Résolution de problème de contrôle optimal en mécanique quantique par des méthodes de continuation et de tir multiple

Conférence MODE 2012 - Dijon
Mathématiques de l'Optimisation et de la décision

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Dijon, 28-30 mars 2012

Introduction - Collaborations

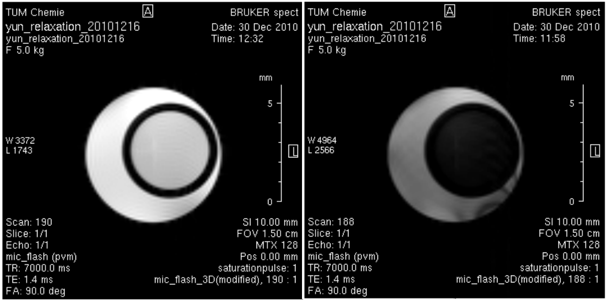

Figure: (LHS) Hard pulse of 90°. (RHS) Optimal solution.

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

Contrast problem

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

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

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

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

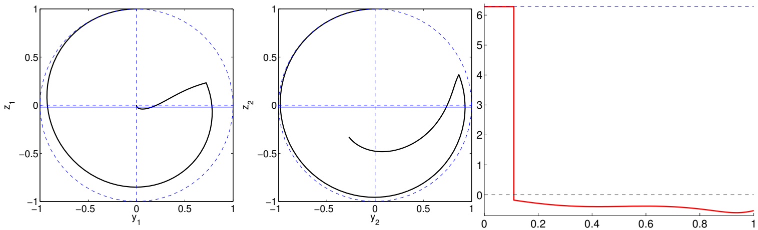


Figure: Trajectories of spin 1, 2 and the control associated for the Blood case.

Single spin problem (see [BCG+11])

$$(P_1)\begin{cases} t_f \to \min \\ \begin{bmatrix} \dot{y} & = & -\Gamma y & - u\, z \\ \dot{z} & = & \gamma(1-z) & + u\, y \end{bmatrix} \\ q(0) = (0,1) \\ q(t_f) = (0,0) \end{cases}$$

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

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

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

The dynamics: $\dot{q} = F(q) + u\, G(q)$

The Hamiltonian: $H(q,u,p) = H_F(q,p) + u\, H_G(q,p),\ H_i =< p, F_i >, i = F, G$

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

[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.

Single spin: singular extremals

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

$$\left.\begin{array}{lllll} H_G & = & <p, G> & = & 0 \\ \dot{H}_G & = & <p, [G, F]> & = & 0 \end{array}\right\} \Rightarrow \det(G, [G, F]) = y(-2\delta z + \gamma) = 0$$

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 $\ddot{H}_G = \{\{H_G, H_F\}, H_F\}(z) + u_s\{\{H_G, H_F\}, H_G\}(z) = 0$.

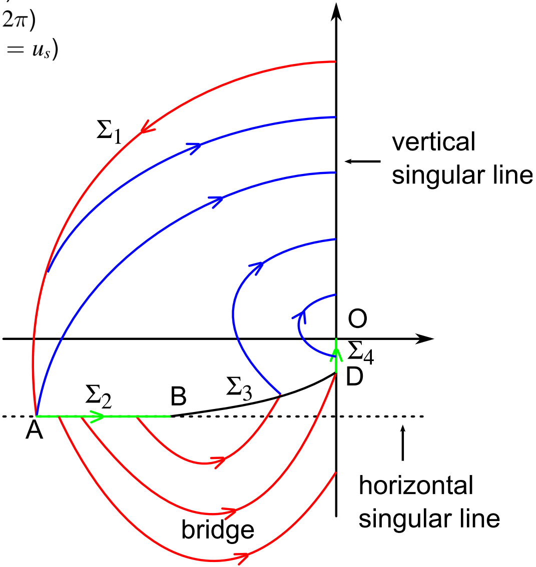
Horizontal line ($z_0 = \frac{\gamma}{2\delta}$): optimal, according to Generalized Legendre-Clebsch condition (see [BC03]) and $u_s(q) = \gamma(2\Gamma - \gamma)/(2\delta y) \Rightarrow u_s \in L^1$, $u_s \notin L^2$

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

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

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.

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

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

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

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

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

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: $H(q,u,p,\lambda)=H_F(q,p)+u\,H_G(q,p)+(1-\lambda)\,|u|^{2-\lambda}$

(P_λ)-extremals are admissible for (P).

Maximum principle

The maximization of the Hamiltonian gives:

$$u(q,p,\lambda) = \underset{w \in U}{argmax} \quad H(q,w,p,\lambda)$$

and we have

$$\lambda < 1 \Rightarrow \begin{cases} u = & sign(H_G).\{\frac{2|H_G|}{((2-\lambda)(1-\lambda))}\}^{\frac{1}{(1-\lambda)}} \quad if\ |u| \leq 2\pi \\ u = 2\pi & sign(H_G) \quad else \end{cases}$$

We call true Hamiltonian the function (which does not depend on u)

$$H_r(q,p,\lambda) = H(q,u(q,p,\lambda),p,\lambda)$$

In order to solve the problem (P) in $\lambda = 1$, we:

1. solve by simple shooting method the problem in $\lambda = 0$ easily,
2. use homotopic method to solve (P_λ), from $\lambda = 0$ to $\lambda = \lambda_f < 1$, to ...
3. ... capture the structure of (P) and initialize the multiple shooting method.

1: Solving in $\lambda = 0$ with simple shooting method

The final time t_f is equal to $1.1T_{min}$ where T_{min} is the minimal time to transfer the spin 1 from $(0, 1)$ to $(0, 0)$.

Blood case:
Spin 1 = (De)oxygenate blood : $T_{11} = 1350$ and $T_{21} = 200$
Spin 2 = Oxygenate blood : $T_{12} = 1350$ and $T_{22} = 50$

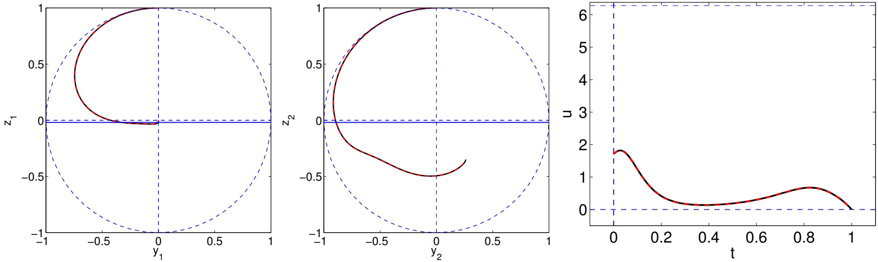


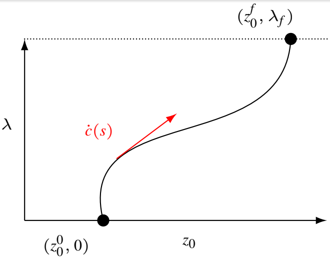
Figure: Solution for $\lambda = 0$ with $L^{2-\lambda}$ regularization. Trajectories of spin 1 and 2 and the control associated.

Let us define the homotopic function

$$h : \mathbf{R}^{2n} \times [0,1] \longrightarrow \mathbf{R}^{2n}$$
$$(z_0, \lambda) \longmapsto S_\lambda(z_0)$$

with $z_0 = (q_0, p_0)$.
Assuming that 0 is a regular value for h, the level set $\{h = 0\}$ is a one dimensional submanifold of $\mathbf{R}^{2n+1}$ called the path of zeros.

We know a zero of $h(., \lambda)$ for $\lambda_0 = 0$ noted z_0^0, and we want to follow this path to reach a zero for a target value of the parameter λ close to 1.



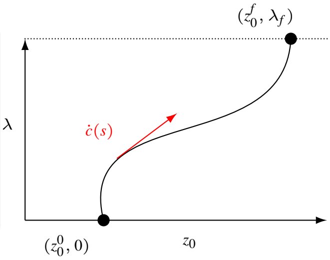
HAMPATH uses DOPRI5 from E. Hairer and G. Wanner [HrW93] [HW], for the numerical integration (without any correction) of:

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

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

Under generic assumptions, $\dot{c}(s) = T(c(s))$ is determined by

1. $h'(c(s))\dot{c}(s) = 0$
2. $|\dot{c}(s)|$=1
3. $\det \begin{pmatrix} h'(c(s)) \\ {}^t\dot{c}(s) \end{pmatrix}$ is of constant sign



[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.`

The path of zeros: $\lambda_f = 0.915$.

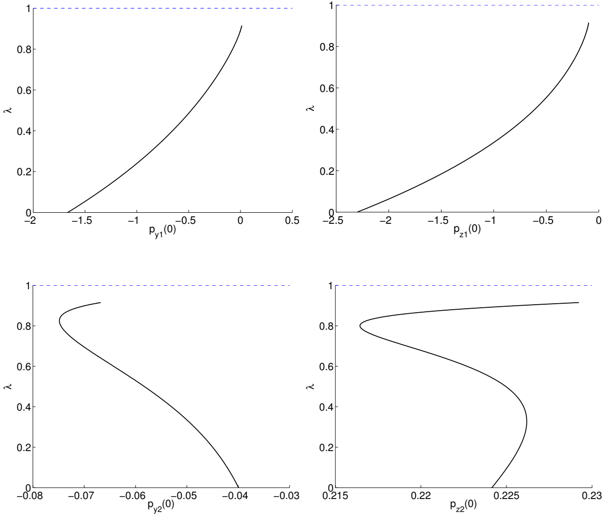
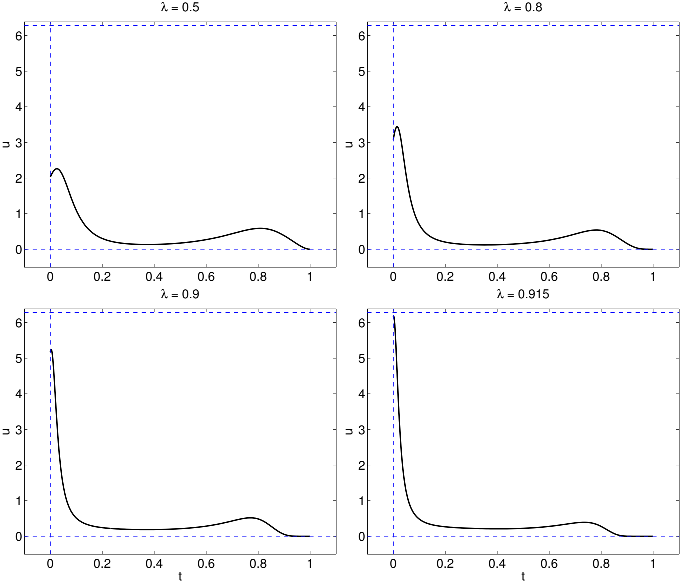
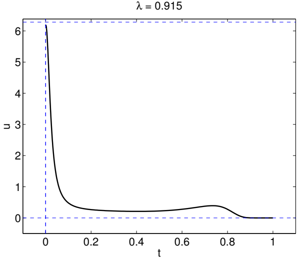


Figure: Homotopic path with $L^{2-\lambda}$ regularization. Initial adjoint vector w.r.t. λ.

Control: $\lambda \in \{0.5, 0.8, 0.9, 0.915\}$





$\longrightarrow$ Bang-Singular structure.

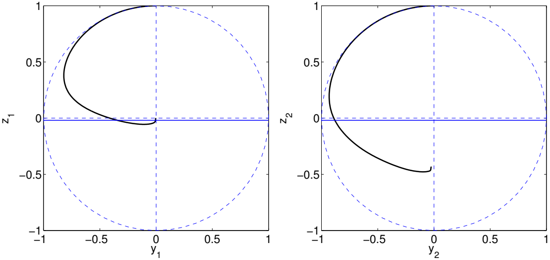


Figure: Solution for $\lambda = 0.915$ with $L^{2-\lambda}$ regularization. Trajectories of spin 1 and 2 and the control associated.

3: multiple shooting

We have a BS structure for $t_f = 1.1T_{min}$. We denote by t_0, t_1, t_f the different instants and by z_0, z_1, 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 :
  $$H(q,u,p) = H_F(q,p) + u\, H_G(q,p), \begin{cases} u = 2\pi & \text{if } t \in [t_0; t_1] \\ u = u_{sing} & \text{if } t \in [t_1; t_f] \end{cases}$$
- Equations (*cf.* [Mau76]) :

$$\begin{array}{lcccl} & \textit{Bang} & & \textit{Sing} & \\ (t_0, z_0) & \longrightarrow & (t_1, z_1) & \longrightarrow & (t_f, z_f) \\ q_1 = (0,1) & & H_G = 0 & & q_1 = (0,0) \\ q_2 = (0,1) & & \dot{H}_G = 0 & & q_2 = p_2 \end{array}$$

with the matching conditions $z(t_1; t_0, z_0) = z_1$.

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

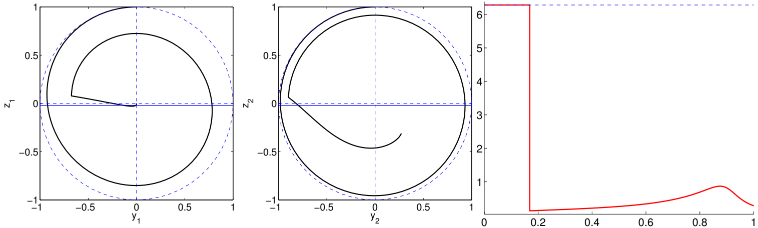


Figure: First solution (contrast of 0.41) from the $L^{2-\lambda}$ regularization.

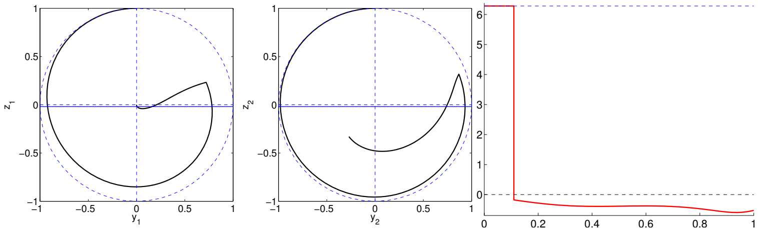


Figure: Second solution (contrast of 0.42) from the $L^{2-\lambda}$ regularization.

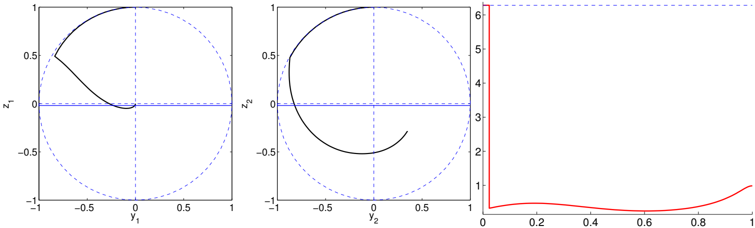


Figure: Best solution (contrast of 0.45) from the $L^{2-\lambda}$ regularization.

Remark: other possible homotopy

Let us define the L^2 regularization : $-\left(y_2^2(t_f) + z_2^2(t_f)\right) + (1-\lambda)\int_0^{t_f} |u|^2(t)dt \to \min$

The Hamiltonian becomes : $H(q,u,p,\lambda) = H_F(q,p) + u\, H_G(q,p) + (1-\lambda)\, |u|^2$

And the maximization of the H gives : $\lambda < 1 \Rightarrow \begin{cases} u = & -\frac{H_G}{2(1-\lambda)p^0} & \textit{if } |u| \leq 2\pi \\ u = & 2\pi\, sign(H_G) & \textit{else} \end{cases}$

We find the same solutions but the structure appears not very clearly during the continuation process.

First conclusion

- We have an optimal control problem with Bang and Singular arcs. The regularizations $L^{2-\lambda}$ and L^2 permit to find solutions satisfying the first order necessary conditions of optimality.
- To solve in $\lambda = 0$ is very easy.
- $L^{2-\lambda}$ captures the BS structure very well compared to L^2.

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

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

$\hookrightarrow$ there is an horizontal asymptote on the contrast plot. The optimal solution in terms of contrast is obtain from $t_f = 1.3T_{min}$.

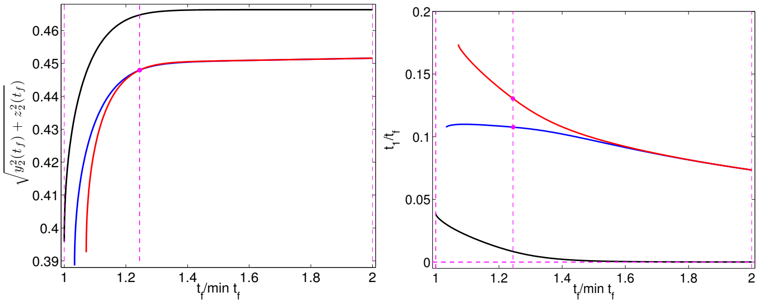


Figure: Best solution in black. (LHS) Contrast w.r.t the transfer duration. (RHS) Normalized duration of the Bang arc.

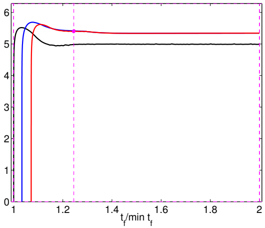


Figure: The minimal distance between the singular control and the saturation with respect to the final time.

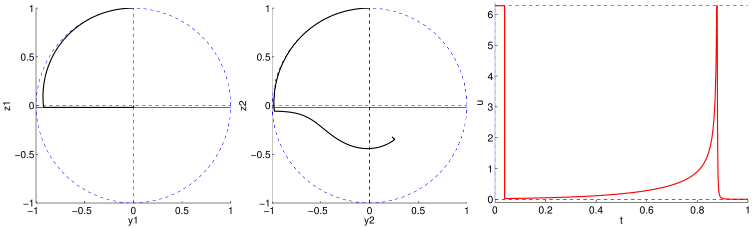


Figure: Best solution for $t_f = 1.000004 \times \min t_f$.

HAMPATH package

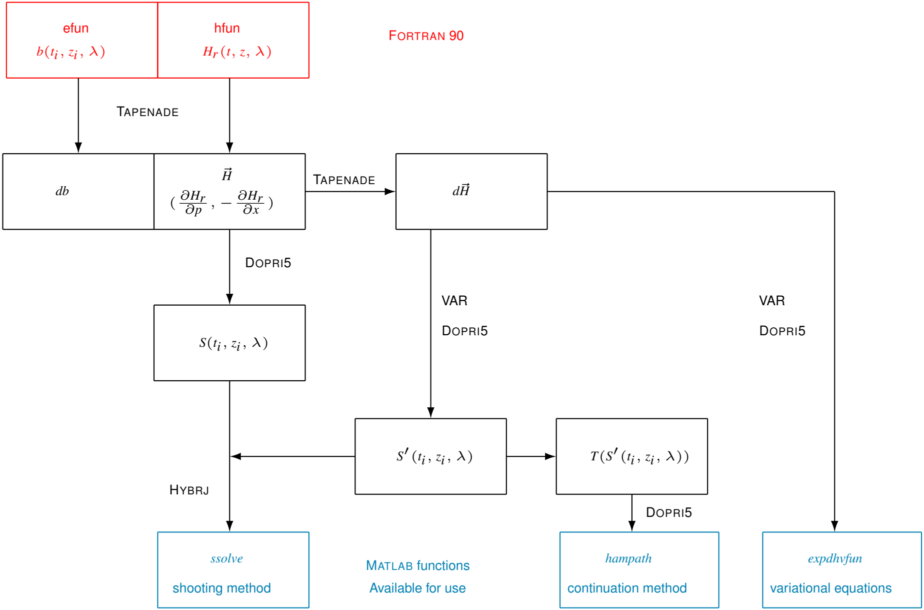
From the true hamiltonian and the boundary, intermediate and transversality conditions, HAMPATH [CCG11]:

- 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 the diagram commutes (the step size control is only made on the state and co-state equations)

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

[CCG11] J.B. Caillau, O. Cots, and J. Gergaud.
Differential pathfollowing for regular optimal control problems. HAMPATH apo.enseeiht.fr/hampath.
Optimization Methods and Software, to appear, 2011.

Global diagram of HAMPATH



Last conclusion

- The HAMPATH package gives tools to solve OCP by indirect methods:
  - Shooting methods: simple and multiple;
  - Homotopic methods: differential without correction;
  - Function which integrate the variationnal equations and permit to check sufficient second order conditions in the smooth case;
  - ...
- The derivatives and the functions are computed accurately and automatically.
- It is very easy to use since only 2 FORTRAN subroutines need to be implemented. Then it is interfaced with MATLAB.

- 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.
- Work in progress:
  - Second order conditions for the contrast problem with BS structure (see [BC12] for details);
  - Convergence of the zeros path to the best solution.

[BC12] B. Bonnard and O. Cots.
Geometric numerical methods and results in the control imaging problem in nuclear magnetic resonance.
submitted to Mathematical Models and Methods in Applied Sciences (M3AS), 2012.

[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.
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[BC12] B. Bonnard and O. Cots.
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Geometric optimal control of the contrast imaging problem in nuclear magnetic resonance.
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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.

[CCG11] J.B. Caillau, O. Cots, and J. Gergaud.
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Optimization Methods and Software, to appear, 2011.

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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.
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