On Life-Cycle-Optimisation Problems in Materials and Deep Neural Network Approach

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Kick-Off Workshop WG 2
Machine Learning for Control Theory,
5 December, 2025

Formal Definition

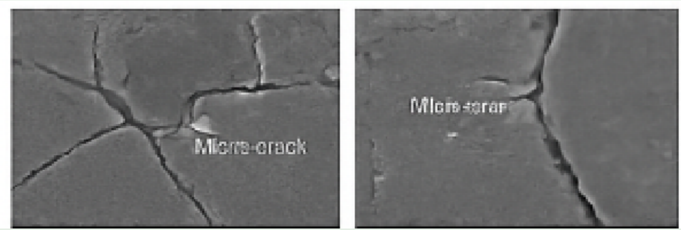
Life cycle optimization typically refers to the integration of objectives calculated using a life-cycle based framework into mathematical optimization problems.

- I. Turner, N. Bamber, J. Andrews, N. Pelletier. *Systematic review of the life cycle optimization literature, and recommendations for performance of life cycle optimization studies*, *Renewable and Sustainable Energy Reviews*, **208** (2025), Id. 115058.

Motivation

Life cycle in materials

Due to corrosion, radiation, external forces, or even age, the life cycle of materials or some their parts may weaken. As a result, some multi-micro cracks, cavities, and other internal damages can appear inside of an elastic body.



Problem 1. How to infer the current state of such objects?

F.N. Airaudo, R. Löhner, R. Wüchner, H. Antil. *Adjoint-based Determination of Weaknesses in Structures*, arXiv:2303.15329, 2023.

Modeling of damage in elastic bodies

Monographs

- M. Fremond, Non-smooth Thermomechanics, Springer, Berlin, 2002.
- M. Shillor, M. Sofonea, J.J. Telega, Models and Analysis of Quasistatic Contact, Lecture Notes in Physics 655, Springer, Berlin, 2004.

The main idea

To model the material damage they propose to use a scalar damage field $\zeta = \zeta(t, x)$ as an internal variable which measures the fractional decrease in the stress-strain response.

(i) When $\zeta = 1$ the material is damage-free;

(ii) When $\zeta = 0$ the material is completely damaged;

(iii) When $0 < \zeta < 1$ the material is partially damaged.

The model for a control process in materials with damage evolution

Mainly following the motivation in Kuttler, we dwell on the following model for the control process:

$$-\operatorname{div}\boldsymbol{\sigma} = \mathbf{f} \quad \text{in} \quad \Omega_T = (0,T)\times\Omega, \tag{1}$$

$$\boldsymbol{\sigma} = \zeta A\mathbf{e}(\mathbf{u}) \quad \text{in} \quad \Omega_T, \tag{2}$$

$$\mathbf{u} = 0 \quad \text{on} \quad (0,T)\times\partial\Omega, \tag{3}$$

$$\zeta' - \kappa\Delta\zeta = \phi(\mathbf{e}(\mathbf{u}),\zeta) \quad \text{in} \quad \Omega_T, \tag{4}$$

$$\zeta(0,\cdot) = \zeta_0 \quad \text{in} \quad \Omega, \tag{5}$$

$$\zeta = 1 \quad \text{on } (0,T)\times\partial\Omega, \tag{6}$$

$$\zeta_* \le \zeta(t,x) \le 1 \quad \text{a.e. in} \quad \Omega_T. \tag{7}$$

where the damage source term $\phi : \Omega\times\mathbb{S}^N\times\mathbb{R}$ satisfies some Lipschitz continuity property and is such that whenever $\zeta > 1$, $\phi(\mathbf{e}(\mathbf{u}),\zeta) \le 0$, and $\zeta_* : \Omega \to [0,1]$ be a given $L^1(\Omega)$-function satisfying

$$\zeta_*^{-1} \in L^1(\Omega), \quad \zeta_*^{-1} \notin L^\infty(\Omega). \tag{8}$$

Solvability Issues

Functional Spaces

- To each $\zeta(t,x)$ we associate the space $W_\zeta(\Omega_T)$ as the set of vector-functions $\mathbf{u}$ for which

$$\|\mathbf{u}\|_\zeta = \Big(\int_0^T \int_\Omega \left(\mathbf{u}^2 + \mathbf{e}^2(\mathbf{u})\zeta\right) dxdt\Big)^{1/2} < \infty. \qquad (9)$$

- For the typical choice of the damage source function

$$\phi(\mathbf{e}(\mathbf{u}),\zeta) = -\lambda_D \left(\frac{1-\zeta}{\zeta}\right) - \frac{1}{2}\lambda_u \mathbf{e}(\mathbf{u})\cdot\mathbf{e}(\mathbf{u}) + \lambda_w,$$

we set $\mathcal{W} = \left\{\zeta \ : \ \zeta \in \mathcal{Z}, \quad \frac{\partial\zeta}{\partial t} \in \mathcal{Z}'\right\}$, where
$\mathcal{Z} = L^2(0,T; W^{1,q}(\Omega))$ for $q < \frac{N}{N-1}$,

Characteristic Features of the Proposed Model

1. The Dirichlet problem for the degenerate elasticity system

$$-\mathrm{div}\,(\zeta A\mathbf{e}(\mathbf{u})) = \mathbf{f} \quad \text{in} \quad \Omega_T,\ \mathbf{u} = 0 \quad \text{on} \quad (0,T)\times\partial\Omega. \tag{10}$$

   is ill-posed even if ζ belongs to the Mackenhoupt class A_2.

2. For some damage field $\zeta(t,x)$ the BVP (10) can exhibit non-uniqueness of weak solutions, the Lavrentieff phenomenon, and other surprising consequences.

3. The initial-boundary value problem for the damage field

$$\zeta' - \kappa\Delta\zeta = \phi(\mathbf{e}(\mathbf{u}),\zeta),\ \zeta(0,\cdot) = \zeta_0, \ \ \zeta = 1 \quad \text{on } (0,T)\times\partial\Omega,$$

   can admit nonuniqueness for distributional solutions.

Open Questions.

Portion 1.

1. Develop the consept of approximating solutions to the elasticity system with damage evolution;
2. Establish the existence and uniqueness of the weak solutions via approximation for the L^1-damage source function

$$\phi(\mathbf{e}(\mathbf{u}), \zeta) = -\lambda_D \left(\frac{1-\zeta}{\zeta} \right) - \frac{1}{2} \lambda_u \mathbf{e}(\mathbf{u}) \cdot \mathbf{e}(\mathbf{u}) + \lambda_w;$$

3. Study the existence of weak solutions to the origonal problem using the following relaxed version of the first equation

$$-\mathrm{div}\ (\zeta A \mathbf{e}(\mathbf{u})) + \varepsilon \mathbf{u} = \mathbf{f} \quad \text{in} \quad \Omega_T;$$

4. Find out whether the strain tensor $\mathbf{e}(\mathbf{u}) = \{\mathbf{e}_{ij}(\mathbf{u})\}$ with

$$\mathbf{e}_{ij}(\mathbf{u}) = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right), \quad \forall\, i,j = 1, \dots, N.$$

possesses the high integrability property, $|\mathbf{e}(\mathbf{u})| \in L^{2(1+\delta)}$ for some $\delta > 0$.

Intuitive Definition of Sustainable Controls

We say that a control (external force) $\mathbf{f} \in L^2\big(0, T; L^2(\Omega)^N\big)$ is sustaible for the elasticity system

$$-\operatorname{div} \boldsymbol{\sigma} = \mathbf{f} \quad \text{in} \quad \Omega_T = (0, T) \times \Omega, \tag{11}$$

$$\boldsymbol{\sigma} = \zeta A \mathbf{e}(\mathbf{u}) \quad \text{in} \quad \Omega_T, \tag{12}$$

$$\mathbf{u} = 0 \quad \text{on} \quad (0, T) \times \partial\Omega, \tag{13}$$

$$\zeta' - \kappa \Delta \zeta = \phi(\mathbf{e}(\mathbf{u}), \zeta) \quad \text{in} \quad \Omega_T, \tag{14}$$

$$\zeta(0, \cdot) = \zeta_0 \quad \text{in} \quad \Omega, \tag{15}$$

$$\zeta = 1 \quad \text{on } (0, T) \times \partial\Omega, \tag{16}$$

$$\zeta_* \leq \zeta(t, x) \leq 1 \quad \text{a.e. in} \quad \Omega_T, \tag{17}$$

if allows to achieve the following two goals:

- it optimizes a desired performance index, say, a tracking a profile;
- it reduces potential internal damage.

The question is how to describe this sort of controls formally.

Possible Statements of Optimization Problems Leading to Sustainable Controls

Variants of the Objective Functionals

$$J_1(\mathbf{f},\mathbf{u},\zeta) = \int_0^T\int_\Omega |\mathbf{u}-\mathbf{u}_d|^2_{\mathbb{R}^N}\,dxdt + \int_0^T\int_\Omega |\zeta - 1|\,dxdt + \int_0^T\int_\Omega \|\mathbf{e}(\mathbf{u})\|^2_{\mathbb{S}^N}\zeta\,dxdt; \quad (18)$$

$$J_2(\mathbf{f},\mathbf{u},\zeta) = \int_0^T\int_\Omega |\mathbf{u}-\mathbf{u}_d|^2_{\mathbb{R}^N}\,dxdt + \int_0^T\int_\Omega |\nabla\zeta|\,dxdt + \int_0^T\int_\Omega \frac{1}{\zeta}\,dxdt + \int_0^T\int_\Omega \|\mathbf{e}(\mathbf{u})\|^2_{\mathbb{S}^N}\zeta\,dxdt; \quad (19)$$

where $\mathbf{f}$ belongs to a weakly compact subset $\mathcal{F}_{ad} \subset L^2(\Omega;\mathbb{R}^N)$.

Characteristic Features of the Optimal Control Problems

1. Undes some special assumptions on the damage source function $\phi = \phi(\mathbf{e}(\mathbf{u}), \zeta)$, the optimization problems on the class of sustainable controls are well-posed whereas the corresponding elasticity system with demage evolution is ill-posed;
2. There are no appropriate a priori estimates for the weak solutions $(\mathbf{u}, \zeta) = (\mathbf{u}(\mathbf{f}, \zeta), \zeta(\mathbf{f}, \mathbf{u}))$ of the degenerate elasticity system;
3. For different admissible controls $\mathbf{f} \in \mathcal{F}_{ad}$ and, therefore, for different admissible damage fields $\zeta : \Omega_T \to [0, 1]$, the corresponding admissible solutions $(\mathbf{f}, \zeta, \mathbf{u})$ of the optimal control problem belong to different weighted spaces.

Open Questions.

Portion 2.

1. Establish the existence of an optimal control provided the damage source function takes the form

$$\phi(\mathbf{e}(\mathbf{u}), \zeta) = -\lambda_D \left(\frac{1-\zeta}{\zeta} \right) - \frac{1}{2} \lambda_u \mathbf{e}(\mathbf{u}) \cdot \mathbf{e}(\mathbf{u}) + \lambda_w;$$

2. Find out whether sustable controls can be attained in the limit as $\varepsilon \to 0$ using the following relaxed version of the first equation

$$-\mathrm{div}\, \left((\zeta)_\varepsilon A \mathbf{e}(\mathbf{u}) \right) = \mathbf{f} \quad \text{in} \quad \Omega_T,$$

where $(\cdot)_\varepsilon$ stands for the Steklov smoothing operator.

3. It is unknown whether there exists a control $\mathbf{f} \in \mathcal{F}_{ad}$ such that the corresponding solutions $(\zeta, \mathbf{u})$ satisfy the equations

$$-\mathrm{div}\, \left(\zeta A \mathbf{e}(\mathbf{u}) \right) = \mathbf{f},$$
$$\zeta' - \kappa \Delta \zeta = \phi(\mathbf{e}(\mathbf{u}), \zeta)$$

in the sense of $L^2(Q_T)$.

Primary Goal

Simplified Version of the Original System

For the coupled system

$$-\operatorname{div}(\zeta\nabla u) = f \quad \text{in} \quad \Omega_T = (0,T)\times\Omega, \tag{20}$$

$$u = 0 \quad \text{on} \quad (0,T)\times\partial\Omega, \tag{21}$$

$$\zeta' - \kappa\Delta\zeta = \phi(\nabla u, \zeta) \quad \text{in} \quad \Omega_T, \tag{22}$$

$$\zeta(0,\cdot) = \zeta_0 \quad \text{in} \quad \Omega, \quad \zeta = 1 \quad \text{on } (0,T)\times\partial\Omega, \tag{23}$$

$$\zeta_* \le \zeta(t,x) \le 1 \quad \text{a.e. in} \quad \Omega_T, \tag{24}$$

the goal is to approximate the solution operator Ψ, which maps (f, ζ_0) to the weak solution (ζ, u) of (20)–(24), by a neural-network–based functional Ψ_θ with trainable parameters θ:

$$\Psi_\theta \approx \Psi : (f, \zeta_0) \mapsto (\zeta, u).$$

Assumption 1
For the source damage function

$$\phi(\nabla u, \zeta) = -\lambda_D \left(\frac{1-\zeta}{\zeta} \right) - \frac{1}{2} \lambda_u \left| \nabla u \right|^2_{\mathbb{R}^N} + \lambda_w;$$

and for given $f \in L^2(\Omega)$ **and** $\zeta_0 \in C^2(\overline{\Omega})$**, there exists a pair** (u, ζ) **such that**

$$u \in C([0,T]; W^{2,2}(\Omega) \cap W_0^{1,2}(\Omega)), \quad 1-\zeta \in C([0,T]; C_0(\overline{\Omega})),$$
$$\zeta_*(x) \le \zeta(t,x) \le 1 \quad \textbf{in} \quad \Omega_T,$$

and

$$-\mathrm{div}\,(\zeta \nabla u) = f \quad \textbf{a.e. in} \quad \Omega_T = (0,T) \times \Omega,$$
$$\zeta(t) = T(t)\zeta_0 + \int_0^t T(t-s)\phi(\nabla u(s), \zeta(s))\, ds, \ \forall\, t \in [0,T],$$

where $T(t)$ **is a** C_0**-semigroup of contractions generated by the Laplacian** $\kappa\Delta$ **in** $C(\overline{\Omega})$**.**

On the Structure of the Neural Network

We propose to consider NNs with a single hidden layer and M hidden units of the class

$$W^M = \left\{ w(t,x) : \mathbb{R}^{N+1} \,\middle|\, w(t,x) = \sum_{i=1}^{M} \alpha_i \sigma \left(\theta_{0,i} t + \sum_{j=1}^{N} \theta_{j,i} x_j + c_i \right) \right\},$$

where σ is a nonlinear bounded smooth activation function, and $\theta^w = \{\alpha_i, \theta_{i,j}, c_i\} \in \mathbb{R}^K$, with $K = M(N+3)$, are the NN's parameters. Setting

$$W = \bigcup_{M \geq 1} W^M,$$

we have the following result:
Theorem. [Hornik, 19991] For every $\varepsilon > 0$ and $\varphi \in C^{1,2}([0,T] \times \overline{\Omega})$ there exists $v \in W$ such that

$$\|\varphi - v\|_{C^{1,2}([0,T]\times\overline{\Omega})} < \varepsilon.$$

The Main Idea of ML Approach

Our main goal is to minimize the following objective functional:

$$\begin{aligned} J(\theta^v, \theta^\xi) = J(v, \xi) &= \|\mathrm{div}\,(\xi \nabla v) + f\|^2_{L^2(\Omega_T)} \\ &+ \|\xi' - \kappa \Delta \xi - \phi(\nabla v, \xi)\|^2_{L^2(\Omega_T)} \\ &+ \|v\|^2_{L^2(0,T;\partial\Omega)} + \|1 - \xi\|^2_{L^2(0,T;\partial\Omega)} \\ &+ \|\xi(0,\cdot) - \zeta_0\|^2_{L2(\Omega)} \Longrightarrow \inf_{v,w \in W^M} . \end{aligned} \tag{25}$$

Open Questions and Expected Results

Portion 1

- Find out whether the existence of the mild solutions to the original system in the sense of Assumption 1 implies the high integrability property of ∇u such that $\phi(\nabla v, \xi) \in L^2(\Omega_T)$.
- Can we assert that, for each $u \in L^2(0, T; W_0^{1,2}(\Omega))$, $\zeta(t, x)$ is a mild solution to

$$\zeta' - \kappa \Delta \zeta = \phi(\nabla u, \zeta) \quad \text{in} \quad \Omega_T,$$
$$\zeta(0, \cdot) = \zeta_0 \quad \text{in} \quad \Omega, \quad \zeta = 1 \quad \text{on } (0, T) \times \partial\Omega$$

  if and only is $\zeta(t, x)$ is a unique duality solution (via approximation of $\phi(\nabla u, \zeta)$ by L^∞-functions)?

Open Questions and Expected Results

Portion 2

- Find out whether there exists an approximation $\{\phi_k\}_{k\in\mathbb{N}} \subset C([0,T]\times\overline{\Omega})$ of

$$\phi(\nabla u, \zeta) = -\lambda_D\left(\frac{1-\zeta}{\zeta}\right) - \frac{1}{2}\lambda_u \left|\nabla u\right|^2_{\mathbb{R}^N} + \lambda_w$$

and elements $(v^M, \xi^M) \in W \times W$ such that

$$J_M(v^M, \xi^M) \to 0 \quad \text{as} \quad M \to \infty, \tag{26}$$

where

$$\begin{aligned} J_M(v,\xi) = {} & \|\mathrm{div}\,(\xi\nabla v) + f\|^2_{L^2(\Omega_T)} \\ & + \|\xi' - \kappa\Delta\xi - \phi_M(\nabla v, \xi)\|^2_{L^2(\Omega_T)} \\ & + \|v\|^2_{L^2(0,T;\partial\Omega)} + \|1-\xi\|^2_{L^2(0,T;\partial\Omega)} \\ & + \|\xi(0,\cdot) - \zeta_0\|^2_{L2(\Omega)}. \end{aligned} \tag{27}$$

Open Questions and Expected Results

Portion 3

- Can we assert that if a sequence $\left\{(v^M, \xi^M)\right\}_{M=1}^{\infty}$ satisfies property

$$J_M(v^M, \xi^M) \to 0 \quad \text{as} \quad M \to \infty, \tag{28}$$

then

$$(v^M, \xi^M) \to (u, \zeta) \quad \text{in} \quad L^2(\Omega_T),$$

where (u, ζ) is a mild solution to the problem

$$-\operatorname{div}(\zeta \nabla u) = f \quad \text{in} \quad \Omega_T = (0,T) \times \Omega, \tag{29}$$

$$u = 0 \quad \text{on} \quad (0,T) \times \partial\Omega, \tag{30}$$

$$\zeta' - \kappa \Delta \zeta = \phi(\nabla u, \zeta) \quad \text{in} \quad \Omega_T, \tag{31}$$

$$\zeta(0,\cdot) = \zeta_0 \quad \text{in} \quad \Omega, \quad \zeta = 1 \quad \text{on } (0,T) \times \partial\Omega, \tag{32}$$

$$\zeta_* \le \zeta(t,x) \le 1 \quad \text{a.e. in} \quad \Omega_T, \tag{33}$$

in the sense of Assumption 1?

That's All!! Thank you for your attention

HAVE A NICE DAY