`scikit-project`: How open source is empowering open science – and vice versa

Nathan Shammah
Theoretical Quantum Physics Lab
Cluster for Pioneering Research
RIKEN, Saitama, Japan

Machine Learning Talks
Spaces Shinagawa
7th November 2019


NathanShammah

Take-Home Message

Open-source and open science empower each other

Open-Source Software

- Reproducible results
- Accelerate discovery
- Coordinate teams, projects

Open Science

- Best practices: *The Scientific Method*, peer review
- Community: ideas, cutting-edge tools
- Subsidize / Support software development

Arguments against open-source software development

A slippery slope

1. **“Competitive advantage”** – you developed some technology over the years
2. **“I’m not interested”** – you only seek the fastest way to do research
3. **Systematic errors** – you are distributing software for others to use
5. **It’s time consuming** – you don’t want to maintain the software

TOOLBOX · 01 JULY 2019

How to support open-source software and stay sane

Releasing lab-built open-source software often involves a mountain of unforeseen work for the developers.

Anna Nowogrodzki

https://www.nature.com/articles/d41586-019-02046-0

Sustainability of the Open-Source Ecosystem

Open-source and open science empower each other

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Non-Profit Org:

NUMFOCUS

OPEN CODE = BETTER SCIENCE

Gig-economy model:

OpenTeams

Outline

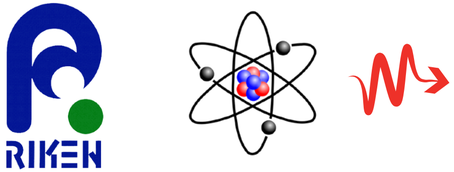
This talk

- My perspective
- Open source in science
- Open source in quantum physics
- Quantum technologies

About me

Nathan Shammah

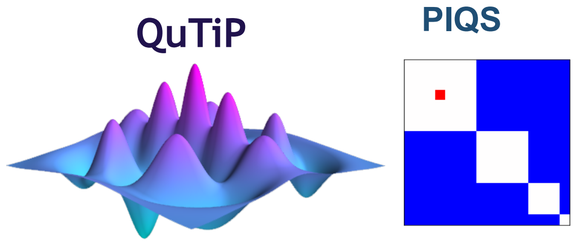
Academic



- Currently: Research Scientist at RIKEN, Wako-shi

Research field: cavity quantum electrodynamics

Education: PhD in Physics at U. of Southampton (UK)
BSc+MSc at U. of Milan (Italy)



PIQS library with S. Ahmed

medium.com/quantum-tech

Monthly newsletter on Quantum Tech

Non-Academic

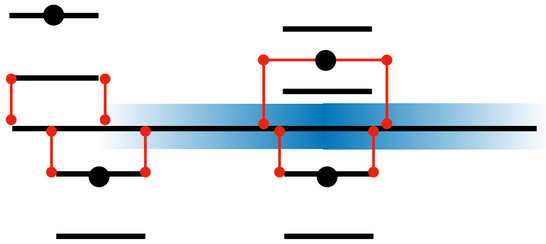
Consulting for investors (VCs), spin-offs. quantika.co

My Research

Cooperative processes in many-body quantum physics

Intersubband Transitions
Polaritons

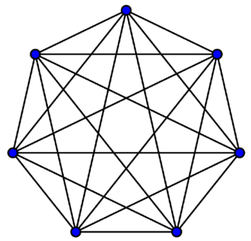
Giant Artificial Atoms



Two-Level Systems
Spins/Qubits

Involvement in Research and Open Source

Hamiltonian



Cooperative phenomena in quantum physics
– A common thread of my research interests

Cooperative behavior in scientific research
– My engagement with quantum open-source development

Open source

A new era for open source

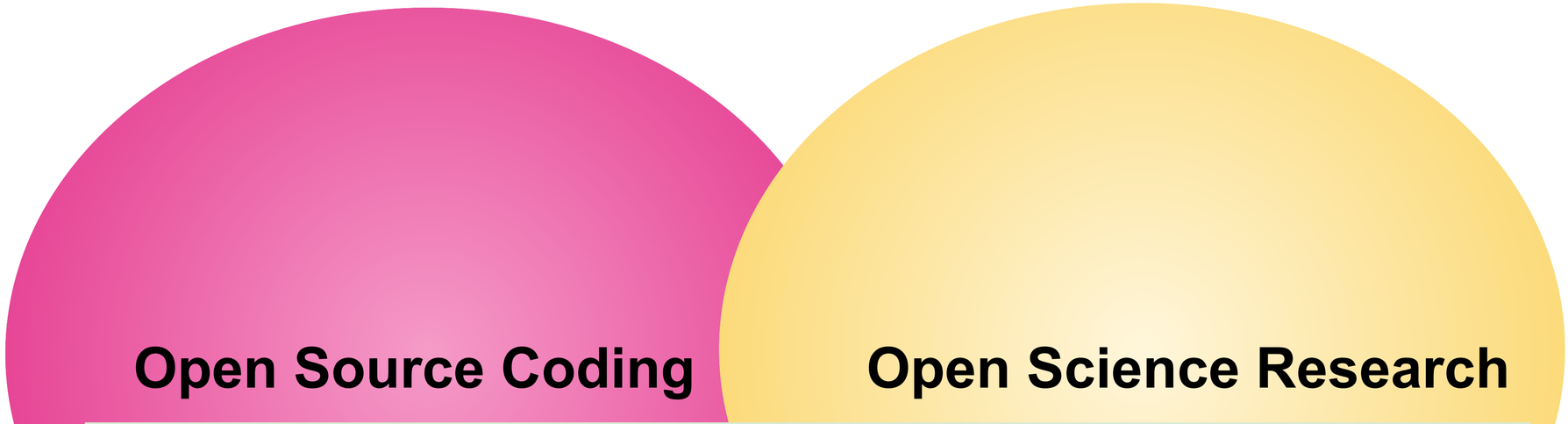
Open-Source Basics
Read. Download. Deploy.
Definition: You can **read** the source code (open-source ≠ free).
Examples of open-source: Linux, Android, FireFox, MySQL, LibreOffice, **Python**.
Open-source deployment is **accelerating** many end-industries applications.

Features for Developers
Learn. Debug. Deploy.
You can **learn** by reading the code and become a better developer.
You can edit the source code (licenses apply) and **collaborate** to existing projects.
You can submit **fixes** to bugs, propose improvements.

Open-source for Businesses
Flexible. Valuable. Growing fast.
Source is generally free but companies can charge for additional services.
GitHub acquired for $7.5 bln (2018).GitLab: $100 mln in funding (2018).
Red Hat acquired by IBM for $34 bln (2019).
Machine learning (‘AI’) is driving **fast**, pervasive adoption of open-source libraries.

Open source for open science

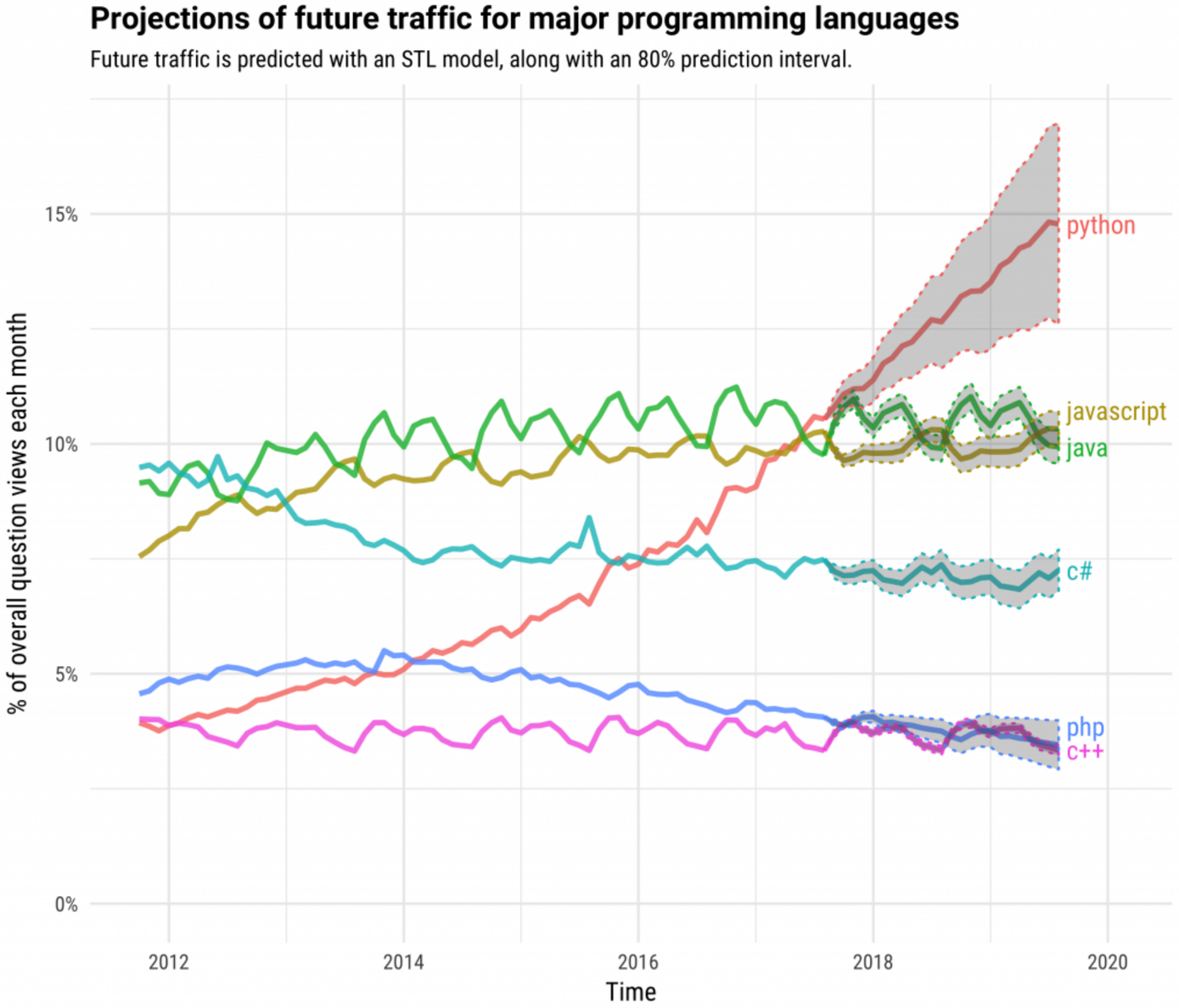
An aligned vision



- Allow **access** to the **research**/project results, sharing knowledge.
- **Coordinate** large and delocalized **teams** working remotely.
- Make supporting data and code available for painless **reproducibility**.

The steady growth of Python

Empowered by a large open-source ecosystem



stackoverflow

Source: David Robinson

Python’s strengths

A community-based programming language

Community

PyCons
Workshops
Sprints
EuroSciPy

Libraries

Tools

Notebooks
LaTeX comments
Interactive code
Jupyter

Jupyter Notebooks

An interactive tool to distill code and research

IPython

Markdown

Below we give basic examples on the use of `qutip.piqs`. In the first example the incoherent emission of N driven TLSs is considered. In tl
two-level system ensemble is a subsystem coupled to another subsystem, a bosonic cavity. Similar considerations apply to the coupling to
subsystems (a single qubit, another two-level system ensmble).

Code blocks

In [1]:
```
import matplotlib.pyplot as plt
import matplotlib as mpl
from matplotlib import cm

from qutip import *
from qutip.piqs import *

import matplotlib.animation as animation
from IPython.display import HTML
from IPython.core.display import Image, display
```

1. N Qubits Dynamics

We study a driven ensemble of N TLSs emitting incoherently,

LaTeX

$$H_{\rm TLS} = \hbar\omega_0 J_z + \hbar\omega_x J_x$$

Plots

$$\dot{\rho} = \mathcal{D}_{\rm TLS}(\rho) = -\frac{i}{\hbar}[H_{\rm TLS}, \rho] + \sum_{n=1}^{N} \frac{\gamma_{\rm E}}{2}\mathcal{L}_{J_{-,n}}[\rho]$$

Notebooks: The new research paper?

A bold stance…

https://www.theatlantic.com/science/archive/2018/04/the-scientific-paper-is-obsolete/556676/

TECHNOLOGY FEATURE · 05 NOVEMBER 2019

Make code accessible with these cloud services

Container platforms let researchers run each other's software – and check the results.

Jeffrey M. Perkel

https://www.nature.com/articles/d41586-019-03366-x

Beyond Reproducibility: Generalization

From reproducible data to reusable code.

Group leader at INRIA in Paris, scikit-learn core developer.

		DATA	
		Same	**Different**
ANALYSIS	**Same**	Reproducible	Replicable
	Different	Robust	Generalizable

Notebooks: The new research paper?

A bold stance…

Jupyter Project: a long evolution and a growing family

One could say it all started in the 1980s with Matlab and Mathematica

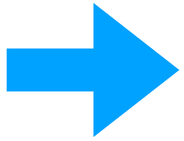
Mathematica

project.nb

MATLAB

project.m

IPython



Jupyter Notebooks

Interactive notebook

JupyterLab

IDE & notebook hybrid

JupyterHub

Set up on your own server

BinderHub

Built on top of JupyterHub

See also:

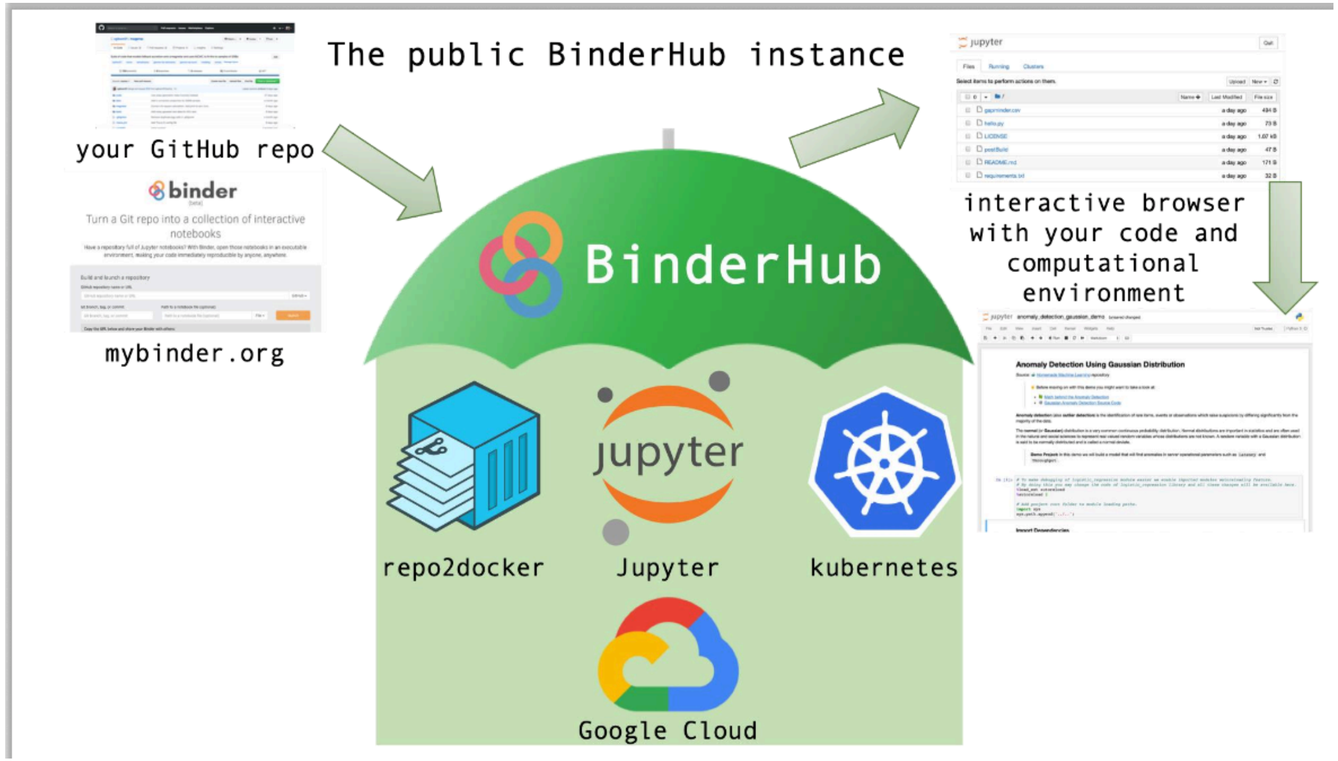
Reproducing Machine Learning Research on Binder | OpenReview

NIPS 2018

My Binder

mybinder.org is a BinderHub for all to use

My Binder: cloud-based notebooks



Github Repository: `environment.yml`

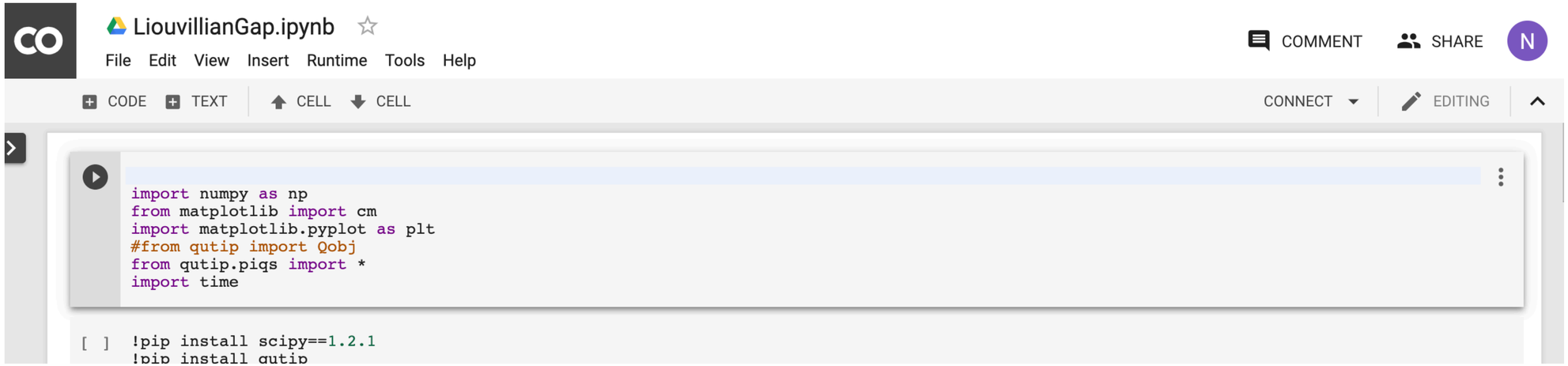
`requirements.txt`

`apt.txt`

Alternative Options for Cloud Notebooks

Various options are becoming available

Option 1. My Binder
Option 2. Google Colab https://colab.research.google.com/notebook



More options: "Six easy ways to run your Jupyter Notebook in the cloud" By Kevin Markham

https://www.kaggle.com/general/87098

Nice Comparison Table https://docs.google.com/spreadsheets/d/12thaaXg1Idr3iWST8QyASNDs08sjdPd6m9mbCGtHFn0/edit

scikit-project: Easy steps to open-source a science project

The tools of open source make your code count

Code & Testing

Documentation

Publication

A Guide to Building Your Open-Source Science Library

A cheatsheet to develop a scientific open-source library from scratch.

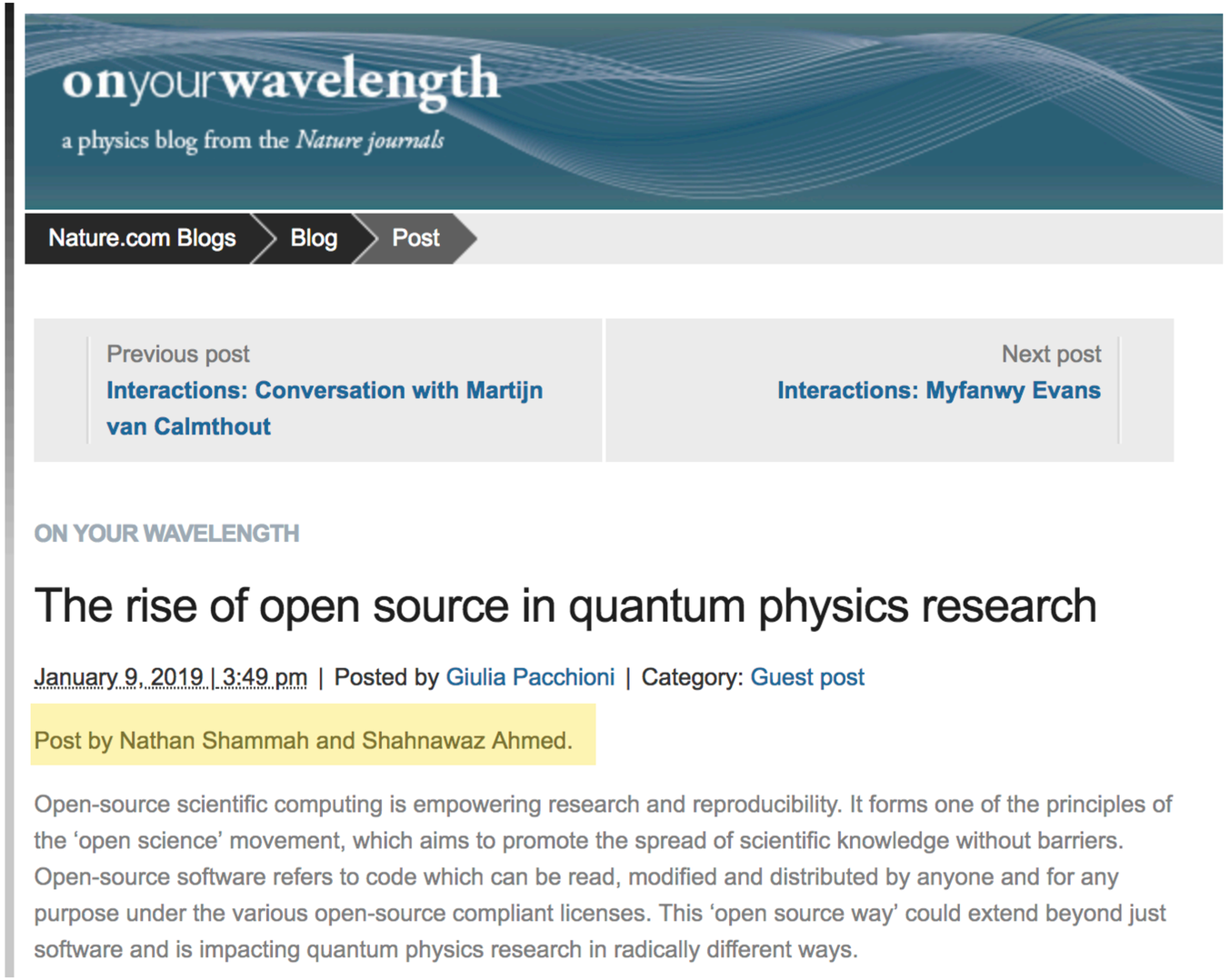
Zero to Library

Here you will find information to design, build, and release an open-source library to perform scientific research in Python from scratch to finish.

https://github.com/nathanshammah/scikit-project

The rise of open source in quantum physics research

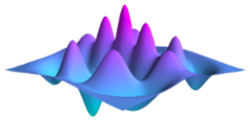
Nathan Shammah and Shahnawaz Ahmed



blogs.nature.com/onyourwavelength

Quantum Tech: Open Source Libraries

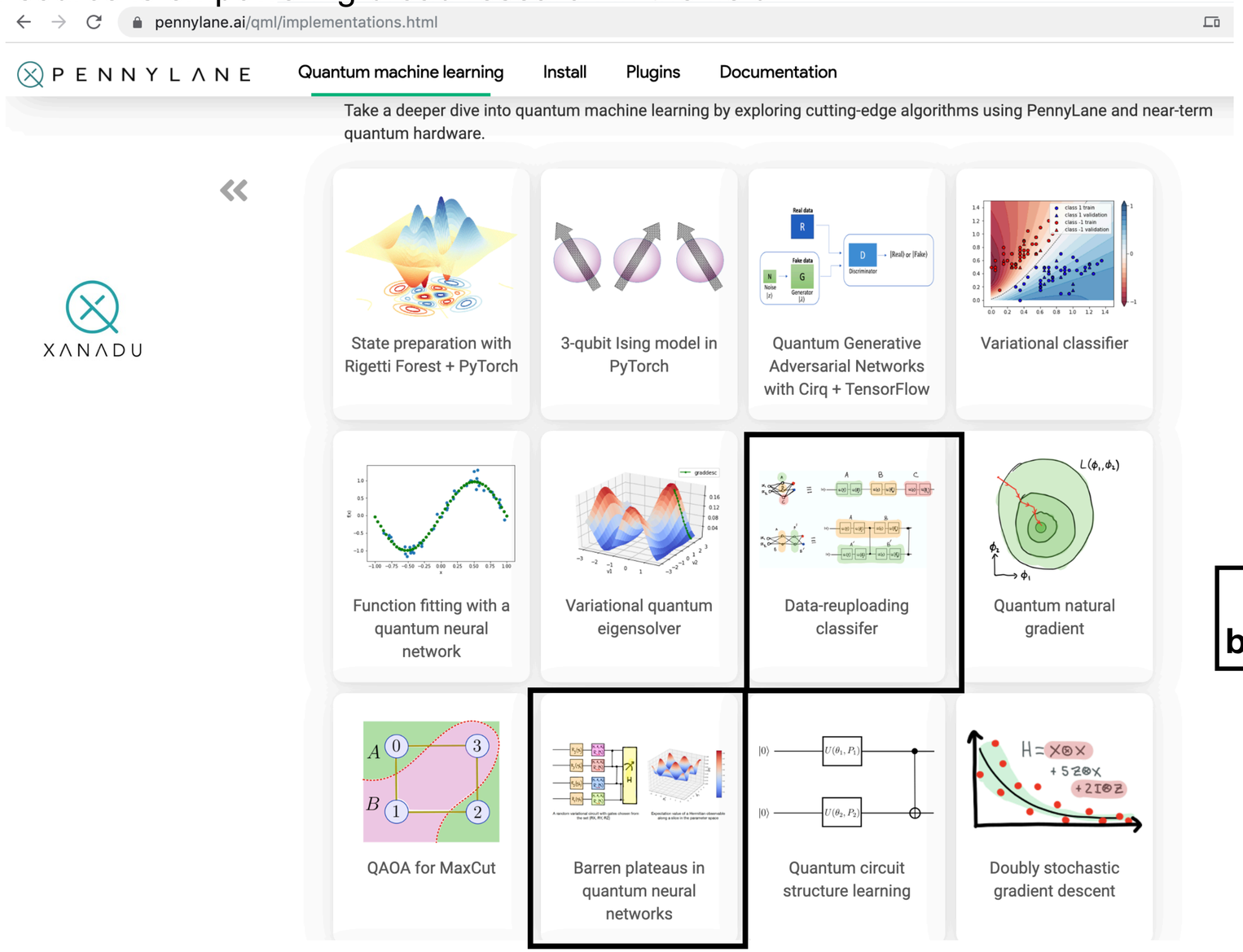
More open-source is empowering broad research in the field

Library	Year	Creators	Institution	Language	Description
 QuTiP Quantum Toolbox in Python	2012	Rob Johannson Paul Nation Franco Nori	RIKEN	**Python**	Simulation of open quantum systems; quantum optics, cavity QED.
 **QNet**	2012	Nikolas Tezak, Michael Goerz Hideo Mabuchi	Stanford	**Python**	Computer algebra package for quantum mechanics and photonic quantum networks
 QuantumOptics.jl	2017	Sebastian Krämer *et al.*	U Innsbruck IQOQI	Julia	Quantum optics and open quantum systems framework inspired by the QO toolbox in Matlab and QuTiP
ProjectQ	2016	Damian S. Steiger Thomas Häner Matthias Troyer	ETH Zurich	**Python**	Hardware-agnostic framework with compiler and simulator with emulation capabilities.
 OpenFermion	2017	Ryan Babbush *et al.*	Google (unofficial)	**Python**	Fermionic potential calculations for quantum chemistry
 **NetKet**	2018	Giuseppe Carleo	The Simons Foundation	C++ **Python**	Studying many-body quantum systems with artificial neural networks and ML techniques.
STRAWBERRY FIELDS PENNYLANE	2018	Nathan Killoran *et al.*	Xanadu Inc	**Python**	Photonic quantum computing And machine learning with continuous-variable optical circuits

Checkout more open-source projects at https://qosf.github.io

Quantum Tech: Open Source Libraries

More open-source is empowering broad research in the field



XANADU

Two notebooks by Shahnawaz Ahmed

Machine Learning and Quantum do not commute

Define: Commutator

$$[A, B] = AB - BA$$

$$[\mathbf{ML}, Quantum] \neq 0$$

MLQ

Machine Learning of Quantum Systems

Apply “standard” Machine Learning to
Study Quantum Physics Systems

J. Carrasquilla & R. Melko, *Nature Phys.* (2017)

QML

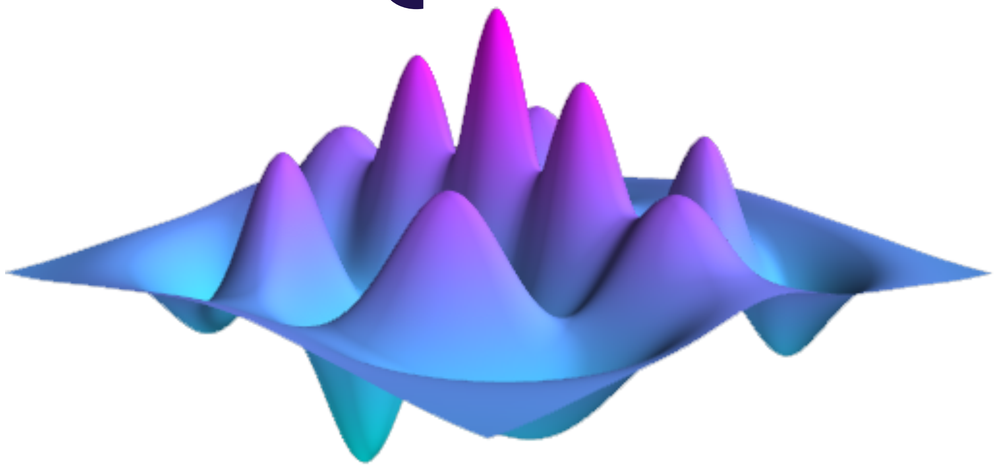
Quantum-enhanced Machine Learning

Exploit quantum correlations
for new algorithms and frameworks (QNN)

J. Biamonte, …, S. Loyd, *Nature* (2017)

The Quantum Toolbox in Python

QuTiP



RIKEN

日本学術振興会
Japan Society for the Promotion of Science

JST Japan Science and Technology Agency

UNIVERSITÉ DE SHERBROOKE

PRIFYSGOL ABERYSTWYTH UNIVERSITY

NUMFOCUS
OPEN CODE = BETTER SCIENCE

Google Summer of Code

Cavity Quantum Electrodynamics (Cavity QED)

Using the **Qu**antum **T**oolbox **i**n **P**ython to study physics

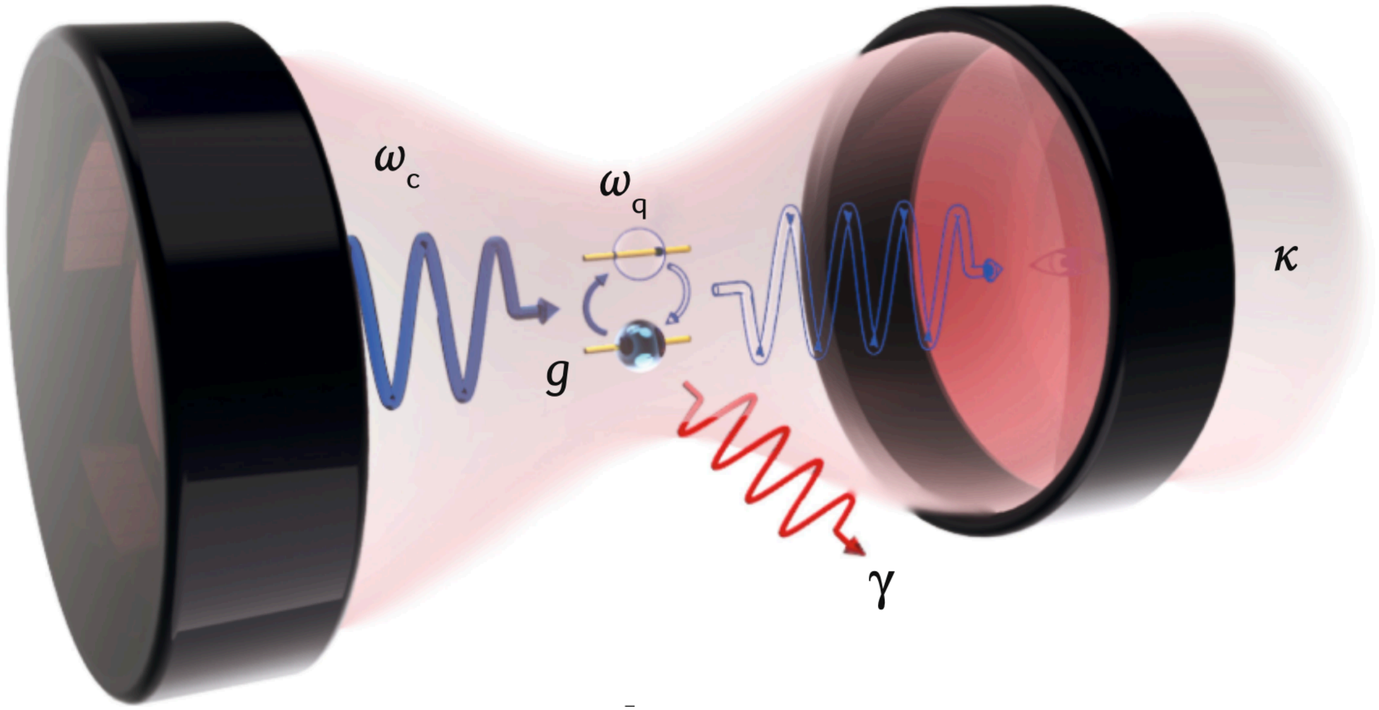
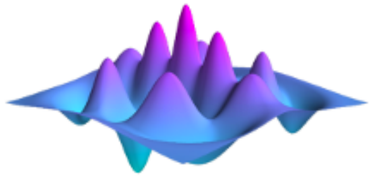


Image Credit: A. F. Kockum, A. Miranowicz, S. De Liberato, S. Savasta & Franco Nori, Nature Reviews Physics, **1** 19 (2019)

Cloud-based Notebooks on Open Quantum Systems

The **Qu**antum **T**oolbox **i**n **P**ython



QuTiP

Quantum Toolbox in Python

You can find an interactive notebook at

https://github.com/nathanshammah/

Repository: interactive-notebooks

You can run the notebooks live

launch binder

Take a snapshot

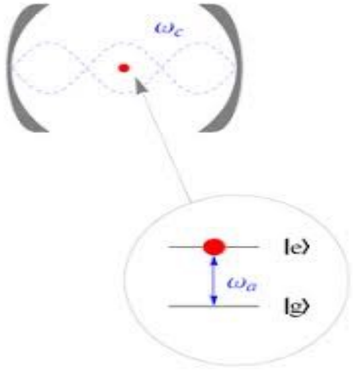
Abdus Salam ICTP
UNESCO, AIEA
Trieste, Italy
July-August 2019

ICTP

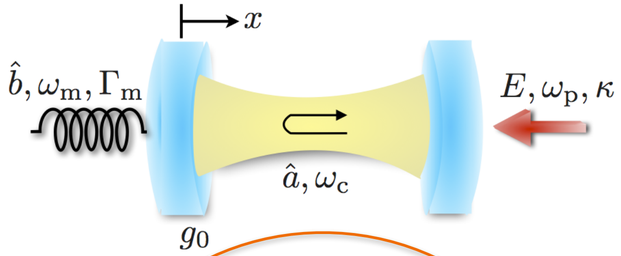
QuTiP: The Quantum *Physics* Simulator

The **Qu**antum **T**oolbox **i**n **P**ython

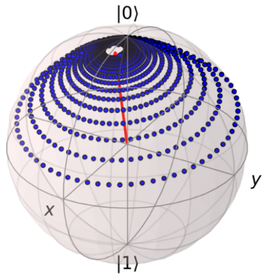
Cavity QED



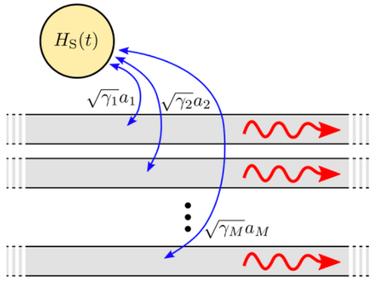
Optomechanics



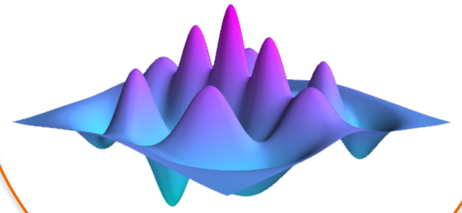
Quantum Optics, QIP



Waveguide QED

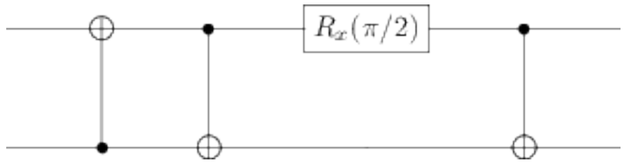


QuTiP



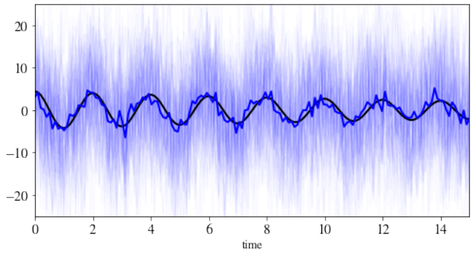
qutip.org

Quantum Circuits

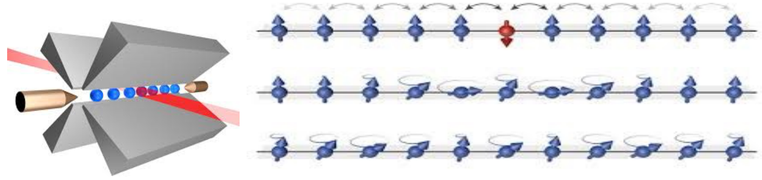


Quantum Optimal Control

Stochastic Dynamics



Spin Lattice Dynamics



QuTiP: History of the project at a glance

The **Qu**antum **T**oolbox **i**n **P**ython

Project Impact

QuTiP
Quantum Toolbox in Python

>**1000** citations (G Scholar)

downloads 130k total (conda forge)

More info at http://qutip.org/

Authors

Comp. Phys. Comm. 183, 1760–1772 (2012); ibid. 184, 1234 (2013).

Code

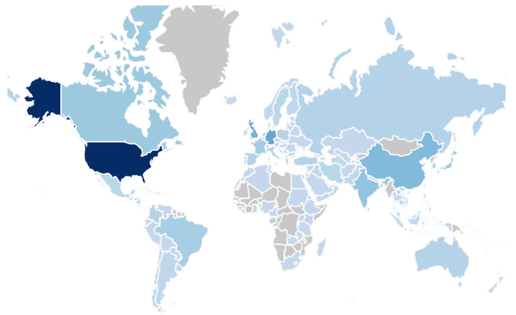
Robert J. Johansson
Rakuten Inc.

Paul D. Nation
IBM Q

Franco Nori
RIKEN / U. Michigan

Users

Distribution of 25k website visitors (2016)



Timeline:

Inspired by the Quantum Toolbox in MatLAB.

- 2011-2012: **QuTiP** 1.0
- Aug 2015: 100 citations
- Aug 2016: 200 citations
- Jan 2017: QuTiP 4.0
- July 2018: QuTiP 4.3
- July 2019: QuTiP 4.4

Previous Lead Developers

Alex Pitchford
Aberystwyth University

Éric Giguère
U. Sherbrooke

Arne Grimsmo
Universite de Sherbrooke

Chris Grenade
University of Sydney

Contributing Developers

- Neill Lambert (RIKEN)
- Denis Vasilyev (Leibniz)
- Kevin Fischer (Stanford)
- Jonathan Zoller (Ulm University)
- Ben Criger (RWTH Aachen)
- …
- Louis Tessler (RIKEN)
- Shahnawaz Ahmed (Chalmers) (**Lead**)
- Nathan Shammah (RIKEN) (**Lead**)

- **GitHub**: 44 contributors, 4k commits

License: BSD

(Berkeley Software Distribution)
Style: PEP8 compliant

Libraries used:

- Scipy
- NumPy
- Cython
- Matplotlib
- SymPy

- Jupyter notebooks
- Online documentation
- Independent testing

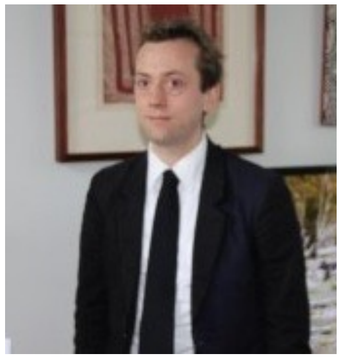
QuTiP Current Lead Developers

Shahnawaz Ahmed
Chalmers, Sweden

Alex Pitchford
Aberystwyth University
United Kingdom

Eric Giguère
U. de Sherbrooke
Canada

Nathan Shammah
RIKEN, Japan



Neill Lambert
RIKEN, Japan

Franco Nori
RIKEN, Japan
U. of Michigan (USA)

日本学術振興会
Japan Society for the Promotion of Science

Japan Science and Technology Agency

RIKEN

JOHN TEMPLETON FOUNDATION

NUMFOCUS
OPEN CODE = BETTER SCIENCE

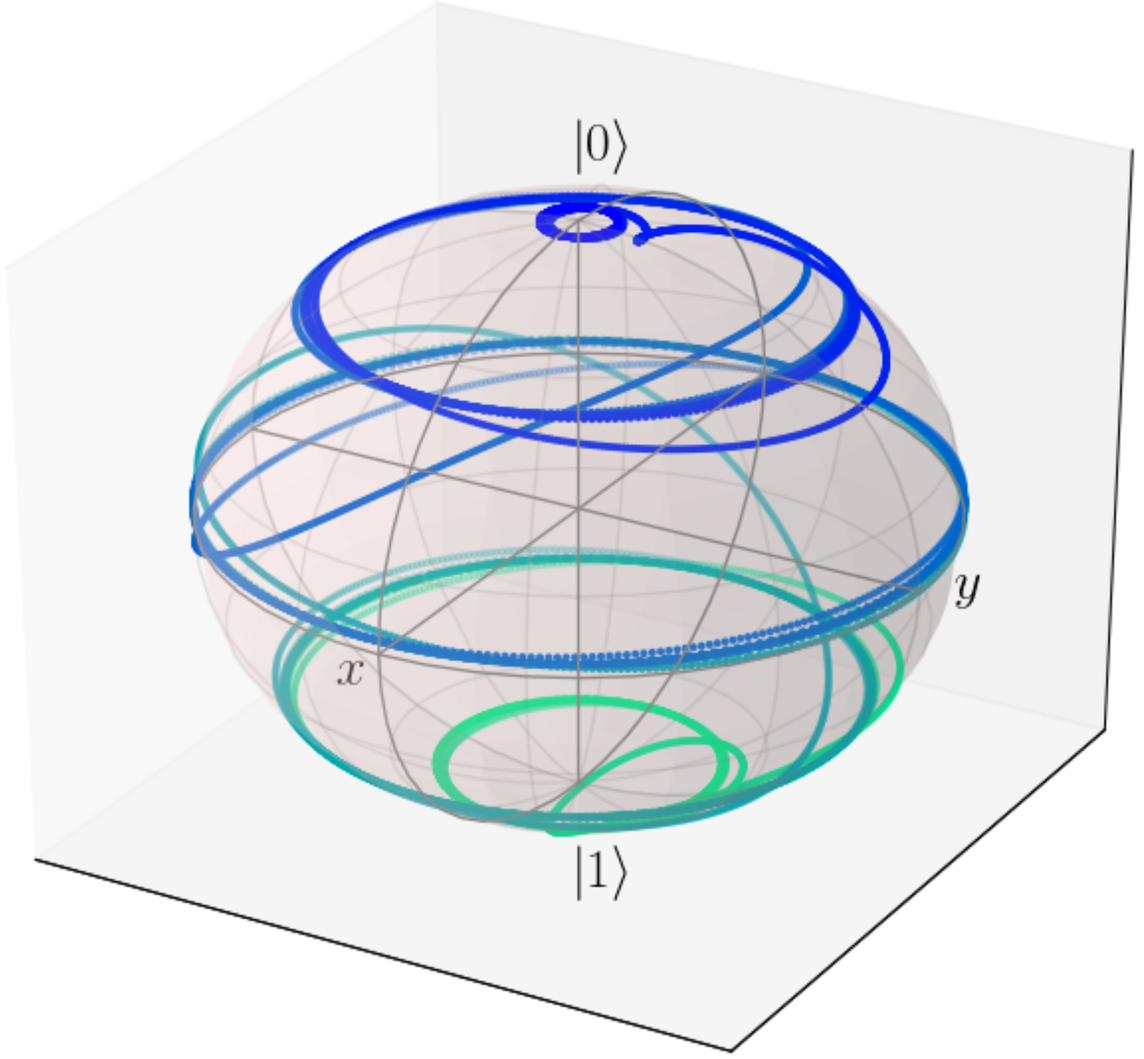
Google Summer of Code

UNIVERSITÉ DE SHERBROOKE
Alexandre Blais's group

PRIFYSGOL ABERYSTWYTH UNIVERSITY

QuTiP: Visualize a qubit

The **Qu**antum **T**oolbox **i**n **P**ython



qutip.org/tutorials

github.com/qutip

launch binder

Take a snapshot

1.Introduction_to_qutip.ipynb

https://github.com/nathanshammah/interactive-notebooks

What does a Schrödinger Cat looks like

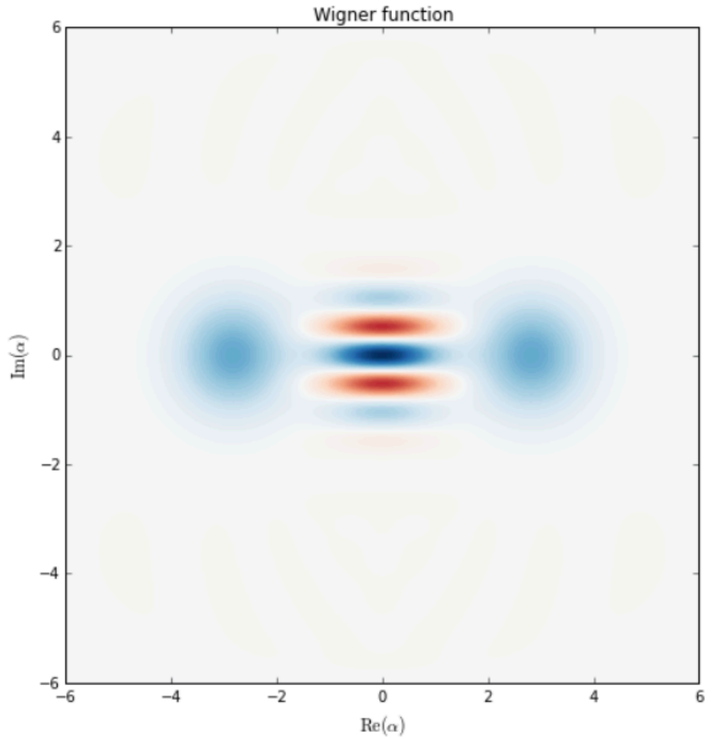
The **Qu**antum **T**oolbox **i**n **P**ython

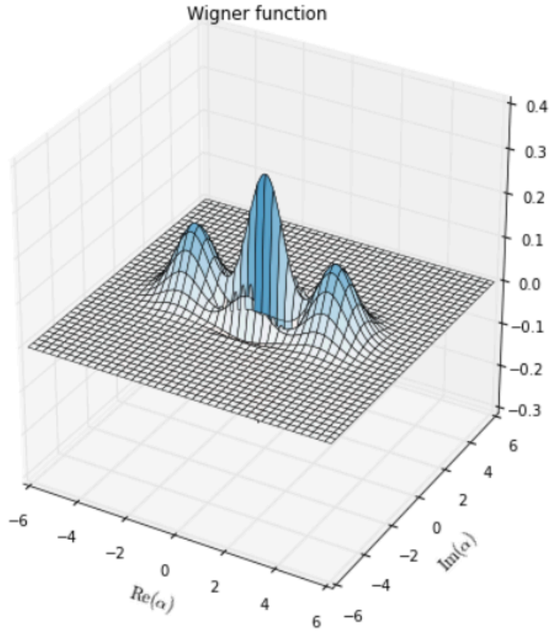
qutip.org/tutorials

Superposition of coherent states

```
In [9]: psi = (coherent(N, -2.0) + coherent(N, 2.0)) / np.sqrt(2)
        plot_wigner_2d_3d(psi)
```

Out[9]:





https://github.com/nathanshammah/interactive-notebooks

Cavity Quantum Electrodynamics (Cavity QED)

Using the **Qu**antum **T**oolbox **i**n **P**ython to study physics. Things are scaling up

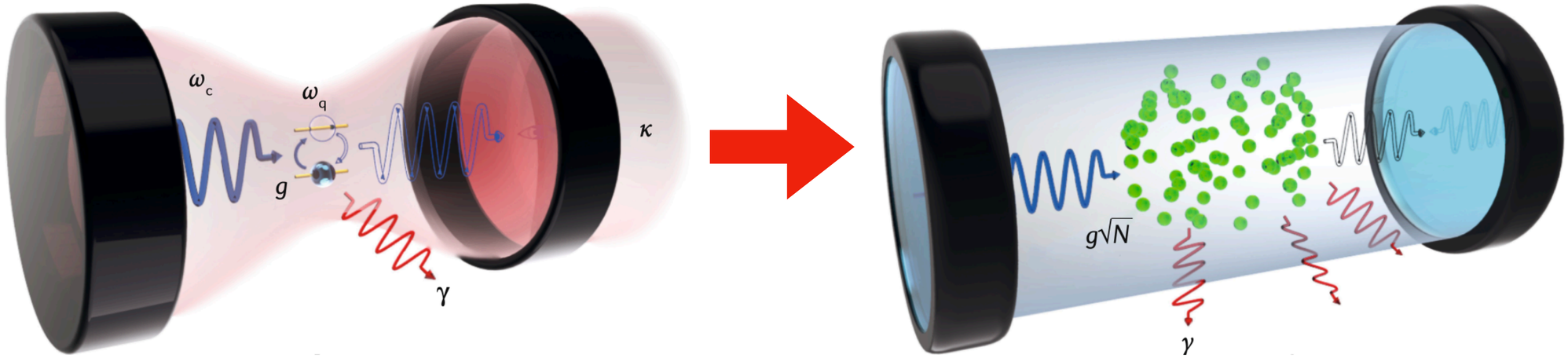


Image Credit: A. F. Kockum, A. Miranowicz, S. De Liberato, S. Savasta & Franco Nori, Nature Reviews Physics, **1** 19 (2019)

Dicke state basis as a visualization tool

Density matrices of collective quantum states

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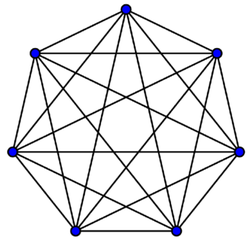
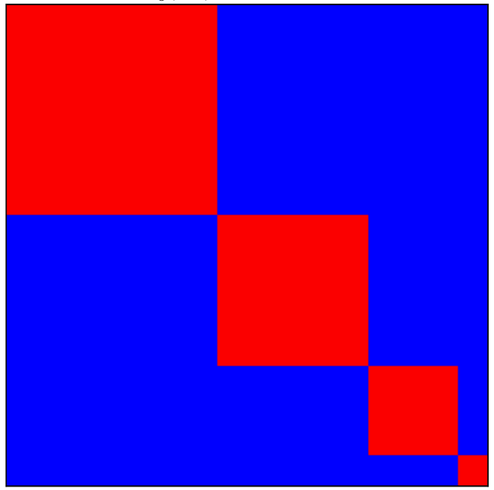
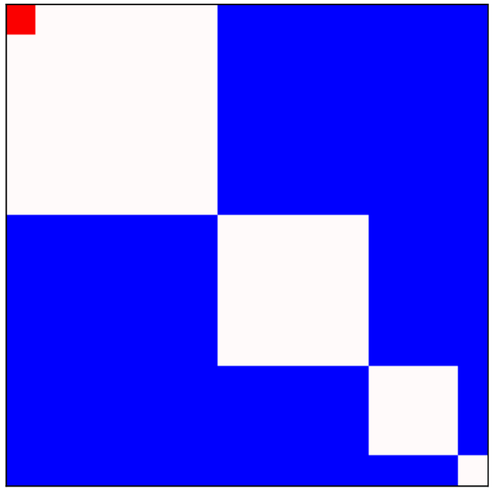


Can also study:
GHZ state
CSS states
Thermal states

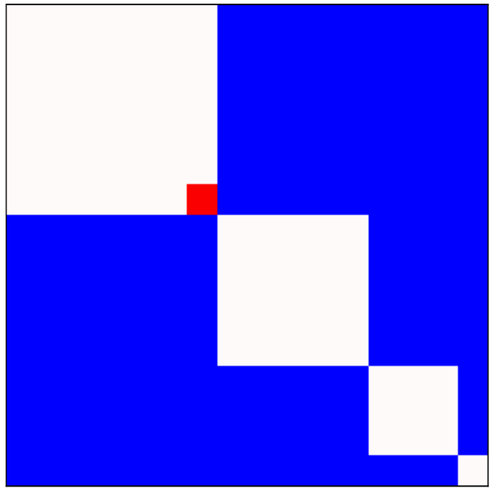
$\rho = \sum_{j,m,m'} |j,m\rangle\langle j,m'|$



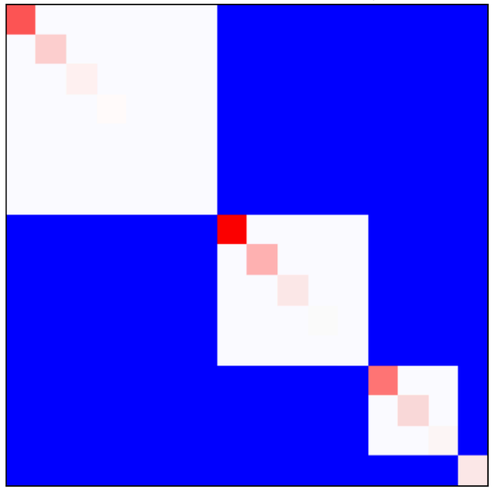
Fully excited state, $|\frac{N}{2},\frac{N}{2}\rangle\langle\frac{N}{2},\frac{N}{2}|$



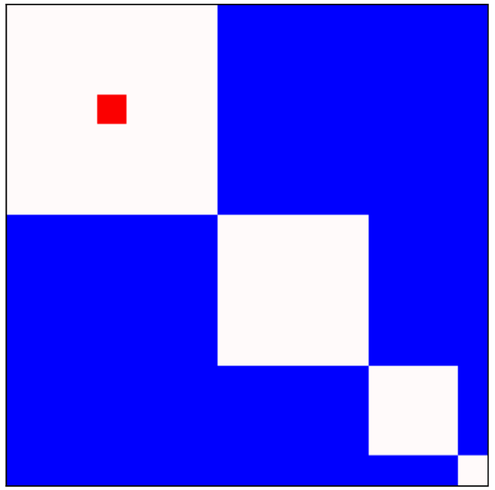
Ground state, $|\frac{N}{2},-\frac{N}{2}\rangle\langle\frac{N}{2},-\frac{N}{2}|$



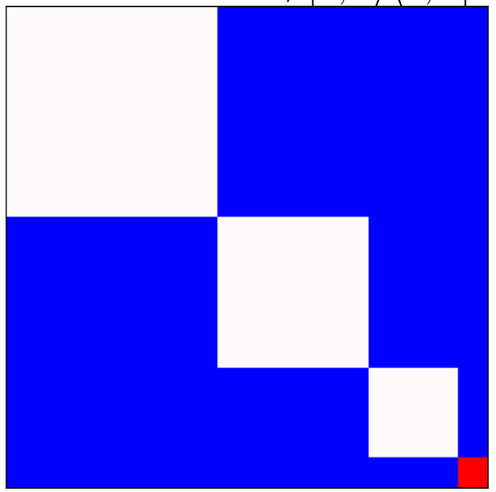
Steady state, $H = J_z$, $\gamma_\downarrow = 0.3\gamma_\uparrow$



Superradiant state, $|\frac{N}{2},0\rangle\langle\frac{N}{2},0|$

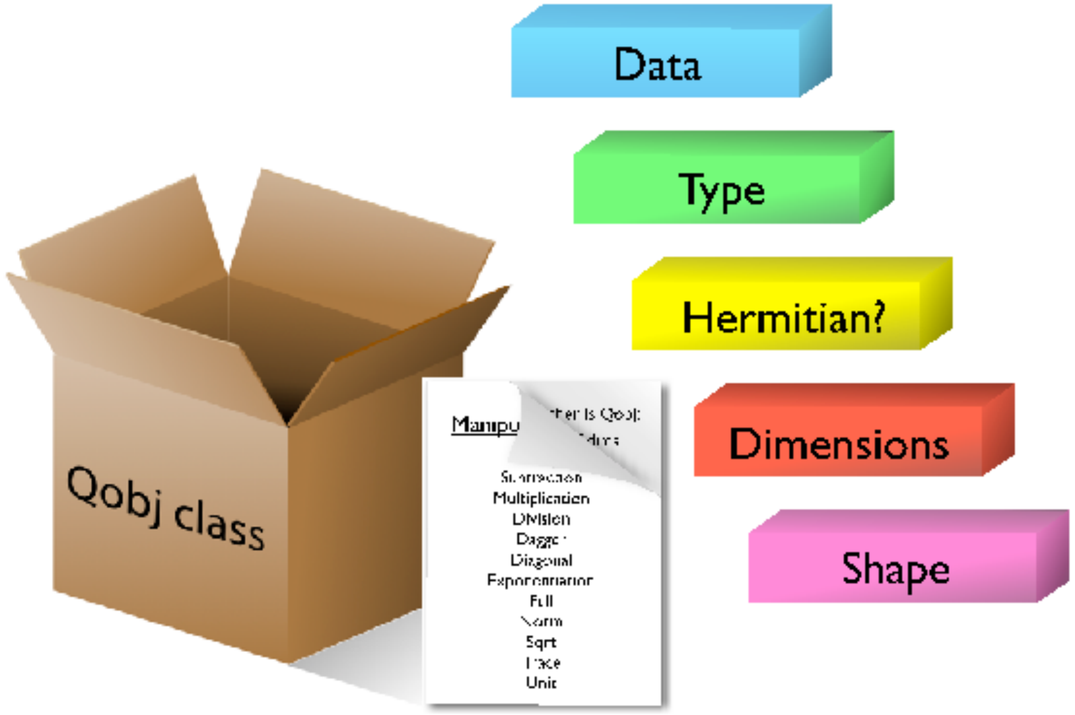


Subradiant state, $|0,0\rangle\langle 0,0|$



QuTiP: The `Qobj` class

The **Qu**antum **T**oolbox **i**n **P**ython



Take a snapshot

J. R. Johansson, P. D. Nation, and F. Nori, Comp. Phys. Comm. **183**, 1760–1772 (2012)
QuTiP: An open-source Python framework for the dynamics of open quantum systems

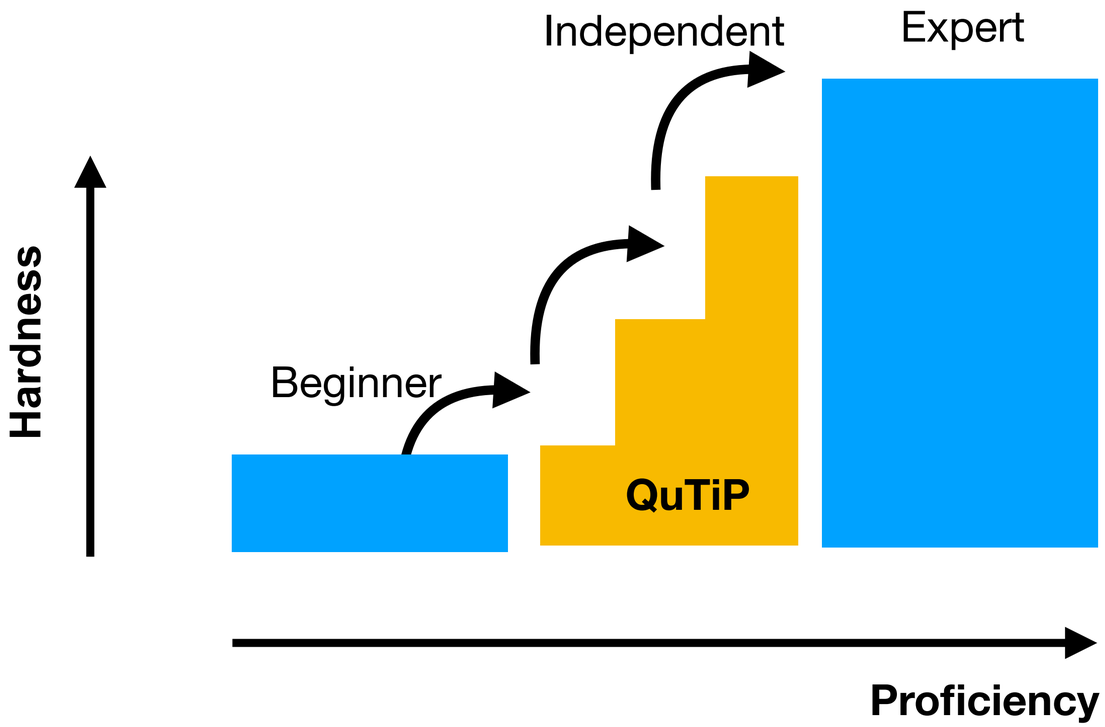
https://github.com/nathanshammah/interactive-notebooks

You can run the notebooks live

QuTiP: A tool to explore quantum mechanics

The **Qu**antum **T**oolbox **i**n **P**ython

Quantum mechanics made easy



Tutorials at qutip.org/tutorials

Python Introduction

- Quick introduction to Python
- Overview of NumPy Arrays
- Brief Introduction to Matplotlib

For a more in depth discussion see: Lectures on scientific computing with Python.

Basics

- Introduction to QuTiP
- Exponential series
- Groundstates: Jaynes-Cumming model in the ultrastrong coupling regime
- Superoperators, Pauli Basis and Channel Contraction

Visualization

- Visualization demos
- Energy-level diagrams
- Bloch-sphere animation
- Bloch Sphere with Colorbar
- Wigner functions
- Pseudo-probability functions
- Process tomography
- Qubism visualizations

Quantum information processing

- Quantum gates and circuits
- Toffoli gate to CNOT
- Spin Chain Qubit model

Time evolution

- Master equation solver: Qubit dynamics
- Master equation solver: Vacuum Rabi oscillations
- Master equation solver: Spin chain
- Monte-Carlo solver: Trilinear oscillators
- Monte-Carlo solver: Birth and Death of Photons in a Cavity
- Bloch-Redfield master equation solver
- Time-dependent Bloch-Redfield Quantum Dot
- Floquet formalism
- Quasi-steadystate of time-dependent (periodic) systems
- Time-dependent master equation: Landau-Zener transitions
- Time-dependent master equation: Landau-Zener-Stuckelberg inteferometry
- Stochastic master equation: Heterodyne detection
- Stochastic master equation: Inefficient detection
- Stochastic master equation: Jaynes-Cumming model with photocurrent detection
- Stochastic master equation: Feedback control
- Steady state solvers: Optomechanical system
- Homodyned Jaynes-Cummings Emission

Optimal control

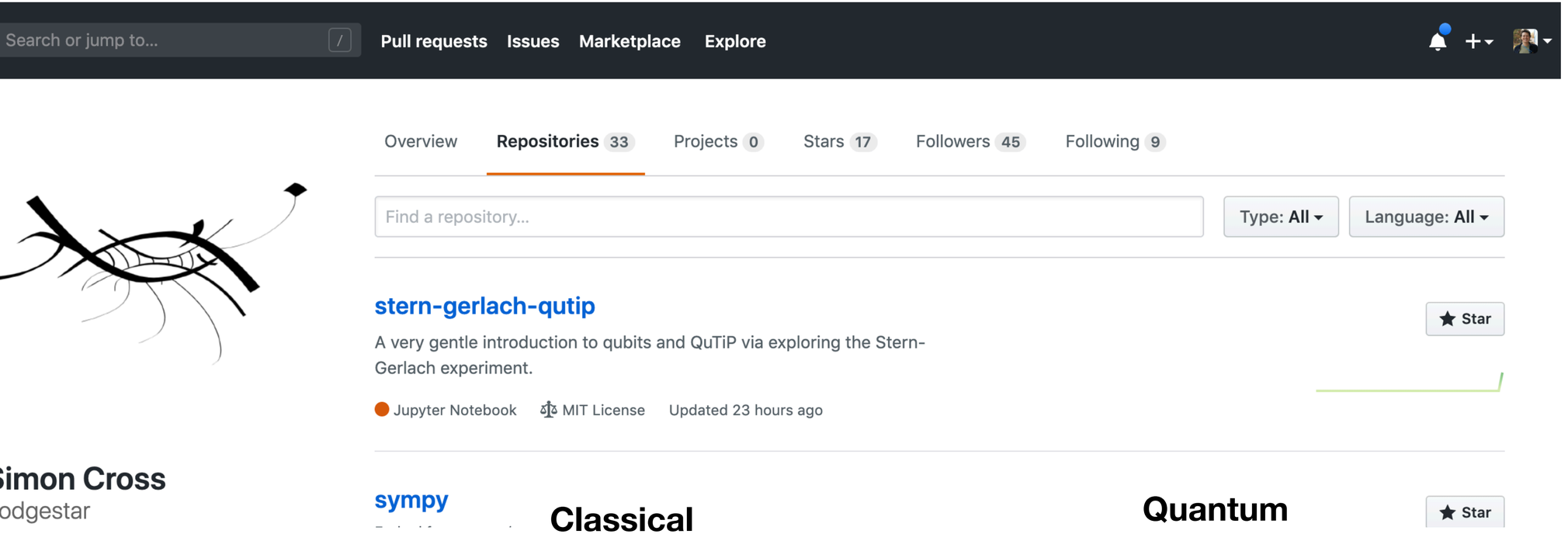
- Overview
- Hadamard
- QFT
- Lindbladian
- Symplectic
- QFT (CRAB)
- state to state (CRAB)
- CNOT
- iSWAP
- Single-qubit rotation
- Toffoli gate

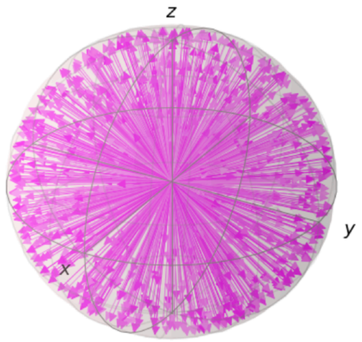
- **Over 60** Jupyter notebook tutorials
- **Over 20** quantum mechanics lectures

launch binder

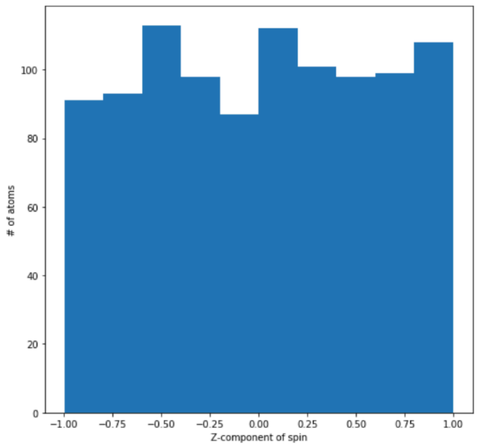
The power of open source: the community

EuroSciPy 2019

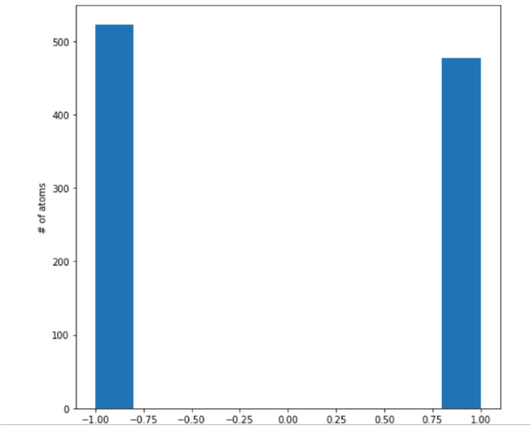




Classical



Quantum



qutip.org/tutorials

QuTiP: A Growing Ecosystem for Quantum Physics

What's going on

- 2018: Joined NumFOCUS, foundation for scientific code (NumPy)

NUMFOCUS
OPEN CODE = BETTER SCIENCE

- 2019: Participating to Google Summer of Code 2019:

Student Applications opened March 26th. Closed April 9th. 3 students working on summer projects.

https://github.com/qutip/qutip/wiki//Google-Summer-of-Code-2019

2019: Applied to 1st Google Season of Docs 2019: Technical writers projects for documentation.

Google Summer of Code

(conda forge)

- 2018-2019: Reaching out to the sci-dev community.

EuroScipy 2018
July 2018
Trento, Italy

PyData 2018
November 2018
Warsaw, Poland

FOSDEM'19 (Quantum Computing)
February 2, 2019,
Brussels, Belgium

1st QuTiP developers workshop
February 19-21, 2019
RIKEN, Wako, Japan

EuroScipy 2019
September 2019
Bilbao, Spain

- 2018-2019: A growing QuTiP ecosystem of satellite libraries:

`piqs`
QuTiP library
Now a qutip module

`krotov`
QuTiP-based quantum optimal control library

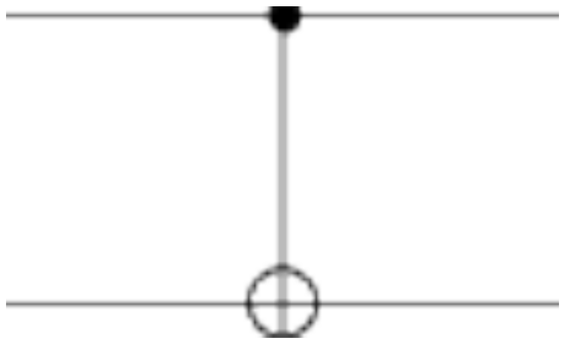
`matsubara`
A qutip plugin for non-Markovian dynamics

QuTiP ecosystem: Like AstroPy, but for Quantum

Quantum Tech: Quantum Circuit Simulators

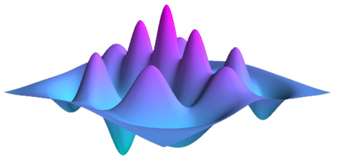
Open-Source Quantum Computing

```
import qutip

q = qutip.QubitCircuit(2)

q.add_gate("CNOT", controls=[0], targets=[1])

q.png
```



https://github.com/nathanshammah/interactive-notebooks

QuTiP ongoing projects (2019)



qutip.nisq

Model noise in quantum information processing (QIP)

QuTiP's QIP module represents ideal quantum circuits.

Student: Boxi Li (ETH Zurich)

Objectives:
- Go beyond gates as instantaneous unitary transformation
- Noise model for realistic devices
- Noise model for dissipative dynamics

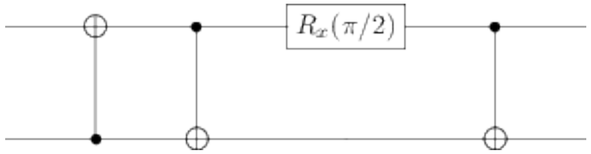
NUMFOCUS
OPEN CODE = BETTER SCIENCE

Google Summer of Code

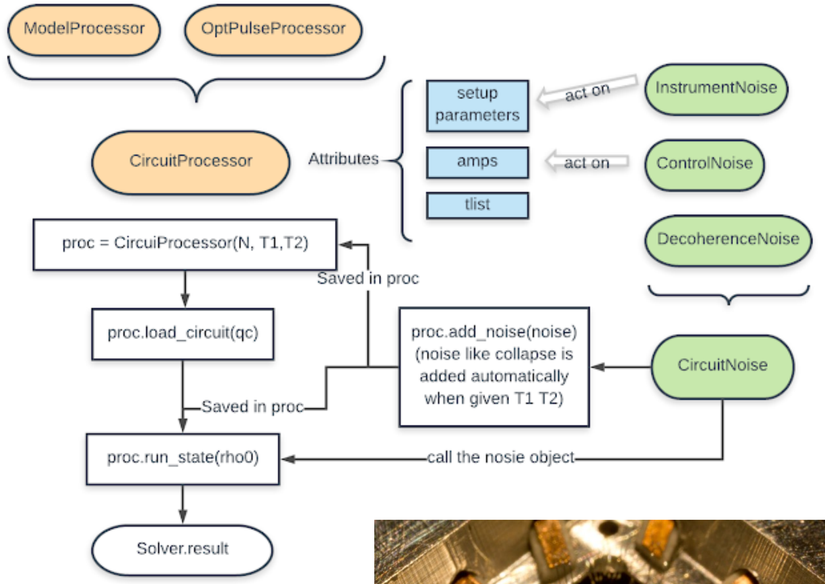
Code: Boxi Li. Github: BoxiLi
Mentors: Alex Pitchford, Neill Lambert, Shahnawaz Ahmed, Nathan Shammah

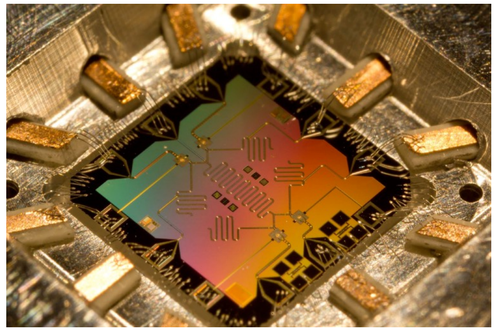
https://gsoc2019-boxili.blogspot.com

Quantum Circuit

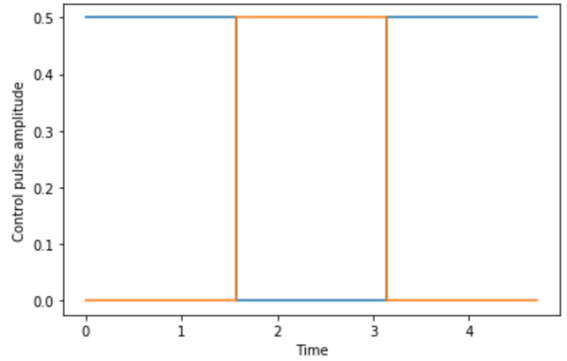


Noise Model



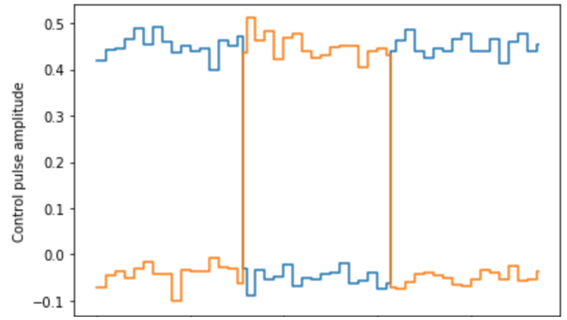


Ideal Pulses




```
[20]: processor_white.plot_pulses(noisy=True)
```

```
[20]: (<Figure size 432x288 with 1 Axes>,
       <matplotlib.axes._subplots.AxesSubplot at 0x269999bb710>)
```



Noisy Pulses

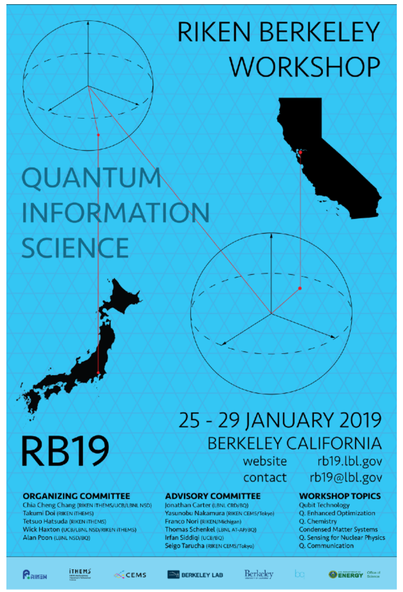
21/12, 2019

Tokyo

Milan

21/1 - 1/2, 2019

California



2/2, 2019

Tokyo

California

Jan 22nd – PsiQuantum

Jan 23rd – Stanford University [Seminar]

Jan 24th – Rigetti Computing [Seminar]

Jan 26th – Berkeley Lab [Invited Talk]

Jan 28th – NASA Ames [Group Seminar]

Jan 29th – Google AI Quantum LA [Seminar]

Jan 31sth – Google AI Quantum SB

Feb 1st – Caltech [IQIM Seminar]

Quantum Tech: Quantum Circuit Simulators

Open-Source Quantum Computing

	Language	Library	Quantum Hardware	Features
D-Wave	Python	qbsolv	“quantum annealing”	Optimization problems.
IBM Q	**Python**	QISKit	Several chips. Up to 53 qubits	**Millions** of experiments from the cloud by online users on the *IBM quantum experience*
Rigetti	**Python**; pyquil	Forest toolkit Grove	19 qubits	Open to research collaborations. Proof-of-concept: clustering
Google	**Python**	Cirq OpenFermion	72-qubit SC chip: Bristlecone 53-qubit SC chip: Sycamore	*Cirq*: an open-source platform for noisy quantum computing Quantum supremacy experiment
Microsoft	**Python**; Q#	Liquid Quantum Dev Kit	NA	Topological quantum computing with Majorana particles
Alibaba	NA	NA	11-qubit SC chip announced unknown architecture	Cloud computing announced

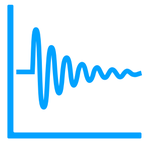
ONLINE

All chips have limited connectivity. Updated to Nov 2019

Open-source cloud quantum labs

Extending the Open-Source Quantum Computing Paradigm

For the first time theorists can run online quantum experiments

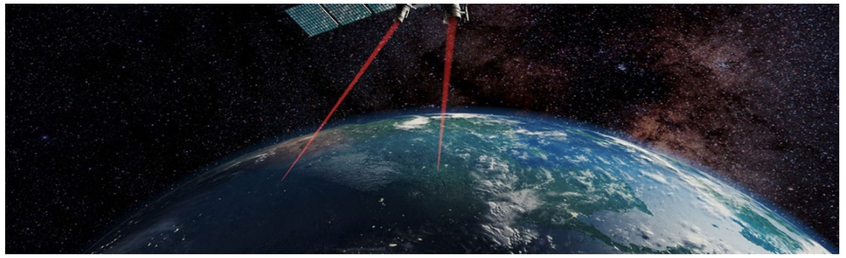
Language	Library		Quantum Experiment	Features
		Actuators Effort $$$ Standards	 	Science acceleration via automation (maybe). Educational value.

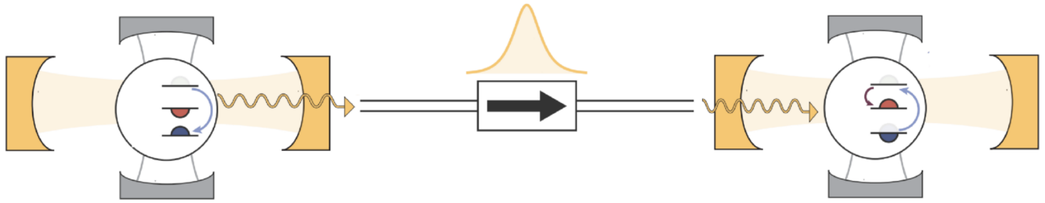
Could academic institutions, physicists replicate this model?

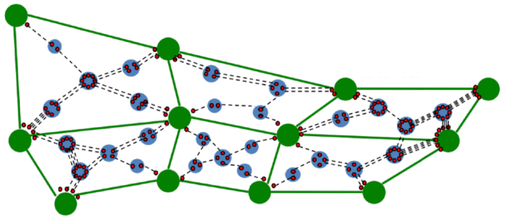
Open Labs, Open Hardware

See: github.com/**SteeleLab**-Delft

SLAB

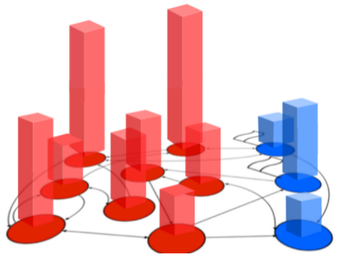




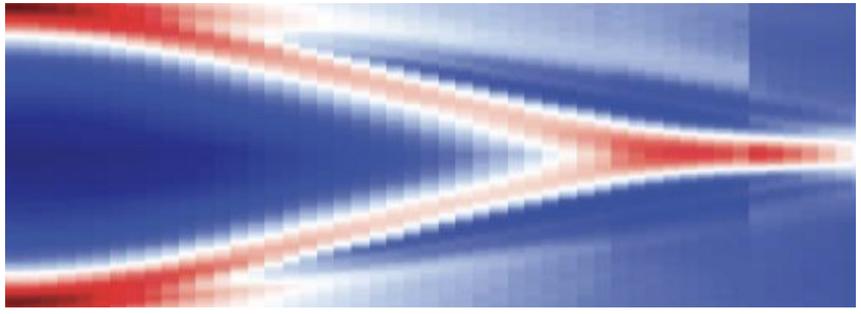


Nathan Shammah
Quantum researcher at RIKEN
Jun 25 · 6 min read

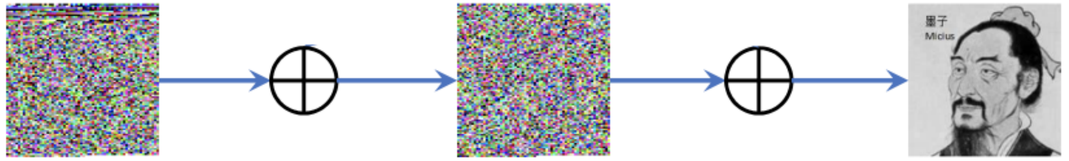
medium.com/quantum-tech



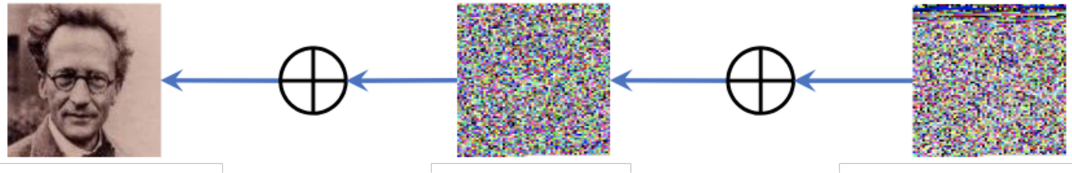
Nathan's Quantum Tech Newsletter: №11



Research Highlights
- Breakthroughs
- Reviews
- Divulgation



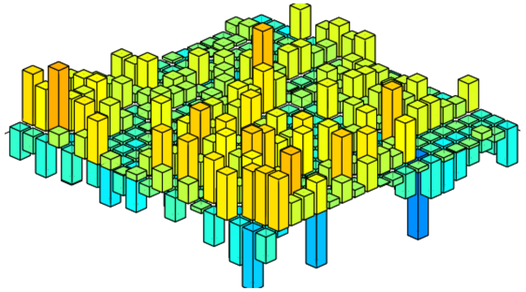
Tech News
- Startup creation, funding rounds
- Corporate Involvement
- Institutional Schemes

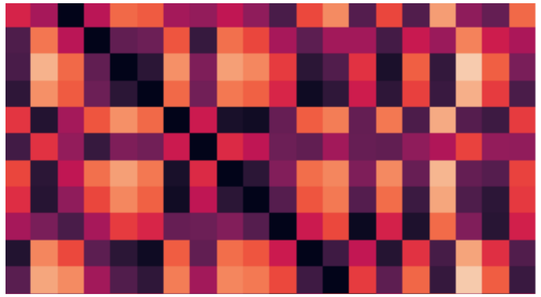


Bonus Links
- Videos
- Long-read popular articles

Sign up: eepurl.com/c10FJz

Focus
- Space Quantum Communication
- Quantum Machine Learning
- Open-Source Quantum Tech
- Quantum Games





Association of Italian Researchers in Japan

www.airj.info

KICK-OFF EVENT: DECEMBER 2019

Thank you

 @NathanShammah

GitHub: nathanshammah
LinkedIn: Nathan Shammah