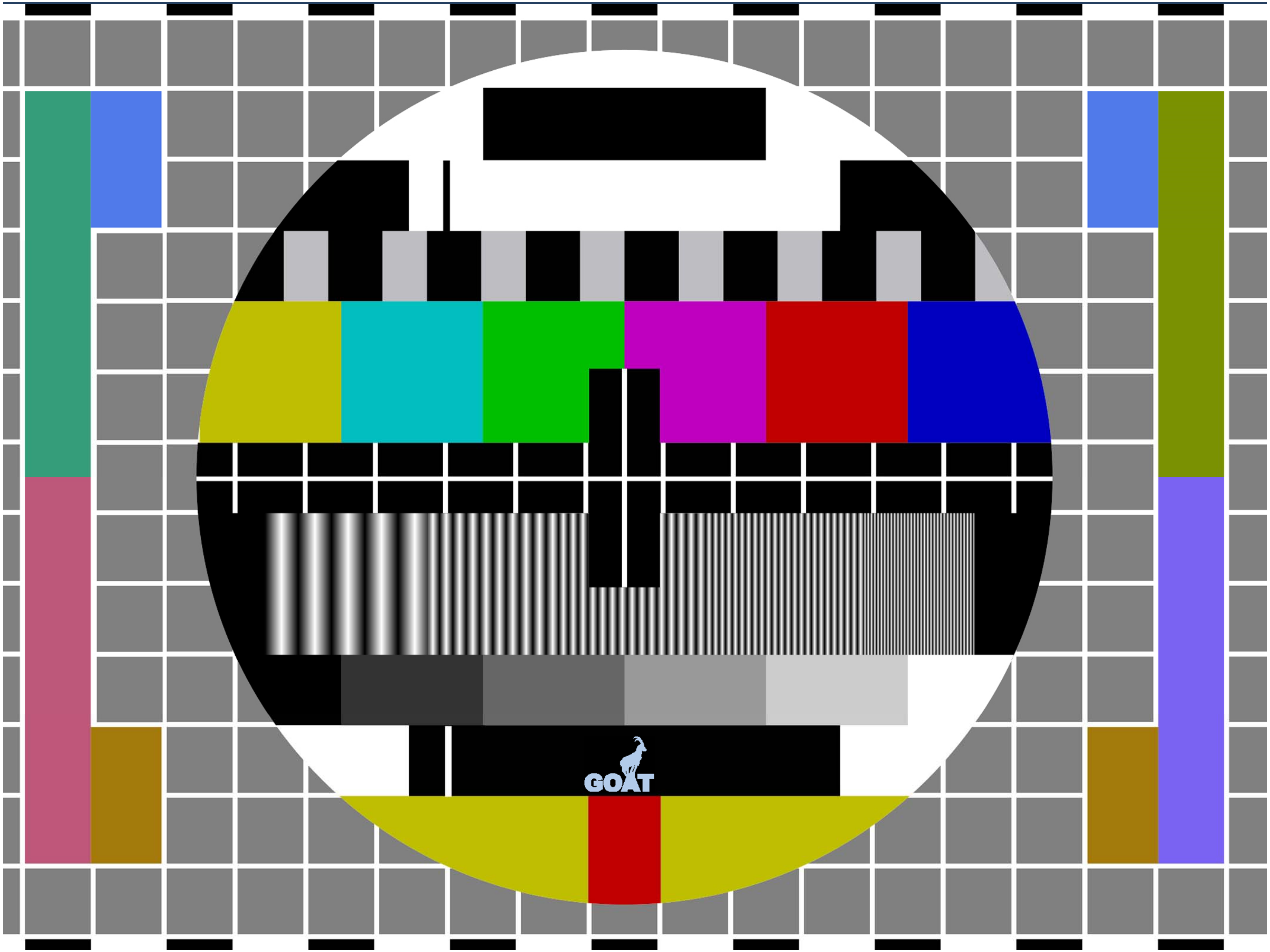

GOAT

UNIVERSITÄT DES SAARLANDES

Introduction to Quantum Optimal Control

Shai Machnes

S. J. Glaser, et al., *The European Physical Journal* D 69.12 (2015): 1-24

C. P. Koch, *Journal of Physics: Condensed Matter* 28.21 (2016): 213001

Overview

- What is Optimal Control
- Quantum Optimal Control
- Controllability
- Speed limits
- Avoiding subspaces
  - Adiabaticity
  - Shortcuts to Adiabaticity
- Optimization landscapes
  - Local traps
  - Dimensionality
- QOC Workflow
- Robustness
- Requirements from QOC
- QOC Dos and Don'ts
- QOC algorithms
  - CRAB
  - PMP
    - GRAPE
    - Krotov
  - GOAT
- Constraints
- Multi-goal optimization
- Example

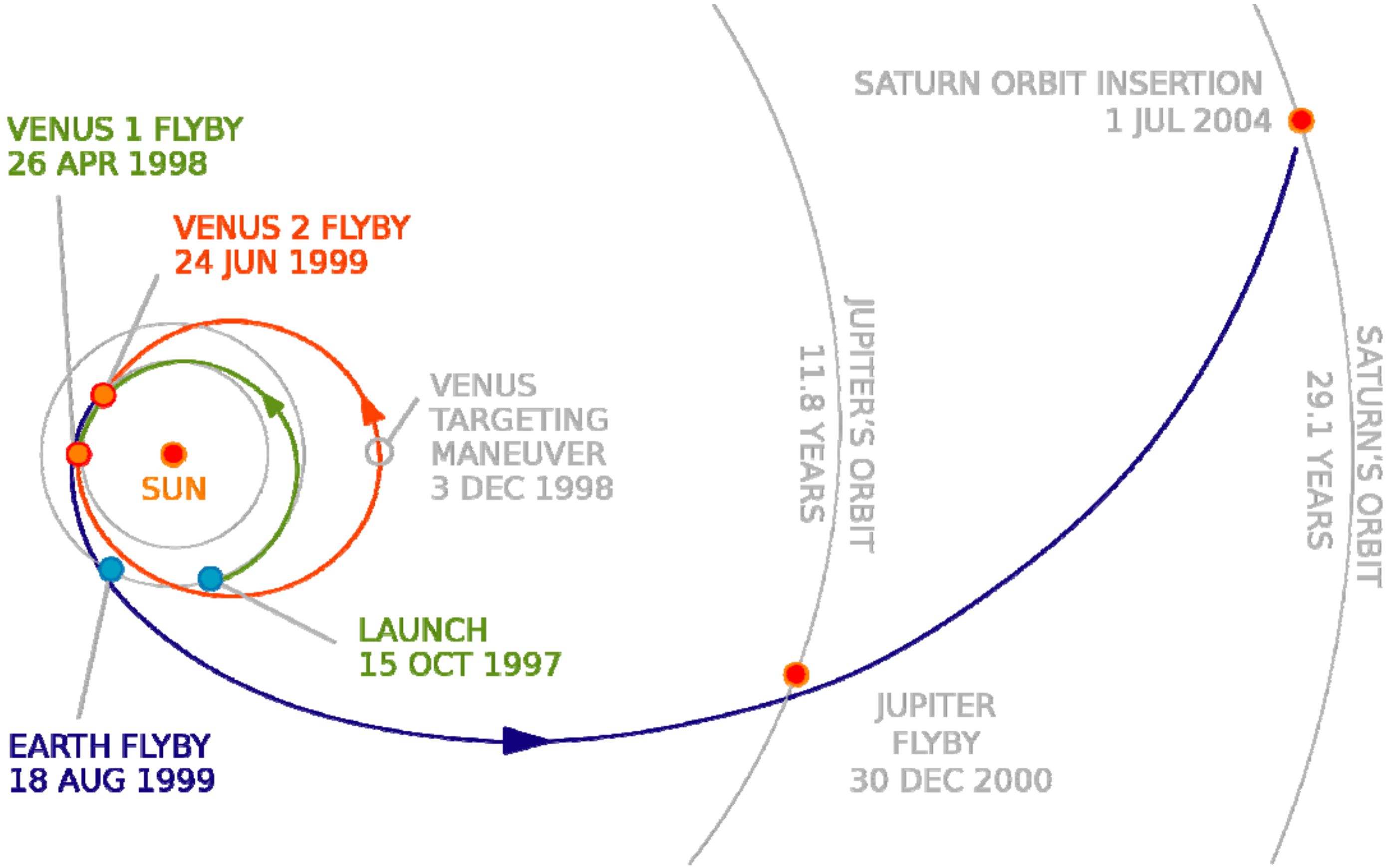
What is Optimal Control?

Congratulations !

You just saved 0.4 seconds

What is Optimal Control?

Reach Saturn, minimize fuel



Cassini Huygens trajectory [NASA / JPL]

What is Optimal Control?

Waiter race (1949)

Quantum Optimal Control

Given

$$H(t) = H_0 + \sum_{k=1}^{K} c_k(t) H_k$$

Find control fields

$$c_k(t)$$

such that we

- transform some initial state to some final state, or
- generate a unitary gate (i.e. rotation of states), or …

Quantum Optimal Control

Given $g(\bar{\alpha}) = 1 - \frac{1}{dim(U)} \left| U^{\dagger}_{goal} U(\bar{\alpha}, T) \right|$

$$U(\bar{\alpha}, T) = \mathbb{T} \exp\left(\int_0^T -\frac{i}{\hbar} H(\bar{\alpha}, t)\, dt \right)$$

$$H(\bar{\alpha}, t) = H_0 + \sum_{k=1}^{K} c_k(\bar{\alpha}, t) H_k$$

$$c_k(\bar{\alpha}, t) = \sum_{j=1}^{m} A_{k,m} \exp\left(-(t - \tau_{k,m})^2 / \sigma^2_{k,m} \right)$$

$$\bar{\alpha} = \{A_{k,m}, \tau_{k,m}, \sigma_{k,m}\}_{k=1\ldots K, j=1\ldots m}$$

$$\left| A_{k,m} \right| \leq 500\text{MHz}$$

Find $\bar{\alpha}$ such that $g(\bar{\alpha})$ is minimal

Controllability

- Can we implement any gate we wish?
- Can we implement a specific gate?

- Coherent dynamics: Closure of H-s:

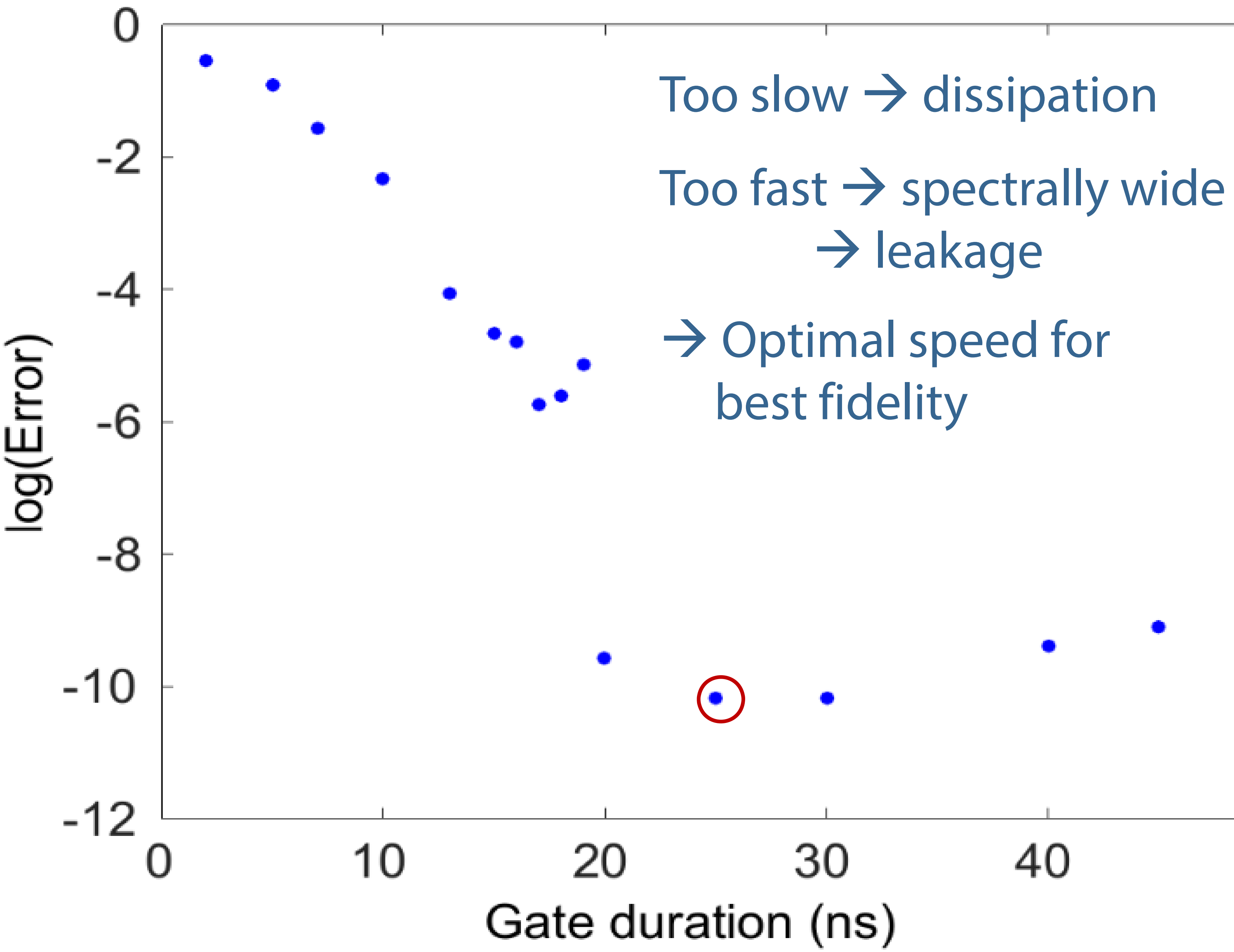
$$\left\{H_j,\ \left[H_j, H_k\right],\ \left[H_j, [H_k, H_m]\right], \ldots\right\}_{j,k,m,\ldots=0\ldots K}$$

$$e^A e^B = e^{A+B+\frac{1}{2}[A,B]+\frac{1}{12}([A,[A,B]]+[[A,B],B])+\ldots}$$

- Open systems: open question

Quantum Speed Limit

- How fast can we rotate state to state?
  Gate = multiple concurrent rotations
- Bounded for time indep systems:
  Mandelstam-Tamm, Margolus-Levitin
- Open systems: open question
- Controllable without drift → no speed limit
- Lindblad ops not controllable → speed limits

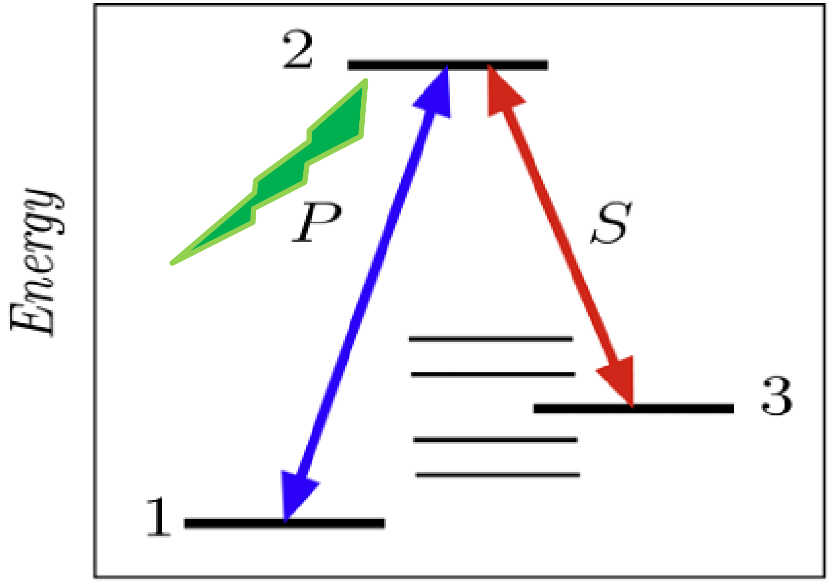


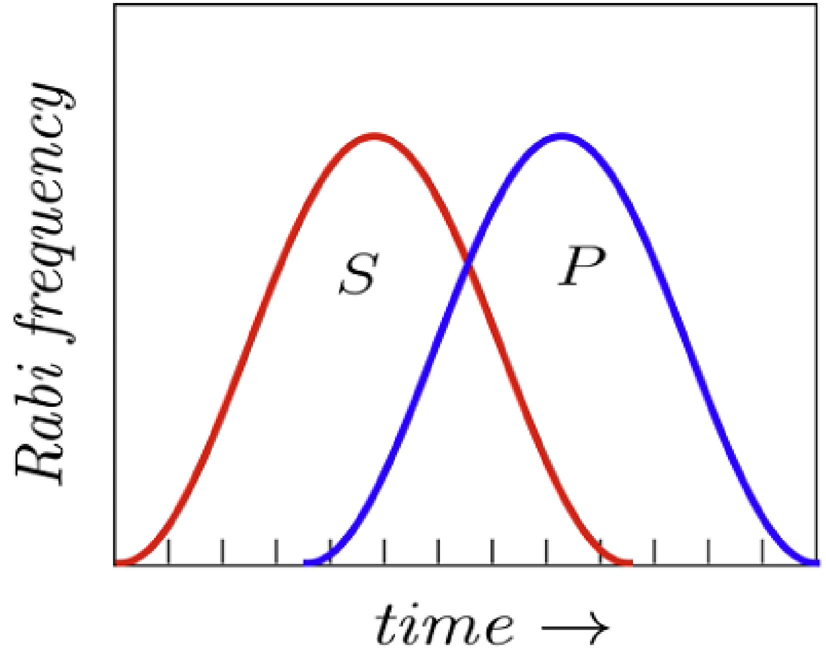
Too slow → dissipation
Too fast → spectrally wide
→ leakage
→ Optimal speed for
best fidelity
log(Error)
Gate duration (ns)
0
-2
-4
-6
-8
-10
-12
0
10
20
30
40
50

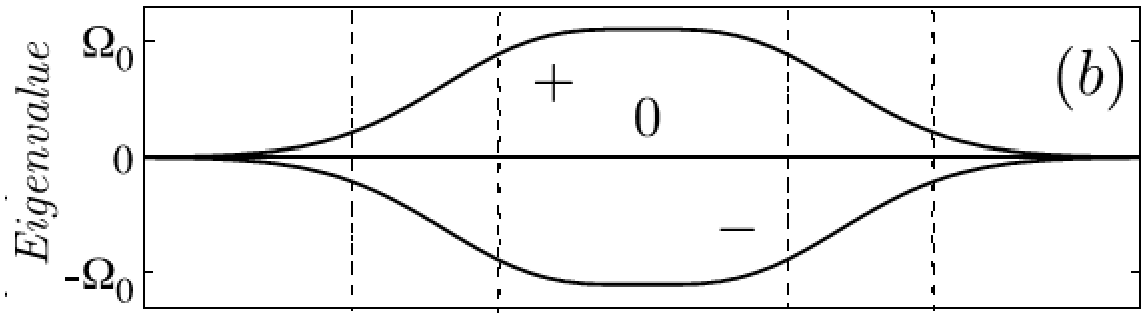
- Poorly characterized
- Dissipative levels

Adiabaticity

STIRAP – Stimulated Raman/Rapid Adiabatic Passage





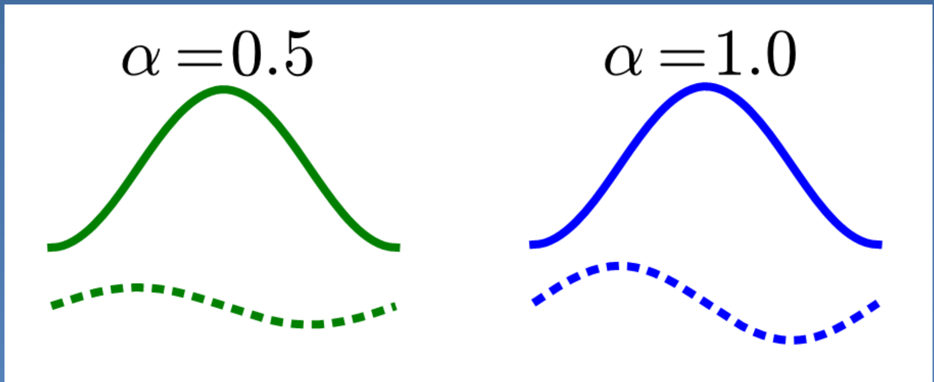


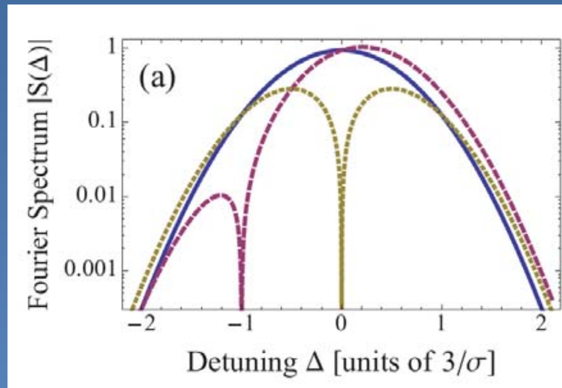
Bergmann, Vitanov and Shore - JCP 142 170901 (2015)

Adiabaticity

- Avoid a subspace (e.g. leaky state)
  - Remain on dark sub-manifolds of the driven system
  - Slow – remain on momentary eigenmodes

- DRAG: Avoid certain frequencies



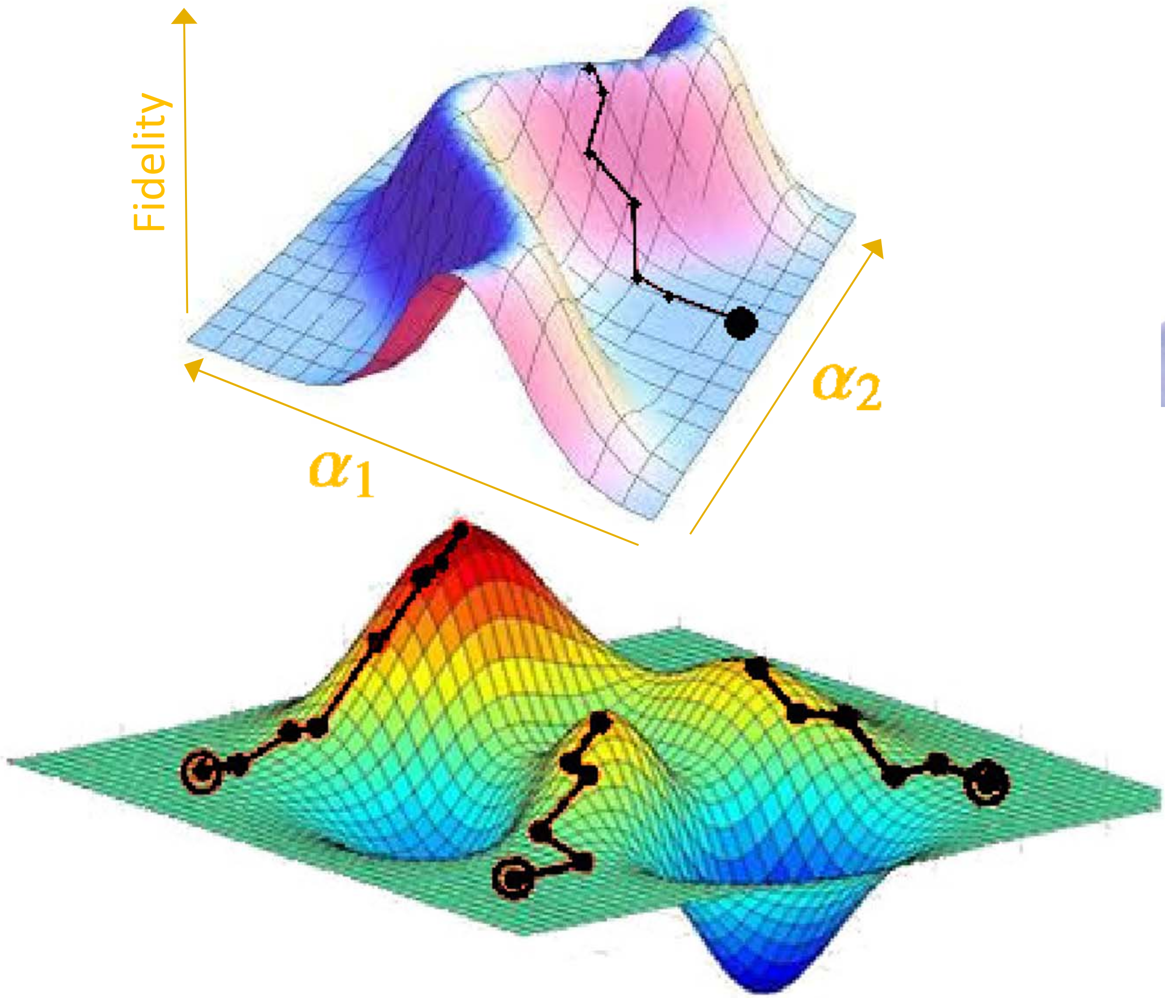


Motzoi, Gambetta, Rebentrost and Wilhelm - PRL 103 110501 (2009)

Shortcuts to Adiabaticity

- Start and end within a subspace
- During the pulse – go wider

Optimization Landscapes




Herschel Rabitz

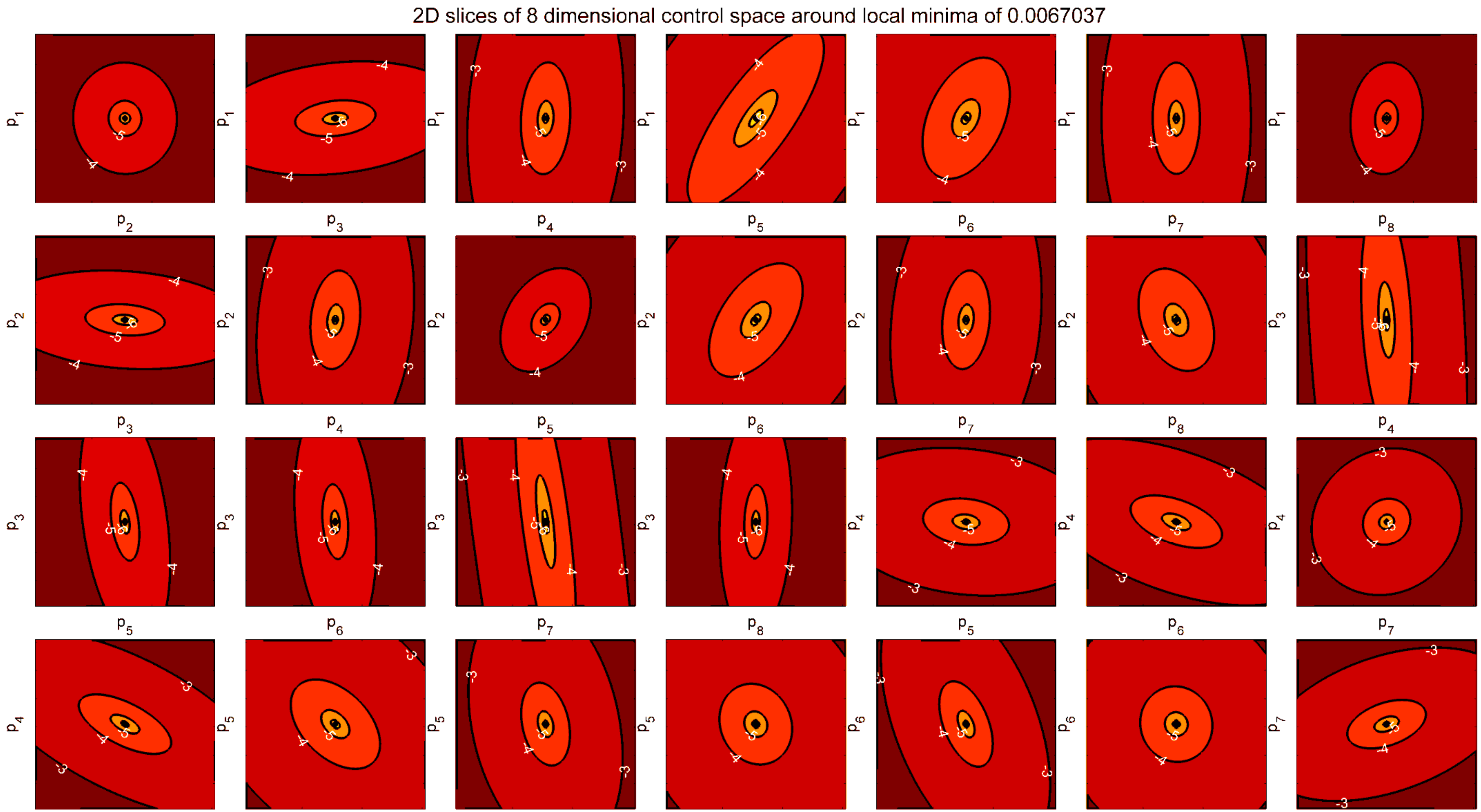
Easy


David Tannor

Hard

B. Russell and H. Rabitz - arXiv 1611.09406 (2016)

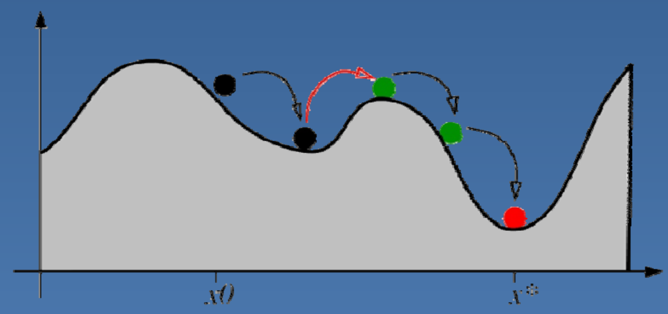
Constrains → Local traps



Strategies for handling local minima

- Repeat search many times, starting at different random points.

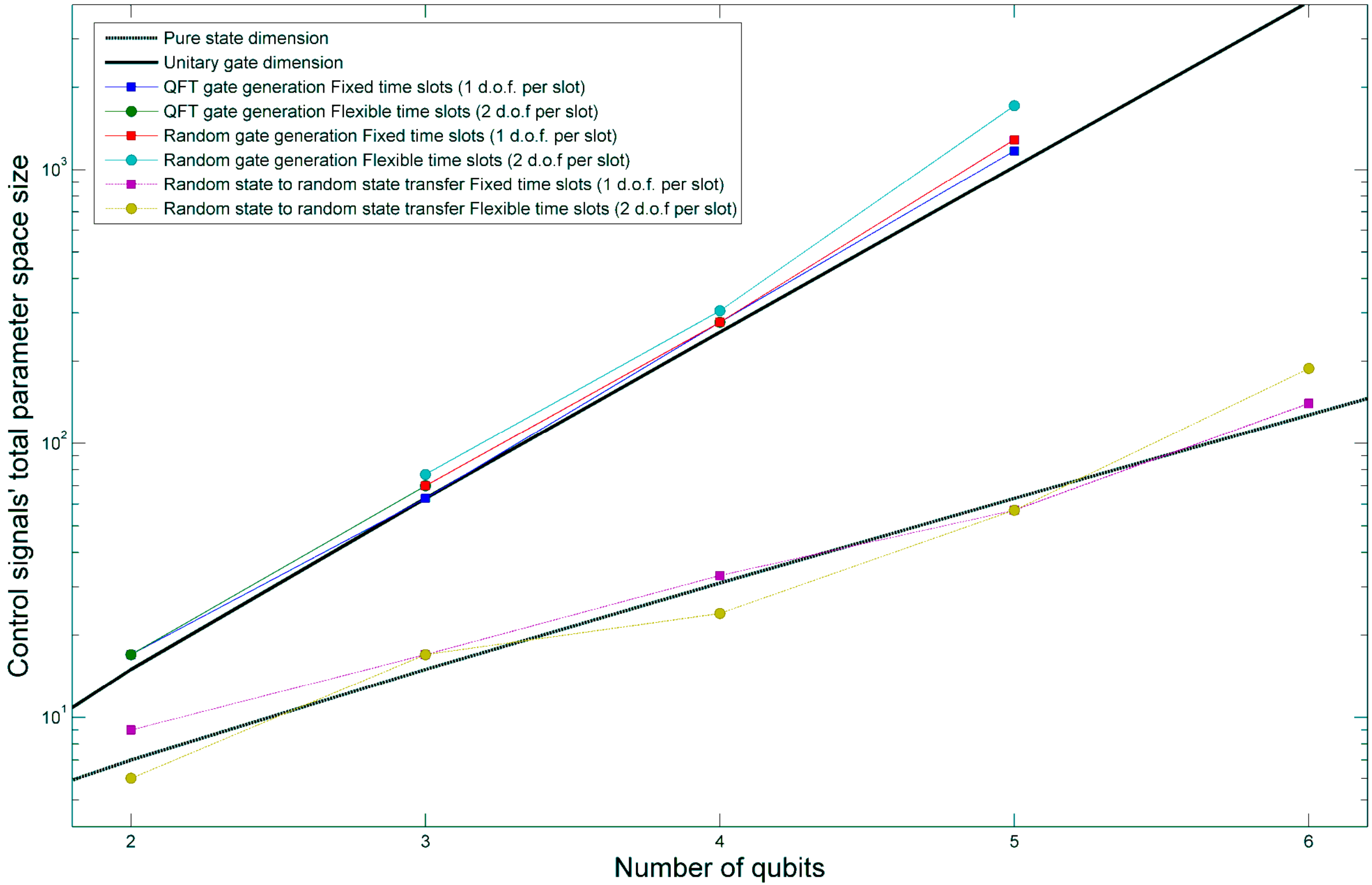
- Use appropriate algorithms
  - Simulated annealing
  - Stochastic tunneling
  - Parallel tempering
  - Genetic algorithms

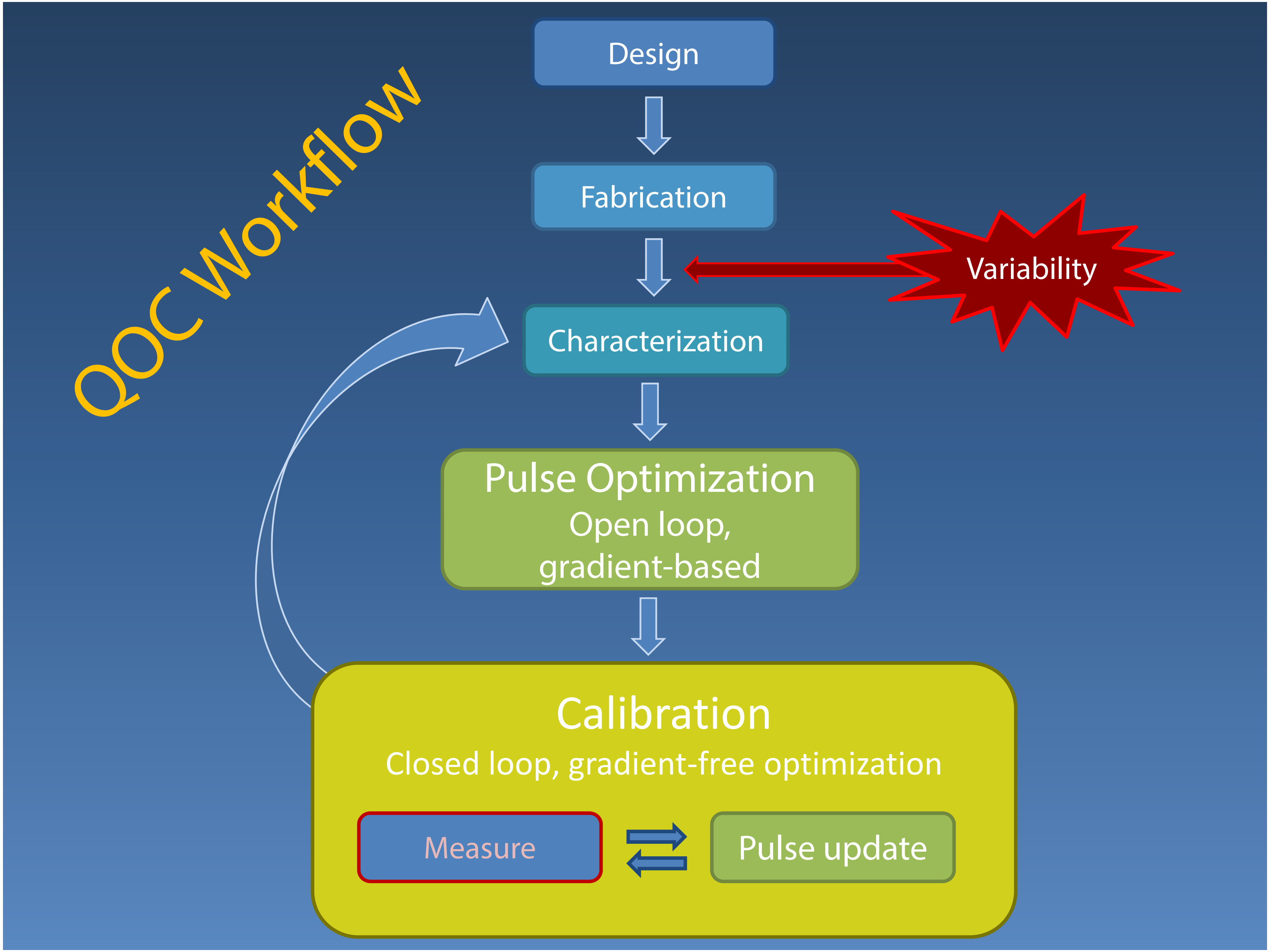


- Use GOAT for
  multi-goal, constrained, optimization

Number of params = Hilbert space size

Dimension of search space




QOC Workflow
Design
Fabrication
Variability
Characterization
Pulse Optimization
Open loop,
gradient-based
Calibration
Closed loop, gradient-free optimization
Measure
Pulse update

Requirements from QOC

- Optimize state transfer, gate generation, etc.
- Unitary, Lindblad, non-Markovian, etc.

- Flexible
  - Any control ansatz and any constraints
  - Filters (Gaussian, band-pass, etc)
  - Multi-goal
  - more

- Quick
- Accurate

Constraints from Experiment and Ansatz

- Experimentally achievable controls (given)
  - Search space must faithfully describe the freedoms / limitations of the experiment.
  - Support for non-linear filters (bandpass, etc).
  - Every parameter is constrained
  - Example: AWG + lowpass filter + IQ mixer
- Control ansatz (chosen)
  - Fourier, Erf, Hann, Gaussian, PWC, etc.
  - Calibration → Use only a few components / pulses

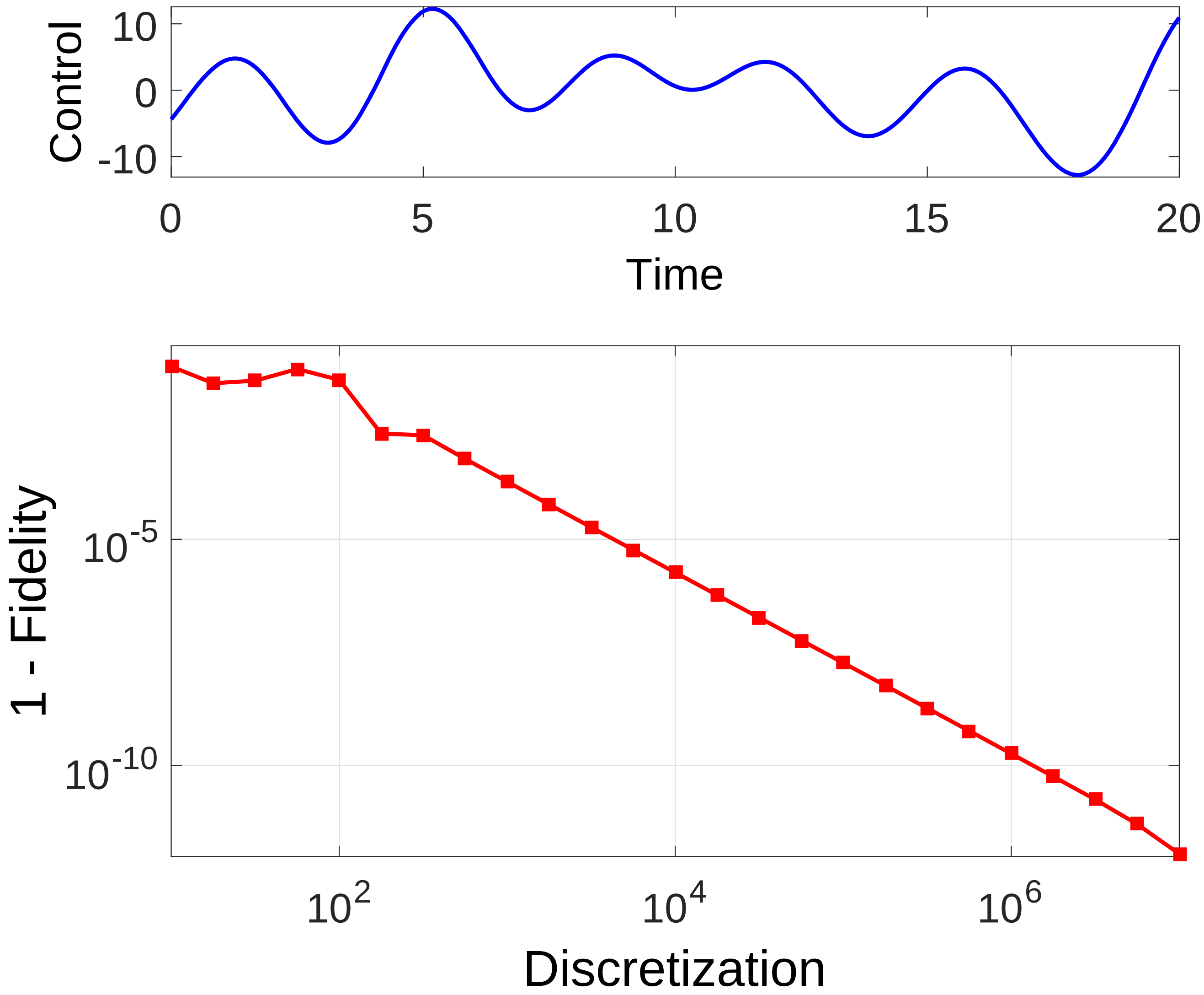
Robustness / Time-scales

- Static = Characterization gaps
  - Fabrication variability
  - Over-simplified model
  - Metrology / tomography gaps
- Slow = Drifts
- Fast = Noise (in controls/system) – Robust pulses
  - Ensemble optimization
  - Multi-goal: Invariability to first-order change of model parameters

QOC– Dos and Don'ts

- Don't
  - Piece-wise-constant (PWC) is a poor approximation for bandwidth-limited controls.
- Do
  - Gradient based optimization is much faster
  - Use analytic controls
    - You only need a few parameters
    - You only want a few parameters
    - Flexible: ansatz and constraints

PWC is a poor approx. of smooth controls



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    - Flexible: ansatz and constraints

QOC Algorithms

- Direct methods - No gradient information
- Variational methods - Gradient based

QOC Algorithms – Direct

Direct methods - No gradient information

- Pro
  - Only require black-box goal function evaluators
    - Closed loop calibration
    - Can use tensor networks propagators (for many-body problems)
  - Relatively simple

- Con
  - Slow
  - Very slow in high dimension search spaces

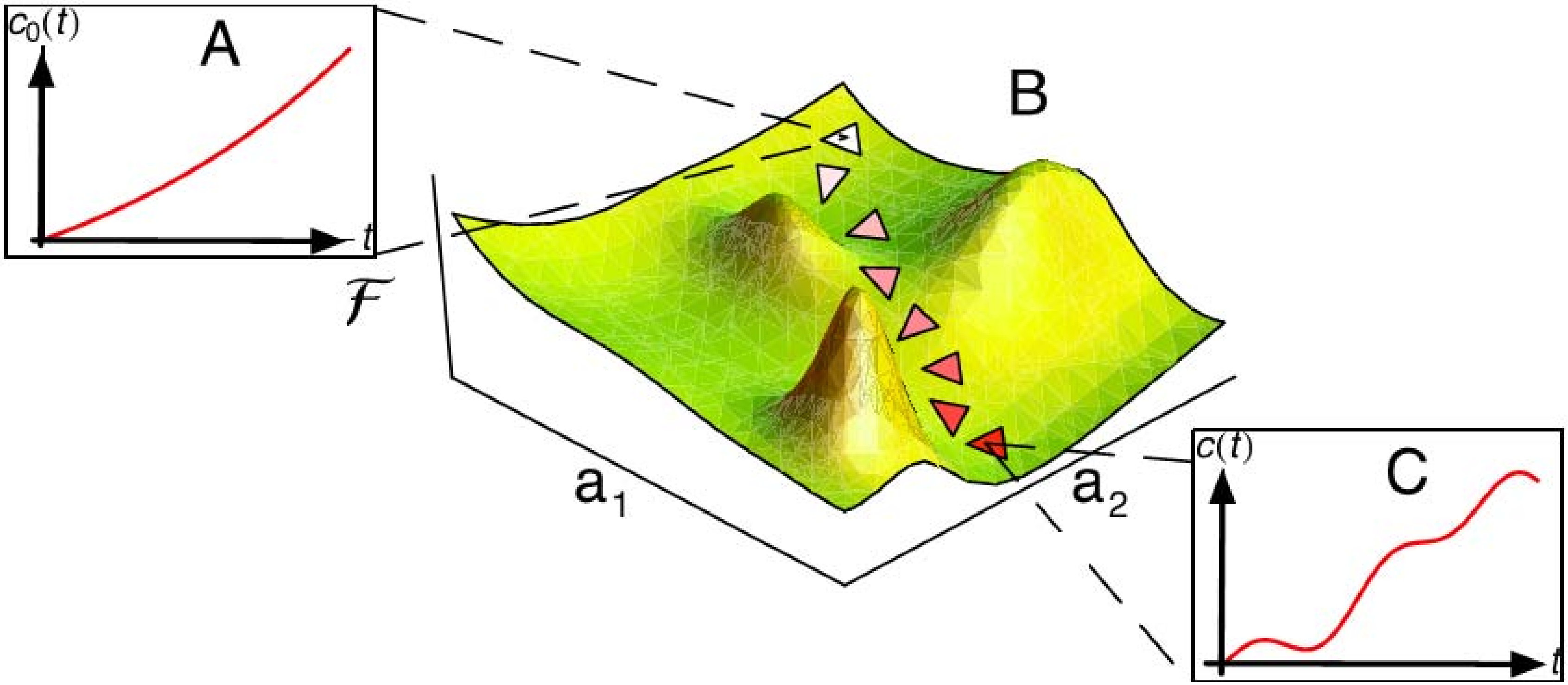
QOC Algorithms - Direct

Direct methods - No gradient information

- Deterministic - CRAB:
  - Simplex search (e.g. Nelder-Mead)
  - Arbitrary analytic controls (normally Fourier basis)
  - Deterministic

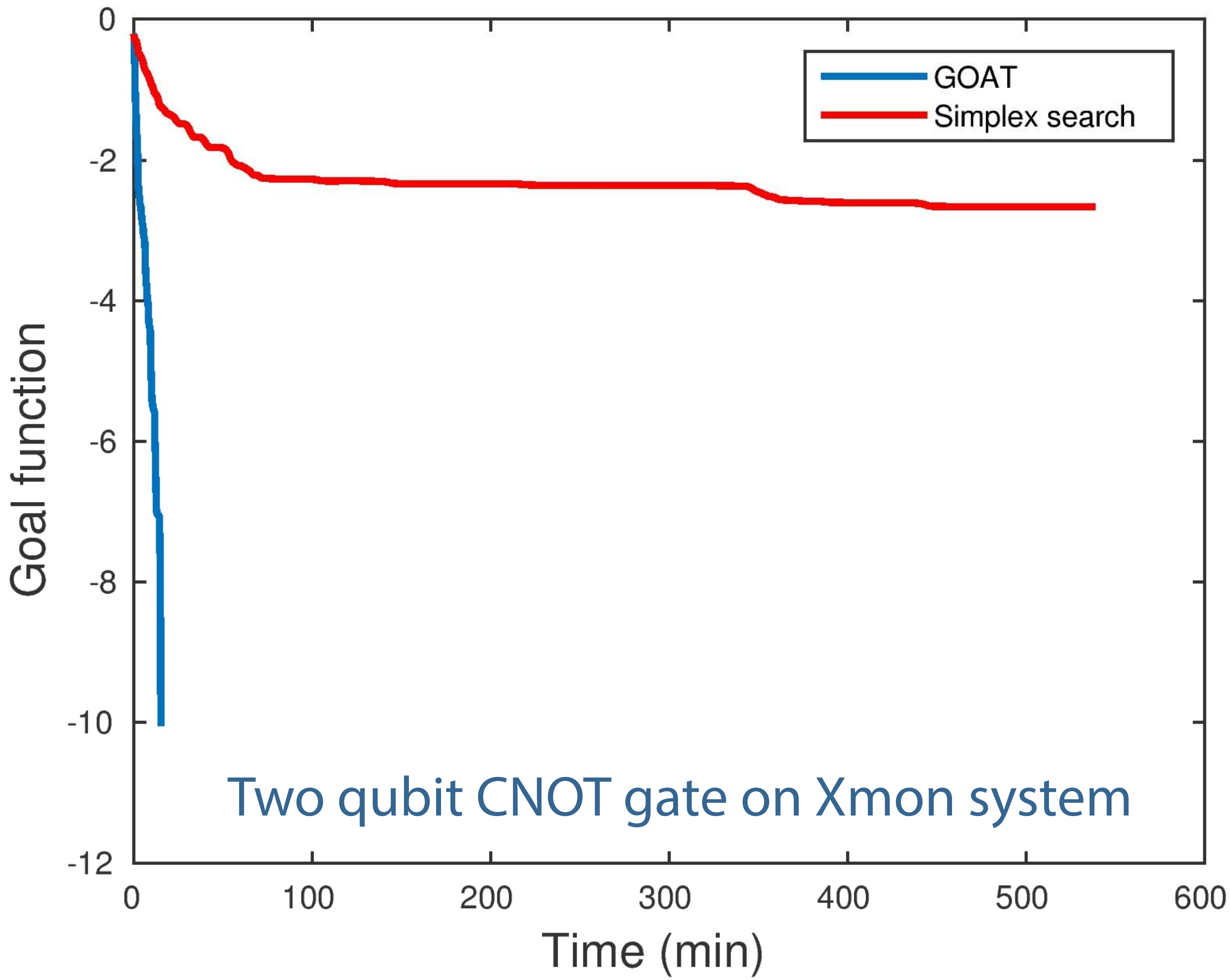
T. Caneva, T. Calarco, and S. Montangero. Phys. Rev. A, 84(2):022326, 2004
P. Doria, T. Calarco, and S. Montangero. Phys. Rev. Lett., 106:190501 (2011)

CRAB



Doria, Calarco and Montangero - PRL 106 190501 (2011)

Gradients allow faster search



QOC Algorithms - Direct

Direct methods - No gradient information

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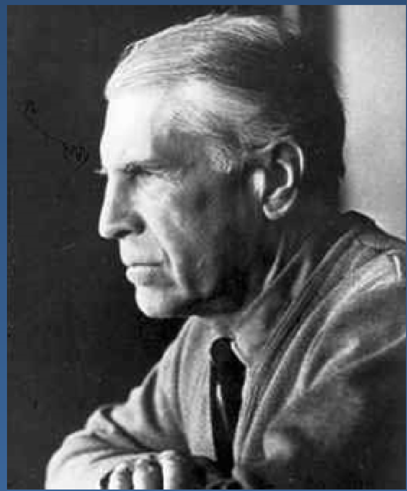
  P. Doria, T. Calarco, and S. Montangero. Phys. Rev. Lett., 106:190501 (2011)

- Stochastic
  - CMA-ES (Covariance Matrix Adaptation Evolution Strategy)
  - NES (Natural Evolution Strategy)
  - Genetic algorithms, Particle swarms

QOC Algorithms - Variational

Variational methods- Gradient based



- Pro
  - Fast
  - Can handle large parameter spaces
  - Optional: Monotonic convergence
- Con
  - Requires gradient of goal w.r.t. control params
  - Usually based on the Pontryagin Max. Principle (PMP)
    - Non-trivial mathematically
    - Requires backwards-in-time propagation of an adjoint state

L. S. Pontryagin, V. G. Bol'tanskii, R. S. Gamkre-lidze, and E. F. Mischenko. The Mathematical Theory of Optimal Processes. Pergamon Press, New York (1964)

Pontryagin Max. Principle (PMP)

Goal $J = \left|\langle\psi(T)|\psi_{\text{goal}}\rangle\right|$

Enforce $\left(i\hbar\frac{\partial}{\partial t} - H(c(t))\right)|\psi(t)\rangle = 0$

Lagrange Multiplier $\left\langle\chi(t)\right| i\hbar\frac{\partial}{\partial t} - H(c(t))\left|\psi(t)\right\rangle$

Functional $\tilde{J} = J + \int_0^T \left\langle\chi(t)\right| i\hbar\frac{\partial}{\partial t} - H(c(t))\left|\psi(t)\right\rangle$

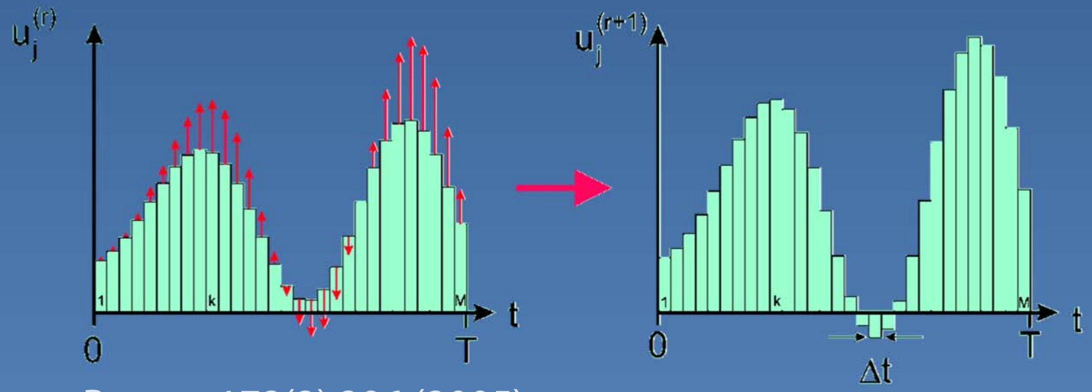
E.o.M for $|\psi(t)\rangle$ forward in time, starting from $|\psi(0)\rangle = |\psi_{\text{init}}\rangle$

E.o.M for $|\chi(t)\rangle$ backward in time, starting from $|\chi(T)\rangle = \left|\psi_{\text{goal}}\right\rangle$

QOC Algorithms - GRAPE

Variational methods- Gradient based

- GRAPE
  - PWC parametrization of control fields
  - Fast gradient-based optimization (L-BFGS)
  - Arbitrary ansatz, constraints, filters: non-trivial



N. Khaneja, et al., J. Magn. Reson., 172(2) 296 (2005)

P. de Fouquieres, S. G. Schirmer, S. J. Glaser, and I. Kuprov, J. Magn. Reson., 212(2) 412 (2011)

S. Machnes, et. al.. PRA, 84 022305 (2011)

QOC Algorithms - Krotov

Variational methods- Gradient based

- Krotov
  - Based on PMP (i.e. required backwards propagation)
  - Mathematically non-trivial
  - Flexible - both PWC and analytic ansatz
  - Monotonic convergence

V. F. Krotov, Global Methods in Optimal Control Theory. Dekker, New York, 1996

D. M. Reich, M. Ndong, and C. P. Koch, JCP 136, 104103 (2012)

R. Eitan, M. Mundt, and D. J. Tannor, Phys. Rev. A, 83(5):053426, 2011

New QOC Algorithm: GOAT

- Gradient based (fast)
- Extremely flexible
  - Any ansatz
  - Any set of constraints
  - Filters (e.g. lowpass)
  - Multi-goal
  - more
- Not based on the PMP – no backpropagation
- SIMPLE

arXiv 1507.04261

Typical optimal control setup

$$g\left(\bar{\alpha}\right) = 1 - \frac{1}{dim(U)} \left| U^{\dagger}_{goal} U\left(\bar{\alpha}, T\right) \right|$$

$$U\left(\bar{\alpha}, T\right) = \mathbb{T} \exp\left(\int_0^T -\frac{i}{\hbar} H\left(\bar{\alpha}, t\right) dt \right)$$

$$H\left(\bar{\alpha}, t\right) = H_0 + \sum_{k=1}^{K} c_k\left(\bar{\alpha}, t\right) H_k$$

$$c_k\left(\bar{\alpha}, t\right) = \sum_{j=1}^{m} A_{k,m} \exp\left(-\left(t - \tau_{k,m}\right)^2 / \sigma^2_{k,m} \right)$$

$$\bar{\alpha} = \left\{ A_{k,m}, \tau_{k,m}, \sigma_{k,m} \right\}_{k=1...K, j=1...m}$$

Find $\partial_{\bar{\alpha}} g\left(\bar{\alpha}\right)$ and follow the gradient.

Deriving GOAT (very simple)

$$g(\bar{\alpha}) = 1 - \frac{1}{dim(U)} \left| U^{\dagger}_{goal} U(\bar{\alpha}, T) \right|$$

$$\partial_{\bar{\alpha}} g(\bar{\alpha}) = -real\left(\frac{g^*}{|g|} \frac{1}{dim(U)} Tr\left(U^{\dagger}_{goal}\, \partial_{\bar{\alpha}} U(\bar{\alpha}, t)\right)\right)$$

$$g = Tr\left(U^{\dagger}_{goal} U(\bar{\alpha}, t)\right)$$

$$\partial_{\bar{\alpha}} U(\bar{\alpha}, t) = ?$$

$\partial_{\bar{\alpha}} U(\bar{\alpha}, t)$ via modified Schrödinger

$$\partial_t U = -\frac{i}{\hbar} H U$$

$$\partial_{\bar{\alpha}} \partial_t U = -\frac{i}{\hbar} \left(\left(\partial_{\bar{\alpha}} H \right) U + H \partial_{\bar{\alpha}} U \right)$$

$\partial_{\bar{\alpha}} U(\bar{\alpha}, t)$ via modified Schrödinger

$$\partial_t U = -\frac{i}{\hbar} H U$$

$$\partial_t \partial_{\bar{\alpha}} U = -\frac{i}{\hbar}\left((\partial_{\bar{\alpha}} H) U + H \partial_{\bar{\alpha}} U\right)$$

$$\partial_t \begin{pmatrix} U \\ \partial_{\bar{\alpha}} U \end{pmatrix} = -\frac{i}{\hbar} \begin{pmatrix} H & 0 \\ \partial_{\bar{\alpha}} H & H \end{pmatrix} \begin{pmatrix} U \\ \partial_{\bar{\alpha}} U \end{pmatrix}$$

This is the GOAT core idea

Deriving GOAT (very simple)

$$\partial_t \begin{pmatrix} U \\ \partial_{\bar{\alpha}} U \end{pmatrix} = -\frac{i}{\hbar} \begin{pmatrix} H & 0 \\ \boxed{\partial_{\bar{\alpha}} H} & H \end{pmatrix} \begin{pmatrix} U \\ \partial_{\bar{\alpha}} U \end{pmatrix}$$

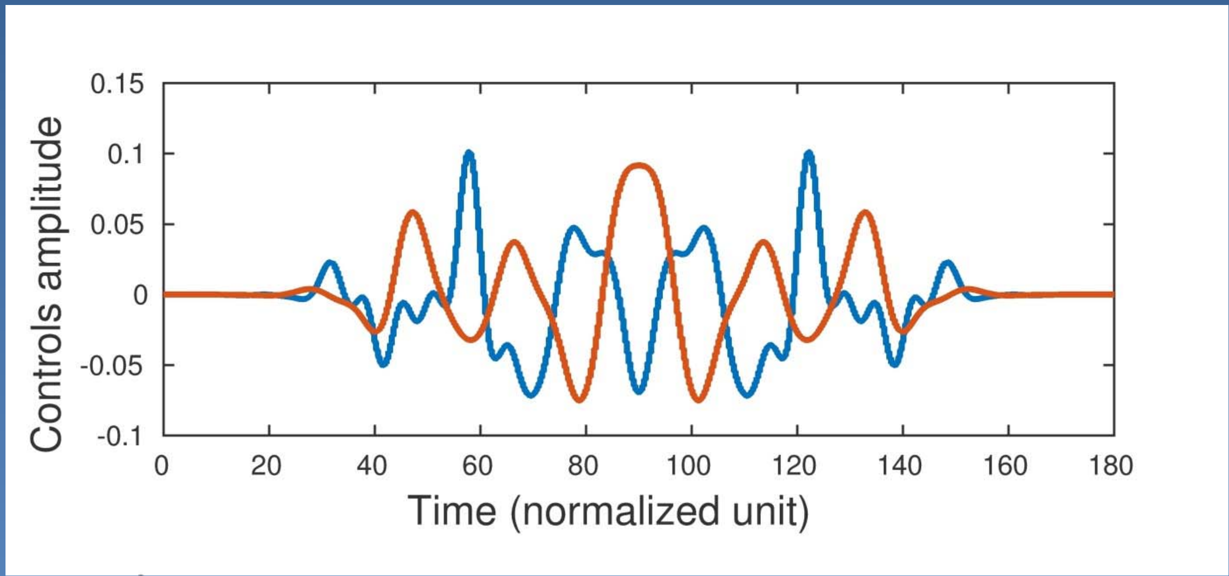
$$H(\bar{\alpha}, t) = H_0 + \sum_{k=1}^{K} c_k(\bar{\alpha}, t) H_k$$

$$\partial_{\bar{\alpha}} H(\bar{\alpha}, t) = \sum_{k=1}^{K} \partial_{\bar{\alpha}} c_k(\bar{\alpha}, t) H_k$$

Constraints?

$$c_k(t) = Ae^{-\frac{(t-\tau)^2}{\sigma^2}} \qquad A = 500\,\text{MHz}\ \frac{\sin(p)+1}{2}$$

Smooth start / finish $\quad c_k(\bar{\alpha}, t) \longrightarrow w(t)\, c_k(\bar{\alpha}, t)$



Local phase freedom

Task: Optimize a gate, ignoring either phases (global phase and local σ_z-s), or, for multi-spin gates, ignoring all local operations.

Example: Generate σ_x rotation up to a phase.

$$U = \begin{pmatrix} u_{00} & u_{01} \\ u_{10} & u_{11} \end{pmatrix} \qquad g = 1 - \left(|u_{01}|^2 + |u_{10}|^2\right)/2$$

General solution

Add the local operations explicitly to the parameter space

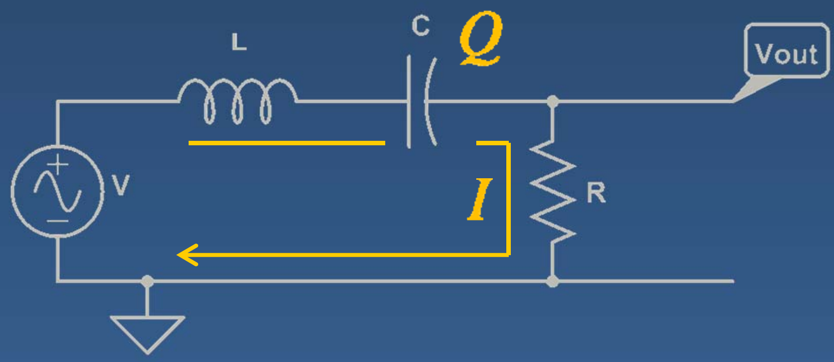
$$U_{\text{total}}\left(\theta_1, \theta_2, \bar{\alpha}, \theta_3, \theta_4, T\right) = e^{i\theta_4 \sigma_{z_b}} e^{i\theta_3 \sigma_{z_a}}\, U\left(\bar{\alpha}, T\right)\, e^{i\theta_2 \sigma_{z_b}} e^{i\theta_1 \sigma_{z_a}}$$

$$g\left(\theta_1, \theta_2, \bar{\alpha}, \theta_3, \theta_4\right) = 1 - \frac{1}{dim(U)} \left| U^{\dagger}_{goal} U_{\text{total}}\left(\ldots\right) \right|$$

Transfer functions

$$V_{in}(\bar{\alpha}, t)$$

$$H(\bar{\alpha}, t) = H_0 + R\, I(\bar{\alpha}, t)\, H_1$$



$$\partial_t Q = I \qquad \partial_t \partial_{\bar{\alpha}} Q = \partial_{\bar{\alpha}} I$$

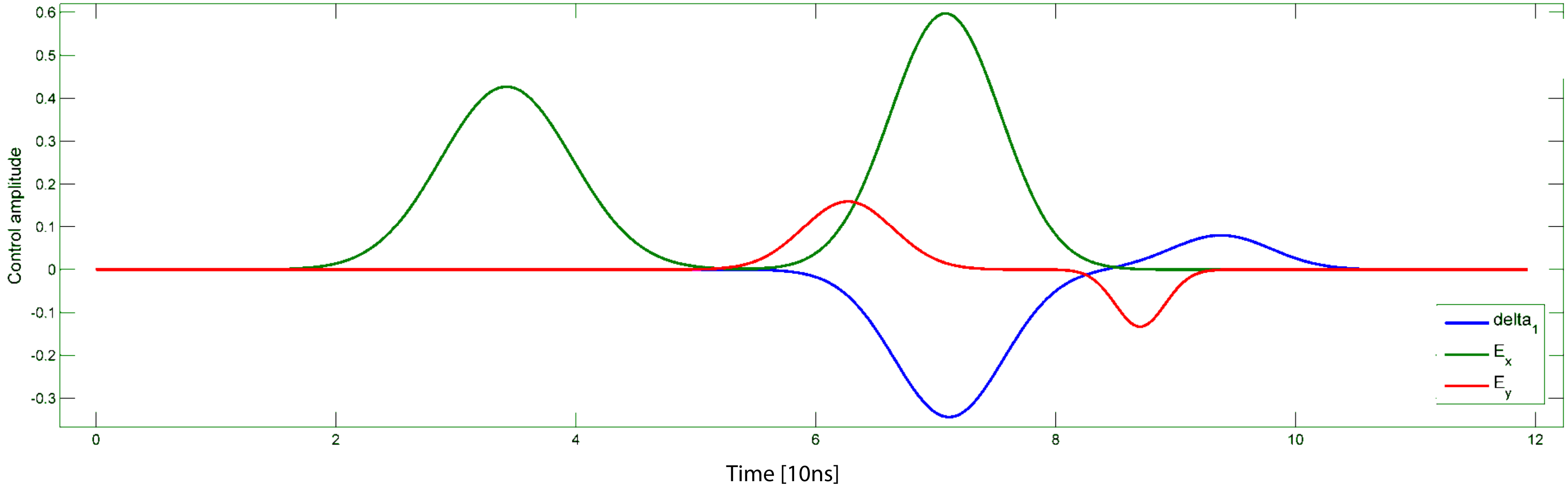
$$\partial_t I = V_{in} - \frac{1}{LC} Q - RI \quad \xRightarrow{\partial_{\bar{\alpha}}} \quad \partial_t \partial_{\bar{\alpha}} I = \partial_{\bar{\alpha}} V_{in} - \frac{1}{LC} \partial_{\bar{\alpha}} Q - R \partial_{\bar{\alpha}} I$$

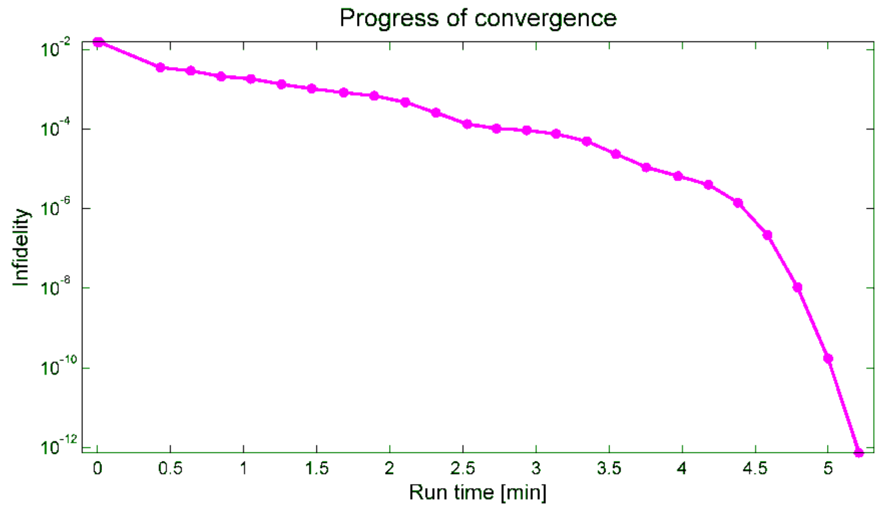
$$\partial_t U = -\frac{i}{\hbar} H U \qquad \partial_t \partial_{\bar{\alpha}} U = -\frac{i}{\hbar} \left((\partial_{\bar{\alpha}} H)\, U + H \partial_{\bar{\alpha}} U \right)$$

See also Hincks, Granade, Borneman, and Cory, *Phys. Rev. Applied* **4** 024012 (2015)

GOAT

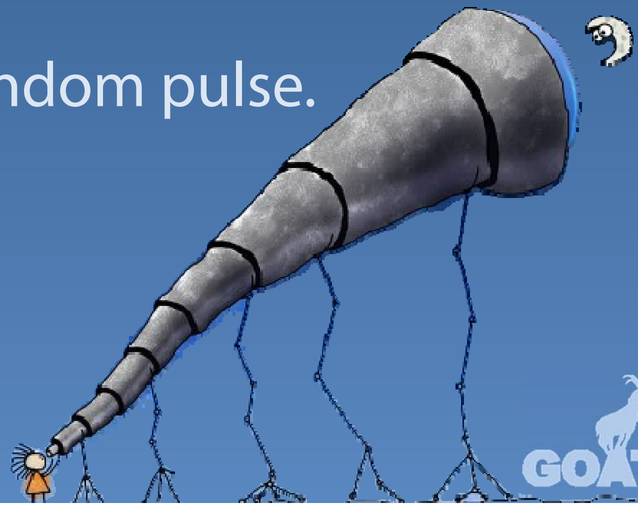
Example: Transmon gates





Searching for the shortest pulse

- Start with long pulse duration, random pulse.
- Optimize pulse until goal fidelity is reached.
- Shorten time repeatedly and re-optimize, until failure rate reaches 100%.
  - Each time start optimization with a random pulse.
  - Use pulse optimized for longer time as starting point (“telescoping”).



Searching for the shortest pulse

- We wish to optimize both fidelity and speed.
- Standard multi-objective approach:

$$g(\bar{\alpha}) = r\, g_1(\bar{\alpha}) + (1-r)\, g_2(\bar{\alpha})$$

and Pareto front.

- Speed interfering at high infidelity.
  Infidelity interfering after it is "good enough"

Searching for the speed limit with GOAT

don't care about speed

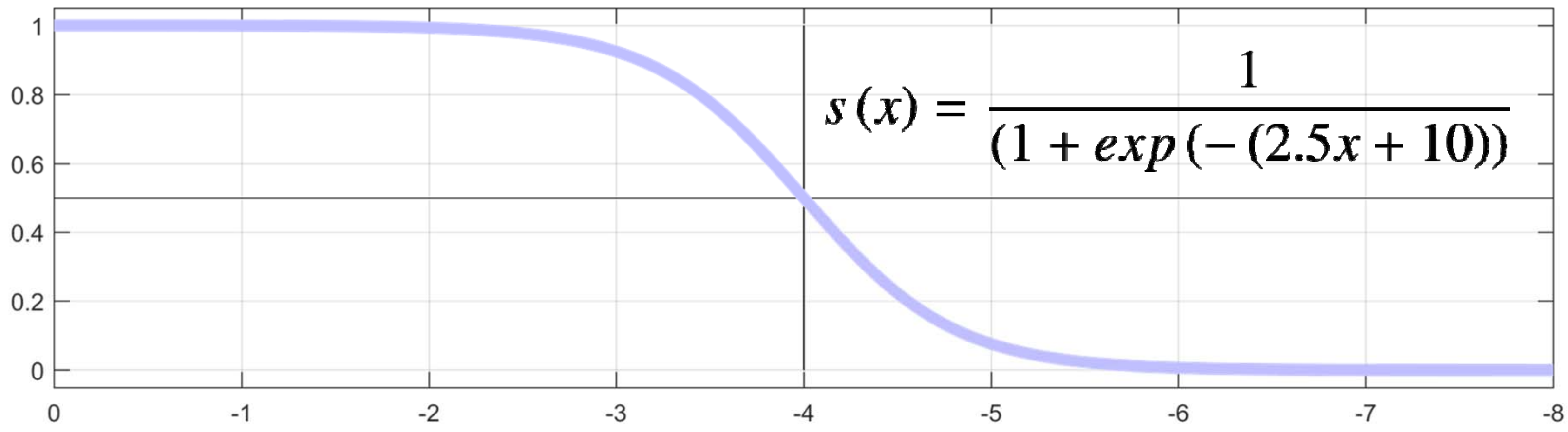
don't care about fidelity

Fidelity

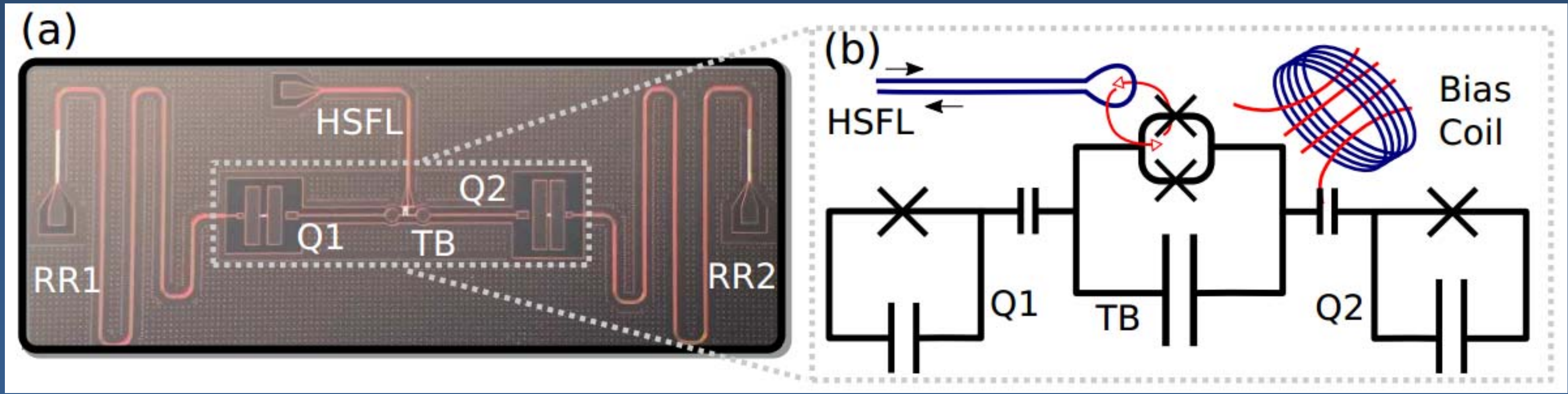
10^{-2} 10^{-6}

$$w = s\left(\log_{10}(g)\right)$$

$$\tilde{g} = w \log_{10}(g) + (1 - w)\, 8 \left(-1 + \frac{t}{T}\right)$$



IBM's Flux Tunable Coupler



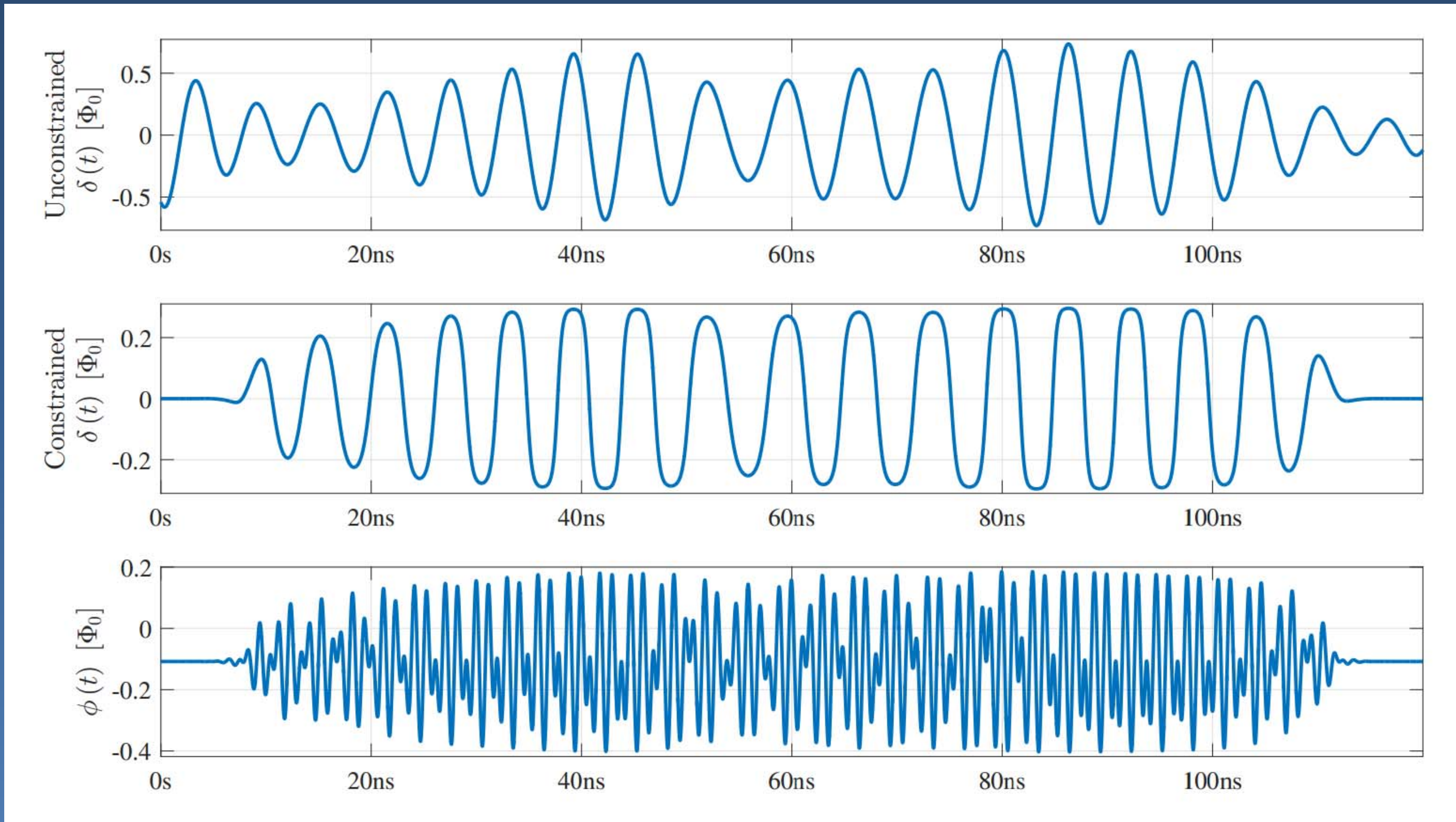
D. McKay, S. Filipp, A. Mezzacapo, E. Magesan, J. Chow, and J. Gambetta, arXiv 1604.0307 (2016)

$$H = \sum_k \omega_k a^\dagger a - \alpha \left|2\right\rangle \left\langle 2\right|_k + \omega_{TB}(\Phi) b^\dagger b + g_k (a_k^\dagger b + b^\dagger a_k)$$

$$\omega_{TB}(\Phi) = \omega_{\mathrm{TB},0} \sqrt{|\cos(\pi\Phi/\Phi_0)|}$$

$$\Phi = \Theta + \delta(t)\cos(\omega_\Phi t)$$

Flux Tunable Coupler



6 Fourier components, full system model

10^{-12} infidelity

Summary

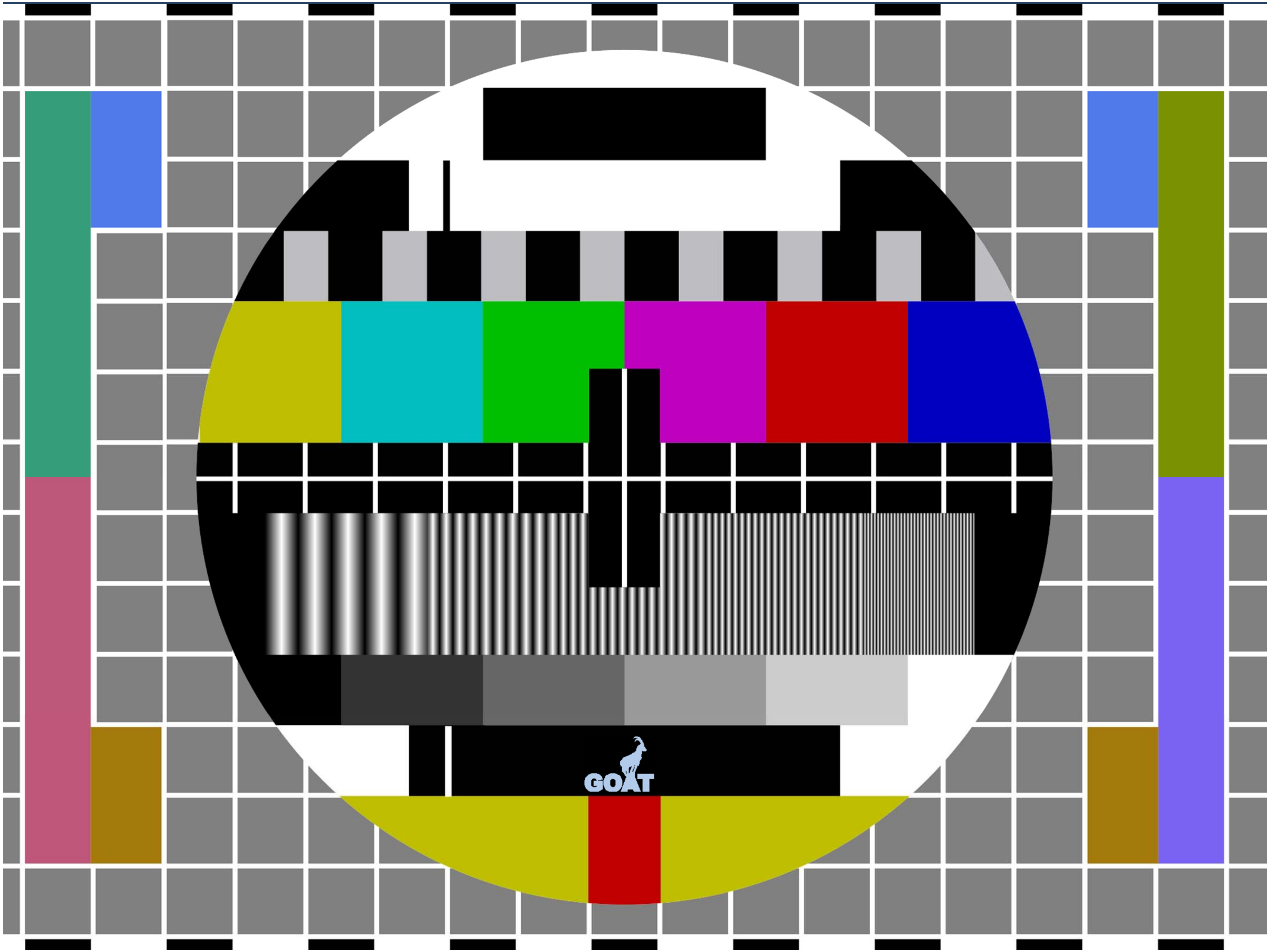
- Quantum optimal control is a critical technology for high-accuracy driving of quantum systems.
- Research in the field of QOC is on-going. Challenges include traps, open systems (esp. non- Markovian), optimal closed-loop, measurements, much much more.
- GOAT is a novel, highly flexible, conceptually simple and easy-to-implement gradient-based optimal control algorithm.

Thank you !

S. J. Glaser, et al.,
The European Physical Journal D 69.12 (2015): 1-24

C. P. Koch,
Journal of Physics: Condensed Matter 28.21 (2016): 213001

GOAT
arXiv 1507.04261


GOAT