



Quantum Dynamics and Control with QuantumControl.jl

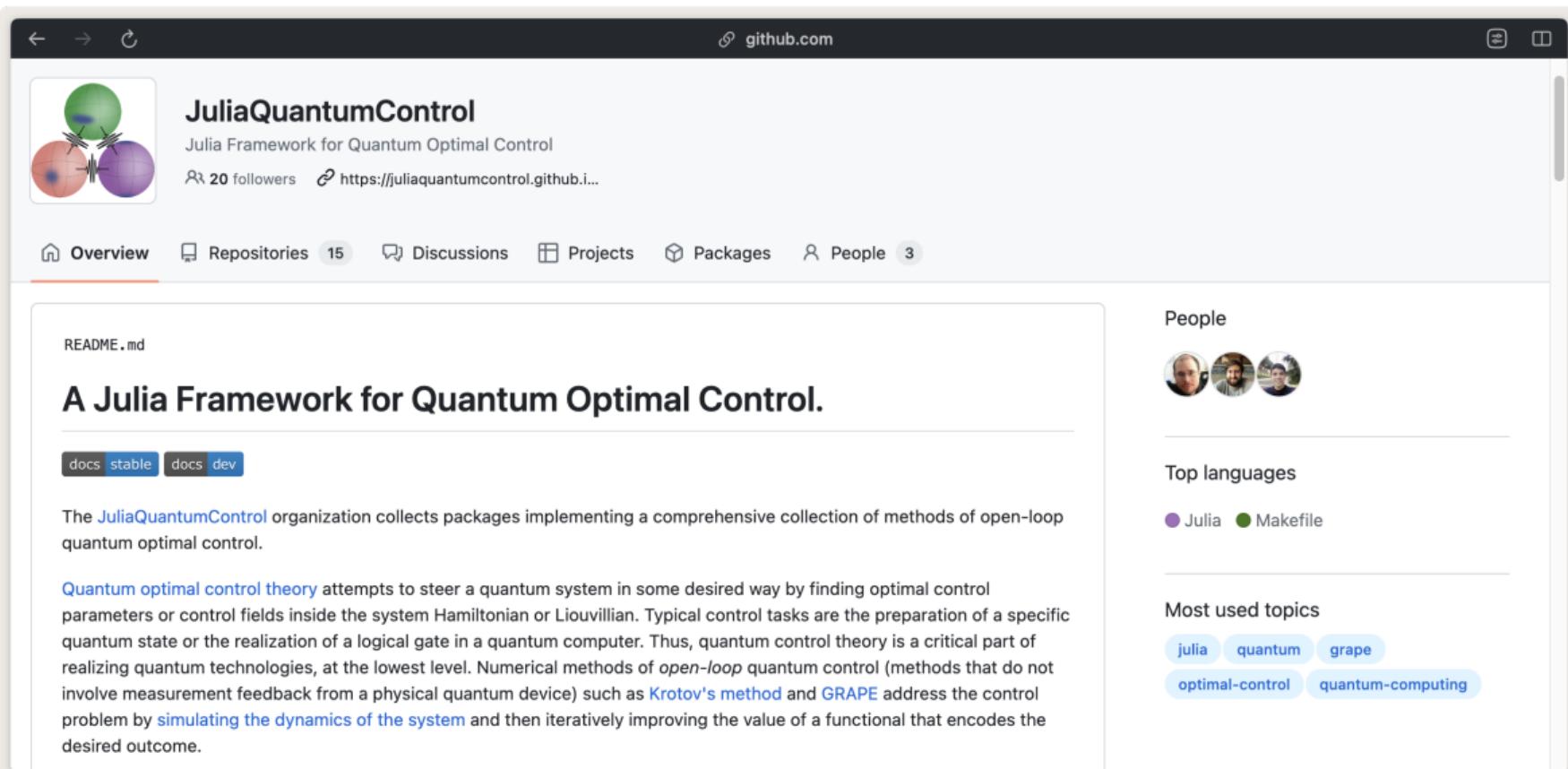
Michael H. Goerz

DEVCOM Army Research Lab

JuliaCon 2023

JuliaQuantumControl

github.com



The image shows a screenshot of a GitHub repository page for 'JuliaQuantumControl'. At the top, there's a header with a logo consisting of three spheres (green, red, and purple) and the text 'JuliaQuantumControl'. Below the header, it says 'Julia Framework for Quantum Optimal Control' and shows 20 followers with a link. The main navigation bar includes 'Overview' (which is active), 'Repositories 15', 'Discussions', 'Projects', 'Packages', and 'People 3'. On the left, there's a 'README.md' section with the heading 'A Julia Framework for Quantum Optimal Control.' and two status badges: 'docs stable' and 'docs dev'. Below this, a paragraph explains that the organization collects packages for quantum optimal control. A detailed text block follows, discussing quantum optimal control theory and its applications. To the right, there are sections for 'People' (with three profile icons), 'Top languages' (Julia and Makefile), and 'Most used topics' (julia, quantum, grape, optimal-control, quantum-computing).

JuliaQuantumControl

Julia Framework for Quantum Optimal Control

20 followers <https://juliaquantumcontrol.github.io...>

Overview Repositories 15 Discussions Projects Packages People 3

README.md

A Julia Framework for Quantum Optimal Control.

docs stable docs dev

The [JuliaQuantumControl](#) organization collects packages implementing a comprehensive collection of methods of open-loop quantum optimal control.

Quantum optimal control theory attempts to steer a quantum system in some desired way by finding optimal control parameters or control fields inside the system Hamiltonian or Liouvillian. Typical control tasks are the preparation of a specific quantum state or the realization of a logical gate in a quantum computer. Thus, quantum control theory is a critical part of realizing quantum technologies, at the lowest level. Numerical methods of *open-loop* quantum control (methods that do not involve measurement feedback from a physical quantum device) such as [Krotov's method](#) and [GRAPE](#) address the control problem by [simulating the dynamics of the system](#) and then iteratively improving the value of a functional that encodes the desired outcome.

People



Top languages

Julia Makefile

Most used topics

julia quantum grape
optimal-control quantum-computing

JuliaQuantumControl

github.com

Packages

Package	Version	CI Status	Coverage	Description
★ QuantumPropagators.jl	May 2023 v0.6.0	 CI passing	 codecov 90%	Simulate the time evolution of quantum systems (docs)
QuantumControlBase.jl	May 2023 v0.8.3	 CI passing	 codecov 89%	Shared methods and data structures (docs)
QuantumGradientGenerators.jl	May 2023 v0.1.2	 CI passing	 codecov 81%	Dynamic Gradients for Quantum Control (docs)
Krotov.jl	Mar 2023 v0.5.3	 CI passing	 codecov 90%	Krotov's method of optimal control (docs)
GRAPE.jl	Mar 2023 v0.5.4	 CI passing	 codecov 79%	Gradient Ascent Pulse Engineering method (docs)
TwoQubitWeylChamber.jl	Mar 2023 v0.1.1	 CI passing	 codecov 97%	Optimizing two-qubit gates in the Weyl chamber (docs)
QuantumControlTestUtils.jl	May 2023 v0.1.5	 CI passing		Tools for testing and benchmarking (docs)
★ QuantumControl.jl	May 2023 v0.8.0	 CI passing	 codecov 78%	Framework for Quantum Dynamics and Control (docs)

[Documentation](#)

What is Quantum Control?

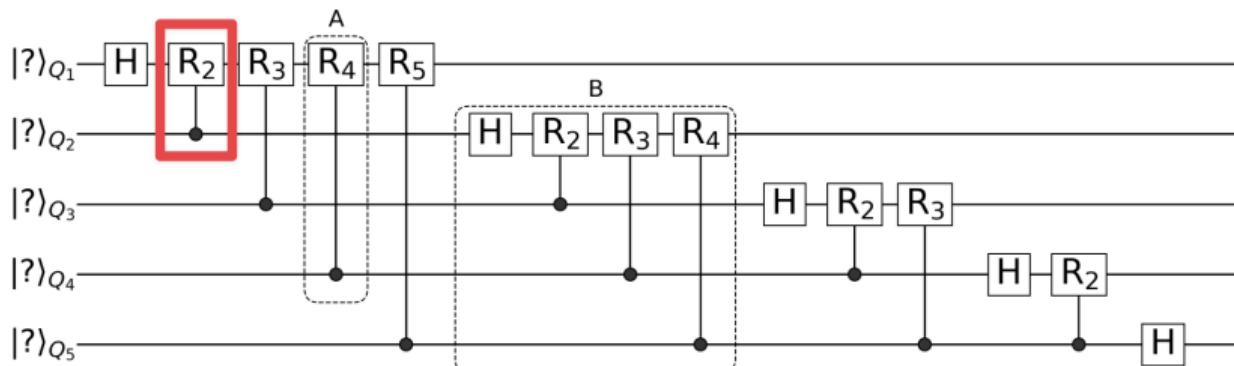
Steer a quantum system in some desired way

Quantum Gates

docs.yaoquantum.org

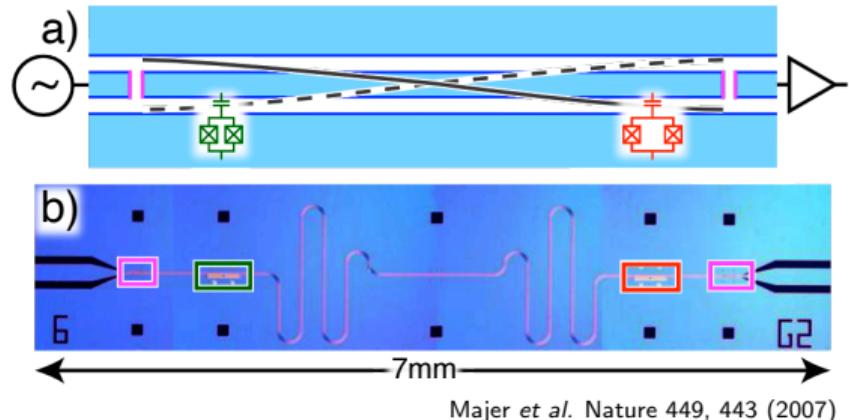
Quantum Fourier Transformation

The Quantum Fourier Transformation (QFT) circuit is to repeat two kinds of blocks repeatedly:



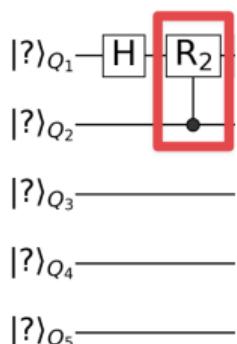
The basic building block control phase shift gate is defined as

Two-Transmon Gate



$$\hat{H} = \hat{H}_0 + \epsilon(t)\hat{H}_1$$

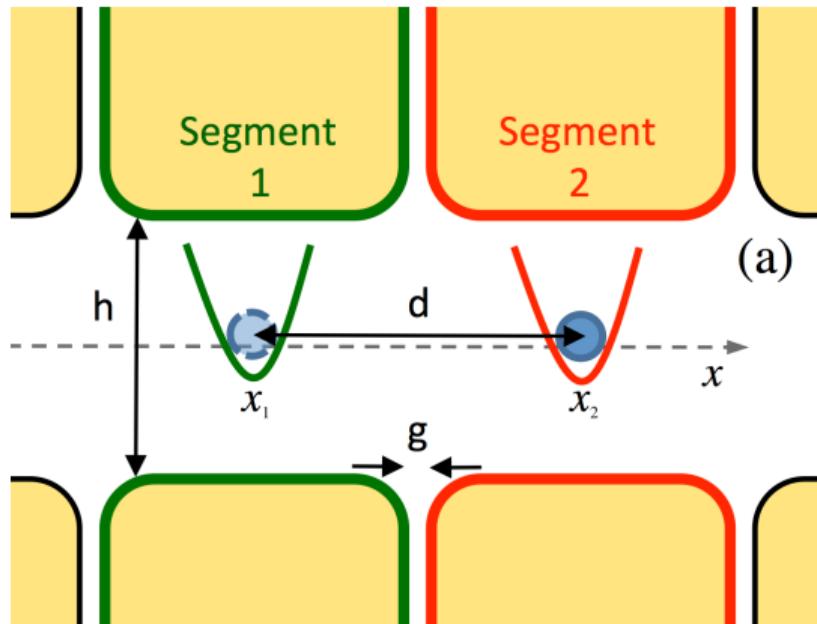
↑
microwave field in transmission line



$$\left. \begin{array}{l} |00\rangle \rightarrow CR_2|00\rangle \\ |01\rangle \rightarrow CR_2|01\rangle \\ |10\rangle \rightarrow CR_2|10\rangle \\ |11\rangle \rightarrow CR_2|11\rangle \end{array} \right\}$$

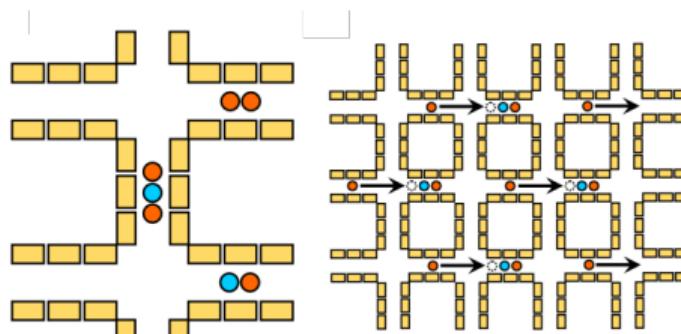
with the same $\epsilon(t)$;
acting on logical subspace

Controlling the transport of an ion



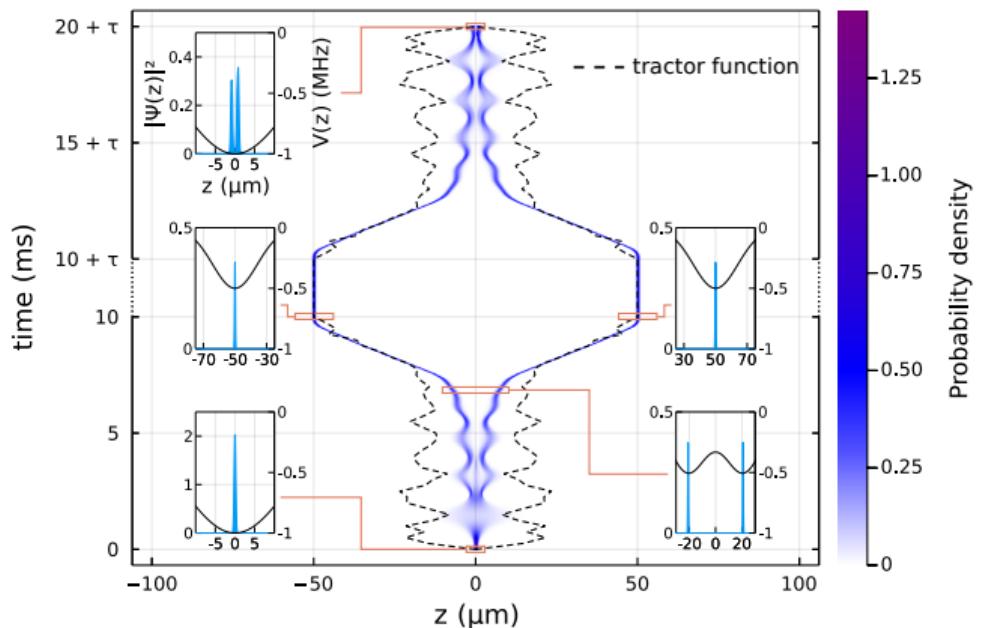
Fürst et al. New J. Phys. 16, 075007 (2014)

Find electrode voltages
to move trapped ions



Bruzewicz et al. npj Quantum Inf 5, 102 (2019)

Tractor atom interferometry

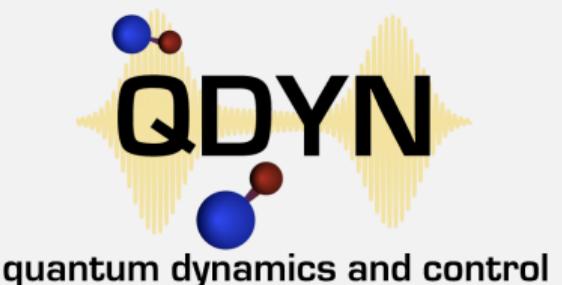


Find non-adiabatic tractor potential closing interferometric path

Raihel et al. Quantum Sci. Technol. 8, 014001 (2022)

Fortran: QDYN library

qdyn-library.net About Developers Collaborations Publications



C. Koch group
FU Berlin

About QDYN

QDYN is a Fortran 95 library and collection of utilities for the simulation of quantum dynamics and optimal control with a focus on both efficiency and precision. Its core features include

- A rich set of data structures for both closed and open quantum systems
- Routines for static system analysis (e.g. diagonalization, emission spectra)
- Propagators for the dynamic equations (Schrödinger equation, master equation) using



Python

github.com

README.rst

🔗 Krotov Python Package

github qucontrol/krotov docs gh-pages pypi v1.2.1 chat on gitter Docs passing
Tests passing codecov 96% License BSD launch binder
DOI 10.21468/SciPostPhys.7.6.080

Python implementation of Krotov's method for quantum optimal control.

This implementation follows the original implementation in the [QDYN Fortran library](#).

The `krotov` package is built on top of [QuTiP](#).

Development happens on [Github](#). You can read the full documentation [online](#) or [download a PDF version](#).

Goerz et al. SciPost Phys. 7, 80 (2019)

Languages



Python 98.5% Makefile 1.5%

Why Julia?

- Flexibility
- Performance
- Expressiveness

QuantumControl.jl examples

[←](#) [→](#) [⟳](#)[🔗 juliaquantumcontrol.github.io](#)

Examples / List of Examples



Examples

Krotov-specific examples

- Optimization of a State-to-State Transfer in a Two-Level-System
- Optimization of a Dissipative Quantum Gate
- Pulse Parametrization
- Optimization for a perfect entangler

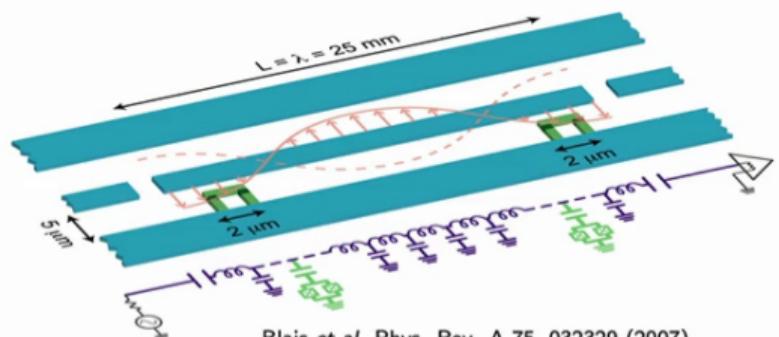
GRAPE-specific examples

- Optimization of a State-to-State Transfer in a Two-Level-System
- Optimization for a perfect entangler

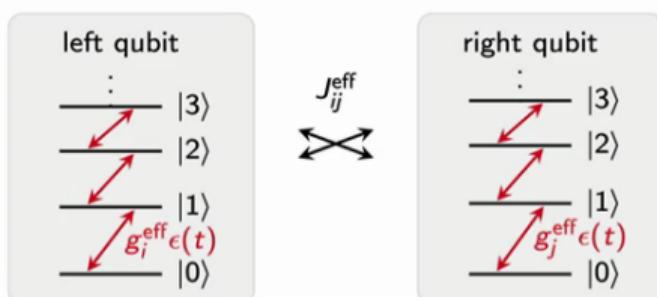
juliaquantumcontrol.github.io/GRAPE.jl/stable/examples/perfect_entanglers

Example: Optimization of Perfectly Entangling Quantum gate

Two Transmon qubits with a shared transmission line ¶



Blais et al. Phys. Rev. A 75, 032329 (2007)

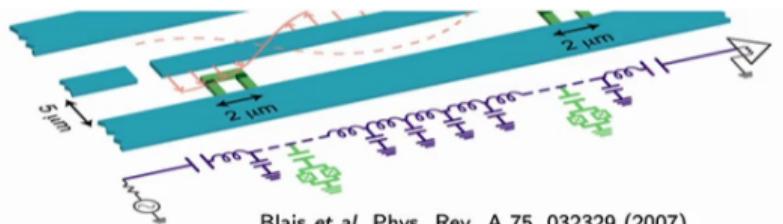


Goerz et al. EPJ Quantum Tech. 2, 21 (2015)

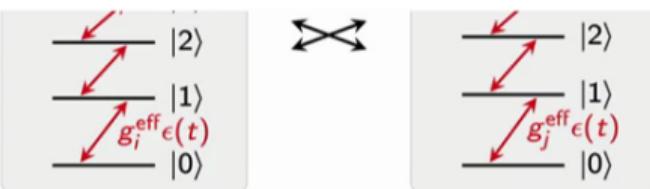
Goerz et al. npj Quantum Information 3, 37 (2017)

Hamiltonian

The system energies are on the order of GHz (angular frequency; the factor 2π is implicit), with dynamics on the order of ns



Blais *et al.*, Phys. Rev. A 75, 032329 (2007)



Goerz et al. EPJ Quantum Tech. 2, 21 (2015)

Goerz et al. npj Quantum Information 3, 37 (2017)

▼ Hamiltonian

The energies system energies are on the order of GHz (angular frequency; the factor 2π is implicit), with dynamics on the order of ns

```
[ ]: const GHz = 2π
      const MHz = 0.001GHz
      const ns = 1.0
      const μs = 1000ns;
      ⊗ = kron;
      const I = 1im;
```

We truncated the Hamiltonian to N levels

```
[ ]: const N = 6; # levels per transmon
```

So the dimension of the total Hilbert space is $N^2 = 36$

The Hamiltonian and parameters are taken from Goerz et al., Phys. Rev. A 91, 062307 (2015); Table 1.

```

w1 - w2 = sparse(w1 * w2), w1-w2 = sparse(w1 * w2)

# rotating frame:  $\omega_1, \omega_2 \rightarrow$  detuning; driving field  $\Omega \in \mathbb{C}$ 
 $\tilde{\omega}_1 = \omega_1 - \omega_d$ ;  $\tilde{\omega}_2 = \omega_2 - \omega_d$ 

 $\hat{H}_0 = \text{sparse}(
    (\tilde{\omega}_1 - \alpha_1 / 2) * \hat{n}_1 +
    (\alpha_1 / 2) * \hat{n}_1^2 +
    (\tilde{\omega}_2 - \alpha_2 / 2) * \hat{n}_2 +
    (\alpha_2 / 2) * \hat{n}_2^2 +
    J * (\hat{b}_1^+ \hat{b}_2 + \hat{b}_1 \hat{b}_2^+)
)$ 
 $\hat{H}_{1\text{re}} = \text{sparse}((1 / 2) * (\hat{b}_1 + \hat{b}_1^+ + \lambda * \hat{b}_2 + \lambda * \hat{b}_2^+))$ 
 $\hat{H}_{1\text{im}} = \text{sparse}((i / 2) * (\hat{b}_1^+ - \hat{b}_1 + \lambda * \hat{b}_2^+ - \lambda * \hat{b}_2))$ 
return hamiltonian( $\hat{H}_0$ , ( $\hat{H}_{1\text{re}}$ ,  $\Omega_{\text{re}}$ ), ( $\hat{H}_{1\text{im}}$ ,  $\Omega_{\text{im}}$ ))
end;

```

Last executed at 2023-07-24 20:13:26 in 11ms

...



Initial driving field

```
[ ]: using QuantumControl.Amplitudes: ShapedAmplitude
using QuantumControl.Shapes: flattop

function guess_amplitudes(; T=400ns, E₀=35MHz, dt=0.1ns, t_rise=15ns)
    tlist = collect(range(0, T, step=dt))
    shape(t) = flattop(t, T=T, t_rise=t_rise)
    Qre = ShapedAmplitude(t -> E₀, tlist; shape)
    Qim = ShapedAmplitude(t -> 0.0, tlist; shape)
    return tlist, Qre, Qim

```

Dynamical Generator

juliaquantumcontrol.github.io

Glossary



Generator – Dynamical generator (Hamiltonian / Liouvillian) for the time evolution of a state, i.e., the right-hand-side of the equation of motion (up to a factor of i) such that $|\Psi(t + dt)\rangle = e^{-i\hat{H}dt}|\Psi(t)\rangle$ in the infinitesimal limit. We use the symbols G , \hat{H} , or L , depending on the context (general, Hamiltonian, Liouvillian). Examples for supported forms a Hamiltonian are the following, from the most general case to simplest and most common case of linear controls,

$$\hat{H} = \overbrace{\hat{H}_0}^{\text{drift term}} + \sum_l \overbrace{\hat{H}_l(\{\epsilon_l(t)\}, t)}^{\text{control term}} \quad (\text{G1})$$

$$\hat{H} = \hat{H}_0 + \sum_l \underbrace{a_l(\{\epsilon_l(t)\}, t)}_{\text{control function}} \hat{H}_l \quad (\text{G2})$$

$$\hat{H} = \hat{H}_0 + \sum_l \overbrace{\epsilon_l(t)}^{\text{control operator}} \underbrace{\hat{H}_l}_{\text{control operator}} \quad (\text{G3})$$

Dynamical Generator

🔗 juliaquantumcontrol.github.io

Glossary



Generator – Dynamical generator (Hamiltonian / Liouvillian) for the time evolution of a state, i.e., the right-hand-side of the equation of motion (up to a factor of i) such that $|\Psi(t + dt)\rangle = e^{-i\hat{H}dt}|\Psi(t)\rangle$ in the infinitesimal limit. We use the symbols G , \hat{H} , or L , depending on the context (general, Hamiltonian, Liouvillian). Examples for supported forms a Hamiltonian are the following, from the most general case to simplest and most common case of linear controls,

```
return hamiltonian(̂H₀, (̂H₁re, Ωre), (̂H₁im, Ωim))
```

$$\hat{H} = \hat{H}_0 + \sum_l \underbrace{a_l(\{\epsilon_l(t)\}, t)}_{\text{control function}} \hat{H}_l \quad (\text{G2})$$

$$\hat{H} = \hat{H}_0 + \sum_l \overbrace{\epsilon_l(t)}^{\text{control amplitude}} \underbrace{\hat{H}_l}_{\text{control operator}} \quad (\text{G3})$$

Generator Interface

[←](#) [→](#) [↻](#)

juliaquantumcontrol.github.io

[API](#) / [Subpackages](#) / [QuantumPropagators](#)

```
@test check_generator(generator; state, tlist,
                      for mutable_state=true, for immutable_state=true,
                      for_expval=true, atol=1e-15)
```



verifies the given generator:

- `get_controls(generator)` must be defined and return a tuple
- all controls returned by `get_controls(generator)` must pass `check_control`
- `evaluate(generator, tlist, n)` must return a valid operator (`check_operator`), with forwarded keyword arguments (including `for_expval`)
- `evaluate!(op, generator, tlist, n)` must be defined
- `substitute(generator, replacements)` must be defined
- If `generator` is a `Generator` instance, all elements of `generator.amplitudes` must pass `check_amplitude`.

[source](#)

QuantumControl.jl is not a modeling framework!



docs.qojulia.org



QuantumOptics.jl

Search docs

Quantum systems

Introduction

Spin

Fock space

N-Level

Particle

States

Operators

Additional functions

Quantum systems / Particle



Particle

```
xmin = -2.  
xmax = 4.  
N = 10  
b_position = PositionBasis(xmin, xmax, N)  
b_momentum = MomentumBasis(b_position)  
  
x0 = 1.2  
p0 = 0.4  
sigma = 0.2  
psi = gaussianstate(b_position, x0, p0, sigma)  
  
x = position(b_position)  
p = momentum(b_position)
```

For particles QuantumOptics.jl provides two different choices - either the calculations can be done in real space or they can be done in momentum space by using [PositionBasis](#) or [MomentumBasis](#) respectively. The definition of these two bases types is:

Initial driving field

```
[41]: using QuantumControl.Amplitudes: ShapedAmplitude
using QuantumControl.Shapes: flattop

function guess_amplitudes(; T=400ns, E₀=35MHz, dt=0.1ns, t_rise=15ns)
    tlist = collect(range(0, T, step=dt))
    shape(t) = flattop(t, T=T, t_rise=t_rise)
    Qre = ShapedAmplitude(t -> E₀, tlist; shape)
    Qim = ShapedAmplitude(t -> 0.0, tlist; shape)
    return tlist, Qre, Qim
end

tlist, Qre_guess, Qim_guess = guess_amplitudes();
```

Last executed at 2023-07-24 20:15:32 in 81ms

```
[ ]: include("includes/plot_complex_pulse.jl")
[ ]: plot_complex_pulse(tlist, Array(Qre_guess))
[ ]: H = transmon_hamiltonian(Qre=Qre_guess, Qim=Qim_guess);
```

Logical basis

```
[ ]: function ket(i::Int64; N=N)
    Ψ = zeros(ComplexF64, N)
    Ψ[i+1] = 1
    return Ψ
end
```

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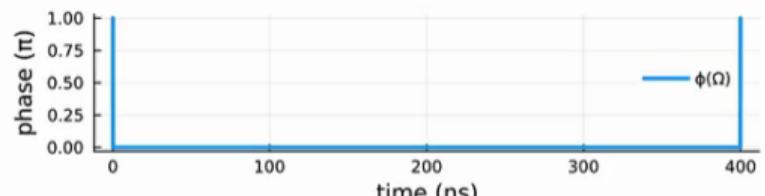
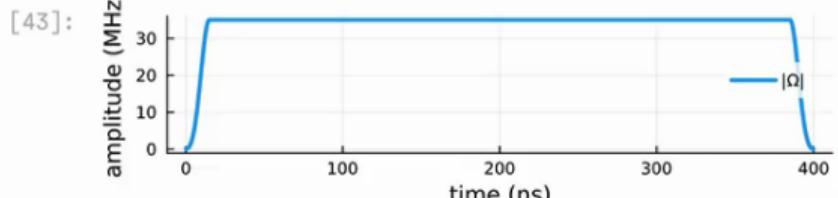
```
[42]: include("includes/plot_complex_pulse.jl")
```

Last executed at 2023-07-24 20:16:27 in 11ms

```
[42]: plot_complex_pulse (generic function with 1 method)
```

```
[43]: plot_complex_pulse(tlist, Array(Qre_guess))
```

Last executed at 2023-07-24 20:16:27 in 74ms



```
[44]: H = transmon_hamiltonian(Qre=Qre_guess, Qim=Qim_guess);
```

Last executed at 2023-07-24 20:16:31 in 65ms

Logical basis



```
[ ]: function ket(i::Int64; N=N)
```

Logical basis

```
[ ]: function ket(i::Int64; N=N)
    Ψ = zeros(ComplexF64, N)
    Ψ[i+1] = 1
    return Ψ
end

function ket(indices::Int64...; N=N)
    Ψ = ket(indices[1]; N=N)
    for i in indices[2:end]
        Ψ = Ψ ⊗ ket(i; N=N)
    end
    return Ψ
end

function ket(label::AbstractString; N=N)
    indices = [parse(Int64, digit) for digit in label]
    return ket(indices...; N=N)
end;
```

```
[ ]: basis = [ket("00"), ket("01"), ket("10"), ket("11")];
```

```
[ ]: ket("01")
```

Dynamics of the guess field

```
[ ]: using QuantumControl: propagate
```

```
[47]: ket("01")
```

Last executed at 2023-07-24 20:20:11 in 6ms

```
[47]: 36-element Vector{ComplexF64}:
```

$0.0 + 0.0im$

$1.9 + 0.0im$

$0.0 + 0.0im$

$0.0 + 0.0im$

$$0.0 + 0.0im$$

0.0 + 0.0im

0.0 + 0.0im

$$0.0 \pm 0.0 \text{im}$$

8.8 ± 0.8im

0.0 ± 0.0im

8.0 + 8.0im

0.0 ± 0.0im

$0.0 + 0.0im$

5.5 + 5.5mm

$\theta_{\text{a}} + \theta_{\text{sim}}$

0.0 + 0.0im

0.0 + 0.0im

0.0 + 0.0im

$$0.0 + 0.0im$$

$0.0 + 0.0i$

$$0.0 + 0.01m$$

$$0.0 + 0.01m$$

$0.0 + 0.0im$

$$0.0 + 0.0im$$

$0.0 + 0.0im$

$0.0 + 0.0im$

$0.0 + 0.0\text{im}$

0.0 + 0.0im
0.0 + 0.0im
0.0 + 0.0im
0.0 + 0.0im
0.0 + 0.0im

Dynamics of the guess field

```
[ ]: using QuantumControl: propagate
```

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三

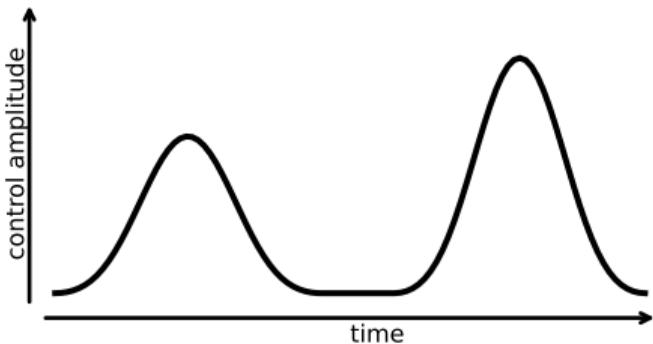
```
[ ]: logical_overlap = [(\psi -> \psi . \phi) for \phi \in basis];
```

```
[ ]: dyn00 = propagate(ket("00"), H, tlist; observables=logical_overlap, storage=true)
dyn01 = propagate(ket("01"), H, tlist; observables=logical_overlap, storage=true)
dyn10 = propagate(ket("10"), H, tlist; observables=logical_overlap, storage=true)
dyn11 = propagate(ket("11"), H, tlist; observables=logical_overlap, storage=true)
```

```
[ ]: U_of_t = [[dyn00[::,n] dyn01[::,n] dyn10[::,n] dyn11[::,n]] for n = 1:length(tlist)];
```

```
[ ]: using TwoQubitWeylChamber: gate_concurrence, unitarity
```

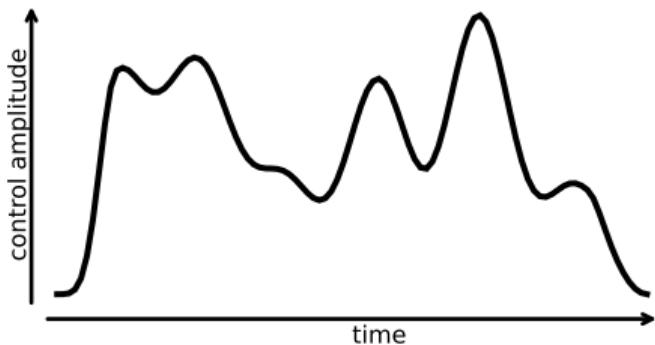
QuantumPropagators.jl



$$i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle = \hat{H}(\{\epsilon_I(t)\}) |\Psi(t)\rangle$$

$$i\hbar \frac{\partial}{\partial t} \hat{\rho}(t) = \mathcal{L}(\{\epsilon_I(t)\}) [\hat{\rho}(t)]$$

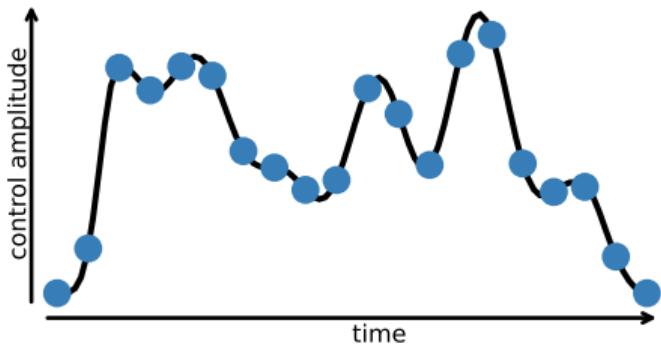
QuantumPropagators.jl



$$i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle = \hat{H}(\{\epsilon_I(t)\}) |\Psi(t)\rangle$$

$$i\hbar \frac{\partial}{\partial t} \hat{\rho}(t) = \mathcal{L}(\{\epsilon_I(t)\}) [\hat{\rho}(t)]$$

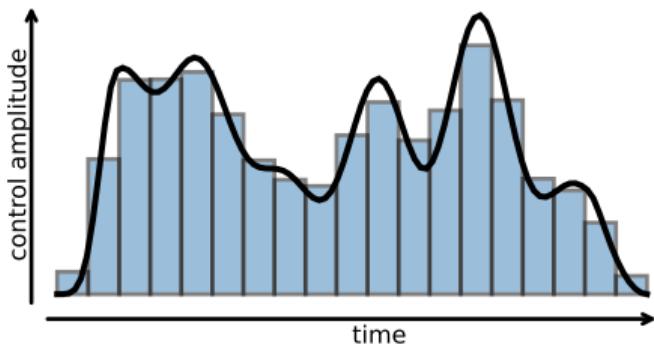
QuantumPropagators.jl



$$i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle = \hat{H}(\{\epsilon_I(t)\}) |\Psi(t)\rangle$$

$$i\hbar \frac{\partial}{\partial t} \hat{\rho}(t) = \mathcal{L}(\{\epsilon_I(t)\}) [\hat{\rho}(t)]$$

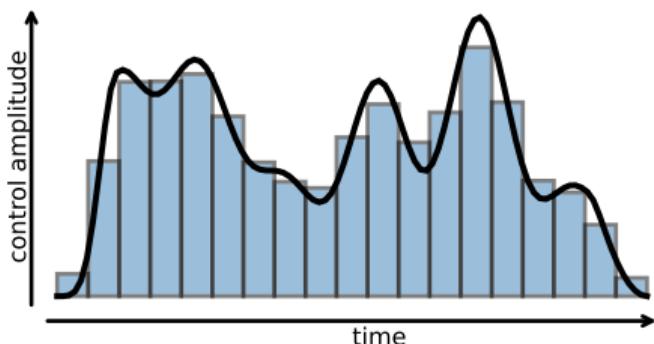
QuantumPropagators.jl



$$i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle = \hat{H}(\{\epsilon_I(t)\}) |\Psi(t)\rangle$$

$$i\hbar \frac{\partial}{\partial t} \hat{\rho}(t) = \mathcal{L}(\{\epsilon_I(t)\}) [\hat{\rho}(t)]$$

QuantumPropagators.jl



$$i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle = \hat{H}(\{\epsilon_I(t)\}) |\Psi(t)\rangle$$

$$i\hbar \frac{\partial}{\partial t} \hat{\rho}(t) = \mathcal{L}(\{\epsilon_I(t)\}) [\hat{\rho}(t)]$$

PWC propagator: $\hat{U}_n = \exp[-\frac{i}{\hbar} \hat{H}_n dt]$ for n 'th time slice

⇒ evaluate $\hat{U}_n |\Psi\rangle$ (or $\mathcal{U}_n[\hat{\rho}]$) as a polynomial expansion

- Hermitian Hamiltonian → Chebychev polynomials
- Non-Hermitian Hamiltonian or Liouvillian → Newton polynomials

Propagator Interface

juliaquantumcontrol.github.io



Overview



The Propagator interface

As a lower-level interface than `propagate`, the `QuantumPropagators` package defines an interface for "propagator" objects. These are initialized via `init_prop` as, e.g.,

```
using QuantumPropagators: init_prop

propagator = init_prop(Ψ₀, H, tlist)
```

The `propagator` is a propagation-method-dependent object with the interface described by `AbstractPropagator`.

The `prop_step!` function can then be used to advance the `propagator`:

```
using QuantumPropagators: prop_step!

Ψ = prop_step!(propagator) # single step
```

Dynamics of the guess field

```
[48]: using QuantumControl: propagate
```

Last executed at 2023-07-24 20:20:23 in 1ms

1

□ ↑ ↓ ± × └

```
[ ]: logical_overlap = [(\Psi -> \Psi + \phi) for \phi \in basis];
```

```
[ ]: dyn00 = propagate(ket("00"), H , tlist; observables=logical_overlap, storage=true)
dyn01 = propagate(ket("01"), H , tlist; observables=logical_overlap, storage=true)
dyn10 = propagate(ket("10"), H , tlist; observables=logical_overlap, storage=true)
dyn11 = propagate(ket("11"), H , tlist; observables=logical_overlap, storage=true)
```

```
[ ]: U_of_t = [[dyn00[ :,n] dyn01[ :,n] dyn10[ :,n] dyn11[ :,n]] for n = 1:length(tlist)];
```

```
[ ]: using TwoQubitWeylChamber; gate_concurrence.unitarity
```

```
0.0 + 0.0im
0.0 + 0.0im
```

Dynamics of the guess field

[48]: `using QuantumControl: propagate`

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...

[49]: `logical_overlap = [(\psi -> \psi * \phi) for \phi \in basis];`

Last executed at 2023-07-24 20:21:22 in 22ms

[50]: `dyn00 = propagate(ket("00"), H, tlist; observables=logical_overlap, storage=true)`
`dyn01 = propagate(ket("01"), H, tlist; observables=logical_overlap, storage=true)`
`dyn10 = propagate(ket("10"), H, tlist; observables=logical_overlap, storage=true)`
`dyn11 = propagate(ket("11"), H, tlist; observables=logical_overlap, storage=true)`

Last executed at 2023-07-24 20:21:29 in 399ms

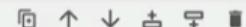
[50]: 4x4001 Matrix{ComplexF64}:

0.0+0.0im	-2.39717e-38+6.02033e-41im	...	-0.235051+0.0535181im
0.0+0.0im	5.01846e-21-1.52469e-19im		-0.00751948+0.0103133im
0.0+0.0im	-6.35138e-21-1.56991e-19im		-0.00120914-0.00378444im
1.0+0.0im	0.999992-0.00125631im		0.549798-0.644815im

[51]: `U_of_t = [[dyn00[:,n] dyn01[:,n] dyn10[:,n] dyn11[:,n]] for n = 1:length(tlist)];`

Last executed at 2023-07-24 20:21:40 in 117ms

[]: `using TwoQubitWeylChamber: gate_concurrence, unitarity`



[]: `CNOT = [`

```
1.0+0.0im      0.999992-0.00125631im      0.549798-0.644815im
```

```
[51]: U_of_t = [[dyn00[:,n] dyn01[:,n] dyn10[:,n] dyn11[:,n]] for n = 1:length(tlist)];
```

Last executed at 2023-07-24 20:21:40 in 117ms

```
[52]: using TwoQubitWeylChamber: gate_concurrence, unitarity
```

Last executed at 2023-07-24 20:21:46 in 3ms

```
[53]: CNOT = [
    1 0 0 0
    0 1 0 0
    0 0 0 1
    0 0 1 1
];
```

Last executed at 2023-07-24 20:22:03 in 2ms

```
[54]: gate_concurrence(CNOT)
```

Last executed at 2023-07-24 20:22:05 in 1ms

```
[54]: 1.0
```

```
[ ]: plot(tlist, gate_concurrence.(U_of_t), xlabel="time (ns)", ylabel="gate concurrence", label="", ylim=(0, 1))
```

```
[ ]: gate_concurrence(U_of_t[end])
```

```
[ ]: plot(tlist, 1 .- unitarity.(U_of_t), xlabel="time (ns)", ylabel="loss from subspace", label="")
```

```
[ ]: 1 - unitarity(U_of_t[end])
```

Maximization of Gate Concurrence

Last executed at 2023-07-24 20:22:05 in 1ms

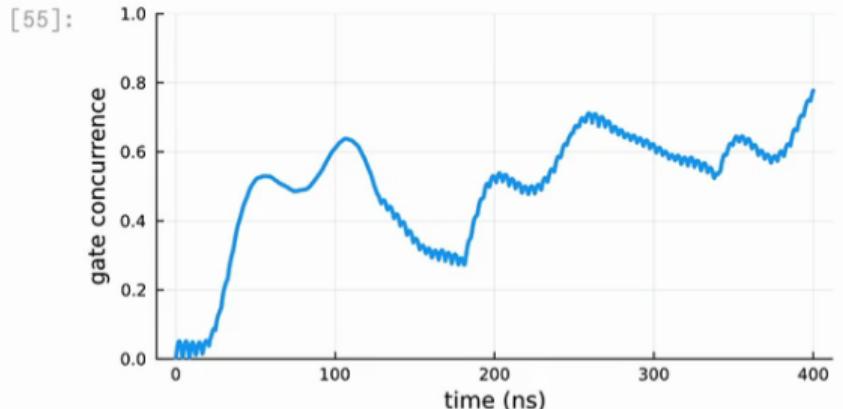
[54]: gate_concurrence(CNOT)

Last executed at 2023-07-24 20:22:05 in 1ms

[54]: 1.0

[55]: plot(tlist, gate_concurrence.(U_of_t), xlabel="time (ns)", ylabel="gate concurrence", label="", ylim=(0, 1))

Last executed at 2023-07-24 20:22:10 in 80ms



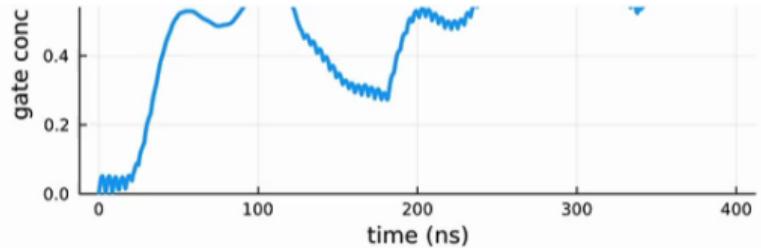
[56]: gate_concurrence(U_of_t[end])

Last executed at 2023-07-24 20:22:20 in 2ms

[56]: 0.7773116198529164

[]: plot(tlist, 1 .- unitarity.(U_of_t), xlabel="time (ns)", ylabel="loss from subspace", label="")

[]: 1 - unitarity(U_of_t)[end]



```
[56]: gate_concurrence(U_of_t[end])
```

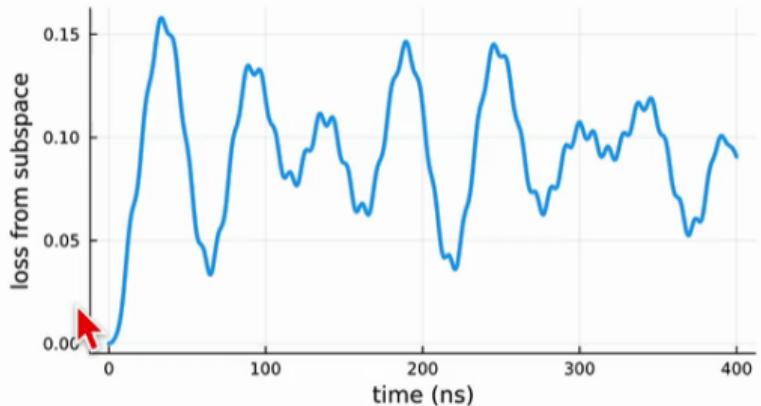
Last executed at 2023-07-24 20:22:20 in 2ms

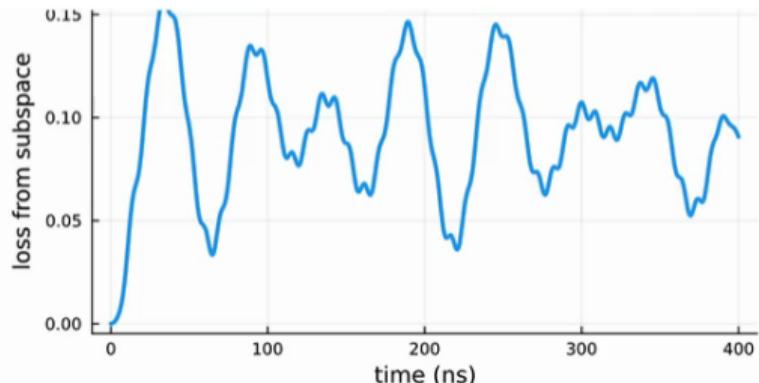
```
[56]: 0.7773116198529164
```

```
[57]: plot(tlist, 1 .- unitarity.(U_of_t), xlabel="time (ns)", ylabel="loss from subspace", label="")
```

Last executed at 2023-07-24 20:22:35 in 37ms

```
[57]:
```





```
[58]: 1 - unitarity(U_of_t[end])
```

Last executed at 2023-07-24 20:22:45 in 2ms

```
[58]: 0.09071664593816564
```

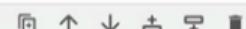
Maximization of Gate Concurrence

```
[59]: using QuantumControl: Objective
```

```
objectives = [Objective(; initial_state=Ψ, generator=H) for Ψ ∈ basis];
```

Last executed at 2023-07-24 20:22:57 in 40ms

```
[ ]: J_T_C = U -> 0.5 * (1 - gate_concurrence(U)) + 0.5 * (1 - unitarity(U));
```



```
[ ]: J_T_C(U_of_t[end])
```

Last executed at 2023-07-24 20:22:40 in 4ms

[58]: 0.09071664593816564

Maximization of Gate Concurrence

[59]:

```
using QuantumControl: Objective
```

```
objectives = [Objective(; initial_state=ψ, generator=H) for ψ ∈ basis];
```

Last executed at 2023-07-24 20:22:57 in 40ms

[60]:

```
J_T_C = U -> 0.5 * (1 - gate_concurrence(U)) + 0.5 * (1 - unitarity(U));
```

Last executed at 2023-07-24 20:23:20 in 4ms

[61]: ~~J_T_C(U_of_t[end])~~

Last executed at 2023-07-24 20:23:36 in 8ms

[61]: 0.1567025130426246

[]:

```
using QuantumControl.Functionals: gate_functional
```



```
J_T = gate_functional(J_T_C);
```

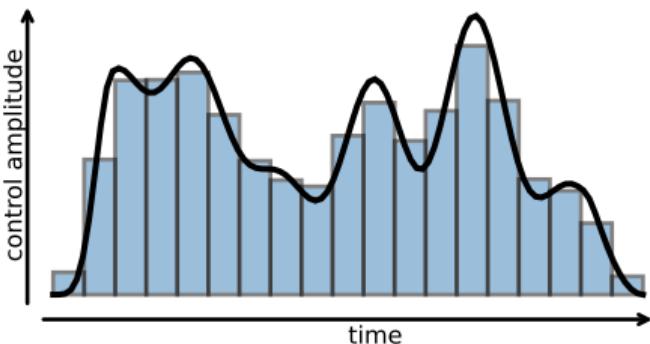
J_T is now a function of the propagated states $|\Psi_{00}(T)\rangle, |\Psi_{01}(T)\rangle, |\Psi_{10}(T)\rangle, |\Psi_{11}(T)\rangle$.

[]:

```
using QuantumControl.Functionals: make_gate_chi
```

```
chi = make_gate_chi(J_T_C, objectives)
```

Gradient-based optimal control



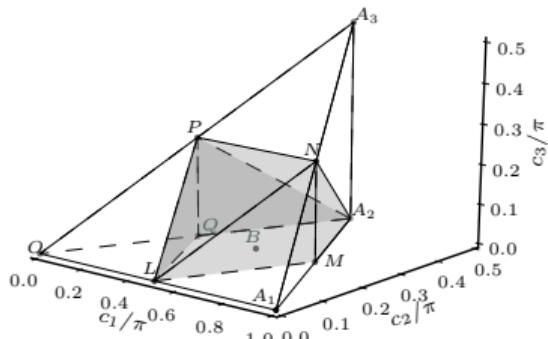
- Control parameters: discretized pulse values ϵ_{nl}
- Gradient $\nabla J_T = \frac{\partial J_T}{\partial \epsilon_{nl}}$
- Tune controls in the direction of the gradient

gate concurrence of two-qubit gate \hat{U}

- 1 $c_1, c_2, c_3 \propto \text{eigvals}(\hat{U}\tilde{U})$; $\tilde{U} = (\hat{\sigma}_y \otimes \hat{\sigma}_y) \hat{U} (\hat{\sigma}_y \otimes \hat{\sigma}_y)$
- 2 $C(\hat{U}) = \max |\sin(c_{1,2,3} \pm c_{3,1,2})|$

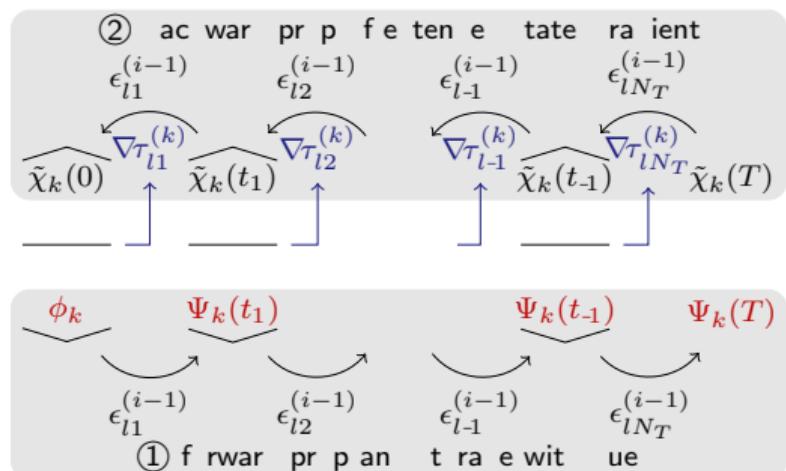
Childs et al. Phys. Rev. A 68, 052311 (2003)

Not analytic!



Semi-automatic differentiation

$$\begin{aligned}\nabla J_T &= \frac{\partial J_T(\{\Psi_k(T)\})}{\partial \epsilon_{nl}} \\ &= 2\text{Re} \left[\sum_k \underbrace{\frac{\partial J_T}{\partial |\Psi_k(T)\rangle}}_{\equiv \langle \chi_k |} \frac{\partial |\Psi_k(T)\rangle}{\partial \epsilon_{nl}} \right] \\ &= 2\text{Re} \left[\sum_k \frac{\partial}{\partial \epsilon_{nl}} \langle \chi_k(T) | \Psi_k(T) \rangle \right]\end{aligned}$$



Goerz et al. Quantum 6, 871 (2022)



Yao Community Seminar:
<https://youtu.be/MQCILD2P89c>

Last executed at 2023-07-24 20:22:40 in 4ms

[58]: 0.09071664593816564

Maximization of Gate Concurrence

[59]:

```
using QuantumControl: Objective
```

```
objectives = [Objective(; initial_state=Ψ, generator=H) for Ψ ∈ basis];
```

Last executed at 2023-07-24 20:22:57 in 40ms

[60]:

```
J_T_C = U -> 0.5 * (1 - gate_concurrence(U)) + 0.5 * (1 - unitarity(U));
```

Last executed at 2023-07-24 20:23:20 in 4ms

[61]:

```
J_T_C(U_of_t[end])
```

Last executed at 2023-07-24 20:23:36 in 8ms

[61]: 0.1567025130426246

[62]:

```
using QuantumControl.Functionals: gate_functional
```

```
J_T = gate_functional(J_T_C);
```

Last executed at 2023-07-24 20:24:02 in 4ms

J_T is now a function of the propagated states $|\Psi_{00}(T)\rangle, |\Psi_{01}(T)\rangle, |\Psi_{10}(T)\rangle, |\Psi_{11}(T)\rangle$.

...

[]:

```
using QuantumControl.Functionals: make_gate_chi
```



```
chi = make_gate_chi(J_T_C, objectives)
```

Last executed at 2023-07-24 20:24:02 in 4ms

J_T is now a function of the propagated states $|\Psi_{00}(T)\rangle, |\Psi_{01}(T)\rangle, |\Psi_{10}(T)\rangle, |\Psi_{11}(T)\rangle$.

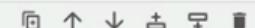
...

```
[63]: using QuantumControl.Functionals: make_gate_chi  
  
chi = make_gate_chi(J_T_C, objectives)
```

Last executed at 2023-07-24 20:25:01 in 71ms

```
[63]: (::QuantumControl.Functionals.var"#zygote_gate_chi!#35"{QuantumControl.Functionals.var"#zygote_gate_chi!#29#36"{Bool, Base.Pairs{Symbol, Union{}, Tuple{}, NamedTuple{(), Tuple{}}}, var"#52#53", Vector{Vector{ComplexF64}}, Int64}})  
(generic function with 1 method)
```

```
[ ]: using QuantumControl: ControlProblem  
  
problem = ControlProblem(;  
    objectives, tlist, J_T, chi,  
    check_convergence=res -> begin  
        (  
            (res.J_T <= 1e-3) &&  
            (res.converged = true) &&  
            (res.message = "Found a perfect entangler")  
        )  
    end,  
    use_threads=true,  
);
```



```
[ ]: using QuantumControl: optimize  
  
res = optimize(problem; method=:GRAPE)
```

t, base,rati~~s~~ly~~g~~mm~~o~~, un~~to~~ll~~s~~, t~~u~~p~~le~~ls, m~~an~~neu~~tu~~re~~l~~, t~~u~~p~~le~~ss~~ss~~, var nu~~z~~uu , v~~e~~c~~t~~o~~l~~z v~~e~~c~~t~~o~~l~~z l~~u~~m~~pl~~ea~~r~~ u~~u~~ss, t~~u~~lu~~u~~ss)
(generic function with 1 method)

```
[64]: using QuantumControl: ControlProblem

problem = ControlProblem();
objectives, tlist, J_T, chi,
check_convergence=res -> begin
    (
        (res.J_T <= 1e-3) &&
        (res.converged = true) &&
        (res.message = "Found a perfect entangler")
    )
end,
use_threads=true,
);
```

Last executed at 2023-07-24 20:25:41 in 44ms

```
[*]: using QuantumControl: optimize

res = optimize(problem; method=:GRAPE)
```

N/A (28.57s)

iter.	J_T	∇J_T	ΔJ_T	FG(F)	secs
0	1.57e-01	1.42e-01	n/a	1(0)	1.4
1	1.46e-01	3.18e-01	-1.05e-02	1(0)	0.3
2	1.30e-01	2.86e-01	-1.61e-02	1(0)	0.3
3	8.10e-02	2.10e-01	-4.91e-02	2(0)	0.5
4	7.66e-02	3.79e-01	-4.41e-03	1(0)	0.2
5	4.89e-02	1.87e-01	-2.77e-02	1(0)	0.2
6	2.64e-02	2.11e-01	-2.25e-02	1(0)	0.2
7	7.54e-03	1.09e-01	-1.89e-02	1(0)	0.3
8	5.86e-03	1.98e-01	-1.68e-03	1(0)	0.3

Execution started at 2023-07-24 20:25:47

```
[65]: using QuantumControl: optimize
```

```
res = optimize(problem; method=:GRAPE)
```

Last executed at 2023-07-24 20:25:52 in 5.02s

iter.	J_T	∇J_T	ΔJ_T	FG(F)	secs
0	1.57e-01	1.42e-01	n/a	1(0)	1.4
1	1.46e-01	3.18e-01	-1.05e-02	1(0)	0.3
2	1.30e-01	2.86e-01	-1.61e-02	1(0)	0.3
3	8.10e-02	2.10e-01	-4.91e-02	2(0)	0.5
4	7.66e-02	3.79e-01	-4.41e-03	1(0)	0.2
5	4.89e-02	1.87e-01	-2.77e-02	1(0)	0.2
6	2.64e-02	2.11e-01	-2.25e-02	1(0)	0.2
7	7.54e-03	1.09e-01	-1.89e-02	1(0)	0.3
8	5.86e-03	1.98e-01	-1.68e-03	1(0)	0.3
9	3.00e-03	4.01e-02	-2.87e-03	1(0)	0.3
10	2.71e-03	2.72e-02	-2.88e-04	1(0)	0.3
11	2.21e-03	2.82e-02	-5.01e-04	1(0)	0.3
12	1.42e-03	2.46e-02	-7.84e-04	1(0)	0.3
13	3.24e-04	2.83e-02	-1.10e-03	1(0)	0.3

```
[65]: GRAPE Optimization Result
```

-
- Started at 2023-07-24T20:25:47.270
- Number of objectives: 4
- Number of iterations: 13
- Number of pure func evals: 0
- Number of func/grad evals: 15
- Value of functional: 3.24322e-04
- Reason for termination: Found a perfect entangler
- Ended at 2023-07-24T20:25:52.287 (5 seconds, 17 milliseconds)

```
cont = res.optimized_controls[1] + i * res.optimized_controls[2]
```

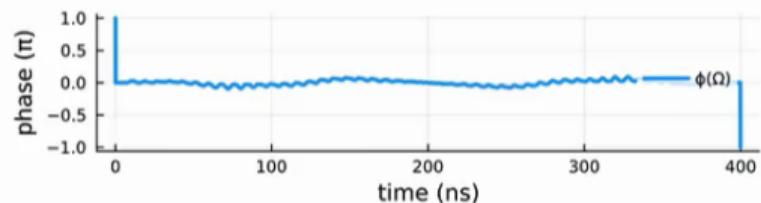
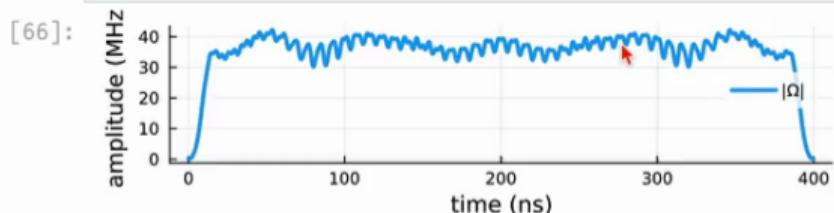


- Started at 2023-07-24T20:25:47.270
- Number of objectives: 4
- Number of iterations: 13
- Number of pure func evals: 0
- Number of func/grad evals: 15
- Value of functional: 3.24322e-04
- Reason for termination: Found a perfect entangler
- Ended at 2023-07-24T20:25:52.287 (5 seconds, 17 milliseconds)

```
[66]: ε_opt = res.optimized_controls[1] + i * res.optimized_controls[2]
Ω_opt = ε_opt .* discretize(Qre_guess.shape, tlist)

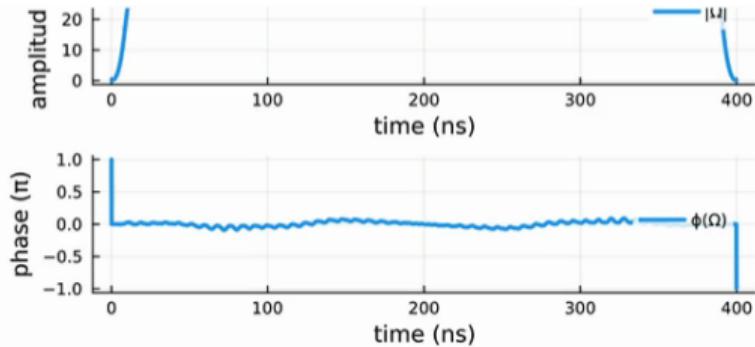
plot_complex_pulse(tlist, Ω_opt)
```

Last executed at 2023-07-24 20:26:09 in 80ms



Dynamics of the optimized field





▼ Dynamics of the optimized field ¶

```
[67]: using QuantumControl.Controls: get_controls
ε_re_guess, ε_im_guess = get_controls(H);
```

Last executed at 2023-07-24 20:26:19 in 3ms

```
[ ]: using QuantumControl.Controls: substitute

H_opt = substitute(
    H,
    IdDict(
        ε_re_guess => res.optimized_controls[1],
        ε_im_guess => res.optimized_controls[2]
    )
);
```



```
[67]: using QuantumControl.Controls: get_controls
      ε_re_guess, ε_im_guess = get_controls(H);
```

Last executed at 2023-07-24 20:26:19 in 3ms

```
[68]: using QuantumControl.Controls: substitute
      H_opt = substitute(
          H,
          IdDict(
              ε_re_guess => res.optimized_controls[1],
              ε_im_guess => res.optimized_controls[2]
          )
      );
```

Last executed at 2023-07-24 20:26:31 in 2ms

```
[69]: dyn00_opt = propagate(ket("00"), H_opt, tlist; observables=logical_overlap, storage=true)
      dyn01_opt = propagate(ket("01"), H_opt, tlist; observables=logical_overlap, storage=true)
      dyn10_opt = propagate(ket("10"), H_opt, tlist; observables=logical_overlap, storage=true)
      dyn11_opt = propagate(ket("11"), H_opt, tlist; observables=logical_overlap, storage=true)
      U_opt_of_t = [[dyn00_opt[:,n] dyn01_opt[:,n] dyn10_opt[:,n] dyn11_opt[:,n]] for n = 1:length(tlist)];
```

Last executed at 2023-07-24 20:26:42 in 417ms

```
[ ]: plot(tlist, gate_concurrence.(U_opt_of_t), xlabel="time (ns)", ylabel="gate concurrence", label="")
      plot!(tlist, gate_concurrence.(U_of_t), label="guess")
```

```
[ ]: gate_concurrence(U_opt_of_t[end])
```

```
[ ]: plot(tlist, 1 .- unitarity.(U_opt_of_t), xlabel="time (ns)", ylabel="loss from subspace", label="")
      plot!(tlist, 1 .- unitarity.(U_of_t), label="guess")
```

```
    )
);
```

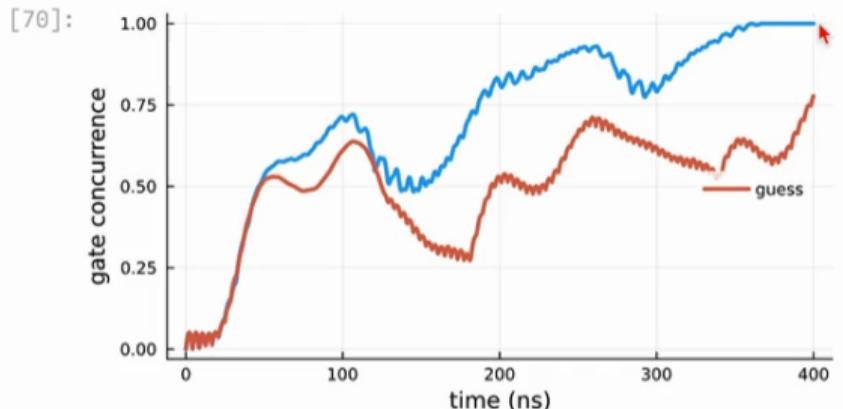
Last executed at 2023-07-24 20:26:31 in 2ms

```
[69]: dyn00_opt = propagate(ket("00"), H_opt , tlist; observables=logical_overlap, storage=true)
dyn01_opt = propagate(ket("01"), H_opt , tlist; observables=logical_overlap, storage=true)
dyn10_opt = propagate(ket("10"), H_opt , tlist; observables=logical_overlap, storage=true)
dyn11_opt = propagate(ket("11"), H_opt , tlist; observables=logical_overlap, storage=true)
U_opt_of_t = [[dyn00_opt[:,n] dyn01_opt[:,n] dyn10_opt[:,n] dyn11_opt[:,n]] for n = 1:length(tlist)];
```

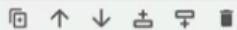
Last executed at 2023-07-24 20:26:42 in 417ms

```
[70]: plot(tlist, gate_concurrence.(U_opt_of_t), xlabel="time (ns)", ylabel="gate concurrence", label="")
plot!(tlist, gate_concurrence.(U_of_t), label="guess")
```

Last executed at 2023-07-24 20:26:47 in 123ms

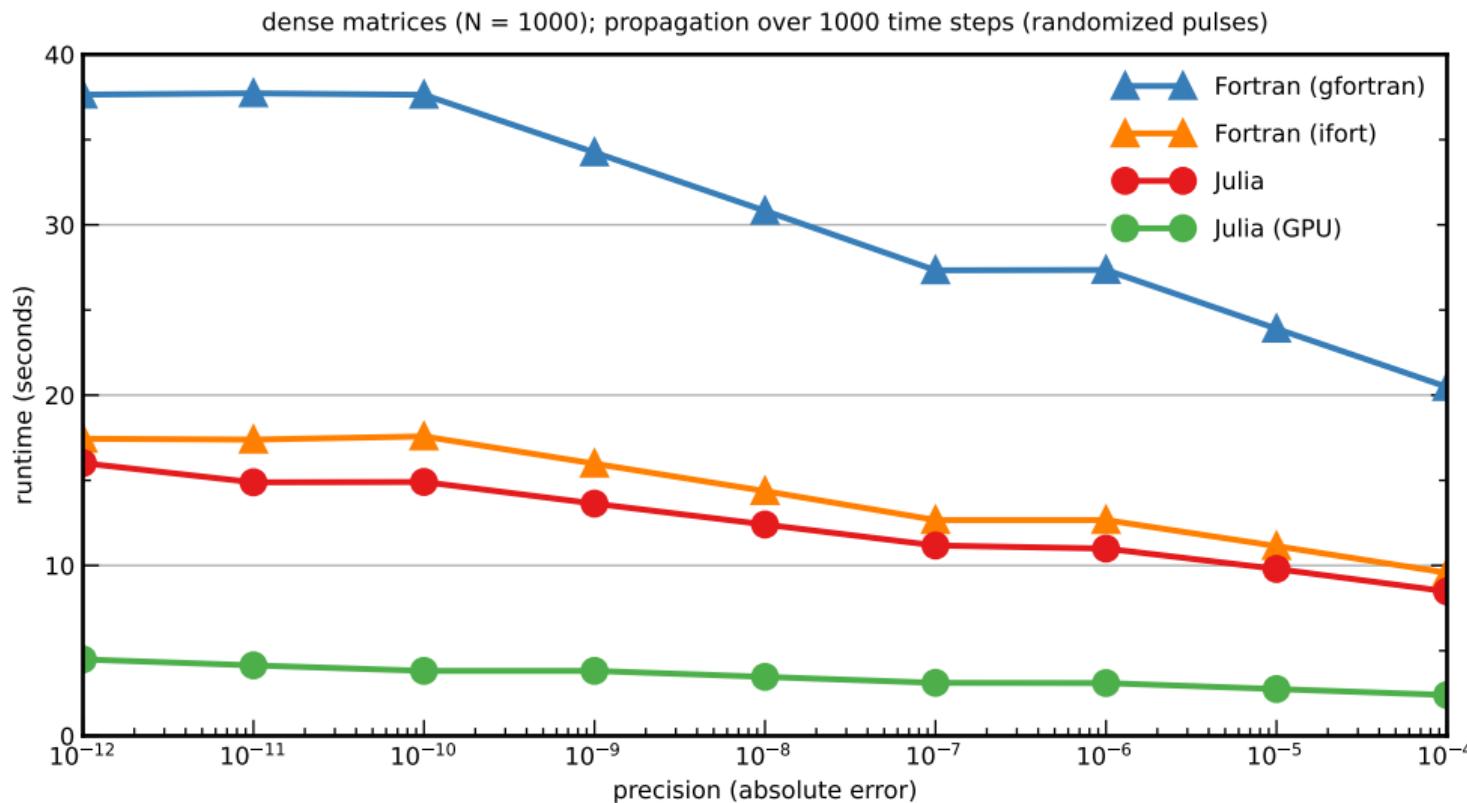


[]: gate_concurrence(U_opt_of_t[end])

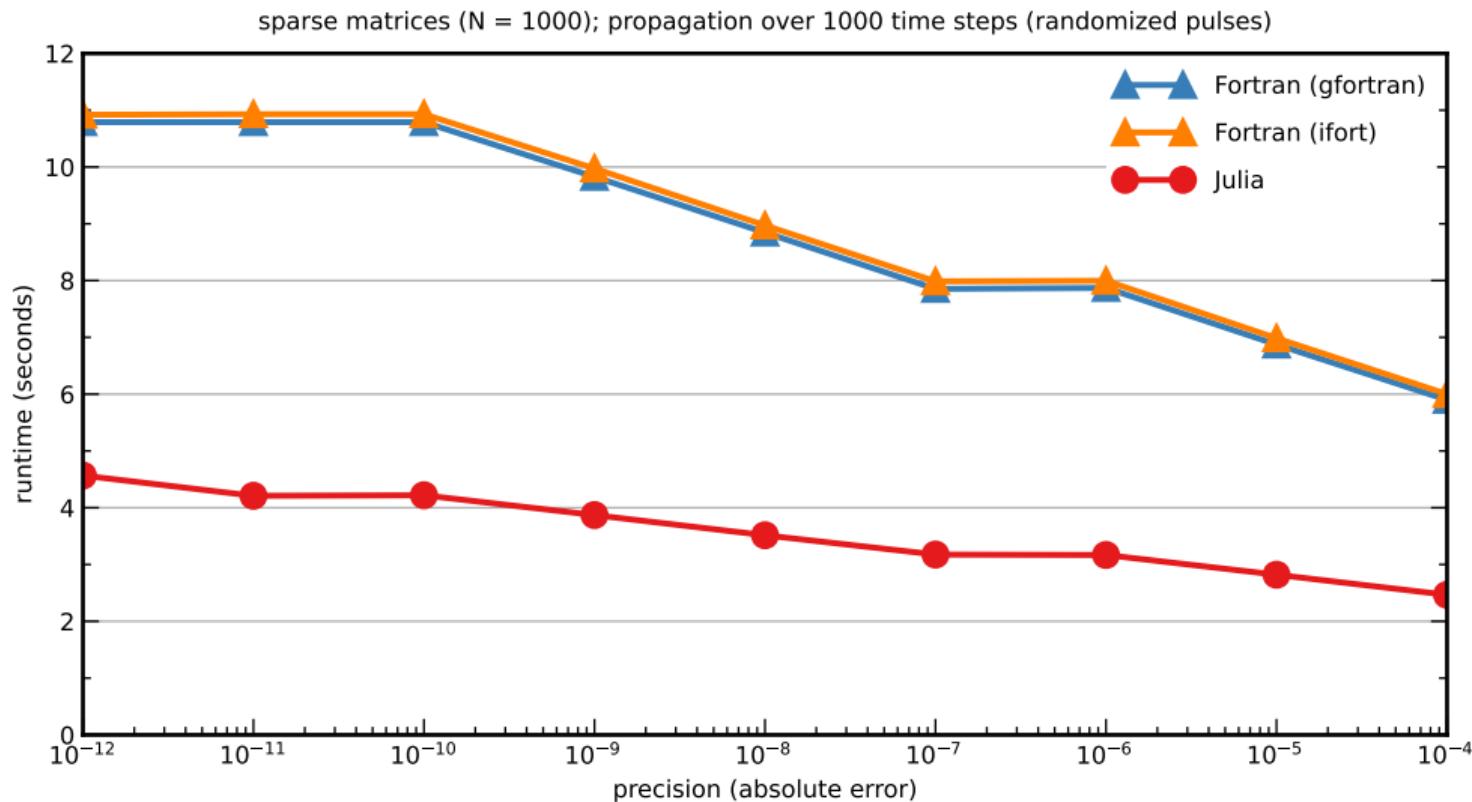


Performance

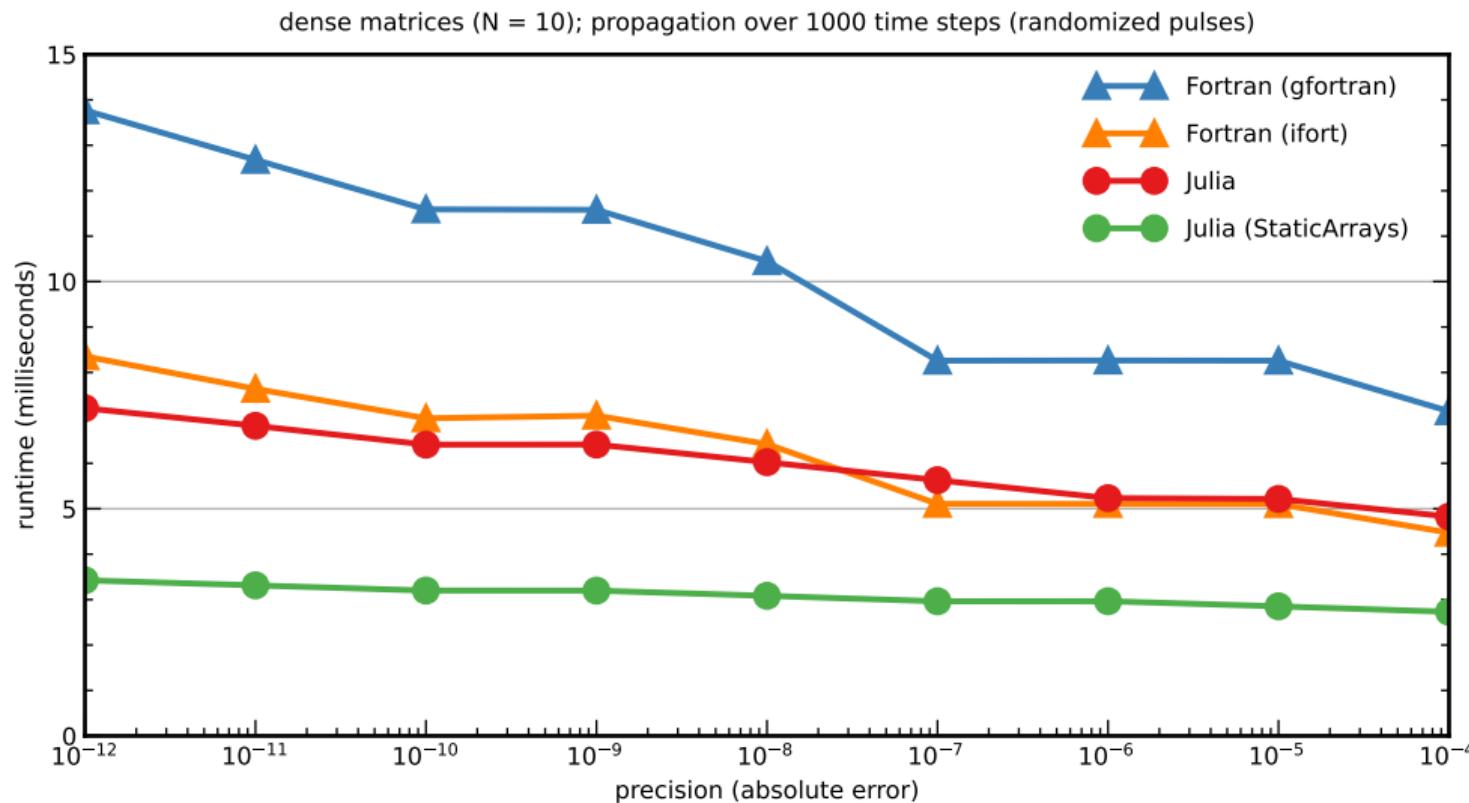
Benchmark for Chebychev Propagator – Large Hilbert Space



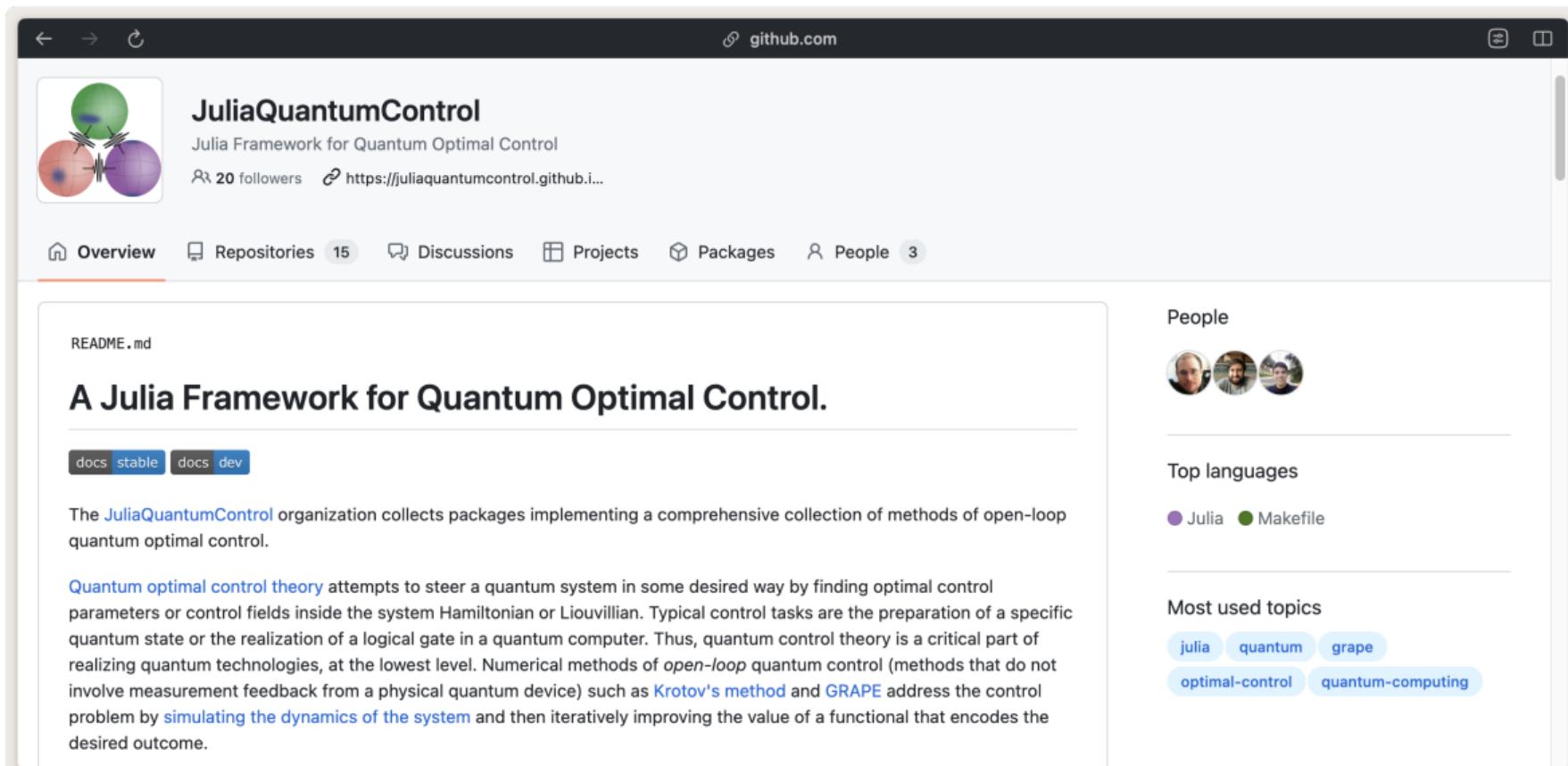
Benchmark for Chebychev Propagator – Large Hilbert Space (sparse)



Benchmark for Chebychev Propagator – Small Hilbert Space



Conclusions



The screenshot shows the GitHub repository page for **JuliaQuantumControl**. The page includes the repository icon (three spheres in green, red, and purple), the repository name, a brief description, follower count, and a link to the repository. Below the header, there are navigation links for Overview, Repositories (15), Discussions, Projects, Packages, and People (3). The main content area displays the README.md file, which contains the title "A Julia Framework for Quantum Optimal Control.", build status badges for docs stable and docs dev, and a paragraph about the organization's purpose. To the right, there are sections for People (showing three profile icons) and Top languages (Julia and Makefile). At the bottom, there is a section for Most used topics (julia, quantum, grape, optimal-control, quantum-computing).

JuliaQuantumControl

Julia Framework for Quantum Optimal Control

20 followers <https://juliaquantumcontrol.github.io...>

Overview Repositories 15 Discussions Projects Packages People 3

README.md

A Julia Framework for Quantum Optimal Control.

docs stable docs dev

The [JuliaQuantumControl](#) organization collects packages implementing a comprehensive collection of methods of open-loop quantum optimal control.

Quantum optimal control theory attempts to steer a quantum system in some desired way by finding optimal control parameters or control fields inside the system Hamiltonian or Liouvillian. Typical control tasks are the preparation of a specific quantum state or the realization of a logical gate in a quantum computer. Thus, quantum control theory is a critical part of realizing quantum technologies, at the lowest level. Numerical methods of *open-loop* quantum control (methods that do not involve measurement feedback from a physical quantum device) such as [Krotov's method](#) and [GRAPE](#) address the control problem by [simulating the dynamics of the system](#) and then iteratively improving the value of a functional that encodes the desired outcome.

People



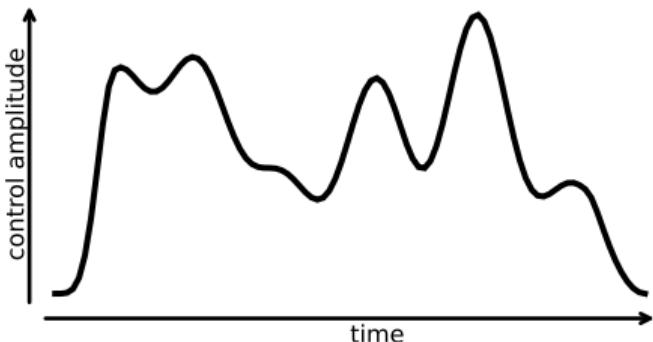
Top languages

Julia Makefile

Most used topics

julia quantum grape
optimal-control quantum-computing

Outlook



piecewise-constant pulses
⇒ parametrized continuous controls

$$\epsilon(t) = \epsilon(\{u_n\}, t)$$

- Adapt to experimental constraints on controls
- No PWC error: use DifferentialEquations as Propagator
- Specialized quantum control methods: CRAB, GROUP, GOAT, etc.
- But: local traps, controllability issues