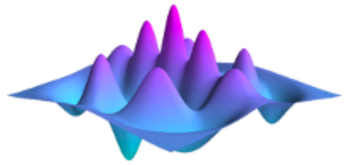
Open-source software for open science: interactive notebooks for generalizable results



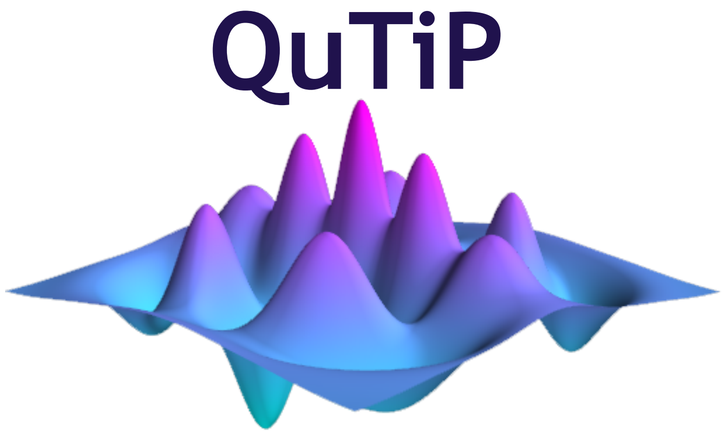
QuTiP
Quantum Toolbox in Python

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

3rd July 2019
CM Seminar
ICTP, Trieste

QuTiP: The Quantum *Physics* Simulator

The **Qu**antum **T**oolbox **i**n **P**ython: A toolbox to study the **open** quantum dynamics of realistic systems.



Interactive Lectures @ ICTP, Leonardo Building

Tue 25th June - 11:45am, Seminar Room –	Driven-dissipative models in quantum physics
Wed 26th June - 11am, Seminar Room –	Quantum Open Source & Introduction to QuTiP
Thur 27th June - 9am, Computer Room –	Hands-on session on QuTiP's main features
Mon 1st July - 9am, Computer Room –	QuTiP stochastic solvers
Tue 2nd July - 9am, Computer Room –	PIQS and How to Build your Own Software
Wed 3rd July - 9am, Computer Room –	**Extra meeting: Interactive notebooks, SISSA/ICTP**

Take a snapshot

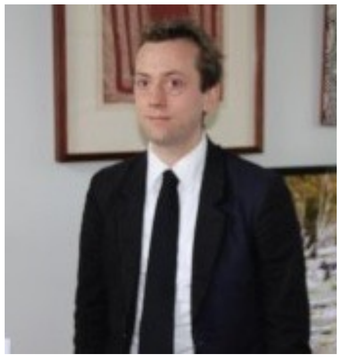
https://github.com/nathanshammah/interactive-notebooks

Acknowledgements and funding

Shahnawaz Ahmed
Chalmers, Sweden
(RIKEN, Japan)

Alex Pitchford
Aberystwyth University
United Kingdom

Eric Giguère
U. de Sherbrooke
Canada



Dr. Neill Lambert
RIKEN, Japan

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

RIKEN

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

JST Japan Science and Technology Agency

THE ROYAL SOCIETY

JOHN TEMPLETON FOUNDATION

NUMFOCUS
OPEN CODE = BETTER SCIENCE

Google Summer of Code

UNIVERSITÉ DE SHERBROOKE

PRIFYSGOL ABERYSTWYTH UNIVERSITY

@NathanShammah

medium.com/quantum-tech

GitHub: nathanshammah
LinkedIn: Nathan Shammah

quantika.co

QuTiP: The project at a glance

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

Project Impact

QuTiP
Quantum Toolbox in Python

>**600** citations (Google Scholar)

downloads 79k total (conda forge)

More info at http://qutip.org/

Authors

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

Code

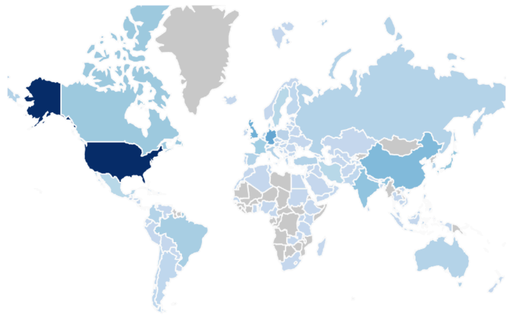
Robert J. Johansson
Rakuten Inc.

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

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)
- Nathan Shammah (RIKEN)

- **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

A Guide to Make your Open Source Scientific Library

GitHub, Inc. [US] | https://github.com/nathanshammah/opensource/blob/master/README.md

https://github.com/nathanshammah/opensource

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.

0 - Open Source for Open Science: Some information about the Python and open source ecosystem, and how they relate to open science are also given.

- StackOverflow

1 - Before Starting Coding: Setting up the working environment on your machine, including the tools you will need to write code efficiently.

- Sublime, Git, GitHub

2 - Developing your Project: A step-by-step guide with best practices for coding, and tips for making code development as effortless as possible.

- PEP 8, PEP 257
- jupyter notebook
- nbconvert

3 - Testing: Especially in software related to scientific research, at start, the destination is not always crystal clear. Code is written, optimized, reorganized. Unit testing is a crucial task to avoid getting lost in the process.

- nose2, pytest

Beyond Reproducibility

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

https://dx.doi.org/10.6084/m9.figshare.7140050

Reproducibility in Science

A bold stance…

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

The Jupyter project

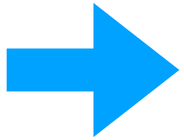
Mathematica

project.nb

MATLAB

project.m

IPython



Jupyter Notebooks

JupyterLab

My Binder

JupyterHub

BinderHub

The Jupyter project

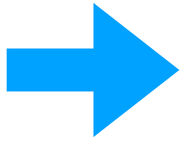
Mathematica

project.nb

MATLAB

project.m

IPython



Jupyter Notebooks

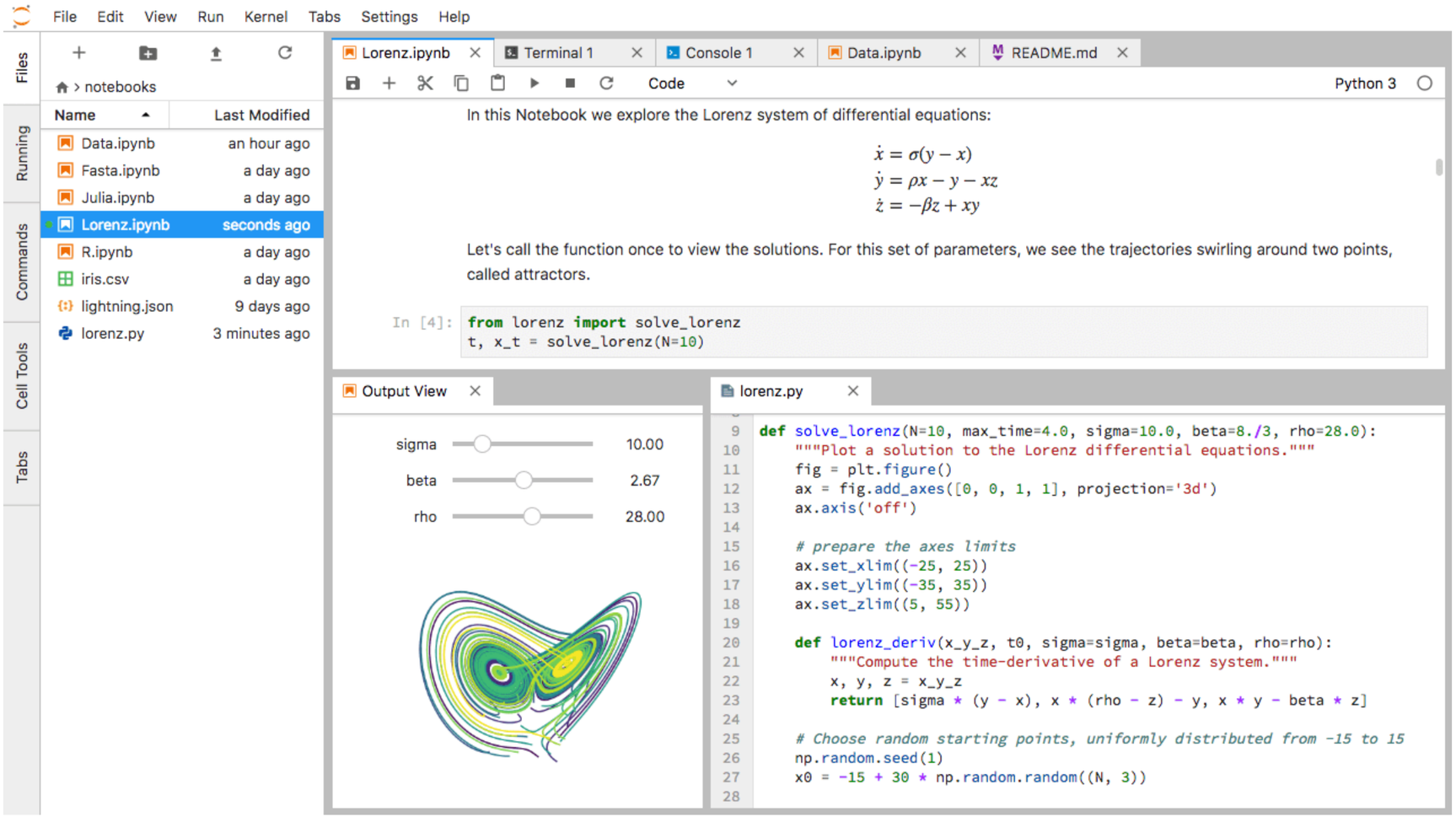
JupyterLab

My Binder

JupyterHub

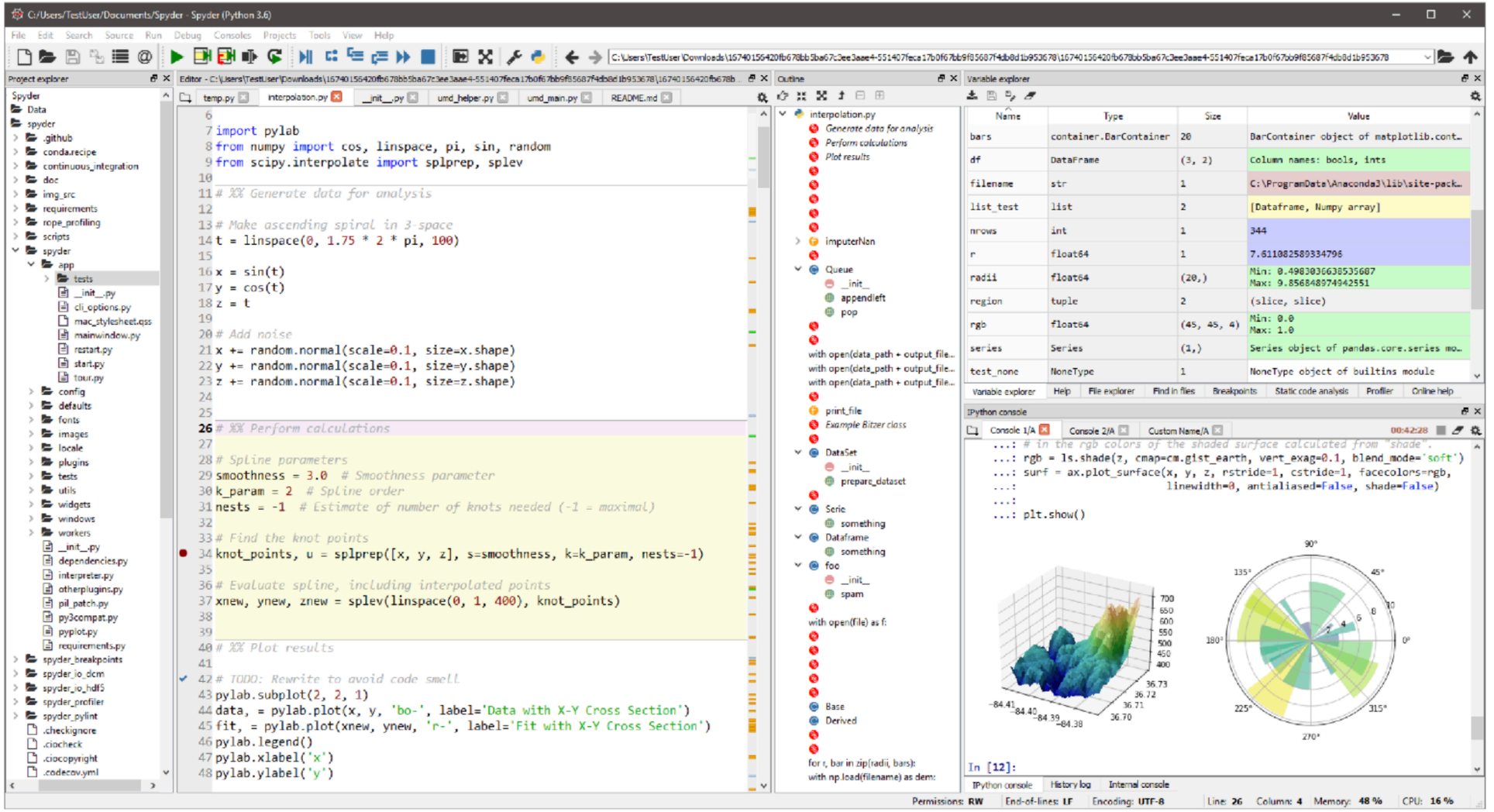
BinderHub

JupyterLab: IDE in the browser



Another option: Spyder

Spyder: IDE in an app



Another option: Spyder https://www.spyder-ide.org/

SPYDER
The Scientific Python Development Environment

Jupyter Notebooks

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,

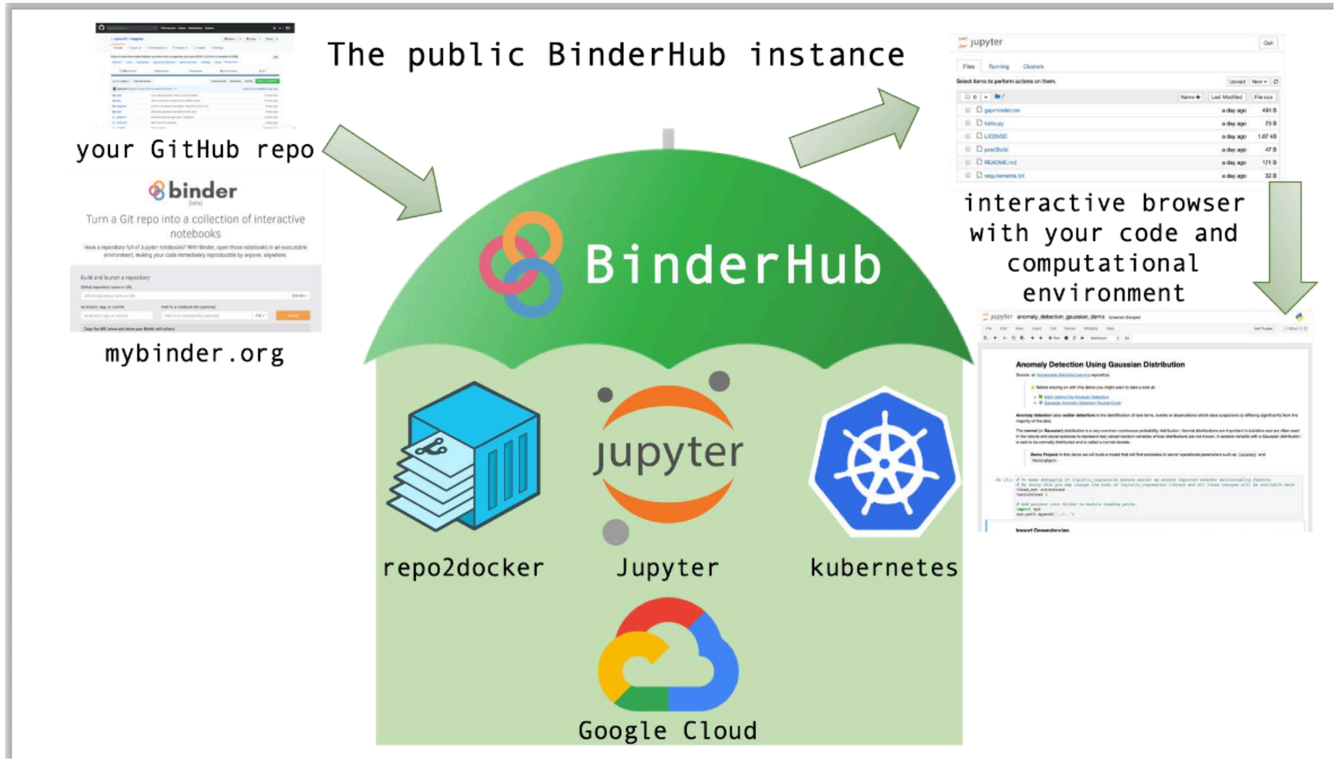
LaTeX

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

Plots

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

My Binder: cloud-based notebooks



Github Repository:

`environment.yml`

`requirements.txt`

`apt.txt`

Reproducibility: Online

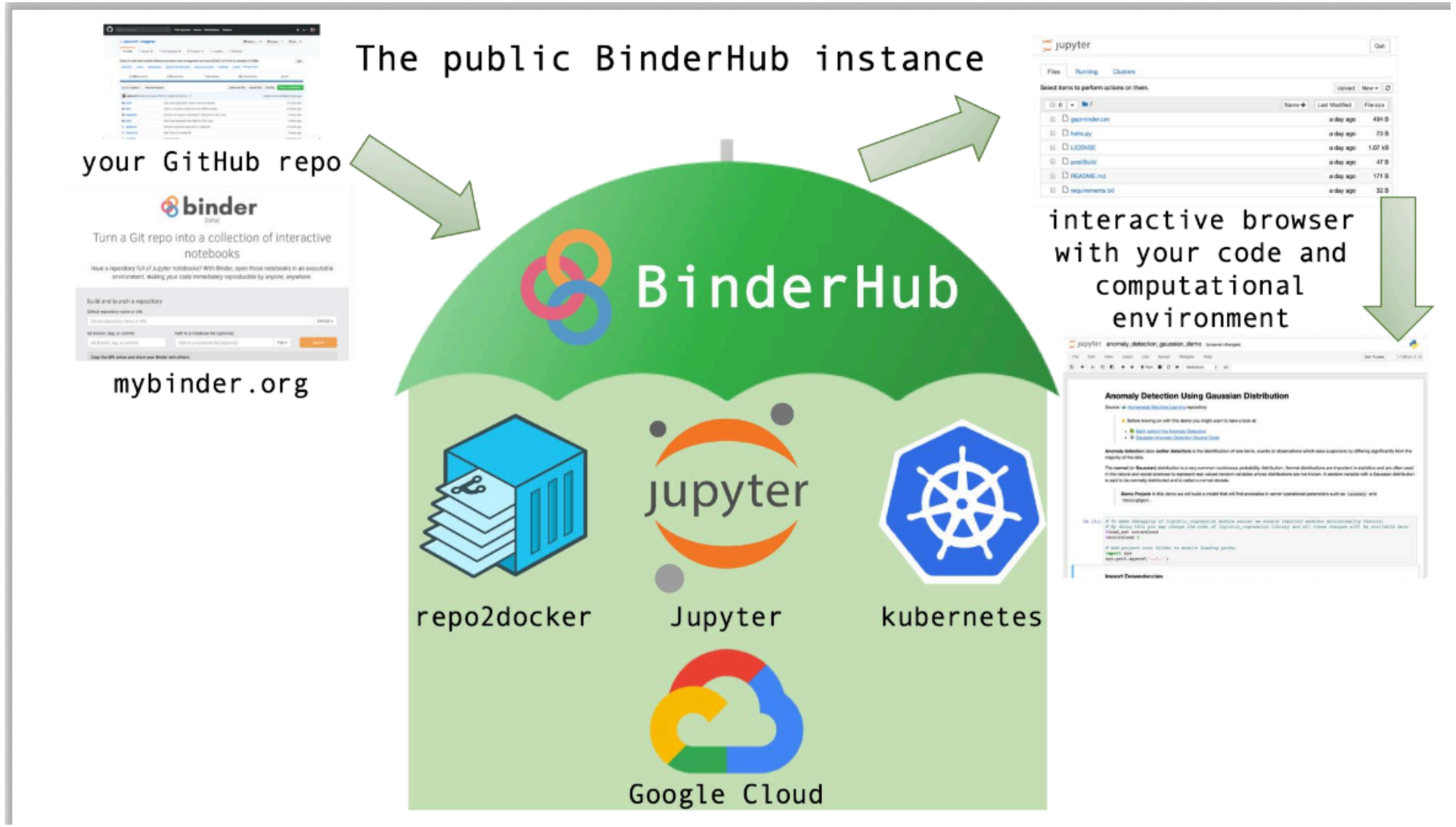


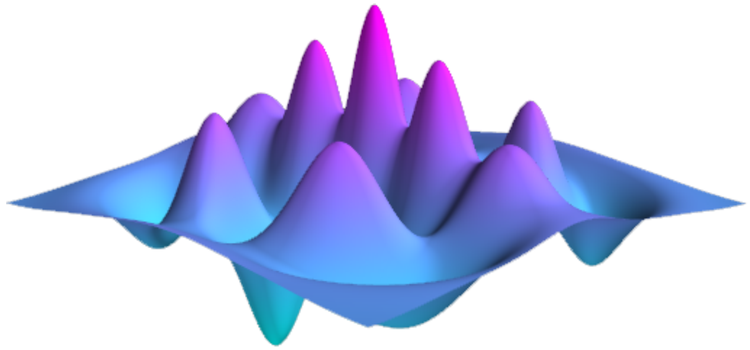
Figure from @TuringInst: Kirstie Whitaker, Why you need a reproducible computing environment

https://zenodo.org/record/2598530#.XQDf8tP7Q5g

QuTiP: Interactive Notebooks

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

QuTiP



You can find an interactive notebook at

https://github.com/nathanshammah/

Repository: **interactive-notebooks**

You can run the notebook live at

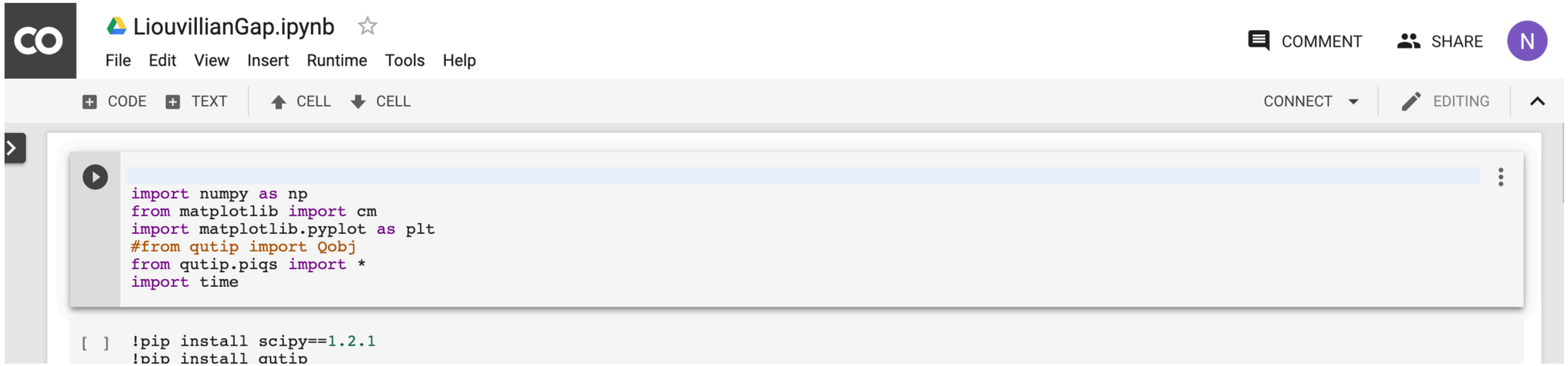
https://mybinder.org/v2/gh/nathanshammah/interactive-notebooks/binder

Take a snapshot

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

Quantum Tech Newsletter

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

medium.com/quantum-tech

Nathan's Quantum Tech Newsletter: №11

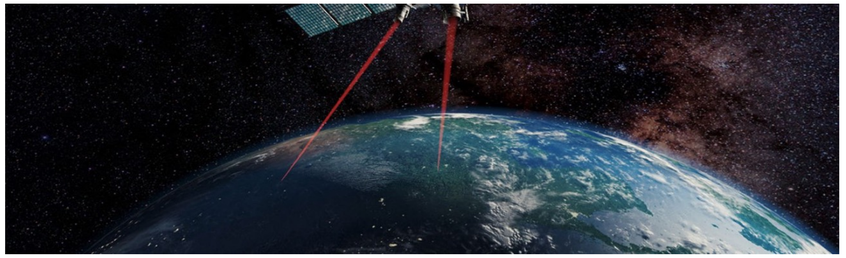
Sign up: eepurl.com/c10FJz

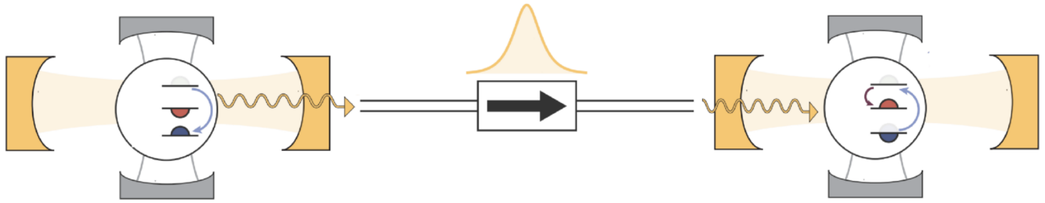
Research Highlights
- Breakthroughs
- Reviews
- Divulgation

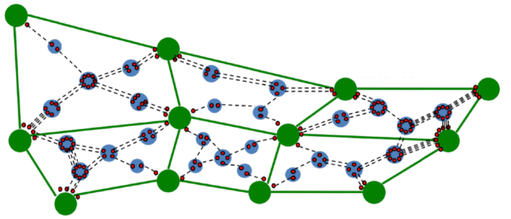
Tech News
- Startup creation, funding rounds
- Corporate Involvement
- Institutional Schemes

Bonus Links
- Videos
- Long-read popular articles

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







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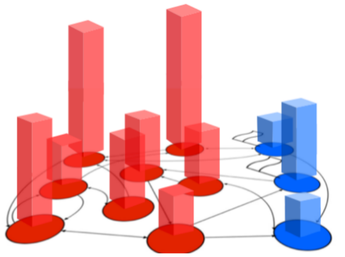
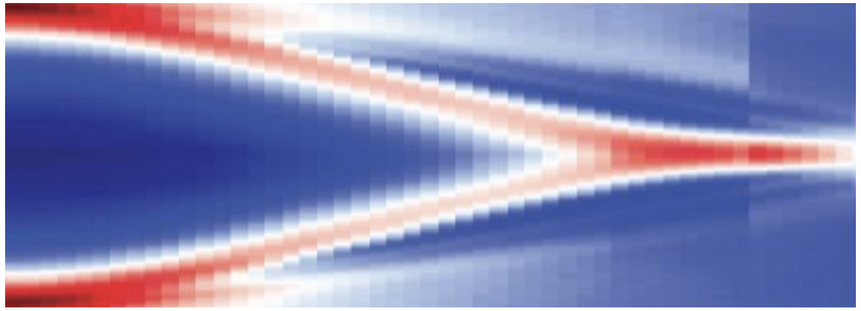
medium.com/quantum-tech



Nathan's Quantum Tech Newsletter: №11



Research Highlights
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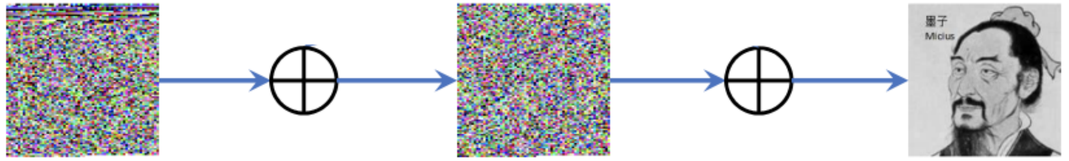

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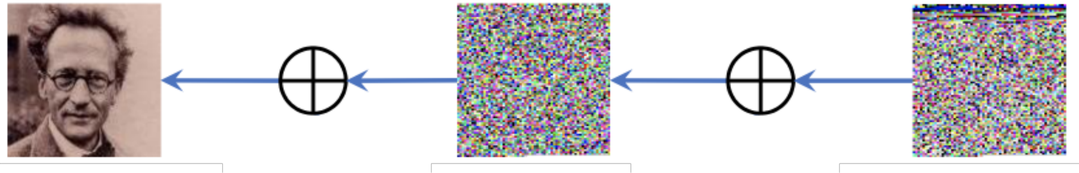

Bonus Links
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Sign up: eepurl.com/c10FJz

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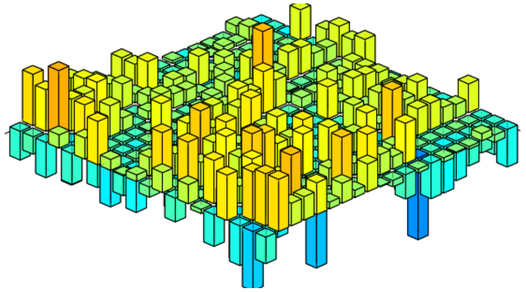

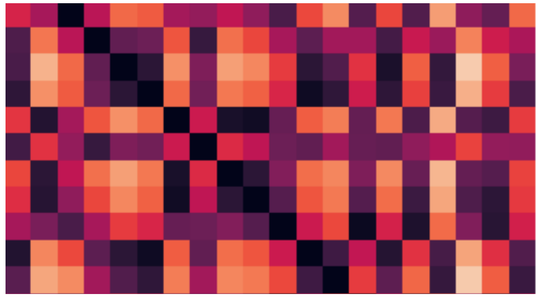

Thank you

 @NathanShammah

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LinkedIn: Nathan Shammah