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Control of Laser Surface Hardening by a Memory Efficient Approach of Second Order

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Outline

1. Optimal control problem
2. Multiple sweep algorithm
3. Nested checkpointing
4. Numerical results
5. Summary and conclusion

1. Optimal control problem

$$\min_{\mathbf{u}\in\mathcal{U}_{ad}} \phi(\mathbf{x}(T)),$$

$$\dot{\mathbf{x}} = f(\mathbf{x}(t), \mathbf{u}(t), t), \qquad \mathbf{x}(0) = \mathbf{x}_0$$

Adjoint problem

$$\dot{\bar{\mathbf{x}}} = -H_{\mathbf{x}}^T = -f_{\mathbf{x}}^T\,\bar{\mathbf{x}}, \qquad \bar{\mathbf{x}}(T) = \phi_{\mathbf{x}}^T(\mathbf{x}(T))$$

First order necessary optimality condition

$$H_{\mathbf{u}}^T = f_{\mathbf{u}}^T\,\bar{\mathbf{x}} = 0, \qquad 0 \le t \le T$$

Express $\mathbf{u}(t)$ in terms of $\mathbf{x}(t)$ and $\bar{\mathbf{x}}(t)$

$$H_{\mathbf{u}}^T = f_{\mathbf{u}}^T\,\bar{\mathbf{x}} = 0 \Rightarrow \mathbf{u}(t) = \mathbf{u}(\mathbf{x}(t), \bar{\mathbf{x}}(t))$$

$\Rightarrow$ BVP with separated BC

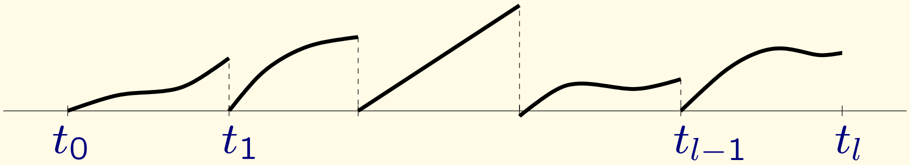
Multiple shooting technique

$$\begin{aligned} \dot{\mathbf{x}} &= f(\mathbf{x}(t), \bar{\mathbf{x}}(t)), & \mathbf{x}(0) &= \mathbf{x}_0 \\ \dot{\bar{\mathbf{x}}} &= f_{\mathbf{x}}^T(\mathbf{x}(t), \bar{\mathbf{x}}(t))\,\bar{\mathbf{x}}, & \bar{\mathbf{x}}(T) &= \phi_{\mathbf{x}}^T(\mathbf{x}(T)) \end{aligned}$$

Coose a mesh

$$0 = t_0 < t_1 < \ldots < t_{l-1} < t_l = T.$$

- Integrate IVP on each subinterval $[t_i, t_{i+1}]$
- Patch resulting solution segments over entire interval $[0, T]$
- Use separated BC and suitable decoupling



— Requires expression for $\mathbf{u}(t) = \mathbf{u}(\mathbf{x}(t), \bar{\mathbf{x}}(t))$
— Requires estimation for $\bar{\mathbf{x}}(0)$

Quasilinearization technique

Step $\delta\mathbf{x}$, $\delta\bar{\mathbf{x}}$, $\delta\mathbf{u}$ satisfy:

$$
\begin{aligned}
\delta\dot{\mathbf{x}} &= f_{\mathbf{x}}\delta\mathbf{x} + f_{\mathbf{u}}\delta\mathbf{u} && \textbf{linearized state} \\
\delta\dot{\bar{\mathbf{x}}} &= -H^T_{\mathbf{x}\mathbf{x}}\delta\mathbf{x} - H^T_{\mathbf{x}\mathbf{u}}\delta\mathbf{u} - H^T_{\mathbf{x}\bar{\mathbf{x}}}\delta\bar{\mathbf{x}} && \textbf{linearized adjoint} \\
0 &= H^T_{\mathbf{u}} + H^T_{\mathbf{u}\mathbf{u}}\delta\mathbf{u} + H^T_{\mathbf{u}\mathbf{x}}\delta\mathbf{x} + H^T_{\mathbf{u}\bar{\mathbf{x}}}\delta\bar{\mathbf{x}} && \textbf{linearized optimality}
\end{aligned}
$$

Separated boundary conditions:

$$
\begin{bmatrix} I & 0 \\ 0 & 0 \end{bmatrix}
\begin{pmatrix} \delta\mathbf{x}(0) \\ \delta\bar{\mathbf{x}}(0) \end{pmatrix}
+
\begin{bmatrix} 0 & 0 \\ -\phi^T_{\mathbf{x}\mathbf{x}}(T) & I \end{bmatrix}
\begin{pmatrix} \delta\mathbf{x}(T) \\ \delta\bar{\mathbf{x}}(T) \end{pmatrix}
=
\begin{bmatrix} \mathbf{x}_0 - \mathbf{x}(0) \\ \phi^T_{\mathbf{x}}(T) - \bar{\mathbf{x}}(T) \end{bmatrix}
$$

$\Rightarrow$ Eliminate $\delta\mathbf{u}$ from **linearized optimality** $(det(H_{\mathbf{u}\mathbf{u}}) \neq 0)$

$\Rightarrow$ Linear BVP for $\delta\mathbf{x}$ & $\delta\bar{\mathbf{x}}$

Linear BVP

$$\begin{pmatrix} \delta\dot{\mathbf{x}}(t) \\ \delta\dot{\bar{\mathbf{x}}}(t) \end{pmatrix} = \begin{pmatrix} A^{11}(t) & A^{12}(t) \\ A^{21}(t) & A^{22}(t) \end{pmatrix} \begin{pmatrix} \delta\mathbf{x}(t) \\ \bar{\mathbf{x}}(t) \end{pmatrix} + \begin{pmatrix} q^1(t) \\ q^2(t) \end{pmatrix}$$

Introduce substitution

$$\begin{pmatrix} \delta\mathbf{x}(t) \\ \delta\bar{\mathbf{x}}(t) \end{pmatrix} = \begin{pmatrix} I & 0 \\ K(t) & I \end{pmatrix} \begin{pmatrix} \delta\mathbf{x}(t) \\ y(t) \end{pmatrix}$$

$$\begin{pmatrix} \delta\dot{\mathbf{x}}(t) \\ \dot{y}(t) \end{pmatrix} = \begin{pmatrix} A^{11} + A^{12}K & A^{12} \\ \star & -KA^{12} + A^{22} \end{pmatrix} \begin{pmatrix} \delta\mathbf{x}(t) \\ y(t) \end{pmatrix} + \begin{pmatrix} g^1(t) \\ g^2(t) \end{pmatrix}$$

$\star = 0 \Rightarrow$ **Riccati equation**

$$\dot{K} = A^{21} - KA^{11} + A^{22}K - KA^{12}K, \qquad K(T) = \phi_{\mathbf{xx}}^T$$

$$\dot{y} = [-KA^{12} + A^{22}]y - Kq^1 + q^2, \qquad y(T) = 0$$

$\Rightarrow$ Decoupling can be realised using size$(\mathbf{u}) << $ size$(\mathbf{x})$

Explicit discretization

$$\min_{\mathbf{x},\mathbf{u}} \phi(\mathbf{x}_l),$$
$$\mathbf{x}_{i+1} = f_i(\mathbf{x}_i, \mathbf{u}_i), \quad i = 0, ..., l-1, \quad \mathbf{x}_0 \text{ fixed},$$

- Apply discrete Riccati approach
- Integration of discrete Riccati equation too expensive

Remedy: change the order of elimination

$$\delta\mathbf{u} = \delta\mathbf{u}(\delta\mathbf{x}, \delta\bar{\mathbf{x}})$$

and substitution

$$\begin{pmatrix} \delta\mathbf{x}_i \\ \delta\bar{\mathbf{x}}_i \end{pmatrix} = \begin{pmatrix} I & 0 \\ K_i & I \end{pmatrix} \begin{pmatrix} \delta\mathbf{x}_i \\ y_i \end{pmatrix}.$$

$\Rightarrow$ Pantoja approach [Pantoja]
$\Rightarrow$ AD implementation [Christianson]

Problem: Implicit discretisation is required
$\Rightarrow$ Straightforward extension of Pantoja algorithm

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Implicit discretization

$$\min_{\mathbf{x},\mathbf{u}} \phi(\mathbf{x}_l),$$
$$F_i(\mathbf{x}_i, \mathbf{x}_{i+1}, \mathbf{u}_i) = 0, \quad i = 0, \ldots, l-1, \quad \mathbf{x}_0 \text{ fixed},$$

Unknown expression: $\mathbf{x}_{i+1} = f_i(\mathbf{x}_i, \mathbf{u}_i)$
Find

$$f_{\mathbf{x},i} = \frac{\partial \mathbf{x}_{i+1}}{\partial \mathbf{x}_i} \quad \text{and} \quad f_{\mathbf{u},i} = \frac{\partial \mathbf{x}_{i+1}}{\partial \mathbf{u}_i}$$

using Implicit Function Theorem:

$$\frac{\partial \mathbf{x}_{i+1}}{\partial \mathbf{x}_i} = -\left(\frac{\partial F_i}{\partial \mathbf{x}_{i+1}}\right)^{-1} \frac{\partial F_i}{\partial \mathbf{x}_i} = H_{\bar{\mathbf{x}}\mathbf{x}}^\top,$$

$$\frac{\partial \mathbf{x}_{i+1}}{\partial \mathbf{u}_i} = -\left(\frac{\partial F_i}{\partial \mathbf{x}_{i+1}}\right)^{-1} \frac{\partial F_i}{\partial \mathbf{u}_i} = H_{\bar{\mathbf{x}}\mathbf{u}}^\top.$$

$\Rightarrow$ Straightforward extension of Pantoja algorithm

2. Multiple sweep algorithm

Input: $\mathbf{u}_i$ for $0 < i < l$, $\mathbf{x}_0$

$\Rightarrow$ **Original sweep:** $i : 0 \rightarrow l-1$

Solve $F_i(\mathbf{x}_i, \mathbf{x}_{i+1}, \mathbf{u}_i) = 0$ for $\mathbf{x}_{i+1}$

Adjoint initialisation:

$\bar{\mathbf{x}}_l = \phi_{\mathbf{x}}^\top(\mathbf{x}_l)$, $K_l = \phi_{\mathbf{xx}}^\top(\mathbf{x}_l)$ and $y_l = 0$

$\Leftarrow$ **Adjoint sweep:** $i : l-1 \rightarrow 0$

$$\bar{\mathbf{x}}_i = \left(\frac{\partial \mathbf{x}_{i+1}}{\partial \mathbf{x}_i}\right)^\top \bar{\mathbf{x}}_{i+1}$$
$$K_i = K(K_{i+1}, \mathbf{x}_i, \bar{\mathbf{x}}_{i+1}),\ y_i = y(y_{i+1}, \mathbf{x}_i, \bar{\mathbf{x}}_{i+1}, K_{i+1})$$

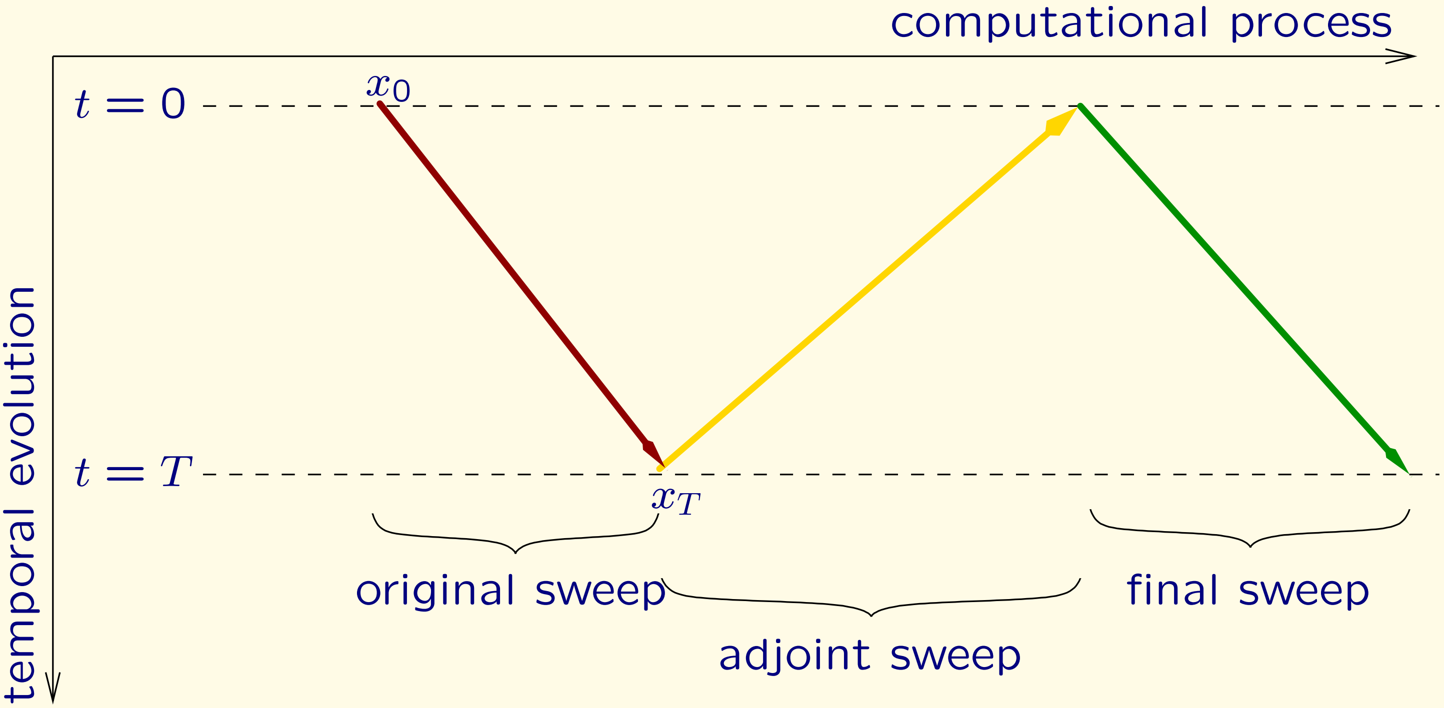
Final initialisation:

$\delta \mathbf{x}_0 = 0$

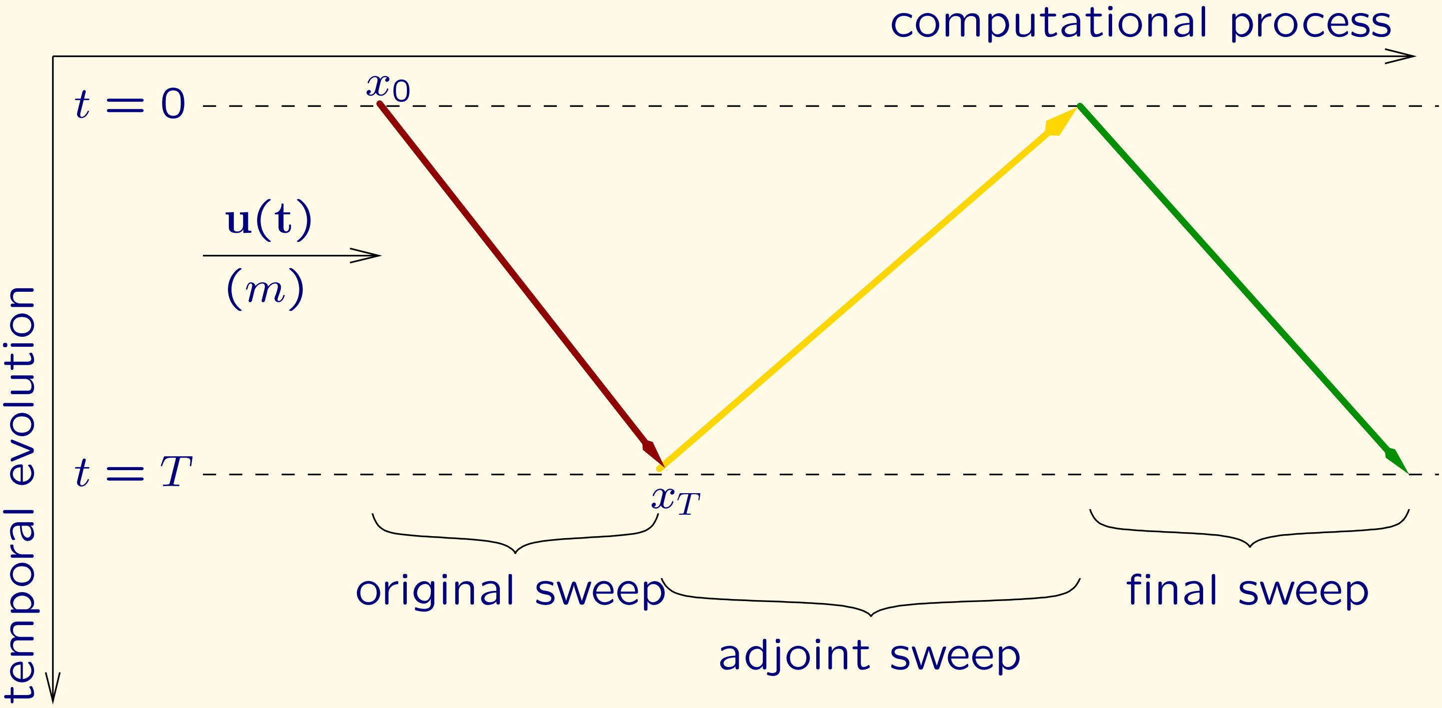
$\Rightarrow$ **Final sweep:** $i : 0 \rightarrow l-1$

$$\delta \mathbf{u}_i = \delta \mathbf{u}(\delta \mathbf{x}_i, \delta \bar{\mathbf{x}}_{i+1}, \mathbf{x}_i, \bar{\mathbf{x}}_{i+1}),\ \delta \mathbf{x}_{i+1} = \frac{\partial \mathbf{x}_{i+1}}{\partial \mathbf{x}_i}\delta \mathbf{x}_i + \frac{\partial \mathbf{x}_{i+1}}{\partial \mathbf{u}_i}\delta \mathbf{u}_i$$
$$\mathbf{u}_i^{j+1} = \mathbf{u}_i + \delta \mathbf{u}_i$$

Information flow by Riccati/Pantoja computation of Newton step



Information flow by Riccati/Pantoja computation of Newton step



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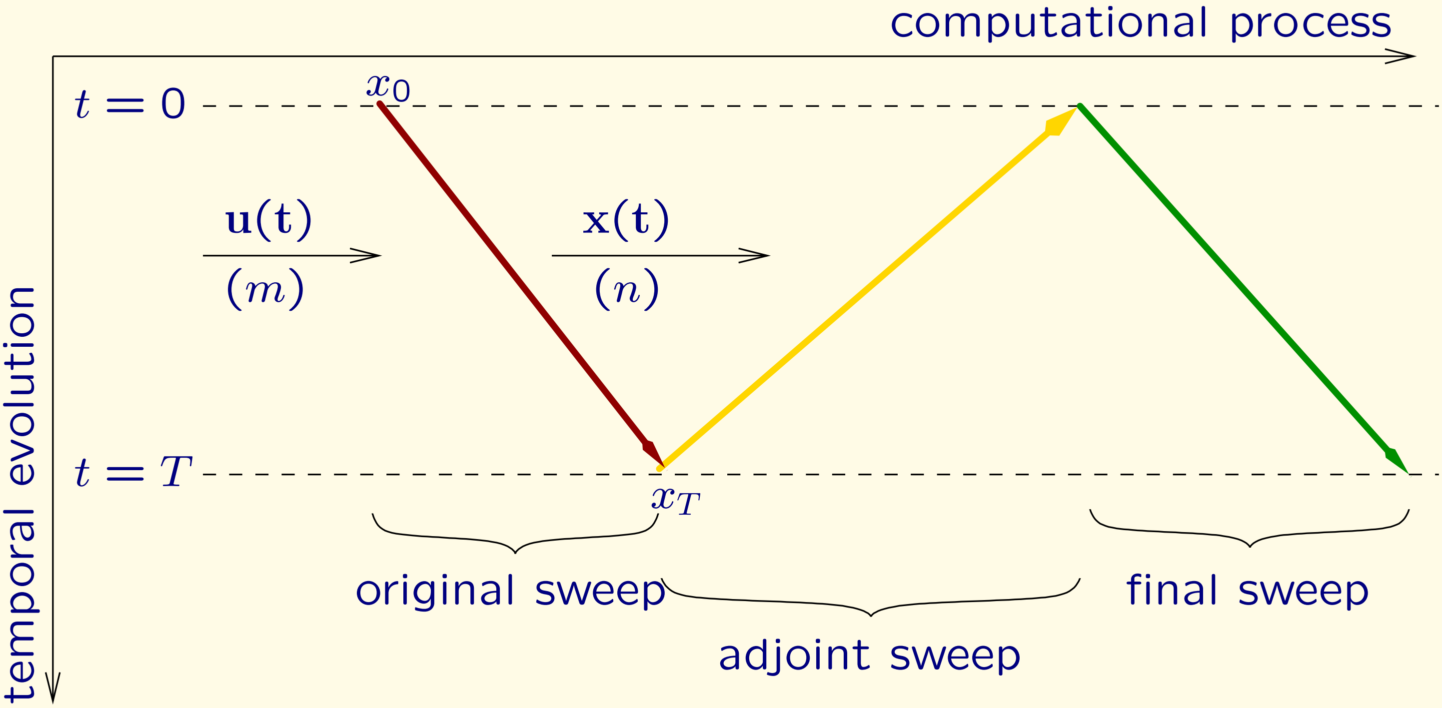
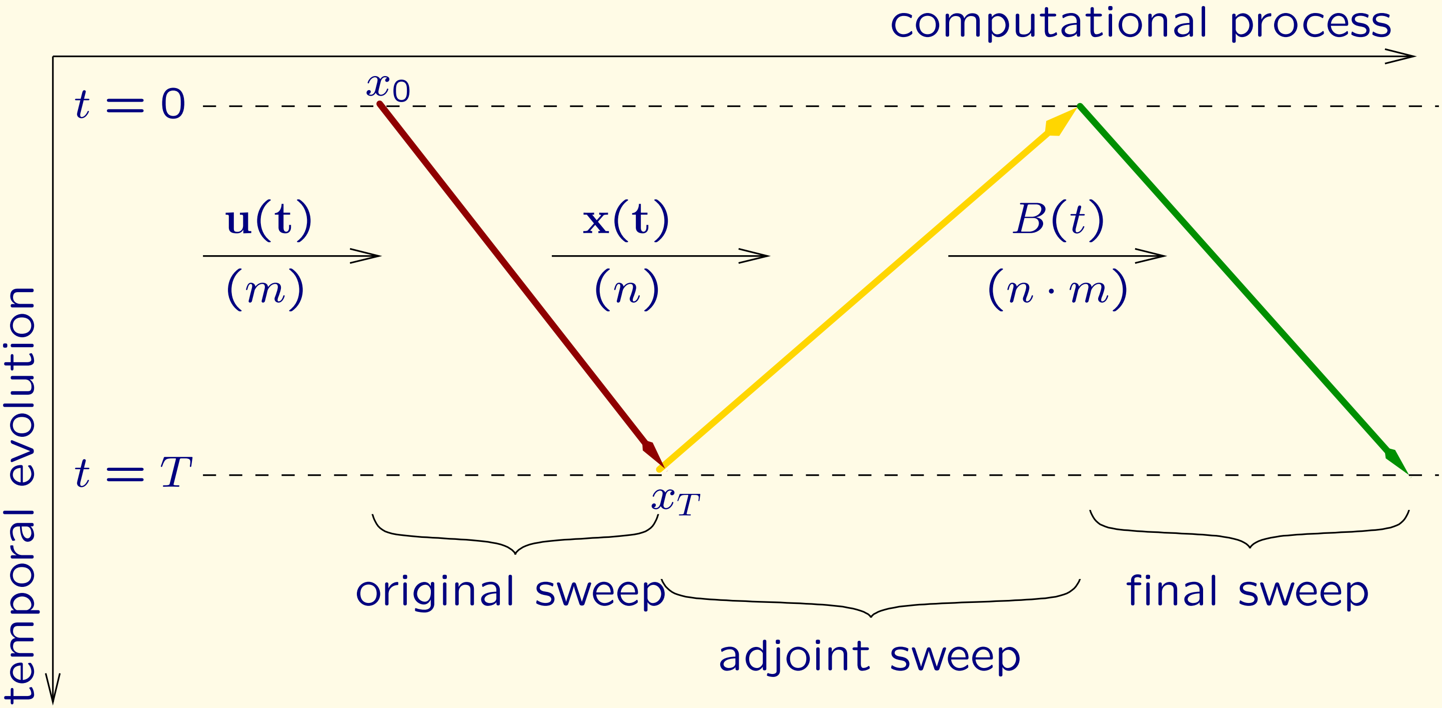


Information flow by Riccati/Pantoja computation of Newton step



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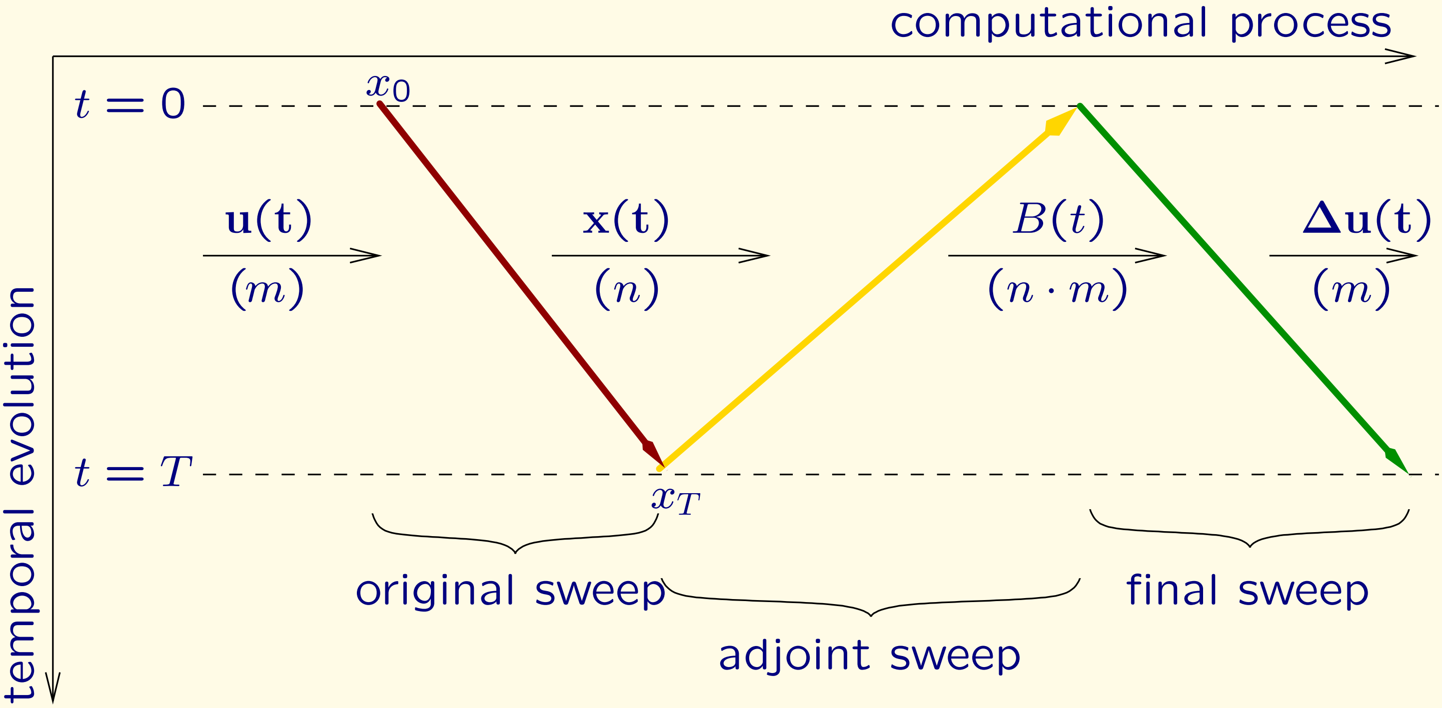
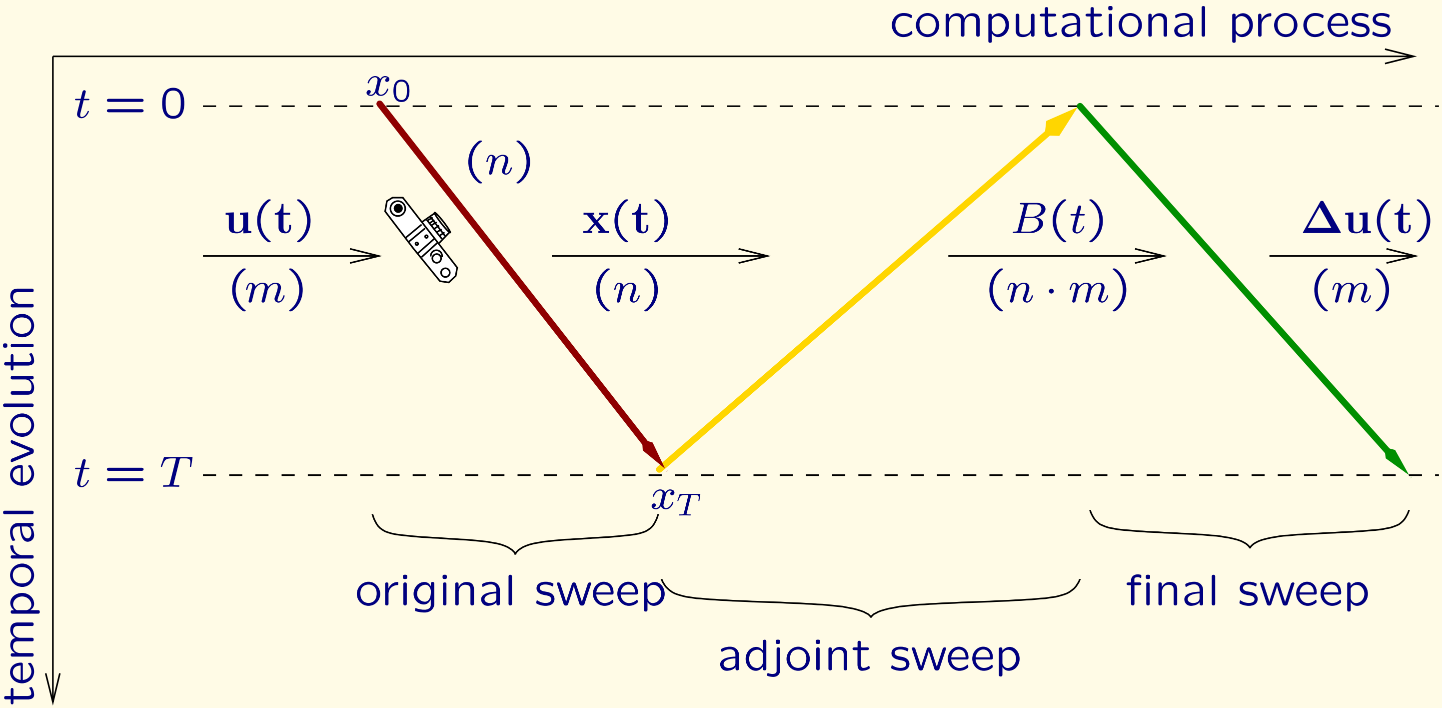
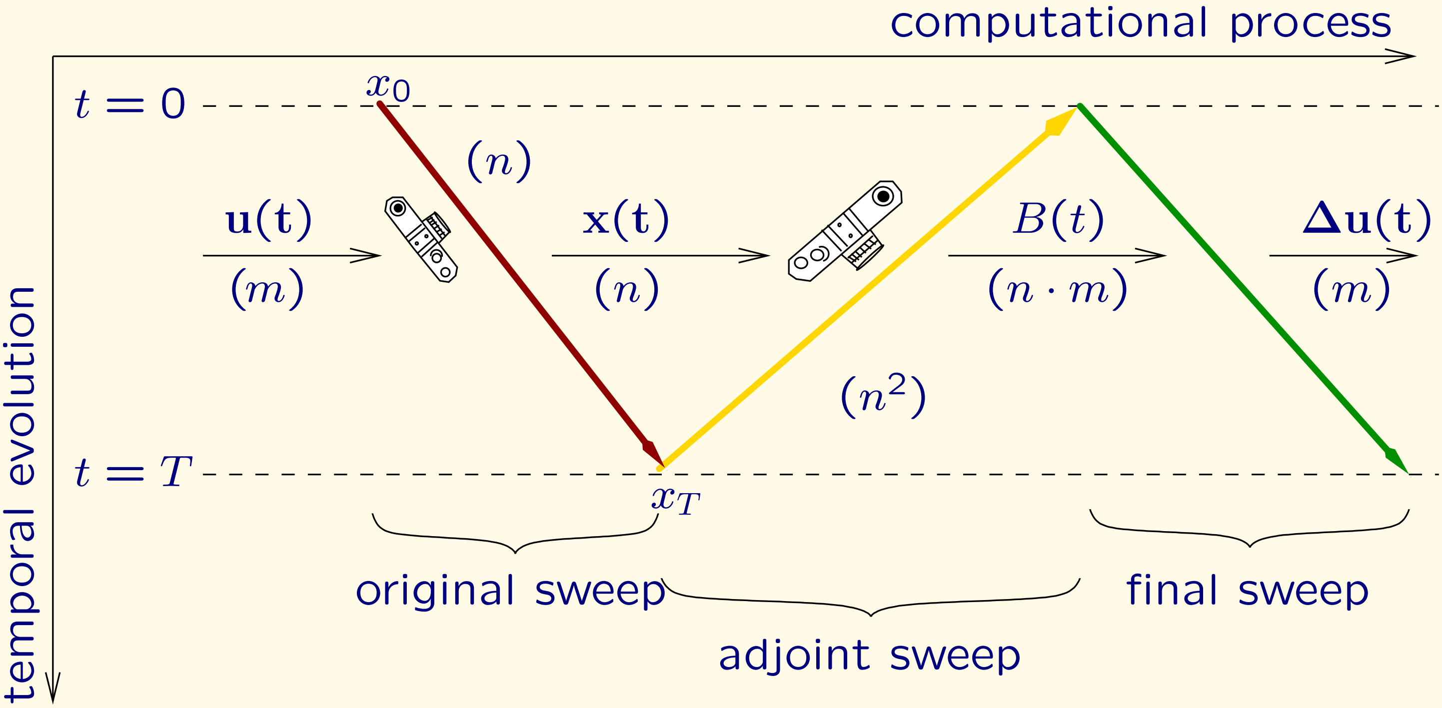


Information flow by Riccati/Pantoja computation of Newton step

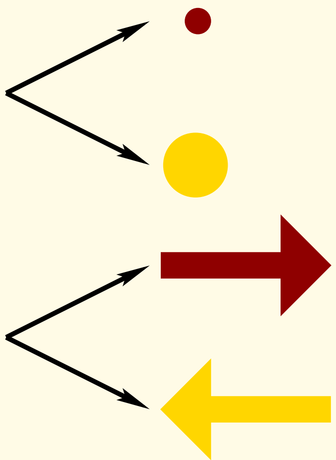


Information flow by Riccati/Pantoja computation of Newton step



3. Nested checkpointing

checkpoints



thin $d = \mathcal{O}(n)$

fat $\bar{d} = \mathcal{O}\left(n^2\right)$

step cost

original $t = \mathcal{O}\left(n^2\right)$

adjoint $\bar{t} = \mathcal{O}\left(n^3\right)$

Available memory is given as number C of fat checkpoints

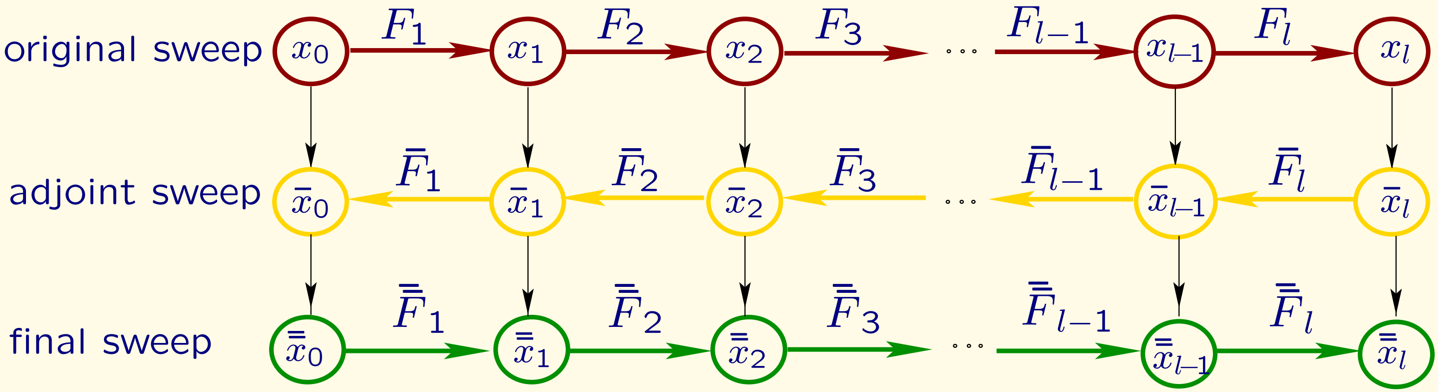
$$\#thin = c \times \#fat = c \times C$$

Find an optimal nested reversal by minimizing

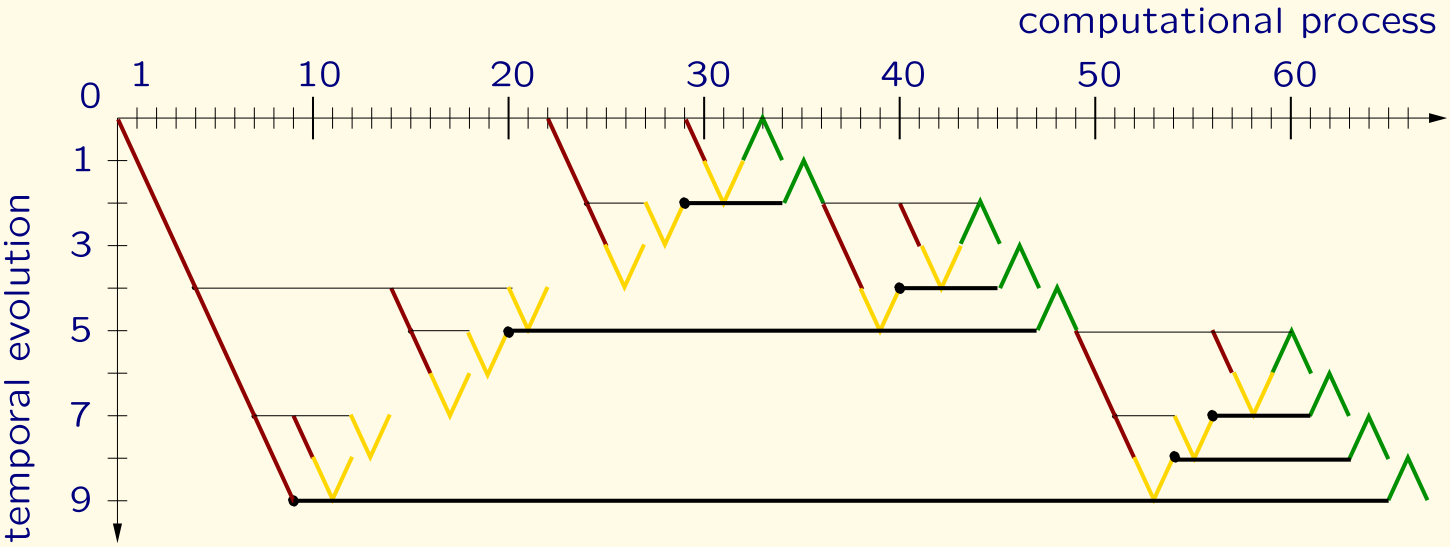
$$\mathbf{T}_{min}(l, C, c, t, \bar{t})$$

over all possible checkpoint distributions

Multiple sweep evolution $\mathcal{E}_{3\times l}$



Example of optimal nested reversal $\mathbf{S}_{min}(9,2)$ with $c = 1$, $t = 1$, and $\bar{t} = 5$



$\Rightarrow$ 23 original steps, 13 adjoint steps, 9 final steps

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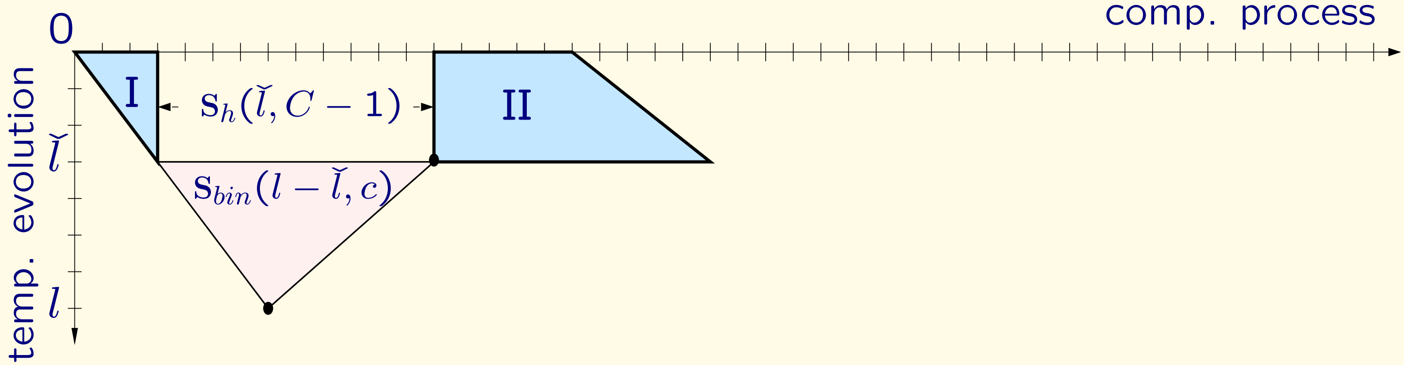
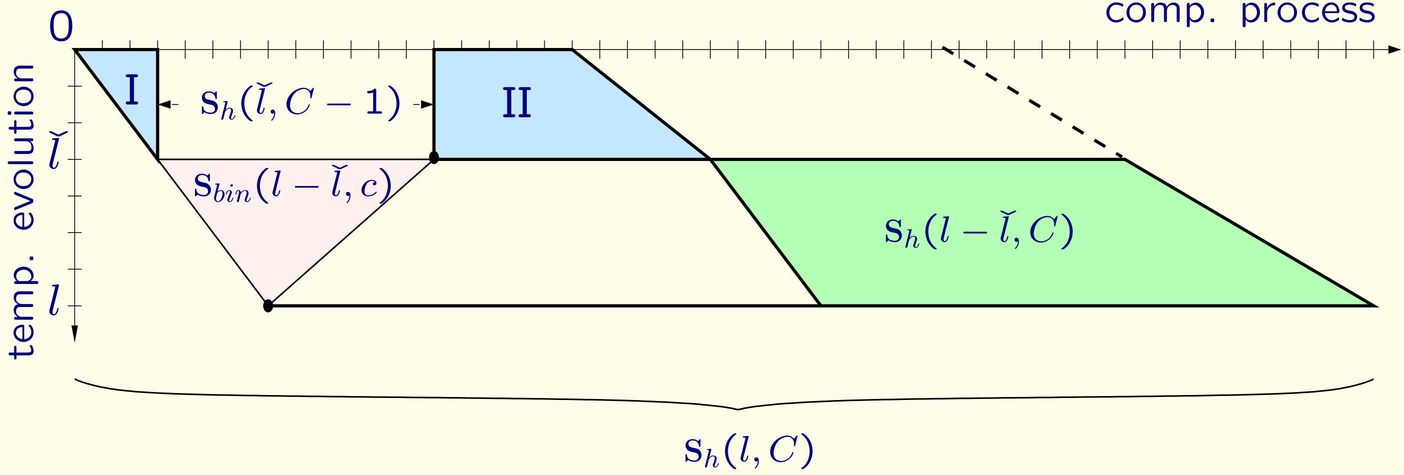
Heuristic

Decomposition of nested reversal schedule $\mathbf{S}_h(l, C)$



Heuristic

Decomposition of nested reversal schedule $\mathbf{S}_h(l, C)$



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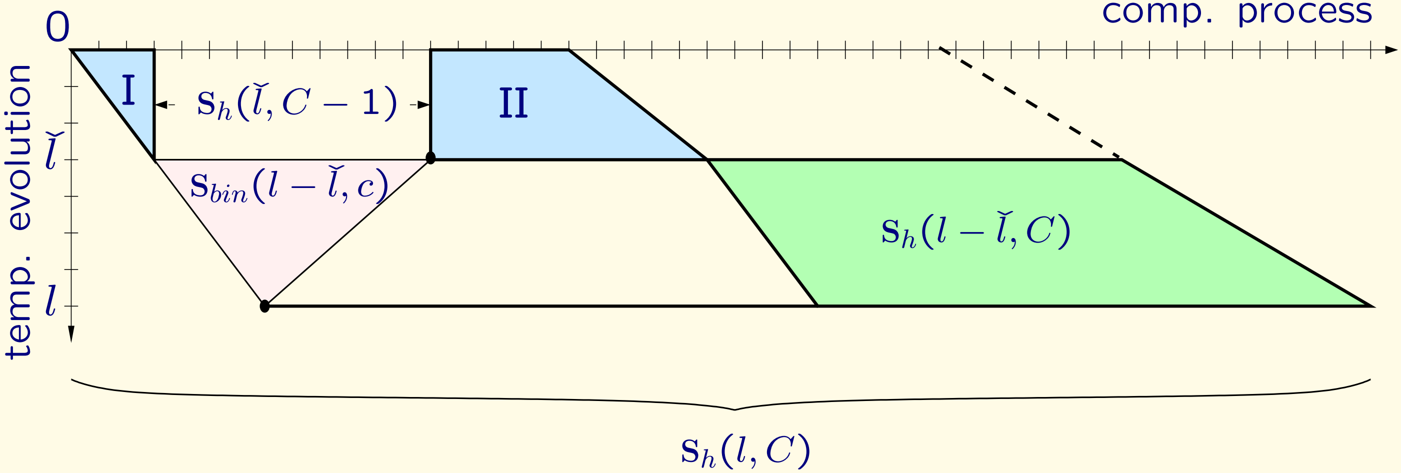
Heuristic

Decomposition of nested reversal schedule $\mathbf{S}_h(l, C)$



Find $\check{l}$ by minimizing

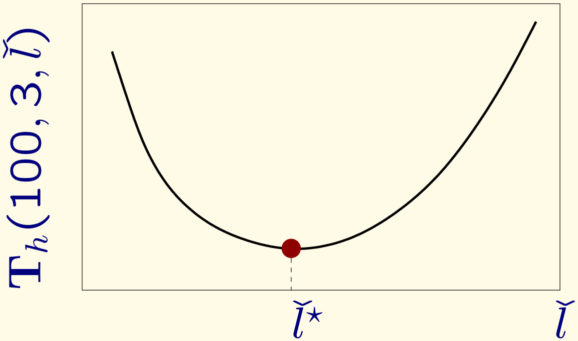
$$\mathbf{T}_h(l, C) = \min_{0<\check{l}<l} \mathbf{T}_h(l, C, \check{l})$$

Use **Linear method**

	Exhaustive search	Linear method
Memory	$\approx \mathcal{O}(l^C)$	$\mathcal{O}(l \times C)$
Run-Time	$\approx \mathcal{O}(l^3)$	$\mathcal{O}(l \times C)$

Linear method

$\mathbf{T}_h(l, C, \check{l})$ convex in dependence of $\check{l}$



$$\mathbf{T}_h(l, C, \check{l}) \searrow \; for\, \check{l} \le \check{l}^\star$$

$$\mathbf{T}_h(l, C, \check{l}) \nearrow \; for\, \check{l} > \check{l}^\star$$

- Find where $\mathbf{T}_h(l, C, \check{l}) - \mathbf{T}_h(l, C, \check{l} - 1)$ changes its sign first time

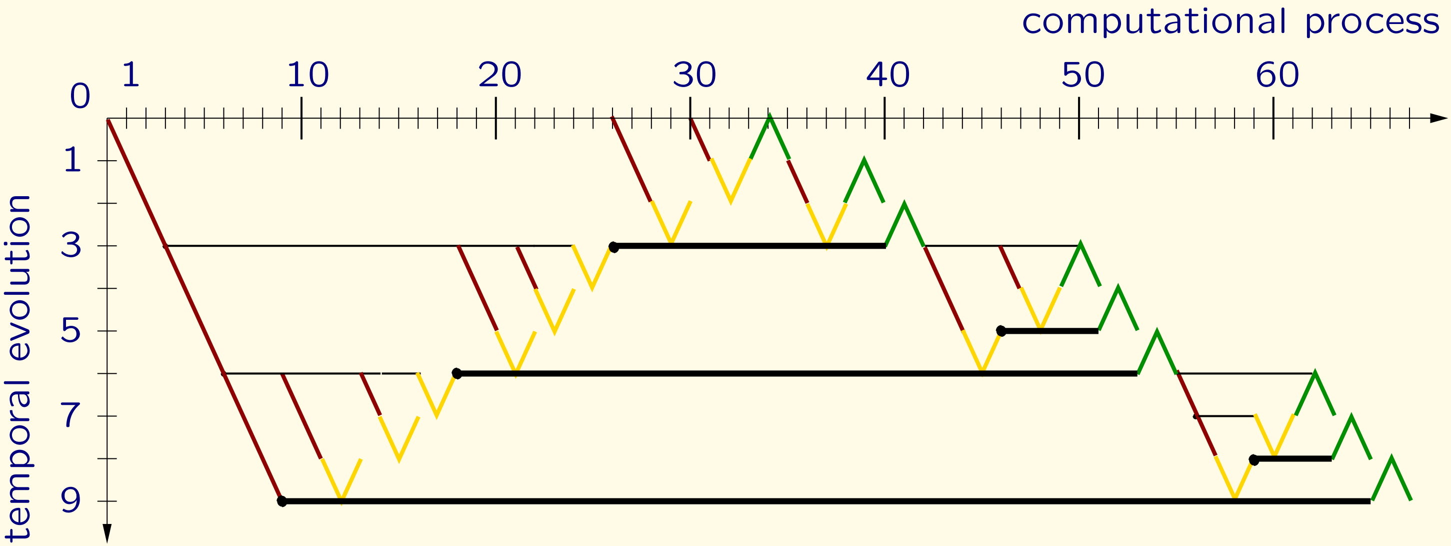
- Find $\mathbf{T}_h(l, C)$ using recursion over l and C

Use:

$$\check{l}^\star = \check{m}^\star \vee \check{l}^\star = \check{m}^\star + 1, \qquad \text{with } m = l - 1$$

$$\mathbf{F}_h(l, C) \equiv \mathbf{T}_h(l, C) - \mathbf{T}_h(l - 1, C)$$

Example of nested reversal $\mathbf{S}_h(9,2)$ with $c = 1$, $t = 1$, and $\bar{t} = 5$

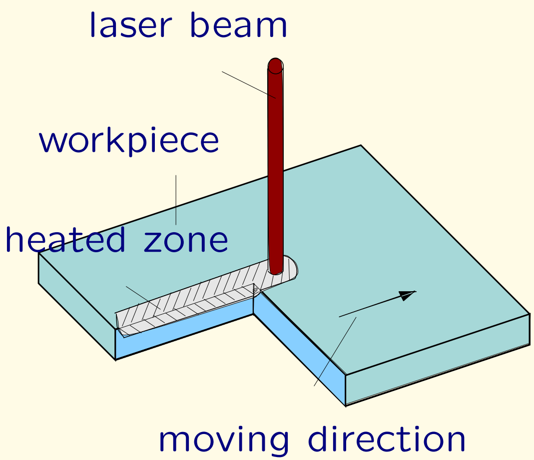


$\Rightarrow$ 24 original steps, 13 adjoint steps, 9 final steps

4. Numerical results

Laser surface hardening [Hömberg, Volkwein]

$Q = \Omega \times (0,T)$, $\Sigma = \partial\Omega \times (0,T)$, $\Omega = [0,5] \times [-1,0]$, $T = 5.25$



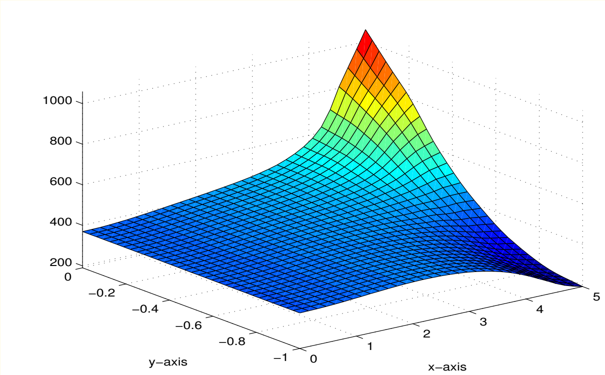
State equations

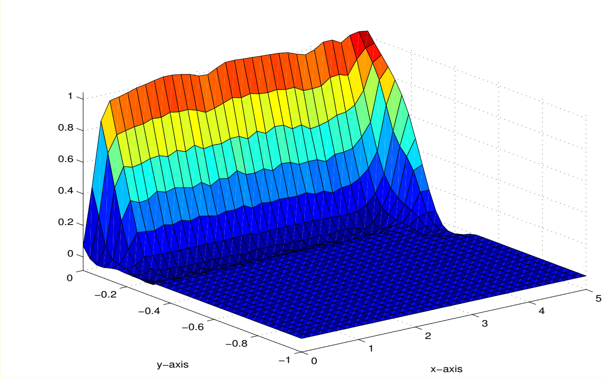
$$
\begin{aligned}
a_t &= \frac{1}{\tau(\theta)}[a_{eq}(\theta) - a]_+, \text{ in } Q \\
a(0) &= 0, \text{ in } \Omega \\
\rho c_\rho \theta_t - k\triangle\theta &= -\rho L a_t + u\alpha, \text{ in } Q \\
\frac{\partial\theta}{\partial\nu} &= 0, \text{ on } \Sigma \\
\theta(0) &= \theta_0, \text{ in } \Omega
\end{aligned}
$$

Cost functional

$$J(a,\theta,u) = \frac{\beta_1}{2}\int_\Omega (a(x,T) - a_d(x))^2 dx + \frac{\beta_2}{2}\int_0^T \int_\Omega [\theta - \theta_m]_+^2 dx\, dt + \frac{\beta_3}{2}\int_0^T u^2 dt$$

FE snapshot for temperature and volume fraction of austenite at $t = T$ $(n = 147)$





Desired state a_d

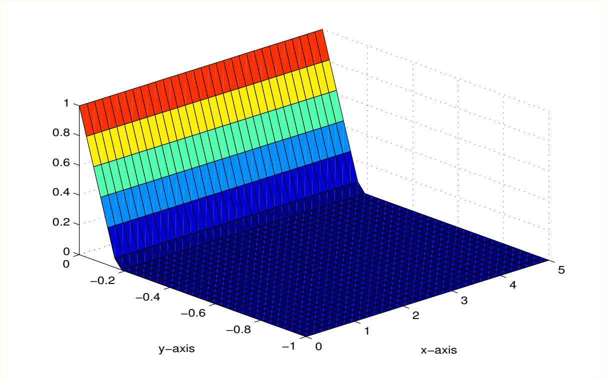


Table 1: Program data

i	λ^i	$J(\mathbf{u}^i)$	$\|\nabla J(\mathbf{u}^i)\|_2$	$\nabla J(\mathbf{u}^i)\delta\mathbf{u}^i$	$\|a^i(T) - a_d\|_{L^2(\Omega)}$	$\|\theta^i\|_{L^\infty(Q)}$	$\Lambda(i) = \frac{\|\delta\mathbf{u}^i\|}{\|\delta\mathbf{u}^i+\mathbf{u}^i\|}$
0	0.000000	670.096247	2.197499	−0.000000	0.158144	1148.594458	0.000000
1	0.001130	665.493535	2.198253	−4275.090081	0.157792	1148.527231	0.019460
2	0.005000	650.324921	2.194708	−3257.726444	0.156671	1148.370625	0.032751
3	0.000034	647.678880	2.194745	−82044.859253	0.156744	1148.433767	0.014622
4	0.000001	647.678880	2.166298	782.845599	0.155249	1147.414625	0.000561
5	0.000000	647.678880	2.136994	2524.100850	0.153778	1146.409009	0.000554
6	0.100000	589.317913	1.864956	−543.282251	0.140428	1141.066647	0.088242
7	0.134720	576.179109	1.824791	−409.596505	0.144286	1134.496470	0.088891
8	0.100000	534.398496	1.378520	−668.869910	0.123036	1201.254915	0.236620
9	0.100000	522.596740	1.229784	−209.076937	0.119931	1185.524519	0.094729
10	0.100000	507.601359	1.066479	−192.808499	0.114103	1178.850090	0.130864
11	1.000000	458.536134	0.463360	−212.394660	0.069952	1219.525080	0.391770
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮
30	1.000000	355.305487	0.019172	−2.436999	0.045926	987.141029	0.052059
31	1.000000	355.106094	0.004853	−0.396550	0.045660	986.614861	0.019979
32	1.000000	355.047319	0.001508	−0.103916	0.045595	986.605644	0.008947
33	1.000000	355.043523	0.000163	−0.008023	0.045628	986.605683	0.003201
34	1.000000	355.043510	0.000006	−0.000185	0.045634	986.605683	0.000582
35	1.000000	355.043510	0.000000	−0.000000	0.045634	986.605683	0.000000

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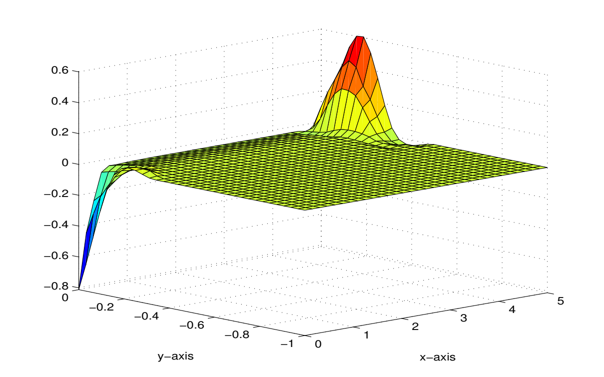
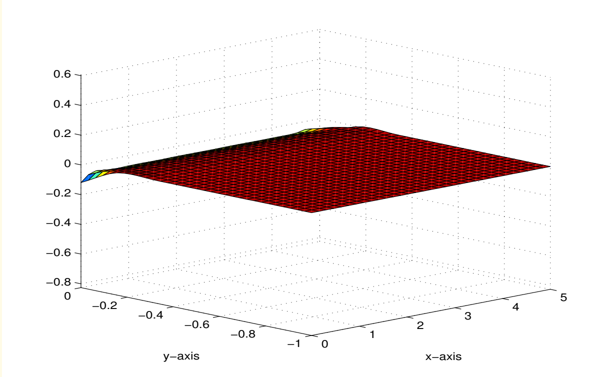
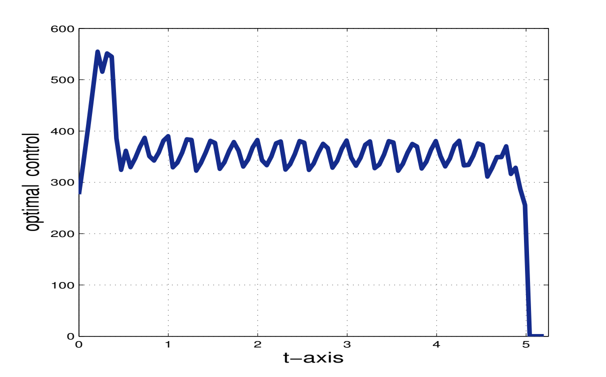
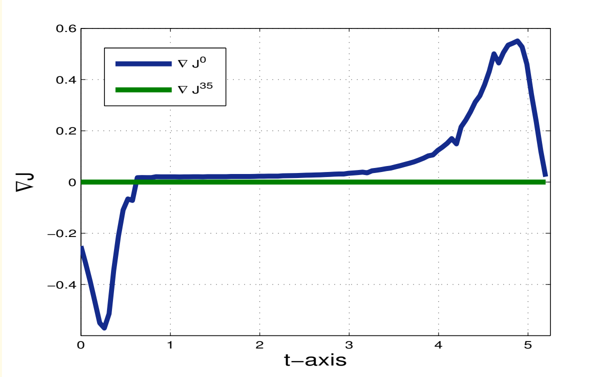
Differences $a^0(T) - a_d$ and $a^{35}(T) - a_d$ for the initial iterate a^0 and for the optimal state a^{35}



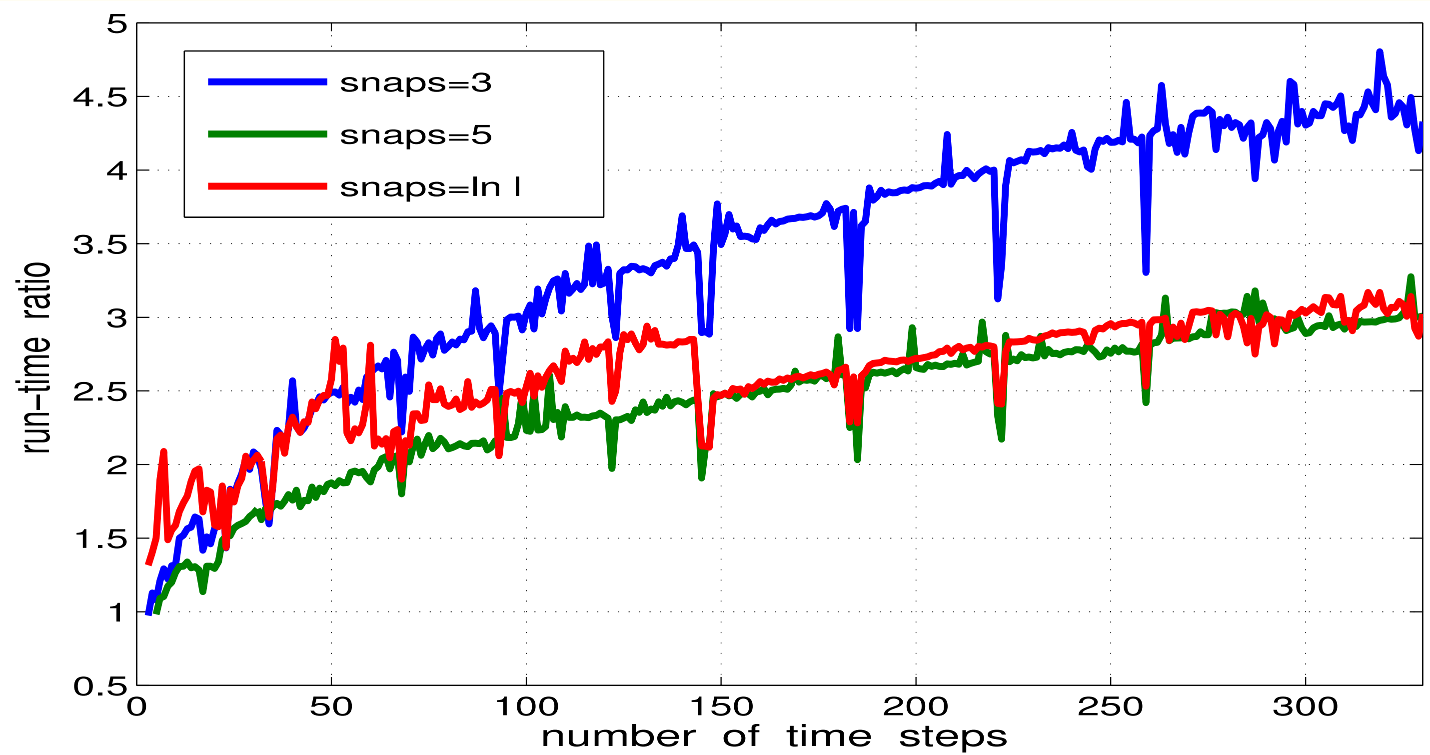


Optimal control $\mathbf{u}^{35}$ and the gradients ∇J^0 and ∇J^{35} of the cost function





Run-time & memory trade-off



5. Summary and conclusion

- Optimal control problems:

  Multiple shooting method

  - Requires expression for $\mathbf{u}(t) = \mathbf{u}(\mathbf{x}(t), \bar{\mathbf{x}}(t))$
  - Requires estimation for $\bar{\mathbf{x}}(0)$

  Newton/Riccati/Pantoja method

  Requires triple sweep

  Enormous memory requirement for its realization

- Nested checkpointing:

  Optimal strategies & heuristic

  Drastic memory reduction

  Run-time $\approx \mathcal{O}\left(l \ln^2 l\right)$