Geometric and numerical methods for the contrast and saturation problems in Magnetic Resonance Imaging

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• **Contrast** and **Saturation** problems in Magnetic Resonance Imaging.
  - Dynamics: Bloch equation
  - Mayer optimal control problems, with 4D, 2D systems and a bounded scalar control

• **Geometric control and algebraic techniques**
  - Pontryagin maximum principle, Optimal syntheses for 2D systems
  - Analysis of the singular flow

• **Numerical methods**
  - Indirect multiple shooting, homotopy methods
  - Direct methods
  - Moments / LMI techniques

• **Softwares:** HamPath, Bocop, GloptiPoly

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Collaborators

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- ...
Magnetic Resonance Imaging

L’IRM anatomique

1. Sans champ magnétique, les spins des protons d’hydrogène du corps sont orientés de manière aléatoire.

2. Le champ magnétique $B_0$ aligne les spins des protons d’hydrogène.

3. Une onde radio $B_1$ fait basculer les protons de la position haute à la position basse et les synchronise.

4. Lorsqu’on éteint cette source $B_1$, les protons d’hydrogène se désynchronisent et restituent l’énergie absorbée. C’est l’analyse de ce signal qui permettra de reconstituer l’image finale.
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Inversion sequence
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Goal: optimize step 3
Bloch equation

Félix Bloch, Nobel Prize (1952)
Magnetic moment

Particles of spin-1/2 (proton, neutron, electron...) have magnetic moment.
There are two possible orientations for a spin-1/2 held in a stationary magnetic field $\vec{B}$. 
The magnetization vector $\vec{M} := (M_x, M_y, M_z)$ is the sum of the magnetic moments. $\vec{M}$ is non-zero and pointing in the same direction as $\vec{B}$. 
Conservative Bloch equation.

\[
\frac{dM(t)}{dt} = \gamma B(t) \wedge M(t),
\]

- Precession around \( B \) (\( \gamma \) is the gyromagnetic ratio).

Nuclear Magnetic Resonance experiments: two magnetic fields.

Intense stationary field: \( B_0 := (0, 0, B_z) \)

Control RF-field: \( B_1(t) := (B_x(t), B_y(t), 0) \)

- \( M(t) \) lives on a sphere.
Dissipative Bloch equation. Two relaxation effects: longitudinal ($T_1$) and transversal ($T_2$)

\[
\dot{M} = R(M, T_1, T_2) + \gamma B \wedge M
\]

Denoting $\omega_0 := -\gamma B_0$ and $(\omega_x(t), \omega_y(t)) := -\gamma (B_x(t), B_y(t))$ the control field, then we have

\[
\frac{d}{dt} \begin{bmatrix} M_x \\ M_y \\ M_z \end{bmatrix} = \begin{bmatrix} -M_x/T_2 \\ -M_y/T_2 \\ (M_0 - M_z)/T_1 \end{bmatrix} + \begin{bmatrix} 0 & -\omega_0 & \omega_y \\ \omega_0 & 0 & -\omega_x \\ -\omega_y & \omega_x & 0 \end{bmatrix} \begin{bmatrix} M_x \\ M_y \\ M_z \end{bmatrix}
\]

$x \ M(t)$ lives in the Bloch ball: $|M(t)| \leq M_0$, with $M_0$ the thermal equilibrium.

In practice, we have to consider perturbations (that is inhomogeneities) in the system:

**$B_0$ inhomogeneity.** $\omega_0 \to \omega_0(X^m, Y^m, Z^m)$

**$B_1$ inhomogeneity.** $\omega(t) := (\omega_x(t), \omega_y(t)) \to a(X^m, Y^m, Z^m) \omega(t)$

with $(X^m, Y^m, Z^m)$ the spatial coordinates of the molecule inside the sample.
Normalized dissipative Bloch equation (in a well chosen rotating frame - no inhomogeneities).

\[
\begin{align*}
\dot{x} &= -\Gamma x + u_2 z \\
\dot{y} &= -\Gamma y - u_1 z \\
\dot{z} &= \gamma (1 - z) + u_1 y - u_2 x
\end{align*}
\]

- State \( q := (x, y, z) := M/M_0 \in B(0, 1) \) : normalized magnetization vector

- Parameters \( \gamma := \frac{1}{T_1 \omega_{\text{max}}} \), \( \Gamma := \frac{1}{T_2 \omega_{\text{max}}} \) : characteristics of the experiment

- Control \( u := (u_1, u_2), \| u \| \leq 1 \) : normalized RF-field

- North Pole \( N := (0, 0, 1) \) : equilibrium

where \( \omega_{\text{max}} \) is the maximal amplitude of the control, that is \( \omega_x(t)^2 + \omega_y(t)^2 \leq \omega_{\text{max}} \).
Medical imaging. The norm of the magnetization vector corresponds to gray scale.
Contrast and Saturation problems
Experiment: two samples (deoxygenated and oxygenated bloods) in two square test tubes, a small one inside a bigger one. In this experiment, the samples are spatially separated.

Equilibrium state $\Rightarrow$ both samples appear white after processing the image.
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Equilibrium state ⇒ both samples appear white after processing the image.

Application of the optimal control law which maximize the contrast ⇒ the first sample appears black while the second is gray.

The figures are inspired from

In the saturation problem, we consider only one sample, that is one Bloch equation.

Thanks to the symmetry of revolution around (Oz), we set $u_2 = 0$ and we obtain the single-input planar control system:

\[
\begin{align*}
\dot{y} &= -\Gamma y - u z \\
\dot{z} &= \gamma (1 - z) + uy
\end{align*}
\]

where $u := u_1$ is the control satisfying $|u| \leq 1$. 
Saturation problem in MRI

Consider the planar Bloch equation. The goal of the saturation problem is to steer the normalized magnetization vector \( q \) from the North Pole \( N = (0, 1) \) to the center \( O := (0, 0) \) of the Bloch ball \( \{ q \in \mathbb{R}^2 \mid \| q \| \leq 1 \} \) in minimum time.
Consider the planar Bloch equation. The goal of the **saturation problem** is to steer the normalized magnetization vector \( q \) from the North Pole \( N = (0, 1) \) to the center \( O := (0, 0) \) of the Bloch ball \( \{ q \in \mathbb{R}^2 \mid \|q\| \leq 1 \} \) in **minimum time**.

The inversion sequence \( \sigma_+ \sigma_s^v \) is the simplest way to go from \( N \) to \( O \). Is it optimal?
Saturation problem and optimal syntheses
Saturation problem: formulation

One 2D Bloch equation.

\[
\begin{align*}
\dot{y} &= -\Gamma y - uz, \\
\dot{z} &= \gamma (1 - z) + uy,
\end{align*}
\]

written in the form \( \dot{q} = F_0(q) + u F_1(q) \), with

\[
F_0(q) := -\Gamma y \frac{\partial}{\partial y} + \gamma (1 - z) \frac{\partial}{\partial z}, \quad F_1(q) := -z \frac{\partial}{\partial y} + y \frac{\partial}{\partial z},
\]

Parameters: \( \{(\gamma, \Gamma) \in \mathbb{R}^2 \mid |\gamma - \Gamma| < 2, \ 0 < \gamma \leq 2\Gamma\} \),

State space: \( \{q \in \mathbb{R}^2 \mid \|q\| \leq 1\} \), \( q := (y, z) \),

Control domain: \( \{u \in \mathbb{R} \mid |u| \leq 1\} \).

Initial state (North Pole). \( q(0) = (0, 1) = N \),

Final state (saturation). \( q(T) = (0, 0) = O \),

Minimum time. minimize the transfer time \( T \).
Saturation problem. The saturation problem we consider here may be written in the following form:

\[ v(q_f) := \inf_{u \in \mathcal{U}} T_u, \quad \text{s.t.} \quad q(T_u, q_0, u) = q_f, \]

where \( \mathcal{U} := \{ u : [0, \infty[ \rightarrow [-1, 1] \mid u \text{ measurable} \} \) is the set of admissible controls and where \( q(T, q_0, u) \) is the solution at time \( T \) of the system (1) with control \( u \), initial condition \( q_0 = N \), and final condition \( q_f = O \).
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Optimal synthesis. For a given reachable state \( q_f \), one can denote by \( u^*(\cdot, q_f) \) the optimal control law (if it is unique). Since we have a single-input 2D affine control problem, we can go further and compute the optimal synthesis, that is compute for any reachable state \( q_f \) the value function \( v(q_f) \) with its associated optimal control law \( u^*(\cdot, q_f) \).

| Remark 1. The optimal synthesis depends on the parameters \( \gamma \) and \( \Gamma \). |

Pontryagin Maximum Principle

Pseudo-Hamiltonian: \( H(q, p, u) := H_0(q, p) + u H_1(q, p) \), \( H_i(q, p) = \langle p, F_i(q) \rangle \).

Necessary conditions of optimality: If \( u(\cdot) \) is optimal, with \( q(\cdot) \) the associated trajectory, then \( \exists p(\cdot): [0, T_u] \to (\mathbb{R}^2)^* \setminus \{0\} \) such that a.e. on \([0, T_u]\):

\[
\dot{q} = \frac{\partial H}{\partial p}, \quad \dot{p} = -\frac{\partial H}{\partial q},
\]

and

\[
H(q(t), p(t), u(t)) = \max_{|w| \leq 1} H(q(t), p(t), w) = \text{cst} \geq 0. \quad \text{Normal case: } H > 0.
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\]

Bang controls: \( u(t) = \text{sign}(H_1(q(t), p(t))) \), when \( H_1(q(t), p(t)) \neq 0 \).

Singular controls. The singular trajectories are contained in the set:
\[
\mathcal{S} := \{ q \mid \det(F_1(q), F_{01}(q)) = 0 \} = \left\{ q = (y, z) \mid z = \frac{\gamma}{2\delta} \text{ or } y = 0 \right\} ,
\]
where \( F_{01} := [F_0, F_1] := F'_1 F_0 - F'_0 F_1 \) and \( \delta := \gamma - \Gamma \).
Singular controls

Computations of singular controls. The singular control $u_s$ is given by solving

$$D_{001}(q) + u D_{101}(q) = 0,$$

with $D_{001} = \det(F_1, F_{001})$ and $D_{101} = \det(F_1, F_{101})$. This gives

$$u_s = \gamma (2\Gamma - \gamma) / (2\delta y)$$

on the horizontal singular line $z = \gamma / 2\delta$,

$$u_s = 0$$

on the vertical singular line $y = 0$.

See the following reference for details:

Symmetry. $(u, y, z) \leftarrow (-u, -y, z)$ still a solution.

Singular set: $z = \frac{\gamma}{2\delta}$ and $y = 0$.

Collinearity set: $\mathcal{C} := \{q \mid \det(F_0, F_1)(q) = 0\}$.

Switching function: $\Phi(t) := H_1(q(t), p(t))$.

Outside the set $\mathcal{C}$, we have $\text{sign}(\dot{\Phi}(t)) = \text{sign}(\alpha(q(t)))$, with

$$\alpha(q) := \frac{\det(F_1, F_{01})(q)}{\det(F_1, F_0)(q)}.$$
Concept of bridge: An arc $\sigma_+$ or $\sigma_-$ corresponding to $u = +1$ or $u = -1$, is called a bridge on $[0, t]$ if the extremities satisfy $\Phi(0) = \dot{\Phi}(0) = \Phi(t) = \dot{\Phi}(t) = 0$. 
**Concept of bridge, bang-bang arcs and optimality status**

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**Optimality status (some tools).**

- Small time optimality of the singular trajectories: generalized Legendre-Clebsch condition.
- Global optimality: outside $\mathcal{C}$, we can use the so-called clock form.
- We use the $\theta$ function, see Boscain & Piccoli (2004), to eliminate the possibility of two consecutive switching times.
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Optimality near the North Pole. The SiCo singularity: only bang-bang trajectories with at most one switching are optimal.

Optimality near the singularity of the singular locus. The horizontal singular line being admissible up to a saturation point, there is a birth of a switching locus connecting the horizontal and vertical singular lines. This is related to the concept of bridge and this phenomenon is referred as the SiSi singularity.
In this example, \((\gamma, \Gamma) = (0.12, 0.5)\). The point \(S_3\) corresponds to the saturation of the singular control on the horizontal singular line.
The optimal synthesis depends on \((\gamma, \Gamma)\)

Case 1: \(S_1 \leq S_2 < S_3\)

Case 2: \(S_2 < S_1 \leq S_3\)

Case 3: \(S_1\) does not exist

Case 1: corresponds to the domain \(C\) (see next slide).

Case 2: corresponds to the domain \(B\) (see next slide).

Case 3: corresponds to the domain \(A\) (see next slide).

Notation. \(S_2\) is one extremity of the bridge joining the horizontal and vertical singular lines.
**Parameters domain**

**Assumptions.** $|\gamma - \Gamma| < 2$, $0 < \gamma \leq 2\Gamma$, $S'_1$ and $S'_3$ below $O$.

The domain of interest of the parameters in white with the sub-domains $A_1$, $A_2$, $B$ and $C$.

**Notation.** $S_2$ is one extremity of the bridge joining the horizontal and vertical singular lines.
Optimal synthesis, case 3: $S_1$ does not exist, i.e. domain $A$

Optimal trajectory from $N$ to $O$: $\sigma_+^N \sigma_s^\psi$. 

\[
\sigma_+^N \sigma_s^\psi 
\]
Optimal synthesis, case 1: $S_1 \leq S_2 < S_3$, i.e. domain $C$

Optimal trajectory from $N$ to $O$: $\sigma^N_+ \sigma_s^h \sigma^b_+ \sigma_s^v$. 
Optimal synthesis, case 2: $S_2 < S_1 \leq S_3$, i.e. domain $B$

Optimal trajectory from $N$ to $O$: $\sigma^N_+ \sigma^v_s$.
**Theorem.** Under our assumptions, the time optimal trajectory for the saturation problem of 1-spin is of the form

\[ \sigma^N + \sigma^h_s \sigma^b_s + \sigma^v, \]

with \( \sigma^h_s \sigma^b_s \) empty if \( S_2 \leq S_1 \) or if \( S_1 \) does not exist.

**Proposition.** For any relaxation times \( T_1, T_2 \) satisfying the physical constraint \( 0 < T_2 \leq 2T_1 \), there exists \( \omega_{\text{max}} > 0 \) such that the associated pair of parameters \((\gamma, \Gamma)\) belongs either to:

- \( C \) if \( 0 < T_2 < \frac{2}{3}T_1 \), or
- \( A \) if \( \frac{2}{3}T_1 \leq T_2 \leq 2T_1 \).

Reminder: \( \gamma = \frac{1}{T_1 \omega_{\text{max}}} \), \( \Gamma = \frac{1}{T_2 \omega_{\text{max}}} \)

Experimental result: inversion sequence vs. optimal sequence for \((\gamma, \Gamma) \in C\).
**Just few words on the Bi-saturation problem**

**Model.** Consider two spins with the same characteristics, that is the same relaxation times, but for which for each, the control field has different intensities, because of $B_1$-inhomogeneities:

\[
\dot{q}_1(t) = F_0(q_1(t)) + u(t) F_1(q_1(t)), \\
\dot{q}_2(t) = F_0(q_2(t)) + u(t) (1 - \varepsilon) F_1(q_2(t)),
\]

where $q_i := (y_i, z_i), \ i = 1, 2,$ denote the coordinates of each system. The term $(1 - \varepsilon), \ \varepsilon > 0$ small, is the rescaling factor of the control maximal amplitude.

**Aim.** Steer from the North Pole, each system to the center of the Bloch ball, in minimum time.

**Difficulties.** 4D nonlinear dynamics with a complex singular flow; Discontinuous optimal control; Many local minima; 3 parameters ($T_1, T_2$ and $\varepsilon$)...

**Methodology.** The same as the one presented next for the contrast problem, see:

Just few words on the Bi-saturation problem

Water case: $\rho = \bar{\rho}$, $\theta = 0.7854$ and $\varepsilon = 0.1$. Trajectories of spins 1 and 2, and control.

Notation. $\bar{\rho} \approx 0.0551$, $\Gamma = \rho \cos \theta$ and $\gamma = \rho \sin \theta$. 
Just few words on the Bi-saturation problem

Fluid case: $\rho = \bar{\rho}, \theta = 0.1489$ and $\varepsilon = 0.1$. Trajectories of spins 1 and 2, and control.

Fat case: $\rho = \bar{\rho}, \theta = 0.4636$ and $\varepsilon = 0.1$. Trajectories of spins 1 and 2, and control.
Contrast problem by saturation

See:


The same methodology as the one presented next for the contrast problem is applied to the bi-saturation problem, see:

Formulation of the contrast problem by saturation

Two Bloch equations. Two 2D systems coupled by the same scalar control.

\[ \dot{q} = F_0 + u F_1 \]

given by

\[
\begin{align*}
\dot{y}_1 &= -\Gamma_1 y_1 - u z_1 \\
\dot{z}_1 &= \gamma_1 (1 - z_1) + u y_1 \\
\dot{y}_2 &= -\Gamma_2 y_2 - u z_2 \\
\dot{z}_2 &= \gamma_2 (1 - z_2) + u y_2
\end{align*}
\]

where \((\gamma_i, \Gamma_i)\) and \(q_i = (y_i, z_i), i = 1, 2\), are the parameters and the state of each species, with \(\|q_i\| \leq 1\) and where the control satisfies \(|u| \leq 1\).

Initial state. \(q_1(0) = q_2(0) = (0, 1)\).

Saturation of the first spin. \(q_1(t_f) = (0, 0)\).

Maximization of the contrast. \(c(q(t_f)) := -\|q_2(t_f)\|^2 \rightarrow \min\).

Fixed final time. The final time is fixed: \(t_f = \lambda T_{\min}, \lambda \geq 1\), where \(T_{\min}\) is the minimum time to steer the first spin from \(N\) to \(O\).
Pontryagin Maximum Principle

Pseudo-Hamiltonian: \( H(q, p, u) := H_0(q, p) + u H_1(q, p), \) \( H_i(q, p) = \langle p, F_i(q) \rangle \).

Necessary conditions of optimality: If \( u(\cdot) \) is optimal, with \( q(\cdot) \) the associated trajectory, then \( \exists p(\cdot): [0, T_u] \rightarrow (\mathbb{R}^4)^* \setminus \{0\} \) such that a.e. on \([0, T_u]\):

\[
\dot{q} = \frac{\partial H}{\partial p}, \quad \dot{p} = -\frac{\partial H}{\partial q}, \quad H(q(t), p(t), u(t)) = \max_{|w|\leq 1} H(q(t), p(t), w),
\]

and

\[ p_2(t_f) = q_2(t_f) \quad \text{(transversality conditions in the normal case)}. \]

Bang controls: \( u(t) = \text{sign}(H_1(q(t), p(t))), \) when \( H_1(q(t), p(t)) \neq 0 \).

Singular controls. \( u(t) = -\frac{H_{001}(q(t), p(t))}{H_{101}(q(t), p(t))}, \) when \( H_1(q(t), p(t)) = 0 \) and \( H_{101}(q(t), p(t)) \neq 0 \), and where:

\[
H_{001}(q, p) := \langle p, F_{001}(q) \rangle, \quad H_{101}(q, p) := \langle p, F_{101}(q) \rangle.
\]
The simplest solution is of the form $\sigma_+\sigma_s$, i.e. Bang-Singular.

Trajectories of spins 1, 2 and the associated Bang-Singular control.

Remark. In this graph, the control is normalized between 0 and $2\pi$ in norm and the time is normalized between 0 and 1.
Summary and difficulties

Summary.

- The simplest possible solution is a Bang-Singular sequence.
- The solution for $t_f = T_{\text{min}}$ is Bang-Singular-Bang-Singular in some cases.

Difficulties.

- The singular flow is very complex: use of algebraic techniques based on Gröbner basis (see Bonnard et al. 2017 preprint).
- Discontinuous optimal control: use of multiple shooting methods combined with regularization techniques or direct methods to determine the structure and initialize the Newton algorithm of the shooting method.
- Many local solutions: use of homotopy methods coupled with LMI validation.
- Many parameters: $\gamma_1, \Gamma_1, \gamma_2, \Gamma_2, t_f$. 
Bang-Singular example. We denote by \( t_0 = 0 \), \( t_1 \) and \( t_f = \lambda T_{\text{min}} \) the initial, switching and final times. We write \( z := (q, p) \) the state-costate vector in \( \mathbb{R}^8 \).

The shooting equations are:

\[
\begin{align*}
(t_0, q_0, p_0) & \quad \text{Bang} \quad (t_1, z_1) & \quad \text{Sing} \quad (t_f, z_f) \\
q_{0,1} = (0, 1) & \quad H_1(z_1) = 0 & \quad q_{f,1} = (0, 0) \\
q_{0,2} = (0, 1) & \quad H_{01}(z_1) = 0 & \quad q_{f,2} = p_{f,2}
\end{align*}
\]

with the matching condition \( z(t_1, t_0, z_0) = z_1 \) to improve numerical stability.

The shooting method consists in solving a nonlinear system of equations of the form

\[
S_\lambda(p_0, t_1, z_1) = 0_{\mathbb{R}^{13}}.
\]

We use for this a Newton-like algorithm which is sensitive to the initial condition.
Method. We use the solution of a direct method to determine the optimal structure and initialize the multiple shooting equation.

Principle of the direct methods. The optimal control problem is transcribed into a Nonlinear Programming Problem (NLP) via a full discretization of the state, control and dynamics. The NLP is then solved by interior point method for instance.

Softwares.

- Direct method: Bocop, see bocop.org.
- Indirect method: HamPath, see hampath.org.
Direct and indirect methods: example

\[ t_f = 1.5 T_{\text{min}} \]

Bocop and HamPath solutions.
Examples of local solutions

Fluid case with \( t_f = 2T_{\text{min}} \).

Species 1: \((y_1, z_1)\) - Cerebrospinal fluid
Species 2: \((y_2, z_2)\) - Water

The contrast is 0.705 for the solution \( \sigma^-\sigma_s\sigma^+\sigma_s \) and 0.702 for the solution \( \sigma^+\sigma_s\sigma^+\sigma_s \).
Contrast w.r.t. $\lambda = \frac{t_f}{T_{\text{min}}}$ between 1 and 3.

Structures of the solutions: 4BS (green), 3BS (red), 2BS (blue).
Sub-optimal synthesis (Fluid case)

\[
\sigma_+ \sigma_+ \sigma_+ \sigma_+ \quad \text{for} \; \lambda \in [1.000, 1.006]
\]

\[
\sigma_+ \sigma_+ \sigma_+ \sigma_- \sigma_- \quad \text{for} \; \lambda \in [1.006, 1.048]
\]

\[
\sigma_+ \sigma_+ \sigma_- \sigma_- \sigma_- \quad \text{for} \; \lambda \in [1.048, 1.351]
\]

\[
\sigma_+ \sigma_- \sigma_- \quad \text{for} \; \lambda \in [1.351, 3.000]
\]
LMI method

NLP or OCP problem
Cost : $C_{OCP}$

LP on measures
Cost : $C_{LP}$

SDP on moments
Cost : $C_{SDP}$

We consider only moments of order less than $d$.

LMI relaxation at order $d$
Cost : $C_{LMI}^d$

Proposition (Monotone convergence.)

$C_{LMI}^d \uparrow C_{SDP} = C_{LP} = C_{OCP}, \quad d \to \infty$

Polynomial criterion and dynamics: measures $\Rightarrow$ moments.

The LMI method gives an upper bound of the contrast.

(Left) Upper bounds (dashed line, LMI) compared to the sub-optimal synthesis (solid line, HamPath). (Right) Relative gap between the upper (LMI) and lower (HamPath) bounds.
Visual representation of a 5% gap in the Fluid case, for a lower bound (left) of 0.7 and an upper bound (right) of 0.74.
Conclusion and perspectives

Conclusion.

- The optimal syntheses for the 2D problem of the saturation of one species gives the minimum time with the optimal control law to steer the system from the North Pole to the origin, and generalize the inversion sequence. The concept of bridge is crucial.

- The methodology combining geometric control theory, algebraic techniques and numerical methods (direct, indirect and LMI) gives a large framework to analyze in details the contrast and saturation problems in MRI.

Perspectives.

- Generalization of the saturation problem to an ensemble of pair of spins where the Bloch equations are coupled and inhomogeneities on the control field $B_1$ are taken into account.

- Cartography of the (ideal) contrast problem where we have two species to discriminate, taking into account the possibility of adding contrast agents.

- Robust control for the contrast problem with $B_0$ and $B_1$ inhomogeneities, that is considering an ensemble of pair of spins, where one ensemble is put to the origin while the other is put far from the origin.