Block iterative algorithms for Parabolic Optimal Control Problems

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28 AÑOS CONSTRUYENDO EL FUTURO

LCCA

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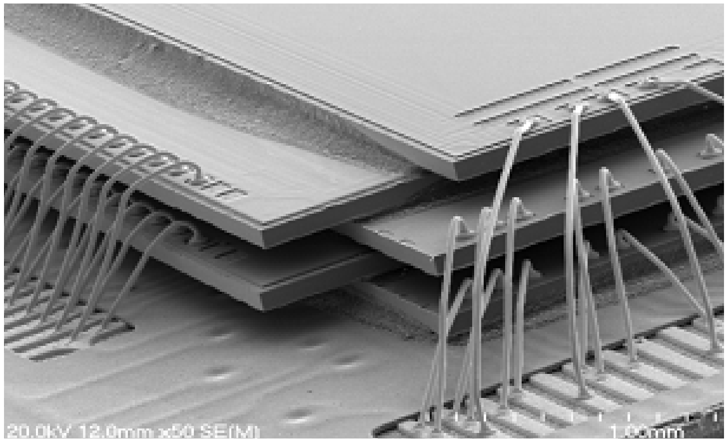
Outline

1. Motivation
2. Modeling
3. Simulation
4. Optimal control problem
5. Discretization all at once - KKT system.
6. Algorithm 1: Elimination of state and adjoint variables.
7. Algorithm 2: Block diagonal preconditioning.
8. Concluding remarks.

ITRS: International Technology Roadmap for Semiconductors: the next 15 years

SiP: System in Package

(ITRS, Assembly and Packaging)

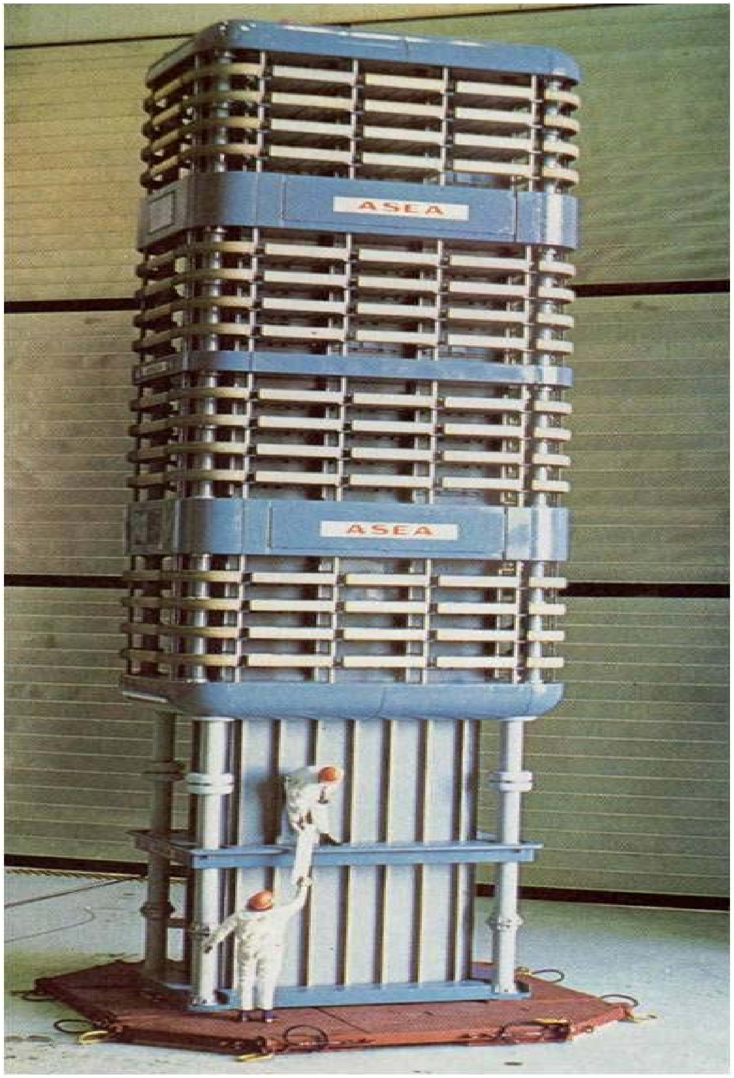


System level integration at the package level poses many **new thermal and mechanical challenges.** Reliable products cannot be built unless we understand these issues and design to **accommodate them**

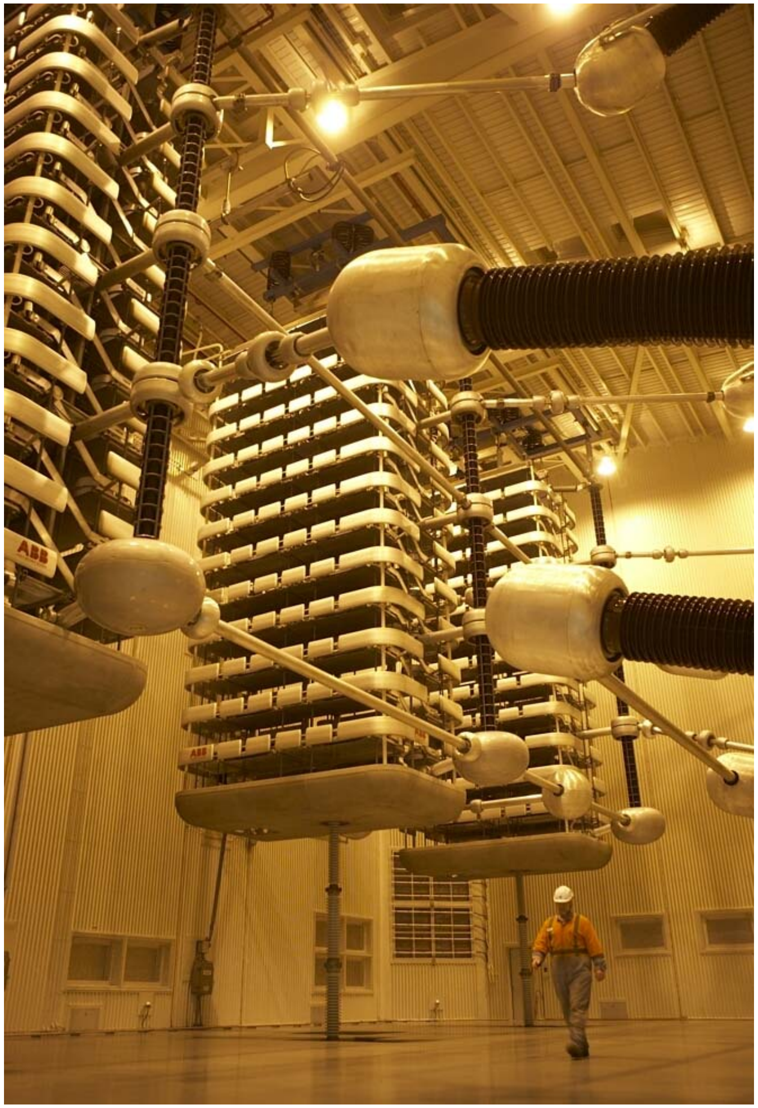
System Level Integration

Figures from ITRS 2007

Power System devices



SCR inverter in a transmission system



Tiristors in HVDC in New Zealand

Heating: Failure in electronic devices

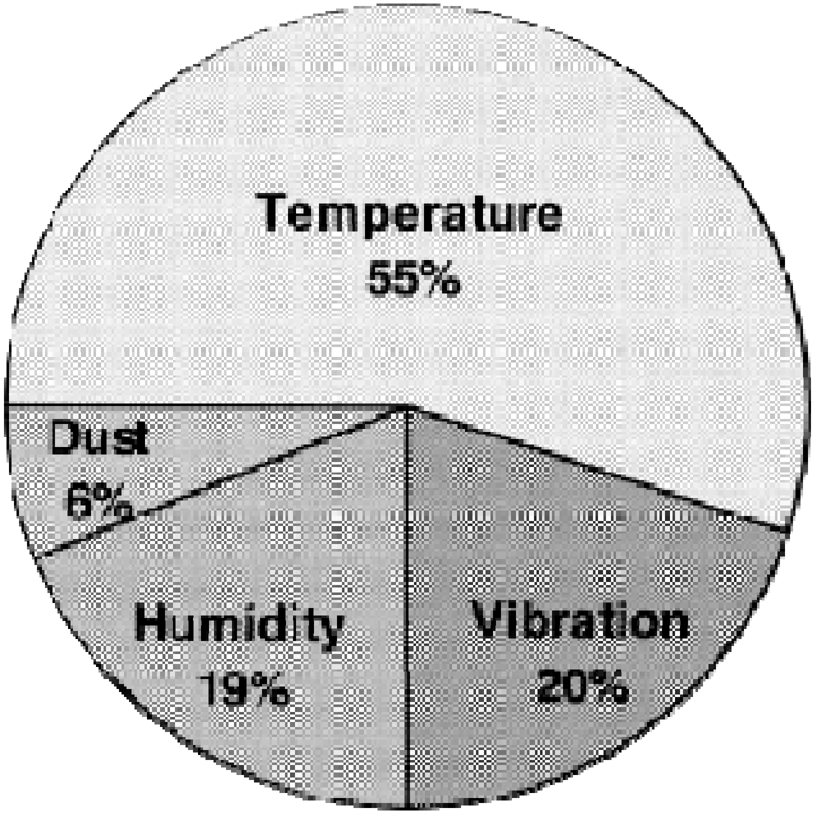


Figure from Art. Modeling electronic circuit radiation cooling using analytical thermal model. M. Janicki y Marcin Napieralski

A Circuit

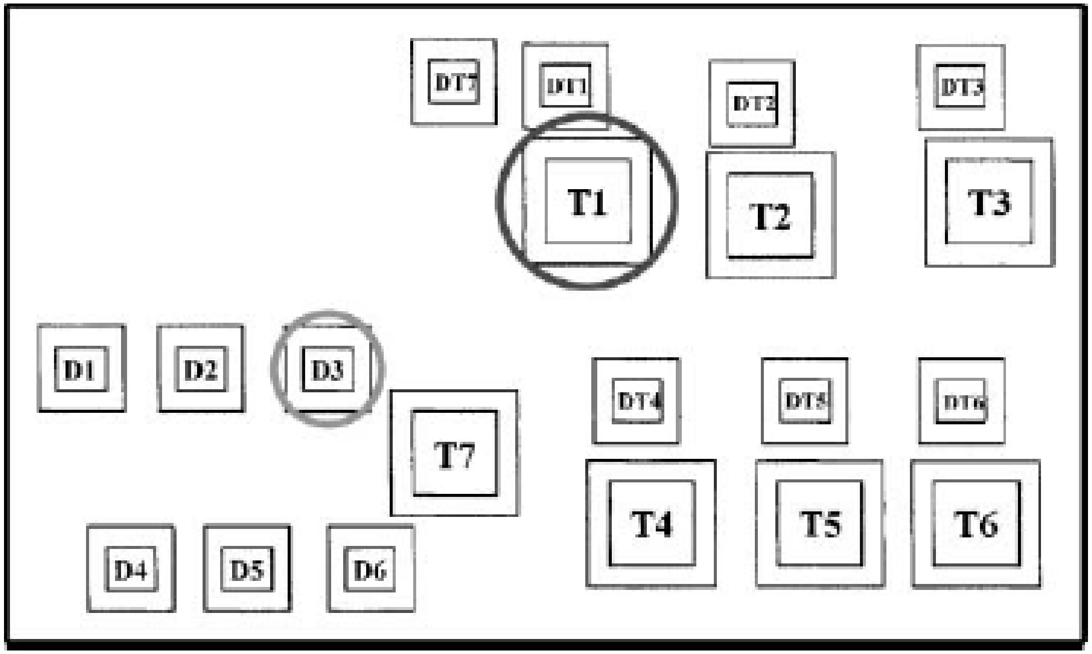


Fig. 1. IGBT module layout.

Ti are power transistors

Constitutive law

- Fourier law for conduction in solids

$$q = -\lambda \nabla y$$

q is heat flux and λ is the thermal conductivity, c_p specific heat and ρ is the density.

- Balance of energy

$$\frac{d}{dt}\int_{\Omega} \rho e d\Omega = \int_{\partial\Omega} q d\Gamma + \int_{\Omega} \rho f$$

Differential equation for heat conduction in solids

$$\rho c_p \frac{\partial y}{\partial t} = -\nabla \cdot \left(\lambda \nabla y \right) + f$$

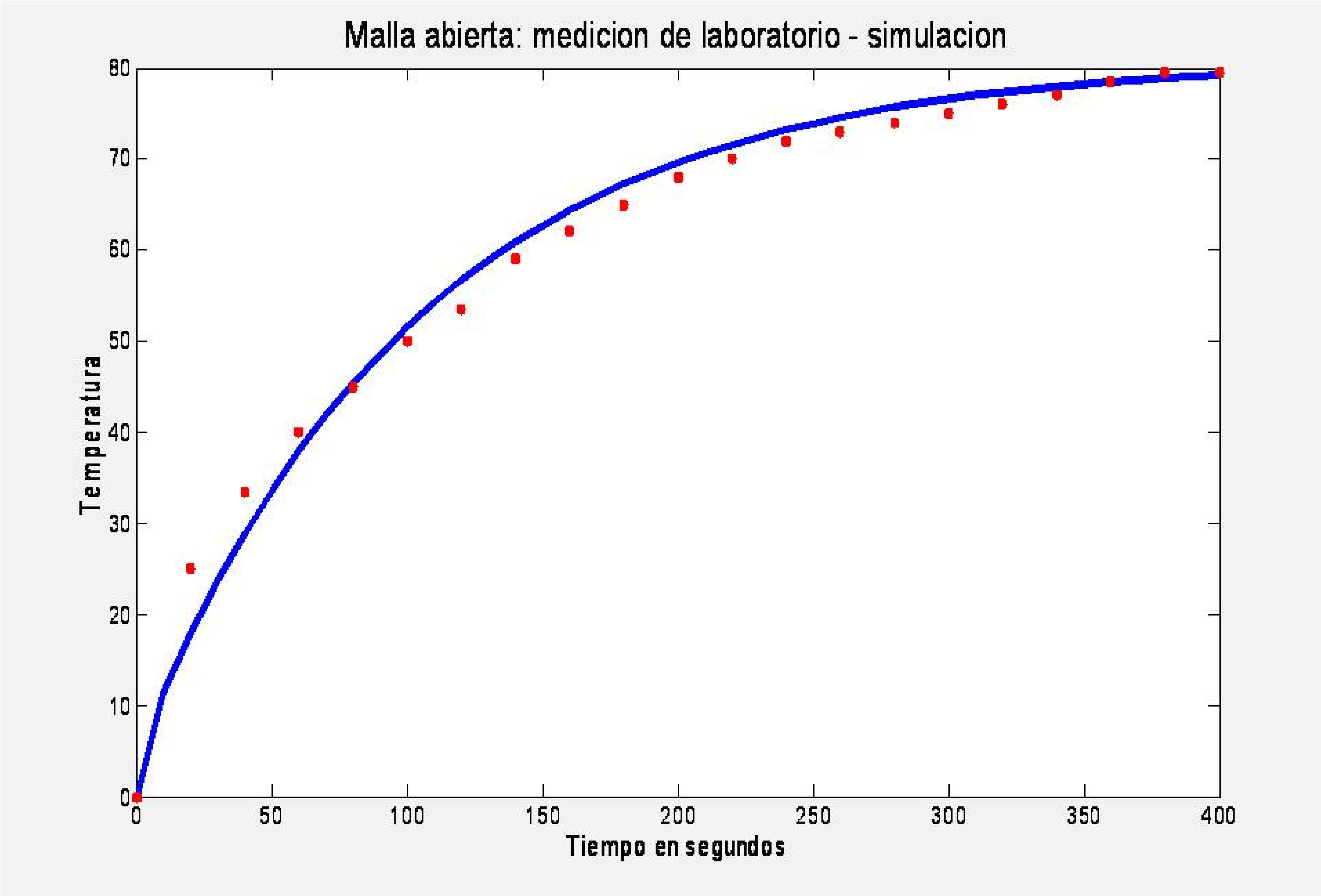
The plant

$$\begin{cases} \rho c_p \dfrac{\partial y}{\partial t} = \nabla \cdot \left(\lambda \nabla y \right) + f & \text{in} \quad \Omega \times \left[t_0,\ t_f \right] \\ y\left(x,\ 0\right) = y_0 & \text{in} \quad \Omega \\ y = 0 & \text{in} \quad \partial\Omega \times \left[t_0,\ t_f \right] \end{cases}$$

$$f = u + g$$

$$\left. \begin{aligned} u = y \quad & \text{in} \quad \partial\Omega \times \left[t_0,\ t_f \right] \\ u = \frac{\partial y}{\partial \eta} \quad & \text{in} \quad \partial\Omega \times \left[t_0,\ t_f \right] \end{aligned} \right\}$$

Comparison with laboratory data

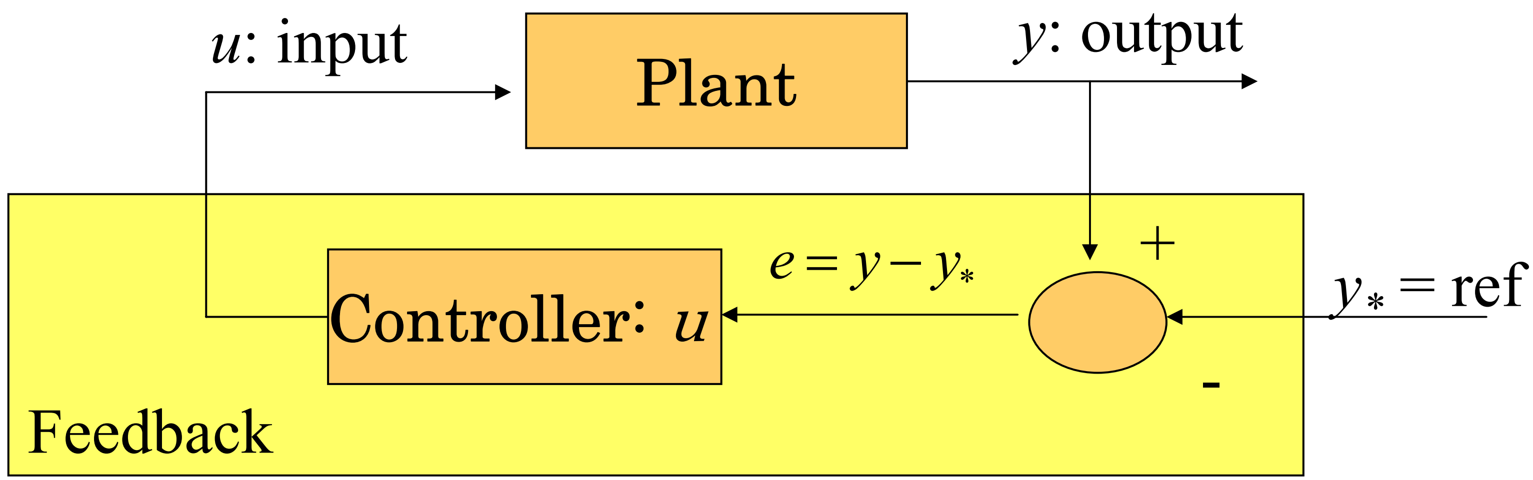


Continuous line is the simulation result and dotted are the laboratory measurements.

Janicki M.; De Mey G.; Napieralski A.; “Transient thermal analysis of multilayered structures using Green’s function”. (Microelectronics Reliability, 42: 1059-1064, 2002).

The control problem: block diagram

Tracking problem



u: input

Plant

y: output

$+$

$e = y - y_*$

Controller: u

$y_* = \text{ref}$

-

Feedback

y: state vector and output

Plant ⇨

$$\begin{aligned}\dot{y}(t) &= A(t)y(t) + B(t)u(t)\\ y(0) &= 0\end{aligned}$$

The aim is to make the output y to behave in the way specified by y_*

u: must be chosen in order to make the error e *small*.

The state equation: Plant

State equation
$$\begin{cases} \partial_t y = Ay + Bu, \quad t \in [0,\, t_f] \\ y(t, \partial\Omega) = 0 \\ y(0, \Omega) = 0 \end{cases}$$

where, y is the state of the system,

A is an uniformly elliptic linear operator from $L^2(0,t_f;V)$ to $L^2(0,t_f;V^*)$.

V is a Hilbert space (in our case $V = H_0^1$), H is a pivot Hilbert space, i.e. $V \subset H \subset V^*$, $H = L^2(\Omega)$.

Distributed control problem

$$u \in U_{\mathrm{ad}} = L^2(0,\, t_f; L^2(\Omega))$$

$$B \in L\ (U_{\mathrm{ad}}\,;\, L^2(0,\, t_f;\, V^{\,*})$$

The optimal control problem

For the system: $\begin{cases} \partial_t y = Ay + Bu \\ \quad i.c. + b.c. \end{cases}$

Find a control *u*(*t*,*x*) which minimize the performance functional:

$$J(y_u,u) := \frac{q}{2}\| Ce \|^2_{L^2(0,t_f;L^2(\Omega))} + \frac{r}{2}\| u \|^2_{L^2(0,t_f;L^2(\Omega))} + \frac{s}{2}\left\| y(t_f,x) - y_*(t_f,x) \right\|^2_{L^2(\Omega)}$$

where $e = y_u - y_*$, y_* is a given target function.

y_u denotes the dependence of the state y of the controller u.

u is the optimal controller

Remark

In the cost function $J(y_u,u)$

$$0<\frac{r}{2}\left\|u\right\|_{L^2\left((0,t_f);L^2(\Omega)\right)} \text{ for } 0<r$$

$$0\leq\frac{q}{2}\left\|Ce\right\|_{L^2\left((0,t_f);L^2(\Omega)\right)} \text{ for } 0\leq \mathrm{q}$$

Then, the optimal control problem is well posed. We consider $C=I$.

J. L. Lions, *Optimal Control of Systems Governed by Partial Differential Equations*, SpringerVerlag, New York, 1971.

The discretization in space

Weak form for the state eq.:

$$(\partial_t y, \eta) = (Ay, \eta) + (Bu, \eta)$$

and choosing $\{\phi_1(x), \cdots, \phi_n(x)\}$ as a nodal basis for $V_h \subset V$, then we can writte

$$y_h(t,x) = \sum_{i=1}^{\hat{m}} \phi_i(x)\xi_i(t) \quad \text{and} \quad u_h(t,x) = \sum_{j=1}^{\hat{p}} \varphi_j(x) u_j(t)$$

$$\hat{M}_h \dot{\xi}(t) = \hat{A}_h \xi(t) + \hat{B}\mathrm{u}(t)$$

y_h is continuous in space and
discontinuous in time
u_h is discontinuous
in space and time

$$\hat{M}_h = U_h^T U_h$$

$$\dot{\mathrm{y}}(t) = \underbrace{U_h^{-T} \hat{A}_h U_h^{-1}}_{A} \mathrm{y}(t) + \underbrace{U_h^{-T} \hat{B}}_{B} \mathrm{u}(t)$$

The linear quadratic

Probably the most celebrated optimal control problem, *Locatelli*.

For the system:
$$\dot{y}(t) = Ay(t) + Bu(t)$$
$$y(0) = 0$$

Find a control *u(t)* which minimize the performance functional:

$$J = \frac{1}{2}\left(\int_0^{t_f}\left((y-y_*)^T Q (y-y_*) + u^T R u \right) dt + (y-y_*)^T S (y-y_*)(t_f)\right)$$

Properties:

1) The final time t_f is given, y_* is the reference function.

2) A, B, Q and R are matrices. $A=A^T < 0$

3) $Q = Q^T \geq 0$, $R=R^T > 0$, $\forall t \in [0, t_f]$.

The continuous saddle point formulation

Introducing a Lagrange multiplier function $p(t)$ we obtain the Lagrangian:

$$L(y,u,p)=\frac{1}{2}\left(\int_0^{t_f}\left((\mathrm{y}-\mathrm{y}_*)^T Q(\mathrm{y}-\mathrm{y}_*)+\mathrm{u}^T R\mathrm{u}\right)dt+(\mathrm{y}-\mathrm{y}_*)^T S(\mathrm{y}-\mathrm{y}_*)(t_f)\right)$$

$$+\int_0^{t_f}\left(\mathrm{p},\dot{\mathrm{y}}-A\mathrm{y}-B\mathrm{u}\right)dt$$

Taking *inf* in y and u and *sup* in p, we obtain the following:

Equations	Boundary conditions
$\dot{\mathrm{y}}-A\mathrm{y}-B\mathrm{u}=0$	$\mathrm{y}(0)=0$
$\dot{\mathrm{p}}+A^T\mathrm{p}-Q(\mathrm{y}-\mathrm{y}_*)=0$	$\mathrm{p}(t_f)=-S(\mathrm{y}-\mathrm{y}_*)(t_f)$
$R\mathrm{u}-B^T\mathrm{p}=0$	

The Hamiltonian form

Because u and p have an algebraic relationship, we eliminate the control variable u, we obtain:

$$\text{Eq.}\quad \begin{cases} \dot{y} = Ay + BR^{-1}B^{T}p \\ \dot{p} = Q(y - y_*) - A^{T}p \end{cases}$$

$$\text{B.C.}\quad \begin{cases} y(0) = 0 \\ p(t_f) = -S(y - y_*)(t_f) \end{cases}$$

Comments:

1) Since there is a coupling on p and y at $t = t_f$, the value of p depends on the whole history of p and y.
2) The value of the controller u at a generic time t depends on the future behavior of the signal to be tracked.
3) Given $y_*(\cdot)\ \forall t \in [0, t_f]$ the problem is well posed, the solution is given via for instance the Riccati equation.

Future work

All at once discretization

The functional

$$J = \frac{1}{2}\left(\int_0^{t_f}\left((\mathrm{y}-\mathrm{y}_*)^T Q(\mathrm{y}-\mathrm{y}_*)+\mathrm{u}^T R\mathrm{u}\right)dt+(\mathrm{y}-\mathrm{y}_*)^T S(\mathrm{y}-\mathrm{y}_*)(t_f)\right)$$

The state equation

$$\dot{\mathrm{y}}(t) = A\mathrm{y}(t) + B\mathrm{u}(t)$$

$$\mathrm{y}(0) = 0$$

Discretization in time θ-scheme

$$\dot{\mathrm{y}} = A\,\mathrm{y} + B\,\mathrm{u} \longrightarrow F_1 \mathrm{y}_{l+1} = F_0 \mathrm{y}_l + \tau\, B\, u_{l+1/2}$$

$$F_0 = \big(I + \tau\,(1-\theta)\,A\big) \text{ and } F_1 = \big(I - \tau\,\theta\,A\big)$$

$$\mathbf{E}\,\mathbf{y} + \mathbf{N}\,\mathbf{u} = \mathbf{f}$$

$$\mathbf{E} = \begin{bmatrix} -F_1 & & \\ F_0 & -F_1 & \\ & F_0 & -F_1 \end{bmatrix} \qquad \mathbf{N} = \tau \begin{bmatrix} B & & \\ & B & \\ & & B \end{bmatrix}$$

The functional

$$J = \frac{1}{2}\left(\int_0^{t_f} \left((\mathrm{y}-\mathrm{y}_*)^T Q (\mathrm{y}-\mathrm{y}_*) + \mathrm{u}^T R \mathrm{u} \right) dt + (\mathrm{y}-\mathrm{y}_*)^T S (\mathrm{y}-\mathrm{y}_*)(t_f) \right)$$

$$\frac{1}{2}\int_0^{t_f} \mathrm{u}^T R \mathrm{u} = \frac{\tau}{2}\sum_{l=1}^{\hat{l}} \mathrm{u}_l^T R \mathrm{u}_l \rightarrow \frac{1}{2}\mathbf{u}^T \mathbf{G}\,\mathbf{u}$$

$$\frac{1}{2}\int_0^{t_f} (\mathrm{y}\text{-}\mathrm{y}_*)^T Q (\mathrm{y}\text{-}\mathrm{y}_*) \rightarrow \frac{1}{2}(\mathbf{y}-\mathbf{y}_*)^T \mathbf{Z} (\mathbf{y}-\mathbf{y}_*)$$

$$\frac{1}{2}(\mathrm{y}-\mathrm{y}_*)^T S (\mathrm{y}-\mathrm{y}_*)(t_f) = \frac{1}{2}(\mathbf{y}-\mathbf{y}_*)^T \overset{\Gamma}{\overset{\big\downarrow}{\begin{bmatrix} 0 & & & \\ & \ddots & & \\ & & 0 & \\ & & & \mathrm{Q} \end{bmatrix}}} (\mathbf{y}-\mathbf{y}_*)$$

All at once minimization problem

$$\min J(\mathbf{y},\mathbf{u})$$

subject to: $\mathbf{E}\;\mathbf{y} + \mathbf{N}\;\mathbf{u} = \mathbf{f}$

where $J(\mathrm{y},\mathrm{u}) = \frac{1}{2}\left(\mathbf{y}-\mathbf{y}_*\right)^T \mathbf{K}\left(\mathbf{y}-\mathbf{y}_*\right) + \frac{1}{2}\mathbf{u}^T\mathbf{G}\mathbf{u}$

The saddle point system

The discrete Lagrangian has the matrix form

$$L_h(\mathbf{y},\mathbf{u},\mathbf{p}) = \frac{1}{2}\left(\mathbf{u}^T\mathbf{G}\mathbf{u} + \left(\mathbf{y}-\mathbf{y}_*\right)^T \mathbf{K}\left(\mathbf{y}-\mathbf{y}_*\right)\right) + \mathbf{p}^T\left(\mathbf{E}\mathbf{y}+\mathbf{N}\mathbf{u}-\mathbf{f}\right)$$

where $\mathbf{K} := \mathbf{Z} + \boldsymbol{\Gamma}$ and $\boldsymbol{\Gamma} = diag(0,\ldots 0,Q)$

The discrete saddle point system has the form:

$$\begin{bmatrix} \mathbf{K} & & \mathbf{E}^{\mathbf{T}} \\ & \mathbf{G} & \mathbf{N}^{\mathbf{T}} \\ \mathbf{E} & \mathbf{N} & \end{bmatrix} \begin{bmatrix} \mathbf{y} \\ \mathbf{u} \\ \mathbf{p} \end{bmatrix} = \begin{bmatrix} \mathbf{K}\mathbf{y}_* \\ \mathbf{0} \\ \mathbf{f} \end{bmatrix}$$

- Evolution matrix E is ill-conditioned.

USAWA method

The discrete saddle point system has the form:

$$\begin{bmatrix} \mathbf{K} & & \mathbf{E}^{\mathrm{T}} \\ & \mathbf{G} & \mathbf{N}^{\mathrm{T}} \\ \mathbf{E} & \mathbf{N} & \end{bmatrix} \begin{bmatrix} \mathbf{y} \\ \mathbf{u} \\ \mathbf{p} \end{bmatrix} = \begin{bmatrix} \mathbf{K}\mathbf{y}_* \\ \mathbf{0} \\ \mathbf{f} \end{bmatrix}$$

$$\left(\mathbf{N}\mathbf{G}^{-1}\mathbf{N}^T + \mathbf{E}\mathbf{K}^{-1}\mathbf{E}^T\right)\mathbf{p} = \mathbf{b}$$

- Classical method for Saddle point systems
- Evolution matrix *E* is ill-conditioned.

Bounds for evolution matrix

Theorem 1: Let A a matrix $\hat{m} \times \hat{m}$ symmetric negative definite $\lambda_m(A)$ with matrices

$$F_0 := I + \tau(1-\theta)A, \quad \text{and} \quad F_1 := I - \tau\theta A, \text{ for } 0 \le \theta \le 1.$$

Matrix EE^T has condition number

$$\mathrm{Cond}(\mathbf{EE}^T) \approx \frac{4(1+\tau\theta\rho_{\max})^2}{(\theta\rho_{\min})^2} \quad \boxed{\approx O\left(h^{-4}\right)}$$

where $\rho_{\max} = \max\left|\lambda_m(A)\right|$ and $\rho_{\min} = \min\left|\lambda_m(A)\right|$.

Stability restrictions for τ are:

if $\theta \ge \frac{1}{2}$ is stable for all τ and if $\theta < \frac{1}{2}$ is conditionally stable for $\tau < \dfrac{2}{(1-2\theta)\max\left|\lambda_m\right|}$

$$\mathbf{EE}^T = \begin{bmatrix} F_1F_1^T & -F_1F_0^T & & & \\ -F_0F_1^T & F_0F_0^T + F_1F_1^T & -F_1F_0^T & & \\ & -F_0F_1^T & F_0F_0^T + F_1F_1^T & -F_1F_0^T & \\ & & \ddots & \ddots & \ddots \\ & & & -F_0F_1^T & F_0F_0^T + F_1F_1^T \end{bmatrix}$$

Using eigendecomposition of A: $\Lambda = Q^T A Q$

$$\Lambda_0 = Q^T F_0 Q = Q^T \left(I - \tau\theta A\right) Q$$

$$\Lambda_1 = Q^T F_1 Q = Q^T \left(I + \tau(1-\theta) A\right) Q$$

We obtain:

$$\mathbf{E}\mathbf{E}^T \quad \rightarrow \begin{bmatrix} \Lambda_1^2 & -\Lambda_1\Lambda_0 & & & \\ -\Lambda_0\Lambda_1 & \Lambda_0^2+\Lambda_1^2 & -\Lambda_1\Lambda_0 & & \\ & -\Lambda_0\Lambda_1 & \Lambda_0^2+\Lambda_1^2 & -\Lambda_1\Lambda_0 & \\ & & \ddots & \ddots & \ddots \\ & & & -\Lambda_0\Lambda_1 & \Lambda_0^2+\Lambda_1^2 \end{bmatrix}$$

We also permute ordering by eigenvalues obtaining

$$\Theta_{\mathrm{m}} = \left(P\mathbf{E}\mathbf{E}^T P^T\right)_m = \begin{bmatrix} a_m^2 & -a_m b_m & & & \\ -a_m b_m & a_m^2+b_m^2 & -a_m b_m & & \\ & -a_m b_m & a_m^2+b_m^2 & -a_m b_m & \\ & & \ddots & \ddots & \ddots \\ & & & -a_m b_m & a_m^2+b_m^2 \end{bmatrix}$$

where $a_m := \left(1 - \tau\theta\lambda_m\right)$ and $b_m := \left(1 + \tau(1-\theta)\lambda_m\right)$

To guarantee stability: $|b_m| \le |a_m|$ using Gershgoring's radius theorem

An lower bound

$$\mu(\Theta_m) \ge \min \left(|a_m|^2 \left(1 - \frac{|b_m|}{|a_m|} \right)^2 \right) = \min \left(\tau |\lambda_m| \right)^2 \qquad \mu(\Theta_m) \ge (\tau \rho_{\min})^2$$

An upper bound $\mu(\Theta_m) \le \max\ 4|a_m|^2 \rightarrow \quad \mu(\Theta_i) \le 4(1 - \tau\theta\rho_{\max})^2$

$$\text{Cond}(EE^T) \approx \frac{4(1 + \tau\theta\rho_{\max})^2}{(\tau\rho_{\min})^2}$$

Remark: for finite element discretization

$$-O\left(\frac{1}{h^2}\right) < \lambda_m < -O(1)$$

$$\text{Cond}(EE^T) \approx \frac{(1 + \tau\theta h^{-2})^2}{(\tau)^2}$$

The Schur complement for **u**

$$\begin{bmatrix} \mathbf{K} & & \mathbf{E}^T \\ & \mathbf{G} & \mathbf{N}^T \\ \mathbf{E} & \mathbf{N} & \end{bmatrix} . \begin{bmatrix} \mathbf{y} \\ \mathbf{u} \\ \mathbf{p} \end{bmatrix} = \begin{bmatrix} \mathbf{K}\mathbf{y}_* - \mathbf{g} \\ \mathbf{0} \\ \mathbf{f} \end{bmatrix}$$

$$\mathbf{p} = -\mathbf{E}^{-T}\mathbf{M}\mathbf{y} + \mathbf{E}^{-T}\mathbf{K}\mathbf{y}_* - \mathbf{E}^{-T}\mathbf{g}$$

$$\mathbf{y} = -\mathbf{E}^{-1}\mathbf{N}\mathbf{u} + \mathbf{E}\mathbf{f}$$

We reduce to the following Schur complement system for **u**

$$\left(\mathbf{G} + \mathbf{N}^T\mathbf{E}^{-T}\mathbf{K}\mathbf{E}^{-1}\mathbf{N}\right)\ \mathbf{u} \quad = \mathbf{b}$$

Properties:

Matrix $\mathbf{G} + \mathbf{N}^T\ \mathbf{E}^{-T}\ \mathbf{K}\ \mathbf{E}^{-1}\mathbf{N}$ is s.p.d.

Does not require $\mathbf{K}^{-1}$ and u could be low dimension.

The application of $\mathbf{E}^{-1}$ is stable.

Bounds for $\mathbf{G} + \mathbf{N}^T \mathbf{E}^{-T} \mathbf{K} \mathbf{E}^{-1}\mathbf{N}$

Conditioning of the matrices $\mathbf{G}, \mathbf{E}, \mathbf{K}, \mathbf{N}, \mathbf{\Gamma}$:

$$\mathrm{c}_1 \; q\tau \; \mathbf{y}^T\mathbf{y} \;\; \le \mathbf{y}^T\mathbf{Z}\mathbf{y} \le \mathrm{c}_2 \; q\tau \; \mathbf{y}^T\mathbf{y},$$

$$\mathrm{c}_3 \; r\tau \; h^d\mathbf{u}^T\mathbf{u} \le \mathbf{u}^T\mathbf{G}\mathbf{u} \le \mathrm{c}_4 \; r\tau \; h^d\mathbf{u}^T\mathbf{u},$$

$$\mathrm{c}_5\tau^2h^d\mathbf{p}^T\mathbf{p} \le \mathbf{p}^T\mathrm{N}\mathbf{N}^T\mathbf{p} \le \mathrm{c}_6\tau^2h^d\mathbf{p}^T\mathbf{p}$$

$$0 \le \mathbf{y}^T\mathbf{\Gamma}\mathbf{y} \le \mathrm{c}_7 \; s \; \mathbf{y}^T\mathbf{y}$$

$$\mathbf{K} = \mathbf{Z} + \mathbf{\Gamma}$$

Then

$$\mathbf{u}^T\mathbf{G}\mathbf{u} \le \mathbf{u}^T\left(\mathbf{G} + \mathbf{N}^T\mathbf{E}^{-T}\mathbf{K}\mathbf{E}^{-1}\mathrm{N}\right)\,\mathbf{u} \le \left(1 + \hat{c}\right)\,\mathbf{u}^T\mathbf{G}\mathbf{u}$$

Because $0 \le \mathbf{u}^T \mathbf{N}^T \mathbf{E}^{-T} \mathbf{M} \mathbf{E}^{-1} \mathbf{N} \mathbf{u}$ we can prove that:

$$\mathbf{u}^T \mathbf{N}^T \mathbf{E}^{-T} \mathbf{K} \mathbf{E}^{-1} \mathbf{N} \mathbf{u} \le \left(c_2 \tau + c_7 s\right) \, \mathbf{u}^T \mathbf{N}^T \mathbf{E}^{-T} \mathbf{E}^{-1} \mathbf{N} \mathbf{u}$$

$$\le \frac{\left(c_2 \tau + c_7 s\right)}{\left(\tau \rho_{\min}\right)^2} \mathbf{u}^T \mathbf{N}^T \mathbf{N} \mathbf{u} \le \frac{\left(c_2 \tau + c_7 s\right) \, \mathrm{c}_6 \tau^2 h^d}{\left(\tau \rho_{\min}\right)^2} \mathbf{u}^T \mathbf{u}$$

$$= \frac{\left(c_2 \tau + c_7 s\right) \, \mathrm{c}_6}{\left(\rho_{\min}\right)^2} \mathbf{u}^T \mathbf{u} \le \frac{\left(c_2 \tau + c_7 s\right) \, c_6}{\left(\rho_{\min}\right)^2 c_3 r \tau} \mathbf{u}^T \mathbf{G} \mathbf{u}$$

$$\hat{c} = \frac{\left(c_2 \tau + c_7 s\right) c_6}{\left(\rho_{\min}\right)^2 c_3 r \tau} \longrightarrow \mathbf{u}^T \mathbf{N}^T \mathbf{E}^{-T} \mathbf{K} \mathbf{E}^{-1} \mathbf{N} \mathbf{u} \le \hat{c} \, r \, \tau \, \mathbf{u}^T \mathbf{u} = \hat{c} \, \mathbf{u}^T \mathbf{G} \mathbf{u}$$

$$\lambda_{\min} \approx O(1)$$

$$\lambda_{\max} \approx O(h^{-4}) \longrightarrow \hat{c} = O\left(1 + \frac{1 + \frac{s}{\tau}}{r}\right)$$

$\hat{c}$ is sharp

Schaerer-Mathew-Sarkis, 2007. LNCS.

A simple example:
OCP for the 1-d heat equation

The equation: $\partial_t y = \partial_{xx} y + u, \quad y(0) = 0$

The performance functional:

$$J(y,u) := \frac{q}{2} \| y - y_* \|^2_{L^2(0,t_f;L^2(\Omega))} + \frac{r}{2} \| u \|^2_{L^2(0,t_f;L^2(\Omega))} + \frac{s}{2} \| y(t_f,x) - y_*(t_f,x) \|^2_{L^2(\Omega)}$$

$q = 1, \ r = 0.0001, \quad s = 0, \ s \neq 0 \quad \Omega = (0,1), \quad t \in (0,1)$

$$\left(\mathbf{G} + \mathbf{N}^T \mathbf{E}^{-T} \mathbf{K} \mathbf{E}^{-1} \mathbf{N} \right) \mathbf{u} = \mathbf{b}$$

$\tau = 1/N_t, \ \ h = 1/N_x \qquad \|\mathbf{r}_j\|_2 / \|\mathbf{r}_0\|_2 \leq 10^{-6} \qquad y_*(t,x) = x(1-x)e^{-x}$

$\hat{c}$ is sharp

$$\hat{c} = O\left(1 + \frac{1 + \frac{s}{\tau}}{r}\right)$$

Condition number

$r \backslash s$	10^4	10^2	10^0	10^{-2}	0
10^{-2}	4.9 10^4	5.0 10^2	6.21	1.9	1.9
10^{-4}	4.7 10^6	4.8 10^4	521	93	93
10^{-6}	4.2 10^8	4.8 10^6	51400	9200	9140

$q = 1, \quad h = 1/32, \quad \tau = 1/64$

CG-iteration numbers

Tolerance: 10^{-6} $s = 0$ ($s = 1$) $\mathbf{G} + \mathbf{N}^T\mathbf{E}^{-T}\mathbf{K}\mathbf{E}^{-1}\mathbf{N}$

$N_x \backslash N_t$	32	64	128	256	512
32	18 (19)	23 (25)	24 (27)	24 (29)	25 (30)
64	17 (19)	23 (25)	24 (27)	24 (29)	25 (30)
128	17 (19)	23 (26)	24 (27)	24 (29)	25 (30)
256	17 (19)	23 (26)	24 (27)	24 (29)	26 (31)
512	17 (19)	23 (26)	25 (27)	25 (29)	26 (31)

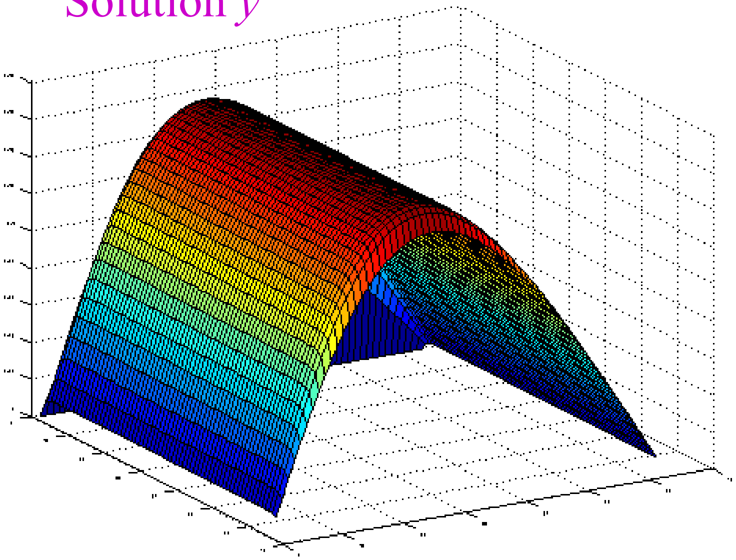
Backward - Euler rule is used for marching in time.

For the test problem studied, the method is scalable in h.

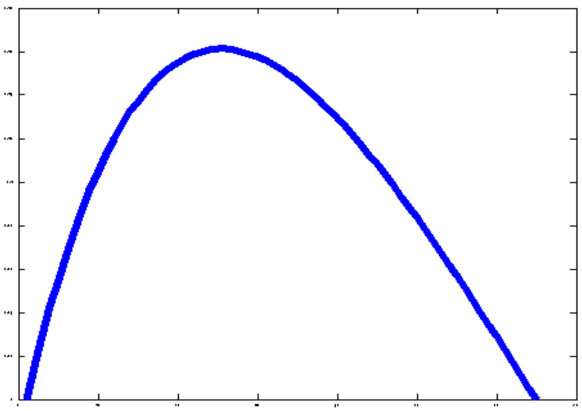
Solutions y and u

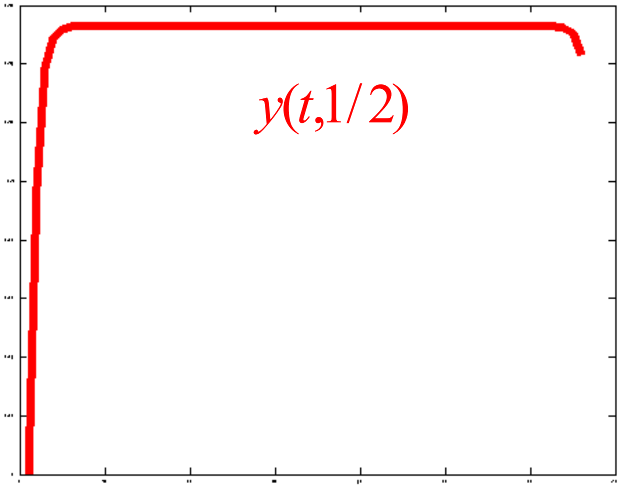
$s=0$

Solution y

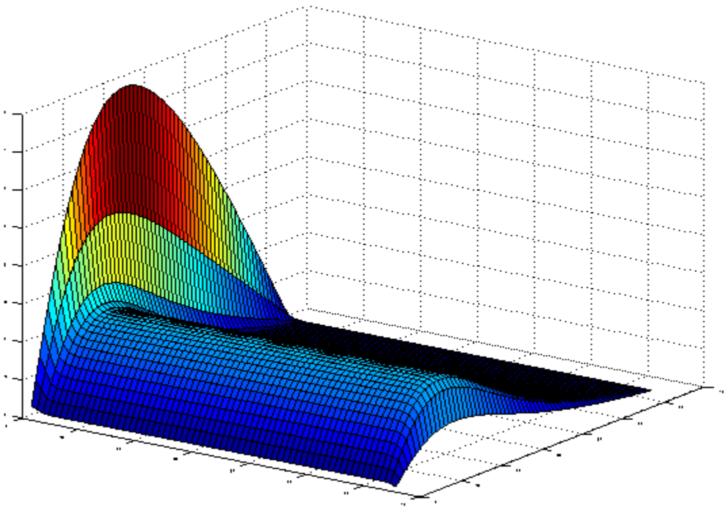


$y_*(t,x) = x(1-x)e^{-x}$



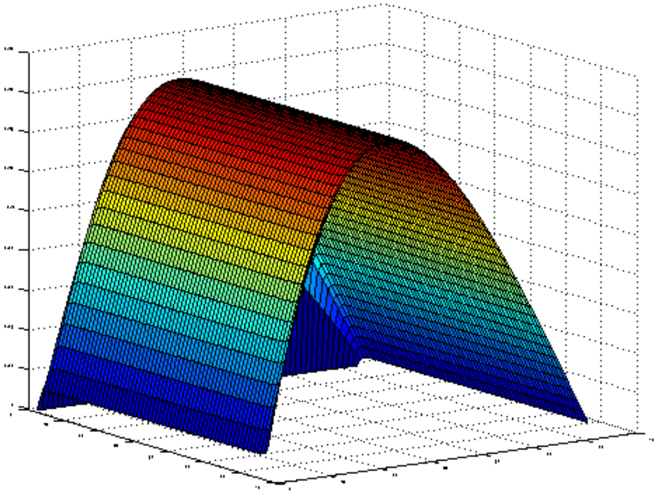

$y(t,1/2)$

Control function u



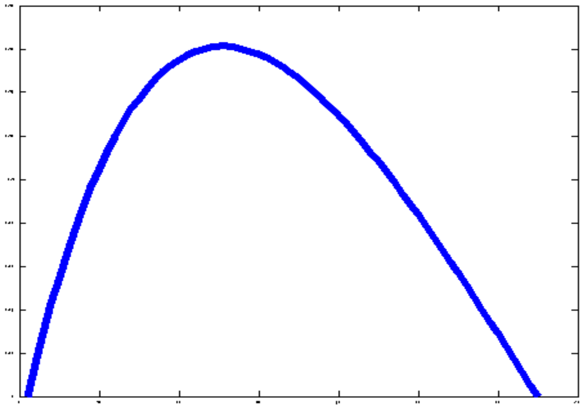
Solutions y and u

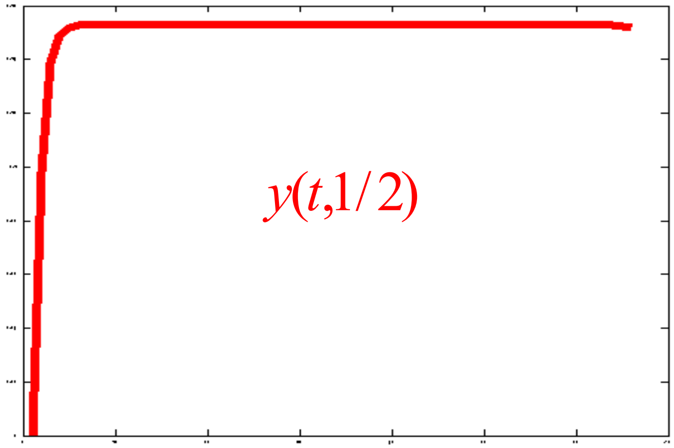
Solution y



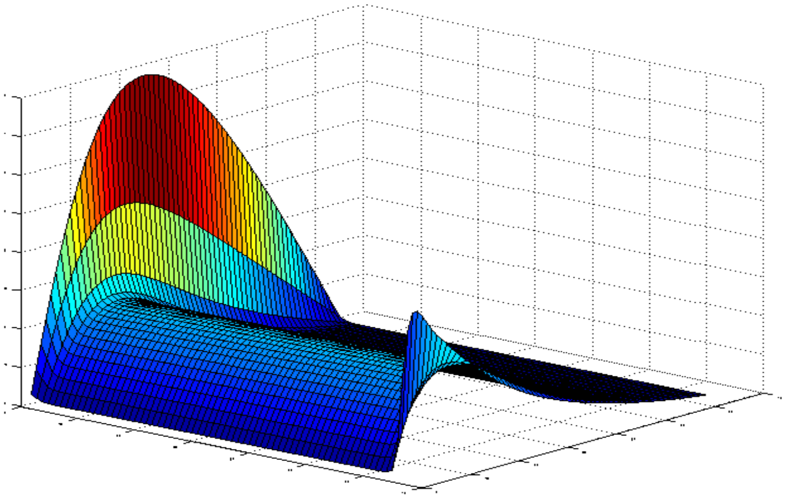
s=10

$y_*(t,x) = x(1-x)e^{-x}$



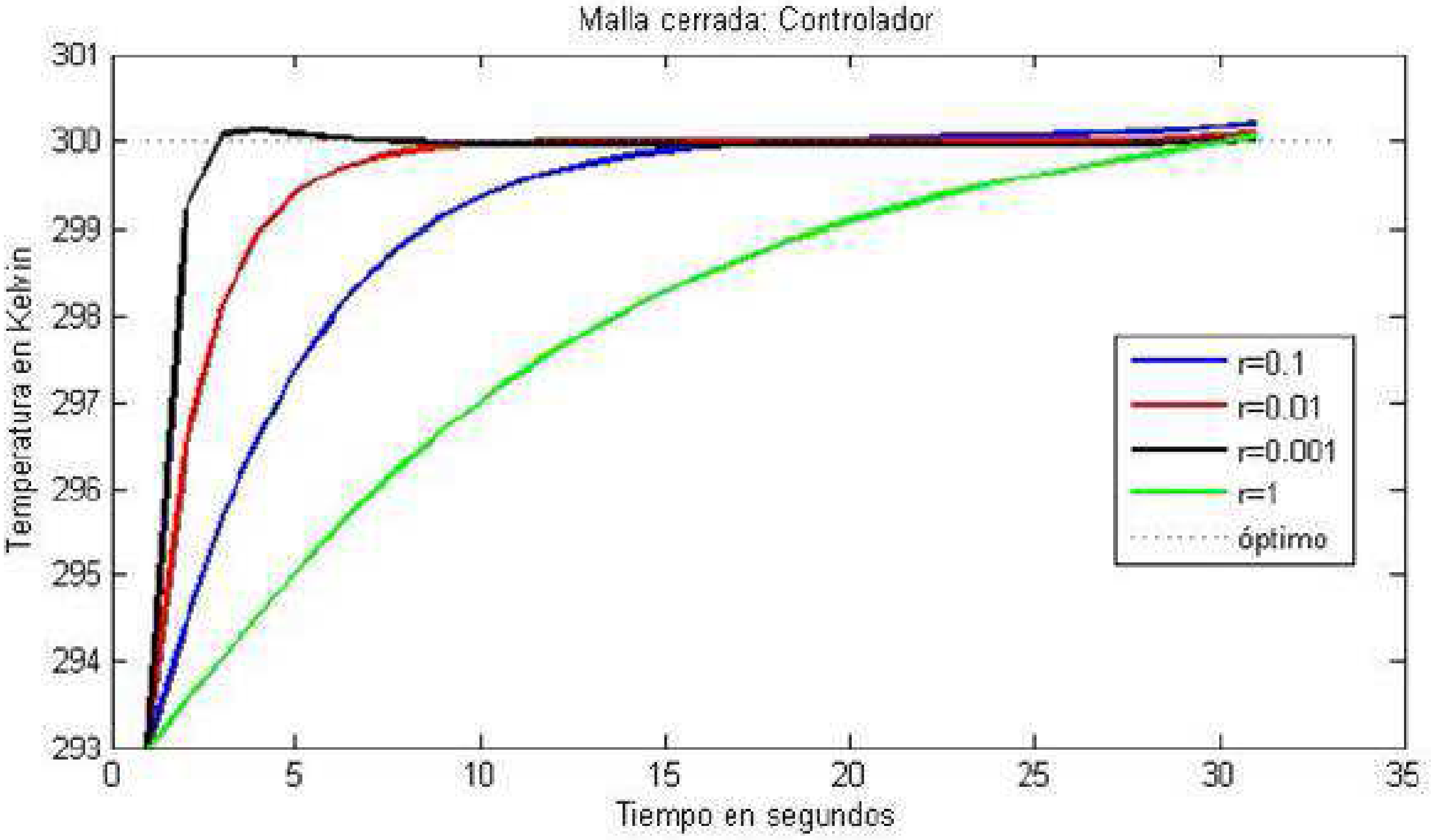


Control function u



Influence of *q* and *r*

Sauer-Feliciangeli-Schaerer, CNMAC



Properties of the reduced Schur complement system for the control variable

Advantages

1. This algorithm is solved by conjugate gradient.
2. The rate of convergence independents of the space discretization and depends weakly on time discretization.
3. r is chosen to adjust the solution to the reference y_* and to avoid oscillations.
3. s large avoids boundary layer.

Drawbacks

1. A double iteration algorithm (exact computation of E^{-1} and E^{-T}).

Next we parallelize in time: Parareal algorithm.

How to deal with the double iteration

$$\left(\mathbf{G} + \mathbf{N}^T \mathbf{E}^{-T} \mathbf{K} \mathbf{E}^{-1} \mathbf{N}\right) \mathbf{u} \quad = \mathbf{b}$$

- Consider inner – outer iteration with inexact solvers (Szyld).
- Consider a preconditioner for $\mathbf{E}^{-T}\mathbf{M}\mathbf{E}^{-1}$

$$\left(\mathbf{G} + \mathbf{N}^{\mathrm{T}} \mathbf{E}_n^{-T} \mathbf{K} \mathbf{E}_n^{-1} \mathbf{N}\right) \tilde{\mathbf{u}} \quad = \mathbf{b}$$

$$\tilde{\mathbf{u}} \to \mathbf{u} \qquad\qquad \mathbf{E}_n \to \mathbf{E}$$

How to apply $\mathbf{E}^{-\mathrm{T}}\mathbf{K}\mathbf{E}^{-1}$

$$\mathbf{v} = \mathbf{E}^{-T}\mathbf{K}\mathbf{E}^{-1}\mathbf{s}$$

1. Solve $\mathbf{Ez}=\mathbf{s}$
2. Multiply $\mathbf{Kz}$
3. Solve $\mathbf{E}^{T}\mathbf{v}=\mathbf{Kz}$

→ $\mathbf{Ez} = \mathbf{s}$

Avoiding double iterations

$$\left(\mathbf{G} + \mathbf{N}^{T}\mathbf{E}^{-T}\mathbf{K}\mathbf{E}^{-1}\mathbf{N}\right)\mathbf{u} \quad = \mathbf{b}$$

$$\mathbf{w} \;=\; -\mathbf{E}^{-T}\mathbf{K}\,\mathbf{E}^{-1}\mathbf{N}\,\mathbf{u}$$

$$\begin{bmatrix} \mathbf{E}^{T}\mathbf{K}^{-1}\mathbf{E} & \mathbf{N} \\ \mathbf{N}^{T} & -\mathbf{G} \end{bmatrix} \begin{bmatrix} \mathbf{w} \\ \mathbf{u} \end{bmatrix} = \begin{bmatrix} \mathbf{0} \\ -\mathbf{b} \end{bmatrix}$$

- The resulting system is symmetric and indefinite.
- It does not require $\mathbf{E}^{-1}$ and $\mathbf{E}^{-T}$.
- Easy to parallelize, however, ill conditioned, needs preconditioning.

Preconditioning

$$\overset{H}{\begin{bmatrix} \mathbf{E}^T\mathbf{K}^{-1}\mathbf{E} & \mathbf{N} \\ \mathbf{N}^T & -\mathbf{G} \end{bmatrix}} \begin{bmatrix} \mathbf{w} \\ \mathbf{u} \end{bmatrix} = \lambda \overset{P}{\begin{bmatrix} \mathbf{E}^T\mathbf{K}^{-1}\mathbf{E} & \\ & \mathbf{G} \end{bmatrix}} \begin{bmatrix} \mathbf{w} \\ \mathbf{u} \end{bmatrix}$$

$$(\lambda - 1)\mathbf{E}^T\mathbf{K}^{-1}\mathbf{E}\ \mathbf{w} = \mathbf{N}\mathbf{u} \quad \text{and} \quad (\lambda + 1)\mathbf{G}\ \mathbf{w} = \mathbf{N}^T\mathbf{u}$$

$$\mathbf{N}^T\mathbf{E}^T\mathbf{K}^{-1}\mathbf{E}\mathbf{N}\ \mathbf{u} = (\lambda^2 - 1)\mathbf{G}\mathbf{u}$$

$$\kappa\left(P^{-1}H\right) = O\left(\left(1 + \frac{1 + s/\tau}{r}\right)^{1/2}\right)$$

MINRES-iterations numbers

Tolerance: 10^{-6} $s = 0$ $(s = 1)$ $\mathbf{P}^{-1}\mathbf{H} = \begin{bmatrix} \mathbf{I} & \mathbf{E}^{-T}\mathbf{K}\mathbf{E}^{-1}\mathbf{N} \\ \mathbf{G}^{-1}\mathbf{N} & -\mathbf{I} \end{bmatrix}$

Nx \ Nt	32	64	128	256	512
32	34 (36)	40 (44)	42 (46)	42 (46)	42 (46)
64	32 (36)	40 (44)	42 (46)	42 (46)	42 (46)
128	32 (36)	40 (44)	42 (46)	42 (46)	42 (46)
256	32 (36)	40 (44)	42 (46)	42 (46)	42 (46)
512	32 (36)	40 (44)	42 (46)	42 (46)	42 (46)

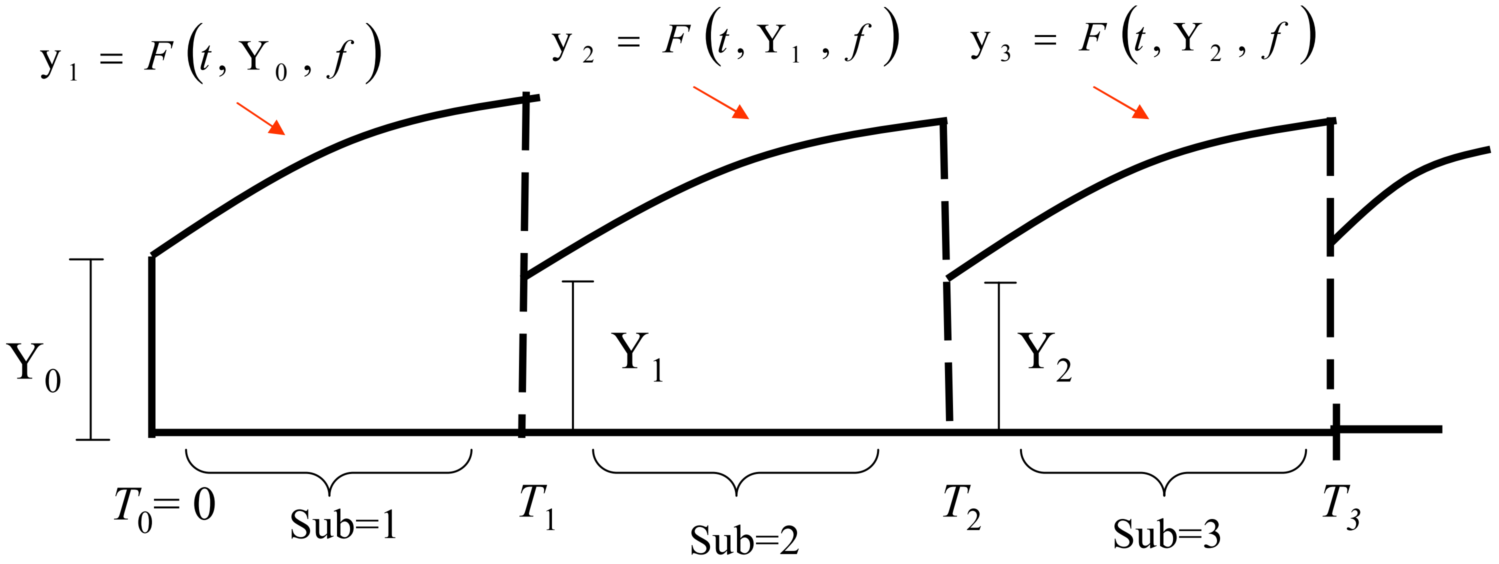
$\mathbf{E}^{-1}$ is sequential.

Still expensive

$$\mathbf{P}^{-1}\mathbf{H} = \begin{bmatrix} \mathbf{I} & \boxed{\mathbf{E}^{-T}\mathbf{K}\mathbf{E}^{-1}\mathbf{N}} \\ \mathbf{G}^{-1}\mathbf{N} & -\mathbf{I} \end{bmatrix}$$

How to parallelize E^{-1} in time:

Parareal-method



$$f = Bu \qquad \begin{cases} \dot{y} = Ay + f \\ y(T_i) = Y_i \end{cases} \quad \rightarrow \quad F(t, Y_i, f) := y(t)$$

Backward Euler

Continuity of solution

$$Y_k - FY_{k-1} = 0, \quad k = 1, \ldots, \hat{k}$$

$$Y_0 = 0$$

Parareal: Lions-Maday-Turinici

Parareal: parallel preconditioner

$$\begin{bmatrix} I & & & \\ -F & I & & \\ & \ddots & \ddots & \\ & & -F & I \end{bmatrix} \begin{bmatrix} Y_0 \\ Y_1 \\ \vdots \\ Y_{\hat{k}} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

F is a fine marching operator

$$\begin{bmatrix} Y_0 \\ Y_1 \\ \vdots \\ Y_{\hat{k}} \end{bmatrix}^{n+1} = \begin{bmatrix} Y_0 \\ Y_1 \\ \vdots \\ Y_{\hat{k}} \end{bmatrix}^{n} - \begin{bmatrix} I & & & \\ -G & I & & \\ & -G & I & \\ & & -G & I \end{bmatrix}^{-1} \left(\begin{bmatrix} I & & & \\ -F & I & & \\ & \ddots & \ddots & \\ & & -F & I \end{bmatrix} \begin{bmatrix} Y_0 \\ Y_1 \\ \vdots \\ Y_{\hat{k}} \end{bmatrix}^{n} \right)$$

G is a coarse marching operator $\quad G = (I - A\Delta T)^{-1}, \quad \Delta T = T_{k+1} - T_k$

Convergence theorem for parabolic equation

The error of the Parareal scheme using backward Euler in both fine and coarse propagators is given by

$$\max_{1\le k\le \hat{k}} \left\| y(T_k) - Y_k^n \right\|_{L^2(\Omega)} \le \rho_n \max_{1\le k\le \hat{k}} \left\| y(T_k) \right\|_{L^2(\Omega)}$$

where

$$\rho_n = \max_{0<\beta<1}\left(\left(e^{1-1/\beta} - \beta\right)^n \frac{1}{n!} \frac{d^{n-1}}{d\beta^{n-1}} \left| \frac{1-\beta^{\hat{k}-1}}{1-\beta} \right| \right) \le \left(\max_{0<\beta<1} \frac{\left(e^{1-1/\beta} - \beta\right)}{1-\beta} \right)^n \le 0.2984^n$$

- Maximum is attained around β_* is independent of n and k.
- For practical problems λ_* defined by $\beta_* = \left(1 - \lambda_* \Delta T\right)^{-1}$ will lie in the interior of the spectrum of eigenvalues of A.

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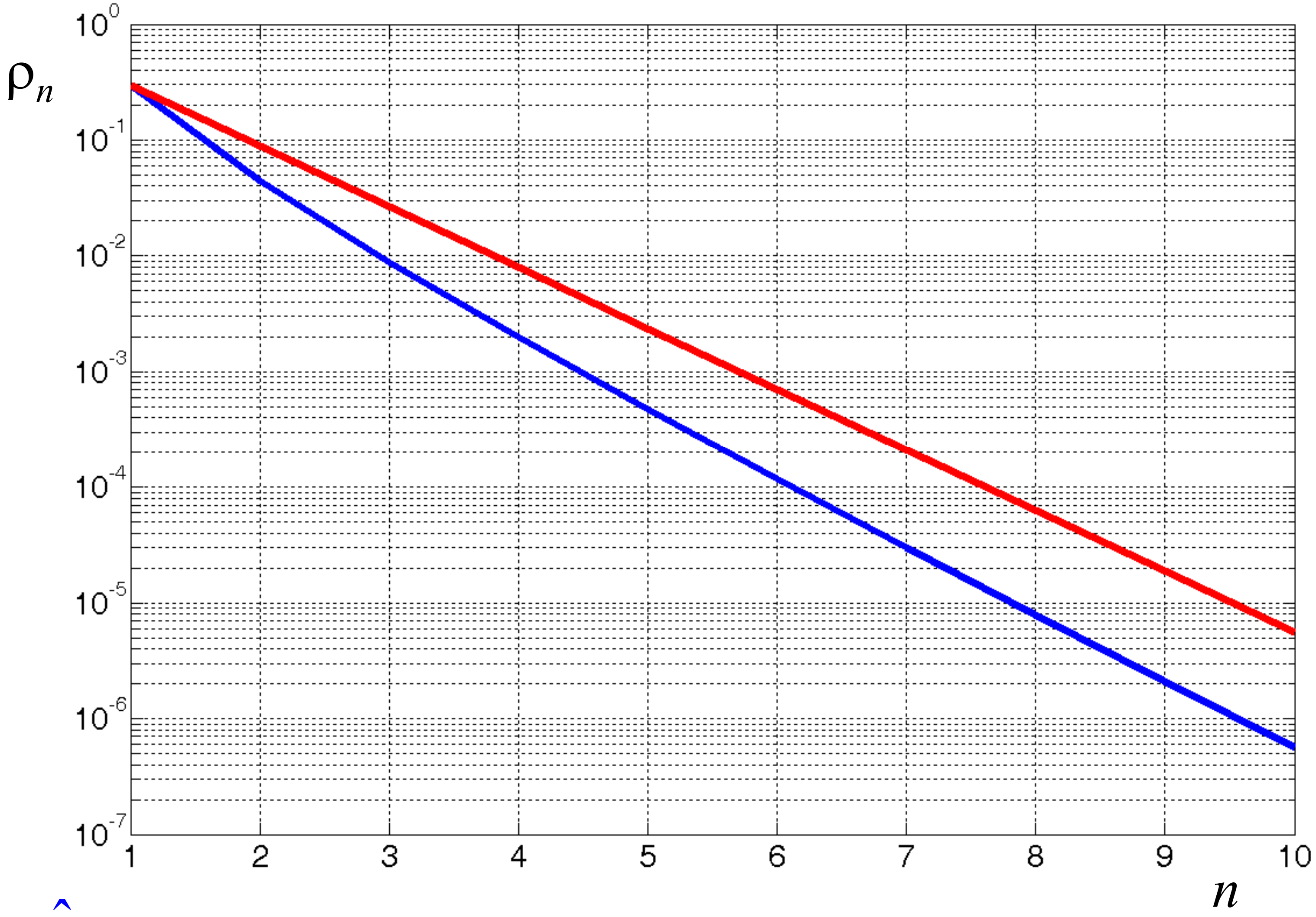
ρ_n in terms of n



$\hat{k} = 160$

Parareal for control

Theorem: Let E_n the n^{th} application of the Parareal scheme, then

$$\gamma_{\min}\left(\mathbf{r},\mathbf{E}^{-T}\mathbf{K}\mathbf{E}^{-1}\mathbf{r}\right)\leq\left(\mathbf{r},\mathbf{E}_n^{-T}\hat{\mathbf{K}}\mathbf{E}_n^{-1}\mathbf{r}\right)\leq\gamma_{\max}\left(\mathbf{r},\mathbf{E}^{-T}\mathbf{K}\mathbf{E}^{-1}\mathbf{r}\right)$$

where $\gamma_{\max}=1+O\left(2\sqrt{\frac{\rho_n t_f}{\tau}}\right)$ and $\gamma_{\min}=1-O\left(2\sqrt{\frac{\rho_n t_f}{\tau}}\right)$

This is a sharp bound

For n small: error on the solution.

Dynamic adapted Krylov method (Sarkis-Schaerer-Szyld: in progress) .

$\gamma_{\max}$ and $\gamma_{\min}$ estimates are sharp

	N_t	200	400	800	1600
$\gamma_{\max}-1$	n=1	0.8644	1.4493	2.4737	4.3717
	n=2	0.0708	0.0979	0.1368	0.1938
	n=3	0.0078	0.0108	0.0151	0.0212
	n=4	0.0009	0.0012	0.0017	0.0024

$\Delta T = 1/20$

$h = 1/10$

Factor $\sqrt{2}$

	N_t	200	400	800	1600
$1-\gamma_{\min}$	n=1	0.4642	0.5663	0.6925	0.7991
	n=2	0.0663	0.0895	0.1217	0.1642
	n=3	0.0077	0.0107	0.0149	0.0207
	n=4	0.0008	0.0012	0.0017	0.0024

How to deal with the double iteration

$$\left(\mathbf{G}+\mathbf{N}^{T}\mathbf{E}^{-T}\mathbf{K}\mathbf{E}^{-1}\mathbf{N}\right)\mathbf{u} \quad =\mathbf{b}$$

- Consider inner – outer iteration with inexact solvers (Szyld).

- Consider a preconditioner for $\mathbf{E}^{-T}\mathbf{M}\mathbf{E}^{-1}$

$$\left(\mathbf{G}+\mathbf{N}^{\mathrm{T}}\mathbf{E}_{n}^{-T}\mathbf{K}\mathbf{E}_{n}^{-1}\mathbf{N}\right)\tilde{\mathbf{u}} \quad =\mathbf{b}$$

$$\tilde{\mathbf{u}}\rightarrow\mathbf{u} \qquad \mathbf{E}_{n}\rightarrow\mathbf{E}$$

CG-iteration numbers: Parareal-6

Tolerance: 10^{-6} $s = 0$ ($s = 1$) $G + N^T E^{-T} M E^{-1} N$

$N_x \backslash N_t$	32	64	128	256	512
32	18 (19)	23 (25)	24 (27)	24 (29)	25 (30)
64	17 (19)	23 (25)	24 (27)	24 (29)	25 (30)
128	17 (19)	23 (26)	24 (27)	24 (29)	25 (30)
256	17 (19)	23 (26)	24 (27)	24 (29)	26 (31)
512	17 (19)	23 (26)	25 (27)	25 (29)	26 (31)

Backward - Euler rule is used for marching in time.

For the test problem studied, the method is scalable in h.

Inexact Case with Daniel Szyld

Block Matrix Algorithms

Alg. 2. Reduction to **u** and $\mathbf{w}=-\mathbf{E}^{-T}\mathbf{K}\mathbf{E}^{-1}\mathbf{N}\mathbf{u}$

$$\begin{bmatrix} \mathbf{E}^{\mathrm{T}}\mathbf{K}^{-1}\mathbf{E} & \mathbf{N} \\ \mathbf{N}^{-T} & -\mathbf{G} \end{bmatrix} \begin{bmatrix} \mathbf{w} \\ \mathbf{u} \end{bmatrix} = \begin{bmatrix} \mathbf{0} \\ -\mathbf{b} \end{bmatrix}$$

$$\mathbf{P} = \begin{bmatrix} \mathbf{E}^{\mathrm{T}}\mathbf{K}^{-1}\mathbf{E} & \\ & \mathbf{G} \end{bmatrix} \qquad \mathbf{P}_n = \begin{bmatrix} \mathbf{E}_n^T\hat{\mathbf{K}}^{-1}\mathbf{E}_n & \\ & \mathbf{G} \end{bmatrix}$$

MINRES-iterations numbers

Tolerance: 10^{-6} $s = 0$ (s = 1) $P^{-1}H = \begin{bmatrix} I & E^{-T}KE^{-1}N \\ G^{-1}N & -I \end{bmatrix}$

Nx \ Nt	32	64	128	256	512
32	34 (36)	40 (44)	42 (46)	42 (46)	42 (46)
64	32 (36)	40 (44)	42 (46)	42 (46)	42 (46)
128	32 (36)	40 (44)	42 (46)	42 (46)	42 (46)
256	32 (36)	40 (44)	42 (46)	42 (46)	42 (46)
512	32 (36)	40 (44)	42 (46)	42 (46)	42 (46)

E^{-1} is sequential.

Parareal cycles vs exact solver

Tolerance: 10^{-6} N_x=64

Stop criteria: $\|\mathbf{r}_j\|_2 / \|\mathbf{r}_0\|_2 \leq 10^{-6}$

MINRES - number of iterations for $\Delta T/\tau = 16$

$\hat{k}$	4	8	16	32
N_t	64	128	256	512
h=1/16	57 / 40 / 40	59 / 54 / 42	63 / 54 / 42	63 / 54 / 44
h=1/32	55 / 40 / 40	59 / 54 / 42	63 / 54 / 42	63 / 54 / 44
h=1/64	55 / 40 / 40	59 / 54 / 42	63 / 54 / 42	63 / 54 / 44

$n = 2/4/6$

$q = 1 \quad r = 10^{-4} \quad s = 0$

Backward Euler for both fine and coarse grid.

For the test problem studied, the method is scalable.

Scalability

Tolerance: 10^{-6} N_x=64 Stop criteria: $\|\mathbf{r}_j\|_2 / \|\mathbf{r}_0\|_2 \leq 10^{-6}$

MINRES - Number of iterations

$\hat{k}$	8	16	32	64
$\Delta T / \tau$	64	32	16	8
h=1/16	66	66	64	63
h=1/32	66	66	64	62
h=1/64	65	64	63	61

$n = 2$ $\tau = 1/512$ $q = 1$ $r = 10^{-4}$ $s = 0$

Backward Euler for both fine and coarse grid.

For the test problem studied, the method is scalable.

Block Matrix Algorithms

- Alg. 1. Reduction to **u**

$$\left(\mathbf{G} + \mathbf{N}^{\mathbf{T}}\mathbf{E}^{\mathbf{-T}}\mathbf{K}\mathbf{E}^{\mathbf{-1}}\mathbf{N}\right)\ \mathbf{u} \quad = \mathbf{b}$$

- Alg. 2. Reduction to **u** and **w = -E**$^{-T}$**KE**$^{-1}$**Nu**

$$\begin{bmatrix} \mathbf{E}^{\mathbf{T}}\mathbf{K}^{-1}\mathbf{E} & \mathbf{N} \\ \mathbf{N}^{-T} & -\mathbf{G} \end{bmatrix}\begin{bmatrix} \mathbf{w} \\ \mathbf{u} \end{bmatrix} = \begin{bmatrix} \mathbf{0} \\ -\mathbf{b} \end{bmatrix}$$

Block Matrix Algorithms

Alg. 2. Reduction to $\mathbf{u}$ and $\mathbf{w}=-\mathbf{E}^{-T}\mathbf{K}\mathbf{E}^{-1}\mathbf{N}\mathbf{u}$

$$\begin{bmatrix} \mathbf{E}^{\mathrm{T}}\mathbf{K}^{-1}\mathbf{E} & \mathbf{N} \\ \mathbf{N}^{-T} & -\mathbf{G} \end{bmatrix} \begin{bmatrix} \mathbf{w} \\ \mathbf{u} \end{bmatrix} = \begin{bmatrix} \mathbf{0} \\ -\mathbf{b} \end{bmatrix}$$

$$\mathbf{P} = \begin{bmatrix} \mathbf{E}^{\mathrm{T}}\mathbf{K}^{-1}\mathbf{E} & \\ & \mathbf{G} \end{bmatrix} \qquad \mathbf{P}_n = \begin{bmatrix} \mathbf{E}_n^T\hat{\mathbf{K}}^{-1}\mathbf{E}_n & \\ & \mathbf{G} \end{bmatrix}$$

Concluding remarks

- We presented two algorithms for solving the parabolic optimal control problem. Sharp analysis were developed.
- A scalable algorithm based on Parareal and block type preconditioning is introduced. It is fully scalable in terms of space and time discretization.

There is much more on the road

On going work:

- Preconditioned for the nonlinear problem.
- Non all at once methods.
- The inexact case.

Future work:

- Parallelization in space and time simultaneously.
- Parallel computations.
- Augmented Lagrangian when M is singular1.

THANK YOU

Robin OCP

Minimize $J(y,u)$

subject to
$$\begin{cases} \rho c_p \dfrac{\partial y}{\partial t} = \nabla \cdot \left(\lambda \nabla y\right) + f & \text{in} \quad \Omega \times \left[t_0,\ t_f\right] \\ y\left(x,\ 0\right) = y_0 & \text{in} \quad \Omega \\ \dfrac{\partial y}{\partial \eta} = -\dfrac{u}{\lambda}\left(y - y_\infty\right) & \text{in} \quad \partial\Omega \times \left[t_0,\ t_f\right] \end{cases}$$

where $J(y,u) = \dfrac{q}{2}\left\|y - y_*\right\|^2_{L^2\left(t_0, t_f; \Omega\right)} + \dfrac{r}{2}\left\|u\right\|^2_{L^2\left(t_0, t_f; \partial\Omega\right)}$

The discretization in space

$$M\dot{\mathrm{y}} = -A\mathrm{y} - C(\mathrm{u})\mathrm{y} + y_{\infty}B\mathrm{u} + \mathrm{f}$$

where:

$$M = \left[\int_{\Omega} \rho c_p \phi_i \phi_j\right]_{ij} \in \mathbb{R}^{\hat{m}\times\hat{m}} \qquad A = \left[\int_{\Omega} \lambda \nabla\phi_i \cdot \nabla\phi_j\right]_{ij} \in \mathbb{R}^{\hat{m}\times\hat{m}}$$

$$C = \left[\int_{\partial\Omega} u \phi_i \phi_j\right]_{ij} \in \mathbb{R}^{\hat{m}\times\hat{m}} \qquad B = \left[\int_{\partial_j} \phi_i\right]_{ij} \in \mathbb{R}^{\hat{m}\times\hat{l}}$$

The discretization in time

Backward Euler

$$\left(M_l + \tau A_l + \tau C_l\right)\mathrm{y}_l - \tau y_\infty B_l \mathrm{u}_{l-1} = \tau f_l + M_l \mathrm{y}_{l-1}$$

we have

$$F_1 \mathrm{y}_{l+1} = F_0 \mathrm{y}_l + \tau \ B \ \mathrm{u}_l + \tau b$$

We obtain

$$\mathbf{E}\left(\mathbf{u}\right)\mathbf{y}+\mathbf{N}\mathbf{u}=\mathbf{f}$$

donde:

$$F_1=\left(M_l+\tau A_l+\tau C_l\right)$$

$$\mathbf{E}=\begin{bmatrix} -F_1 & & \\ F_0 & -F_1 & \\ & F_0 & -F_1 \end{bmatrix}$$

$$F_0=M_l$$

All at once discretization

$$\min J(\mathbf{y},\mathbf{u})$$

subject to: $\mathbf{E}(\mathbf{u})\ \mathbf{y} + \mathbf{N}\ \mathbf{u} = \mathbf{f}$

where $J(\mathrm{y},\mathrm{u}) = \frac{q}{2}\left(\mathbf{y}-\mathbf{y}_*\right)^T \mathbf{K}\left(\mathbf{y}-\mathbf{y}_*\right)+\frac{r}{2}\mathbf{u}^T\mathbf{G}\mathbf{u}$

KKT-conditions

$$L(\mathbf{y},\mathbf{u},\mathbf{p}) = \frac{q}{2}\left(\mathbf{y}-\mathbf{y}_*\right)^T \mathbf{K}\left(\mathbf{y}-\mathbf{y}_*\right) + \frac{r}{2}\mathbf{u}^T\mathbf{G}\mathbf{u} + \left\langle \mathbf{p}, \mathbf{E}(\mathbf{u})\,\mathbf{y} + \mathbf{N}\,\mathbf{u} - \mathbf{f} \;\right\rangle$$

$$F(\mathbf{y},\mathbf{u},\mathbf{p}) = \begin{cases} \partial_{\mathbf{y}-\mathbf{y}_*} L = q\mathbf{K}\left(\mathbf{y}-\mathbf{y}_*\right) + \mathbf{E}^T(\mathbf{u})\mathbf{p} = \mathbf{0} \\ \partial_{\mathbf{u}} L = r\mathbf{G}\mathbf{u} + \partial_{\mathbf{u}}\left(\mathbf{p}^T\mathbf{E}(\mathbf{u})\mathbf{y}\right) + \mathbf{N}^T\mathbf{p} = \mathbf{0} \\ \partial_{\mathbf{p}} L = \mathbf{E}(\mathbf{u})\mathbf{y} + \mathbf{N}\mathbf{u} - \mathbf{f} = \mathbf{0} \end{cases}$$

Solving the nonlinear system

$$\begin{bmatrix} \mathbf{y} \\ \mathbf{u} \\ \mathbf{p} \end{bmatrix}_{k+1} = \begin{bmatrix} \mathbf{y} \\ \mathbf{u} \\ \mathbf{p} \end{bmatrix}_{k} - F^{-1}(\mathbf{y},\mathbf{u},\mathbf{p})F(\mathbf{y}_k,\mathbf{u}_k,\mathbf{p}_k)$$

$$F = \begin{bmatrix} \partial_{\mathbf{y}}\left(\mathbf{K}\left(\mathbf{y}-\mathbf{y}_*\right)+\mathbf{E}^T(\mathbf{u})\mathbf{p}\right) & \partial_{\mathbf{u}}\left(\mathbf{K}\left(\mathbf{y}-\mathbf{y}_*\right)+\mathbf{E}^T(\mathbf{u})\mathbf{p}\right) & \partial_{\mathbf{p}}\left(\mathbf{K}\left(\mathbf{y}-\mathbf{y}_*\right)+\mathbf{E}^T(\mathbf{u})\mathbf{p}\right) \\ \partial_{\mathbf{y}}\left(\mathbf{G}\mathbf{u}+\partial_{\mathbf{u}}\left(\mathbf{p}^T\mathbf{E}(\mathbf{u})\mathbf{y}\right)+\mathbf{N}^T\mathbf{p}\right) & \partial_{\mathbf{u}}\left(\mathbf{G}\mathbf{u}+\partial_{\mathbf{u}}\left(\mathbf{p}^T\mathbf{E}(\mathbf{u})\mathbf{y}\right)+\mathbf{N}^T\mathbf{p}\right) & \partial_{\mathbf{p}}\left(\mathbf{G}\mathbf{u}+\partial_{\mathbf{u}}\left(\mathbf{p}^T\mathbf{E}(\mathbf{u})\mathbf{y}\right)+\mathbf{N}^T\mathbf{p}\right) \\ \partial_{\mathbf{y}}\left(\mathbf{E}(\mathbf{u})\mathbf{y}+\mathbf{N}\mathbf{u}-\mathbf{f}\right) & \partial_{\mathbf{u}}\left(\mathbf{E}(\mathbf{u})\mathbf{y}+\mathbf{N}\mathbf{u}-\mathbf{f}\right) & \partial_{\mathbf{p}}\left(\mathbf{E}(\mathbf{u})\mathbf{y}+\mathbf{N}\mathbf{u}-\mathbf{f}\right) \end{bmatrix} = \mathbf{0}$$

$$F = \begin{bmatrix} \mathbf{K} & & \mathbf{E}^T(\mathbf{u}) \\ & \mathbf{G} & \mathbf{N}^T \\ \mathbf{E}(\mathbf{u}) & \mathbf{N} & \mathbf{0} \end{bmatrix}$$

Resultados del control

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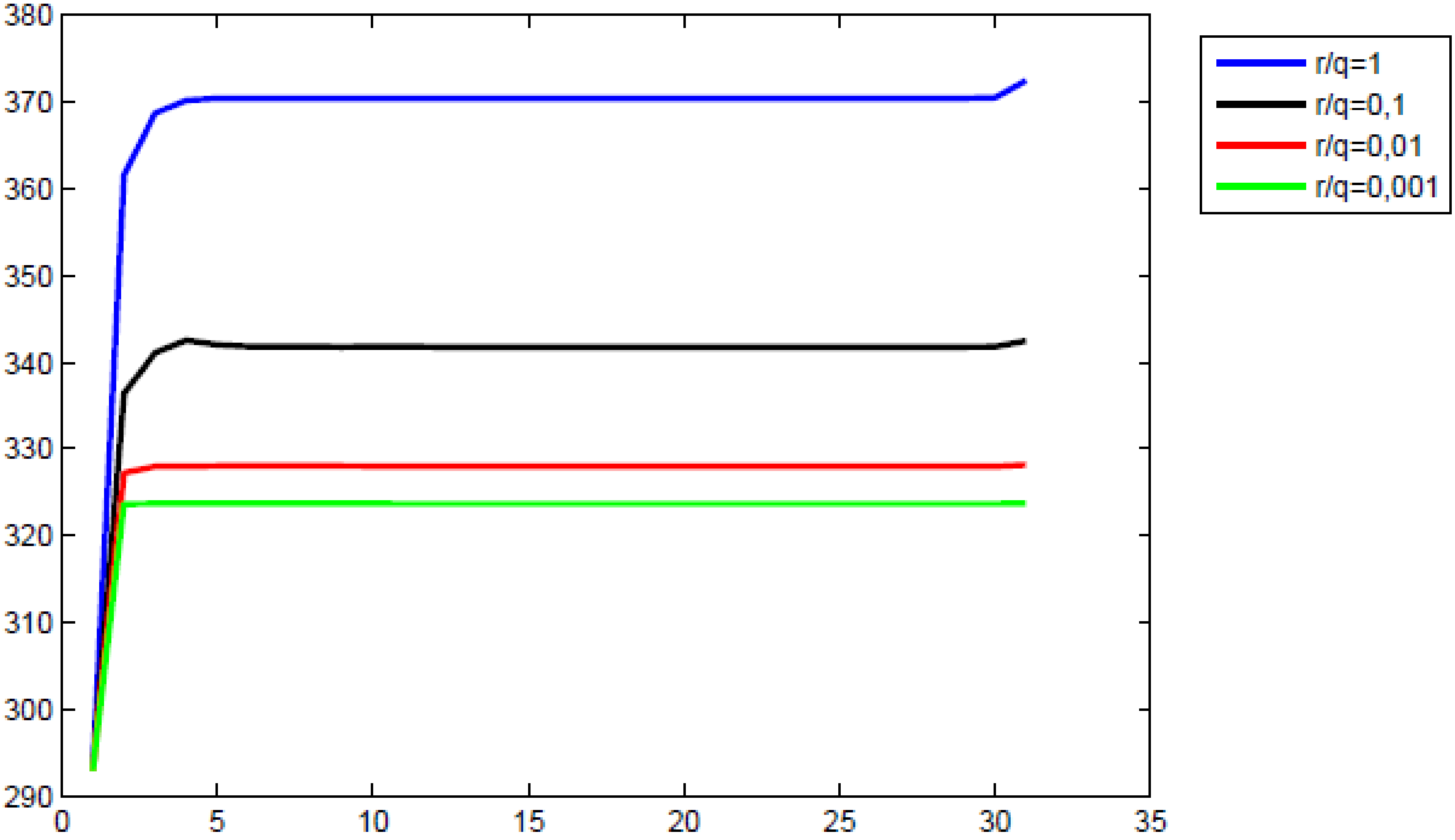
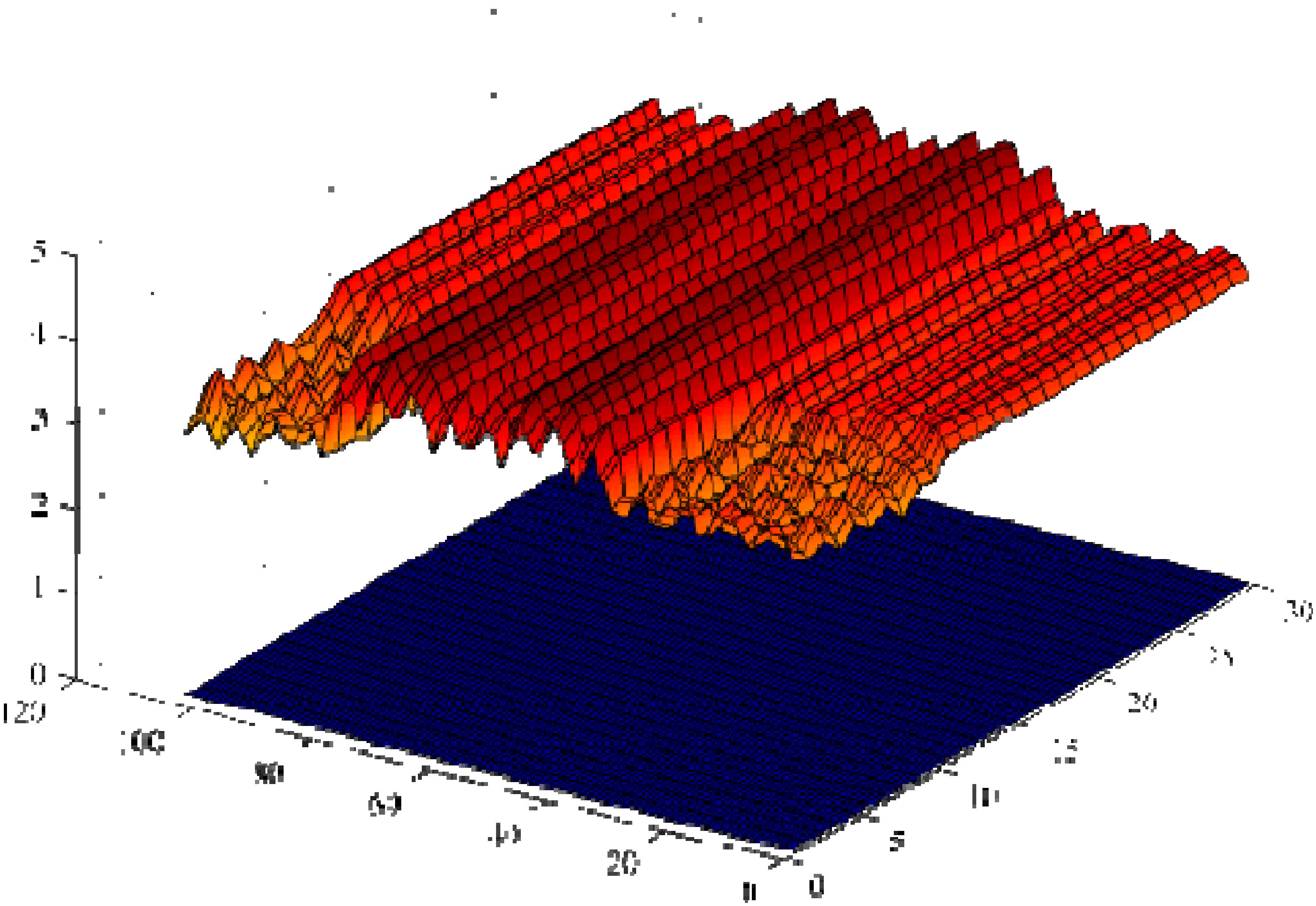


RESULTADOS DEL CONTROL



Then we obtain

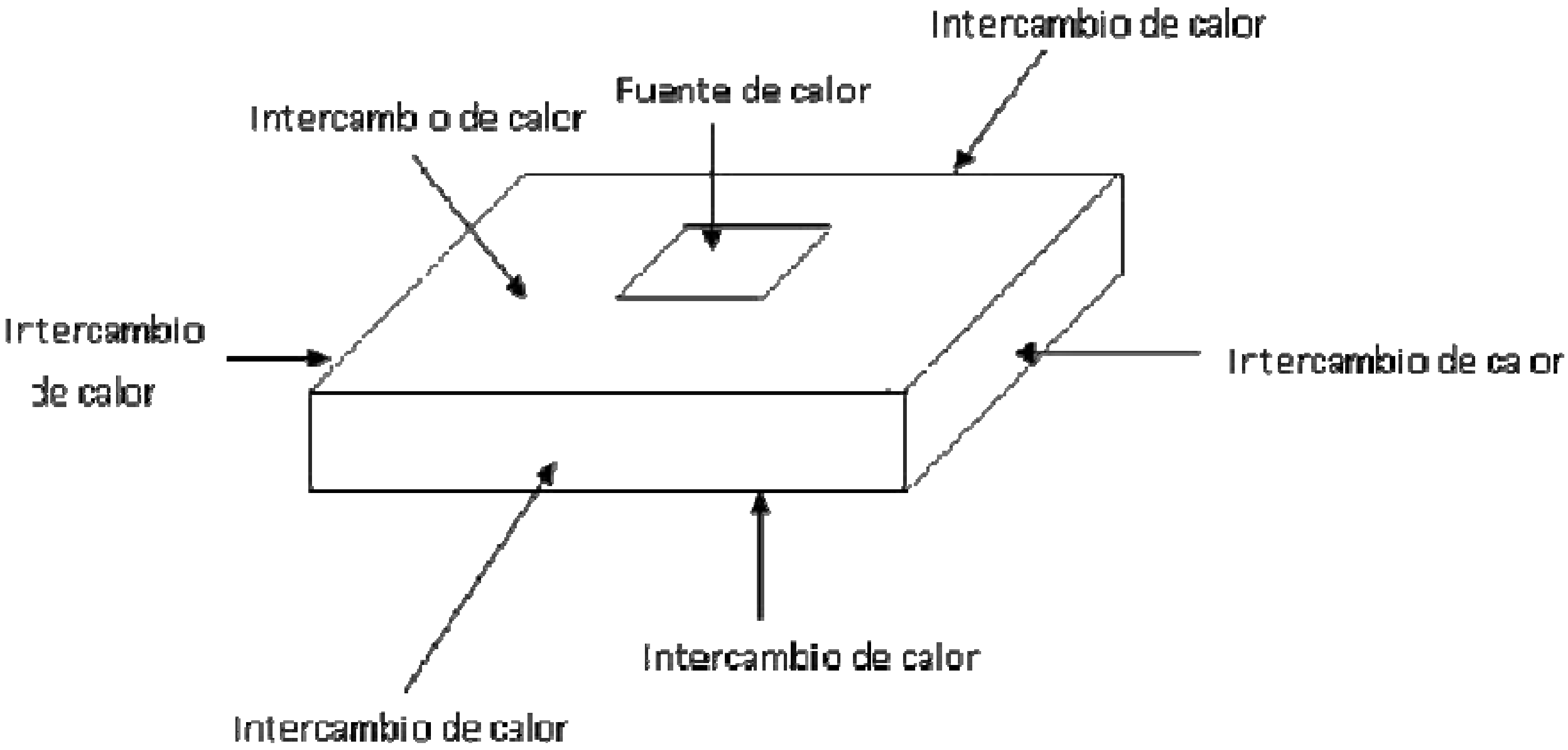
$$\left\{\begin{array}{llll} \rho c_p \dfrac{\partial y}{\partial t} & = & \nabla \cdot \left(\lambda \nabla y\right) + f & \text{in} \quad \Omega \times \left[t_0,\ t_f\right] \\ y\left(x,\ 0\right) & = & y_0 & \text{in} \quad \Omega \\ \dfrac{\partial y}{\partial \eta} & = & -\dfrac{u}{\lambda}\left(y - y_\infty\right) & \text{in} \quad \partial\Omega \times \left[t_0,\ t_f\right] \end{array}\right.$$

u is the convection coefficient and the control variable to dissipate the heat.

Simplifications in the model

- Physical properties are piecewise constant in space and time.
- Isotropic material.
- Perfect contact.
- Initial the linear case.

Modeling


Intercambio de calor
Fuante de calor
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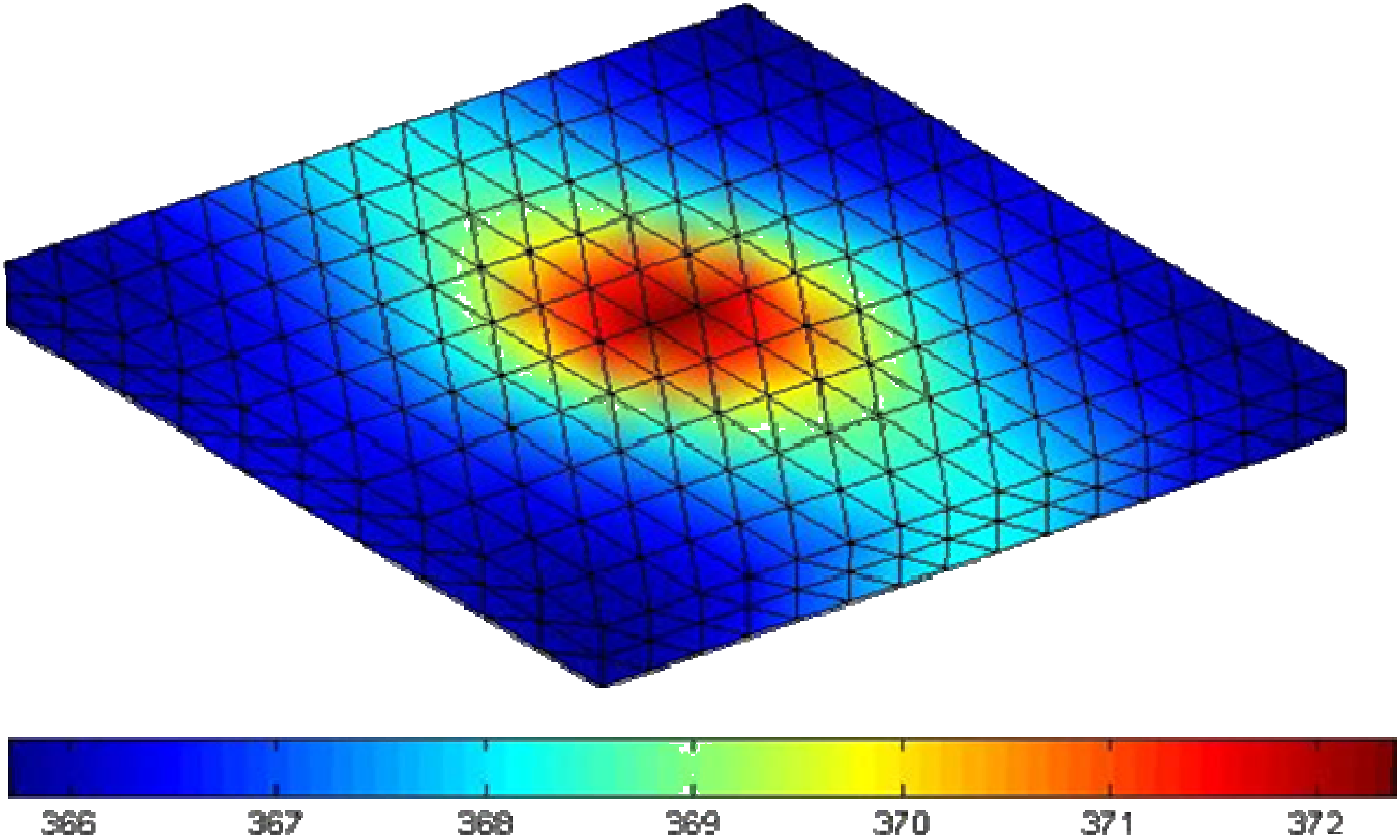
Intercambio de calor
Intercambio de calor

Numerical result



Past and Future: necessity for simulation

In the past, we could build **physical prototypes** and characterize those prototypes to ensure they met performance and reliability requirements.

Today, the consumer dominated market demands short lead time and low cost.

The only possibility for meeting these demands and delivering the required performance and reliability is to do the prototype build and characterization through **modeling and simulation**

ITRS 2007 Assembly & Packaging

New technologies

The introduction of low-κ dielectrics with low thermal conductivity increases the **need for thermal analysis**.

Simulation of **heat generation and removal and thermal dissipation is even more important** than for standard CMOS due to the higher power densities typically present in the wide bandgap semiconductors and wafer thinning used.

Advanced modeling tools covering the related electrical, **thermal**, and mechanical aspects are needed to support the development and optimization of these technologies

ITRS 2007 Modeling & Simulation

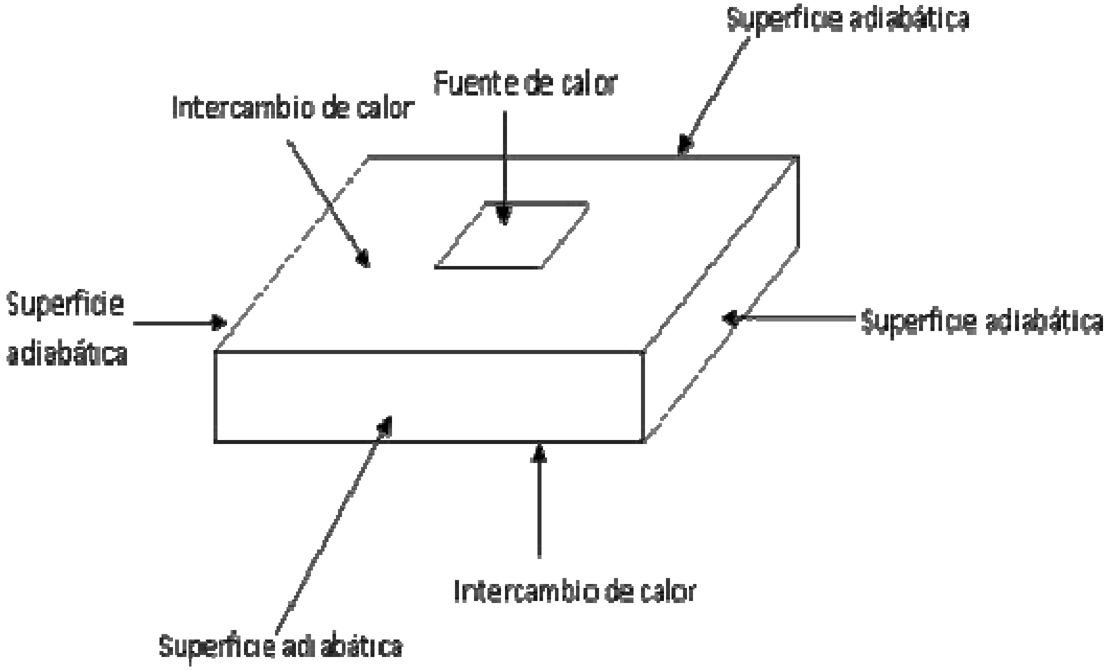
Then we obtain

$$\begin{cases} \rho c_p \dfrac{\partial y}{\partial t} = \nabla \cdot (\lambda \nabla y) + f & \text{in} \quad \Omega \times [t_0,\ t_f] \\ y(x,\ 0) = y_0 & \text{in} \quad \Omega \\ \dfrac{\partial y}{\partial \eta} = -\dfrac{u}{\lambda}(y - y_\infty) & \text{in} \quad \partial\Omega \times [t_0,\ t_f] \end{cases}$$

We are going to consider first Dirichlet and Neumann B.C.

u is the convection coefficient and the control variable to dissipate the heat.

Practical case: a circuit



<u>Dimensiones placa:</u>

- 7,5 cm x 5 cm y 1,5mm.

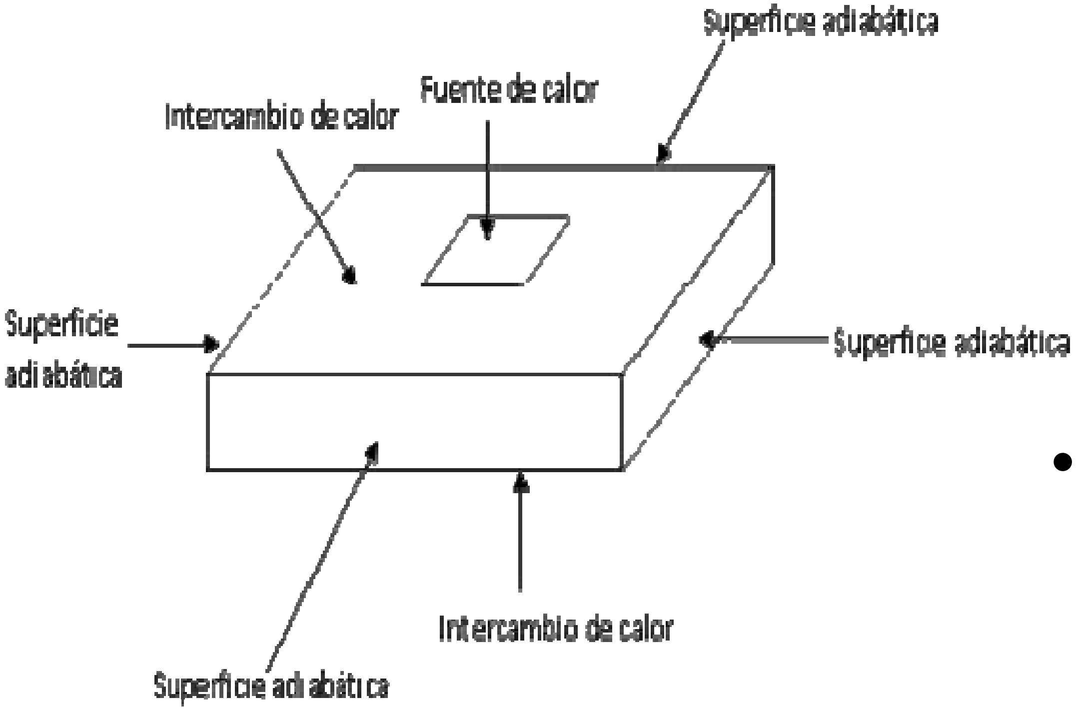
<u>Dimensiones del chip:</u>

- 2 cm x 1 cm y 1,5mm.

- Despreciamos el intercambio de calor en las superficies laterales.
- Tenemos la temperatura inicial:
- Tomamos temperatura ambiente:

$$\begin{cases} y(x,0) & = & y_\infty \\ y_\infty & = & 293\,\mathrm{K} \end{cases}$$

Model parameters



- En el cuerpo generador de calor tenemos:

$$\lambda_1 = 1,5 \frac{W}{mK}$$

$$\rho_1 c_{p1} = 1,67 \times 10^7 \frac{J}{m^3 K}$$

- En la placa tenemos:

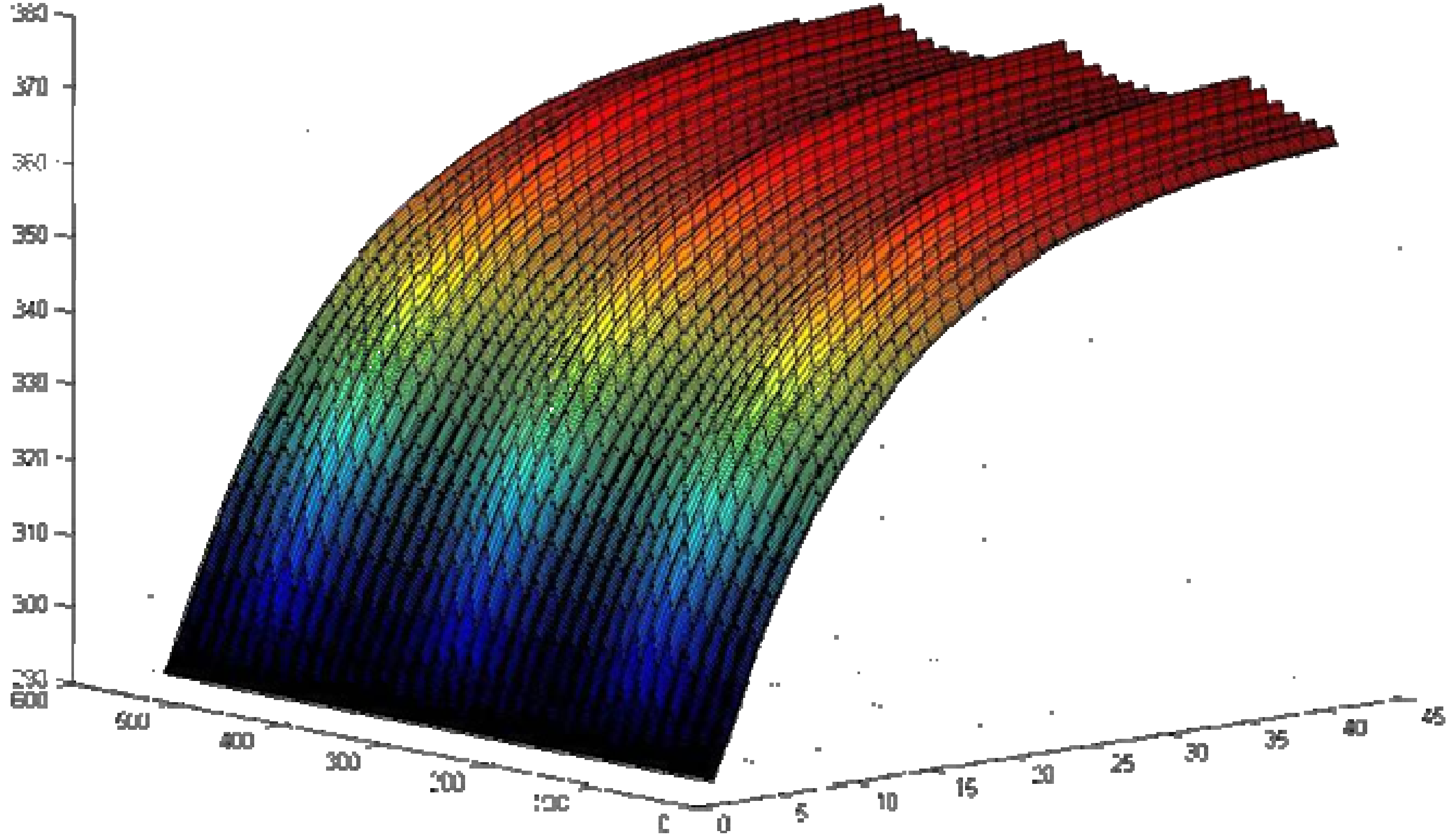
$$\lambda_2 = 240 \frac{W}{mK}.$$

$$\rho_2 c_{p2} = 240 \times 10^4 \frac{J}{m^3 K}$$

- El coeficiente de convección: $u = 17,8 \frac{W}{m^2 K}$

- Calor generado por el chip: $9,4W$

Numerical result: cont.



Computing optimality cond.

Is a derivative in the Gâteaux sense

$$\partial_{\mathbf{u}}\left(\mathbf{p}^{T}\mathbf{E}(\mathbf{u})\mathbf{y}\right)=\mathbf{p}^{T}\partial_{\mathbf{u}}\mathbf{E}(\mathbf{u})\mathbf{y}$$

i.e. if we have **u** with two entries we have

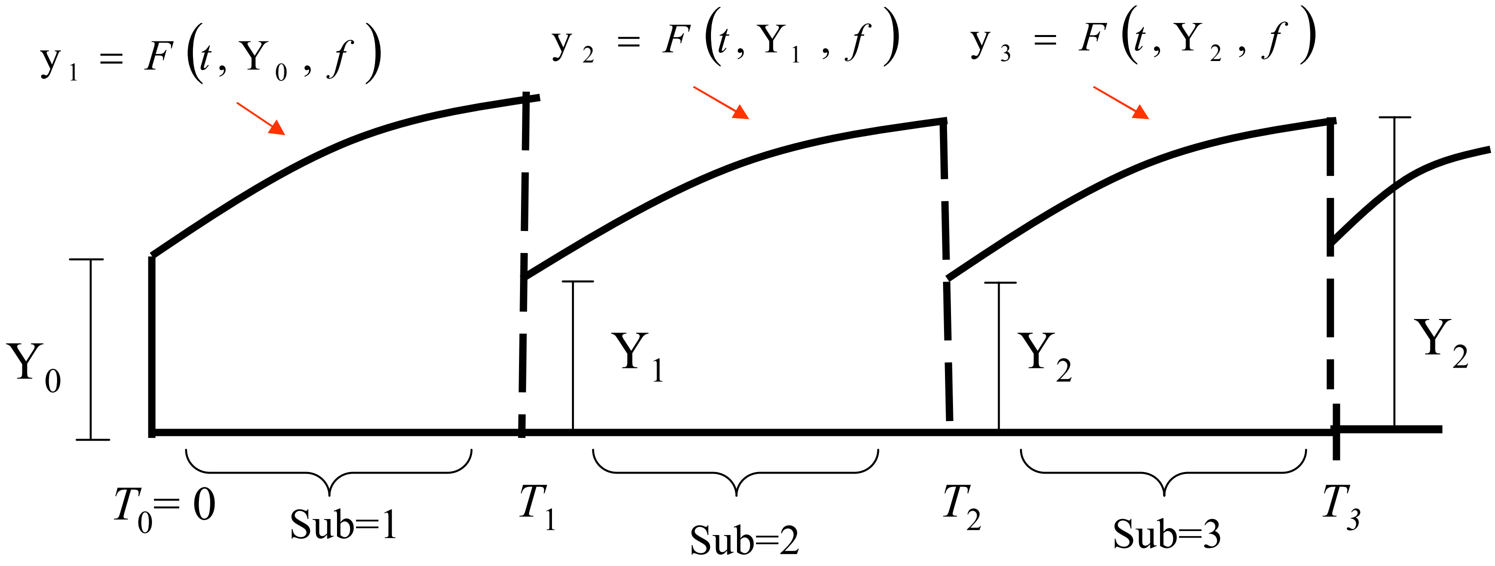
$$\partial_{\mathbf{u}}\left(\mathbf{p}^{T}\mathbf{E}(\mathbf{u})\mathbf{y}\right)=\mathbf{p}^{T}\left[\partial_{\mathbf{u}_1}\mathbf{E}(\mathbf{u})+\partial_{\mathbf{u}_2}\mathbf{E}(\mathbf{u})\right]\mathbf{y}$$

Still expensive

$$P^{-1}H = \begin{bmatrix} I & \boxed{E^{-T}KE^{-1}N} \\ G^{-1}N & -I \end{bmatrix}$$

How to parallelize E^{-1} in time:

Parareal-method



$$f = Bu \qquad \begin{cases} \dot{y} = Ay + f \\ y(T_i) = Y_i \end{cases} \quad \rightarrow \quad F(t, Y_i, f) := y(t)$$

Backward Euler

Continuity of solution

$$Y_k - FY_{k-1} = 0, \quad k = 1, \ldots, \hat{k}$$
$$Y_0 = 0$$

Parareal: Lions-Maday-Turinici

Parareal for control

Theorem: Let E_n the n^{th} application of the Parareal scheme, then

$$\gamma_{\min}\left(\mathbf{r}, E^{-T} K E^{-1}\mathbf{r}\right) \le \left(\mathbf{r}, E_n^{-T} K E_n^{-1}\mathbf{r}\right) \le \gamma_{\max}\left(\mathbf{r}, E^{-T} K E^{-1}\mathbf{r}\right)$$

where $\gamma_{\max} = 1 + O\left(2\sqrt{\frac{\rho_n t_f}{\tau}}\right)$ and $\gamma_{\min} = 1 - O\left(2\sqrt{\frac{\rho_n t_f}{\tau}}\right)$

This is a sharp bound

For n small: error on the solution.

Dynamic adapted Krylov method (Sarkis-Schaerer-Szyld: in progress) .

MINRES-iterations numbers

Tolerance: 10^{-6} $s = 0$ (s = 1) $P^{-1}H = \begin{bmatrix} I & E^{-T}KE^{-1}N \\ G^{-1}N & -I \end{bmatrix}$

Nx \ Nt	32	64	128	256	512
32	34 (36)	40 (44)	42 (46)	42 (46)	42 (46)
64	32 (36)	40 (44)	42 (46)	42 (46)	42 (46)
128	32 (36)	40 (44)	42 (46)	42 (46)	42 (46)
256	32 (36)	40 (44)	42 (46)	42 (46)	42 (46)
512	32 (36)	40 (44)	42 (46)	42 (46)	42 (46)

E^{-1} is sequential.

Parareal cycles vs exact solver

Tolerance: 10^{-6} N_x=64

Stop criteria: $\|\mathbf{r}_j\|_2 / \|\mathbf{r}_0\|_2 \leq 10^{-6}$

MINRES - number of iterations for $\Delta T/\tau = 16$

$\hat{k}$	4	8	16	32
N_t	64	128	256	512
h=1/16	57 / 40 / 40	59 / 54 / 42	63 / 54 / 42	63 / 54 / 44
h=1/32	55 / 40 / 40	59 / 54 / 42	63 / 54 / 42	63 / 54 / 44
h=1/64	55 / 40 / 40	59 / 54 / 42	63 / 54 / 42	63 / 54 / 44

$n = 2/4/exact\ solver$

$q=1 \quad r=10^{-4} \quad s=0$

Backward Euler for both fine and coarse grid.

For the test problem studied, the method is scalable.

Scalability

Tolerance: 10^{-6} N_x=64

Stop criteria: $\|\mathbf{r}_j\|_2 / \|\mathbf{r}_0\|_2 \leq 10^{-6}$

MINRES - Number of iterations

$\hat{k}$	8	16	32	64
$\Delta T / \tau$	64	32	16	8
h=1/16	66	66	64	63
h=1/32	66	66	64	62
h=1/64	65	64	63	61

$n = 2$ $\tau = 1/512$ $q = 1$ $r = 10^{-4}$ $s = 0$

Backward Euler for both fine and coarse grid.

For the test problem studied, the method is scalable.

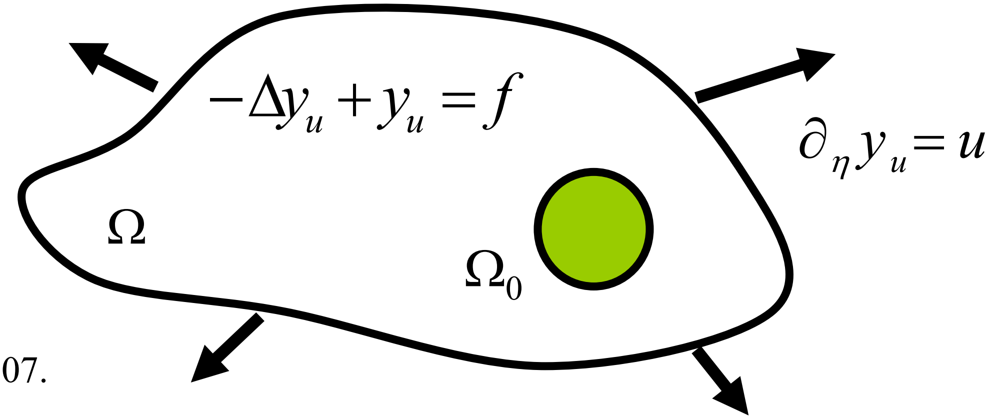
Elliptic optimal control problem

Given $y^* \in L^2(\Omega_0),\ \ \Omega_0 \subset \Omega,\ \ \alpha_1,\ \alpha_2$

$$\underset{y,u}{Min}\ \ \frac{1}{2}\left\| y - y^* \right\|^2_{L^2(\Omega_0)} + \begin{cases} \dfrac{\alpha_1}{2}\left\| u \right\|^2_{L^2(\partial\Omega)} \\ \dfrac{\alpha_2}{2}\left\| u \right\|^2_{H^{-1/2}(\partial\Omega)} \end{cases}$$

subject to $\begin{cases} -\Delta y + y = f \\ \partial_\eta y = u \end{cases}$

$\alpha_1,\ \alpha_2 \geq 0$



Mathew-Sarkis-Schaerer: Num. Lin. Alg. w Applic. 2007.

FEM Formulation

$$y, p \in V_h = V_h(\Omega) \longrightarrow P_1 \text{ conf. FEM}$$

$$u \in V_h(\partial\Omega) \qquad y = \sum_{j \in \Omega_h} \mathrm{y}_j \varphi_j \qquad u = \sum_{k \in \partial\Omega_h} \mathrm{u}_k \varphi_k$$

$$\int_\Omega \nabla\varphi_i \nabla\varphi_j + \int_\Omega \varphi_i \varphi_j \rightarrow \mathrm{A} \qquad \int_{\partial\Omega} \varphi_i \varphi_j \rightarrow \mathrm{B} = \begin{pmatrix} 0 \\ \mathrm{Q} \end{pmatrix}$$

Interior variables

Boundary variables

$$\mathrm{A\,y + B\,u = f}$$

Min Max condition

$$\underset{y,u}{\text{Min}} \quad \frac{1}{2}\left(y-y^*\right)^T M\left(y-y^*\right)+u^T G u$$

$$\text{Subject to} \; : \quad Ay+Bu=f$$

$$\text{where } \; G=\begin{cases}\alpha_1 Q \\ \alpha_2 B^T A^{-1} B\end{cases}$$

M is a mass matrix on Ω_0

$$\underset{y,u}{\text{Min}} \; \underset{p}{\text{Max}} \; \frac{1}{2}\left(y - y^*\right)^T M\left(y - y^*\right)+\frac{1}{2}u^T G u+p^T\left(Ay+Bu-f\right)$$

KKT system

$$\begin{pmatrix} M & & A \\ & G & B \\ A & B & \end{pmatrix} \begin{pmatrix} y \\ u \\ p \end{pmatrix} = \begin{pmatrix} f_1 \\ f_2 \\ f_3 \end{pmatrix}$$

1. Ker M might be large
2. $\mathrm{Ker}\begin{pmatrix} M & \\ & G \end{pmatrix} \cap \mathrm{Ker}\begin{pmatrix} A & B \end{pmatrix} = \varnothing$ and $A^{-1},\ G^{-1}$ exist

Approaches

- Reduction to u: PCG (double iterations).

$$\left(G + B^{T} A^{-T} M A^{-1} B\right) u = g$$

- Biros & Ghattas (PGMRES)

$$\begin{pmatrix} M & & A^{T} \\ & G & B^{T} \\ A & B & \end{pmatrix} = \begin{pmatrix} MA^{-1} & & I \\ & I & B^{T}A^{-1} \\ I & & \end{pmatrix} \begin{pmatrix} A & B & \\ & H & \\ & -MA^{-1}B & A^{T} \end{pmatrix}$$

- Heinkenschloss & Nguyen (PGMRES)

Neumann-Neumann (Mandel)

$$\begin{pmatrix} M & A^{T} \\ A & \frac{-1}{\alpha_1}\begin{pmatrix} 0 & 0 \\ 0 & Q \end{pmatrix} \end{pmatrix} \begin{pmatrix} y \\ p \end{pmatrix}$$

Two-level OSM (Cai & Widlund)

$$\begin{pmatrix} A^{T} & M \\ \frac{-1}{\alpha_1}\begin{pmatrix} 0 & 0 \\ 0 & \tilde{Q} \end{pmatrix} & A \end{pmatrix}$$

Approach adopted (PCG, PMINRES)

- Reduction to u

$$G + B^{T} A^{-T} M A^{-1} B$$

- Block diagonal preconditioner for

$$\begin{pmatrix} M & & A^{T} \\ & G & B^{T} \\ A & B & \end{pmatrix}$$

Block diagonal precon. MINRES

Block triangular precon. (CG)

Mathew, Sarkis, Schaerer 2006

Similarities

1. Dim M small (few selected nodes)

Use Sherman-Morrison-Woodbury formula

$$G + \boxed{B^T A^{-T} M A^{-1} B} \quad \text{Low rank}$$

2. If M is invertible. Define $\mu = -A^{-T} M A^{-1} B u$

$$\begin{pmatrix} AMA & B \\ B^T & -G \end{pmatrix} \begin{pmatrix} \mu \\ u \end{pmatrix} \quad \text{same as before}$$

The Schur complement

Employ the partition $y = \left(y_I^T \quad y_B^T \right)^T$ to obtain

$$B^T A^{-1} B = \begin{bmatrix} 0 \\ Q \end{bmatrix}^T \begin{bmatrix} A_{II} & A_{IB} \\ A_{IB}^T & A_{BB} \end{bmatrix} \begin{bmatrix} 0 \\ Q \end{bmatrix} = Q^T \left(A_{BB} - A_{IB}^T A_{II}^{-1} A_{IB} \right)^{-1} Q$$

where $S = \left(A_{BB} - A_{IB}^T A_{II}^{-1} A_{IB} \right)$ is the Schur complement for the boundary variables.

Properties for G

$G = \alpha_1 Q$ or $\alpha_2 B^T A^{-1} B$

$$u^T B^T A^{-1} B u = u^T Q^T S^{-1} Q u = \left\| S^{-1/2} Q u \right\|^2 =$$

$$= \sup_{v \in \Re^m} \frac{\left(S^{-1/2} Qu, v \right)^2}{\left\| v \right\|^2} = \sup_{v \in \Re^m} \frac{\left(Qu, S^{-1/2} v \right)^2}{\left\| v \right\|^2} = \sup_{w \in \Re^m} \frac{\left(Qu, w \right)^2}{\left\| S^{1/2} w \right\|^2}$$

$$\approx \sup_{w \in V_h(\partial\Omega)} \frac{\left\langle u_h, w_h \right\rangle^2_{L^2(\partial\Omega)}}{\left\| w \right\|^2_{H^{1/2}}} \approx \sup_{w \in H^{1/2}} \frac{\left\langle u_h, w \right\rangle^2_{L^2(\partial\Omega)}}{\left\| w \right\|^2_{H^{1/2}}}$$

$$= \left\| u_h \right\|^2_{H^{1/2}(\partial\Omega)} \le \left\| u_h \right\|^2_{L^2(\partial\Omega)} = u^T Q u$$

$$\tilde{c} h \, u^T Q u \le u^T B^T A^{-1} B u \le \hat{c} \, u^T Q u$$

where $\hat{c}$ and $\tilde{c}$ are independent of the mesh size.

Two possibilities

a) If $\alpha_i = O(1)$

$$u^T\ B^T A^{-T} M A^{-1} B\,u \quad \leq \quad \gamma\, u^T\ B^T A^{-T} A A^{-1} B\,u \ =$$

$$\gamma\, u^T\ B^T A^{-1} B\,u \quad \leq \quad \tilde{\gamma}\, u^T\ G\,u$$

$$G \ \leq \ G \ + \ B^T A^{-T} M A^{-1} B \ \leq \ \left(1+\tilde{\gamma}\right) G$$

G optimal preconditioner.

b) If α_i is small and $\Omega_{\mathrm{o}} \equiv \Omega$

$$\mathrm{v} = \mathrm{A}^{-1}\mathrm{Bu} \quad \longrightarrow \quad \begin{cases} -\Delta \mathrm{v} + \mathrm{v} = 0 \\ \qquad \partial_\eta \mathrm{v} = \mathrm{u} \quad \text{on } \partial\Omega \end{cases}$$

$$\mathrm{w} = \mathrm{v}\big|_{\partial\Omega} \qquad \mathrm{w} = \mathrm{S}^{-1}\mathrm{Qu} \qquad \approx \begin{cases} -\Delta \mathrm{v} + \mathrm{v} = 0 \\ \qquad \mathrm{v} = \mathrm{w} \quad \text{on } \partial\Omega \end{cases}$$

$$\mathrm{u}^{\mathrm{T}}\ \mathrm{B}^{\mathrm{T}}\mathrm{A}^{-\mathrm{T}}\mathrm{M}\mathrm{A}^{-1}\mathrm{B}\ \mathrm{u} \ = \ \mathrm{v}^{\mathrm{T}}\ \mathrm{M}\ \mathrm{v} \ = \ \|\mathrm{v}\|^2_{L^2(\Omega)} \approx \|\mathrm{w}\|^2_{H^{-1/2}(\partial\Omega)}$$

$$\approx \ \mathrm{w}^{\mathrm{T}}\mathrm{Q}^{\mathrm{T}}\mathrm{S}^{-1}\mathrm{Q}\mathrm{w} \ = \ \mathrm{v}^{\mathrm{T}}\mathrm{Q}^{\mathrm{T}}\mathrm{S}^{-1}\mathrm{Q}\mathrm{S}^{-1}\mathrm{Q}^{\mathrm{T}}\mathrm{S}^{-1}\mathrm{Q}\ \mathrm{v} \approx \ h^4\mathrm{S}^{-3}$$

Peisker 88’: Ω convex $\quad \|\mathrm{v}\|_{L^2(\Omega)} \approx \|\mathrm{w}\|_{H^{-1/2}(\partial\Omega)}$

Eigenvalues distributions

$$Q \approx hI \approx (h,h)$$

$$S^{-1} = S^{-1} \approx (1,1/h)$$

$$B^T A^{-1} B \approx h^2 S^{-1} \approx (h^2, h)$$

$$B^T A^{-T} M A^{-1} B \approx h^4 S^{-3} \approx (h^4, h) \qquad H_0 = B^T A^{-T} M A^{-1} B$$

Conclusion

$$G = \alpha_1 Q$$

$$G + H_0 \approx h\left(\alpha_1 I + h^3 S^{-3}\right)$$

$$G = \alpha_2 B^T A^{-1} B$$

$$G + H_0 \approx h\left(\alpha_2 h S^{-1} + h^3 S^{-3}\right)$$

$\alpha_1 \succ 1 \quad H_0 \prec G$ $\longleftrightarrow$ G optimal prec. $\longleftrightarrow$ $\alpha_2 \succ 1 \quad H_0 \prec G$

$\alpha_1 \prec h^3 \quad G \prec H_0$ $\longleftrightarrow$ H_0 optimal prec. $\longleftrightarrow$ $\alpha_2 \prec h^2 \quad G \prec H_0$

Intermediate α_i case

Simultaneous spectral approximation for I, S, S^{-1}, S^{-2}, S^{-3}, etc...

$$\begin{array}{lllll} V_0(\partial\Omega) \subset & V_1(\partial\Omega) \subset & V_2(\partial\Omega) \subset & \ldots \subset & V_q(\partial\Omega) \\ \updownarrow & \updownarrow & \updownarrow & & \updownarrow \\ h_0 \approx 1 & h_1 & h_2 & & h_\mathrm{q} = h \end{array}$$

Multilevel refinements

$\mathrm{P}_i :\ L_2(\partial\Omega) -$ orthogonal projection of $V_h(\partial\Omega)$

onto $V_i(\partial\Omega)$

$$(\mathrm{P}_i\mathrm{u},\mathrm{Qv}_i) = (\mathrm{u},\mathrm{Qv}_i) \qquad \mathrm{v}_i \in V_i(\partial\Omega)$$

Oswald 94’, Bramble , Pasciak, Vassilevsky 00’
Nepomnyaschikh 95’.

L_2 projection

$$\mathrm{I} = \mathrm{P}_0 + \left(\mathrm{P}_1 - \mathrm{P}_0\right) + \cdots + \left(\mathrm{P}_q - \mathrm{P}_{q-1}\right)$$

$$\mathrm{Q} = \mathrm{Q}\,\mathrm{P}_0 + \mathrm{Q}\left(\mathrm{P}_1 - \mathrm{P}_0\right) + \cdots + \mathrm{Q}\left(\mathrm{P}_q - \mathrm{P}_{q-1}\right)$$

$$\mathrm{Q} \approx h\,\mathrm{P}_0 + h\left(\mathrm{P}_1 - \mathrm{P}_0\right) + \cdots + h\left(\mathrm{P}_q - \mathrm{P}_{q-1}\right)$$

$$\mathrm{S} \approx \frac{h}{h_0}\mathrm{P}_0 + \frac{h}{h_1}\left(\mathrm{P}_1 - \mathrm{P}_0\right) + \cdots + \frac{h}{h_q}\left(\mathrm{P}_q - \mathrm{P}_{q-1}\right)$$

$$\mathrm{S}^{-1} \approx \frac{h_0}{h}\mathrm{P}_0 + \frac{h_1}{h}\left(\mathrm{P}_1 - \mathrm{P}_0\right) + \cdots + \frac{h_q}{h}\left(\mathrm{P}_q - \mathrm{P}_{q-1}\right)$$

$$\mathrm{S}^{-3} \approx \frac{h_0^3}{h^3}\mathrm{P}_0 + \frac{h_1^3}{h^3}\left(\mathrm{P}_1 - \mathrm{P}_0\right) + \cdots + \frac{h_q^3}{h^3}\left(\mathrm{P}_q - \mathrm{P}_{q-1}\right)$$

For quasi L_2 projections BPV 00’

Multilevel preconditioning for H

$$\mathrm{H} = \alpha_1 \mathrm{Q} + \mathrm{B}^{\mathrm{T}} \mathrm{A}^{-\mathrm{T}} \mathrm{M} \mathrm{A}^{-1} \mathrm{B} \approx h\left(\alpha_1 \mathrm{I} + h^3 \mathrm{S}^{-3}\right)$$

$$\approx h\left[\left(\alpha_1 + h_0^3\right)\mathrm{P}_0 + \left(\alpha_1 + h_1^3\right)\left(\mathrm{P}_1 - \mathrm{P}_0\right) + \cdots + \left(\alpha_1 + h_q^3\right)\left(\mathrm{P}_q - \mathrm{P}_{q-1}\right)\right]$$

$$\mathrm{H}^{-1} \approx \frac{1}{h}\left[\frac{1}{\left(\alpha_1 + h_0^3\right)}\mathrm{P}_0 + \frac{1}{\left(\alpha_1 + h_1^3\right)}\left(\mathrm{P}_1 - \mathrm{P}_0\right) + \cdots + \frac{1}{\left(\alpha_1 + h_q^3\right)}\left(\mathrm{P}_q - \mathrm{P}_{q-1}\right)\right]$$

If $\alpha_1 \succ 1 \approx h_0$, $\quad \mathrm{H}_0 \prec \mathrm{G}$ G optimal prec.

If $\alpha_1 \prec h^3 \approx h_q^3$, $\quad \mathrm{H}_0 \succ \mathrm{G}$ H_0 optimal prec.

Multilevel preconditioning for H

$$\mathrm{H} = \alpha_2 \mathrm{B}^{\mathrm{T}}\mathrm{A}^{-1}\mathrm{B} + \mathrm{B}^{\mathrm{T}}\mathrm{A}^{-\mathrm{T}}\mathrm{M}\mathrm{A}^{-1}\mathrm{B} \approx h\left(\alpha_2 h \mathrm{S}^{-1} + h^3 \mathrm{S}^{-3}\right)$$

$$\approx h\left[\left(\alpha_2 h_0 + h_0^3\right)\mathrm{P}_0 + \left(\alpha_2 h_1 + h_1^3\right)\left(\mathrm{P}_1 - \mathrm{P}_0\right) + \cdots + \left(\alpha_1 h_q + h_q^3\right)\left(\mathrm{P}_q - \mathrm{P}_{q\text{-}1}\right)\right]$$

$$\mathrm{H}^{-1} \approx \frac{1}{h}\left[\frac{1}{\left(\alpha_2 h_0 + h_0^3\right)}\mathrm{P}_0 + \frac{1}{\left(\alpha_2 h_1 + h_1^3\right)}\left(\mathrm{P}_1 - \mathrm{P}_0\right) + \cdots + \frac{1}{\left(\alpha_2 h_q + h_q^3\right)}\left(\mathrm{P}_q - \mathrm{P}_{q\text{-}1}\right)\right]$$

If $\alpha_2 \succ 1 \approx h_0, \quad \mathrm{H}_0 \prec \mathrm{G}$ G optimal prec.

If $\alpha_2 \prec h^2 \approx h_q^2, \quad \mathrm{H}_0 \succ \mathrm{G}$ H_0 optimal prec.

Conclusions

- If $\Omega_0 = \Omega$, optimal preconditioners independent of h and α_i.
- If $\Omega_0 \subset\subset \Omega$, optimal preconditioner independent of h. They do not require M to be invertible.
- Open problem: $\Omega_0 \subset\subset \Omega$ and α_i independent preconditioners.

Remarks

1. Dim M small (few selected nodes)

Use Sherman-Morrison-Woodbury formula

$$G \; + \; B^T A^{-T} M A^{-1} B \qquad \text{Low rank}$$

2. If M is invertible. Define $\mu = -A^{-T} M A^{-1} B u$

$$\begin{pmatrix} AMA & B \\ B^T & -G \end{pmatrix} \begin{pmatrix} \mu \\ u \end{pmatrix} \qquad \text{same as before}$$

3. $\int_{\partial\Omega} \left(y-y^*\right)^T G \left(y-y^*\right) \rightarrow B^T A^{-T} \begin{pmatrix} 0 & \\ & Q \end{pmatrix} A^{-1} B \approx h^3 S^{-2}$

4. Ker M small $\rightarrow$ FETI approach

Outline

1. Optimal control problem for PDE of parabolic type.
2. Discretization all at once - KKT system.
3. Algorithm 1: Elimination of state and adjoint variables.
4. Saddle point formulation (2 x 2 block with control and auxiliary variables).
5. Algorithm 2: Block diagonal preconditioning.
6. Parareal for PDE of parabolic type.
7. Algorithm 3: Using Parareal for the control problems.
8. Conclusions and future work.

MODELADO Y DISCRETIZACIÓN

Formulación débil

Utilizando la primera identidad de Green, dada por:

$$\int_\Omega \phi \nabla^2 \varphi dV = -\int_\Omega (\nabla \varphi \cdot \nabla \phi) \, dV + \oint_{\partial\Omega} \phi \, (\nabla \varphi \cdot \mathbf{n}) \, dS$$

Y la condición de contacto perfecto, se tiene la siguiente formulación débil

$$\left\{ \begin{array}{rcll} \int_\Omega \rho c_p \eta \frac{\partial T}{\partial t} & = & -\int_\Omega \lambda \nabla \eta \cdot \nabla T + \oint_{\partial\Omega} \lambda \eta \partial_n T + \int_\Omega f \eta & \text{en} \quad \Omega \times [t_0, t_f] \\ T(x, 0) & = & T_0 & \text{en} \quad \Omega \\ \frac{\partial T}{\partial \eta} & = & -\frac{h}{\lambda} (T - T_\infty) & \text{en} \quad \partial\Omega \times [t_0, t_f] \end{array} \right.$$

MODELADO Y DISCRETIZACIÓN

Discretización temporal

$$E\left(\hat{\mathbf{u}}\right)\hat{\mathbf{z}} + N\hat{\mathbf{u}} = \mathbf{f}$$

Donde:

$$\hat{A} = \begin{pmatrix} \tau_1 A_1 & 0 & \cdots & \cdots & 0 \\ 0 & \ddots & & & \vdots \\ \vdots & & \tau_n A_n & & \vdots \\ \vdots & & & \ddots & \vdots \\ 0 & \cdots & \cdots & 0 & \tau_{\hat{n}} A_{\hat{n}} \end{pmatrix} \in \mathbb{R}^{\hat{m}\cdot\hat{n}\times\hat{m}\cdot\hat{n}}$$

MODELADO Y DISCRETIZACIÓN

Discretización temporal

$$E\left(\hat{\mathbf{u}}\right)\hat{\mathbf{z}} + N\hat{\mathbf{u}} = \mathbf{f}$$

Donde:

$$\hat{B} = \begin{pmatrix} -B_1 & 0 & \cdots & \cdots & \cdots & 0 \\ -B_2 & B_2 & & & & \vdots \\ 0 & \ddots & \ddots & & & \vdots \\ \vdots & & -B_n & B_n & & \vdots \\ \vdots & & & \ddots & \ddots & 0 \\ 0 & \cdots & \cdots & 0 & -B_{\hat{n}} & B_{\hat{n}} \end{pmatrix} \in \mathbb{R}^{\hat{m}\cdot\hat{n}\times\hat{m}\cdot\hat{n}}$$

MODELADO Y DISCRETIZACIÓN

Discretización temporal

$$E\left(\hat{\mathbf{u}}\right)\hat{\mathbf{z}} + N\hat{\mathbf{u}} = \mathbf{f}$$

Donde:

$$\hat{C} = \begin{pmatrix} \tau_1 C_1 & 0 & \cdots & \cdots & 0 \\ 0 & \ddots & & & \vdots \\ \vdots & & \tau_n C_n & & \vdots \\ \vdots & & & \ddots & \vdots \\ 0 & \cdots & \cdots & 0 & \tau_{\hat{n}} C_{\hat{n}} \end{pmatrix} \in \mathbb{R}^{\hat{m}\cdot\hat{n}\times\hat{m}\cdot\hat{n}}$$

MODELADO Y DISCRETIZACIÓN

Discretización temporal

$$E\left(\hat{\mathbf{u}}\right)\hat{\mathbf{z}} + N\hat{\mathbf{u}} = \mathbf{f}$$

Donde:

$$\hat{N} = \begin{pmatrix} \tau_1 y_\infty D_1 & 0 & \cdots & \cdots & 0 \\ 0 & \ddots & & & \vdots \\ \vdots & & \tau_n y_\infty D_n & & \vdots \\ \vdots & & & \ddots & \vdots \\ 0 & \cdots & \cdots & 0 & \tau_{\hat{n}} y_\infty D_{\hat{n}} \end{pmatrix} \in \mathbb{R}^{\hat{m}\cdot\hat{n}\times\hat{l}\cdot\hat{n}}$$

MODELADO Y DISCRETIZACIÓN

Discretización temporal

$$E\left(\hat{\mathbf{u}}\right)\hat{\mathbf{z}} + N\hat{\mathbf{u}} = \mathbf{f}$$

Donde:

$$\hat{\mathbf{z}} = \left[\mathbf{z}_1^T \ \ldots \ \mathbf{z}_n^T \ \ldots \ \mathbf{z}_{\hat{n}}^T\right]^T \in \mathbb{R}^{\hat{m}\times\hat{n}}$$

$$\hat{\mathbf{u}} = \left[\mathbf{u}_1^T \ \ldots \ \mathbf{u}_n^T \ \ldots \ \mathbf{u}_{\hat{n}}^T\right]^T \in \mathbb{R}^{\hat{l}\times\hat{m}}$$

$$\hat{\mathbf{f}} = \left[\left(b_1 + B_1\mathbf{z}_0\right)^T \ \ldots \ b_2^T \ \ldots \ b_n^T \ \ldots \ b_{\hat{n}}^T\right]^T \in \mathbb{R}^{\hat{m}\times\hat{n}}$$

CONTROL ÓPTIMO

El problema discreto

Análogamente a $$T(x,t) = \sum_{m=1}^{\hat{m}} z_m(t)\,\eta_m(x)$$

Obtenemos $$T^*(x,t) = \sum_{m}^{\hat{m}} z_m^*(t)\,\eta_m(x)$$

Entonces

$$\| T - T^* \|_{L^2(t_o,t_f,\Omega)}^2 = \int_{t_0}^{t_f} \int_{\Omega} \Big(\sum_j z_j(t)\,\eta_j(x) - \sum_j z_j^*(t)\,\eta_j(x)\Big)^2 dx\,dt$$

CONTROL ÓPTIMO

El problema discreto:

$$\| T - T^* \|^2_{L^2(t_o,t_f,\Omega)} = \int_{t_0}^{t_f} \sum_i \sum_j (z_i - z_i^*)(z_j - z_j^*)\left(\int_\Omega \eta_j \eta_i \, dx\right) dt$$

O equivalentemente

$$\| T - T^* \|^2_{L^2(t_o,t_f,\Omega)} = \int_{t_0}^{t_f} (\mathbf{z} - \mathbf{z}^*)^T B (\mathbf{z} - \mathbf{z}^*) \, dt$$

Donde

$$\mathbf{z} = \begin{bmatrix} z_1 & \dots & z_j & \dots & z_{\hat{m}} \end{bmatrix}^T \quad , \mathbf{z}^* = \begin{bmatrix} z_1^* & \dots & z_m^* & \dots & z_{\hat{m}}^* \end{bmatrix}^T$$

y

$$B = \left[\int_\Omega \rho c_p \eta_i \eta_j\right]_{ij} \in \mathbb{R}^{\hat{m} \times \hat{m}}$$

CONTROL ÓPTIMO

El problema discreto

Utilizando $h(x,t) = \sum_{j=1}^{l} h_j(t)\,\sigma_j(x)$

donde $\sigma_l(x) = \begin{cases} 1 & \text{si } x \in \partial_l\Omega \\ 0 & \text{si } x \notin \partial_l\Omega \end{cases}$

Se tiene $\| h(x,t) \|^2_{L^2(t_0,t_f,\partial\Omega)} = \int_{t_0}^{t_f} \int_{\partial\Omega} \sum_i h_i\sigma_i \sum_j h_j\sigma_j \, dx \, dt$

CONTROL ÓPTIMO

El problema discreto

$$\| h(x,t) \|^2_{L^2(t_o,t_f,\partial\Omega)} = \int_{t_0}^{t_f} \sum_i \sum_j h_i h_j \left(\int_{\partial\Omega} \sigma_i \sigma_j \, dx \right) dt$$

Equivalentemente

$$\| h(x,t) \|^2_{L^2(t_o,t_f,\partial\Omega)} = \int_{t_0}^{t_f} \mathbf{h}^{\mathrm{T}} \, Q \, \mathbf{h} \, dt.$$

Donde

$$\mathbf{h} = \begin{bmatrix} h_1 & \dots & h_l & \dots & h_{\hat{i}} \end{bmatrix}^T \in \mathbb{R}^{\hat{i}} \qquad , Q = \left[\int_{\partial\Omega} \sigma_i \sigma_j \right]_{ij} \in \mathbb{R}^{\hat{i}\times\hat{i}}$$

CONTROL ÓPTIMO

El problema discreto

$$J = \frac{q}{2}\int_{t_0}^{t_f} (\mathbf{z}-\mathbf{z}^*)^T \, B \, (\mathbf{z}-\mathbf{z}^*)\,dt + \frac{r}{2}\int_{t_0}^{t_f} \mathbf{h}^{\mathrm{T}} Q \,\mathbf{h}\,dt$$

Discretizando en el tiempo

$$\int_{t_0}^{t_f} (\mathbf{z}-\mathbf{z}^*)^T \, B \, (\mathbf{z}-\mathbf{z}^*)\,dt = \tau \sum_{n=1}^{\hat{n}} (\mathbf{z}_\mathbf{n}-\mathbf{z}_\mathbf{n}^*)^T \, B \, (\mathbf{z}_\mathbf{n}-\mathbf{z}_\mathbf{n}^*)$$

$$\int_{t_0}^{t_f} \mathbf{h}^{\mathrm{T}} Q \,\mathbf{h}\,dt = \tau \sum_{n=1}^{\hat{n}} \mathbf{h}_\mathbf{n}{}^T \, Q \, \mathbf{h}_\mathbf{n}$$

CONTROL ÓPTIMO

El problema discreto

$$J = \frac{q}{2}\left(\hat{\mathbf{z}} - \hat{\mathbf{z}}^{*}\right)^{T} M \left(\hat{\mathbf{z}} - \hat{\mathbf{z}}^{*}\right) + \frac{r}{2}\hat{\mathbf{h}}^{T} G\, \hat{\mathbf{h}}$$

Donde

$$M = \begin{bmatrix} \tau B & 0 & \cdots & 0 \\ 0 & \tau B & & \vdots \\ \vdots & & \ddots & 0 \\ 0 & \cdots & 0 & \tau B \end{bmatrix} \in \mathbb{R}^{\hat{m}\cdot\hat{n}\times\hat{m}\cdot\hat{n}} \quad G = \begin{bmatrix} \tau Q & 0 & \cdots & 0 \\ 0 & \tau Q & & \vdots \\ \vdots & & \ddots & 0 \\ 0 & \cdots & 0 & \tau Q \end{bmatrix} \in \mathbb{R}^{\ddot{l}\cdot\hat{n}\times\ddot{l}\cdot\hat{n}}$$

$$\hat{\mathbf{z}}^{*} = \begin{bmatrix} \mathbf{z}_{1}^{*\mathbf{T}} & \ldots & \mathbf{z}_{\mathbf{n}}^{*\mathbf{T}} & \ldots & \mathbf{z}_{\hat{\mathbf{n}}}^{*\mathbf{T}} \end{bmatrix}^{T} \in \mathbb{R}^{\hat{m}\cdot\hat{n}}$$

IMPLEMENTACIÓN NUMÉRICA

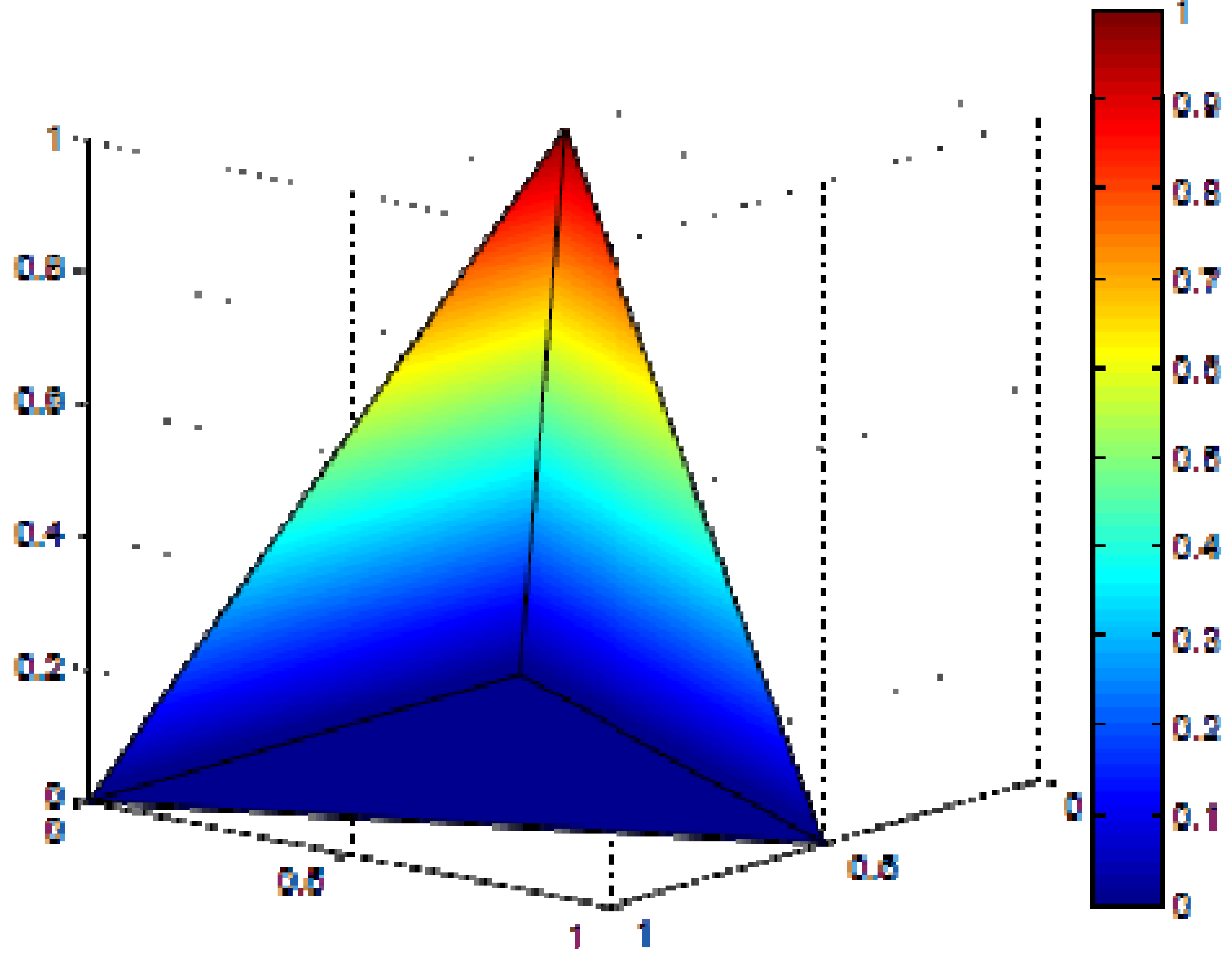
Método de los elementos finitos

- Elementos conformes
- Funciones sombrero lineales
- Matrices locales y globales

IMPLEMENTACIÓN NUMÉRICA

Método de los elementos finitos

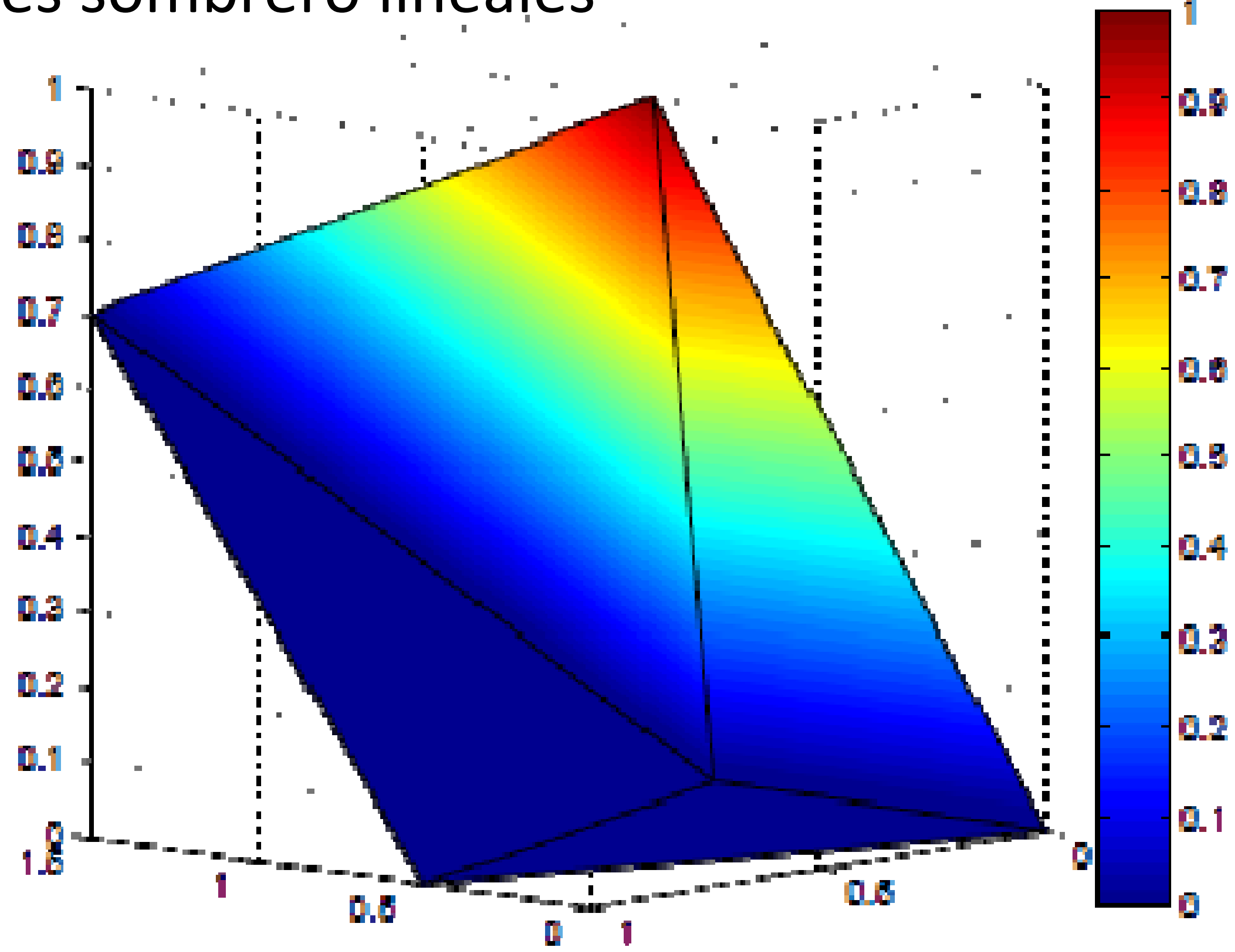
Funciones sombrero lineales



IMPLEMENTACIÓN NUMÉRICA

Método de los elementos finitos

Funciones sombrero lineales



To guarantee stability: $|b_m| \le |a_m|$ using Gershgoring's radius theorem

An lower bound

$$\mu(\Theta_m) \ge \min \left(|a_m|^2 \left(1 - \frac{|b_m|}{|a_m|} \right)^2 \right) = \min \left(\tau \, |\lambda_m|\right)^2 \qquad \mu(\Theta_m) \ge (\tau \; \rho_{\min})^2$$

An upper bound $\mu(\Theta_m) \le \max \; 4|a_m|^2 \rightarrow \quad \mu(\Theta_i) \le 4(1 - \tau\theta\rho_{\max})^2$

$$\text{Cond}(EE^T) \approx \frac{4(1+\tau\theta\rho_{\max})^2}{(\tau\rho_{\min})^2}$$

Remark: for finite element discretization

$$-O\left(\frac{1}{h^2}\right) < \lambda_m < -O(1)$$

$$\text{Cond}(EE^T) \approx \frac{(1+\tau\theta h^{-2})^2}{(\tau)^2}$$

Robin boundary condition

$$\begin{cases} \int_\Omega \rho c_p \phi \dfrac{\partial y}{\partial t} & = & -\int_\Omega \lambda \nabla \phi \cdot \nabla y + \oint_{\partial\Omega} \lambda \phi \, \partial_\eta y + \int_\Omega f\phi & \text{in} \quad \Omega \times \left[t_0,\, t_f\right] \\ y(x,\, 0) & = & y_0 & \text{in} \quad \Omega \\ \quad \dfrac{\partial y}{\partial \eta} & = & -\dfrac{u}{\lambda}\left(y - y_\infty\right) & \text{in} \quad \partial\Omega \times \left[t_0,\, t_f\right] \end{cases}$$

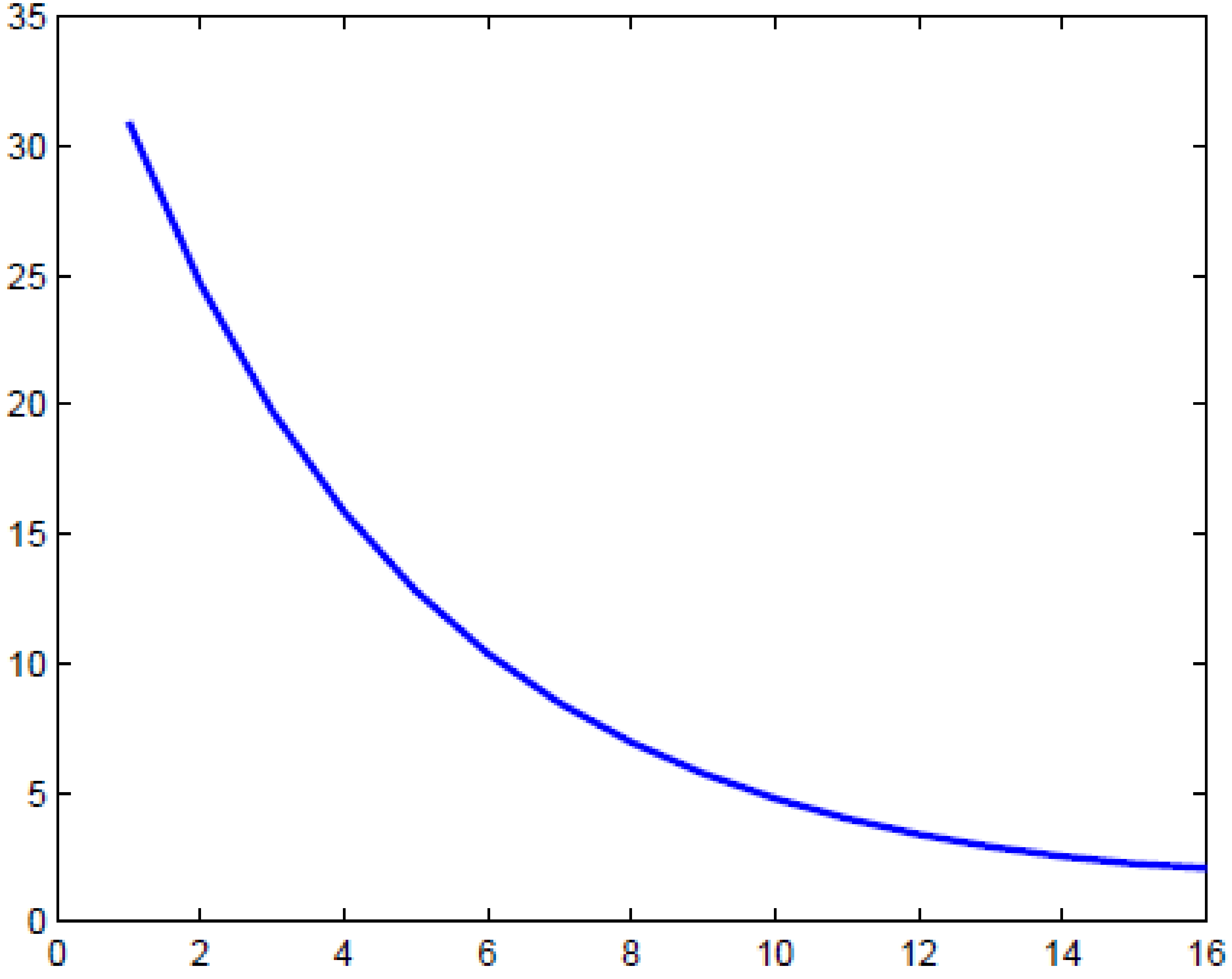
- Separación de variables

$$y(x, t) = \sum_{m=1}^{\hat{m}} z_m(t)\, \phi_m(x)$$

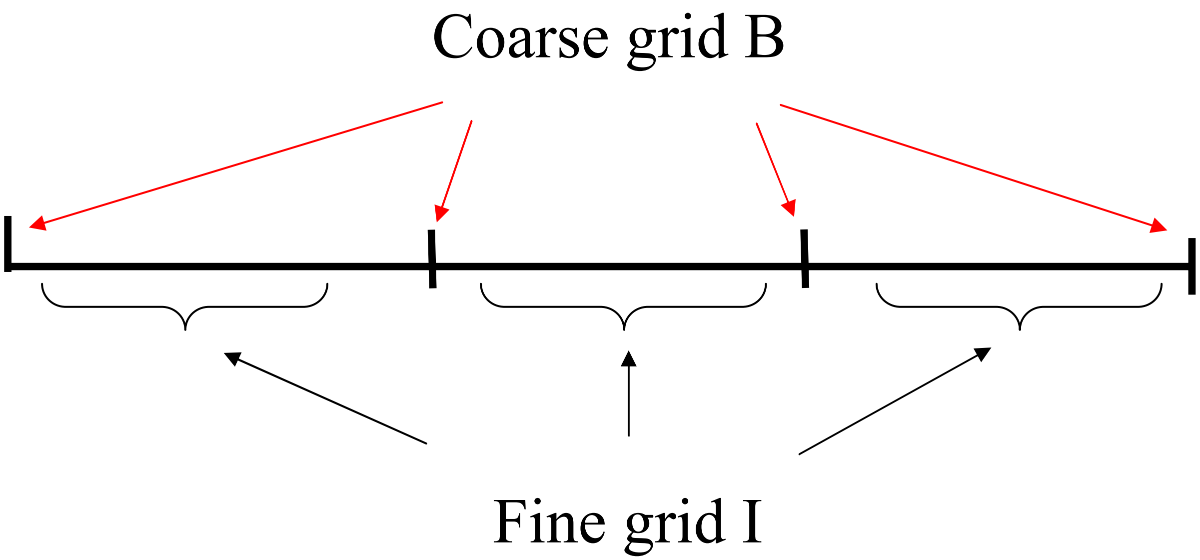
- Espacio de dimensión finita

$$\int_\Omega \rho c_p \phi_i \left(\sum_j \dot{z}_j \phi_j \right) = -\int_\Omega \lambda \nabla \phi_i \cdot \nabla \left(\sum_j z_j \phi_j \right) - \int_{\partial\Omega} u\phi_i \left(\sum_j z_j \phi_j \right) + y_\infty \int_{\partial\Omega} u\phi_i + \int_\Omega f\phi_i$$

RESULTADOS DEL CONTROL



Domain decomposition

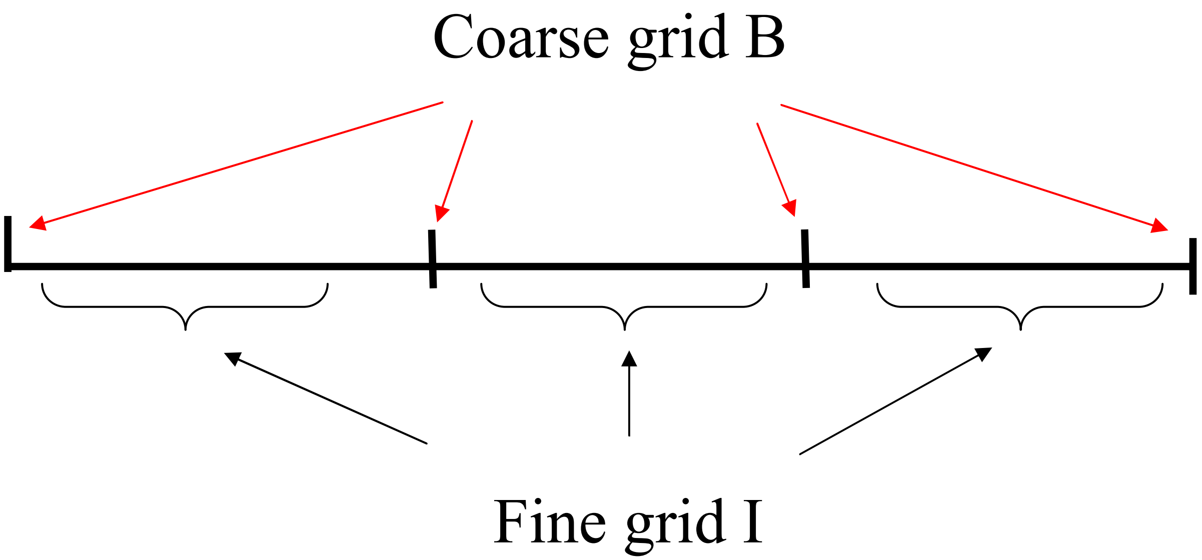


Coarse grid B

Fine grid I

Permute to organize the unknown $\begin{bmatrix} \mathbf{y}_{\mathrm{I}} \\ \mathbf{y}_{\mathrm{B}} \end{bmatrix}$

How to parallelize E^{-1} in time: Parareal-method



Coarse grid B

Fine grid I

$$\begin{bmatrix} \mathbf{E}_{\mathrm{II}} & \mathbf{E}_{\mathrm{IB}} \\ \mathbf{E}_{\mathrm{BI}} & \mathbf{E}_{\mathrm{BB}} \end{bmatrix} \begin{bmatrix} \mathbf{y}_{\mathrm{I}} \\ \mathbf{y}_{\mathrm{B}} \end{bmatrix} = \begin{bmatrix} \mathbf{s}_{\mathrm{I}} \\ \mathbf{s}_{\mathrm{B}} \end{bmatrix}$$

Schur complement for $\mathbf{y}_{\mathrm{B}}$

$$\begin{bmatrix} \mathbf{E}_{\mathrm{II}} & \mathbf{E}_{\mathrm{IB}} \\ \mathbf{E}_{\mathrm{BI}} & \mathbf{E}_{\mathrm{BB}} \end{bmatrix} \begin{bmatrix} \mathbf{y}_{\mathrm{I}} \\ \mathbf{y}_{\mathrm{B}} \end{bmatrix} = \begin{bmatrix} \mathbf{s}_{\mathrm{I}} \\ \mathbf{s}_{\mathrm{B}} \end{bmatrix}$$

$$\mathbf{E}_{\mathrm{II}} = \begin{bmatrix} \mathbf{E}_{\mathrm{II}}^{1} & & \\ & \ddots & \\ & & \mathbf{E}_{\mathrm{II}}^{\hat{k}} \end{bmatrix}$$

This matrix is easy
to solve in parallel

Schur complement $\mathbf{S}\ \mathbf{y}_{\mathrm{B}} = \left(\mathbf{s}_{\mathrm{B}} - \mathbf{E}_{\mathrm{BI}} \mathbf{E}_{\mathrm{II}}^{-1} \mathbf{s}_{\mathrm{I}} \right)$

where $\mathbf{S} = \left[\mathbf{E}_{\mathrm{BB}} - \mathbf{E}_{\mathrm{BI}} \mathbf{E}_{\mathrm{II}}^{\text{-1}} \mathbf{E}_{\mathrm{IB}} \right]$

Parareal algorithm

$$\begin{bmatrix} \mathbf{E}_{\mathrm{II}} & \mathbf{E}_{\mathrm{IB}} \\ \mathbf{E}_{\mathrm{BI}} & \mathbf{E}_{\mathrm{BB}} \end{bmatrix} \begin{bmatrix} \mathbf{y}_{\mathrm{I}} \\ \mathbf{y}_{\mathrm{B}} \end{bmatrix} = \begin{bmatrix} \mathbf{s}_{\mathrm{I}} \\ \mathbf{s}_{\mathrm{B}} \end{bmatrix}$$

$$\mathbf{y}_{\mathrm{I}}^{\mathrm{n}} = \left(\mathbf{E}_{\mathrm{II}}^{-1} \mathbf{s}_{\mathrm{I}} \right)$$

$$\mathbf{y}_{\mathrm{I}}^{\mathrm{n+1}} = \mathbf{E}_{\mathrm{II}}^{-1} \left(\mathbf{s}_{\mathrm{I}} - \mathbf{E}_{\mathrm{IB}} \mathbf{y}_{\mathrm{B}}^{\mathrm{n}} \right)$$

$$\mathbf{y}_{\mathrm{B}}^{\mathrm{n+1}} = \mathbf{y}_{\mathrm{B}}^{\mathrm{n+1}} + \tilde{\mathbf{S}}^{-1} \left(\mathbf{s}_{\mathrm{B}} - \mathbf{E}_{\mathrm{BI}} \mathbf{y}_{\mathrm{I}}^{\mathrm{n+1}} - \mathbf{E}_{\mathrm{BB}} \mathbf{y}_{\mathrm{B}}^{\mathrm{n}} \right)$$

$$\mathbf{y} := \begin{bmatrix} \mathbf{y}_{\mathrm{I}} \\ \mathbf{y}_{\mathrm{B}} \end{bmatrix}$$

Using Gershgoring’s radius theorem we have

$$\left|\mu(\Theta_m) - a_m^2\right| \leq \left|a_m b_m\right| \quad \text{or} \quad \left|\mu(\Theta_m) - a_m^2 - b_m^2\right| \leq 2\left|a_m b_m\right|$$

To guarantee stability: $\left|b_m\right| \leq \left|a_m\right|$

An lower bound

$$\mu(\Theta_m) \geq \min\left(\left|a_m\right|^2\left(1 - \frac{\left|b_m\right|}{\left|a_m\right|}\right)^2\right) = \min\left(\tau\left|\lambda_m\right|\right)^2 \longrightarrow \quad \mu(\Theta_m) \geq \left(\tau\rho_{\min}\right)^2$$

An upper bound

$$\mu(\Theta_m) \leq \max\ 4\left|a_m\right|^2 \rightarrow \quad \mu(\Theta_i) \leq 4\left(1 - \tau\theta\rho_{\max}\right)^2$$

Condition for $\mathbf{EE}^T$

An lower bound $\mu(\Theta_m) \geq (\tau \ \rho_{\min})^2$

An upper bound $\mu(\Theta_i) \leq 4(1 - \tau\theta\rho_{\max})^2$

$$\text{Cond}(EE^T) \approx \frac{4(1+\tau\theta\rho_{\max})^2}{(\tau\rho_{\min})^2}$$

Remark: for finite element discretization

$$-O\left(\frac{1}{h^2}\right) < \lambda_m < -O(1)$$

$$\text{Cond}(\mathbf{EE}^T) \approx \frac{(1+\tau\theta h^{-2})^2}{(\tau)^2}$$

Boundary condition

- Newton law for heat convection transfer

$$\frac{\partial y}{\partial \eta} = -\frac{u}{\lambda}\left(y - y_{\infty}\right)$$

u is the convection coefficient and the control variable to dissipate the heat.

$\gamma_{\max}$ and $\gamma_{\min}$ estimates are sharp

	N_t	200	400	800	1600
$\gamma_{\max} - 1$	n=1	0.8644	1.4493	2.4737	4.3717
	n=2	0.0708	0.0979	0.1368	0.1938
	n=3	0.0078	0.0108	0.0151	0.0212
	n=4	0.0009	0.0012	0.0017	0.0024

$\Delta T = 1/20$

$h = 1/10$

Factor $\sqrt{2}$

	N_t	200	400	800	1600
$1 - \gamma_{\min}$	n=1	0.4642	0.5663	0.6925	0.7991
	n=2	0.0663	0.0895	0.1217	0.1642
	n=3	0.0077	0.0107	0.0149	0.0207
	n=4	0.0008	0.0012	0.0017	0.0024