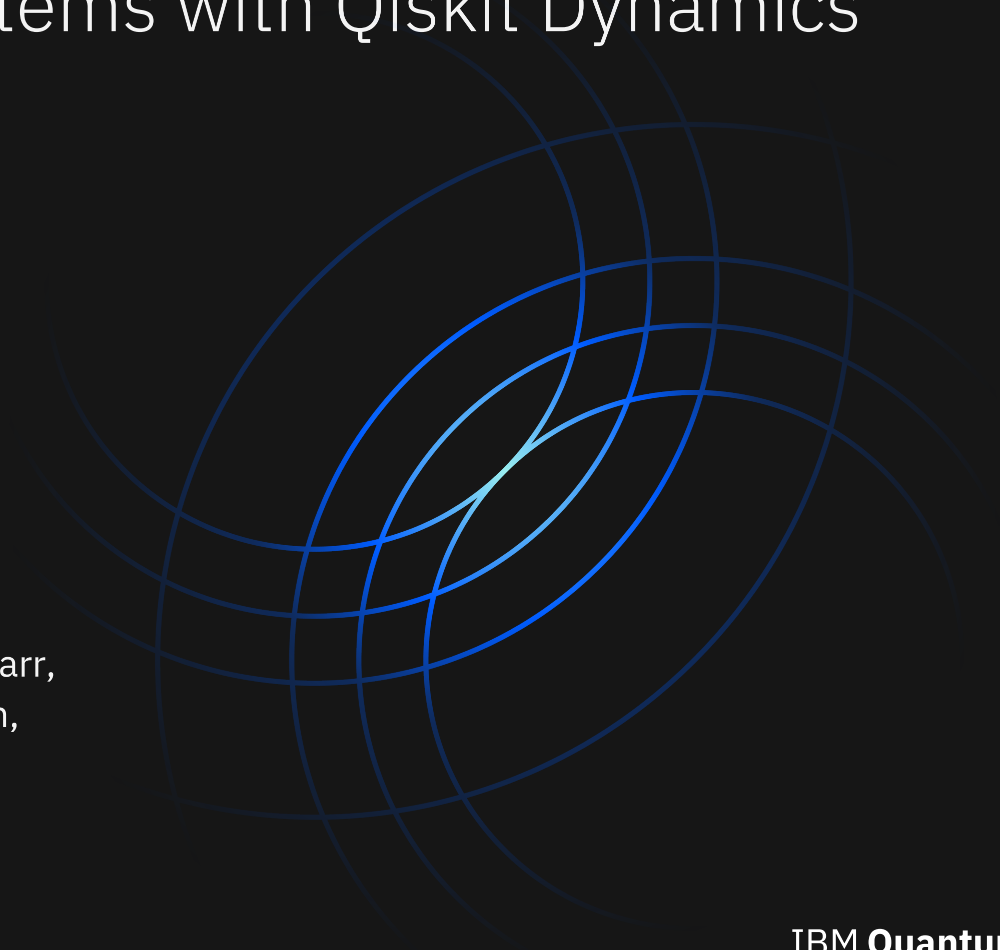
Simulating quantum systems with Qiskit Dynamics

Daniel Puzzuoli
IBM Quantum



Dynamics contributors:

Daniel Egger, Ian Hincks, Haggai Landa, Avery Parr, Daniel Puzzuoli, Benjamin Rosand, R. K. Rupesh, Matthew Treinish, Christopher J. Wood

Outline

- Intro: Simulate what, why?
- Simulation package landscape
  - Helpful features
  - Open-source packages
- Qiskit Dynamics
  - General feature description
  - Common code examples
  - Performance comparison
  - Advanced feature: numerical perturbation theory

Simulate *what*?

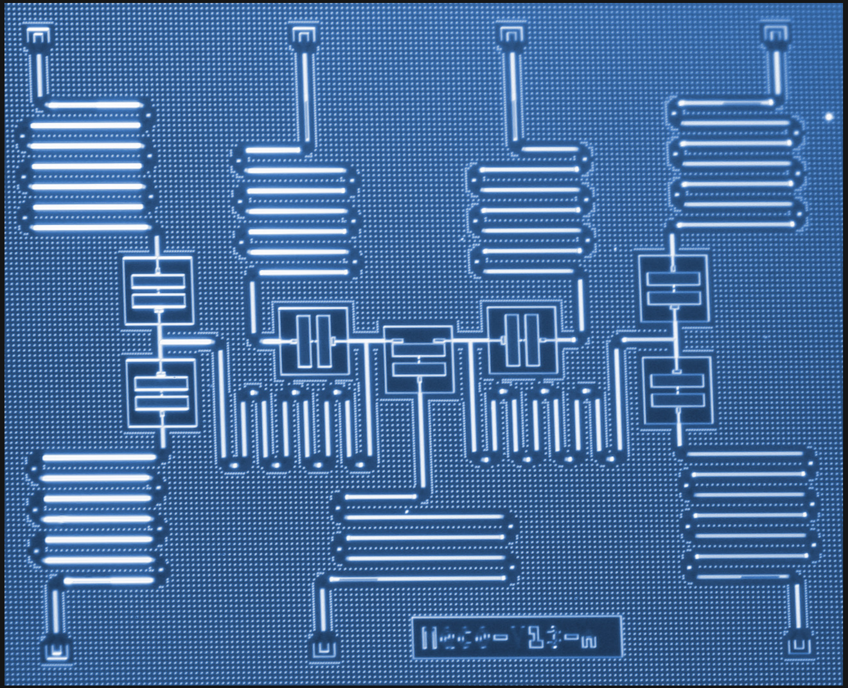
- Quantum devices are quantum systems
- Schrodinger equation

$$\boxed{\dot{U}(t) = -iH(t)U(t)}$$

- Lindblad equation

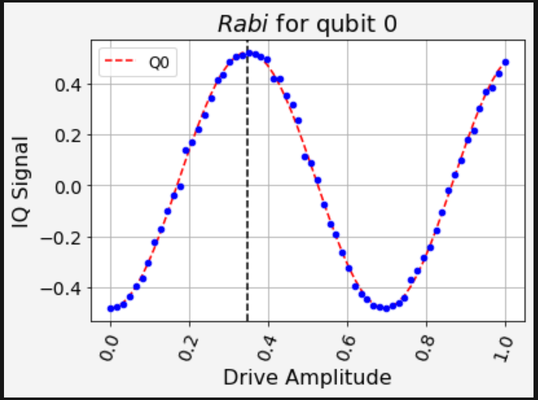
$$\boxed{\dot{\rho}(t) = -i[H(t), \rho(t)] + \sum_j L_j \rho(t) L_j^\dagger - \frac{1}{2}\{L_j^\dagger L_j, \rho(t)\}}$$

- Others (e.g. Bloch-Redfield)

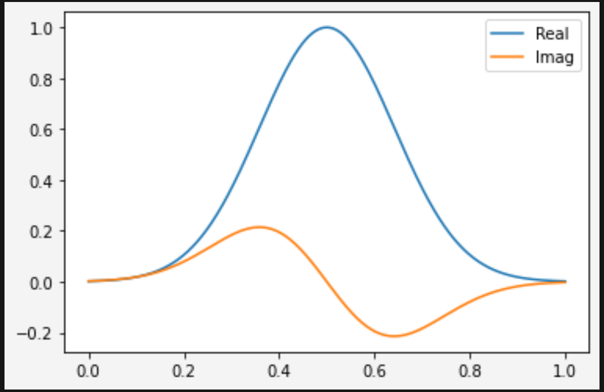


Simulation workflows

Building device models



Control design



Optimize chip design
“virtual prototyping”

Welcome to Qiskit Metal!

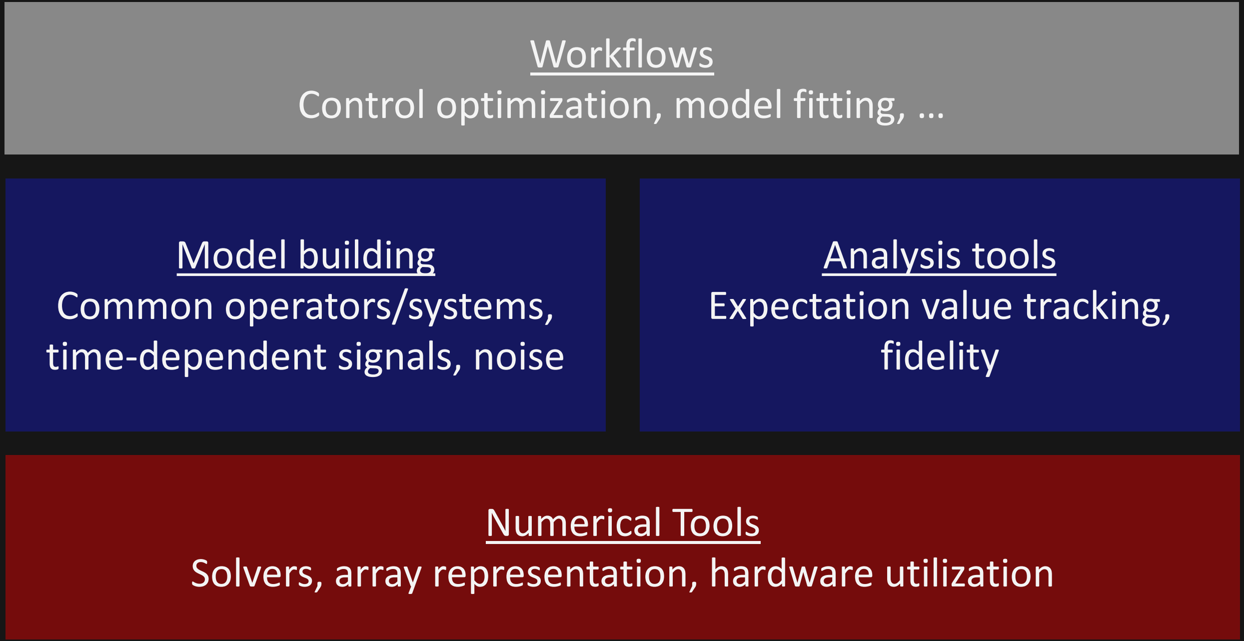
v0.0.3

Tip: All component widget: Double click a component to zoom into it!

Faster is better

- Faster simulation accelerates research
  - Models simulated 1000s of times
- Challenge: curse of dimensionality
  - Hilbert space dimension grows exponentially in number of subsystems
- Challenge: the *other* curse of dimensionality
  - Even small systems can have *a lot of model parameters*
  - Exploring parameter space is expensive
- Faster simulation enables more complex workflows
  - Enables asking more complicated questions

Components of a simulation package



Workflows

Control optimization, model fitting, …

Model building

Common operators/systems, time-dependent signals, noise

Analysis tools

Expectation value tracking, fidelity

Numerical Tools

Solvers, array representation, hardware utilization

Critical technical capabilities:

- Speed
- Flexible/general core
- For optimization:
  - Compilation
  - Automatic differentiation

Open-source packages (non-exhaustive)

Python packages

QuTiP
Quantum Toolbox in Python


C^3 - An integrated tool-set for control, calibration and characterization

Torch Quantum

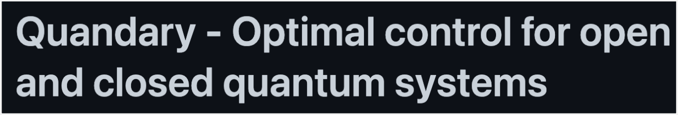

qiskit-community / **lindbladmpo**

Julia

HOQST

BLOQADE

C++


Quandary - Optimal control for open and closed quantum systems

Matlab

Spinach A Fast and General Spin Dynamics Simulation Library

Qiskit Dynamics

- New Qiskit package (Python) for Hamiltonian and Lindblad simulation
- Central applications of interest
  - Optimization applications (control, model fitting)
  - Virtual prototyping
- General feature goals
  - Configurability, configurability, configurability (every problem is different)
  - Compilable and automatically differentiable
  - Integration with Qiskit ecosystem

Qiskit Dynamics status
Current version 0.3.0

IBM **Quantum**

Numerical Tools

Solvers
ODE solvers
“Geometric” solvers

Array types
Dense/sparse
Numpy/scipy/JAX

JAX integration
JIT compile
Autodiff
GPU

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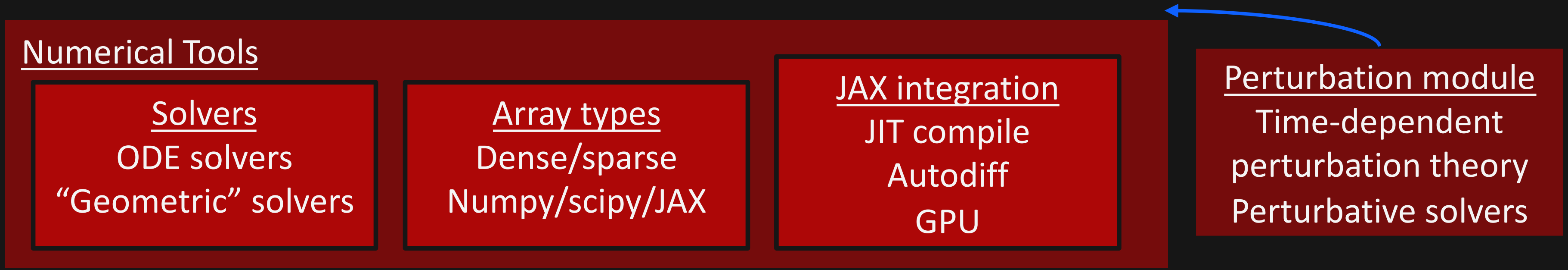

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Perturbation module
Time-dependent perturbation theory
Perturbative solvers

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Model building

General decompositions

$$H(t) = H_0 + \sum_j s_j(t) H_j$$

$$s_j(t) = Re[f_j(t) e^{i\omega_j t}]$$

Automated Model transformations

Rotating Frames

$$H(t) \mapsto e^{iH_F t}(H(t) - H_F) e^{-iH_F t}$$

RWA: $H(t) \approx H_{RWA}(t)$

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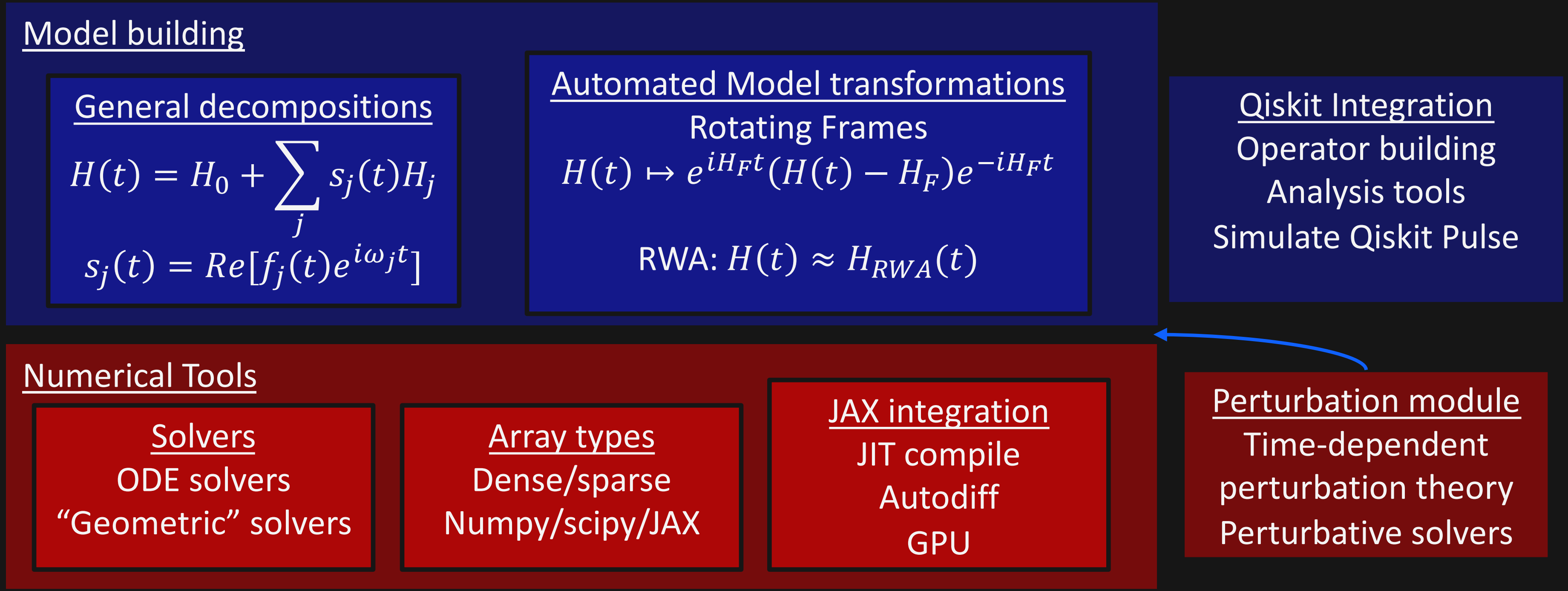

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Operator building
Analysis tools
Simulate Qiskit Pulse

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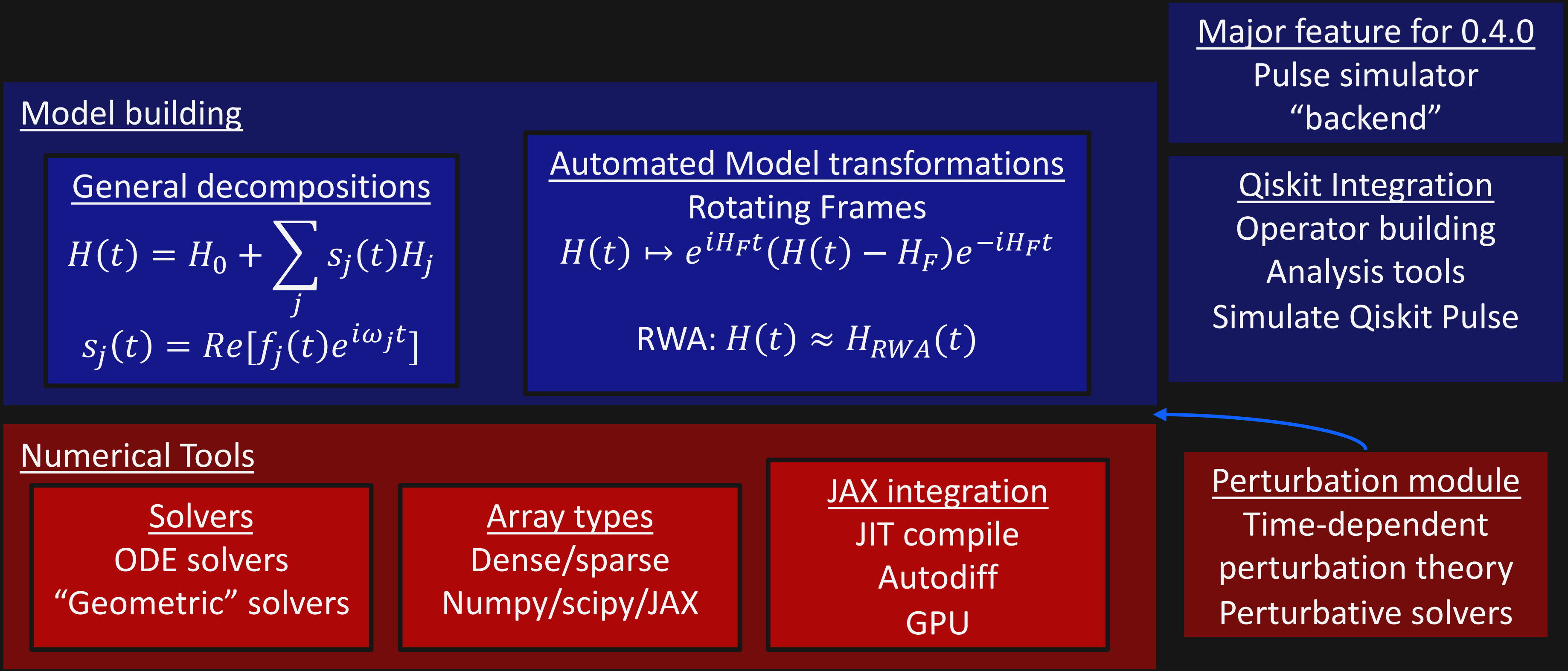

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Major feature for 0.4.0

Pulse simulator
“backend”

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Workflows

To come

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Getting started with Qiskit-Dynamics

- Simulate a Hamiltonian $H(t) = H_0 + s_1(t)H_1$

```
Array.set_default_backend('jax')

solver = Solver(
    static_hamiltonian=H0,
    hamiltonian_operators=[H1],
    evaluation_mode='dense',
    rotating_frame=H0
)

s1 = Signal(envelope=f, carrier_freq=fdr)

result = solver.solve(
    signals=[s1],
    t_span=[times[0], times[-1]],
    y0=y0,
    t_eval=times,
    method='jax_odeint',
    atol=1e-10,
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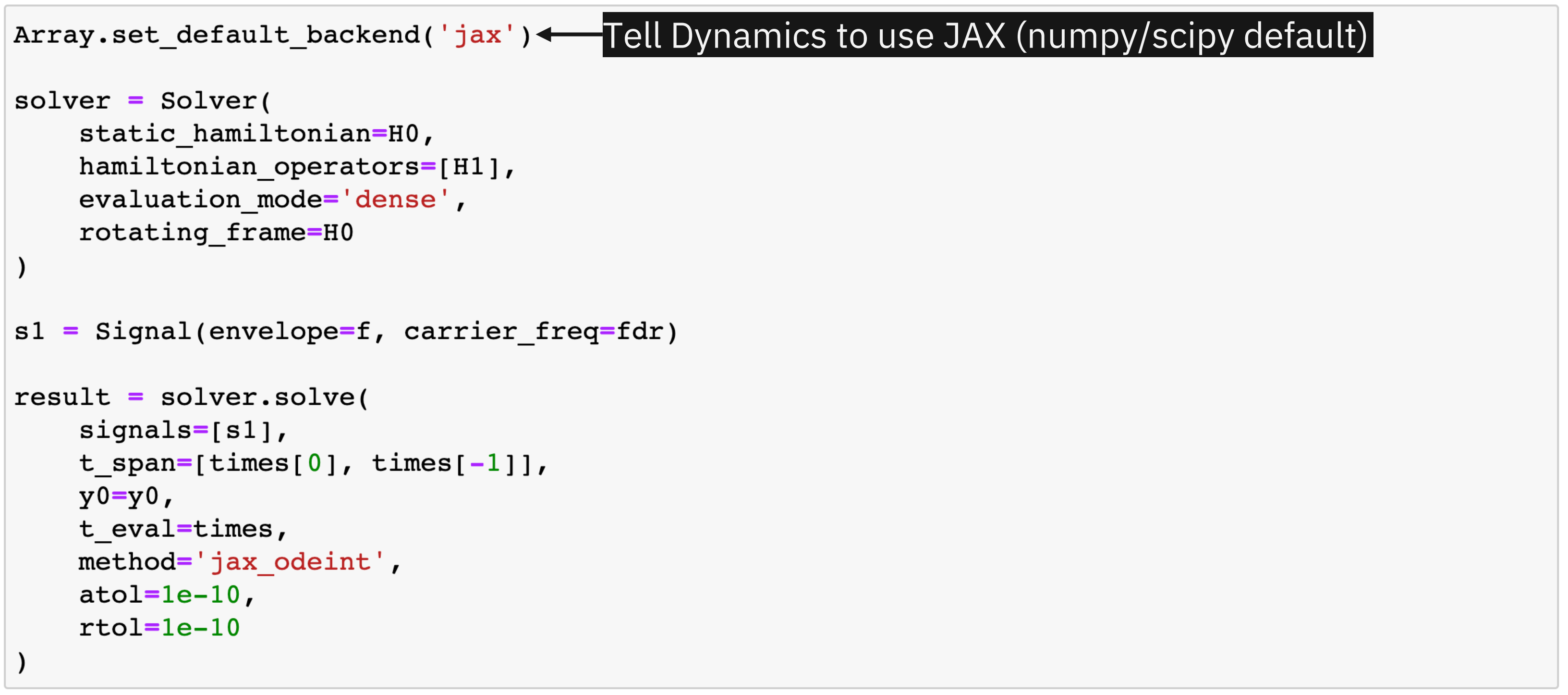

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Tell Dynamics to use JAX (numpy/scipy default)

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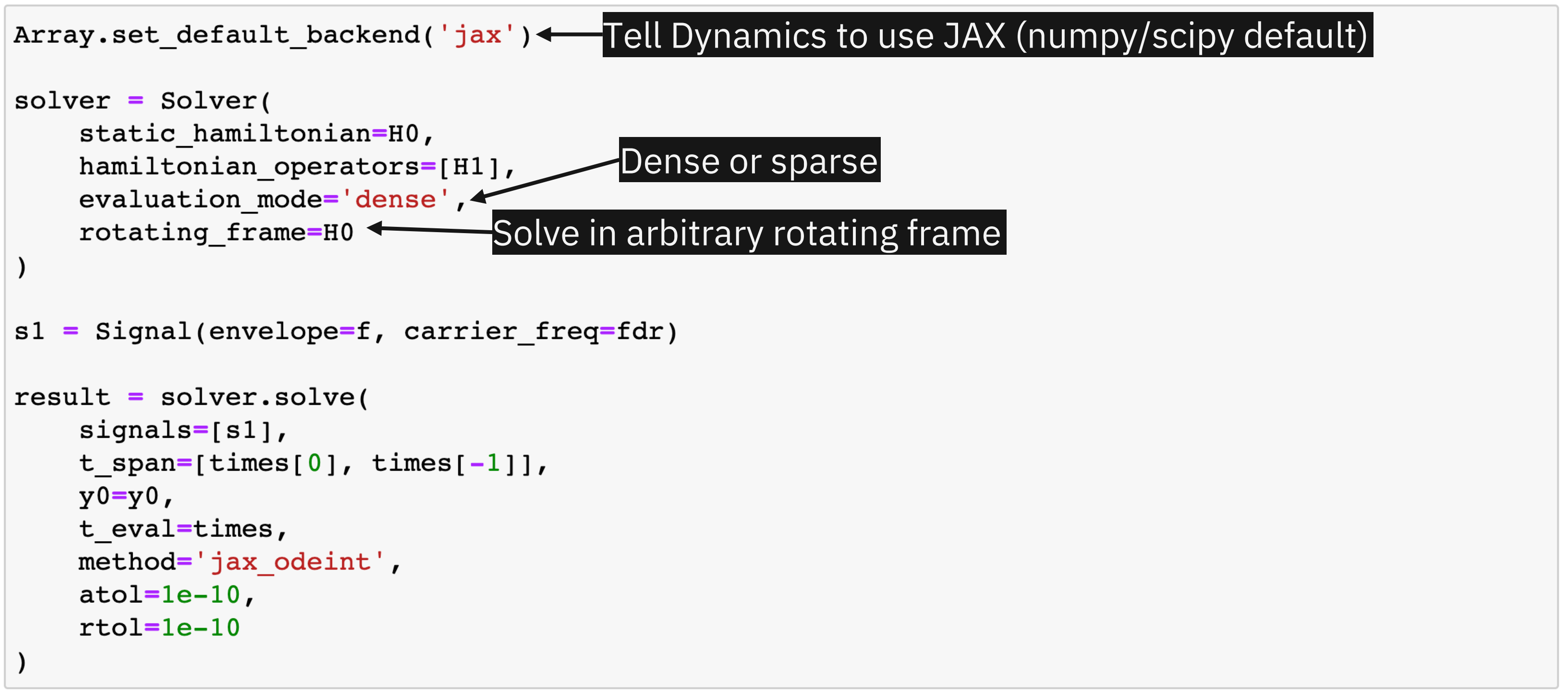

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Dense or sparse

Solve in arbitrary rotating frame

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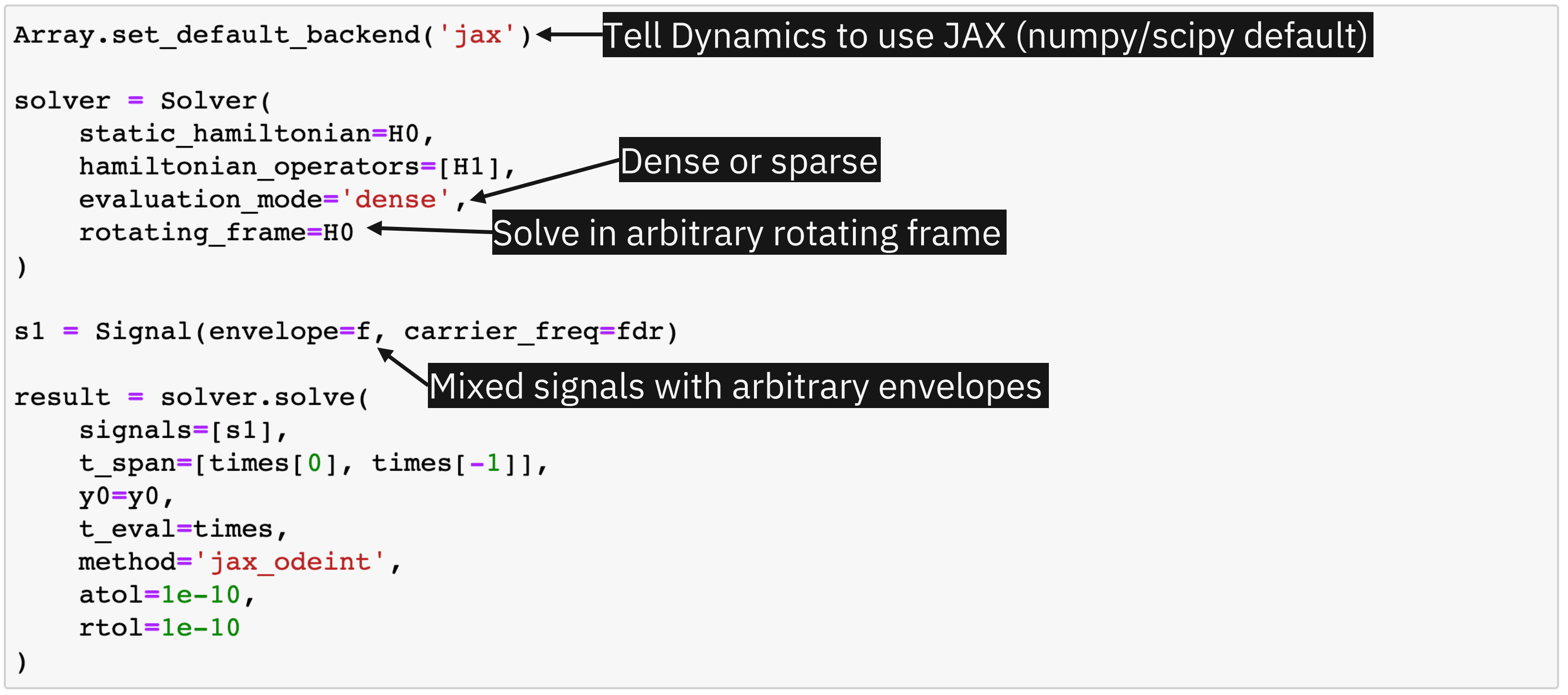

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Mixed signals with arbitrary envelopes

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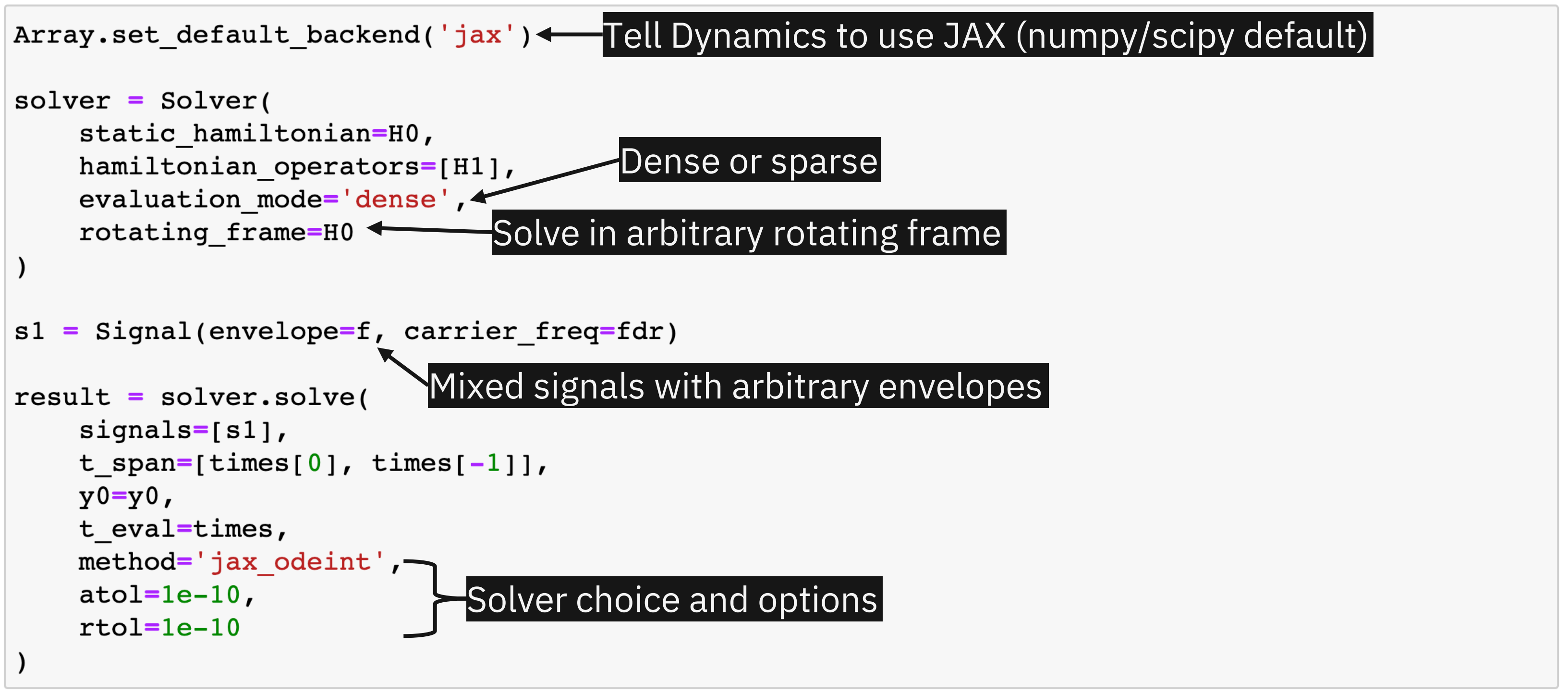

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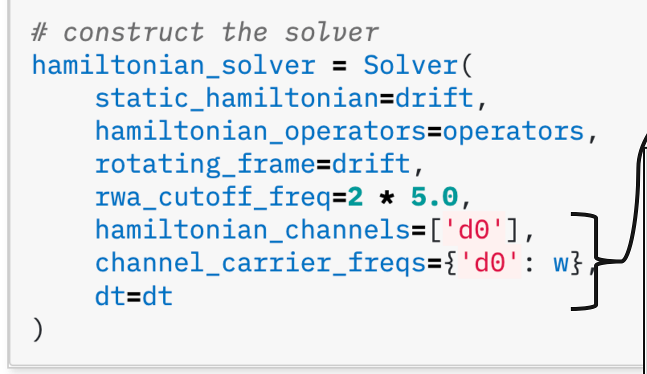
Solver choice and options

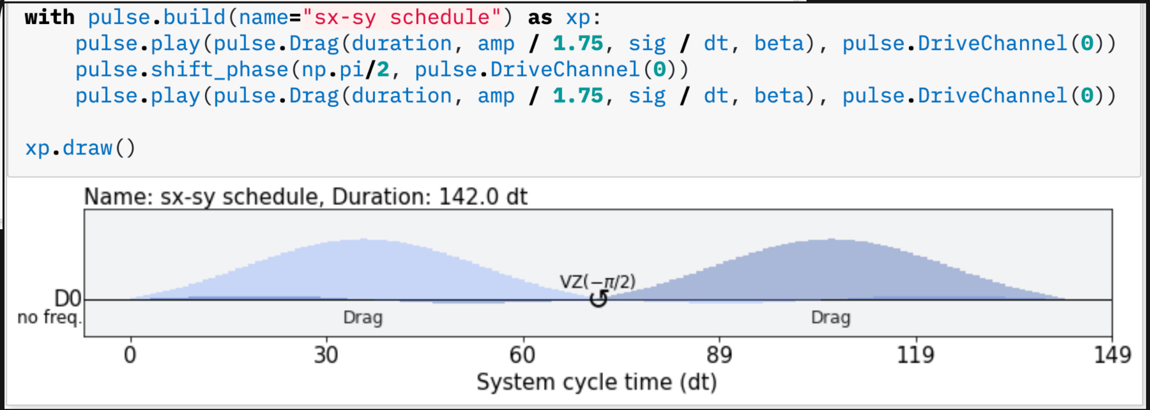
Qiskit Pulse simulation

- Can configure Solver to solve Qiskit Pulse schedules



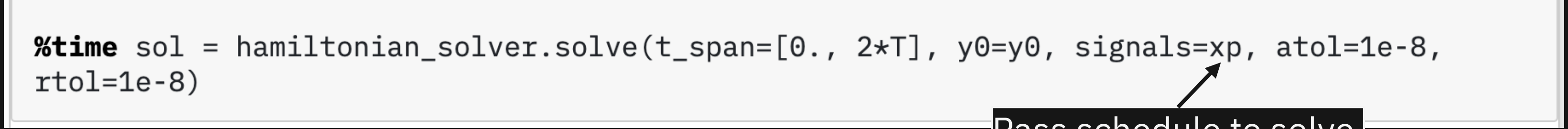
```
# construct the solver
hamiltonian_solver = Solver(
    static_hamiltonian=drift,
    hamiltonian_operators=operators,
    rotating_frame=drift,
    rwa_cutoff_freq=2 * 5.0,
    hamiltonian_channels=['d0'],
    channel_carrier_freqs={'d0': w},
    dt=dt
)
```

Add pulse configuration information to model structure



```
with pulse.build(name="sx-sy schedule") as xp:
    pulse.play(pulse.Drag(duration, amp / 1.75, sig / dt, beta), pulse.DriveChannel(0))
    pulse.shift_phase(np.pi/2, pulse.DriveChannel(0))
    pulse.play(pulse.Drag(duration, amp / 1.75, sig / dt, beta), pulse.DriveChannel(0))

xp.draw()
```

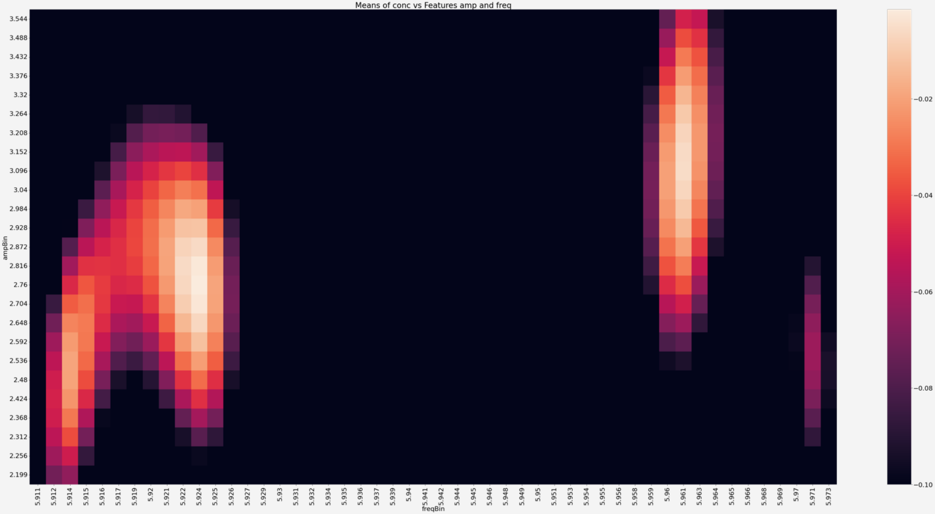


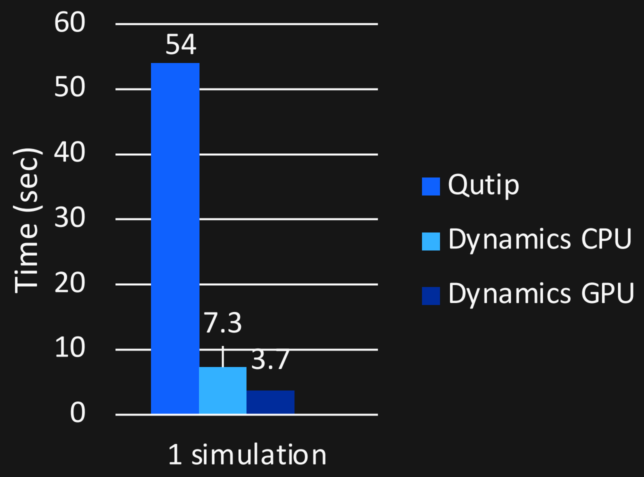
```
%time sol = hamiltonian_solver.solve(t_span=[0., 2*T], y0=y0, signals=xp, atol=1e-8,
rtol=1e-8)
```

Pass schedule to solve

QuTiP v.s. Dynamics speed comparisons

- Using Dynamics to tune gate parameters in a 3 transmon model
  - Dimension 160

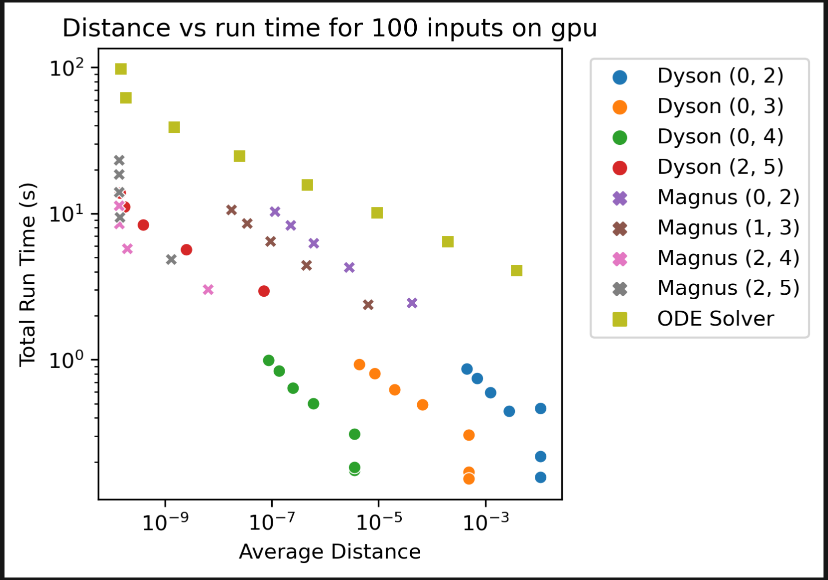




- 1000 sims on GPU w/vmap $\approx 147\ s$
  - Equiv to ≈ 25 sims in parallel at single sim speed

Advanced feature: Perturbation theory

- Numerical perturbation theory module added in 0.3.0
  - Algorithms for perturbative analysis and simulation of quantum dynamics (arxiv.org/abs/2210.11595)
    D. Puzzuoli, S. F. Lin, M. Malekakhlagh, E. Pritchett, B. Rosand, C. J. Wood
- Perturbative solvers, based on Dyson series and Magnus expansion
  - Simulating 100 different pulse parameter values for 2 qubit gate on GPU for system with dimension 25



Variation of solvers in:
Shillito et al. Fast and differentiable simulation of driven quantum systems, *Phys. Rev. Research*, 3(3):033266

Closing

- Package overview recap
  - Current version 0.3.0: Core numerical foundation, automatic model transformations, JIT, autodiff
  - Future version 0.4.0: Full Qiskit Pulse integration, simulator backend
  - Beyond: Tools for building optimization workflows
- Please submit issues, ask for help, and/or contribute!
  - Github: github.com/Qiskit/qiskit-dynamics
  - Documentation: qiskit.org/documentation/dynamics/
  - Slack: Qiskit workspace, #qiskit-dynamics
- Thank you!

Workshop closing

Thanks to all our participants and attendees!

Jens Koch
Katarina Cicak
Angela Kou
John Teufel
Archana Kamal
Amir Safavi-Naeini
Holger Haas
Michael Hush
Ziwen Huang

Thanks to all my co-organizers:
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https://brosand.github.io/DSSQ-2022-IEEE-QuantumWeek/