Parareal methods for optimal control II.

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Optimal control and time-parallelization

Optimal control problems: *Minimize*

$$J(c) = F(u(T)) + \int_0^T G(u(t), c(t)) \, dt,$$

with the constraint $\dot{u} = f(u, c)$.

Context: We already have an optimal control solver. **Question:** *How to parallelize it ?*

Outline

1 The Intermediate States Method

- **2** Quantum control problems
- **3** Various optimization solvers
- 4 Full efficiency ?



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Linear or Nonlinear ??

"Non-linear control" or "Bilinear control"

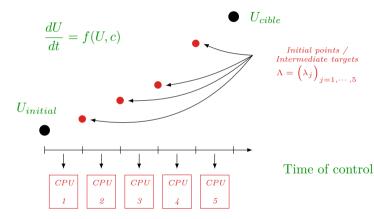
	Linear eq.	Non-linear eq.
"Linear" control	$\dot{y} = Ay + Bc$	$\dot{y} = f(y) + Bc$
Non-linear control	$\dot{y} = A(c)y$	$\dot{y} = f(y,c)$

•
$$y = y(t, x)$$
 state
• $a = a(t)$ or $a(t, x)$ conv

• c = c(t) or c(t, x) control

The Intermediate States Method

Schematic description



Disclaimer : not a parareal algorithm.

The Intermediate States Method

Schematic description

And it follows:

• Independent sub-problems

$$J \to \left(J_j\right)_{j=1,\cdots,N},$$

• Need for an update formula for the intermediate states

$$\Lambda = (\lambda_j)_{j=1,\cdots,N}.$$

The Intermediate States Method

Schematic description

Algorithm:

Given c^k , Λ^k (intermediate targets) at step k:

1 solve <u>in parallel</u> on $[T_j, T_{j+1}]$

$$\max_{c_j} J_j(c_j) \to c_j^{k+1},$$

- 2) define c^{k+1} as the concatenation of c_j^{k+1} ,
- **3** define Λ^{k+1} in a "relevant way" with c^{k+1} , so that the consistency lemma holds.

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Example of quantum control: Schrödinger Equation:

$$i\frac{\partial\psi(x,t)}{\partial t} = \left[-\frac{\hbar}{2m}\Delta + V(x) - \mu(x)\mathbf{c(t)}\right]\psi(x,t)$$

Cost functional:

$$J(c) = 2\Re \langle \psi_{target} | \psi(.,T) \rangle - \int_0^T \alpha(t) c^2(t) dt$$

$$\left(=2 - \|\psi_{target} - \psi(.,T)\|_{L^2}^2 - \int_0^T \alpha(t)c^2(t)dt\right)$$

...to be maximized.

$$J(c,\psi,\chi) = 2\Re \langle \psi_{target} | \psi(.,T) \rangle - \int_0^T \alpha(t) c^2(t) dt$$
$$-2\Re \int_0^T \langle \chi(.,t) | \partial_t + iH - \mu c(t) | \psi(.,t) \rangle dt.$$

Optimality system:

$$\nabla_{\chi} J \rightarrow \begin{cases} i \frac{\partial}{\partial t} \psi(x,t) = (H - c(t)\mu(x))\psi(x,t) \\ \psi(x,t=0) = \psi_0(x) \end{cases}$$
$$\nabla_{\psi} J \rightarrow \begin{cases} i \frac{\partial}{\partial t} \chi(x,t) = (H - c(t)\mu(x))\chi(x,t) \\ \chi(x,t=T) = \psi_{target}(x) \end{cases}$$
$$\nabla_c J \rightarrow \quad \alpha(t)c(t) = -\Im < \chi(.,t)|\mu|\psi(.,t) > \end{cases}$$

Parallelization setting:

Define $\lambda_0 = \psi_0$, $\lambda_N = \psi_{target}$, $c_j = c_{|[T_j, T_{j+1}]}$ and $\beta_j = \frac{T}{T_{j+1} - T_j}$.

$$J_{\parallel}(c,\Lambda) = \sum_{j=0}^{N-1} \beta_j J_j(c_j,\lambda_j,\lambda_{j+1})$$

where J_j are the parareal cost functionals:

$$J_j(c_j, \lambda_j, \lambda_{j+1}) = \|\psi_j(T_{j+1}^-) - \lambda_{j+1}\|_{L^2}^2 + \int_{T_j}^{T_{j+1}} \alpha'_j(t) c_j(t)^2 dt,$$
$$\alpha'_j(t) = \frac{\alpha(t)}{\beta_j}, \ \psi_j(T_j^+) = \lambda_j.$$

The Intermediate States Method Quantum Control

Theorem: Given c, with the previous notations, let us define $\Lambda^c = (\lambda_j^c)_{j=1,\dots,N-1}$ by:

$$\lambda_j^c = (1 - \gamma_j)\psi(T_j) + \gamma_j\chi(T_j),$$

where $\gamma_j = \frac{T_j}{T}$. Then :

$$\Lambda^c = \operatorname{argmin}_{\Lambda} (J_{\parallel}(c, \Lambda)).$$

Moreover we have:

$$J_{\parallel}(c,\Lambda^c) = J(c).$$

Y. Maday, J. Salomon, G. Turinici, SIAM J. Num. Anal., 45 (6) (2007)

Convergence?

$$\begin{aligned} J_{\parallel}(c^{k+1},\Lambda^{k+1}) - J_{\parallel}(c^{k},\Lambda^{k}) &= J_{\parallel}(c^{k+1},\Lambda^{k+1}) - J_{\parallel}(c^{k},\Lambda^{k+1}) \\ J_{\parallel}(c^{k},\Lambda^{k+1}) - J_{\parallel}(c^{k},\Lambda^{k}) \end{aligned}$$

Convergence?

$$\begin{split} J_{\parallel}(c^{k+1},\Lambda^{k+1}) - J_{\parallel}(c^{k},\Lambda^{k}) &= & J_{\parallel}(c^{k+1},\Lambda^{k+1}) - J_{\parallel}(c^{k},\Lambda^{k+1}) \\ & & J_{\parallel}(c^{k},\Lambda^{k+1}) - J_{\parallel}(c^{k},\Lambda^{k}) \\ &\geq & J_{\parallel}(c^{k+1},\Lambda^{k+1}) - J_{\parallel}(c^{k},\Lambda^{k+1}). \end{split}$$

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 \Rightarrow The proof of convergence is reduced to the one of the optimization solver.

Quantum control problems Nuclear Magnetic Resonance

Another example: Nuclear Magnetic Resonance



<u>Aim</u> : control spin using Magnetic fields.

Applications :

- Medical imaging
- Quantum computing
- Porous media identification

• ...

Quantum control problems Nuclear Magnetic Resonance

Toy model : Bloch equations

$$i\partial_t U(t) = [H_0 + \sum_{\ell}^L \omega_{\ell}(t)H_{\ell}]U(t)$$
$$U(t=0) = U_0.$$

Optimal control problem:

find $\Omega^{\star}(t) = (\omega_1^{\star}(t), \cdots, \omega_L^{\star}(t))$, that solves

$$\Omega^{\star} = \operatorname{argmax} \left(J(\Omega) \right) = \operatorname{argmax} \left(Re \langle U(T), U_{target} \rangle \right).$$

K. Riahi, J. Salomon, D. Sugny, Physical Review A (2016).

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5 Conclusion

Various optimization solvers Standard Gradient method

What about the optimization solver ? We can show that :

$$\nabla J(\mathbf{c})_{|[T_j,T_{j+1}]} = \frac{T_{j+1} - T_j}{T} \nabla J_j(\mathbf{c}_{|[T_j,T_{j+1}]}).$$

FOR EVERY *c* !

 \Rightarrow the intermediate target method provides a **decomposition of the gradient** that enables parallelization.

Various optimization solvers Standard Gradient method

Constant step gradient method \Rightarrow Full efficiency !

Algebraic identity:

$$J(c') - J(c) = \int_0^T (c(t) - c'(t)) \Big(\alpha(t) (c(t) + c'(t)) + 2\Im \langle \chi(.,t) | \mu | \psi'(.,t) \rangle \Big) dt$$

Algebraic identity:

$$\begin{split} J(c') - J(c) &= \int_0^T \left(c(t) - c'(t) \right) \Big(\alpha(t) \left(c(t) + c'(t) \right) \\ &+ 2 \Im \langle \chi(.,t) | \mu | \psi'(.,t) \rangle \Big) dt \\ &\longrightarrow c^{k+1} = -\frac{1}{\alpha(t)} \Im \langle \chi^k(.,t) | \mu | \psi^{k+1}(.,t) \rangle \end{split}$$

Algebraic identity:

$$J(c') - J(c) = \int_0^T (c(t) - c'(t)) \left(\alpha(t) (c(t) + c'(t)) + 2\Im \langle \chi(.,t) | \mu | \psi'(.,t) \rangle \right) dt$$

$$\Rightarrow J(c^{k+1}) - J(c^k) = \int_0^T \alpha(t) (c^{k+1}(t) - c^k(t))^2 dt \ge 0$$

Convergence?

$$\begin{aligned} J_{\parallel}(c^{k+1},\Lambda^{k+1}) - J_{\parallel}(c^{k},\Lambda^{k}) &= & J_{\parallel}(c^{k+1},\Lambda^{k+1}) - J_{\parallel}(c^{k},\Lambda^{k+1}) \\ & & J_{\parallel}(c^{k},\Lambda^{k+1}) - J_{\parallel}(c^{k},\Lambda^{k}) \\ &\geq & J_{\parallel}(c^{k+1},\Lambda^{k+1}) - J_{\parallel}(c^{k},\Lambda^{k+1}) \end{aligned}$$

Convergence?

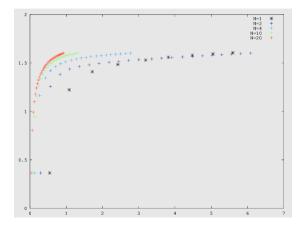
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 \Rightarrow Monotonicity preserved by the parallelization.

Monotonic algorithm



N	$\frac{Time_{seq}}{N \cdot Time_{\parallel}}$
1	-
2	41.7%
4	45.8%
10	39.4%
20	27.2%

Various optimization solvers Newton method

Newton

Here, our parallelization method not only improves the Newton convergence makes it possible .

N	$N \cdot Time_{\parallel}$
1	-
2	-
4	33.722
10	3.2544
20	0.72559

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Full efficiency ?

The optimization is achieved in parallel, but $\psi(t)$ and $\chi(t)$ seem to require solving on [0, T] (full propagation) ?

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NO $!!! \rightarrow \text{only } \psi(t_j) \text{ and } \chi(t_j) \text{ are required.}$

 \Rightarrow For low dimensional systems, the propagators $t_j \rightarrow t_{j+1}$ can be computed in parallel, when computing the gradient !

Full efficiency ?

For large systems:

• Use the parareal algorithm to achieve full propagations, see

"Parareal in time intermediate targets methods for optimal control problem", Y. Maday, J. Salomon, K. Riahi, Proc. of " Control and Optimization of PDEs ", (Birkhäuser, Basel)

• Use model reduction...

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Conclusion

- Generic approach with respect to the solver,
- Definition of the intermediate states depends on the problem,
- Limit preserving parallelization strategy,
- Full efficiency obtained in some cases.

Merci !