

# Optimal Control for Quantum Networks

Michael Goerz

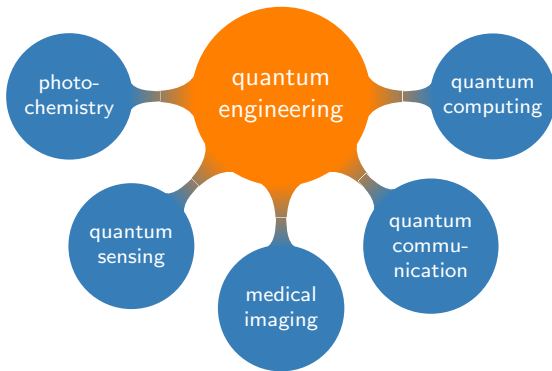
Stanford University / Army Research Lab

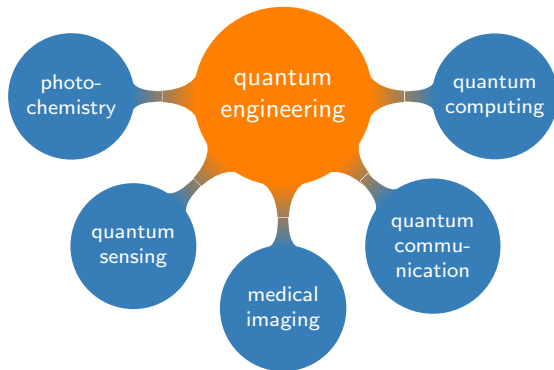
CECAM Workshop

Numerical methods for optimal control of open quantum systems

Berlin

September 27, 2016





scalable systems  $\Rightarrow$  quantum networks

# the software toolbox

## Modeling

QNET



Design and analysis of photonic circuit models

- QHDL model
- SLH formalism
- symbolic quantum algebra
- circuit component library
- visualization

yields Master equation of quantum network

<https://github.com/mabuchilab/qnet>

## Simulation & Optimization

QDYN

Fortran

high performance quantum simulation and optimal control

- Spectral methods
- Chebychev/Newton propagator
- Krotov's method
- Grape/LBFGS

Solves equation of motion and control problems

<https://github.com/goerz/qdynpylib>  
<http://bitly.com/agkoch-kassel>

## Python Ecosystem

jupyter

sympy

matplotlib

```
1 SLH Description
In [8]: from twi_node_xik import qnet_node_system, setup_qnet_sys
In [9]: n_cavity = 2
In [10]: sys, sys1, opt1, sys2, opt2 = setup_qnet_sys(n_cavity=n_cavity)
In [11]: sys.s
Out[11]: 
$$\begin{aligned} & \frac{d}{dt} \begin{pmatrix} \langle a_1 \rangle \\ \langle a_2 \rangle \end{pmatrix} + i \begin{pmatrix} \omega_{c1} \\ \omega_{c2} \end{pmatrix} \begin{pmatrix} \langle a_1 \rangle \\ \langle a_2 \rangle \end{pmatrix} - i \begin{pmatrix} \omega_{s1} \\ \omega_{s2} \end{pmatrix} \begin{pmatrix} \langle a_1 \rangle \\ \langle a_2 \rangle \end{pmatrix} - \frac{d}{dt} \begin{pmatrix} \langle a_1 \rangle \\ \langle a_2 \rangle \end{pmatrix} + \frac{d}{dt} \begin{pmatrix} \langle a_1 \rangle \\ \langle a_2 \rangle \end{pmatrix} \\ & + \frac{d}{dt} \begin{pmatrix} \langle a_1 \rangle \\ \langle a_2 \rangle \end{pmatrix} + \frac{d}{dt} \begin{pmatrix} \langle a_1 \rangle \\ \langle a_2 \rangle \end{pmatrix} \end{aligned}$$

```

QSD



Quantum Trajectories solver

<https://github.com/mabuchilab/qsd-mpi>

clusterjob



Drive HPC compute jobs

<https://github.com/goerz/clusterjob>

QuTip



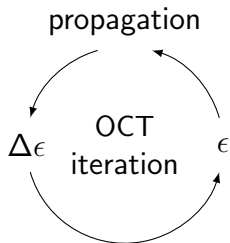
## optimization functional

$$J_T = 1 - \frac{1}{d^2} \left| \sum_{k=1}^d \langle \phi_k^{\text{tgt}} | \phi_k(T) \rangle \right|^2 \longrightarrow 0$$

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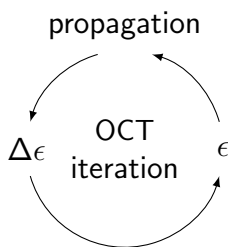
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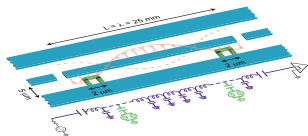
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Applications:

- state preparation
- quantum gates, entanglement creation
- robustness to qu. and classical noise
- performance bounds (QSL, *parameter exploration*)

# mapping the design parameter landscape of cQED

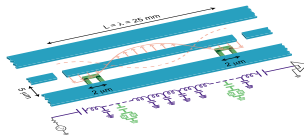


[Blais et al, PRA 75, 032329 (2007)]

transmon qubits:  
optimal system  
parameters?

- qubit  
frequency,  
anharmonicity
- qubit-cavity  
coupling,  
detuning

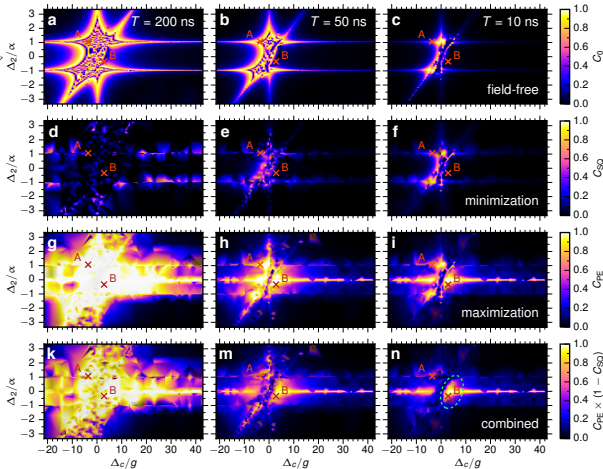
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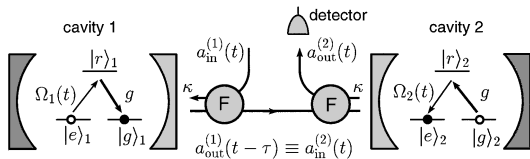


identify new parameter regime!

arXiv:1606.08825 (2016)

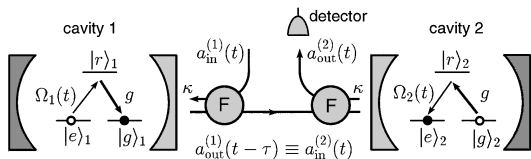
# quantum networks

# a two-node network



[Cirac et al, PRL 78, 3221 (1997)]

# a two-node network

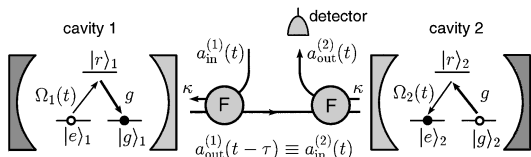


[Cirac et al, PRL 78, 3221 (1997)]

- each node  $j$  (after adiabatic elimination):
  - $\hat{H}_j = -\delta \hat{\mathbf{a}}_j^\dagger \hat{\mathbf{a}}_j - ig_j(t)(\hat{\sigma}_+ \hat{\mathbf{a}}_j - \hat{\sigma}_- \hat{\mathbf{a}}_j^\dagger)$
  - Lindblad operator  $\sqrt{2\kappa} \hat{\mathbf{a}}_j$



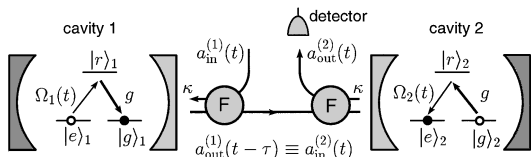
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- input-output theory (SLH framework): [Gough, James]
  - $\hat{H} = \hat{H}_1 + \hat{H}_2 + i\kappa(\hat{\mathbf{a}}_1^\dagger \hat{\mathbf{a}}_2 - \hat{\mathbf{a}}_1 \hat{\mathbf{a}}_2^\dagger)$
  - Lindblad operator  $\sqrt{2\kappa}(\hat{\mathbf{a}}_1 + \hat{\mathbf{a}}_2)$

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challenges:

- large combined Hilbert spaces (for larger networks)
- inherently dissipative (at the same scale as interactions!)

# a two-node network

```
Mabuchi_PRL78.3221 x
localhost:47962/notebooks/Mabuc
File Edit View Insert Cell Kernel
In [8]: from two_node_slh import qnet
In [9]: n_cavity = 2
In [10]: SYS = setup_qnet_sys(n_cavity)
In [11]: SYS.H
Out[11]: 
$$-\frac{g_1^2}{\Delta_1} a_{cav_1}^\dagger a_{cav_1} + ika_{cav_1}^\dagger a_{cav_2} - \frac{g_2^2}{\Delta_2} a_{cav_2}^\dagger a_{cav_2} - ika_{cav_1}^\dagger a_{cav_2} - \frac{i\Omega_1 g_1}{2\Delta_1} \sigma_{e,g}^{atom_1} a_{cav_1} + \frac{i\Omega_1 g_1}{2\Delta_1} \sigma_{e,g}^{atom_2} a_{cav_2} + \frac{g_2^2}{2\Delta_2} \Pi_g^{atom_2} a_{cav_2}^\dagger a_{cav_2}$$

In [12]: SYS.L
Out[12]:  $(\sqrt{2}\sqrt{\kappa}a_{cav_1} + \sqrt{2}\sqrt{\kappa}a_{cav_2})$ 
```

```
Default
def node_hamiltonian():
    H = -6*Op_n + (g**2/Delta)*Op_n*Op_gg \
        -I * (g/(2*Delta)) * Omega * (Op_eg*Op_a - Op_ge*Op_a_dag)
    return H

def setup_qnet_sys():
    Sym1, Op1 = qnet_node_system('1', n_cavity,
                                zero_phi=zero_phi, keep_delta=keep_delta)
    H1 = node_hamiltonian(Sym1, Op1,
                          stark_shift=stark_shift, zero_phi=zero_phi,
                          keep_delta=keep_delta)
    Sym2, Op2 = qnet_node_system('2', n_cavity,
                                zero_phi=zero_phi, keep_delta=keep_delta)
    H2 = node_hamiltonian(Sym2, Op2,
                          stark_shift=stark_shift, zero_phi=zero_phi,
                          keep_delta=keep_delta)
    S = identity_matrix(1)
    L1 = sympy.sqrt(2*kappa) * Op1['a']
    L2 = sympy.sqrt(2*kappa) * Op2['a']
    SLH1 = SLH(S, [L1,], H1)
    SLH2 = SLH(S, [L2,], H2)
    components = [SLH1, SLH2]
    connections = [((0,0), (1,0)), ]
    return connect(components, connections), Sym1, Op1, Sym2, Op2

NORMAL slh.py 36% ¶ 14/38: 5 python utf-8[unix] ← master
Neomake: pyflakes completed with exit code 1
```

# quantum trajectories

**Quantum trajectory:** specific realization of an evolution in Hilbert space, and (bath) measurement record

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... or a **numerical tool** for the ensemble dynamics!  
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... or a **numerical tool** for the ensemble dynamics!  
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## ensemble dynamics

$$\hat{\rho}(t) = \frac{1}{N} \sum_{n=1}^{N \rightarrow \infty} |\Psi_n(t)\rangle \langle \Psi_n(t)|$$
$$\langle \hat{\mathbf{O}}(t) \rangle = \text{tr} [\rho^\dagger \hat{\mathbf{O}}(t)] = \frac{1}{N} \sum_{n=1}^{N \rightarrow \infty} \langle \hat{\mathbf{O}}(t) \rangle_n$$

# the quantum jump (MCWF) method

for each trajectory  $|\Psi_n\rangle$ :

[Dum et al. PRA 4879 (1992); Mølmer et al. JOSAB 10, 524 (1993)]

**1** effective Hamiltonian  $H_{\text{eff}} = \hat{H} - \frac{i\hbar}{2} \sum_i \hat{L}_i^\dagger \hat{L}_i$



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- 3** Apply an instantaneous quantum jump  $|\Psi(t_j)\rangle \rightarrow \hat{L}_n |\Psi(t_j)\rangle$  use  $\hat{L}_n$  with relative probability  $\langle \Psi(t_j) | \hat{L}_n^\dagger \hat{L}_n | \Psi(t_j) \rangle$ .

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Can we optimize over individual trajectories  $|\Psi_n\rangle$ ?

# optimal control of quantum trajectories

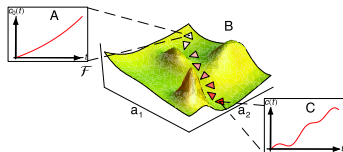
gradient-free: relies *only* on evaluation of functional

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- CRAB: truncate the search space

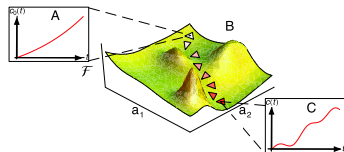


[Doria et al, PRL 106, 190501 (2011)]

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[Doria et al, PRL 106, 190501 (2011)]

Works great when there are only a handful of control parameters.

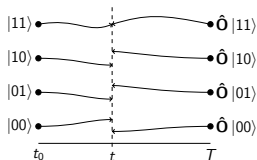
Good for obtaining guess pulses!



# methods of optimal control – gradient-based

typical functional:  $J_T(\{\tau_k\})$ ,

$$\tau_k = \left\langle k^{\text{tgt}} \left| \hat{\mathbf{U}}(T, 0) \right| k \right\rangle$$



- Grape/LBFGS: use gradient  $\frac{\partial J_T}{\partial \epsilon_j}$

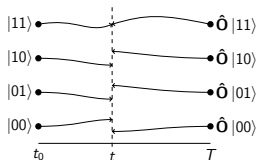
[Khaneja et al, JMR 172, 296 (2005); de Fouquières et al, JMR 212, 412 (2011)]

$$\frac{\partial \tau_k}{\partial \epsilon_j} = \left\langle k^{\text{tgt}} \left| \hat{\mathbf{U}}_{nt-1} \dots \hat{\mathbf{U}}_{j+1} \frac{\partial \hat{\mathbf{U}}_j}{\partial \epsilon_j} \hat{\mathbf{U}}_{j-1} \dots \hat{\mathbf{U}}_1 \right| k \right\rangle = \left\langle \chi_k(t_{j+1}) \left| \frac{\partial \hat{\mathbf{U}}_j}{\partial \epsilon_j} \right| \phi_k(t_j) \right\rangle,$$

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- Krotov's method: constructive pulse update (time-continuous)

$$\Delta \epsilon(t) \propto \sum_{k=1}^N \left\langle \chi_k^{(i)}(t) \left| \left( \frac{\partial \hat{\mathbf{H}}}{\partial \epsilon} \right) \Big|_{\epsilon^{(i+1)}(t)} \right| \phi_k^{(i+1)}(t) \right\rangle; \quad \left| \chi_k^{(i)}(T) \right\rangle = - \frac{\partial J_T}{\partial \langle \phi_k |} \Big|_{\phi_k^{(i)}(T)}$$

[Zhu et al, JCP 108, 1953 (1998); Palao, Kosloff, PRA 68 062308 (2003);  
Reich et al, JCP 136, 104103 (2012)]

# gradient-based trajectory optimization

**Grape/LBFGS:**  $\frac{\partial \hat{U}_j}{\partial \epsilon_j} \rightarrow \dots ?$

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Krotov optimization procedure

Each trajectory contributes to pulse update  $\Delta \epsilon(t) \rightarrow$  average

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cf. “ensemble optimization” for robustness  
[Goerz et al., PRA 90, 032329 (2014)]

# gradient-based trajectory optimization

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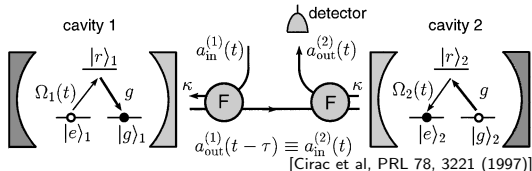
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[Goerz et al., PRA 90, 032329 (2014)]

$$J_{T,sm} = \frac{1}{N^2} \left| \sum_k \tau_k \right|^2 \rightarrow - \left. \frac{\partial J_{T,sm}}{\partial \langle \phi_k |} \right|_{\phi_k^{(i)}(T)} = \left( \frac{1}{N^2} \sum_{l=1}^N \tau_l \right) |k^{\text{tgt}}\rangle,$$

$$J_{T,re} = \frac{1}{N} \Re \sum_k \tau_k \rightarrow - \left. \frac{\partial J_{T,re}}{\partial \langle \phi_k |} \right|_{\phi_k^{(i)}(T)} = \frac{1}{2N} |k^{\text{tgt}}\rangle$$

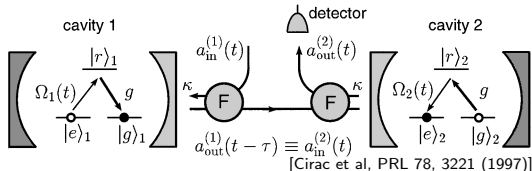
# example: directional state transfer



$$\hat{H} = \hat{H}_1 + \hat{H}_2 + i\kappa(\hat{\mathbf{a}}_1^\dagger \hat{\mathbf{a}}_2 - \hat{\mathbf{a}}_1 \hat{\mathbf{a}}_2^\dagger), \quad \hat{L} = \sqrt{2\kappa}(\hat{\mathbf{a}}_1 + \hat{\mathbf{a}}_2)$$

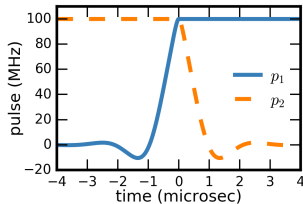
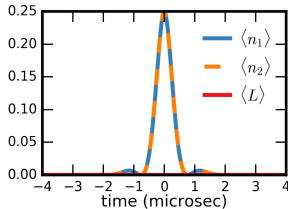
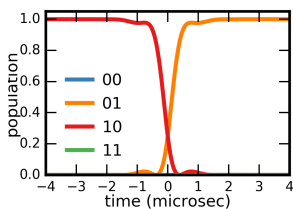


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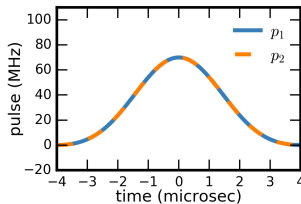
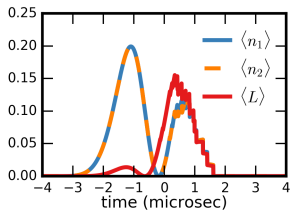
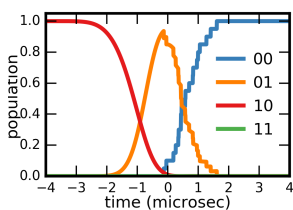
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Time-symmetric solution to  $|10\rangle \rightarrow |01\rangle$   
 with **dark state condition**  $\hat{L}|\Psi(t)\rangle = 0$



# optimal control solution for state transfer

**density matrix optimization:**  $|10\rangle\langle 10| \rightarrow |01\rangle\langle 01|$  [Y. Ohtsuki]

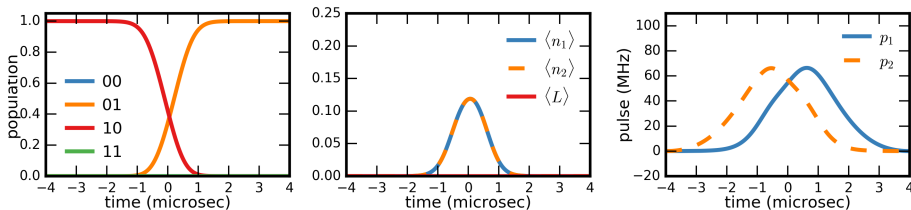


# optimal control solution for state transfer

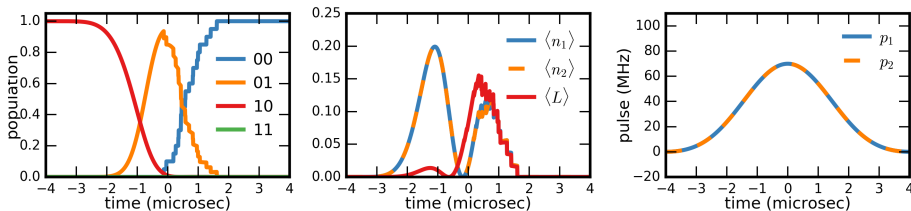
**density matrix optimization:**  $|10\rangle\langle 10| \rightarrow |01\rangle\langle 01|$  [Y. Ohtsuki]

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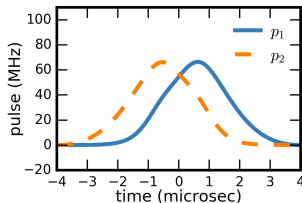
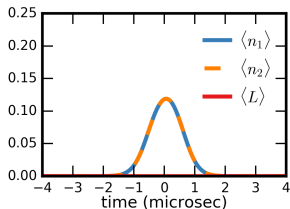
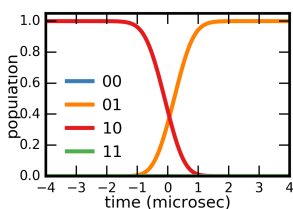


**MCWF optimization:**  $|10\rangle \rightarrow |01\rangle$



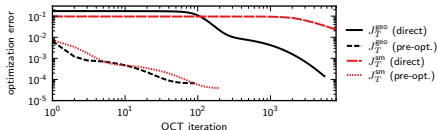
# optimal control solution for state transfer

**density matrix optimization:**  $|10\rangle\langle 10| \rightarrow |01\rangle\langle 01|$  [Y. Ohtsuki]



**MCWF optimization:**  $|10\rangle \rightarrow |01\rangle$

- “Hybrid optimization” (combine gradient-free and gradient-based methods); pulse smoothing



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

- Optimize with non-Hermitian Hamiltonian

$$\hat{H}_{\text{eff}} = \hat{H} - \frac{i\hbar}{2} \sum_i \hat{\mathbf{L}}_i^\dagger \hat{\mathbf{L}}_i$$

for weak dissipation and unitary target

- Optimize dark state condition  $\langle \hat{\mathbf{L}}^\dagger \hat{\mathbf{L}} \rangle = 0$

[Palao et al, PRA 77, 063412 (2008)]

$\Rightarrow$  Second order Krotov, inhomogeneous bw-propagation

[Reich et al, JCP 136, 104103 (2012)]

# summary & conclusion

- Quantum trajectories are highly scalable approach to simulating open quantum systems (MPI!)
- Toolbox: QNET (Stanford) and QDYN (Kassel)
- Krotov's method allows for trajectory optimization (for any large open quantum system, not just networks)
- Grape/LBFGS: open question

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Thank you!