Optimal energy harvesting with a piezoelectric device, modeled by Preisach operators

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joint work with

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Overview

- physical background
- thermodynamic consistency
- Preisach operators and hysteresis potentials
- a thermodynamically consistent material law for ferroelectricity and ferroelasticity
- energy harvesting: a simple harvester model
- optimization
- gradient computation

physical background

Piezoelectric Transducers

Direct effect: apply mechanical force $\rightarrow$ measure electric voltage

Indirect effect: impress electric voltage $\rightarrow$ observe mechanical displacement

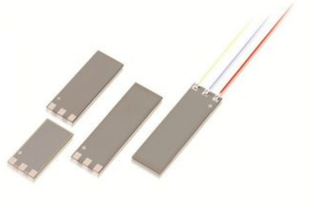
Piezoelectric Transducers

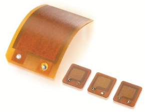
Direct effect: apply mechanical force → measure electric voltage

Indirect effect: impress electric voltage → observe mechanical displacement

Application Areas:

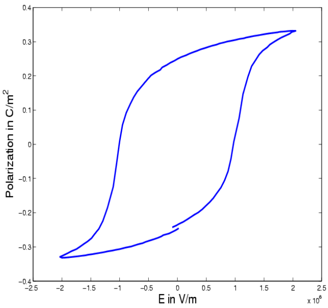
- ultrasound (imaging, therapy)
- force- and acceleration Sensors
- actor injection valves
- SAW sensors
- energy harvesting
- ...

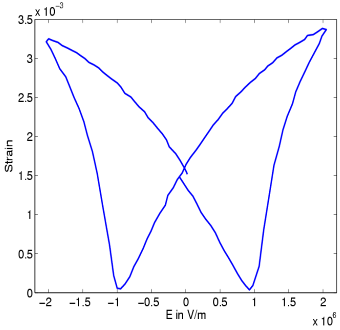




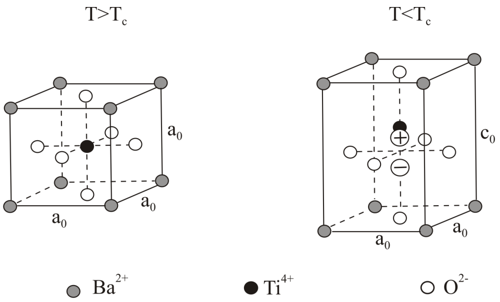
Hysteresis of Piezoelectric Materials

e.g. ferroelectric hysteresis:
dielectric displacement and mechanical strain
at high electric field intensities ($E \sim 2MV/m$):





Piezoelectricity and Ferroelectricity on Unit Cell Level

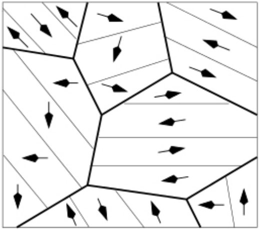


Unit cell of $BaTiO_3$ above (left) and below (right) Curie temperature T_c, the latter exhibiting sponaneos polarization and strain

courtesy to M.Kamlah

[Kamlah, Continuum Mech. Thermodyn., 2001]

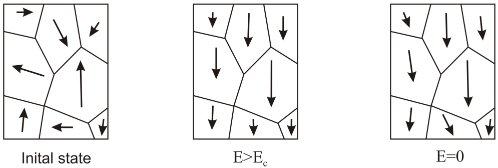
Grain and Domain Structure



Grains with same unit cell orientation
domains with same polarization direction

courtesy to M.Kamlah

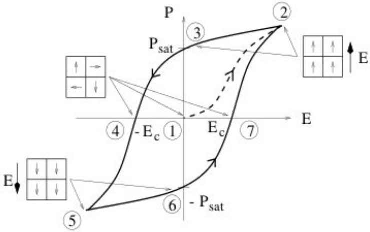
Poling Process



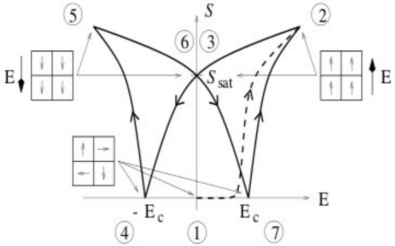
Orientation of the total polarization of the grains at initial state (left), due to a strong external electric field (middle) and after switching it off, leading to a remanent polarization and strain (right)

courtesy to M.Kamlah

Ferroelectricity



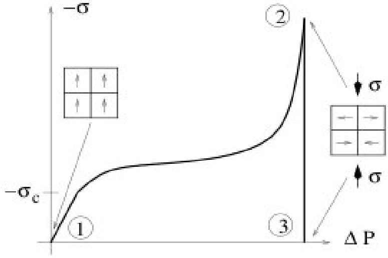
polarization hysteresis



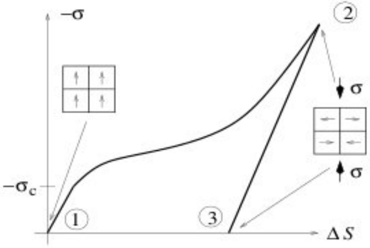
strain hysteresis (butterfly)

courtesy to M.Kamlah

Ferroelasticity



mechanical depolarization
$\Delta P = P_{\text{max}} - P$



stress-strain relation
$\Delta S = S_{\text{max}} - S$

courtesy to M.Kamlah

Piezoelectricity – Ferroelectricity – Ferroelasticity

Piezoelectricity
. . . linear coupling between electric and mechanical fields
(reversible)

Ferroelectricity
. . . external electric field influences polarization
(irreversible, hysteretic)

Ferroelasticity
. . . external mechanical field influences polarization
(irreversible, hysteretic)

1. *Thermodynamically consistent models*
   macroscopic view, 2nd law of thermodynamics
   Bassiouny&Ghaleb'89, Kamlah&Böhle'01, Landis'04, Schröder&Romanowski'05, Su&Landis'07, Linnemann&Klinkel&Wagner'09, Mielke&Timofte'06, Alber&Kraynyukova'12, ...
2. *Micromechanical models*
   Huber&Fleck'01, Fröhlich'01, Delibas&Arockiarajan&Seemann'05, Belov&Kreher'06, Huber'06, McMeeking&Landis&Jimeneza'07, ...
3. *Phase field models*
   Wang&Kamlah&Zhang'10, Xu&Schrade&Müller&Gross&Granzow&Rödel'10, Schrade&Müller&Gross&Keip&Thai&Schrder'14, ...
4. *Multiscale models*
   Schröder&Keip'10, '12, Miehe&Kiefer&Rosato&'12, Miehe&Zäh&Rosato&'12, ...
5. *Phenomenological models using hysteresis operators*
   from input-output description for control purposes
   Hughes&Wen'95, Kuhnen'01, Cimaa&Laboure&Muralt'02, Smith&Seelecke&Ounaies&Smith'03, Pasco&Berry04, Kuhnen&Krejčí'07, Ball&Smith&Kim&Seelecke'07, Hegewald&BK&MK&Lerch'08,'09, ...

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thermodynamic consistency

Thermodynamic Consistency

$\underline{\sigma}$ . . . mechanical stress
$\underline{\varepsilon}$ . . . mechanical strain
$\vec{E}$. . . electic field
$\vec{D}$. . . dielectic displacement
$\mathcal{W}$. . . work done by electric and mechanical forces
$\mathcal{F}$. . . Helmholtz free energy
$\mathcal{D}$. . . energy dissipation

$$\mathcal{W}(t_1, t_2) = \int_{t_1}^{t_2} \dot{\underline{\varepsilon}}(t) : \underline{\sigma}(t) + \dot{\vec{D}}(t) \cdot \vec{E}(t)\, dt$$

2nd law of thermodynamics:

$$\mathcal{D}(t_1, t_2) = \mathcal{W}(t_1, t_2) - (\mathcal{F}(t_2) - \mathcal{F}(t_1)) \geq 0$$

differential form (Clausius Duhem inequality):

$$\dot{\underline{\varepsilon}} : \underline{\sigma} + \dot{\vec{D}} \cdot \vec{E} - \dot{\mathcal{F}} \geq 0$$

A Class of Thermodynamically Consistent Material Laws

split ε and D as well as constitutive relations into reversible and irreversible part:

$$\begin{cases} \varepsilon = \underline{s}\sigma + d^T E + S \\ D = d\sigma + \kappa E + P \\ \mathcal{F} = \frac{1}{2}\sigma : (\underline{s}\sigma) + \frac{1}{2} E \cdot (\kappa E) + \sigma : (dE) + \Psi(S, P) \end{cases}$$

$\underline{s}$ . . . compliance tensor
κ . . . dielectric coefficients
d . . . piezoelectric coupling coefficients
S. . . irreversible strain
P. . . polarization

linear part: piezoelectric coupling
nonlinear hysteretic part: ferroelectricity and ferroelasticity

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Clausius Duhem inequality:

$$\underline{\dot{\varepsilon}} : \underline{\sigma} + \dot{\vec{D}} \cdot \vec{E} - \dot{\mathcal{F}} \geq 0$$

leads to

$$\dot{S} : \left(\sigma - \frac{\partial \Psi}{\partial S}\right) + \dot{P} \cdot \left(E - \frac{\partial \Psi}{\partial P}\right) \geq 0$$

$\rightsquigarrow$ evolution system for irreversible strain and polarization:

$$\begin{pmatrix} \dot{S} \\ \dot{P} \end{pmatrix} \in \partial \Phi \begin{pmatrix} \sigma - \frac{\partial \Psi}{\partial S} \\ E - \frac{\partial \Psi}{\partial P} \end{pmatrix}$$

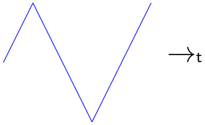
with Φ a proper convex function such that $\Phi(x) - \Phi(0) \geq 0$ (e.g., $\Phi = \delta_K$ indicator function).

[Kraynyukova&Nesenenko'13]: existence of measure valued solutions

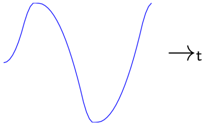
Preisach operators
and hysteresis potentials

Hysteresis and Hysteresis Operators

input:



output:



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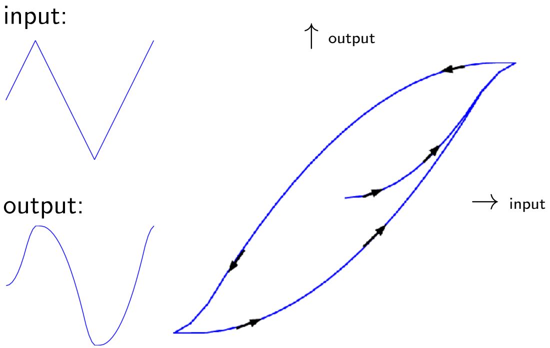

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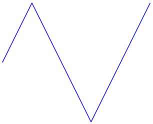

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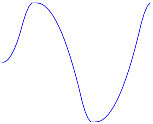
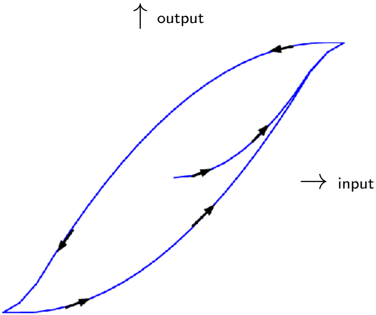


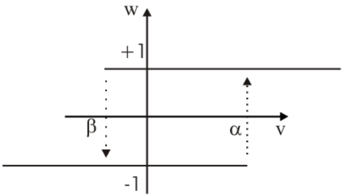


- magnetics
- ferroelectricity
- plasticity
- . . .

* memory
* Volterra property
* rate independence

Krasnoselksii-Pokrovskii (1983), Mayergoyz (1991), Visintin (1994), Krejčí (1996), Brokate-Sprekels (1996)

A Simple Example I: The Relay

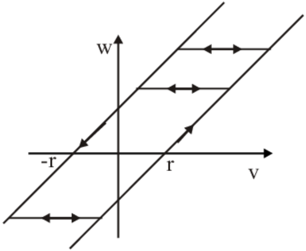


$$\mathfrak{r}_{\beta,\alpha}[\mathrm{v}](t) = \mathrm{w}(t)$$

$$= \begin{cases} +1 & \text{if } \mathrm{v}(t) > \alpha \text{ or } (\mathrm{w}(t_i) = +1 \wedge \mathrm{v}(t) > \beta) \\ -1 & \text{if } \mathrm{v}(t) < \beta \text{ or } (\mathrm{w}(t_i) = -1 \wedge \mathrm{v}(t) < \alpha) \end{cases} \qquad t \in [t_i, t_{i+1}]$$

$t_0, t_1, t_2, \ldots$ sequence of local extrema of v,
i.e., v monotone on $[t_i, t_{i+1}]$.

A Simple Example II: The Mechanical Play



$$\mathfrak{p}_r[\mathrm{v}](t) = \mathrm{w}(t) = \max\{\mathrm{v}(t) - r, \min\{\mathrm{v}(t) + r, \mathrm{w}(t_i)\}\} \quad t \in [t_i, t_{i+1}]$$

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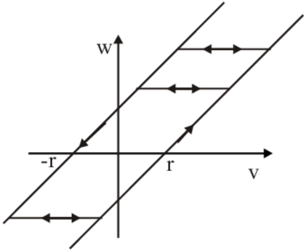

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characterization via variational inequality:

$$\begin{cases} |\mathrm{v}(t) - \mathrm{w}(t)| \leq r & \forall t \in [0, T], \\ \dot{\mathrm{w}}(t)(\mathrm{v}(t) - \mathrm{w}(t) - z) \geq 0 & \text{a. e.} \quad \forall |z| \leq r \end{cases}$$

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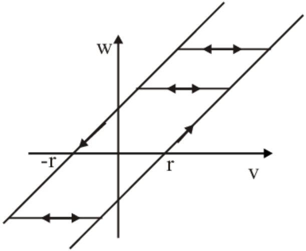

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Relation to Relay operator: $\mathfrak{p}_r[\mathrm{v}](t) = \frac{1}{2} \int_{-\infty}^{\infty} \mathfrak{r}_{s-r,s+r}[\mathrm{v}](t)\, ds$

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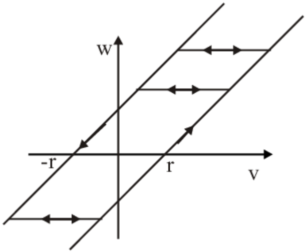

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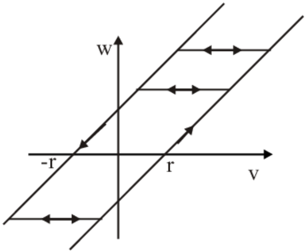

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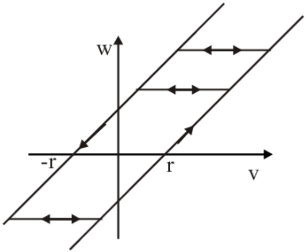

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where $\delta_{[-r,r]}(z) = \begin{cases} 0 \text{ if } |z| \le r \\ \infty \text{ else} \end{cases}$:

A General Hysteresis Model: the Preisach Operator

$$\mathcal{P}[\mathrm{v}](t) = \int\int_{\beta<\alpha} \omega(\beta,\alpha)\mathfrak{r}_{\beta,\alpha}[\mathrm{v}](t)\, d(\beta,\alpha)$$
$$= \int_0^\infty g(\mathfrak{p}_r[\mathrm{v}](t), r)\, dr$$

with $g(s,r) = 2\int_0^s \omega(\sigma - r, \sigma + r)\, d\sigma$

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- ± high dimensionality
- \+ can model minor loops
- \+ can model saturation
- \+ highly efficient evaluation

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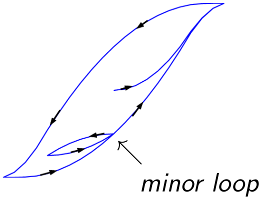

Hysteresis Potentials

clockwise:

$$\mathcal{P}[\mathrm{v}](t)\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{v}(t) - \frac{\mathrm{d}}{\mathrm{d}t}\mathcal{U}[\mathrm{v}](t) \geq 0 \quad \text{for all inputs } \mathrm{v}$$

counterclockwise:

$$\mathrm{v}(t)\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{P}[\mathrm{v}](t) - \frac{\mathrm{d}}{\mathrm{d}t}\mathcal{U}[\mathrm{v}](t) \geq 0 \quad \text{for all inputs } \mathrm{v}$$

v . . . input
$\mathcal{P}$ . . . hysteresis operator
$\mathcal{U}$ . . . hysteresis potential

Hysteresis Potentials for Preisach Operators

For the Preisach hysteresis operator defined by

$$\mathcal{P}[\mathrm{v}](t) = \int\int_{\beta<\alpha} \omega(\beta,\alpha)\mathfrak{r}_{\beta,\alpha}[\mathrm{v}](t)d(\beta,\alpha) = \int_0^\infty g(\mathfrak{p}_r[\mathrm{v}](t),r)\,dr$$

with nonnegative symmetric weight function ω,
a counterclockwise hysteresis potential is given by

$$\mathcal{U}[\mathrm{v}](t) = \int\int_{\beta<\alpha} \frac{|\beta+\alpha|}{2}\omega(\beta,\alpha)\mathfrak{r}_{\beta,\alpha}[\mathrm{v}](t)d(\beta,\alpha) = \int_0^\infty G(\mathfrak{p}_r[\mathrm{v}](t),r)\,dr$$

where

$$G(\sigma,r) = \int_0^\sigma \tau\partial_1 g(\tau,r)\,d\tau$$

Krejčí (1996), Brokate-Sprekels (1996)

Hysteresis Potential for the Play Operators

For the play operator

$$\mathcal{P}[\mathrm{v}](t) = \mathfrak{p}_r[\mathrm{v}](t) = \mathrm{w}(t)$$

a counterclockwise hysteresis potential is given by

$$\mathcal{U}[\mathrm{v}](t) = \frac{1}{2}\mathrm{w}(t)^2$$

where

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where

$$\dot{\mathrm{w}} \in \partial\delta_{[-r,r]}(\mathrm{v}(t) - \mathrm{w}(t))$$

where $\delta_{[-r,r]}(z) = \begin{cases} 0 \text{ if } |z| \leq r \\ \infty \text{ else} \end{cases}$:

A thermodynamically consistent material law for ferroelectricity and ferroelasticity

A Thermodynamically Consistent Material Law using Hysteresis Operators and Potentials

see [Davino&Krejčí&Visone'13] for magnetostriction

Ansatz: $$\begin{cases} \sigma = \underline{c}\varepsilon + a\mathcal{P}[q] + b\mathcal{U}[q] \\ D = \kappa E + c\mathcal{P}[q] + d\mathcal{U}[q] \\ \mathcal{F} = \frac{c}{2}\varepsilon^2 + \frac{\kappa}{2}E^2 + \xi\mathcal{P}[q] + \eta\mathcal{U}[q] \end{cases}$$

$q = q(\varepsilon, E)$ . . . internal variable

$a = a(\varepsilon, E)$, $b = b(\varepsilon, E)$, $c = c(\varepsilon, E)$, $d = d(\varepsilon, E)$, $\xi = \xi(\varepsilon, E)$, $\eta = \eta(\varepsilon, E)$ . . . coefficient functions

$\mathcal{U}$ . . . counterclockwise hysteresis potential for $\mathcal{P}$

linear part

nonlinear hysteretic part

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$\eta = \eta(\varepsilon, E)$ ... coefficient functions

$\mathcal{U}$ ... counterclockwise hysteresis potential for $\mathcal{P}$

linear part

nonlinear hysteretic part

Choose q, a, b, c, d, e, ξ, η such that thermodynamic consistency holds:

$$\dot{\underline{\varepsilon}} : \underline{\sigma} + \dot{\vec{D}}(t) \cdot \vec{E} - \dot{\mathcal{F}} \geq 0$$

A Thermodynamically Consistent Material Law

$$\text{Ansatz:} \quad \begin{cases} \sigma = \underline{c}\varepsilon + a\mathcal{P}[q] + b\mathcal{U}[q] \\ D = \kappa E + c\mathcal{P}[q] + d\mathcal{U}[q] \\ \mathcal{F} = \frac{\underline{c}}{2}\varepsilon^2 + \frac{\kappa}{2}E^2 + \xi\mathcal{P}[q] + \eta\mathcal{U}[q] \end{cases}$$

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A Thermodynamically Consistent Material Law

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$q = q(\varepsilon, E)$ ... internal variable
$a = a(\varepsilon, E)$, $b = b(\varepsilon, E)$, $c = c(\varepsilon, E)$, $d = d(\varepsilon, E)$, $\xi = \xi(\varepsilon, E)$,
$\eta = \eta(\varepsilon, E)$ ... coefficient functions
$\mathcal{U}$ ... counterclockwise hysteresis potential for $\mathcal{P}$

thermodynamically consistent, for any choice of scalar valued functions $f = f(\varepsilon, E) \in \mathbb{R}^+$, $g = g(\varepsilon, E) \in \mathbb{R}$:

$$a = \frac{\partial g}{\partial \varepsilon} \qquad b = \frac{\partial f}{\partial \varepsilon} \qquad c = -\frac{\partial g}{\partial E} \quad d = -\frac{\partial f}{\partial E}$$

$$\xi = g + cE \quad \eta = f + dE \quad q = -\frac{g}{f}$$

e.g., $f(\varepsilon, E) = f(\varepsilon) > 0$, $g(\varepsilon, E) = E$.

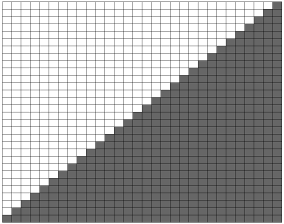
A Thermodynamically Consistent Material Law: An Example

$f : \mathbb{R} \to \mathbb{R}^+$

$$\begin{cases} \sigma = \underline{c}\varepsilon + f'(\varepsilon)\mathcal{U}[\frac{E}{f(\varepsilon)}] \\ D = \kappa E + \mathcal{P}[\frac{E}{f(\varepsilon)}] \\ \mathcal{F} = \frac{\underline{c}}{2}\varepsilon^2 + \frac{\kappa}{2}E^2 + f(\varepsilon)\mathcal{U}[\frac{E}{f(\varepsilon)}] \end{cases}$$

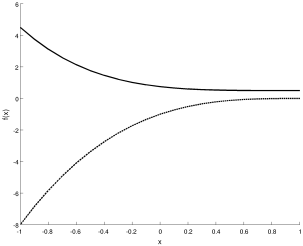
A Simple Test

Preisach weight function ω:



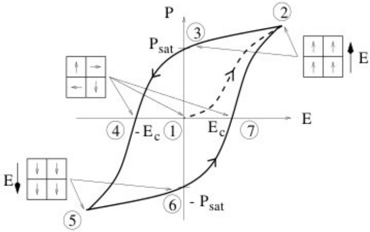
$$\omega(\beta, \alpha) \equiv 0.5$$

function f, f':

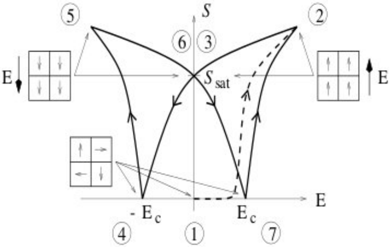


$$f(x) = \frac{2+(x-1)^4}{4}$$
$$-1 \leq x \leq 1$$

Ferroelectricity



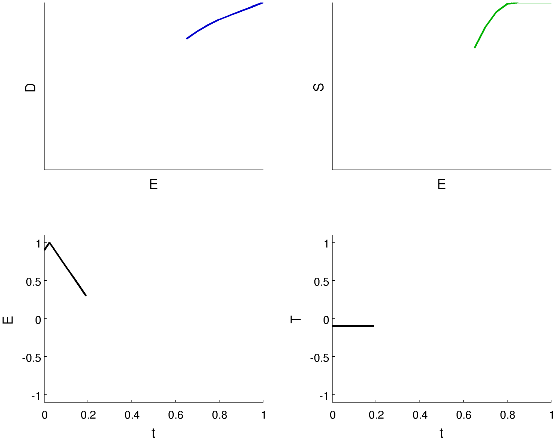
polarization hysteresis



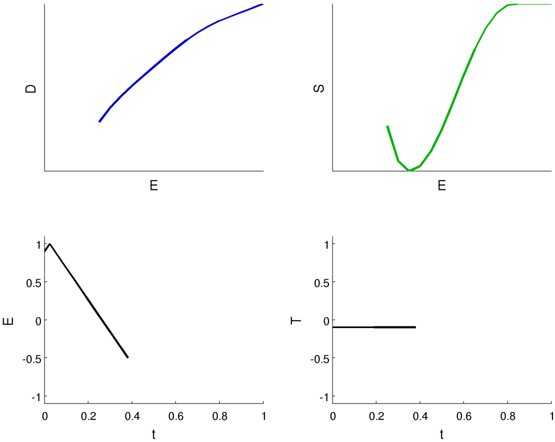
strain hysteresis (butterfly)

courtesy to M.Kamlah

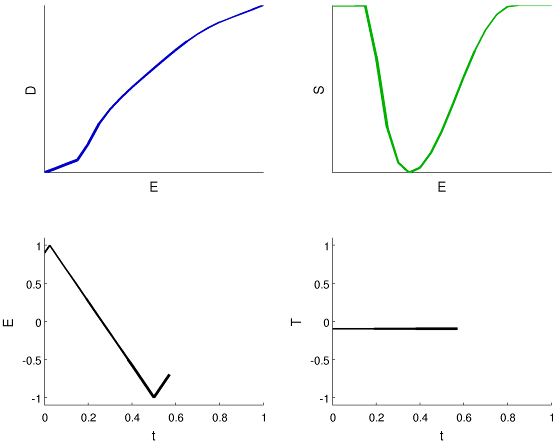
Ferroelectricity



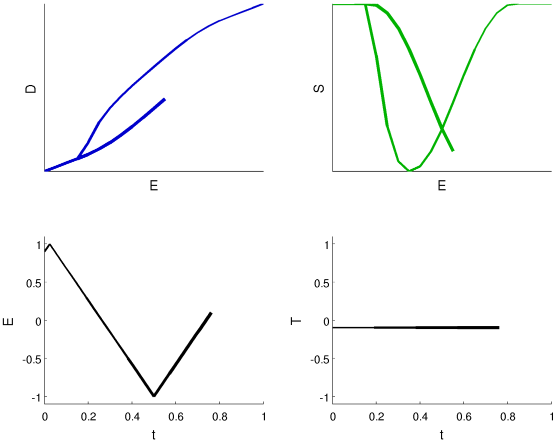
Ferroelectricity



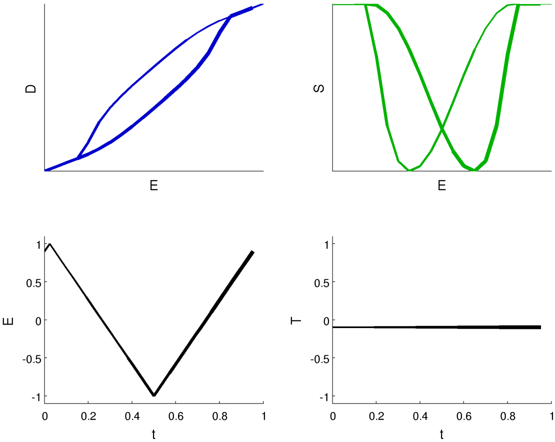
Ferroelectricity



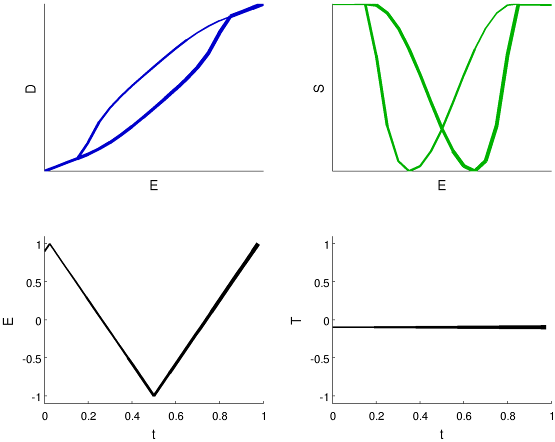
Ferroelectricity



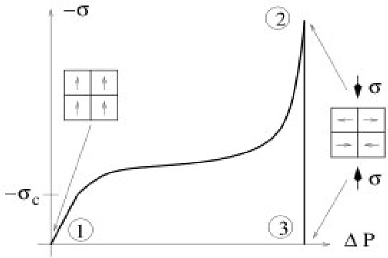
Ferroelectricity

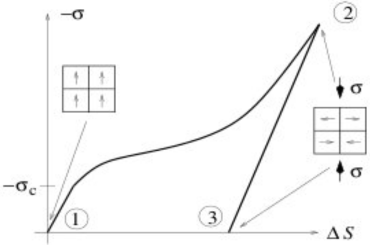


Ferroelectricity



Ferroelasticity





mechanical depolarization

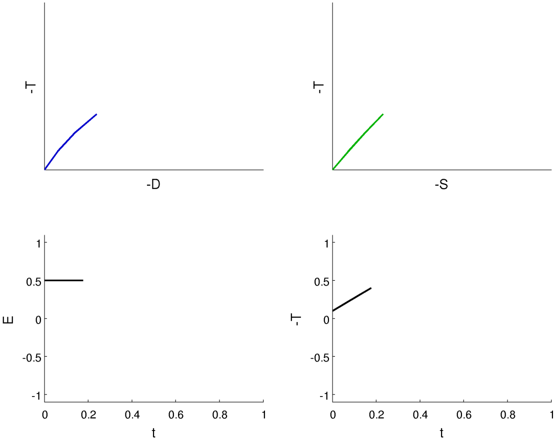
$\Delta P = P_{\max} - P$

stress-strain relation

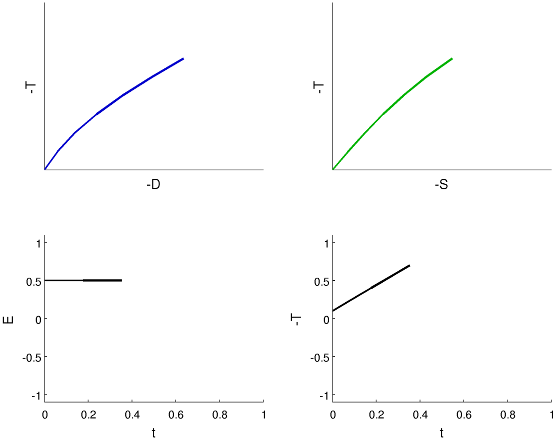
$\Delta S = S_{\max} - S$

courtesy to M.Kamlah

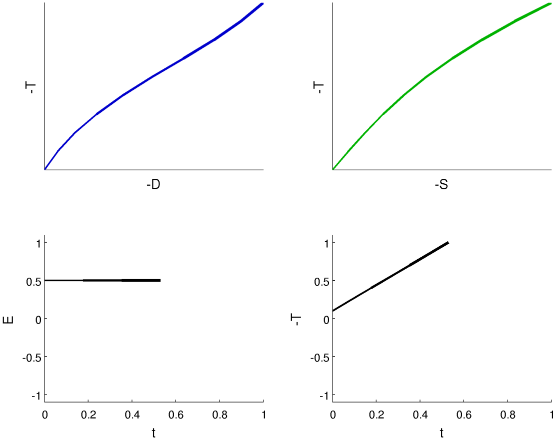
Ferroelasticity



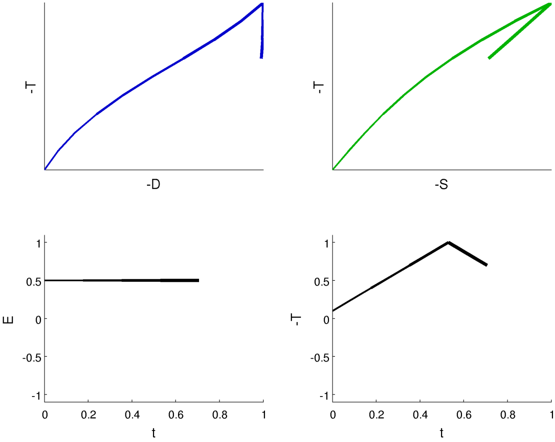
Ferroelasticity



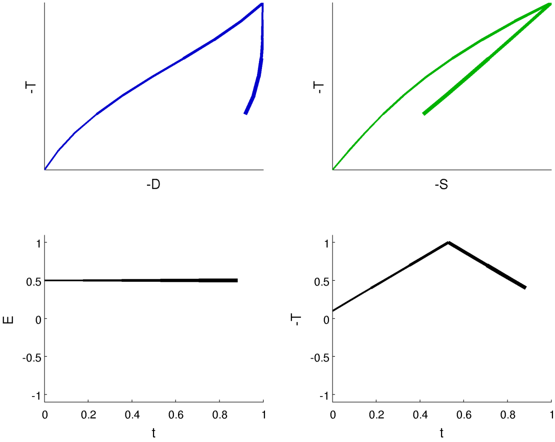
Ferroelasticity



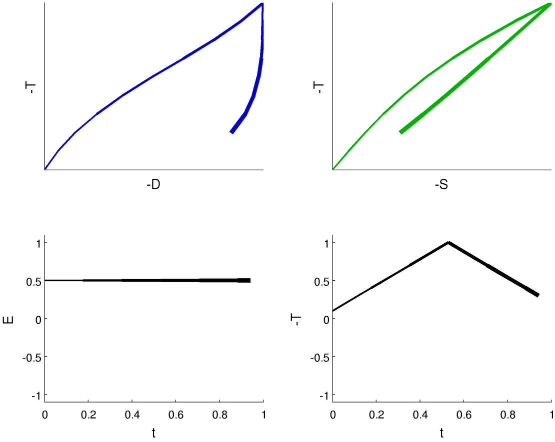
Ferroelasticity



Ferroelasticity



Ferroelasticity



An Alternative Thermodynamically Consistent Material Law

$f : \mathbb{R} \to \mathbb{R}_0^+$

$$\begin{cases} \varepsilon = \underline{s}\sigma + f'(\sigma)\mathcal{U}[E] \\ D = \kappa E + f(\sigma)\mathcal{P}[E] \\ \mathcal{F} = \frac{\underline{c}}{2}\varepsilon^2 + \frac{\kappa}{2}E^2 - f(\varepsilon)\mathcal{U}[E] \end{cases}$$

with $-\mathcal{U}$ clockwise hysteresis potential for $-\mathcal{P}$

An Alternative Thermodynamically Consistent Material Law

$f : \mathbb{R} \to \mathbb{R}_0^+$

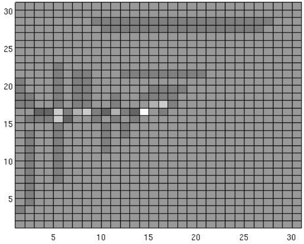
$$\begin{cases} \varepsilon = \underline{s}\sigma + f'(\sigma)\mathcal{U}[E] \\ D = \kappa E + f(\sigma)\mathcal{P}[E] \\ \mathcal{F} = \frac{\underline{c}}{2}\varepsilon^2 + \frac{\kappa}{2}E^2 - f(\varepsilon)\mathcal{U}[E] \end{cases}$$

with $-\mathcal{U}$ clockwise hysteresis potential for $-\mathcal{P}$

- additive decomposition of strain and dielectric displacement into reversible and irreversible parts
- models only ferroelectric hysteresis;
  but also general verison with $q = q(\sigma, E)$ . . . internal variable
  $a = a(\sigma, E)$, $b = b(\sigma, E)$, $c = c(\varepsilon, E)$, $d = d(\sigma, E)$,
  $\xi = \xi(\sigma, E)$, $\eta = \eta(\sigma, E)$ . . . coefficient functions possible
  (see [Davino&Krejčí&Visone'13] for magnetostriction)

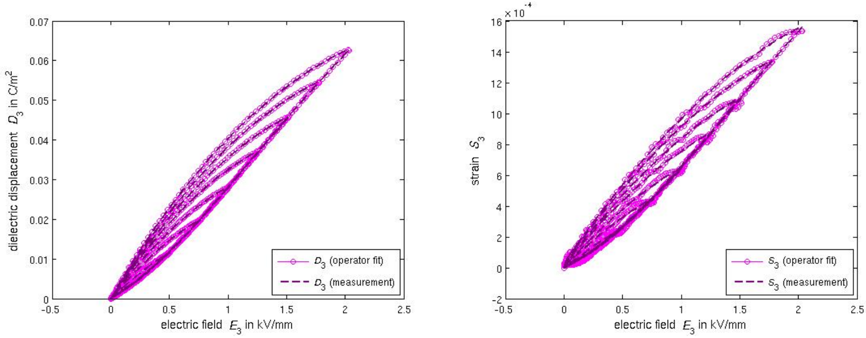
Numerical Results: Stack Actuator

Identified Preisach weight function:



Numerical Results: Stack Actuator

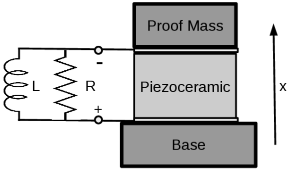
ferroelectric hysteresis
comparison measurement – simulation
with fitted Preisach operators:



energy harvesting

A Simple Harvester Model

$$\frac{m}{A}\ddot{x} + \bar{\sigma} = 0$$
$$\ddot{D} + \frac{1}{R}\dot{\phi} + \frac{1}{L}\phi = 0$$



or, without inductance

$$\frac{m}{A}\ddot{x} + \bar{\sigma} = 0$$
$$\dot{D} + \frac{1}{R}\phi = 0$$

x	displacement
$\bar{\sigma}$	total stress $= \sigma_{piezo} + \sigma_{visc} + \sigma_{imp}$
ϕ	voltage
D	dielectric displacement
m	mass
A	contact area
R	electric resistance
L	inductance
d	thickness of piezo

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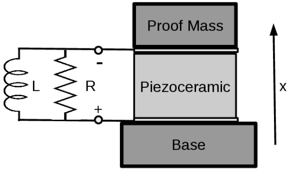

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$$\frac{m}{A}\ddot{x} + \bar{\sigma} = 0$$

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x	displacement $\quad \varepsilon = \frac{x}{d}$ strain
$\bar{\sigma}$	total stress $= \sigma_{piezo} + \sigma_{visc} + \sigma_{imp}$
ϕ	voltage $\quad E = \frac{\phi}{d}$ electric field
D	dielectric displacement
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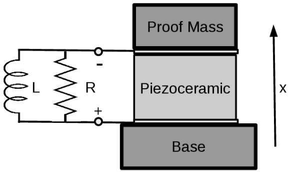

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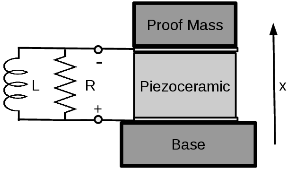

[Renno&Daqaq&Inman09]

linear constitutive law:

$$\sigma_{visc} = \nu\dot{\varepsilon},$$

$$\sigma_{piezo} = c\varepsilon - eE,$$

$$D = e\varepsilon + \kappa E$$

ν	viscosity,
c	elasticity modulus,
e	piezoelectric coupling coeff.,
κ	dielectric constant.

A Simple Harvester Model

$$\frac{md}{A}\ddot{\varepsilon} + \bar{\sigma} = 0$$
$$\ddot{D} + \frac{d}{R}\dot{E} + \frac{d}{L}E = 0$$

or, without inductance

$$\frac{md}{A}\ddot{\varepsilon} + \bar{\sigma} = 0$$
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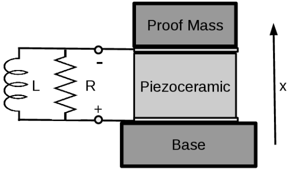

x	displacement $\quad \varepsilon = \frac{x}{d}$ strain
$\bar{\sigma}$	total stress $= \sigma_{piezo} + \sigma_{visc} + \sigma_{imp}$
ϕ	voltage $\quad E = \frac{\phi}{d}$ electric field
q	internal variable
D	dielectric displacement
m	mass
A	contact area
R	electric resistance
L	inductance

hysteretic constitutive law:

$$\sigma_{visc} = \nu\dot{\varepsilon},$$
$$\sigma_{piezo} = c\varepsilon - eE + f'(\varepsilon)\mathcal{U}[q] + \frac{b'(\varepsilon)}{2}\mathcal{P}^2[q],$$
$$D = e\varepsilon + \kappa E + \mathcal{P}[q],$$
$$q = \frac{1}{f(\varepsilon)}(E - b(\varepsilon)\mathcal{P}[q]),$$

ν	viscosity,
c	elasticity modulus,
e	piezoelectric coupling coeff.,
κ	dielectric constant
b, f	real functions

Thermodynamic Consistency

$$\begin{cases} \sigma_{piezo} = c\varepsilon - eE + f'(\varepsilon)\mathcal{U}[q] + \frac{b'(\varepsilon)}{2}\mathcal{P}^2[q], \\ D = e\varepsilon + \kappa E + \mathcal{P}[q], \\ \mathcal{F} = \frac{c}{2}\varepsilon^2 + \frac{\kappa}{2}E^2 + f(\varepsilon)\mathcal{U}[q] + \frac{b(\varepsilon)}{2}\mathcal{P}^2[q] \end{cases}$$

where $q = \frac{1}{f(\varepsilon)}(E - b(\varepsilon)\mathcal{P}[q])$.

Thermodynamic Consistency

$$\begin{cases} \sigma_{piezo} = c\varepsilon - eE + f'(\varepsilon)\mathcal{U}[q] + \frac{b'(\varepsilon)}{2}\mathcal{P}^2[q], \\ D = e\varepsilon + \kappa E + \mathcal{P}[q], \\ \mathcal{F} = \frac{c}{2}\varepsilon^2 + \frac{\kappa}{2}E^2 + f(\varepsilon)\mathcal{U}[q] + \frac{b(\varepsilon)}{2}\mathcal{P}^2[q] \end{cases}$$

where $q = \frac{1}{f(\varepsilon)}(E - b(\varepsilon)\mathcal{P}[q])$.
This model satisfies

$$\dot{D}E + \dot{\varepsilon}\sigma_{piezo} - \frac{\mathrm{d}}{\mathrm{d}t}\mathcal{F}[\varepsilon, E] \geq 0$$

provided $\mathcal{U}$ is a (counterclockwise) hysteresis potential for $\mathcal{P}$

$$v\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{P}[v] - \frac{\mathrm{d}}{\mathrm{d}t}\mathcal{U}[v] \geq 0 \quad \text{for all inputs v}$$

Evolutionary System

From balance equations and material laws we get

$$\rho\ddot{\varepsilon} + \nu\dot{\varepsilon} + c\varepsilon - eE + f'(\varepsilon)\mathcal{U}[q] + \tfrac{1}{2}b'(\varepsilon)\mathcal{P}^2[q] = -\sigma_{imp},$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\Big(e\varepsilon + \kappa E + \mathcal{P}[q]\Big) + \alpha E = 0,$$

$$q + \tfrac{b(\varepsilon)}{f(\varepsilon)}\mathcal{P}[q] = \tfrac{E}{f(\varepsilon)},$$

with $\rho = \frac{md}{A}$, $\alpha = \frac{d}{R}$, and initial conditions

$$\varepsilon(0) = \varepsilon_0, \quad \dot{\varepsilon}(0) = \varepsilon_1, \quad E(0) = E_0$$

Evolutionary System

$$\rho\ddot{\varepsilon} + \nu\dot{\varepsilon} + c\varepsilon - eE + f'(\varepsilon)\mathcal{U}[q] + \tfrac{1}{2}b'(\varepsilon)\mathcal{P}^2[q] = -\sigma_{imp},$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\Big(\underbrace{e\varepsilon + \kappa E + \mathcal{P}[q]}_{D}\Big) + \alpha E = 0,$$

$$q + \tfrac{b(\varepsilon)}{f(\varepsilon)}\mathcal{P}[q] = \tfrac{E}{f(\varepsilon)},$$

with initial conditions

$$\varepsilon(0) = \varepsilon_0, \quad \dot{\varepsilon}(0) = \varepsilon_1, \quad E(0) = E_0$$

Evolutionary System

$$\rho\ddot{\varepsilon} + \nu\dot{\varepsilon} + c\varepsilon - eE + f'(\varepsilon)\mathcal{U}[q] + \tfrac{1}{2}b'(\varepsilon)\mathcal{P}^2[q] = -\sigma_{imp},$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\Big(\underbrace{e\varepsilon + \kappa E + \mathcal{P}[q]}_{D}\Big) + \alpha E = 0,$$

$$q + \tfrac{b(\varepsilon)}{f(\varepsilon)}\mathcal{P}[q] = \tfrac{E}{f(\varepsilon)},$$

with initial conditions

$$\varepsilon(0) = \varepsilon_0, \quad \dot{\varepsilon}(0) = \varepsilon_1, \quad E(0) = E_0$$

...use D instead of E as a variable, by expressing E in terms of D:

$$D = e\varepsilon + \kappa E + \mathcal{P}[q] \;\Leftrightarrow\; E = \tfrac{1}{\kappa}(D - e\varepsilon - \mathcal{P}[q])$$

$\rightsquigarrow$

Evolutionary System

$$\rho\ddot{\varepsilon} + \nu\dot{\varepsilon} + c\varepsilon - \tfrac{e}{\kappa}(D - e\varepsilon - \mathcal{P}[q]) + f'(\varepsilon)\mathcal{U}[q] + \tfrac{1}{2}b'(\varepsilon)\mathcal{P}^2[q] = -\sigma_{imp},$$

$$\dot{D} + \tfrac{\alpha}{\kappa}(D - e\varepsilon - \mathcal{P}[q]) = 0,$$

$$q + \tfrac{1+\kappa b(\varepsilon)}{\kappa f(\varepsilon)}\mathcal{P}[q] = \tfrac{D-e\varepsilon}{\kappa f(\varepsilon)},$$

with initial conditions

$$\varepsilon(0) = \varepsilon_0, \quad \dot{\varepsilon}(0) = \varepsilon_1, \quad D(0) = D_0$$

Evolutionary System

$$\rho\ddot{\varepsilon} + \nu\dot{\varepsilon} + c\varepsilon - \frac{e}{\kappa}(D - e\varepsilon - \mathcal{P}[q]) + f'(\varepsilon)\mathcal{U}[q] + \frac{1}{2}b'(\varepsilon)\mathcal{P}^2[q] = -\sigma_{imp},$$
$$\dot{D} + \frac{\alpha}{\kappa}(D - e\varepsilon - \mathcal{P}[q]) = 0,$$
$$q + \frac{1+\kappa b(\varepsilon)}{\kappa f(\varepsilon)}\mathcal{P}[q] = \frac{D - e\varepsilon}{\kappa f(\varepsilon)},$$

with initial conditions

$$\varepsilon(0) = \varepsilon_0, \quad \dot{\varepsilon}(0) = \varepsilon_1, \quad D(0) = D_0$$

... resolve implicit relation for q

$\rightsquigarrow$

Evolutionary System

$$\rho\ddot{\varepsilon} + \nu\dot{\varepsilon} + c\varepsilon - \frac{e}{\kappa}(D - e\varepsilon - \mathcal{P}[q]) + f'(\varepsilon)\mathcal{U}[q] + \frac{1}{2}b'(\varepsilon)\mathcal{P}^2[q] = -\sigma_{imp},$$

$$\dot{D} + \frac{\alpha}{\kappa}(D - e\varepsilon - \mathcal{P}[q]) = 0,$$

$$q = \mathcal{W}[\varepsilon, D],$$

with initial conditions

$$\varepsilon(0) = \varepsilon_0, \quad \dot{\varepsilon}(0) = \varepsilon_1, \quad D(0) = D_0$$

Evolutionary System

$$\rho\ddot{\varepsilon} + \nu\dot{\varepsilon} + c\varepsilon - \frac{e}{\kappa}(D - e\varepsilon - \mathcal{P}[q]) + f'(\varepsilon)\mathcal{U}[q] + \frac{1}{2}b'(\varepsilon)\mathcal{P}^2[q] = -\sigma_{imp},$$
$$\dot{D} + \frac{\alpha}{\kappa}(D - e\varepsilon - \mathcal{P}[q]) = 0,$$
$$q = \mathcal{W}[\varepsilon, D],$$

with initial conditions

$$\varepsilon(0) = \varepsilon_0, \quad \dot{\varepsilon}(0) = \varepsilon_1, \quad D(0) = D_0$$

... rewrite as a first order system by setting
$v = \rho\dot{\varepsilon} + \nu\varepsilon$

Evolutionary System

$$\underbrace{\rho\ddot{\varepsilon} + \nu\dot{\varepsilon}}_{:=\dot{v}} + c\varepsilon - \frac{e}{\kappa}(D - e\varepsilon - \mathcal{P}[q]) + f'(\varepsilon)\mathcal{U}[q] + \frac{1}{2}b'(\varepsilon)\mathcal{P}^2[q] = -\sigma_{imp},$$

$$\dot{D} + \frac{\alpha}{\kappa}(D - e\varepsilon - \mathcal{P}[q]) = 0,$$

$$q = \mathcal{W}[\varepsilon, D],$$

with initial conditions

$$\varepsilon(0) = \varepsilon_0, \quad \dot{\varepsilon}(0) = \varepsilon_1, \quad D(0) = D_0$$

. . . rewrite as a first order system by setting

$v = \rho\dot{\varepsilon} + \nu\varepsilon \quad \Leftrightarrow \quad \dot{\varepsilon} = \frac{1}{\rho}(v - \nu\varepsilon)$

$\rightsquigarrow$

Evolutionary System

$$
\begin{aligned}
\dot{\varepsilon} &= \frac{1}{\rho}(v - \nu\varepsilon) \\
\dot{v} + c\varepsilon - \frac{e}{\kappa}(D - e\varepsilon - \mathcal{P}[q]) + f'(\varepsilon)\mathcal{U}[q] + \frac{1}{2}b'(\varepsilon)\mathcal{P}^2[q] &= -\sigma_{imp}, \\
\dot{D} + \frac{\alpha}{\kappa}(D - e\varepsilon - \mathcal{P}[q]) &= 0, \\
q &= \mathcal{W}[\varepsilon, D],
\end{aligned}
$$

with initial conditions

$$
\varepsilon(0) = \varepsilon_0, \quad v(0) = v_0, \quad D(0) = D_0
$$

Evolutionary System

$$\begin{aligned}
\dot{\varepsilon} &= \frac{1}{\rho}(v - \nu\varepsilon) \\
\dot{v} + c\varepsilon - \frac{e}{\kappa}(D - e\varepsilon - \mathcal{P}[q]) + f'(\varepsilon)\mathcal{U}[q] + \frac{1}{2}b'(\varepsilon)\mathcal{P}^2[q] &= -\sigma_{imp}, \\
\dot{D} + \frac{\alpha}{\kappa}(D - e\varepsilon - \mathcal{P}[q]) &= 0, \\
q &= \mathcal{W}[\varepsilon, D],
\end{aligned}$$

with initial conditions

$$\varepsilon(0) = \varepsilon_0, \quad v(0) = v_0, \quad D(0) = D_0$$

$\varepsilon, v, D \ldots$ state variables, $\quad q \ldots$ internal variable

optimization

Optimization Problem

maximize the total harvested energy in a given time interval $[0, T]$

$$\int_0^T P_{el}\,\mathrm{d}t = \int_0^T \phi\, i\,\mathrm{d}t = \frac{\alpha d}{\kappa^2}\int_0^T (D - e\varepsilon - \mathcal{P}[q])^2\,\mathrm{d}t\,.$$

where we have used

$$i = \frac{\phi}{R} = \frac{dE}{R} = \frac{\alpha}{\kappa}(D - e\varepsilon - \mathcal{P}[q])\,, \quad \phi = dE = \frac{d}{\kappa}(D - e\varepsilon - \mathcal{P}[q])$$

Optimization Problem

maximize the total harvested energy in a given time interval $[0, T]$

$$\int_0^T P_{el}\,\mathrm{d}t = \int_0^T \phi\, i\,\mathrm{d}t = \frac{\alpha d}{\kappa^2}\int_0^T (D - e\varepsilon - \mathcal{P}[q])^2\,\mathrm{d}t\,.$$

where we have used

$$i = \frac{\phi}{R} = \frac{dE}{R} = \frac{\alpha}{\kappa}(D - e\varepsilon - \mathcal{P}[q])\,, \quad \phi = dE = \frac{d}{\kappa}(D - e\varepsilon - \mathcal{P}[q])$$

$\nu, c, e, \kappa, f, b, \mathcal{P}, \mathcal{U}$ ... fixed material properties,

σ_{imp} ... given excitation,

$\rightsquigarrow \rho, \alpha, d$ as design variables.

Optimization Problem

maximize the total harvested energy in a given time interval $[0, T]$

$$\int_0^T P_{el}\,\mathrm{d}t = \int_0^T \phi\, i\,\mathrm{d}t = \frac{\alpha d}{\kappa^2}\int_0^T (D - e\varepsilon - \mathcal{P}[q])^2\,\mathrm{d}t\,.$$

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$$i = \tfrac{\phi}{R} = \tfrac{dE}{R} = \tfrac{\alpha}{\kappa}(D - e\varepsilon - \mathcal{P}[q])\,, \quad \phi = dE = \tfrac{d}{\kappa}(D - e\varepsilon - \mathcal{P}[q])$$

$\nu, c, e, \kappa, f, b, \mathcal{P}, \mathcal{U}$ ... fixed material properties,
σ_{imp} ... given excitation,
$\rightsquigarrow$ ρ, α, d as design variables.

$$\begin{cases} \max_{\varepsilon, v, D, q;\, \rho,\alpha\geq 0} \; J(v, \varepsilon, D, q, \rho, \alpha) \\ \text{s.t. } (\varepsilon, v, D, q) \text{ solves evolutionary system with parameters } \rho, \alpha \end{cases}$$

where

$$J(\varepsilon, v, D, q; \rho, \alpha) := \alpha \int_0^T \Big(D - e\varepsilon - \mathcal{P}[q]\Big)^2\,\mathrm{d}t\,.$$

Optimization Problem

$$\begin{cases} \max_{\varepsilon,v,D,q;\,\rho,\alpha\geq 0} \ \alpha \int_0^T \Big(D - e\varepsilon - \mathcal{P}[q]\Big)^2 \,\mathrm{d}t \\ \text{ s.t. } (\varepsilon, v, D, q) \text{ solves} \\ \qquad \dot{\varepsilon} = \frac{1}{\rho}(v - \nu\varepsilon) \\ \qquad \dot{v} + c\varepsilon - \frac{e}{\kappa}(D - e\varepsilon - \mathcal{P}[q]) + f'(\varepsilon)\mathcal{U}[q] + \frac{1}{2}b'(\varepsilon)\mathcal{P}^2[q] = -\sigma_{imp}, \\ \qquad \dot{D} + \frac{\alpha}{\kappa}(D - e\varepsilon - \mathcal{P}[q]) = 0, \\ \qquad q = \mathcal{W}[\varepsilon, D], \end{cases}$$

Optimization Problem

$$\begin{cases} \max_{\varepsilon,v,D,q;\,\rho,\alpha\geq 0} \ \alpha \int_0^T \Big(D - e\varepsilon - \mathcal{P}[q]\Big)^2 \,\mathrm{d}t \\ \text{ s.t. } (\varepsilon, v, D, q) \text{ solves} \\ \qquad \begin{aligned} \dot{\varepsilon} &= \tfrac{1}{\rho}(v - \nu\varepsilon) \\ \dot{v} + c\varepsilon - \tfrac{e}{\kappa}(D - e\varepsilon - \mathcal{P}[q]) + f'(\varepsilon)\mathcal{U}[q] + \tfrac{1}{2}b'(\varepsilon)\mathcal{P}^2[q] &= -\sigma_{imp}, \\ \dot{D} + \tfrac{\alpha}{\kappa}(D - e\varepsilon - \mathcal{P}[q]) &= 0, \\ q &= \mathcal{W}[\varepsilon, D], \end{aligned} \end{cases}$$

For the play operator

$$\mathcal{P}[q](t) = \lambda \mathfrak{p}_r[q](t) = \mathrm{w}(t)$$

we have

$$\mathcal{U}[q](t) = \frac{\lambda}{2}\mathrm{w}(t)^2$$

where

$$\dot{\mathrm{w}} \in \partial\delta_{[-r,r]}(u(t) - \mathrm{w}(t))$$

Optimization Problem

$$\begin{cases} \max_{\varepsilon,v,D,q;\,\rho,\alpha\geq 0} \;\alpha \int_0^T \Big(D - e\varepsilon - \mathcal{P}[q]\Big)^2 \,\mathrm{d}t \\ \text{ s.t. } (\varepsilon, v, D, q) \text{ solves} \\ \qquad \begin{aligned} \dot{\varepsilon} = \tfrac{1}{\rho}(v - \nu\varepsilon) & \\ \dot{v} + c\varepsilon - \tfrac{e}{\kappa}(D - e\varepsilon - \mathcal{P}[q]) + f'(\varepsilon)\mathcal{U}[q] + \tfrac{1}{2}b'(\varepsilon)\mathcal{P}^2[q] &= -\sigma_{imp}, \\ \dot{D} + \tfrac{\alpha}{\kappa}(D - e\varepsilon - \mathcal{P}[q]) &= 0, \\ q = \mathcal{W}[\varepsilon, D], & \end{aligned} \end{cases}$$

For the play operator

$$\mathcal{P}[q](t) = \lambda\mathfrak{p}_r[q](t) = \mathrm{w}(t)$$

we have

$$\mathcal{U}[q](t) = \frac{\lambda}{2}\mathrm{w}(t)^2 \text{ and } \mathcal{W}[\varepsilon, D] = A(\varepsilon, D) - \lambda B(\varepsilon)\mathrm{w}(t)$$

where

$$\dot{\mathrm{w}} \in \partial\delta_{[-r,r]}(u(t) - \mathrm{w}(t))$$

Optimization Problem in case of the Play Operator

$$
\begin{cases}
\max_{\varepsilon,v,D,\mathrm{w};\,\rho,\alpha\geq 0}\ \alpha\int_0^T\Big(D-e\varepsilon-\mathcal{P}[q]\Big)^2\,\mathrm{d}t \\
\text{ s.t. } (\varepsilon,v,D,\mathrm{w}) \text{ solves} \\
\qquad \begin{aligned} \dot\varepsilon = \tfrac{1}{\rho}(v-\nu\varepsilon) & \\ \dot v + c\varepsilon - \tfrac{e}{\kappa}(D-e\varepsilon-\lambda\mathrm{w}) + \tfrac{\lambda(f'(\varepsilon)+\lambda b'(\varepsilon))}{2}\,\mathrm{w}^2 &= -\sigma_{imp}, \\ \dot D + \tfrac{\alpha}{\kappa}(D-e\varepsilon-\lambda\mathrm{w}) &= 0 \\ \dot{\mathrm{w}} \in \partial\delta_{[-1,1]}\big(\tfrac{C(\varepsilon,D)-\mathrm{w}}{R(\varepsilon)}\big) & \end{aligned}
\end{cases}
$$

where $C(\varepsilon,D)=\frac{A(\varepsilon,D)}{1+\lambda B(\varepsilon)}$ and $R(\varepsilon)=\frac{r}{1+\kappa B(\varepsilon)}$

Optimization Problem in case of the Play Operator

$$
\begin{cases}
\max_{\varepsilon, v, D, \mathrm{w};\, \rho, \alpha \geq 0} \ \alpha \int_0^T \Big(D - e\varepsilon - \mathcal{P}[q] \Big)^2 \, \mathrm{d}t \\
\text{ s.t. } (\varepsilon, v, D, \mathrm{w}) \text{ solves} \\
\begin{aligned}
\dot{\varepsilon} = \tfrac{1}{\rho}(v - \nu\varepsilon) & \\
\dot{v} + c\varepsilon - \tfrac{e}{\kappa}(D - e\varepsilon - \lambda \mathrm{w}) + \tfrac{\lambda(f'(\varepsilon) + \lambda b'(\varepsilon))}{2} \mathrm{w}^2 & = -\sigma_{imp}, \\
\dot{D} + \tfrac{\alpha}{\kappa}(D - e\varepsilon - \lambda \mathrm{w}) & = 0 \\
\dot{\mathrm{w}} \in \partial \delta_{[-1,1]}\big(\tfrac{C(\varepsilon, D) - \mathrm{w}}{R(\varepsilon)} \big) &
\end{aligned}
\end{cases}
$$

where $C(\varepsilon, D) = \frac{A(\varepsilon, D)}{1 + \lambda B(\varepsilon)}$ and $R(\varepsilon) = \frac{r}{1 + \kappa B(\varepsilon)}$

. . . abbreviate

$y = \varepsilon, v, D$ . . . state,

$\theta = (\rho, \alpha)$ . . . parameters,

$a = \frac{C(\varepsilon, D) - \mathrm{w}}{R(\varepsilon)}$ . . . internal variable

$\rightsquigarrow$

General Optimization Problem

$$
\begin{cases}
\min_{y,a,\theta} \ \int_0^T L(t, y(t), a(t); \theta) \, \mathrm{d}t + j_0(\theta) =: \mathcal{J}(y, a, \theta) \\
\text{s.t. } (y, a) \text{ solves} \\
\qquad \dot{y}(t) = F(t, y(t), a(t); \theta) \,, \ t \in (0, T) \,, \quad y(0) = y_0 \,, \\
\dot{a}(t) + \partial\delta_{[-1,1]}(a(t)) \ni g(t, y(t), a(t); \theta) \,, \ t \in (0, T) \,, \quad a(0) = a_0 \,, \\
\qquad \theta \in \Theta \subseteq \mathbb{R}^k,
\end{cases}
$$

with given functions
$L : [0, T] \times \mathbb{R}^n \times \mathbb{R} \times \Theta \to \mathbb{R}^n$,
$F : [0, T] \times \mathbb{R}^n \times \mathbb{R} \times \Theta \to \mathbb{R}^n$,
$g : [0, T] \times \mathbb{R}^n \times \mathbb{R} \times \Theta \to \mathbb{R}$,
$j_0 : \Theta \to \mathbb{R}$,
$\Theta \subset \mathbb{R}^k$,
and given initial conditions
$y_0 \in \mathbb{R}^n$, $a_0 \in [-1, 1]$

General Optimization Problem

$$
\begin{cases}
\min_{y,a,\theta} \;\int_0^T L(t, y(t), a(t); \theta)\,\mathrm{d}t + j_0(\theta) =: \mathcal{J}(y, a, \theta) \\
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\qquad \dot{y}(t) = F(t, y(t), a(t); \theta)\,, \; t \in (0, T)\,, \quad y(0) = y_0\,, \\
\dot{a}(t) + \partial\delta_{[-1,1]}(a(t)) \ni g(t, y(t), a(t); \theta)\,, \; t \in (0, T)\,, \quad a(0) = a_0\,, \\
\qquad \theta \in \Theta \subseteq \mathbb{R}^k,
\end{cases}
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$j_0 : \Theta \to \mathbb{R}$,
$\Theta \subset \mathbb{R}^k$,
and given initial conditions
$y_0 \in \mathbb{R}^n$, $a_0 \in [-1, 1]$

challenges:

- evolutionary system as a constraint $\Rightarrow$ infinite dimensional optimization problem

General Optimization Problem

$$
\begin{cases}
\min_{y,a,\theta} \int_0^T L(t, y(t), a(t); \theta)\, \mathrm{d}t + j_0(\theta) =: \mathcal{J}(y, a, \theta) \\
\text{s.t. } (y, a) \text{ solves} \\
\qquad \dot{y}(t) = F(t, y(t), a(t); \theta)\,, \quad t \in (0, T)\,, \quad y(0) = y_0\,, \\
\dot{a}(t) + \partial\delta_{[-1,1]}(a(t)) \ni g(t, y(t), a(t); \theta)\,, \quad t \in (0, T)\,, \quad a(0) = a_0\,, \\
\qquad \theta \in \Theta \subseteq \mathbb{R}^k,
\end{cases}
$$

with given functions
$L : [0, T] \times \mathbb{R}^n \times \mathbb{R} \times \Theta \to \mathbb{R}^n$,
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and given initial conditions
$y_0 \in \mathbb{R}^n$, $a_0 \in [-1, 1]$

challenges:

- evolutionary system as a constraint $\Rightarrow$ infinite dimensional optimization problem
- nonsmoothness due to indicator function $\delta_{[-1,1]}$

General Optimization Problem

$$\begin{cases} \min_{y,a,\theta} \int_0^T L(t, y(t), a(t); \theta)\, \mathrm{d}t + j_0(\theta) =: \mathcal{J}(y, a, \theta) \\ \text{s.t. } (y, a) \text{ solves} \\ \qquad \dot{y}(t) = F(t, y(t), a(t); \theta), \; t \in (0, T), \quad y(0) = y_0, \\ \dot{a}(t) + \partial\delta_{[-1,1]}(a(t)) \ni g(t, y(t), a(t); \theta), \; t \in (0, T), \quad a(0) = a_0, \\ \qquad \theta \in \Theta \subseteq \mathbb{R}^k, \end{cases}$$

with given functions
$L : [0, T] \times \mathbb{R}^n \times \mathbb{R} \times \Theta \to \mathbb{R}^n$,
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$g : [0, T] \times \mathbb{R}^n \times \mathbb{R} \times \Theta \to \mathbb{R}$,
$j_0 : \Theta \to \mathbb{R}$,
$\Theta \subset \mathbb{R}^k$,
and given initial conditions
$y_0 \in \mathbb{R}^n$, $a_0 \in [-1, 1]$

challenges:

- evolutionary system as a constraint $\Rightarrow$ infinite dimensional optimization problem
- nonsmoothness due to indicator function $\delta_{[-1,1]}$
- gradient computation?

gradient computation

General Optimization Problem: The smooth case

$$
\begin{cases}
\min_{y,\theta} \; \int_0^T L(t, y(t); \theta) \,\mathrm{d}t + j_0(\theta) =: \mathcal{J}(y, \theta) \\
\text{s.t.} \; \begin{cases} y \text{ solves } \dot{y}(t) = F(t, y(t); \theta)\,, \; t \in (0, T)\,, \quad y(0) = y_0\,, \\ \theta \in \Theta \subseteq \mathbb{R}^k, \end{cases}
\end{cases}
$$

with given functions
$L : [0, T] \times \mathbb{R}^n \times \Theta \to \mathbb{R}^n$,
$F : [0, T] \times \mathbb{R}^n \times \Theta \to \mathbb{R}^n$,
$\Theta \subset \mathbb{R}^k$,
and given initial conditions
$y_0 \in \mathbb{R}^n$

General Optimization Problem: The smooth case

$$\begin{cases} \min_{y,\theta} \ \int_0^T L(t, y(t); \theta) \, \mathrm{d}t + j_0(\theta) =: \mathcal{J}(y, \theta) \\ \text{s.t.} \ \begin{cases} y \text{ solves } \dot{y}(t) = F(t, y(t); \theta)\,, \ t \in (0, T)\,, \quad y(0) = y_0\,, \\ \theta \in \Theta \subseteq \mathbb{R}^k, \end{cases} \end{cases}$$

General Optimization Problem: The smooth case

$$\begin{cases} \min_{y,\theta} \int_0^T L(t, y(t); \theta)\, \mathrm{d}t + j_0(\theta) =: \mathcal{J}(y, \theta) \\ \text{s.t.} \begin{cases} y \text{ solves } \dot{y}(t) = F(t, y(t); \theta)\,, \; t \in (0, T)\,, \quad y(0) = y_0\,, \\ \theta \in \Theta \subseteq \mathbb{R}^k, \end{cases} \end{cases}$$

is equivalent to the reduced formulation

$$\min_{\theta \in \Theta} j(\theta)$$

with

$$j(\theta) = \mathcal{J}(y^\theta, \theta)\,, \qquad \dot{y}^\theta(t) = F(t, y^\theta(t); \theta)\,, \; t \in (0, T)\,, \; y^\theta(0) = y_0$$

General Optimization Problem: The smooth case

$$\begin{cases} \min_{y,\theta} \int_0^T L(t, y(t); \theta) \, \mathrm{d}t + j_0(\theta) =: \mathcal{J}(y, \theta) \\ \text{s.t.} \begin{cases} y \text{ solves } \dot{y}(t) = F(t, y(t); \theta), \; t \in (0, T), \quad y(0) = y_0, \\ \theta \in \Theta \subseteq \mathbb{R}^k, \end{cases} \end{cases}$$

is equivalent to the reduced formulation

$$\min_{\theta \in \Theta} j(\theta)$$

with

$$j(\theta) = \mathcal{J}(y^\theta, \theta), \qquad \dot{y}^\theta(t) = F(t, y^\theta(t); \theta), \; t \in (0, T), \; y^\theta(0) = y_0$$

. . . computation of gradient (e.g., for numerical optimization)

$\rightsquigarrow$

Gradient computation via sensitivities

$$\min_{\theta \in \Theta \subseteq \mathbb{R}^k} j(\theta)$$

with

$$j(\theta) = \mathcal{J}(y^\theta, \theta)\,, \qquad \dot{y}^\theta(t) = F(t, y^\theta(t); \theta)\,,\ t \in (0, T)\,,\ y^\theta(0) = y_0$$

Gradient computation via sensitivities

$$\min_{\theta\in\Theta\subseteq\mathbb{R}^k} j(\theta)$$

with

$$j(\theta) = \mathcal{J}(y^\theta, \theta)\,, \qquad \dot{y}^\theta(t) = F(t, y^\theta(t); \theta)\,,\ t \in (0, T)\,,\ y^\theta(0) = y_0$$

gradient of j

$$\frac{\partial j}{\partial \theta_i}(\theta) = \int_0^T \Big(\partial_{\theta_i} L(t, y(t); \theta) + \partial_y L(t, y(t); \theta) Y_i(t)\Big)\, \mathrm{d}t + \partial_{\theta_i} j_0(\theta)$$

where for each $i \in \{1, \dots, k\}$, Y_i solves the sensitivity equation

$$\dot{Y}_i(t) = \partial_y F(t, y(t); \theta) Y_i(t) + \partial_{\theta_i} F(t, y(t); \theta)\,,\ t \in (0, T)\,, \qquad Y(0) = 0$$

Gradient computation via sensitivities

$$\min_{\theta \in \Theta \subseteq \mathbb{R}^k} j(\theta)$$

with

$$j(\theta) = \mathcal{J}(y^\theta, \theta), \qquad \dot{y}^\theta(t) = F(t, y^\theta(t); \theta), \; t \in (0, T), \; y^\theta(0) = y_0$$

gradient of j

$$\frac{\partial j}{\partial \theta_i}(\theta) = \int_0^T \Big(\partial_{\theta_i} L(t, y(t); \theta) + \partial_y L(t, y(t); \theta) Y_i(t) \Big) \, \mathrm{d}t + \partial_{\theta_i} j_0(\theta)$$

where for each $i \in \{1, \dots, k\}$, Y_i solves the sensitivity equation

$$\dot{Y}_i(t) = \partial_y F(t, y(t); \theta) Y_i(t) + \partial_{\theta_i} F(t, y(t); \theta), \; t \in (0, T), \qquad Y(0) = 0$$

Gradient computation via adjoint equation

$$\min_{\theta \in \Theta} j(\theta)$$

with

$$j(\theta) = \mathcal{J}(y^\theta, \theta)\,, \qquad \dot{y}^\theta(t) = F(t, y^\theta(t); \theta)\,,\ t \in (0, T)\,,\ y^\theta(0) = y_0$$

Gradient computation via adjoint equation

$$\min_{\theta \in \Theta} j(\theta)$$

with

$$j(\theta) = \mathcal{J}(y^\theta, \theta)\,, \qquad \dot{y}^\theta(t) = F(t, y^\theta(t); \theta)\,,\ t \in (0, T)\,,\ y^\theta(0) = y_0$$

gradient of j (e.g., for numerical optimization)

$$\frac{\partial j}{\partial \theta_i}(\theta) = \int_0^T \Big(\partial_{\theta_i} L(t, y(t); \theta) - \partial_{\theta_i} F(t, y(t); \theta)^T P(t) \Big) \,\mathrm{d}t + \partial_{\theta_i} j_0(\theta)$$

where P solves the adjoint equation

$$-\dot{P}(t) = \partial_y F(t, y(t); \theta)^T P(t) - \partial_y L(t, y(t); \theta)\,,\ t \in (0, T)\,, \quad P(T) = 0$$

Lagrange functional:

$$\mathcal{L}(y, p, \theta) = \int_0^T L(t, y(t); \theta) \,\mathrm{d}t + j_0(\theta) + \int_0^T \Big(\dot{y}(t) - F(t, y(t); \theta) \Big) p(t) \,\mathrm{d}t$$

General Optimization Problem

$$
\begin{cases}
\min_{y,a,\theta} \int_0^T L(t,y(t),a(t);\theta)\,\mathrm{d}t + j_0(\theta) =: \mathcal{J}(y,a,\theta) \\
\text{s.t. } (y,a) \text{ solves} \\
\dot{y}(t) = F(t,y(t),a(t);\theta)\,,\ t \in (0,T)\,, \quad y(0) = y_0\,, \\
\dot{a}(t) + \partial\delta_{[-1,1]}(a(t)) \ni g(t,y(t),a(t);\theta)\,,\ t \in (0,T)\,, \quad a(0) = a_0\,, \\
\theta \in \Theta \subseteq \mathbb{R}^k,
\end{cases}
$$

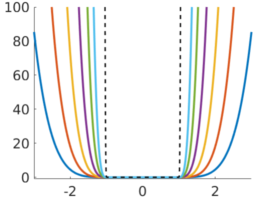
with given functions
$L : [0,T] \times \mathbb{R}^n \times \mathbb{R} \times \Theta \to \mathbb{R}^n$,
$F : [0,T] \times \mathbb{R}^n \times \mathbb{R} \times \Theta \to \mathbb{R}^n$,
$g : [0,T] \times \mathbb{R}^n \times \mathbb{R} \times \Theta \to \mathbb{R}$,
$j_0 : \Theta \to \mathbb{R}$,
$\Theta \subset \mathbb{R}^k$,
and given initial conditions
$y_0 \in \mathbb{R}^n$, $a_0 \in [-1,1]$

General Optimization Problem

$$\begin{cases} \min_{y,a,\theta} \int_0^T L(t,y(t),a(t);\theta)\,\mathrm{d}t + j_0(\theta) =: \mathcal{J}(y,a,\theta) \\ \text{s.t. } (y,a) \text{ solves} \\ \qquad \dot{y}(t) = F(t,y(t),a(t);\theta)\,,\ t\in(0,T)\,, \quad y(0)=y_0\,, \\ \dot{a}(t) + \partial\delta_{[-1,1]}(a(t)) \ni g(t,y(t),a(t);\theta)\,,\ t\in(0,T)\,, \quad a(0)=a_0\,, \\ \qquad \theta\in\Theta\subseteq\mathbb{R}^k, \end{cases}$$

with given functions
$L : [0,T]\times\mathbb{R}^n\times\mathbb{R}\times\Theta\to\mathbb{R}^n$,
$F : [0,T]\times\mathbb{R}^n\times\mathbb{R}\times\Theta\to\mathbb{R}^n$,
$g : [0,T]\times\mathbb{R}^n\times\mathbb{R}\times\Theta\to\mathbb{R}$,
$j_0 : \Theta\to\mathbb{R}$,
$\Theta\subset\mathbb{R}^k$,
and given initial conditions
$y_0\in\mathbb{R}^n$, $a_0\in[-1,1]$

- approximate $\delta_{[-1,1]}(x)$ by $\frac{1}{6\gamma}\max\{(x^2-1),0\}^3$



- take limit as $\gamma\to 0$

General Optimization Problem: Gradient computation

$$\begin{cases} \min_{y,a,\theta} \int_0^T L(t, y(t), a(t); \theta)\, \mathrm{d}t + j_0(\theta) =: \mathcal{J}(y, a, \theta) \\ \text{s.t. } (y, a) \text{ solves} \\ \qquad \dot{y}(t) = F(t, y(t), a(t); \theta)\,, \quad t \in (0, T)\,, \quad y(0) = y_0\,, \\ \dot{a}(t) + \partial\delta_{[-1,1]}(a(t)) \ni g(t, y(t), a(t); \theta)\,, \quad t \in (0, T)\,, \quad a(0) = a_0\,, \\ \qquad \theta \in \Theta \subseteq \mathbb{R}^k, \end{cases}$$

$$\partial_{\theta_i} j(\theta) = \int_0^T \Big(\partial_{\theta_i} L(t, y^\theta, a^\theta; \theta) - \partial_{\theta_i} F(t, y^\theta, a^\theta; \theta) \cdot p^\theta - \partial_{\theta_i} g(t, y^\theta, a^\theta; \theta) q^\theta \Big)(t)\, \mathrm{d}t + \partial_{\theta_i} j_0(\theta).$$

where

$$- \dot{p}^\theta(t) = \partial_y F(t, y^\theta(t), a^\theta(t); \theta) \cdot p^\theta(t) + \partial_y g(t, y^\theta(t), a^\theta(t); \theta)\, q^\theta(t)$$
$$\qquad - \partial_y L(t, y^\theta(t), a^\theta(t); \theta) \quad \text{for} \quad t \in (0, T), \qquad p^\theta(T) = 0,$$
$$- \dot{q}^\theta(t) = \partial_a g(t, y^\theta(t), a^\theta(t); \theta)\, q^\theta(t) + \partial_a F(t, y^\theta(t), a^\theta(t); \theta) \cdot p^\theta(t)$$
$$\qquad - \partial_a L(t, y^\theta(t), a^\theta(t); \theta) \quad \text{for a. e.} \quad t \in \{s \in (0, T) : |a^\theta(s)| < 1\}, \qquad q^\theta(T) = 0,$$
$$q^\theta(t)\, g(t, y^\theta(t), a^\theta(t); \theta) = 0 \quad \text{for a. e.} \quad t \in \{s \in (0, T) : |a^\theta(s)| = 1\}.$$

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- so far only uniaxial case
  $\rightsquigarrow$ extend by replacing $[-1, 1]$ in $\delta_{[-1,1]}$ by a higher dimensional convex set, see [Brokate& Krejčí, DCDS 2013] for an optimal control problem

Thank you for your attention!