Résolution d’un problème de contraste en imagerie par Résonance Magnétique Nucléaire

SMAI 2011

O. Cots

Guidel, Bretagne, 23-27 mai 2011

Introduction - Collaborations

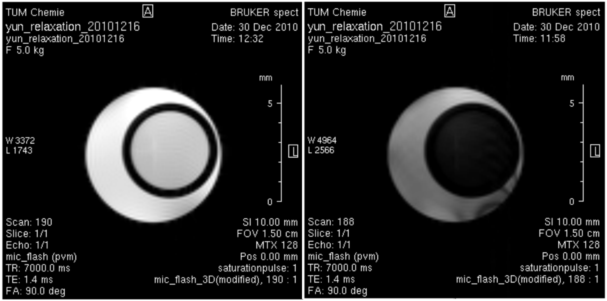


FIGURE: (LHS) Hard pulse of 90˚. (RHS) Optimal solution.

- Bernard Bonnard (Univ. Bourgogne)
- Jean-Baptiste Caillau (Univ. Bourgogne)
- Joseph Gergaud (N7 - IRIT)
- Steffen J. Glaser (Univ. Munich)
- Dominique Sugny (Univ. Bourgogne)
- ...

Contrast problem

$$(P)\begin{cases} |q_2(t_f)|^2 = \left(y_2^2(t_f) + z_2^2(t_f)\right) \to \max \\ \left[\begin{array}{lclll} \dot{y}_1 & = & -\ \Gamma_1\, y_1 & - & u\, z_1 \\ \dot{z}_1 & = & \gamma_1(1-z_1) & + & u\, y_1 \end{array}\right. \\ \left[\begin{array}{lclll} \dot{y}_2 & = & -\ \Gamma_2\, y_2 & - & u\, z_2 \\ \dot{z}_2 & = & \gamma_2(1-z_2) & + & u\, y_2 \end{array}\right. \\ q_1(0) = (0,1) = q_2(0) \\ q_1(t_f) = (0,0) \end{cases}$$

$$q_i = (y_i, z_i),\ |q_i| \leq 1,\ i = 1, 2$$

$$\gamma_i = 1/(32.3\ T_{i1})$$
$$\Gamma_i = 1/(32.3\ T_{i2})$$

$$|u| \leq 2\pi$$

$$H(q,u,p) = H_0(q,p) + u\, H_1(q,p)$$

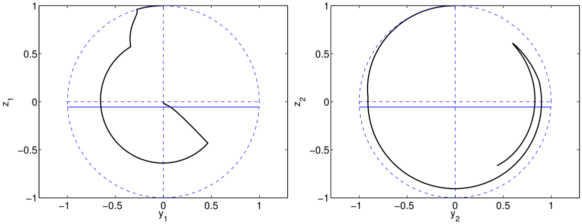


FIGURE: Trajectories of spin 1 (LHS) and spin 2 (RHS) for the Fluid/Water case.

Single spin problem

$$(P_1)\begin{cases} t_f \to \min \\ \left[\begin{array}{lllll} \dot y & = & -\Gamma y & - & u\,z \\ \dot z & = & \gamma(1-z) & + & u\,y \end{array}\right. \\ q(0) = (0,1) \\ q(t_f) = (0,0) \end{cases}$$

$$q = (y,z),\ |q| \le 1$$

$$\frac{3\gamma}{2} < \Gamma$$

$$|u| \le 2\pi$$

The dynamics : $\dot q = F_0(q) \quad + u\, F_1(q)$

The Hamiltonian : $H(q,u,p) = H_0(q,p) + u\, H_1(q,p),\ H_i =< p, F_i >, i = 0, 1.$

$\Rightarrow$ The singular extremals are those contained in $H_1 = 0$.

Single spin : singular extremals

$\Rightarrow$ The singular extremals are those contained in $H_1 = 0$.

$$\left.\begin{array}{rclcl} H_1 & = & < p, F_1 > & = & 0 \\ \dot{H}_1 & = & < p, [F_1, F_0] > & = & 0 \end{array}\right\} \Rightarrow \det(F_1, [F_1, F_0]) = y(-2\delta z + \gamma) = 0$$

with $\delta = \gamma - \Gamma$.

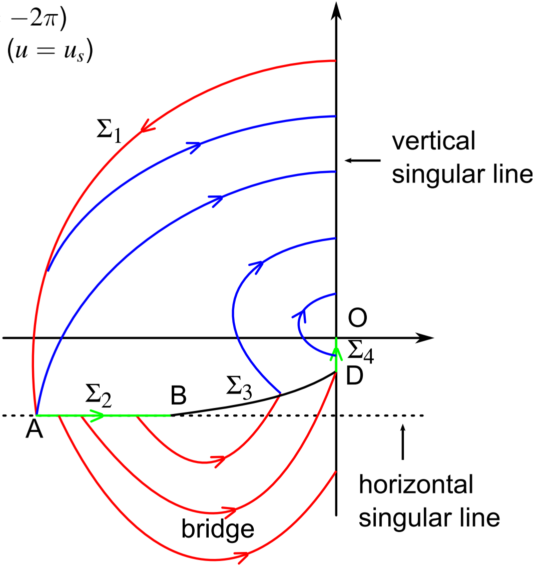
The singular lines are $y = 0$ and $z_0 = \frac{\gamma}{2\delta}$. The singular control $u_s(q,p)$ is computed from $\ddot{H}_1 = \{\{H_1, H_0\}, H_0\}(z) + u_s\{\{H_1, H_0\}, H_1\}(z) = 0$.

Horizontal line ($z_0 = \frac{\gamma}{2\delta}$) : optimal, according to Generalized Legendre-Clebsch condition (see [BC03]) and $u_s(q) = \gamma(2\Gamma - \gamma)/(2\delta y)$ $\Rightarrow u_s \in L^1$, $u_s \notin L^2$

Vertical line ($y = 0$) : optimal for $z_0 < z < 1$ (GLC) and $u_s(q) = 0$.

Single spin : global synthesis

Red : bang ($u = 2\pi$)
Blue : bang ($u = -2\pi$)
Green : singular ($u = u_s$)
B : saturation



Single spin => contrast problem

- We need to start with a bang.
- Singular extremals are expected for the contrast problem.
- Possibility of bridge phenomenon (Singular-Bang-Singular), before saturation.

To solve the contrast problem, we use an indirect method (multiple shooting)

$\Rightarrow$ we need to know the structure a priori.

$\Rightarrow$ we use an homotopic approach to capture the structure and initialize the multiple shooting method.

Homotopy

$$(P_\lambda)\begin{cases} -\left(y_2^2(t_f)+z_2^2(t_f)\right)+(1-\lambda)\int_0^{t_f} u^{2-\lambda}(t)dt \to \min \\ \left[\begin{array}{lcll} \dot{y}_1 & = & -\Gamma_1\, y_1 & -\; u\, z_1 \\ \dot{z}_1 & = & \gamma_1(1-z_1) & +\; u\, y_1 \\ \dot{y}_2 & = & -\Gamma_2\, y_2 & -\; u\, z_2 \\ \dot{z}_2 & = & \gamma_2(1-z_2) & +\; u\, y_2 \end{array}\right. \\ q_1(0)=(0,1)=q_2(0) \\ q_1(t_f)=(0,0) \end{cases}$$

$$q_i=(y_i,z_i),\ |q_i|\le 1,\ i=1,2$$

$$\gamma_i = 1/(32.3\ T_{i1})$$
$$\Gamma_i = 1/(32.3\ T_{i2})$$

$$|u|\le 2\pi$$

Homotopy (P_λ) : $-\left(y_2^2(t_f)+z_2^2(t_f)\right)+(1-\lambda)\int_0^{t_f} u^{2-\lambda}(t)dt \to \min$

The Hamiltonian : $H(q,u,p)=H_0(q,p)+u\,H_1(q,p)+(1-\lambda)\,u^{2-\lambda}$

- (P_λ)-extremals are admissible for (P).
- $\lambda<1 \Rightarrow \begin{cases} u = sign(H_1).\{2|H_1|/((2-\lambda)(1-\lambda))\}^{1/(1-\lambda)} & if\ |u|\le 2\pi \\ u = 2\pi\ sign(H_1) & else \end{cases}$

Regularized problem : homotopic method

We use HAMPATH [CCG] to perform a differential continuation on λ from 0 to 0.93, for $t_f = 2T_{min}$.

- T_{min} : the minimal time to transfer the spin 1 from $(0, 1)$ to $(0, 0)$.

Existing contrast results (with GRAPE, from S. Glaser et al) :

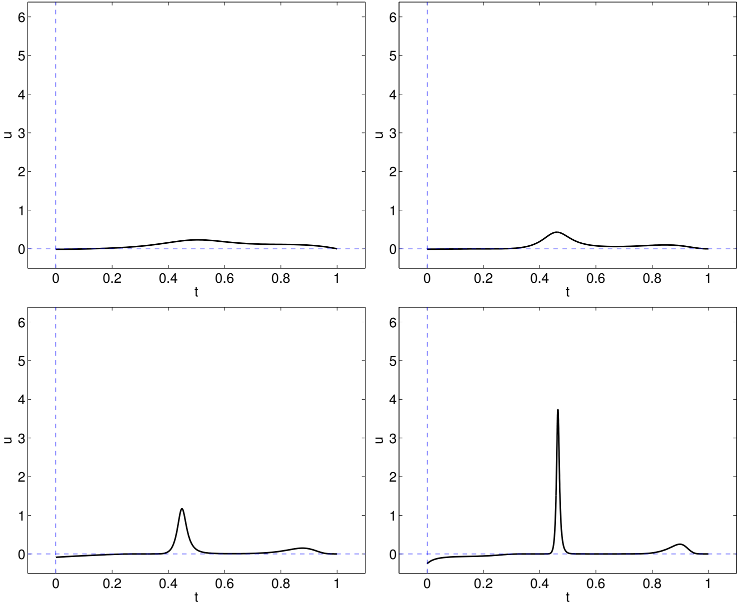
		spin 1	spin 2		
fluid/water case	-	$T_{11} = 2000$	$T_{21} = 2500$	-	contrast $\simeq 0.65$
		$T_{12} = 200$	$T_{22} = 2500$		

[CCG] J.B. Caillau, O. Cots, and J. Gergaud.
HAMPATH `apo.enseeiht.fr/hampath`.

Control : fluid/water case ($\lambda \in \{0, 0.6, 0.8, 0.9\}$)

$\lambda = 0$

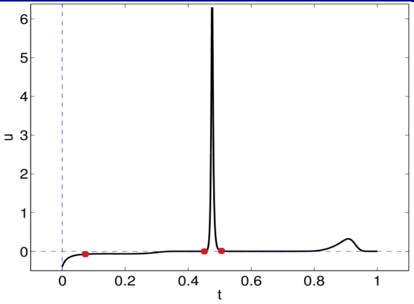
$\lambda = 0.6$

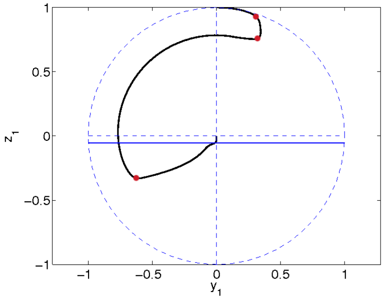


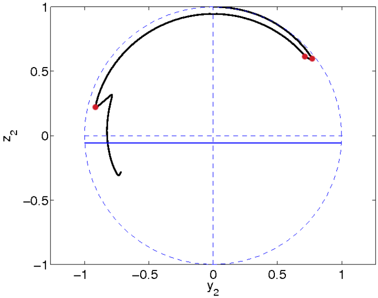
$\lambda = 0.8$

$\lambda = 0.9$

States-Control : fluid/water case $(\lambda = 0.93)$







Contrast problem : multiple shooting description

We have a BSBS structure for $t_f = 2T_{min}$. We denote by t_0, t_1, t_2, t_3, t_f the different instants and by z_0, z_1, z_2, z_3, z_f the state-costate variables associated ($z = (q_1, q_2, p_1, p_2) \in \mathbf{R}^4 \times \mathbf{R}^4$).

- Hamiltonian :

$$H(q,u,p) = H_0(q,p) + u\, H_1(q,p), \begin{cases} u = 2\pi & \textit{if } t \in [t_0;t_1] \textit{ or } t \in [t_2;t_3] \\ u = u_{sing} & \textit{if } t \in [t_1;t_2] \textit{ or } t \in [t_3;t_f] \end{cases}$$

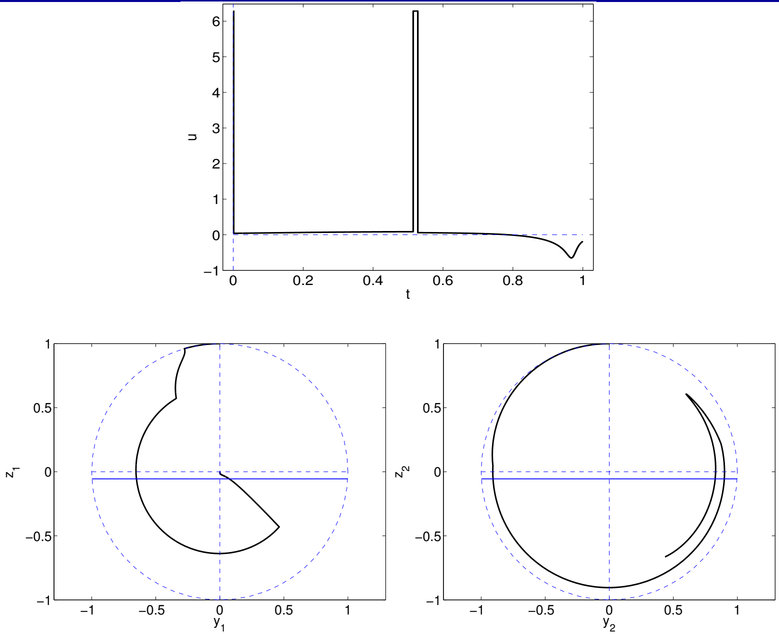
- Equations (*cf.* [Mau76]) :

$$\begin{array}{ccccccccc} & \textit{Bang} & & \textit{Sing} & & \textit{Bang} & & \textit{Sing} & \\ (t_0, z_0) & \longrightarrow & (t_1, z_1) & \longrightarrow & (t_2, z_2) & \longrightarrow & (t_3, z_3) & \longrightarrow & (t_f, z_f) \\ q_1 = (0,1) & & H_1 = 0 & & & & H_1 = 0 & & q_1 = (0,0) \\ q_2 = (0,1) & & \dot{H}_1 = 0 & & & & \dot{H}_1 = 0 & & q_2 = p_2 \end{array}$$

with the matching conditions :

$z(t_1; t_0, z_0) = z_1$, $z(t_2; t_1, z_1) = z_2$ and $z(t_3; t_2, z_2) = z_3$.

[Mau76] H Maurer. . . .
Numerical solution of singular control problems using multiple shooting techniques.
Journal of optimization theory and applications, Jan 1976.

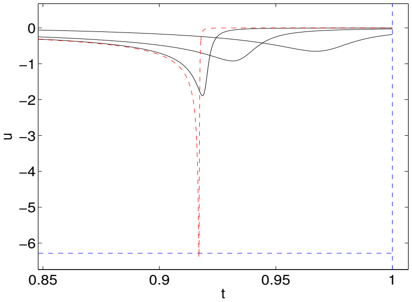

u
t
0
0.2
0.4
0.6
0.8
1
6
5
4
3
2
1
0
–1
z1
y1
z2
y2
0.5
–0.5

Contrast problem : continuation on t_f

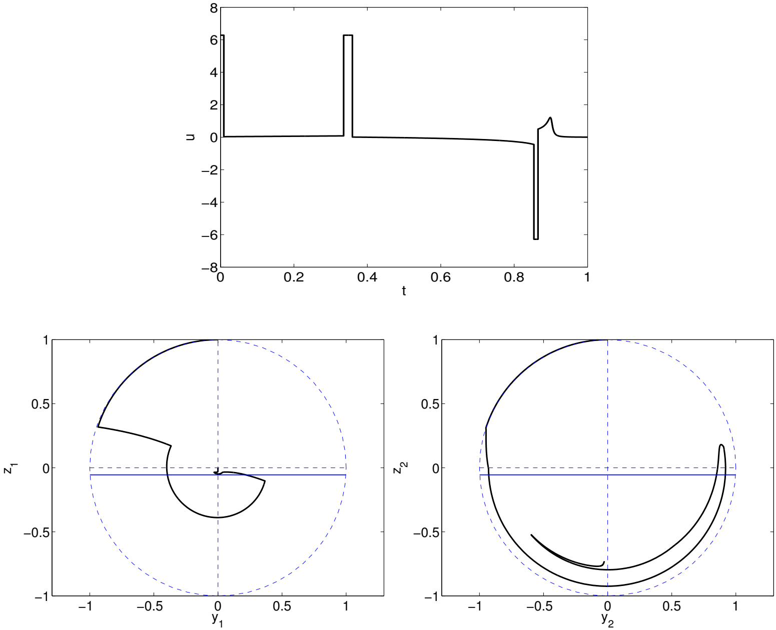
We use HAMPATH to perform a differential continuation on t_f from $2T_{min}$ to $T_{min} + \varepsilon$.

- T_{min} : the minimal time to transfer the spin 1 from $(0, 1)$ to $(0, 0)$.

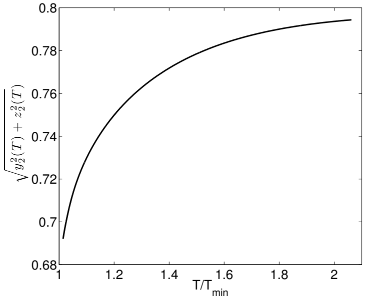
$\Rightarrow$ Problem for $t_f = 1.22T_{min}$. The norm of the second singular control becomes greater than the boundary 2π. The structure changes. We need one more bang arc.

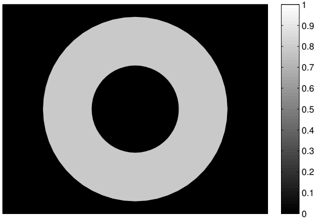


Contrast problem : BSBSBS structure, $t_f = 1.1T_{min}$



Contrast problem : contrast vs t_f





Introduction to homotopic method

We want to compute the zeros path of the homotopic function

$$\begin{array}{rcl} S : \mathbf{R}^{2n} \times [0,1] & \longrightarrow & \mathbf{R}^{2n} \\ (z_0, \lambda) & \longmapsto & S(z_0, \lambda) \end{array}$$

S is nonlinear and smooth. Assuming that 0 is a regular value for S, the solution set of $S(c) = 0$ is made of smooth curves.

Path following techniques :

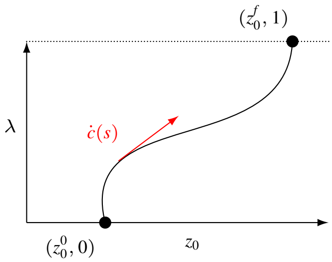
- Prediction-Correction (ALLGOWER AND GEORG. [AG03])
- HAMPATH for optimal control [CCG]

[AG03] E.L. Allgower and K. Georg.
Introduction to numerical continuation methods, volume 45 of *Classics In Applied Mathematics*.
SIAM, 2003.

Differential algorithms

HAMPATH [CCG] uses DOPRI5 from E. Hairer and G. Wanner [HrW93] [HW], for the numerical integration (without any correction) of :

$$(IVP)\left\{\begin{array}{l}\dot{c}(s) = T(c(s))\\ c(0) = (z_0^0, 0)\end{array}\right.$$



Until s_f such as $\lambda(s_f) = 1$ (dense output).

[HrW93] E. Hairer, S.P. Nørsett, and G. Wanner.
Solving Ordinary Differential Equations I, Nonstiff Problems, volume 8 of *Springer Serie in Computational Mathematics*.
Springer-Verlag, second edition, 1993.

[HW] E. Hairer and G. Wanner.
DOPRI5 http://www.unige.ch/~hairer/prog/nonstiff/dopri5.f.

HAMPATH

From the true hamiltonian and the boundary and intermediate conditions, HAMPATH :

- produces automatically the state-costate equations (thanks TAPENADE)
- computes the shooting function by numerical integration (thanks DOPRI5)
- provides the variationnal equations used in the jacobian of the shooting function (thanks TAPENADE)
- integrates the variationnal equations so that this diagram commutes

$$\begin{array}{ccc} (IVP) & \xrightarrow{\text{Numerical integration}} & S(z_0,\lambda) \\ \text{Derivative} \downarrow & & \downarrow \text{Derivative} \\ (VAR) & \xrightarrow{\text{Numerical integration}} & \frac{\partial S}{\partial z_0}(z_0,\lambda) \end{array}$$

Conclusions

- Homotopic method gave us the right structure and a good initial point for the contrast problem ;
- We could compute the solution with accuracy thanks to multiple shooting ;
- What about the second order conditions ;
- Treat the case of C^1-piecewise control.

[AG03] E.L. Allgower and K. Georg.
Introduction to numerical continuation methods, volume 45 of *Classics In Applied Mathematics*.
SIAM, 2003.

[BC03] B Bonnard and M Chyba.
Singular trajectories and their role in control theory, mathématiques & applications, vol. 40.
lavoisier.fr, Jan 2003.

[BCG+11] B Bonnard, Olivier Cots, S Glaser, M Lapert, and Dominique Sugny. . . .
Geometric optimal control of the contrast imaging problem in nuclear magnetic resonance.
math.u-bourgogne.fr, 2011.

[BCS09] B Bonnard, M Chyba, and Dominique Sugny. . . .
Time-minimal control of dissipative two-level quantum systems : the generic case.
Automatic Control, Jan 2009.

[BS09] B Bonnard and Dominique Sugny. . . .
Time-minimal control of dissipative two-level quantum systems : the integrable case.
SIAM J. Control Optim, Jan 2009.

[CCG] J.B. Caillau, O. Cots, and J. Gergaud.
HAMPATH `apo.enseeiht.fr/hampath`.

[HrW93] E. Hairer, S.P. Nørsett, and G. Wanner.
Solving Ordinary Differential Equations I, Nonstiff Problems, volume 8 of *Springer Serie in Computational Mathematics*.
Springer-Verlag, second edition, 1993.

[HW] E. Hairer and G. Wanner.
DOPRI5 `http://www.unige.ch/~hairer/prog/nonstiff/dopri5.f`.

[LZB+10] M Lapert, Y Zhang, M Braun, S Glaser, and Dominique Sugny. . . .
Singular extremals for the time-optimal control of dissipative spin 1/2 particles.
Physical review letters, Jan 2010.

[Mau76] H Maurer. . . .
Numerical solution of singular control problems using multiple shooting techniques.
Journal of optimization theory and applications, Jan 1976.