Energy-dissipation functionals in fracture mechanics

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Systems with evolving microstructure

\[ \partial \psi (\dot{u}) + D E (t, u) = 0, \]
\[ \begin{cases} \psi \equiv \text{dissipation potential} \\ E \equiv \text{energy} \end{cases} \]

- Systems of interest are time-dependent, dissipative, irreversible and hysteretic.
- The behavior of the system is governed by both energy and kinetics.
- However: Energies of interest often lack differentiability and lower-semicontinuity.
- Meaning of ‘solutions’ in the presence of evolving fine microstructure?
- One approach: Time-discretized variational problems.
Classical rate variational problems

- Rate potential: $G : [0, T] \times Y \times Y \to \mathbb{R}$, e. g.,
  \[ G(t, u, v) \equiv \Psi(v) + DE(t, u)(v) \]
- Potential energy:
  \[ E(t, u) = \int_{\Omega} [W(u, \nabla u) - f(t) \cdot u] \, dx \]
- Dissipation potential:
  \[ \Psi(v) = \int_{\Omega} \psi(v, \nabla v) \, dx \]
- IBV problem: For $t \in [0, T]$,
  \[ v(t) \in \text{argmin} \ G(t, u(t), \cdot) \]
  \[ \dot{u}(t) = v(t), \ u(0) = u_0 \]
Rate problems – Time discretization

• Incremental functional: $u \in Y$

$$F(u_{n+1}; u_n) = \inf_{\text{paths}} \int_{t_n}^{t_{n+1}} G(t, u(t), \dot{u}(t)) \, dt$$

• Example: $G(t, u, v) \equiv \Psi(v) + DE(t, u) v$

$$F(u_{n+1}; u_n) = \Delta t \psi \left( \frac{u_{n+1} - u_n}{\Delta t} \right) + E(u_{n+1}) - E(u_n)$$

• Incremental problem: For $t_0, \ldots, t_n, t_{n+1}, \ldots$

$$u(t_0) = u_0,$$

$$\inf_{u_{n+1} \in Y} F(u_{n+1}; u_n)$$
Rate problems – Time discretization

• IBVP reduced to a sequence of minimization problems to be solved sequentially:

\[ \inf_{u_1 \in Y} F(u_1; u_0) \rightarrow u_1 \]
\[ \inf_{u_2 \in Y} F(u_2; u_1) \rightarrow u_2 \]
\[ \ldots \]

• But incremental problems may lack attainment!
• Initial conditions for next minimum problem may be ill-defined → scheme breaks down
• Instead: Devise a single minimum principle for entire trajectories
Energy-dissipation functionals

- Energy-dissipation functional: $\lambda_n > 0$, $u \in Y^N$,
  \[
  F(u) \equiv \sum_{n=0}^{N-1} \lambda_{n+1} F(u_{n+1}; u_n)
  \]
- But *causality* demands: $\lambda_1 \gg \lambda_2 \gg \ldots$
- Introduce function $\lambda_\epsilon(t) > 0$, $\epsilon \geq 0$, s. t.
  \[
  \lim_{\epsilon \to 0} \frac{\lambda_\epsilon(t_{n+1})}{\lambda_\epsilon(t_n)} = 0
  \]
- Sequence of functionals:
  \[
  F_\epsilon(u) \equiv \sum_{n=0}^{N-1} \lambda_\epsilon(t_{n+1}) F(u_{n+1}; u_n)
  \]
Energy-dissipation functionals

- Suppose: \( G(t, u, \nu) = \Psi(\nu) + DE(t, u)(\nu) \)

- Sequence of energy-dissipation functionals:
  \[
  F_c(u) = \sum_{n=0}^{N-1} \lambda_c(t_{n+1}) \left\{ \Psi \left( \frac{\Delta u}{\Delta t} \right) + \frac{\Delta E}{\Delta t} \right\} \Delta t
  \]

- Formally, as \( \Delta t \to 0 \), \( u : [0, T] \to Y \),
  \[
  F_\varepsilon(u) = \int_0^T \lambda_\varepsilon(t) \left[ \Psi(\dot{u}) + \dot{E} \right] dt
  \]

- Minimum principle: \( \mathbb{Y} = \{ u : [0, T] \to Y \} \),
  \[
  \inf_{u \in \mathbb{Y}} F_\varepsilon(u)
  \]
Energy-dissipation functionals

- Particular choice: $\lambda_\epsilon(t) = e^{-t/\epsilon}$,

$$\Gamma_\epsilon(u) = \int_0^T e^{-t/\epsilon} \left[ \Psi(\dot{u}) + \dot{E} \right] dt$$

- Alternatively, integrating by parts,

$$\Gamma_\epsilon(u) = \int_0^T e^{-t/\epsilon} \left[ \Psi(\dot{u}) + \frac{1}{\epsilon} E(t, u) \right] dt + \left[ e^{-t/\epsilon} E \right]_0^T$$

- Euler-Lagrange equations:

$$-\epsilon D^2 \Psi(\dot{u}) \ddot{u} + D\Psi(\dot{u}) + D E(t, u) = 0$$

- Evolutionary problem is (formally) recovered in the limit of $\epsilon \to 0$. 
Energy-dissipation functionals

- Energy-dissipation functionals represent **elliptic regularizations** of the evolutionary problem.
- The system is endowed with a small amount of ‘foresight’ over small time intervals of size $\epsilon$.

$$F_{\epsilon}(u) = \int_0^T e^{-t/\epsilon} \left[ \psi(\dot{u}) + \frac{1}{\epsilon} E(t, u) \right] dt + [e^{-t/\epsilon} E]_0^T$$

- “Arrow of time”

- Minimizers do not define a gradient flow: $E = E(u)$, $\epsilon D\psi(\dot{u})(\ddot{u}) + D\psi(\dot{u})(\ddot{u}) + \dot{E} = 0$
Energy-dissipation functionals

• Minimization of energy-dissipation functionals characterizes *entire trajectories* of the system
• ‘Solutions’, understood as *minimizers*, make sense even when the energy is not differentiable
• ‘Solutions’, understood as *minimizing sequences*, make sense even when the energy lacks lower semicontinuity
• *Existence* of solutions at fixed $\varepsilon$?
• *Causal* limit $\varepsilon \to 0$?
• Limiting behavior of trajectories of *sequences* of energy-dissipation functionals?
Causal limit – Rate-independent case

- Banach spaces $Z$, $X$ compactly embedded.
- Sequences of functionals $\Psi_k$ (rate indep.), $E_k$.
- Energy-dissipation functionals:

$$\Gamma_{c,k}(u) = \int_0^T e^{-t/\varepsilon} [\Psi_k(\dot{u}) + \frac{1}{\varepsilon} E_k(t, u)] \, dt + [e^{-t/\varepsilon} E_k]_0^T$$

- Coercivity:

$$\Psi(v) \geq c \|v\|_Z.$$

$$E(t, u) \geq c \|u\|_X^\alpha - C$$

- Power control:

$$|\partial_t E(t, u)| \leq c_1^E (E(t, u) + c_0^E)$$

- IC stability:

$$E(0, u_0) \leq E(0, \tilde{u}) + \Psi(\tilde{u} - u_0)$$
Causal limit – Rate-independent case

- Weak continuous convergence of $\Psi_k$:
  $$\nu_k \rightharpoonup \nu \Rightarrow \Psi_k(\nu_k) \rightharpoonup \Psi(\nu)$$

- Weak $\Gamma$-convergence of $E_k$:
  $$E = \Gamma-\lim_{k \to \infty} E_k, \text{ weakly in } X$$

- Weak continuity of external power:
  $$u_k \rightharpoonup u \quad E'_k(t, u_k) \rightharpoonup E(t, u) \quad \Rightarrow \partial_t E_k(t, u_k) \rightharpoonup \partial_t E(t, u)$$
Causal limit – Rate-independent case

**Theorem** (A. Mielke & MO) Let assumptions (A) and (B) hold uniformly in $k$. Then:

i) Any family $u_{c,k}$ of minimizers of $F_{c,k}$ is weakly precompact in $\mathcal{Y} \equiv L^\infty([0, T], X) \cap BV([0, T], Z)$.

ii) Any limit point $u \in \mathcal{Y}$ of $u_{c,k}$ is a solution of the energetic formulation

\[
\forall v \in X: E(t, u(t)) \leq E(t, v) + \Psi(v-u(t)),
\]

\[
E(t, u(t)) + \int_0^t \Psi(du) = E(0, u(0)) + \int_0^t \partial_s E(s, u(s)) ds
\]
The rate problem of LEFM

- Assume regularity, smoothness . . .

- Load increment, crack extension:

\[-\Delta E = \int_{\Delta C} [DW (\nabla u_t) \mathbf{n}] \cdot [u_t + \Delta t] \ d\mathcal{H}^2 + h.o.t.\]
The rate problem of LEFM

- Energy-release rate:
  \[ G = \lim_{\Delta t \to 0} \frac{\Delta E}{\Delta t} = \int_F f(n) \, v \, d\mathcal{H}^1 \]

- Driving force:
  \[ f(n) = \lim_{\Delta t \to 0} \frac{1}{\Delta t} [D \mathcal{W}(\nabla u_t) \cdot n] \cdot [u_t + \Delta t] \]

- Crack-tip equation of motion:
  \[ f = \partial \psi(v) \]

- Dissipation:
  \[ \psi(v) = \int_F \psi(v) \, d\mathcal{H}^1 \]
The rate problem of LEFM

Crack-tip equation of motion for fatigue crack growth

Crack-growth data for 2024-T3 aluminum alloy (P. Paris and F. Erdogan, ASME Trans (1963))
The rate problem of LEFM

Crack-growth data for 2024-T3 aluminum alloy (P. Paris and F. Erdogan, ASME Trans (1963))

\[ v \sim f^2 \]
The rate problem of LEFM

Dynamic crack-tip equation of motion

The rate problem of LEFM

- Rate problem: \( \inf_{v,n} \int_F [\psi(v) - f(n) v] \, d\mathcal{H}^1 \)

\[ \Rightarrow \left\{ \begin{array}{l} \partial\psi(v) = f(n) \\ \partial\psi^*(f(n)) = 0 \end{array} \right\} \longrightarrow (v, n) \\
\text{(maximum driving force)} \]
LEFM rate problem – Numerical analysis

Xu, Bower and Ortiz, *IJSS* (1994)
LEFM rate problem – Numerical analysis

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Xu, Bower and Ortiz, *IJSS* (1994)
LEFM rate problem – Numerical analysis

Fiber debonding in composites

Xu, Bower and Ortiz, *JMPS* (1998)
LEFM rate problem — Dynamics

\[ f(n) \text{ (driving force)} \]

\[ v > v_c \]

\[ v = v_c \sim 0.6c_s \]

\[ v < v_c \]

\[ \sim -65^\circ \quad \sim +65^\circ \]

\[ \omega \text{ (kinking angle)} \]

E.H. Yoffe, *Phil. Mag.* (1951)
LEFM rate problem — Dynamics

Subcritical crack growth in Homalite-100

I. Arias et al., CMAME (2007)
LEFM rate problem — Dynamics

Supercritical crack growth in Homalite-100
I. Arias et al., CMAME (2007)
LEFM energy-dissipation functionals

- Crack set: \( C, 0 < \mathcal{H}^{n-1}(C') < +\infty \).
- Crack-front measure: \( \forall \varphi \in C^1_0([0, T]), \forall f \in C_0(\Omega) \),
  \[
  \int_0^T \dot{\varphi} \int_{C(t)} f d\mathcal{H}^{n-1} \, dt = - \int_0^T \varphi \int_{\Omega} f d\mu_t(x) \, dt
  \]
- Crack front, velocity: \( d\mu_t = v_t d\mathcal{H}^{n-2}[F(t)] \).
LEFM energy-dissipation functionals

- **Path**: $p := (u, C)$.

- **Energy-dissipation functional**:

  $$F_\varepsilon(p) := \int_0^T e^{-t/\varepsilon} \left\{ \Psi(v) + \frac{1}{\varepsilon} E(u) \right\} \, dt$$

- **Energy**: $E(u) = \int_\Omega W(\nabla u) \, dx$

- **Dissipation**: $\Psi(v) = \int_{F(l)} (\alpha + v^p) \, d\mathcal{H}^{n-1}$

  - nucleation energy
  - rate-dependent crack-tip equation of motion
LEFM energy-dissipation functionals

- Assume $\Omega \subset \mathbb{R}^2$.
- Minimize $F_\varepsilon(\mathcal{P})$ over the class $\mathcal{P}$ of paths:
  
  i) $u(\cdot, t) \in SBV(\Omega), \forall t \in [0, T]$.
  
  ii) $u(\cdot, t) = g \in L^\infty(\Omega)$ on $\partial \Omega \setminus C(t), \forall t \in [0, T]$.
  
  iii) $C : [0, T] \rightarrow \{ K : K \subset \bar{\Omega}, \mathcal{H}^1(K) < \infty \}$ s. t.:
    
    iii.a) $C$ nondecreasing: $\forall \tau < t, C(\tau) \subseteq \mathcal{H}^1 \subseteq C(t)$.
    
    iii.b) $\forall \tau < t, S(u(\tau)) \subseteq C(t)$.
    
    iii.c) $\exists$ CFM $d\mu_t = \nu_t d\mathcal{H}^0|F(t)$, $F : [0, T] \rightarrow 2^\Omega, \nu(t) : F(t) \rightarrow \mathbb{R}$. 

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LEFM energy-dissipation functionals

- Failure of l.s.c.: For \( u \leq \left( \frac{\alpha}{1 - 2^{1-p}} \right)^{1/p} \),

\[
\alpha + u^p = \liminf_{i \to \infty} \Psi(p_i) \leq \Psi(p) = 2\alpha + \left(\frac{u}{2}\right)^p
\]
LEFM energy-dissipation functionals

Theorem (C. Larsen, MO, C.L. Richardson) The lower semicontinuous envelop of $F_\epsilon$ in $\mathcal{P}$ is:

$$sc^- F_\epsilon(p) = \int_0^T e^{-t/\epsilon} \left\{ \frac{1}{\epsilon} \int_{\Omega} W(\nabla u) dx + \gamma \int_{F(t)} \nu d\mathcal{H}^0 \right\} dt$$

where: $\gamma = p \left( \frac{\alpha}{p - 1} \right)^{\frac{p-1}{p}}$

- Relaxed energy-dissipation functional is rate-independent!
LEFM energy-dissipation functionals

Sketch of proof:

1. Consider an arbitrary $p \in \mathcal{P}$. The plan is to construct a sequence $p_i \to p$ such that $p_i$ builds the crack set of $p$ with minimal dissipation.

2. Break up $[0, T]$ into increments of size $\frac{1}{i}$.

3. For each increment, use rectifiability to finely cover the crack set with balls in which the crack set is close to a segment.

4. Use the Besicovitch covering theorem to get a countable disjoint subcover that covers almost all of the crack set.
LEFM energy-dissipation functionals

**Sketch of proof** (continued):

5. Calculate the minimal dissipation required to build such a hyperplane, and construct the configuration of fronts that achieves the minimum.

6. Define the crack set for $p_i$ locally in space by this construction, on each time increment.
LEFM energy-dissipation functionals

Sketch of proof: Mother-daughter mechanism:

- Twin daughters (optimal by Jensen’s inequality):

\[ \Psi = n\alpha + n \left( \frac{v}{n} \right)^p \rightarrow \min \Rightarrow \]

\[ n_{\text{min}} = \left( \frac{p - 1}{\alpha} \right)^{1/p} v, \quad \Psi_{\text{min}} = p \left( \frac{\alpha}{p - 1} \right)^{1-1/p} v \]
Concluding remarks

• Energy-dissipation functionals provide a useful tool for understanding microstructure evolution within the framework of the calculus of variations.

• The application to fracture requires a careful analysis of the crack front. The dissipation attendant to crack growth is concentrated on the crack front.

• Calculus of variations tools should be most effective for understanding complex fracture processes and defining effective problems, including:
  – Crack branching, fragmentation phenomena
  – Crack propagation through heterogeneous media

• Calculus of variations tools could be useful for understanding the convergence of numerical methods for fracture mechanics.