through this classical perspective, we endeavor to foster a deeper understanding and appreciation of the transformative potential of quantum computing in our digital landscape.

Focus Semester on Quantum Information

Saarland University, Saarbruecken, Germany

Title: Quantum Computing for AI Applications (30 min, list of talks)

Absract: Quantum computing represents a promising alternative to cope with the need to analyze ever-increasing amounts of information. This talk introduces the domain of Quantum Artificial Intelligence, with a focus on how quantum computation can help to improve classical AI methods in solving challenging tasks with demanding computational requirements. In particular, we will discuss some typical AI problems in the context of machine learning, multi-agent systems, scheduling and planning, and we will examine several quantum approaches, with particular care to the advantages with respect to their classical counterparts.

Talks from over 5 years ago

8th Italian Workshop on Machine Learning and Data Mining

AI*IA Conference, Cosenza, Italy

Title: Quantum Machine Learning with Linear Models

Abstract: This talk highlights the HHL algorithm's role in solving linear equations in logarithmic time and its application in Quantum Machine Learning. We examine Ridge Regression (RR) and spline interpolation, which exploit HHL's exponential speedup to enhance parameter estimation in linear models. RR reduces condition numbers for a more quantum-friendly approach, while spline interpolation fits non-linear functions by utilizing quantum computing's ability to handle low-rank linear systems efficiently. Our aim is to showcase RR and spline methods as effective solutions to the HHL algorithm's limitations, demonstrating their potential to make quantum machine learning applications more efficient by optimizing quantum resources.

7^{th} Italian Workshop on Machine Learning and Data Mining

AI*IA Conference, Trento, Italy

Title: Machine Learning in Quantum Computing: State of the art and challenges

Quantum Machine Learning (QML) leverages quantum mechanics for faster problem-solving compared to classical algorithms. Quantum parallelism, enabled by qubit superposition, allows the simultaneous evaluation of functions on multiple inputs. QML can be approached in two ways, either combining classical and quantum computation or using purely quantum computation. Challenges in QML include adapting supervised learning to quantum computing, addressing various aspects of data clustering, and developing quantum neural network models for handling of large datasets.

CERTIFICATIONS

IBM Certified Associate Developer (Verify my badge)

IBM Quantum Qiskit Advocate (Verify my badge)

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December 2021 September 2020

November 2019

November 2018

December 2022

References

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- [2] Luca Clissa, Antonio Macaluso, Roberto Morelli, Alessandra Occhinegro, Emiliana Piscitiello, Ludovico Taddei, Marco Luppi, Roberto Amici, Matteo Cerri, Timna Hitrec, et al. "Fluorescent Neuronal Cells v2: multi-task, multi-format annotations for deep learning in microscopy". In: *Scientific Data* 11.1 (2024), p. 184. DOI: 10.1038/s41597-024-03005-9.
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