

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

SMAI 2011

O. Cots



Guidel, Bretagne, 23-27 mai 2011

Introduction - Collaborations

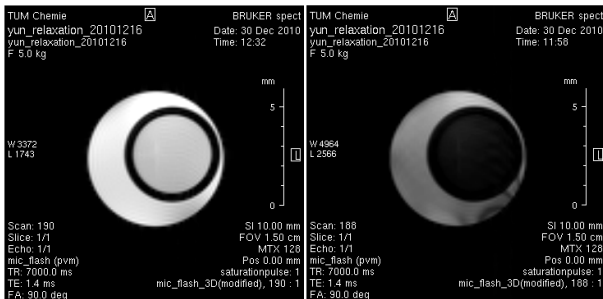


FIGURE: (LHS) Hard pulse of 90° . (RHS) Optimal solution.

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

Contrast problem

$$(P) \left\{ \begin{array}{l} |q_2(t_f)|^2 = (y_2^2(t_f) + z_2^2(t_f)) \rightarrow \max \\ \begin{cases} \dot{y}_1 = -\Gamma_1 y_1 - u z_1 \\ \dot{z}_1 = \gamma_1(1 - z_1) + u y_1 \\ \dot{y}_2 = -\Gamma_2 y_2 - u z_2 \\ \dot{z}_2 = \gamma_2(1 - z_2) + u y_2 \end{cases} \\ q_1(0) = (0, 1) = q_2(0) \\ q_1(t_f) = (0, 0) \end{array} \right. \quad \begin{array}{l} q_i = (y_i, z_i), |q_i| \leq 1, i = 1, 2 \\ \gamma_i = 1/(32.3 T_{i1}) \\ \Gamma_i = 1/(32.3 T_{i2}) \\ |u| \leq 2\pi \\ H(q, u, p) = H_0(q, p) + u H_1(q, p) \end{array}$$

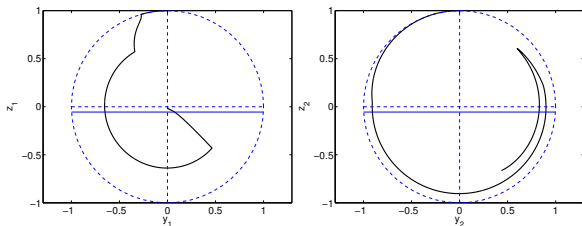


FIGURE: Trajectories of spin 1 (LHS) and spin 2 (RHS) for the Fluid/Water case.

Single spin problem

$$(P_1) \left\{ \begin{array}{l} t_f \rightarrow \min \\ \left[\begin{array}{l} \dot{y} = -\Gamma y - u z \\ \dot{z} = \gamma(1-z) + u y \end{array} \right. \\ q(0) = (0, 1) \\ q(t_f) = (0, 0) \end{array} \right. \quad \begin{array}{l} q = (y, z), |q| \leq 1 \\ \frac{3\gamma}{2} < \Gamma \\ |u| \leq 2\pi \end{array}$$

The dynamics : $\dot{q} = F_0(q) + u F_1(q)$

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

⇒ The **singular extremals** are those contained in $H_1 = 0$.

Single spin : singular extremals

⇒ The **singular extremals** are those contained in $H_1 = 0$.

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

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 $u_s(q) = \gamma(2\Gamma - \gamma)/(2\delta y)$
⇒ $u_s \in L^1$, $u_s \notin L^2$

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

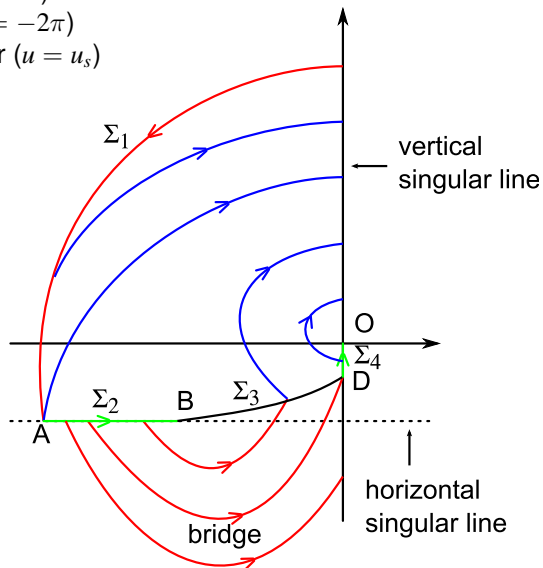
Single spin : global synthesis

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)

⇒ we need to know the **structure a priori**.

⇒ we use an **homotopic approach** to capture the structure and initialize the multiple shooting method.

Homotopy

$$(P_\lambda) \left\{ \begin{array}{l} - (y_2^2(t_f) + z_2^2(t_f)) + (1 - \lambda) \int_0^{t_f} u^{2-\lambda}(t) dt \rightarrow \min \\ \left[\begin{array}{l} \dot{y}_1 = - \Gamma_1 y_1 - u z_1 \\ \dot{z}_1 = \gamma_1 (1 - z_1) + u y_1 \\ \dot{y}_2 = - \Gamma_2 y_2 - u z_2 \\ \dot{z}_2 = \gamma_2 (1 - z_2) + u y_2 \end{array} \right. \quad \begin{array}{l} q_i = (y_i, z_i), |q_i| \leq 1, i = 1, 2 \\ \gamma_i = 1/(32.3 T_{i1}) \\ \Gamma_i = 1/(32.3 T_{i2}) \end{array} \\ q_1(0) = (0, 1) = q_2(0) \\ q_1(t_f) = (0, 0) \end{array} \right. \quad |u| \leq 2\pi$$

Homotopy $(P_\lambda) : - (y_2^2(t_f) + z_2^2(t_f)) + (1 - \lambda) \int_0^{t_f} u^{2-\lambda}(t) dt \rightarrow \min$

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) .
- $\lambda < 1 \Rightarrow \begin{cases} u = \text{sign}(H_1) \cdot \{2|H_1|/((2 - \lambda)(1 - \lambda))\}^{1/(1-\lambda)} & \text{if } |u| \leq 2\pi \\ u = 2\pi \text{ sign}(H_1) & \text{else} \end{cases}$

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) :

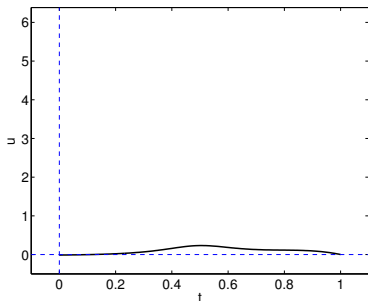
spin 1 spin 2

fluid/water case	-	$\begin{array}{ l} T_{11} = 2000 \\ T_{12} = 200 \end{array}$	$\begin{array}{ l} T_{21} = 2500 \\ T_{22} = 2500 \end{array}$	-	contrast \simeq 0.65
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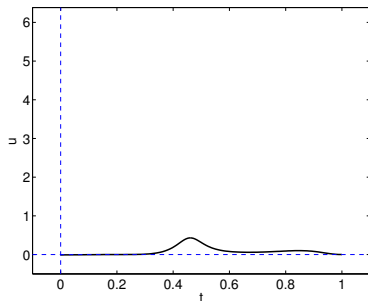
[CCG] J.B. Caillaud, O. Cots, and J. Gergaud.
HAMPATH apo.enseeiht.fr/hampath.

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

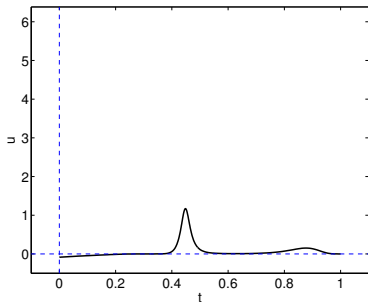
$\lambda = 0$



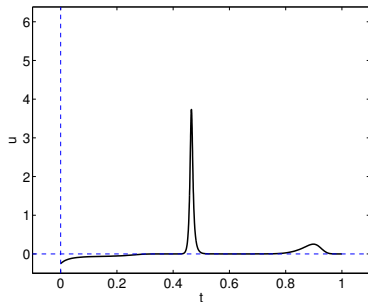
$\lambda = 0.6$



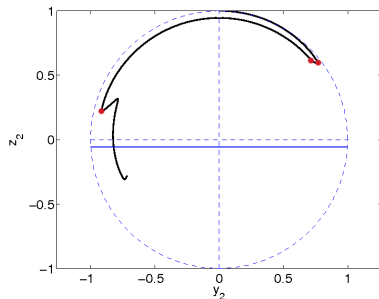
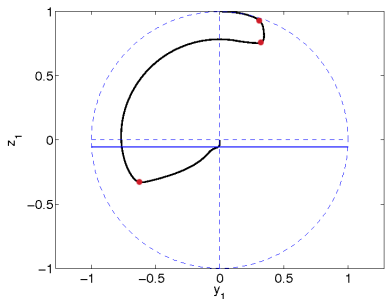
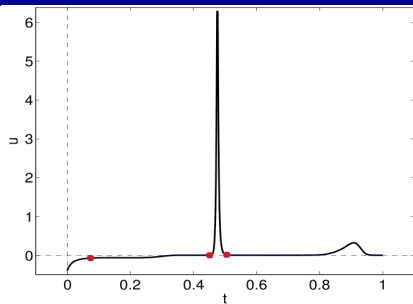
$\lambda = 0.8$



$\lambda = 0.9$



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 :**

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

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

	<i>Bang</i>		<i>Sing</i>		<i>Bang</i>		<i>Sing</i>	
(t_0, z_0)	\longrightarrow	(t_1, z_1)	\longrightarrow	(t_2, z_2)	\longrightarrow	(t_3, z_3)	\longrightarrow	(t_f, z_f)
$q_1 = (0, 1)$		$H_1 = 0$				$H_1 = 0$		$q_1 = (0, 0)$
$q_2 = (0, 1)$		$\dot{H}_1 = 0$				$\dot{H}_1 = 0$		$q_2 = p_2$

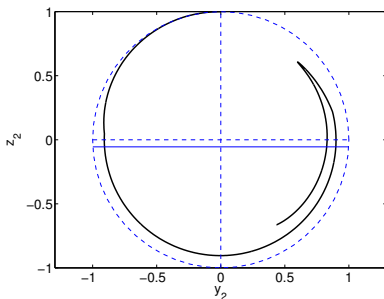
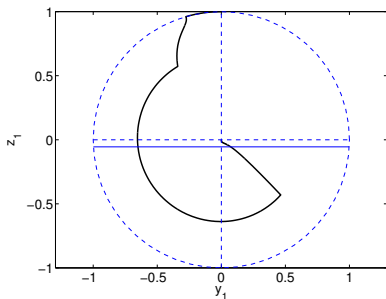
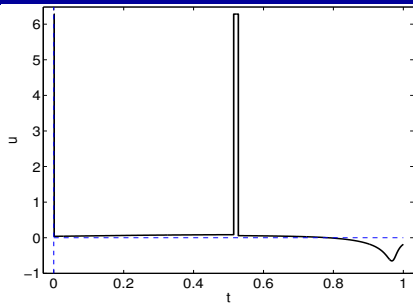
with the matching conditions :

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

[Mau76] H Maurer. . .

Numerical solution of singular control problems using multiple shooting techniques.
Journal of optimization theory and applications, Jan 1976.

States-Control : fluid/water case ($\lambda = 1.0$)

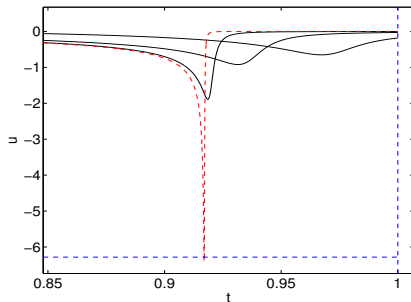


Contrast problem : continuation on t_f

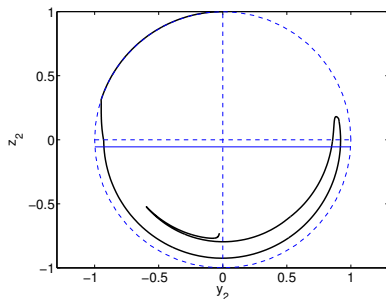
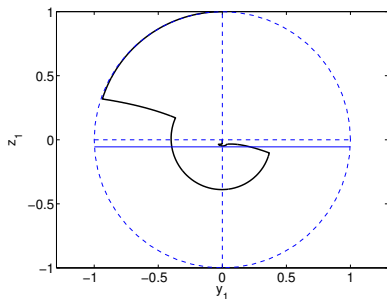
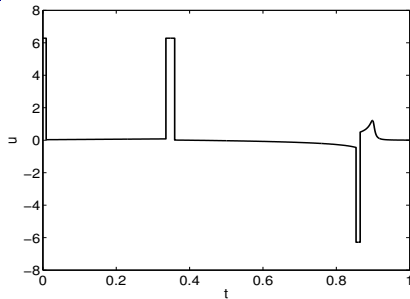
We use HAMPATH to perform a differential continuation on t_f from $2T_{min}$ to $T_{min} + \varepsilon$.

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

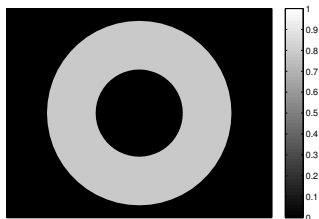
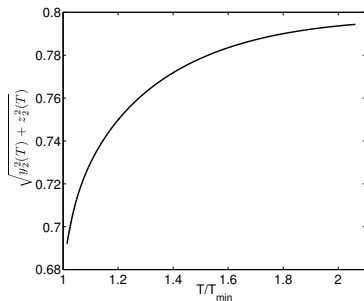
\Rightarrow Problem for $t_f = 1.22T_{min}$. The norm of the second singular control becomes greater than the boundary 2π . The structure changes. We need one more bang arc.



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

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

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.

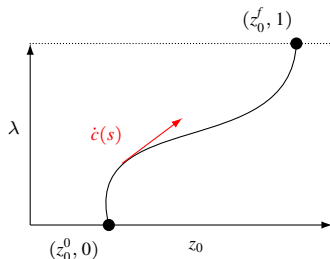
Introduction to numerical continuation methods, volume 45 of *Classics In Applied Mathematics*.
SIAM, 2003.

Differential algorithms

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

$$(IVP) \begin{cases} \dot{c}(s) = T(c(s)) \\ c(0) = (z_0^0, 0) \end{cases}$$

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.

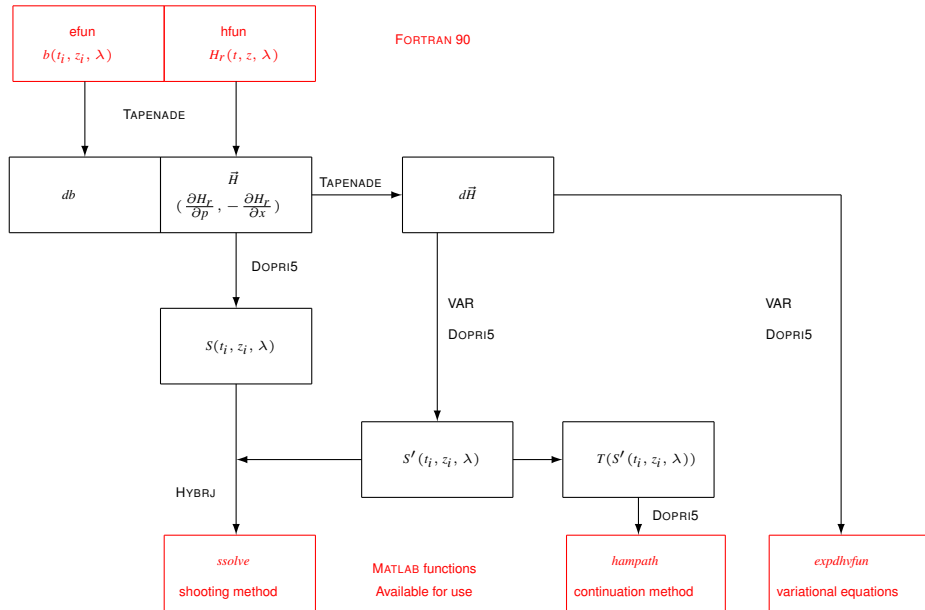
[HW] E. Hairer and G. Wanner. DOPRI5 <http://www.unige.ch/~hairer/prog/nonstiff/dopri5.f>.

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 **variational equations** used in the jacobian of the shooting function (thanks **TAPENADE**)
- integrates the variational equations so that this **diagram commutes**

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

Global diagram



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. Caillaud, O. Cots, and J. Gergaud.
HAMPATH apo.enseeiht.fr/hamopath.
- [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.