Theoretical and numerical aspects of quantum control problems

Alfio Borzì

Dipartimento e Facoltà di Ingegneria, Università degli Studi del Sannio, Italy
Institute for Mathematics and Scientific Computing
Karl-Franzens-University, Graz, Austria
Application fields of quantum control methodologies

1. Quantum control: state transitions, laser induced chemistry, magnetic and optical trapping.
2. Quantum computing: qubits, data operations.
3. Quantum transport, superfluids of atoms, vortices.
4. Construction of barriers, channels, etc. for few atoms.
5. Amplification of material waves: laser of atoms.
The possibility to manipulate states of atoms and molecules by means of laser pulses or magnetic fields opens new technological perspectives.

The solution of quantum control problems poses new challenges involving optimal control theory, numerical analysis, and scientific computing.

Quantum control models define an important class of nonlinear control mechanisms.
Quantum mechanical models

- **One-particle Schrödinger equation**, \( \psi = \psi(x, t) \) or \( \psi = \psi(t) \)

\[
i \frac{\partial}{\partial t} \psi = (H_0 + V) \psi
\]

- **BEC Condensate Gross-Pitaevskii equation**, \( \psi = \psi(x, t) \)

\[
i \frac{\partial}{\partial t} \psi = \left( -\frac{1}{2} \nabla^2 + V + g |\psi|^2 \right) \psi
\]

- **Time-dependent Kohn-Sham equation**, \( \psi_i = \psi_i(x, t) \)

\[
i \frac{\partial}{\partial t} \psi_i = \left( -\frac{1}{2} \nabla^2 + V_{\text{ext}} + V_{\text{Hartree}}(\rho) + V_{\text{exc}}(\rho) + V_{\text{laser}} \right) \psi_i
\]

where \( \psi_i, i = 1, \ldots, N \) are the K-S orbitals; \( \rho = \sum_{i=1}^{N} |\psi_i|^2 \) is the one-electron density.

- **Multi-particle \((n)\) Schrödinger equation**, \( \psi = \psi(x_1, x_2, \ldots, x_n, t) \)

\[
i \frac{\partial}{\partial t} \psi = \left( -\frac{1}{2} \sum_{i=1}^{n} \nabla_i^2 + \sum_{i=1}^{n} V_i + \sum_{i,j=1}^{n} U_{ij} + V_{\text{laser}} \right) \psi
\]
Quantum mechanics structure and objectives

Dynamically stable systems exist with confining potentials $V_0$

$$\left\{ -\nabla^2 + V_0(x) - E_j \right\} \phi_j(x) = 0, \quad j = 1, 2, \ldots,$$

where $\phi_j(x)$ represent the eigenstates and $E_j$ represent the energy.

Control may be required to drive state transitions $\phi_i \rightarrow \phi_j$.

The expectation value of a physical observable $A$ when the system is in a state $\psi$ is given by $(\psi, A\psi)$.

Control may be required to maximize observable expectation.

An Hermitian operator $O$ may represent a transformation regardless of initial and final states (e.g., quantum gates).

Control may be required to obtain best performance of $O$. 
Quantum control mechanisms

Laser pulses, electric fields, and magnetic fields represent physically meaningful control mechanisms. They are represented by potentials that sum up to the stationary ones

\[ V(x, t) = V_0(x) + V_{control}(x, t) \]

The dipole approximation of the electric control field modeling a laser pulse results in the form

\[ V_{control}(x, t) = u(t) x \]

where \( u : (0, T) \rightarrow \mathbb{R} \) is the modulating control amplitude.

A magnetic potential for manipulating a BEC is given by

\[ V_{control}(x, \lambda(t)) = -\frac{\lambda(t)^2 d^2}{8c} x^2 + \frac{1}{c} x^4 \]

where \( \lambda \) is the control function.
Mathematical issues of quantum control problems

- **Finite- and infinite-dimensional quantum systems**
  Finite-level systems are characterized by $H_0, V \in \mathbb{C}^{n \times n}$, while $H_0$ is unbounded in $\infty$-dim systems and $V : \Omega \times (0, T) \to \mathbb{R}$.

- **Existence and uniqueness of optimal control**
  Existence of optimal solutions can usually be proven. Uniqueness usually does not occur: for dipole control if $u(t)$ is a minimizer, then so is $-u(t)$.

- **Exact and approximate controllability**
  A finite-level system is controllable iff $\text{Lie}\{i H_0, i V\} = u(n)$, the Lie algebra of traceless skew-Hermitian $n \times n$ matrices. For infinite-dimensional systems, see K. Beauchard and J.M. Coron’s result.

- **Accurate and fast solution schemes**
  Gradient schemes, monotonic schemes, multigrid schemes, Newton schemes.
Optimal control of a finite-level quantum system

Quantum systems with a finite number of states model artificial atoms (semiconductor quantum dots) and quantum devices (quantum gates). Consider a Λ-type three-level system with two stable states $\psi_1$ and $\psi_2$ (conservative), and one unstable state $\psi_3$ (dissipative).
Finite-level quantum models

Governed by Schrödinger-type equations for a $n$-component wave function $\psi : [0, T] \rightarrow \mathbb{C}^n$ as follows

$$i \dot{\psi}(t) = H(u(t)) \psi(t), \quad \psi(0) = \psi_0,$$

for $t \in [0, T]$ and $T > 0$ is a given terminal time.

The function $u : [0, T] \rightarrow \mathbb{C}^m$ represents the external control field.

The linear Hamiltonian $H(u) = H_0 + V(u)$, consists of

A free Hamiltonian $H_0 \in \mathbb{C}^{n \times n}$ describing the unperturbed (uncontrolled) system;

A control Hamiltonian $V : \mathbb{C} \rightarrow \mathbb{C}^{n \times n}$ modeling the coupling of the quantum state to the control field $u$. 
The objective of the quantum control

Control is applied to reach a target state at \( t = T \).
One needs to avoid population of dissipative states during the control process, while having limited laser resources.
These modeling requirements may result in the following

\[
J(\psi, u) = \frac{1}{2} |\psi(T) - \psi_d|^2_{C^n} + \frac{\gamma}{2} \|u\|^2_{L^2(0, T; \mathbb{C})} + \frac{\mu}{2} \|\dot{u}\|^2_{L^2(0, T; \mathbb{C})} + \frac{1}{2} \sum_{j \in J} \alpha_j \|\psi_j\|^2_{L^2(0, T; \mathbb{C})}
\]

where \( \psi_d \) is the desired terminal state; \( \gamma > 0 \) and \( \mu, \alpha_i \geq 0 \) are weighting factors; \( \psi_j \) denotes the \( j \)-th (dissipative) component of \( \psi \).
First-order necessary optimality conditions

For the quantum optimal control problem

\[ \min J(\psi, u), \text{ subject to } i\dot{\psi}(t) = H(u(t)) \psi(t), \quad \psi(0) = \psi_0 \]

**Theorem**

*Suppose that* \( x = (\psi, u) \in X \) *is a local solution to the optimal control problem. Then there exist (unique) Lagrange multipliers* 

\[ p \in H^1(0, T; \mathbb{C}^n) \quad (\mu > 0) \]

*satisfying*

\[
i\dot{\psi} = H(u(\cdot))\psi
\]

\[
i\dot{p} = H(u(\cdot))^* p - \alpha_j(\psi)_j
\]

\[ -\mu \ddot{u} + \gamma u = \Re(p \cdot (V_r'(u)\psi)^*) + i \Re(p \cdot (V_i'(u)\psi)^*) \]

*where*

\[ \psi(0) = \psi_0, \quad i p(T) = \psi(T) - \psi_d, \quad u(T) = u(0) = 0. \]
Second-order optimality conditions

Consider the following optimal control problem

\[
\begin{align*}
\min_u J(\psi, u) &:= \frac{1}{2} |\psi(T) - \psi_d|^2 + \frac{\gamma}{2} \|\dot{u}\|^2 \\
c(\psi, u) &:= i\psi - a\psi - u\psi = 0
\end{align*}
\]

We obtain

\[
(\nabla^2 \hat{J} \delta u, \delta u) = (W\delta u)(W\delta u)^* + 2\text{Re}(p\delta u, W\delta u) + \gamma(\dot{\delta} u, \dot{\delta} u).
\]

where \( W = W(\psi(u), u) = c_\psi(\psi(u), u)^{-1} c_u(\psi(u), u) \).

Since \( p(t) \) is unitary, we have \( |p(t)| = |p(T)| = |\psi(T) - \psi_d| \).

Using this result we obtain that \( |\text{Re}(p\delta u, W\delta u)| \leq C |\psi(T) - \psi_d| \|\delta u\|^2 \),

for some \( C > 0 \) depending on \( u \).

For sufficiently small values of tracking \( |\psi(T) - \psi_d| \) positiveness of the reduced Hessian is obtained.
Control of a Λ-type three-level model

Free Hamiltonian

\[
H_0 = \frac{1}{2} \begin{pmatrix}
  -\delta & 0 & 0 \\
  0 & \delta & 0 \\
  0 & 0 & -i\Gamma_o
\end{pmatrix}
\]

where the term \(-i\Gamma_o\) accounts for environment losses (spontaneous photon emissions, scattering of gamma rays from crystals).

The coupling to the external field is given by

\[
V(u) = -\frac{1}{2} \begin{pmatrix}
  0 & 0 & \mu_1 u \\
  0 & 0 & \mu_2 u \\
  \mu_1 u^* & \mu_2 u^* & 0
\end{pmatrix}
\]

where \(\mu_1\) and \(\mu_2\) describe the coupling strengths of states \(\psi_1\) and \(\psi_2\) to the inter-connecting state \(\psi_3\) (e.g., optical dipole matrix elements).

Initial and final states are given by

\[
\psi_0 = \begin{pmatrix}
  1 \\
  0 \\
  0
\end{pmatrix} \quad \text{and} \quad \psi_d = \begin{pmatrix}
  0 \\
  e^{-i\delta T} \\
  0
\end{pmatrix}
\]
Importance of optimization parameters

Smaller values of $\gamma$ result in smaller $|\psi(T) - \psi_d|_{C^3}$. As $\mu$ increases, $|\psi(T) - \psi_d|_{C^3}$ increases: additional smoothness of the control function (slightly) reduces the capability of tracking. Larger $\mu$ makes the problem behaving better, resulting in a smaller number of iterations. By taking $\alpha = \alpha_3 > 0$, dissipation is reduced and therefore better tracking is achieved.

| $\gamma$ | $\mu$ | $\alpha$ | $|\psi(T) - \psi_d|_{C^3}$ | $J$ | CPU |
|----------|-------|----------|------------------------|-----|-----|
| $10^{-7}$ | $10^{-7}$ | 0.05 | $8.6 \cdot 10^{-4}$ | $2.37 \cdot 10^{-3}$ | 19.6 |
| $10^{-7}$ | $10^{-9}$ | 0.05 | $3.7 \cdot 10^{-4}$ | $5.46 \cdot 10^{-4}$ | 55.6 |
| $10^{-7}$ | $0$ | 0.05 | $6.9 \cdot 10^{-5}$ | $1.41 \cdot 10^{-4}$ | 424.8 |
| $10^{-7}$ | $0$ | 0 | $1.2 \cdot 10^{-3}$ | $2.33 \cdot 10^{-6}$ | 763.1 |
| $10^{-4}$ | $10^{-4}$ | 0.05 | $3.3 \cdot 10^{-2}$ | $6.52 \cdot 10^{-2}$ | 47.3 |
| $10^{-4}$ | $10^{-6}$ | 0.05 | $4.4 \cdot 10^{-3}$ | $9.03 \cdot 10^{-3}$ | 42.3 |
| $10^{-4}$ | $0$ | 0.05 | $2.7 \cdot 10^{-3}$ | $5.68 \cdot 10^{-3}$ | 17.2 |
| $10^{-4}$ | $0$ | 0 | $8.3 \cdot 10^{-3}$ | $3.34 \cdot 10^{-4}$ | 5.5 |
Optimal solutions

With $\delta = 10$, $\Gamma_0 = 0.01$, $\mu_1 = \mu_2 = 1$, and $\gamma = 10^{-4}$, $\alpha_3 = 0.01$. We have $\mu = 0$ (top) and $\mu = 10^{-6}$ (bottom). Control (left) and state evolution (right).
Monotonic schemes have been initially introduced by Krotov. They are a special case of gradient based methods. Monotonic schemes have been further developed by Tannor, Zhu & Rabitz, Maday, Turinici & Salomon.

Consider two fields $u$ and $u'$, and the corresponding $\psi$ and $\psi'$, and $p$ and $p'$. We have

$$\tilde{J}(u') - \tilde{J}(u) = \int_0^T \Re (p(s)^* \cdot (V(u'(s)) - V(u(s)))\psi'(s))$$

$$- \frac{\gamma}{2} (|u'(s)|^2 - |u(s)|^2) \, ds + \frac{1}{2} \langle \psi' - \psi, \Lambda(\psi' - \psi) \rangle_{L^2(0,T;\mathbb{C}^n)}.$$

This formula is the starting point for the design of monotonic schemes.
Crank-Nicholson monotonic schemes

CNMS schemes represent a recent advance in monotonic schemes, supported by theoretical results on convergence properties.

Algorithm (CNMS)

Given an initial control amplitude \( u^0 \) and its associated state \( \psi^0 \) and Lagrange multiplier \( p^0 \), suppose that \( \psi^k, p^k, u^k \), have already been computed. The derivation of \( \psi^{k+1}, p^{k+1}, u^{k+1} \), is done as follows.

Forward propagation: Given \( \psi^{k+1}_0 = \psi_0 \), compute \( \psi^{k+1}_\ell \) from \( \psi^k_\ell \) by

\[
\begin{pmatrix}
  u^{k+1}_{\text{Re}, \ell} \\
  u^{k+1}_{\text{Im}, \ell}
\end{pmatrix} = \begin{pmatrix}
  u^k_{\text{Re}, \ell} \\
  u^k_{\text{Im}, \ell}
\end{pmatrix} + \frac{1}{2} \left(-\frac{\delta t}{4} \text{Im} B_k + \frac{\gamma}{2} I_2\right)^{-1} \left(\frac{1}{2} \text{Re} A_k - \gamma \begin{pmatrix}
  u^k_{\text{Re}, \ell} \\
  u^k_{\text{Im}, \ell}
\end{pmatrix}\right).
\]

Step 2. Compute \( \psi^{k+1}_{\ell+1} \) by

\[
\psi_{\ell+1} = \left(I_d - \frac{\delta t H_\ell}{2i}\right)^{-1} \left(I_d + \frac{\delta t H_\ell}{2i}\right) \psi_\ell
\]  

Backward propagation: Given \( p^{k+1}_N = i \psi_d \), compute \( p^{k+1}_\ell \) from \( p^{k+1}_{\ell+1} \).
Nonlinear conjugate gradient schemes

Gradient schemes are commonly used methods in computational physics. A first advance in gradient-based schemes has been the extension of NCG methods to problems defined on complex Hilbert spaces. A sufficient descent condition

\[ \Re \langle g_k, d_k \rangle \leq -c \| g_k \|^2 \]

**Step 1.** Given \( k = 1, u_1, d_1 = -g_1 \), if \( \| g_1 \| < tol \) then stop.

**Step 2.** Compute \( \tau_k > 0 \) satisfying the standard Wolfe conditions.

**Step 3.** Let \( u_{k+1} = u_k + \tau_k d_k \).

**Step 4.** Compute \( g_{k+1} = \nabla \hat{J}(u_{k+1}) \).

If \( \| g_{k+1} \| < tol_{abs} \) or \( \| g_{k+1} \| < tol_{rel} \| g_1 \| \) or \( k = k_{max} \) then stop.

**Step 5.** Compute \( \beta_k \) using Dai-Yuan or Hager-Zhang schemes.

**Step 6.** Let \( d_{k+1} = -g_{k+1} + \beta_k d_k \).

**Step 7.** Set \( k = k + 1 \), goto Step 2.
Cascadic acceleration of NCG schemes

The cascadic approach results from combining nested iteration techniques with a (one-grid) iterative scheme. $k = k_0, \ldots, k_f$ index of grid hierarchy. $u_{k_0}$ given starting approximation on the coarsest grid. $I_k^{k+1}$ interpolation operator from $k$ to $k+1$. $NCG_k(u_k)$ the basic iteration; $\ast$ denotes the resulting solution.

Algorithm (Cascadic NCG method)

Step 1. Given $k = k_0, u_{k_0}^\ast$.
Step 2. Compute $u_k = NCG_k(u_k^\ast)$.
Step 3. If $k = k_f$ then stop.
Step 4. Else if $k < k_f$ then interpolate $u_{k+1}^\ast = I_k^{k+1}u_k$.
Step 5. Set $k = k + 1$, goto Step 2.

Theoretical and numerical aspects of quantum control problems
The NCG scheme provides better performance while refining the computational mesh. There is a lack of robustness of the CNMS scheme for small $\gamma = 10^{-3}$ and severe convergence criteria $\|\nabla \hat{J}\| < tol_{abs}$.

<table>
<thead>
<tr>
<th>$tol_{abs}$</th>
<th>$N = 2048$</th>
<th>$N = 4096$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>CPU(NCG)</td>
<td>CPU(CNMS)</td>
</tr>
<tr>
<td>$10^{-4}$</td>
<td>1.17</td>
<td>1.28</td>
</tr>
<tr>
<td>$10^{-5}$</td>
<td>4.32</td>
<td>12.63</td>
</tr>
<tr>
<td>$10^{-6}$</td>
<td>5.01</td>
<td>48.00</td>
</tr>
</tbody>
</table>

Dramatic improvement with the Cascadic-NCG version

<table>
<thead>
<tr>
<th>$\gamma = 10^{-4}$</th>
<th>$\gamma = 10^{-6}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$N$</td>
<td>CPU(NCG)</td>
</tr>
<tr>
<td>4096</td>
<td>40.54</td>
</tr>
<tr>
<td>8192</td>
<td>112.57</td>
</tr>
<tr>
<td>16384</td>
<td>312.17</td>
</tr>
</tbody>
</table>

Computational effort to solve for $tol_{abs} = 10^{-6}; \gamma_0 = 0.01, \alpha_3 = 0.05$; in C-NCG coarsest level $N = 1024$.  

Alfio Borzì  
Theoretical and numerical aspects of quantum control problems
Optimal control of infinite-dimensional quantum systems
Bose Einstein condensates

Consider a bosonic gas (e.g. Rubidium) trapped in a magnetic field. By lowering the confining potential, atoms with higher energy escape (evaporation) while the remaining atoms condensate to a lower temperature (ca. 10 sec, 50 micron).

Courtesy W. Ketterle, MIT
Bose Einstein condensates model

The mean-field dynamics of the condensate is described by the Gross-Pitaevskii equation (GPE)

\[ i \frac{\partial}{\partial t} \psi(\mathbf{r}, t) = \left( -\frac{1}{2} \nabla^2 + V(\mathbf{r}, \lambda(t)) + g |\psi(\mathbf{r}, t)|^2 \right) \psi(\mathbf{r}, t) \]

We consider \( V(\mathbf{r}, \lambda(t)) \) is a three-dimensional potential produced by a magnetic microtrap. The control function \( \lambda(t) \) describes the variation of the confining potential with time.
Total control of matter waves

Trapping and coherent manipulation of cold neutral atoms in microtraps near surfaces of atomic chips is the focus of the present research towards total control of matter waves at small scales.

This achievement has boosted developments in the atomic interferometry, the construction of quantum gates, the microscopic magnetic field imaging, quantum data encoding, etc..

At the base of all these developments is the ability to manipulate Bose-Einstein condensates (BEC) subject to a control potential $V(x, \lambda(t))$ where $\lambda(t)$ parameterizes the trapping field.

We consider the problem to split and transport a BEC being confined in a single well $V(x, 0)$ at $t = 0$ to a double well $V(x, 1)$ at time $t = T$. We have

$$V(x, \lambda(t)) = -\frac{\lambda(t)^2 d^2}{8c} x^2 + \frac{1}{c} x^4$$

where $c = 40$ and $d$ is the width of the double well potential.
Optimal control formulation and optimality system

Consider a BEC at the initial state \( \psi_0 \) and a target state \( \psi_d \).

\[
J(\psi, \lambda) = \frac{1}{2} \left(1 - |\langle \psi_d | \psi(T) \rangle|^2 \right) + \frac{\gamma}{2} \int_0^T (\dot{\lambda}(t))^2 \, dt
\]

Optimal control problem: Minimize the cost function \( J(\psi, \lambda) \) subject to the condition that \( \psi \) fulfills the Gross-Pitaevskii equation. The optimal solution is characterized by the optimality system

\[
i \frac{\partial}{\partial t} \psi = \left(-\frac{1}{2} \nabla^2 + V(\lambda) + g |\psi|^2 \right) \psi
\]

\[
i \frac{\partial}{\partial t} p = \left(-\frac{1}{2} \nabla^2 + V(\lambda) + 2g |\psi|^2 \right) p + g \psi^2 p^*
\]

\[
\gamma \ddot{\lambda} = -\Re \langle \psi | \frac{\partial V(\lambda)}{\partial \lambda} | p \rangle,
\]

where \( \langle u, v \rangle = \int_\Omega u(x)^* v(x) \, dx \). We have the initial and terminal conditions

\[
\psi(0) = \psi_0 \quad \text{and} \quad ip(T) = -\langle \psi_d | \psi(T) \rangle \psi_d
\]

\[
\lambda(0) = 0, \quad \lambda(T) = 1.
\]
The choice of the control space and the gradient

For a given potential $V(x, \lambda(t))$, we have a unique $\psi(\lambda) = \psi(x, t)$. In terms of $\lambda$ we have the reduced objective $\hat{J}(\lambda) = J(\psi(\lambda), \lambda)$. The Taylor series of $\hat{J}(\lambda)$ in a Hilbert space $X$ is

$$\hat{J}(\lambda + \epsilon \varphi) = \hat{J}(\lambda) + \epsilon \left( \nabla \hat{J}(\lambda), \varphi \right)_X + \frac{\epsilon^2}{2} \left( [\nabla^2 \hat{J}(\lambda)] \varphi, \varphi \right)_X + O(\epsilon^3)$$

For $X = L^2(0,T;\mathbb{R})$, the reduced gradient is given

$$\nabla \hat{J}_{L^2}(\lambda) = -\gamma \ddot{\lambda} - \text{Re} \langle \psi | \frac{\partial V_\lambda}{\partial \lambda} | p \rangle,$$

In the case $X = H^1(0,T;\mathbb{R})$ formulation, we have that

$$-\frac{d^2}{dt^2} \left[ \nabla \hat{J}_{H^1}(\lambda) \right] = -\gamma \ddot{\lambda} - \text{Re} \langle \psi, \frac{\partial V_\lambda}{\partial \lambda} | p \rangle,$$

with $[\nabla \hat{J}(\lambda)](0) = 0$ and $[\nabla \hat{J}(\lambda)](T) = 0$.

The $H^1$ gradient $\nabla \hat{J}_{H^1}(\lambda)$ has the same regularity as $\lambda$, while the $L^2$ gradient does not.
Optimal controls obtained on different $X$ spaces

Figure: Dependence of the optimal control function on the regularization parameter $\gamma$ for the $L^2$ and $H^1$ spaces. More oscillating controls are obtained with smaller $\gamma$. $M = 3200$ time steps with $g = 10$ and $T = 7.5$. 
Hager-Zhang Nonlinear conjugate gradient on $X$ space

Step 1. Given $k = 1$, $\lambda_1$, $d_1 = -g_1$, if $\|g_1\|_X < tol$ then stop.

Step 2. Compute $\tau_k > 0$ satisfying the Armij-Wolfe conditions

$$\hat{J}(\lambda_k + \tau_k d_k) \leq \hat{J}(\lambda_k) + \delta \tau_k (g_k, d_k)_X$$
$$ (g(\lambda_k + \tau_k d_k), d_k)_X > \sigma (g_k, d_k)_X, \quad 0 < \delta < \sigma < 1/2$$

Step 3. Let $\lambda_{k+1} = \lambda_k + \tau_k d_k$.

Step 4. Compute $g_{k+1} = \nabla \hat{J}_X(\lambda_{k+1})$.

If $\|g_{k+1}\|_X < tol_{abs}$ or $\|g_{k+1}\|_X < tol_{rel} \|g_1\|_X$ or $k = k_{max}$ then stop.

Step 5. Compute $\beta_k$ by

$$\beta_k = \frac{(\sigma_k, g_{k+1})_X}{(d_k, y_k)_X}, \quad \sigma_k = y_k - 2d_k \frac{(y_k, y_k)_X}{(y_k, d_k)_X}, \quad y_k = g_{k+1} - g_k$$

Step 6. Let $d_{k+1} = -g_{k+1} + \beta_k d_k$.

Step 7. Set $k = k + 1$, goto Step 2.
BFGS on \(X\) space

With BFGS the search direction is given by \(p_k = -H_k \nabla \hat{J}(\lambda_k)\).

By the Sherman-Morrison-Woodbury formula, we establish a recurrence for \(H\).

\[
H_{k+1} = H_k + \frac{s_k^T y_k + y_k^T H_k y_k}{(s_k^T y_k)^2} (s_k s_k^T) - \frac{H_k y_k s_k^T + s_k y_k^T H_k}{s_k^T y_k}
\]

where \(s_k = \tau_k p_k\). Supposing \(X\) is either \(L^2(0, T; \mathbb{R})\) or \(H^1(0, T; \mathbb{R})\), the function space analog of the outer product is a dyadic operator \(x \otimes y : X \rightarrow X\). The action of this operator on a third element \(v \in X\) can be expressed in terms of the inner product \((x \otimes y) v = (y, z)_X v\).

From the recursion relation for \(H\), we obtain

\[
p_k = -H_0 g_k - \sum_{j=0}^{k-1} c_j [d_j (s_j, g_k)_X s_j - (z_j, g_k)_X s_j - (s_j, g_k)_X z_j]
\]

where \(c_j = (s_j, y_j)_X^{-1}\), \(d_j = 1 + c_j (y_j, z_j)\), and for \(z_k = H_k y_k\), we have

\[
z_k = H_0 y_k + \sum_{j=0}^{k-1} c_j \left\{ [d_j (s_j, y_k)_X - (z_j, y_k)_X] s_j - (s_j, y_k)_X z_j \right\}.
\]
Results with HZ-NCG and BFGS on $H^1$ space

<table>
<thead>
<tr>
<th>mesh</th>
<th>$\hat{J}_{min}$</th>
<th>$|\nabla \hat{J}_{min}|$</th>
<th>iterations</th>
<th>CPU time (sec)</th>
</tr>
</thead>
<tbody>
<tr>
<td>400</td>
<td>$1.6605 \times 10^{-2}$</td>
<td>$1.4288 \times 10^{-1}$</td>
<td>15</td>
<td>$3.8407 \times 10^1$</td>
</tr>
<tr>
<td>800</td>
<td>$5.5963 \times 10^{-4}$</td>
<td>$4.5284 \times 10^{-2}$</td>
<td>62</td>
<td>$2.8107 \times 10^2$</td>
</tr>
<tr>
<td>1600</td>
<td>$2.9634 \times 10^{-4}$</td>
<td>$1.0733 \times 10^{-2}$</td>
<td>30</td>
<td>$3.6334 \times 10^2$</td>
</tr>
<tr>
<td>3200</td>
<td>$1.0562 \times 10^{-4}$</td>
<td>$3.6378 \times 10^{-3}$</td>
<td>37</td>
<td>$9.6153 \times 10^2$</td>
</tr>
</tbody>
</table>
MultiGrid OPTimization framework

The MGOPT solution to the optimization problem \( \min_\lambda \hat{J}(\lambda) \) requires to define a hierarchy of minimization problems

\[
\min_{\lambda_k} \hat{J}_k(\lambda_k) \quad k = 1, 2, \ldots, L
\]

where \( \lambda_k \in X_k \) and \( \hat{J}_k(\cdot) \) is the reduced objective.

Among spaces \( X_k \), restriction operators \( I_{k-1}^k: X_k \to X_{k-1} \) and prolongation operators \( I_k^{k-1}: X_{k-1} \to X_k \) are defined.

Require that \( (I_{k-1}^k u, v)_{k-1} = (u, I_k^{k-1} v)_k \) for all \( u \in X_k \) and \( v \in X_{k-1} \).

We also choose an optimization scheme as 'smoother'

\[
\lambda_k^{\ell} = O_k(\lambda_k^{\ell-1})
\]

That provides sufficient reduction

\[
\hat{J}_k(O_k(\lambda_k^{\ell})) < \hat{J}_k(\lambda_k^{\ell}) - \eta \| \nabla \hat{J}_k(\lambda_k^{\ell}) \|^2
\]

for some \( \eta \in (0, 1) \).
MGOP Algorithm

Initialize $\lambda_0$. If $k = 1$, solve $\min_{\lambda_k} \hat{J}_k(\lambda_k) - (f_k, \lambda_k)_k$ and return. Else if $k > 1$,

1. **Pre-optimization**: $\lambda^\ell_k = O_k(\lambda^{\ell-1}_k, f_k)$, $\ell = 1, 2, \ldots, \gamma_1$

2. **Coarse grid problem**
   - Restrict the solution: $\lambda^{\gamma_1}_{k-1} = I^{k-1}_k \lambda^{\gamma_1}_k$
   - Fine-to-coarse correction: $\tau_{k-1} = \nabla \hat{J}_{k-1}(\lambda^{\gamma_1}_{k-1}) - I^{k-1}_k \nabla \hat{J}_k(\lambda^{\gamma_1}_k)$
   - $f_{k-1} = I^{k-1}_k f_k + \tau_{k-1}$
   - Apply MGOPT to the coarse grid problem:

   $$\min_{\lambda_{k-1}} \hat{J}_{k-1}(\lambda_{k-1}) - (f_{k-1}, \lambda_{k-1})_{k-1}$$

3. **Coarse grid correction**
   - Prolongate the error: $d = I^{k-1}_{k-1}(\lambda_{k-1} - \lambda^{\gamma_1}_{k-1})$
   - Perform a line search in the direction $d$ to obtain a step length $\alpha_k$.
   - Coarse grid correction: $\lambda^{\gamma_1+1}_k = \lambda^{\gamma_1}_k + \alpha_k d$

4. **Post-optimization**: $\lambda^\ell_k = O_k(\lambda^{\ell-1}_k, f_k)$, $\ell = \gamma_1 + 2, \ldots, \gamma_1 + \gamma_2 + 1$
Computational performance of CNCG and MGOPT

| $\gamma$  | $\frac{1}{2} \left(1 - \left| \langle \psi_d, \psi(T) \rangle \right|^2 \right)$ | CPU | $\frac{1}{2} \left(1 - \left| \langle \psi_d, \psi(T) \rangle \right|^2 \right)$ | CPU |
|-----------|-------------------------------------------------|-----|-------------------------------------------------|-----|
| $10^{-2}$ | $2.23 \cdot 10^{-2}$                             | 17  | $9.69 \cdot 10^{-4}$                             | 116 |
| $10^{-4}$ | $4.54 \cdot 10^{-4}$                             | 202 | $6.01 \cdot 10^{-4}$                             | 82  |
| $10^{-6}$ | $1.38 \cdot 10^{-2}$                             | 14  | $8.78 \cdot 10^{-4}$                             | 78  |

**Table:** Computational performance of the CNCG and MGOPT schemes; $T = 7.5$. Mesh $128 \times 1250$, $f = 256 \times 2500$.

| $g$ | $\frac{1}{2} \left(1 - \left| \langle \psi_d, \psi(T) \rangle \right|^2 \right)$ | CPU | $\frac{1}{2} \left(1 - \left| \langle \psi_d, \psi(T) \rangle \right|^2 \right)$ | CPU |
|-----|-------------------------------------------------|-----|-------------------------------------------------|-----|
| 25  | $3.89 \cdot 10^{-4}$                             | 53  | $7.08 \cdot 10^{-4}$                             | 149 |
| 50  | $2.35 \cdot 10^{-3}$                             | 80  | $9.84 \cdot 10^{-3}$                             | 76  |
| 75  | $5.54 \cdot 10^{-3}$                             | 90  | $1.85 \cdot 10^{-3}$                             | 163 |
| 100 | $4.94 \cdot 10^{-1}$                             | 50  | $5.44 \cdot 10^{-3}$                             | 257 |

**Table:** Computational performance of the CNCG and MGOPT schemes for different values of $g$; $T = 7.5$, $\gamma = 10^{-4}$, mesh $128 \times 1250$. 

Alfio Borzì
Theoretical and numerical aspects of quantum control problems
Time evolution for linear and optimized $\lambda$ control

The linear $\lambda(t) = t/T$ is the standard choice for the optimal control (left).

Tracking and control profile

Figure: The function $|\psi(x, t)|$ on the space-time domain (top) for the linear (left) and optimized (right) control. The corresponding profiles at $t = T$ (bottom, continuous line) compared to the desired state (dashed line). The tracking error $\frac{1}{2} \left(1 - |\langle \psi_d, \psi(T) \rangle|^2\right)$ results $6.26 \times 10^{-2}$ (lin) and $1.22 \times 10^{-3}$ (opt). MGOPT, Mesh $128 \times 1250; \gamma = 10^{-4}$.
Dipole quantum control
Electronic states of a charged particle in a well potential

The control of quantum electronic states has a host of applications such as control of photochemical processes and semiconductor lasers.

Consider a confining potential \( V_0(x) \) with a 'well' envelope. The eigenproblem

\[
\{-\partial_x^2 + V_0(x) - E_j\} \phi_j(x) = 0, \quad j = 1, 2, \ldots ,
\]

defines eigenfunctions representing the eigenstates with energy \( E_j \).

A representative potential with applications in semiconductor nanostructures is the infinite barrier well potential where \( V_0(x) = 0 \) for \( x \in (0, \ell) \) and \( V_0(0) = +\infty \) and \( V_0(\ell) = +\infty \).

The infinite barrier condition is equivalent to homogeneous Dirichlet boundary conditions for the wavefunction and thus we have

\[
E_j = \frac{j^2\pi^2}{\ell^2} \quad \text{and} \quad \phi_j(x) = \sin\left(j\pi x / \ell\right).
\]
Electric dipole transitions and a GaAs quantum well

Transitions $\phi_j \rightarrow \phi_k$
Electric dipole control

Consider a **control field modeling a laser pulse**. Using the dipole approximation results in the following

\[ V(x, t) = V_0(x) + u(t) x \]

where \( u : (0, T) \rightarrow \mathbb{R} \) is the **modulating control amplitude**.

The quantum state of a charged particle subject to this potential is governed by the time-dependent Schrödinger equation \((c(\psi, u) = 0)\)

\[ i \frac{\partial}{\partial t} \psi(x, t) = \left\{ -\frac{\partial}{\partial x^2} + V(x, t) \right\} \psi(x, t), \quad (x, t) \in Q = \Omega \times (0, T), \]

**Objective of the control**

\[ J(\psi, u) := \frac{1}{2} \left( 1 - \|P\psi(\cdot, T)\|_{\mathcal{H}}^2 \right) + \frac{\gamma}{2} \|u\|_{\mathcal{U}}^2 \]

where the projector \( P\psi = (\psi_d, \psi)_{\mathcal{H}} \psi_d \) and \( \|u\|_{\mathcal{U}}^2 = \|u\|^2 + \alpha \|\dot{u}\|^2 \)
Dipole control optimality system

Introduce the Lagrangian

\[ L(\psi, u, p) = J(\psi, u) + \Re e \int_0^T \int_\Omega p^*(x, t)c(\psi, u)(x, t) \, dx \, dt \]

where \( p \) is the Lagrange multiplier. The following first-order optimality system characterizes the optimal solution

\[
\begin{align*}
\{ i\partial_t + \partial_x^2 - V_0(x) - u(t) x \} \psi(x, t) &= 0 \\
\{ i\partial_t + \partial_x^2 - V_0(x) - u(t) x \} p(x, t) &= 0
\end{align*}
\]

\[-\gamma u + \gamma \alpha \ddot{u} + \Re e \int_\Omega p^*(x, t) x \psi(x, t) \, dx = 0\]

with homogeneous Dirichlet boundary conditions, and initial and terminal conditions given by

\[
\begin{align*}
\psi(x, 0) &= \psi_0(x) \\
p(x, T) &= i (\psi_d(\cdot), \psi(\cdot, T))_x \psi_d(x) \\
u(0) &= 0, \quad u(T) &= 0
\end{align*}
\]
Discretization: modified Crank-Nicholson scheme

Our MCN scheme results in the following

\[ \psi_k - \psi_{k-1} = -\frac{i\delta t}{4}[H(t_k) + H(t_{k-1})][\psi_k + \psi_{k-1}] . \]

Spatial discretization \( H_k \) of the Hamiltonian \( H(t_k) \) is by linear FEM. We have that \( H_k = H_k^\top \), which is important for preserving unitarity of the time-stepping method. Let \( A_k = \frac{\delta t}{4}[H_k + H_{k-1}] \).

\[
B_k = \begin{pmatrix} I & A_k \\ -A_k & I \end{pmatrix}.
\]

This gives the following representation of the equality constraint

\[ c_k(y, u) = B_k y_k - B_k^\top y_{k-1}, \quad y_k = \begin{pmatrix} \Re \psi_k \\ \Im m[\psi_k] \end{pmatrix}, \]

where \( y \) is a compact notation for the set of state vectors at each time step \( y_1, \ldots, y_{N_t} \) and similarly for \( u \).
Discrete optimality system

Let $S$ corresponds to multiplication by $i$. We have that

$$S = \begin{pmatrix} 0 & -I \\ I & 0 \end{pmatrix}, \quad (\psi_d, \psi)_\mathcal{H} \text{ corresponds to } \begin{pmatrix} y_d^\top \\ y_d^\top S \end{pmatrix} y$$

In this representation, we can rewrite the objective in the form

$$J(y, u) = \frac{1}{2} \left[ 1 - y_{N_t}^\top \left( \begin{array}{cc} y_d & -Sy_d \end{array} \right) \begin{pmatrix} y_d^\top \\ y_d^\top S \end{pmatrix} y_{N_t} \right] + \frac{\gamma}{2} u^\top Ku$$

The matrix $K$ is the discretization of $I - \alpha \partial_t^2$. We have the Lagrangian

$$L(y, u, p) = J(y, u) + \sum_{k=1}^{N_t} p_k^\top c_k(y, u)$$

Differentiating this Lagrangian with respect to its arguments and setting the derivatives to zero gives the discrete optimality system

$$B_k y_k = B_k^\top y_{k-1}$$
$$B_k^\top p_k = B_{k+1} p_{k+1}$$
$$\gamma Ku = f$$
Results with globalized Newton method: optimal controls

Optimal controls for transitions from the first state to the second, the third, and the fifth states.
Results with globalized Newton method: minimization

<table>
<thead>
<tr>
<th>Iteration</th>
<th>$J_{SD} - J^*$</th>
<th>$J_{NCG} - J^*$</th>
<th>$J_{KN} - J^*$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$2.4969 \times 10^{-1}$</td>
<td>$2.4969 \times 10^{-1}$</td>
<td>$2.4969 \times 10^{-1}$</td>
</tr>
<tr>
<td>2</td>
<td>$1.3070 \times 10^{-2}$</td>
<td>$1.3070 \times 10^{-2}$</td>
<td>$1.5346 \times 10^{-2}$</td>
</tr>
<tr>
<td>3</td>
<td>$6.4184 \times 10^{-3}$</td>
<td>$6.4184 \times 10^{-3}$</td>
<td>$5.1099 \times 10^{-3}$</td>
</tr>
<tr>
<td>4</td>
<td>$5.5337 \times 10^{-3}$</td>
<td>$5.3438 \times 10^{-3}$</td>
<td>$2.2381 \times 10^{-4}$</td>
</tr>
<tr>
<td>5</td>
<td>$4.8170 \times 10^{-3}$</td>
<td>$3.1011 \times 10^{-3}$</td>
<td>$1.8383 \times 10^{-4}$</td>
</tr>
<tr>
<td>6</td>
<td>$4.2081 \times 10^{-3}$</td>
<td>$2.3384 \times 10^{-3}$</td>
<td>$1.6253 \times 10^{-5}$</td>
</tr>
<tr>
<td>7</td>
<td>$3.6768 \times 10^{-3}$</td>
<td>$1.2475 \times 10^{-3}$</td>
<td>$2.7534 \times 10^{-6}$</td>
</tr>
<tr>
<td>8</td>
<td>$3.2177 \times 10^{-3}$</td>
<td>$9.1869 \times 10^{-5}$</td>
<td>$3.3921 \times 10^{-7}$</td>
</tr>
<tr>
<td>9</td>
<td>$2.8141 \times 10^{-3}$</td>
<td>$5.9258 \times 10^{-5}$</td>
<td>$4.7022 \times 10^{-9}$</td>
</tr>
</tbody>
</table>

**Table**: Convergence of the SteepestDescent scheme, the NonlinearCG scheme, and the KrylovNewton scheme to reach the optimal cost $J^* = J(u^*)$. 

Alfio Borzi  
Theoretical and numerical aspects of quantum control problems
References


Joint work with

Greg von Winckel (University of Graz), quantum modeling, Newton and quasi-Newton methods, sparse grids, uncertainty.

Stefan Volkwein (University of Konstanz), theory of quantum control problems.

Ulrich Hohenester (University of Graz), theoretical physics, quantum optics, nanophysics.

Julien Salomon (University of Dauphine, Paris), monotonic schemes.

Georg Stadler (University of Texas, Austin), theory of quantum control problems.

Partially funded by FWF Austrian Science Fund SFB Project Fast multigrid methods for inverse problems and FWF Project Quantum optimal control of semiconductor nanostructures
Thanks for your attention