COMPUTATIONAL APPROACHES TO RATE-INDEPENDENT PROCESSES

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with computational contributions by
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Introduction, rate-independent processes, discretization.
- General ansatz.
- Definition of energic solution.
- Approximate solution.
- Two-sided approximate energy balance

Convergence analysis outlined
- Assumptions
- Convergence.
- Further developments: stability through Γ-convergence
- Numerics conceptually

Some applications outlined
- Plasticity with hardening
- Damage
- Delamination/debonding.
- Shape-memory alloys

Beyond rate independency

Quasistatic rate-independent processes:

$$\partial_u \mathcal{E}(t, u, z) = 0, \tag{1a}$$

$$\partial_{\frac{\mathrm{d}z}{\mathrm{d}t}} \mathcal{R}\Big(z, \frac{\mathrm{d}z}{\mathrm{d}t}\Big) + \partial_z \mathcal{E}(t, u, z) \ni 0. \tag{1b}$$

with
$u \in \mathcal{U}$ a "fast" variable,
$z \in \mathcal{Z}$ an "slow" variable with activated evolution,
$\mathcal{E} : [0, T] \times \mathcal{U} \times \mathcal{Z} \to \mathbb{R} \cup \{\infty\}$ the stored energy,
$\mathcal{R} : \mathcal{Z} \times \mathcal{Z} \to \mathbb{R} \cup \{\infty\}$ the dissipation pseudopotential
$\mathcal{R}(z, \cdot)$ (positively) homogeneous degree-1

Functional-analytical ansatz: $\mathcal{U}$, $\mathcal{Z}$ Banach spaces,
$u : [0, T] \to \mathcal{U}$,
$z : [0, T] \to \mathcal{Z}$,
$\mathcal{R}$ and $\mathcal{E}$ coercive.

Initial-value problem: $z(0) = z_0$ (and also $u(0) = u_0$).

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Treatment of the general ansatz:
General theory of rate-independent processes based on dissipation distance:

$$\mathcal{D}(z_0, z_1) := \inf \left\{ \int_0^1 \mathcal{R}\Big(\widetilde{z}(t), \frac{\mathrm{d}\widetilde{z}}{\mathrm{d}t}(t)\Big)\mathrm{d}t; \quad \widetilde{z} \in C^1([0,1]; \mathcal{V}),\ \widetilde{z}(0) = z_0,\ \widetilde{z}(1) = z_1 \right\}$$

In principle, $\mathcal{D}$ the dissipation distance can be treated as itself even without referring to $\mathcal{R}$ and without any linear structure on $\mathcal{Z}$.

But we will not pursue this high generality here.

Simplification: $\mathcal{R}(z, \frac{\mathrm{d}z}{\mathrm{d}t}) = \mathcal{R}(\frac{\mathrm{d}z}{\mathrm{d}t})$.
Then $\mathcal{D}(z_0, z_1) = \mathcal{R}(z_1 - z_0)$ is translation invariant
and we assume $\mathcal{R} : \mathcal{Z} \to \mathbb{R} \cup \{\infty\}$ homogeneous degree-1 and coercive.

We call $q=(u,z):[0,T]\to\mathcal{Q}=\mathcal{U}\times\mathcal{Z}$ an energetic solution to the problem (1) with the initial conditions if

$$z:[0,T]\to\mathcal{Z}\ \text{ with } z([0,T]) \text{ relatively compact,}$$
$$\mathrm{Var}_{\mathcal{R}}(z;0,T)=(\text{the variation of } z \text{ over } [0,T] \text{ w.r.t. } \mathcal{R})\quad<\infty\ ,$$
$$t\mapsto\partial_t\mathcal{E}(t,u(t),z(t))\ \text{ is integrable on } [0,T],$$

and if

- the energy equality holds, i.e.

$$\mathcal{E}\big(T,u(T),z(T)\big)+\mathrm{Var}_{\mathcal{R}}(z;0,T)=\mathcal{E}\big(0,u_0,z_0\big)+\int_0^T\partial_t\mathcal{E}(t,u(t),z(t))\mathrm{d}t,$$

- the stability holds for all $\tilde{u}\in\mathcal{U}$, $\tilde{z}\in\mathcal{Z}$ and for $t\in I$:

$$\mathcal{E}\big(t,u(t),z(t)\big)\le\mathcal{E}\big(t,\tilde{u},\tilde{z}\big)+\mathcal{R}\big(\tilde{z}-z(t)\big)$$

- the initial conditions $u(0)=u_0$ and $z(0)=z_0$ are satisfied.

Advantage: no $\frac{\mathrm{d}z}{\mathrm{d}t}$ and $\partial_u\mathcal{E}$ and $\partial_z\mathcal{E}$ explicitly involved.
Convexity of $\mathcal{E}(t,\cdot,\cdot)$: energetic solutions with $\frac{\mathrm{d}z}{\mathrm{d}t}\in L^1(I;\mathcal{Z})$ solve $\partial_u\mathcal{E}(t,u,z)=0$ and $\partial\mathcal{R}\big(\frac{\mathrm{d}z}{\mathrm{d}t}\big)+\partial_z\mathcal{E}(t,u,z)\ni 0$.

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$$\mathcal{E}\big(T, u(T), z(T)\big) + \mathrm{Var}_{\mathcal{R}}(z; 0, T) \\ = \mathcal{E}\big(0, u_0, z_0\big) + \int_0^T \partial_t \mathcal{E}(t, u(t), z(t))\mathrm{d}t,$$

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But it works even without convexity:

maximum-dissipation principle (or Levitas' realizability principle) competing with minimum-stored-energy principle.

Discretization in time by a fully implicit formula:

$$\partial_u \mathcal{E}_\tau^k(u_\tau^k, z_\tau^k) = 0,$$
$$\partial \mathcal{R}\Big(\frac{z_\tau^k - z_\tau^{k-1}}{\tau}\Big) + \partial_z \mathcal{E}_\tau^k(u_\tau^k, z_\tau^k) \ni 0$$

where $\mathcal{E}_\tau^k(u,z) := \mathcal{E}_\tau(k\tau, u, z)$ with $\mathcal{E}_\tau(t,u,z) := \frac{1}{\tau}\int_{-\tau}^0 \mathcal{E}(t+\xi, u, z)\mathrm{d}\xi$, for $k = 1, ..., T/\tau$ and using, for $k = 1$,

$$z_\tau^0 = z_0,$$

The existence of the discrete solution (u_τ^k, z_τ^k):

the direct method: (u_τ^k, z_τ^k) can be taken as a solution to:

$$\left.\begin{array}{ll} \text{minimize} & \tau\mathcal{R}\Big(\dfrac{z - z_\tau^{k-1}}{\tau}\Big) + \mathcal{E}_\tau^k(u,z) \\ \text{subject to} & (u,z) \in \mathcal{Q} = \mathcal{U} \times \mathcal{Z}. \end{array}\right\} \qquad (P_\tau^k)$$

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- Comparing values (P_τ^k) at the level k with those in a general $(\tilde{u},\tilde{z})$ and using degree-1 homogeneity of $\mathcal{R}$, we obtain the discrete stability:

$$\begin{aligned}\mathcal{E}_\tau^k(u_\tau^k,z_\tau^k) &\leq \mathcal{E}_\tau^k(\tilde{u},\tilde{z})+\mathcal{R}(\tilde{z}-z_\tau^{k-1})-\mathcal{R}(z_\tau^k-z_\tau^{k-1})\\ &\leq \mathcal{E}_\tau^k(\tilde{u},\tilde{z})+\mathcal{R}(\tilde{z}-z_\tau^k);\end{aligned}$$

we thus get the stability for the discrete solution, i.e.:

$$\bar{\mathcal{E}}_\tau\big(t,\bar{u}_\tau(t),\bar{z}_\tau(t)\big)\leq\bar{\mathcal{E}}_\tau\big(t,\tilde{u},\tilde{z}\big)+\mathcal{R}\big(\tilde{z}-\bar{z}_\tau(t)\big)$$

holds for all $\tilde{u}\in\mathcal{U}$, $\tilde{z}\in\mathcal{Z}$, and $t\in[0,T]$.

- Comparing values of (P_τ^k) at the level k with those in $(u_\tau^{k-1}, z_\tau^{k-1})$ gives an upper estimate of the energy balance:

$$\mathcal{E}_\tau^k(u_\tau^k, z_\tau^k) + \mathcal{R}(z_\tau^k - z_\tau^{k-1}) - \mathcal{E}_\tau^{k-1}(u_\tau^{k-1}, z_\tau^{k-1})$$
$$\leq \mathcal{E}_\tau^k(u_\tau^{k-1}, z_\tau^{k-1}) + \mathcal{R}(z_\tau^{k-1} - z_\tau^{k-1}) - \mathcal{E}_\tau^{k-1}(u_\tau^{k-1}, z_\tau^{k-1})$$
$$= \int_{(k-1)\tau}^{k\tau} \frac{\partial}{\partial t}\mathcal{E}(t, u_\tau^{k-1}, z_\tau^{k-1})\mathrm{d}t.$$

- Eventually, written the stability at the level $k-1$ and test it by $(\tilde{u}, \tilde{z}) = (u_\tau^k, z_\tau^k)$ gives a lower estimate of the energy balance:

$$\mathcal{E}_\tau^k(u_\tau^k, z_\tau^k) + \mathcal{R}(z_\tau^k - z_\tau^{k-1}) - \mathcal{E}_\tau^{k-1}(u_\tau^{k-1}, z_\tau^{k-1})$$
$$= \mathcal{E}_\tau^{k-1}(u_\tau^k, z_\tau^k) + \int_{(k-1)\tau}^{k\tau} \frac{\partial}{\partial t}\mathcal{E}(t, u_\tau^k, z_\tau^k)\mathrm{d}t + \mathcal{R}(z_\tau^k - z_\tau^{k-1}) - \mathcal{E}_\tau^{k-1}(u_\tau^{k-1}, z_\tau^{k-1})$$
$$\geq \int_{(k-1)\tau}^{k\tau} \frac{\partial}{\partial t}\mathcal{E}(t, u_\tau^k, z_\tau^k)\mathrm{d}t.$$

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$$\mathcal{E}_\tau^{k-1}(u_\tau^k, z_\tau^k) + \mathcal{R}(z_\tau^k - z_\tau^{k-1}) - \mathcal{E}_\tau^{k-1}(u_\tau^{k-1}, z_\tau^{k-1}) + \int_{(k-1)\tau}^{k\tau} \frac{\partial}{\partial t}\mathcal{E}(t, u_\tau^k, z_\tau^k)\mathrm{d}t$$

$$\geq \int_{(k-1)\tau}^{k\tau} 0.$$

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&\ge \int_{(k-1)\tau}^{k\tau} \frac{\partial}{\partial t}\mathcal{E}(t, u_\tau^k, z_\tau^k)\mathrm{d}t.
\end{aligned}$$

Summing it for $k = 1, ..., s/\tau \in \mathbb{N}$, we get the
two-sided approximate energy balance:

$$\mathcal{E}\big(0, u_0, z_0\big) + \int_0^s \partial_t \mathcal{E}_\tau\big(t, \overline{u}_\tau(t), \overline{z}_\tau(t)\big)\mathrm{d}t$$
$$\leq \mathcal{E}\big(s, u_\tau(s), z_\tau(s)\big) + \mathrm{Var}_{\mathcal{R}}\big(z_\tau; 0, s\big)$$
$$\leq \mathcal{E}\big(0, u_0, z_0\big) + \int_0^s \partial_t \mathcal{E}_\tau\big(t, \underline{u}_\tau(t), \underline{z}_\tau(t)\big)\mathrm{d}t,$$

where

u_τ := piecewise affine interpolation of $\{u_\tau^k\}_{k=0}^{T/\tau}$,
$\overline{u}_\tau$:= "forward" piecewise constant interpolation of $\{u_\tau^k\}_{k=0}^{T/\tau}$,
$\underline{u}_\tau$:= "backward" piecewise constant interpolation of $\{u_\tau^k\}_{k=0}^{T/\tau}$,
and similarly for z_τ, $\overline{z}_\tau$, and $\underline{z}_\tau$.

Possibility of a-posteriori check:
if not satisfied, optimization algorithm for (P_τ^k) may have failed
$\Rightarrow$ return back and run it with different initial guess
energy-based "backtracking" strategy (A.Mielke, T.R., J.Zeman, 2007)
possibly with a multigrid strategy in space diescretization (B.Benešová, 2009)

Standard assumptions on:
coercivity,
lower semicontinuity,
compactness of level sets, etc.

An essential assumption:
existence of a joint recovery sequence in the sense

$$\forall (t_\ell, u_\ell, z_\ell) \to (t, u, z) \ \ \forall (\widetilde{u}, \widetilde{z}) \in \mathcal{U} \times \mathcal{Z} \quad \exists (\widetilde{u}_\ell, \widetilde{z}_\ell)_{\ell \in \mathbb{N}} :$$

$$\limsup_{\ell \to \infty} \big(\mathcal{E}(t_\ell, \widetilde{u}_\ell, \widetilde{z}_\ell) + \mathcal{R}(\widetilde{z}_\ell - z_\ell) - \mathcal{E}(t_\ell, u_\ell, z_\ell)\big) \leq \mathcal{E}(t, \widetilde{u}, \widetilde{z}) + \mathcal{R}(\widetilde{z} - z) - \mathcal{E}(t, u, z).$$

Possibly, we also benefit from assuming a uniform monotonicity of $\partial_u \mathcal{E}(t, \cdot, z)$.

Step 1: a-priori estimates: from the approximate energy balance by Gronwall inequality:

$$\big\|u_\tau\big\|_{L^\infty([0,T];\mathcal{U})} \le C_1, \tag{5a}$$

$$\max_{t\in[0,T]} \bar{\mathcal{E}}_\tau(t,\bar{u}_\tau(t),\bar{z}_\tau(t)) \le C_2, \tag{5b}$$

$$\big\|z_\tau\big\|_{L^\infty([0,T];\mathcal{Z})} \le C_3; \tag{5c}$$

$$\mathrm{Var}_{\mathcal{R}}(\bar{z}_\tau;0,T) \le C_4. \tag{5d}$$

Step 2: selection of subsequences

weakly* converging (Banach's selection principle) to some u and z,

pointwise converging (Helly's selection principle):

$$z_\tau(t) \to z(t) \text{ weakly in } \mathcal{Z} \text{ for all } t.$$

in case of a uniform monotonicity of $\partial_u\mathcal{E}(t,\cdot,z)$ also

$$u_\tau \to u \text{ strongly in } L^p([0,T];\mathcal{U}).$$

Step 3: limit passage in the stability:
using the joint-recovery-sequence condition for the (integrated) approximate stability

$$\int_0^T \bar{\mathcal{E}}_\tau\big(t, \bar{u}_\tau(t), \bar{z}_\tau(t)\big)\mathrm{d}t \le \int_0^T \bar{\mathcal{E}}_\tau\big(t, \tilde{u}(t), \tilde{z}(t)\big) + \mathcal{R}\big(\tilde{z}(t) - \bar{z}_\tau(t)\big)\mathrm{d}t$$

to get the limit stability

$$\int_0^T \mathcal{E}\big(t, u(t), z(t)\big)\mathrm{d}t \le \int_0^T \mathcal{E}\big(t, \tilde{u}(t), \tilde{z}(t)\big) + \mathcal{R}\big(\tilde{z}(t) - z(t)\big)\mathrm{d}t$$

for all $(\tilde{u}, \tilde{z}) \in L^\infty([0, T]; \mathcal{U} \times \mathcal{Z})$.

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to get the limit stability and desintegrating it

$$\int_0^T \mathcal{E}\big(t, u(t), z(t)\big)\mathrm{d}t \le \int_0^T \mathcal{E}\big(t, \tilde{u}(t), \tilde{z}(t)\big) + \mathcal{R}\big(\tilde{z}(t) - z(t)\big)\mathrm{d}t$$

for all $(\tilde{u}, \tilde{z}) \in \mathcal{U} \times \mathcal{Z}$ and a.a. $t \in [0, T]$.

Step 4: limit passage in the upper energy inequality:

$$\mathcal{E}\big(T, u_\tau(T), z_\tau(T)\big) + \mathrm{Var}_{\mathcal{R}}\big(z_\tau; 0, T\big) \leq \mathcal{E}\big(0, u_0, z_0\big) + \int_0^T \partial_t \mathcal{E}_\tau\big(t, u_\tau(t), z_\tau(t)\big)\mathrm{d}t.$$

by lower semicontinuity in the l.h.s. and continuity in the r.h.s.

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Step 5: the lower energy inequality:

stability (suffices a.e.) allows

by Riemann-sum approximation of Lebesgue integral to show

the opposite inequality $\Rightarrow$ the energy equality!

Step 6: Improved convergence.

$$\forall\, t \in [0,T]:\ \mathrm{Var}_{\mathcal{R}_1}(z_\tau;[0,t]) \to \mathrm{Var}_{\mathcal{R}_1}(z;[0,t]);$$

$$\forall\, t \in [0,T]:\ \mathcal{E}(t,u_\tau(t),z_\tau(t)) \to \mathcal{E}(t,u(t),z(t));$$

$$\partial_t\mathcal{E}(\cdot,u_\tau(\cdot),z_\tau(\cdot)) \to \partial_t\mathcal{E}(\cdot,u(\cdot),z(\cdot)) \text{ in } L^1((0,T)).$$

Stability under data perturbation:

- Γ-convergence of $\{\mathcal{E}_\ell(\tilde{t},\cdot,\cdot)\}_{\ell\in\mathbb{N},\tilde{t}\to t}$ towards $\mathcal{E}_\infty(t,\cdot,\cdot)$, i.e.

$$(u_\ell,z_\ell)\to(u,z) \implies \mathcal{E}_\infty(t,u,z)\le\liminf_{\tilde{t}\to t,\ell\to\infty}\mathcal{E}_\ell(\tilde{t},u_\ell,z_\ell),$$

$$\forall(\widehat{u},\widehat{z})\in\mathcal{U}\times\mathcal{Z}\ \exists\{(\widehat{u}_\ell,\widehat{z}_\ell)\}_{\ell\in\mathbb{N}} \text{ with } (\widehat{u}_\ell,\widehat{z}_\ell)\to(\widehat{u},\widehat{z}): \quad \mathcal{E}_\infty(t,u,z)\ge\limsup_{\tilde{t}\to t,\ell\to\infty}\mathcal{E}_\ell(\tilde{t},\widehat{u}_\ell,\widehat{z}_\ell),$$

- Γ-convergence of $\{\mathcal{R}_\ell\}_{\ell\in\mathbb{N}}$ towards $\mathcal{R}_\infty$ and
- joint-recovery-sequence condition before:

$$\forall(t_\ell,u_\ell,z_\ell)\to(t,u,z)\ \forall(\widetilde{u},\widetilde{z})\in\mathcal{U}\times\mathcal{Z}\quad\exists(\widetilde{u}_\ell,\widetilde{z}_\ell)_{\ell\in\mathbb{N}}:$$

$$\limsup_{\ell\to\infty}\big(\mathcal{E}_\ell(t_\ell,\widetilde{u}_\ell,\widetilde{z}_\ell)+\mathcal{R}_\ell(\widetilde{z}_\ell-z_\ell)-\mathcal{E}_\ell(t_\ell,u_\ell,z_\ell)\big)\le\mathcal{E}_\infty(t,\widetilde{u},\widetilde{z})+\mathcal{R}_\infty(\widetilde{z}-z)-\mathcal{E}_\infty(t,u,z).$$

Energetic solutions to $(\mathcal{U}\times\mathcal{Z},\mathcal{E}_\ell,\mathcal{R}_\ell)$ converge (as subsequences) to energetic solutions to $(\mathcal{U}\times\mathcal{Z},\mathcal{E}_\infty,\mathcal{R}_\infty)$

(A. Mielke, T.R., U. Stefanelli, 2008)

Stability under data perturbation:

- Γ-convergence of $\{\mathcal{E}_\ell(\tilde{t},\cdot,\cdot)\}_{\ell\in\mathbb{N},\tilde{t}\to t}$ towards $\mathcal{E}_\infty(t,\cdot,\cdot)$, i.e.

$$(u_\ell,z_\ell)\to(u,z) \quad\Longrightarrow\quad \mathcal{E}_\infty(t,u,z)\le\liminf_{\tilde{t}\to t,\ell\to\infty}\mathcal{E}_\ell(\tilde{t},u_\ell,z_\ell),$$

$$\forall\,(\widehat{u},\widehat{z})\in\mathcal{U}\times\mathcal{Z}\;\exists\,\{(\widehat{u}_\ell,\widehat{z}_\ell)\}_{\ell\in\mathbb{N}}\text{ with }(\widehat{u}_\ell,\widehat{z}_\ell)\to(\widehat{u},\widehat{z}):$$

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- Γ-convergence of $\{\mathcal{R}_\ell\}_{\ell\in\mathbb{N}}$ towards $\mathcal{R}_\infty$ and
- joint-recovery-sequence condition now:

$$\forall(t_\ell,u_\ell,z_\ell)\to(t,u,z)\;\;\forall\,(\widetilde{u},\widetilde{z})\in\mathcal{U}\times\mathcal{Z}\quad\exists\,(\widetilde{u}_\ell,\widetilde{z}_\ell)_{\ell\in\mathbb{N}}:$$

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- Γ-convergence of $\{\mathcal{R}_\ell\}_{\ell\in\mathbb{N}}$ towards $\mathcal{R}_\infty$ and
- joint-recovery-sequence condition now:

$$\forall(t_\ell,u_\ell,z_\ell)\to(t,u,z)\ \ \forall\,(\widetilde u,\widetilde z)\in\mathcal{U}\times\mathcal{Z}\quad\exists\,(\widetilde u_\ell,\widetilde z_\ell)_{\ell\in\mathbb{N}}:$$

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(A.Mielke, T.R., U.Stefanelli, 2008)

Combination with time-discretization:
$(u^k_{\ell,\tau}, z^k_{\ell,\tau})$ can be taken as a solution to:

$$\left.\begin{array}{ll}\text{minimize} & \mathcal{R}_\ell\big(z-z^{k-1}_\tau\big) + \big[\mathcal{E}_\ell\big]^k_\tau(u,z) \\ \text{subject to} & (u,z)\in\mathcal{Q}=\mathcal{U}\times\mathcal{Z}.\end{array}\right\} \qquad (P^k_{\ell,\tau})$$

Then $(\bar{u}_{\ell,\tau}, \bar{z}_{\ell,\tau})$ converges for $\ell\to\infty$ and $\tau\to 0$ (as subsequences) to solutions to $(\mathcal{U}\times\mathcal{Z}, \mathcal{E}_\infty, \mathcal{R}_\infty)$.

Numerics:

$\mathrm{dom}\mathcal{E}_\ell(t,\cdot,\cdot)$ a (time-independent) finite-dimensional subspace of $\mathcal{U}\times\mathcal{Z}$.

Then $(P^k_{\ell,\tau})$:

- computationally implementable,
  Mosco's type transformation if $\mathrm{epi}(\mathcal{R}_\ell)$ polyhedral,
- energy-based backtracking at disposal for global optimization
- convergence analysis at disposal.

Particular examples of joint-recovery-sequence conditions:

1. $\{\mathcal{E}_\ell(\tilde{t},\cdot,\cdot)\}_{\ell\in\mathbb{N},\tilde{t}\to t}$ Γ-converges to $\mathcal{E}_\infty(t,\cdot,\cdot)$ and
   $\mathcal{R}_\ell \to \mathcal{R}_\infty$ continuously
   (j.r.s. just the same as for $\mathcal{E}_\ell \to \mathcal{E}_\infty$)
2. $\mathcal{R}_\ell = \mathcal{R}_\infty = \mathcal{R}_0 + \delta_K$ for a cone $K \subset \mathcal{Z}$
   - (i) $\mathcal{E}_\ell = \mathcal{E}_0 + \delta_{Q_\ell}$ with $\mathcal{E}_0(t,\cdot,\cdot)$ quadratic and $Q_\ell \subset \mathcal{U}\times\mathcal{Z}$ finite-dimensional:
     j.r.s. by "binomial trick"
   - (ii) general $\mathcal{E}_\infty$ and $\mathcal{E}_\ell$: case by case
     (e.g. holomic constraints in $\mathcal{E}_\infty$ needs penalization etc.).

(A.Mielke, T.R. in M2AN, 2009)

Error estimates in case 2(i):

A.Mielke, L.Paoli, A.Petrov, U.Steffanelli, 2009.

Linearized plasticity with hardening of Prager/Ziegler's type at small strains:

$\Omega \subset \mathbb{R}^d$ a bounded domain,
$u =$ displacement,
$z = (\pi, \eta) =$ the plastic deformation and the hardening parameter,
$\mathcal{U} = W^{1,2}(\Omega; \mathbb{R}^d)$,
$\mathcal{Z} = L^2(\Omega; \mathbb{R}^{d\times d}_{\mathrm{sym},0} \times \mathbb{R})$,
with $\mathbb{R}^{d\times d}_{\mathrm{sym},0} := \{A \in \mathbb{R}^{d\times d};\ A^\top = A,\ \mathrm{tr}(A) = 0\}$,

$$\mathcal{E}(t, u, \pi, \eta) = \int_\Omega \frac{1}{2}\mathbb{C}\big(e(u) - \pi\big):\big(e(u) - \pi\big) + \frac{1}{2}\mathbb{H}\pi:\pi + \frac{b}{2}\eta^2 - f(t)\cdot u \,\mathrm{d}x,$$

with $e(u) = \frac{1}{2}(\nabla u)^\top + \frac{1}{2}\nabla u$ small-strain tensor,
$b > 0$ isotropic-hardening coefficient,
$\mathbb{H} \geq 0$ kinematic-hardening coefficient (a $d\times d$-tensor),

$$\mathcal{R}(\dot\pi, \dot\eta) = \int_\Omega \delta^*_S(\dot\pi, \dot\eta)\,\mathrm{d}x,$$

with $S \subset \mathbb{R}^{n\times n}_{\mathrm{sym},0} \times \mathbb{R}$ be a convex closed neighbourhood of the origin,
δ_S is its indicator function, and δ^*_S the conjugate functional to δ_S.

Main features (the case "2a"):
$\mathcal{R}$ discontinous but $\mathcal{E}(t,\cdot,\cdot,\cdot)$ convex and quadratic.
Joint recovery sequence by the "binominal trick" ($\mathbb{H}=0$ for simplicity):

$$\limsup_{\ell\to\infty}\Big(\mathcal{E}(t_\ell,\widetilde{u}_\ell,\widetilde{z}_\ell)+\mathcal{R}(\widetilde{z}_\ell-z_\ell)-\mathcal{E}(t_\ell,u_\ell,z_\ell)\Big)$$

$$=\limsup_{\ell\to\infty}\bigg(\int_\Omega\Big(\frac12\mathbb{C}(e(\widetilde{u}_\ell+u_\ell)-\pi_\ell-\widetilde{\pi}_\ell):(e(\widetilde{u}_\ell-u_\ell)+\pi_\ell-\widetilde{\pi}_\ell)+\frac12 b(\widetilde{\eta}_\ell+\eta_\ell)(\widetilde{\eta}_\ell-\eta_\ell)\mathrm{d}x+\mathcal{R}(\widetilde{\pi}_\ell-\pi_\ell,\widetilde{\eta}_\ell-\eta_\ell)\bigg)$$

$$=\int_\Omega\Big(\frac12\mathbb{C}(e(\widetilde{u}+u)-\pi-\widetilde{\pi})\Big):(e(\widetilde{u}-u)+\pi-\widetilde{\pi})+\frac12 b(\eta+\widetilde{\eta})(\eta-\widetilde{\eta})\mathrm{d}x+\mathcal{R}(\widetilde{\pi}-\pi,\widetilde{\eta}-\eta)$$

$$=\mathcal{E}(t,\widetilde{u},\widetilde{z})+\mathcal{R}(\widetilde{z}-z)-\mathcal{E}(t,u,z),$$

if we choose $\widetilde{u}_\ell:=\widetilde{u}-u+u_\ell$, $\widetilde{\pi}_\ell:=\widetilde{\pi}-\pi+\pi_\ell$ and $\widetilde{\eta}_\ell:=\widetilde{\eta}-\eta+\eta_\ell$.

Numerics: P1-FEM for u, P0-FEM for π and η.
Similar results by H.-D.Alber, C.Carstensen, C.Chelminski, W.Han & D.Reddy, A.Mielke, at al.

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Sample calculations:
twisting experiment, steel specimen, loading by hard device (=Dirichlet b.c.):

twist-grid

Calculations and visualization: courtesy of Soeren Bartels (Univ. Bonn).

No hardening ($\mathbb{H} = 0$ and $b = 0$):
Prandtl-Reuss elastic/perfectly plastic model

classical books:
Nečas, Hlaváček, 1981
Lovíšek, Nečas, Hlaváček, Haslinger

newest treatment, BD-space, energetic solutions
G. Dal Maso, A. DeSimone, M.G. Mora (in ARMA, 2006)

limit for $\mathbb{H} \to 0$ and $b \to 0$
S.Bartels, A.Mielke, T.R. (in progress)

Gradient damage (partial) at small strains:

$\Omega \subset \mathbb{R}^d$ a bounded domain,
$u =$ displacement,
$z =$ a scalar damage parameter,
$\mathcal{U} = W^{1,2}(\Omega;\mathbb{R}^d)$,
$\mathcal{Z} = W^{1,p}(\Omega)$,

$$\mathcal{E}_\ell(t,u,z) = \int_\Omega \frac{z}{2}\mathbb{C}e(u){:}e(u) + \delta_{[\frac{1}{\ell},1]}(z) + b|\nabla z|^p - f(t)\cdot u\,\mathrm{d}x,$$

with $b > 0$ nonlocal-influence parameter,

$$\mathcal{R}(\dot z) = \int_\Omega \delta_{(-\infty,0]}(\dot z) - \kappa \dot z\,\mathrm{d}x,$$

with $\kappa > 0$ the energy per d-dimensional volume dissipated by damage.

Main features (the case "2b"):

$\mathcal{R}$ discontinous and $\mathcal{E}_\ell(t,\cdot,\cdot)$ nonconvex
but $\partial_u\mathcal{E}(t,\cdot,z)$ uniformly monotone.

Joint recovery sequence (for $p>d$):

$\widetilde{u}_\ell := \widetilde{u}, \quad \widetilde{z}_\ell := \Pi_\ell\Big(\big(\widetilde{z} - \|z_\ell - z\|_{L^\infty(\Omega)}\big)^+\Big);$ Π_ℓ a projector $\mathcal{Z}\to\mathcal{Z}_\ell$

note that $0\le\widetilde{z}_\ell\le z_\ell$ a.e. (if $\widetilde{z}\le z$ because $p>d$) and $\widetilde{z}_\ell\to\widetilde{z}$.
A.Mielke & T.R.

For $p\le d$ a more complicated construction: A.Mielke & M.Thomas, 2009.

Numerics: both $\mathcal{U}_\ell$ and $\mathcal{Z}_\ell$ P1-FEM.

After having the energetic solution of the regularized problem, passage $\ell\to\infty$ to the complete damage possible because $\mathcal{E}_\ell$ Γ-converges to $\mathcal{E}_\infty$
One trouble: lost of coercivity $\Rightarrow$
only the bulk-load $f=0$ and hard-device load must be used.
u and $e(u)$ loose a sense where $z=0$, only $\mathbb{C}e$ and $\mathbb{C}e{:}e$ have a good sense.
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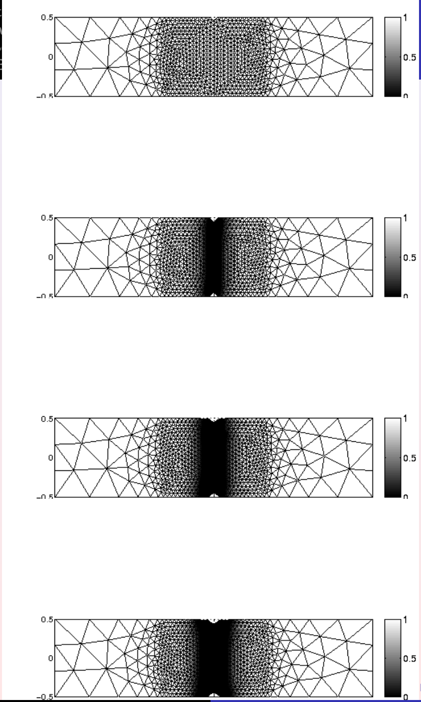
2D-numerical experiments:



Courtesy:
J.Zeman
(Czech Technical Univ.,
Prague).

Delamination/debonding at small strains: Griffith-type model:
$\Omega \subset \mathbb{R}^d$ a bounded domain,
Γ a $d-1$ dimensional manifold inside Ω,
$u =$ displacement,
$z =$ a scalar delamination parameter,
$\mathcal{U} = W^{1,2}(\Omega \setminus \Gamma; \mathbb{R}^d)$,
$\mathcal{Z} = L^\infty(\Gamma)$,

$$\mathcal{E}_\infty(t,u,z) = \begin{cases} \displaystyle\int_\Omega \frac{\mathbb{C}e(u){:}e(u)}{2} - f\cdot u \,\mathrm{d}x & \text{if } u|_{\Gamma_{\rm Dir}} = u_{\rm Dir}(t) \text{ on } \Gamma_{\rm Dir}, \\ & [u(x)]_\Gamma = 0 \text{ if } z(x) > 0, \\ & [u]\cdot\nu \geq 0 \text{ and } 0 \leq z \leq 1 \text{ on } \Gamma, \\ +\infty & \text{elsewhere.} \end{cases}$$

with ν the normal to Γ,

$$\mathcal{R}(\dot z) = \int_\Gamma \delta_{(-\infty,0]}(\dot z) - \kappa \dot z \,\mathrm{d}S, \quad \text{with}$$

$\kappa > 0$ the energy per $d-1$-dimensional surface dissipated by delamination.

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Delamination/debonding at small strains: regularized model:
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Γ a $d-1$ dimensional manifold inside Ω,
$u =$ displacement,
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$\mathcal{U} = W^{1,2}(\Omega \setminus \Gamma; \mathbb{R}^d)$,
$\mathcal{Z} = L^\infty(\Gamma)$,

$$\mathcal{E}_\ell(t,u,z) = \begin{cases} \displaystyle\int_\Omega \frac{\mathbb{C}e(u):e(u)}{2} - f\cdot u\,\mathrm{d}x + \ell\int_\Gamma z[u]_\Gamma^2\,\mathrm{d}S & \text{if } u|_{\Gamma_{\rm Dir}} = u_{\rm Dir}(t) \text{ on } \Gamma_{\rm Dir}, \\ & [u]\cdot\nu\geq 0 \text{ and } 0\leq z\leq 1 \text{ on } \Gamma, \\ +\infty & \text{elsewhere.} \end{cases}$$

with ν the normal to Γ,

$$\mathcal{R}(\dot z) = \int_\Gamma \delta_{(-\infty,0]}(\dot z) - \kappa\dot z\,\mathrm{d}S, \text{ with}$$

$\kappa > 0$ the energy per $d-1$-dimensional surface dissipated by delamination.

Main features (the case "2b"):

$\mathcal{R}$ discontinous and $\mathcal{E}_\infty(t,\cdot,\cdot)$ nonconvex discontinuous,
$\mathcal{E}_\ell(t,\cdot,\cdot)$ nonconvex continuous,

but we benefit from compactness of trace operator on Γ
($\Rightarrow$ no gradient of z nedeed),

$\partial_u\mathcal{E}(t,\cdot,z)$ uniformly monotone.

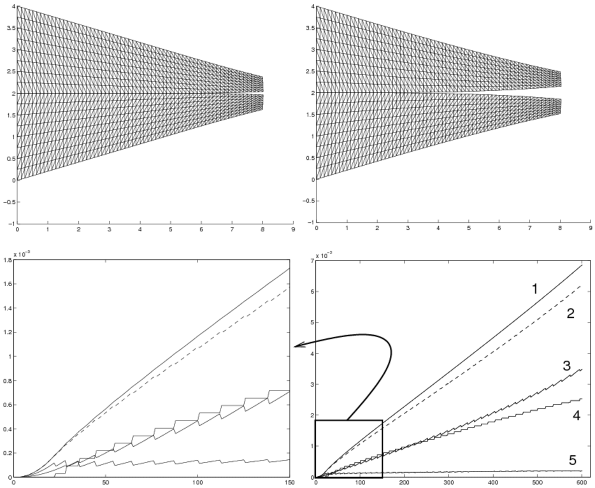
Γ-limit of $\mathcal{E}_\ell$ towards $\mathcal{E}_\infty$ for $\ell\to\infty$: a joint recovery sequence:

$$\widetilde{u}_\ell := \widetilde{u}, \qquad \widetilde{z}_\ell := \begin{cases} z_\ell\widetilde{z}/z & \text{where } z>0,\\ 0 & \text{where } z=0.\end{cases}$$

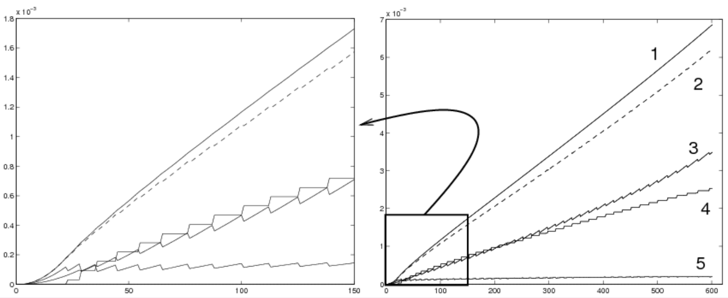
T.R. & L.Scardia & C.Zanini, 2008.

Numerics: P1-FEM for u, P0-FEM for z.

Delamination 2D-experiments documenting energetics (including Clapeyron's effect)



Calculations & visualisation: M. Kočvara (Acad. Sci. Prague, now Univ. Birmingham)



Meaning of particular curves:

(1) work done by loading calculated as $\int_0^t \frac{\partial}{\partial t}\mathcal{E}(t, y(t), z(t))\,\mathrm{d}t$,

(2) work done by loading calculated as $\mathcal{E}(t) + \mathcal{R}(z(t) - z_0) - \mathcal{E}(0)$,

(3) energy stored in the bulk,

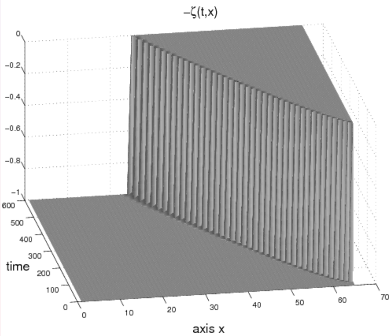
(4) energy dissipated thru delamination,

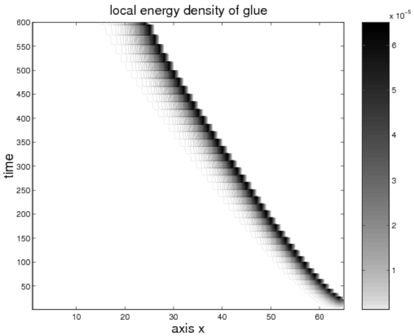
(5) energy stored in the adhesive.

Clapeyron's effect: work done splits to 50% stored and 50% dissipated energy.
i.e. here: (1) $= \frac{1}{2}$ (3) $= \frac{1}{2}$ (4) (at least at some occasions)

Calculations & visualisation: M. Kočvara (Acad. Sci. Prague, now Univ. Birmingham)

Left figure: The delamination parameter takes mostly values 0 or 1:
Righ figure: Active debonding area is localized on the crack tip:

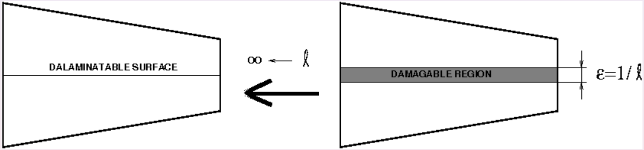




Calculations & visualisation: M. Kočvara (Acad. Sci. Prague, now Univ. Birmingham)

From 3D to 2D:

1. From damage to delamination:



Suitable scalling: $\mathcal{R}_\ell$: damage activation threshold $\sim \ell$,
$\mathcal{E}_\ell$: smart choice of a nonlinear material.
(M.Thomas & T.R., in progress.)

2. From damage in the bulk to damage in the plate: Kirchhoff-Love plates.
(T.R. & G.Tomassetti, in progress too.)

3. From delamination in the bulk to cracks in a Kirchhoff-Love plate.
(L.Fredi, R.Paroni, T.R. & C.Zanini, in progress too.)

4. From plasticity in the bulk to plasticity in a Kirchhoff-Love plate.
(M.Liero & A.Mielke, 2009)

Example of an multiscale modelling: microstructure evolution in shape-memory alloys:

"Micro-level": $u := y$=large deformation,
$z :=$ volume fraction.

Multi-well stored energy: St.Venant-Kirchhoff form of each well:

$$\mathcal{E}_\ell(t,y,z) := \begin{cases} \displaystyle\int_\Omega \min_{\kappa=1,..,K} \left(\frac{\mathbb{C}^\kappa \varepsilon^\kappa : \varepsilon^\kappa}{2} + c_\kappa \right) + \frac{1}{\ell} |\nabla^2 y|^2 \mathrm{d}x & \text{if } z = \mathcal{L}(\nabla y), \\ +\infty & \text{elsewhere} \end{cases}$$

where $\varepsilon^\kappa := \frac{(U_\kappa^\top)^{-1} \nabla y^\top \nabla y U_\kappa^{-1} - \mathrm{I}}{2}$ with U_κ the stretch tensor of the particular variant, and $\mathcal{L} : \mathbb{R}^{d\times d} \to \mathbb{R}^K$.

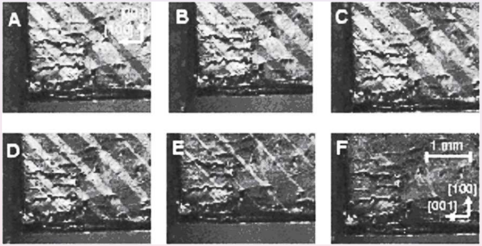
Dissipation:

$$\mathcal{R}(z) := \int_\Omega |\mathcal{S} z| \mathrm{d}x,$$

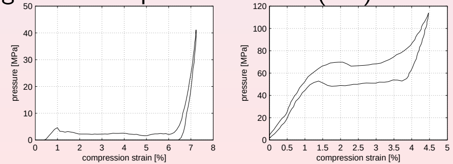
with $\mathcal{S}$ a "smoothening" compact operator like $(I - \epsilon\Delta)^{-1}$ with $\epsilon > 0$ small. Then $\mathcal{R}$ continuous.

Existence + numerical approximation of energetic solutions (the case "1").

Experiments by L.Straka, V.Novák, M.Landa, O.Heczko, 2004:
Compression experiment: reorientation of tetragonal martensite in a (001)-oriented singlecrystal NiMnGa under temperature 293 K:



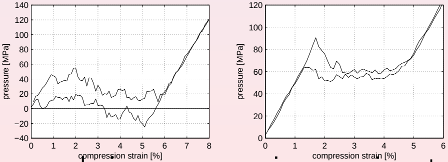
Stress-strain diagram at temperature 293 K (left) and 323 K (right):



Computational simulations:

Compression experiment with NiMnGa (001)-oriented singlecrystal

Reorientation of martensite during a compression experiment at 293 K.



Stress/strain response during a compression experiment at 293 K and at 323 K.

Calculations, visualizations: courtesy of Marcel Arndt, Univ. Bonn (presently in Munich

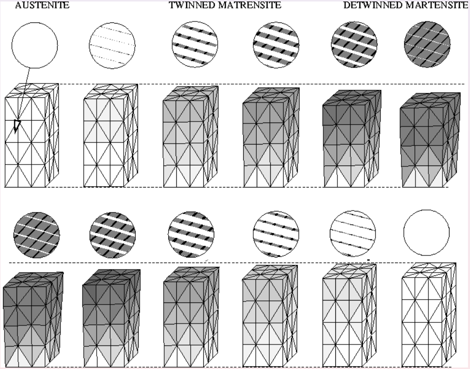
Fighting with multiscales: the limit passage $\ell \to \infty$:
"Meso-level": $u := (y, \nu)$=large deformation×a gradient Young measure,
$z :=$ volume fraction.

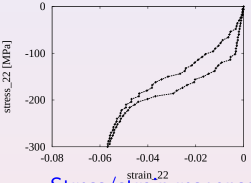
$$\mathcal{E}_\infty(t, y, \nu, z) := \begin{cases} \Big[\displaystyle\int_\Omega \min_{\kappa=1,..,K} \Big(\frac{\mathbb{C}^\kappa \varepsilon^\kappa : \varepsilon^\kappa}{2} + c_\kappa \Big) \Big] (F) \mathrm{d}\nu_x(F) \mathrm{d}x & \text{if } z = \displaystyle\int_{\mathbb{R}^{d\times d}} \mathcal{L}(F) \mathrm{d}\nu_x(F) \\ +\infty & \text{elsewhere} \end{cases}$$

Γ-limit $\mathcal{E}_\ell \to \mathcal{E}_\infty$.

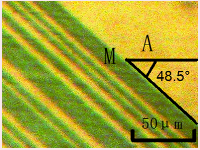
Numerics: P1-FEM for y, P0-FEM for z, element-wise homogeneous laminates for k-th order for ν. Convergence to an energetic solution.
(M.Kružík, A.Mielke, T.R., 2005)

Computational experiments with CuAlNi (1,0,0)-oriented single crystal based on 2nd-order laminate.





Stress/strain response.



A lab experiment.

1. compression: austenite ⟶ twinned martensite,
2. more compression: twinned martensite ⟶ detwinned martensite,
3. and back.

Calculations: courtesy of Martin Kružík.
Experiment: courtesy of Yongzhong Huo.

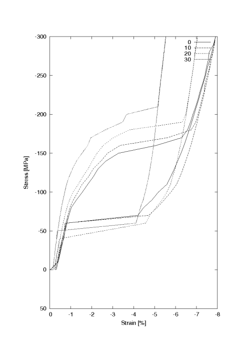
Computational experiments with CuAlNi (1,0,0)-oriented single crystal based on 2nd-order laminate.

CuAlNi

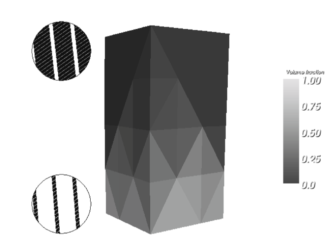
1. compression: austenite $\longrightarrow$ twinned martensite,
2. more compression: twinned martensite $\longrightarrow$ detwinned martensite,
3. and back.

Calculations: courtesy of Martin Kružík.
Visualization: courtesy of Jan Koutný.

Different orientations of the CuAlNi single crystal give different response:



Stress-strain response under cyclic compression load of a (0,tgα,1)-oriented single-crystal depends substantially on α. Here $\alpha = 0^\circ$, 10°, 20°, and 30° is depicted.



Specimen, here (0,tg10°,1)-oriented CuAlNi single crystal, under compression loading at 200 MPa.

Calculations & visualization: courtesy of Jan Koutný.

Computational experiments with NiTi (1,0,0)-oriented single crystal based on 2nd-order laminate, cubic/rhomboedric phase transformation between austenite and R-phase (1 to 4 variants):

NiTi

1. compression: austenite ⟶ austenite co-existing with twinned R-phase,
2. more compression: austenite is vanishing.

Calculations and visualization: courtesy of Barbora Benešová.

A detail of reconstructed microstructure:

NiTi

Calculations and visualization: courtesy of Barbora Benešová.

Beyond rate independency:

Inertia and viscosity:
Combination of rate-independent processes vs. rate-dependent processes.

$$\mathcal{T}'\frac{\mathrm{d}^2 u}{\mathrm{d}t^2} + \mathcal{R}_2'\frac{\mathrm{d}u}{\mathrm{d}t} + \partial_u\mathcal{E}(t,u,z) = 0, \tag{7a}$$

$$\partial_{\frac{\mathrm{d}z}{\mathrm{d}t}}\mathcal{R}_1\big(z,\frac{\mathrm{d}z}{\mathrm{d}t}\big) + \partial_z\mathcal{E}(t,u,z) \ni 0. \tag{7b}$$

with
$u \in \mathcal{U}$ a "displacement" determined essentially by z
$z \in \mathcal{Z}$ an "internal" variable with activated evolution,
$\mathcal{E} : \mathcal{U} \times \mathcal{Z} \to \mathbb{R} \cup \{\infty\}$ the stored energy,
$\mathcal{R}_1 : \mathcal{Z} \times \mathcal{Z} \to \mathbb{R} \cup \{\infty\}$ the dissipation pseudopotential
$\mathcal{R}_1(z,\cdot)$ (positively) homogeneous degree-1
$\mathcal{R}_2 : \mathcal{V} \to \mathbb{R}$ the dissipation pseudopotential of viscous forces, quadratic
$\mathcal{T} : \mathcal{H} \to \mathbb{R}$ the kinetic energy, quadratic

Beyond rate independency:

Inertia and viscosity:
Combination of rate-independent processes vs. rate-dependent processes.

$$\mathcal{T}'\frac{\mathrm{d}^2 u}{\mathrm{d}t^2} + \mathcal{R}_2'\frac{\mathrm{d}u}{\mathrm{d}t} + \partial_u\mathcal{E}(t,u,z) = 0, \tag{7a}$$

$$\partial_{\frac{\mathrm{d}z}{\mathrm{d}t}}\mathcal{R}_1\big(z,\frac{\mathrm{d}z}{\mathrm{d}t}\big) + \partial_z\mathcal{E}(t,u,z) \ni 0. \tag{7b}$$

with
$u \in \mathcal{U}$ a "displacement" evolving "viscously"
$z \in \mathcal{Z}$ an "internal" variable with activated evolution,
$\mathcal{E} : \mathcal{U}\times\mathcal{Z} \to \mathbb{R}\cup\{\infty\}$ the stored energy,
$\mathcal{R}_1 : \mathcal{Z}\times\mathcal{Z} \to \mathbb{R}\cup\{\infty\}$ the dissipation pseudopotential
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Beyond rate independency:

Inertia and viscosity:
Combination of rate-independent processes vs. rate-dependent processes.

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$$\partial_{\frac{\mathrm{d}z}{\mathrm{d}t}}\mathcal{R}_1\big(z,\frac{\mathrm{d}z}{\mathrm{d}t}\big) + \partial_z\mathcal{E}(t,u,z) \ni 0. \tag{7b}$$

with
$u \in \mathcal{U}$ a "displacement" evolving "viscously" and "inertially"
$z \in \mathcal{Z}$ an "internal" variable with activated evolution,
$\mathcal{E} : \mathcal{U} \times \mathcal{Z} \to \mathbb{R} \cup \{\infty\}$ the stored energy,
$\mathcal{R}_1 : \mathcal{Z} \times \mathcal{Z} \to \mathbb{R} \cup \{\infty\}$ the dissipation pseudopotential
$\mathcal{R}_1(z,\cdot)$ (positively) homogeneous degree-1
$\mathcal{R}_2 : \mathcal{V} \to \mathbb{R}$ the dissipation pseudopotential of viscous forces, quadratic
$\mathcal{T} : \mathcal{H} \to \mathbb{R}$ the kinetic energy, quadratic

Thermodynamical expansion possible:

$\mathcal{E} = \mathcal{E}_0 + \theta\mathcal{E}_1$ temperature dependent,
heat-transfer equation of the type:

$$c_v(\theta)\frac{\partial\theta}{\partial t} - \mathrm{div}\big(\mathbb{K}(\theta,u,z)\nabla\theta\big) = \underbrace{\mathcal{R}_1\Big(\frac{\partial z}{\partial t}\Big) + 2\mathcal{R}_2\Big(\frac{\partial u}{\partial t}\Big)}_{\text{dissipative heat}} + \underbrace{\theta[\mathcal{E}_1]'_u\frac{\partial u}{\partial t} + \theta[\mathcal{E}_1]'_z\frac{\partial z}{\partial t}}_{\text{adiabatic heat}}\,.$$

- Fully implicit time discretization does not yield an incremental problem with a variational structure (existence by Schauder fixed point only)
- energetic-solution concept important (weak convergence of the dissipative heat source)
- L^1-theory for heat equation (Boccardo, Galouët, et al.) and interpolation of the adiabatic-heat term (Gagliardo, Nirenberg)

Example: Thermo-visco-elasticity with rate-independent plasticity:
temperature evolution during heating:

temp

Calculations and visualization: courtesy of Soeren Bartels (Univ. Bonn).

Example: Thermo-visco-elasticity with rate-independent plasticity:
stress evolution during heating - residual stresses after plasticizing visible:

stress

Calculations and visualization: courtesy of Soeren Bartels (Univ. Bonn).

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More on: `www.karlin.mff.cuni.cz/~roubicek/trpublic.htm`

Thanks a lot for your attention.