Minimum principles for characterizing the trajectories and microstructural evolution of dissipative systems

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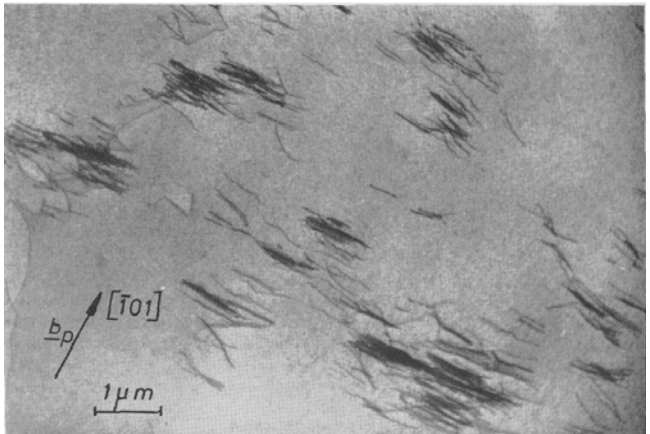
Geometric Analysis, Elasticity and PDEs
Edinburgh, June 26, 2008

Evolving microstructures − Dislocations

Copper single crystal
(Mughrabi, Phil. Mag. **23**, 869, 1971)



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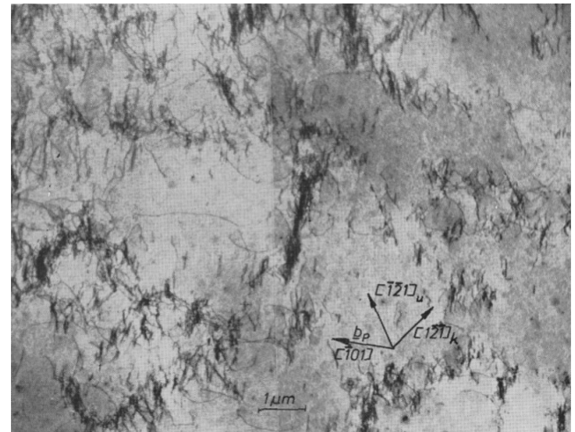

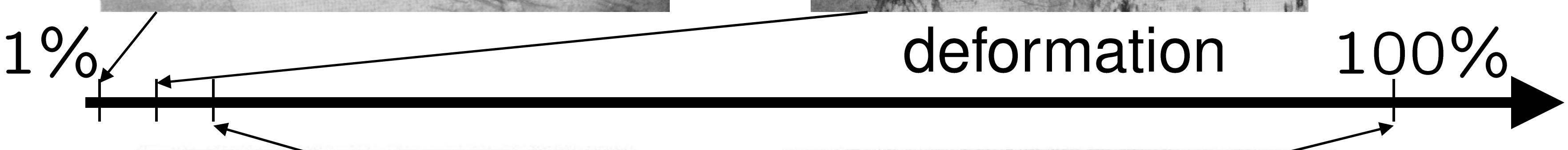

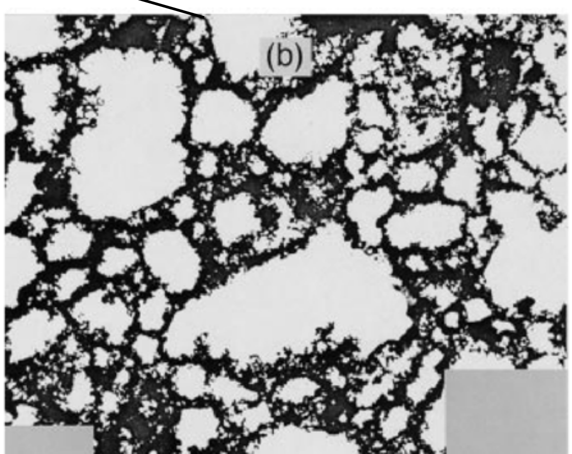

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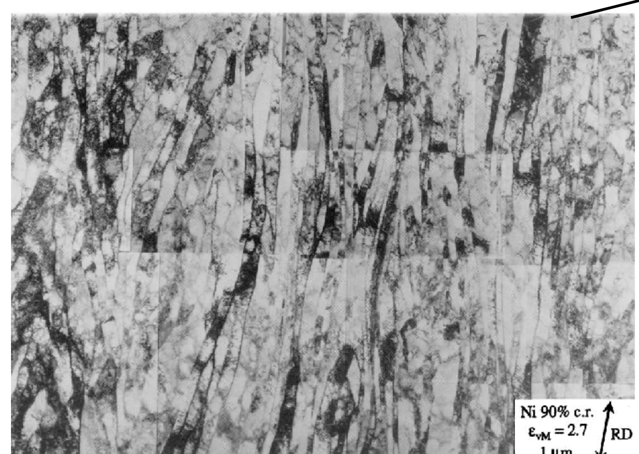


90% cold-rolled Ni (Hansen, Huang and Hughes, Mat. Sci. Engin. A **317**, 3, 2001)

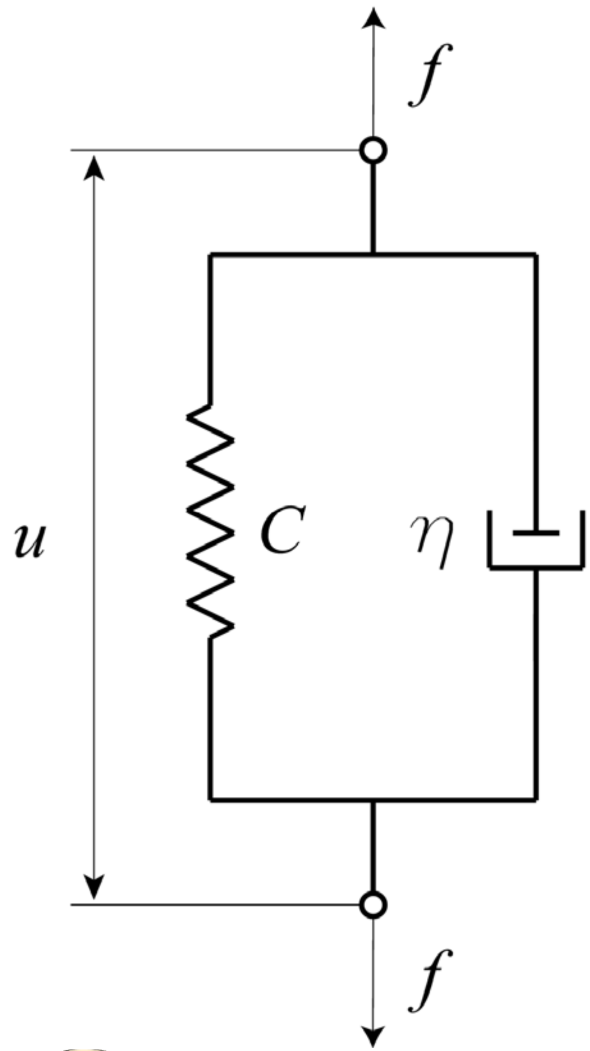
Systems with evolving microstructure

- The behavior of the systems of interest is governed by both energy and kinetics, e. g., through an **equation of evolution** of the form

$$\partial\Psi(\dot{u}) + DE(t,u) = 0, \begin{cases} \Psi \equiv \textit{dissipation potential} \\ E \equiv \textit{energy} \end{cases}$$

- However: Energies of interest often lack differentiability and lower-semicontinuity.
- Meaning of equation of evolution, ‘solutions’, time-discretized incremental problems?
- Wanted: Minimum principles that describe ***entire trajectories*** of the system

Classical rate variational problems



- Kelvin solid IV problem:

$$\left.\begin{aligned} &\eta\dot{u}(t) + Cu(t) = f(t) \\ &u(0) = u_0 \end{aligned}\right\}$$

- Potential energy:

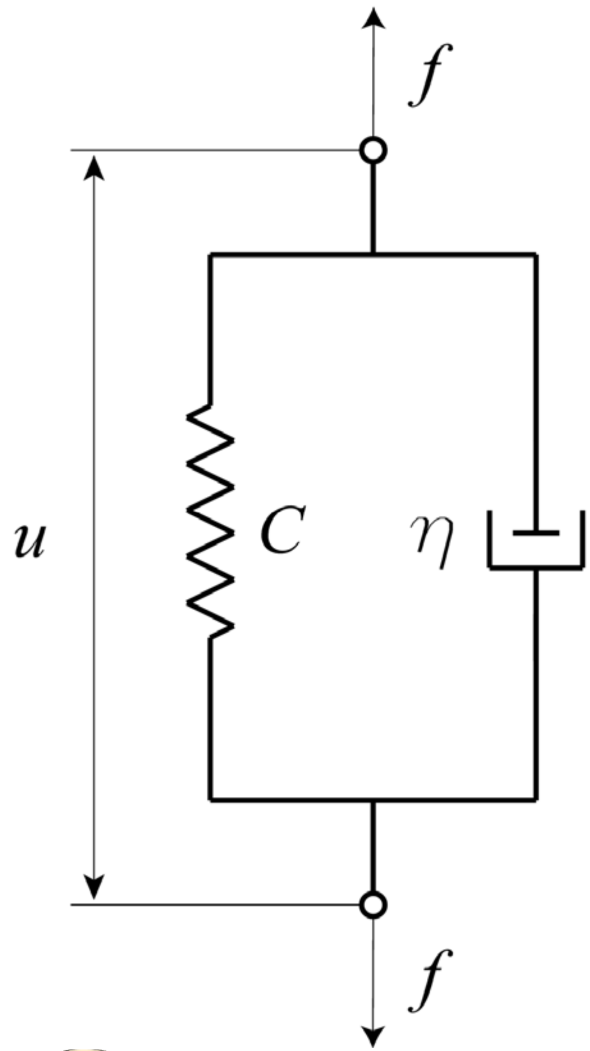
$$E(t,u) = \frac{C}{2}u^2 - f(t)u$$

- Dissipation potential: $\Psi(v) = \frac{\eta}{2}v^2$

- Force equilibrium:

$$\partial\Psi(\dot{u}(t)) + DE(t,u(t)) = 0$$

Classical rate variational problems



- Rate potential:

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

- Rate problem: Given t, u,

$$\min_v G(t, u, v)$$

- Euler-Lagrange equations:

$$\partial\Psi(v) + DE(t, u) = 0$$

- IV problem: For $t \in [0, T]$,

$$\left.\begin{aligned} & v(t) \in \operatorname{argmin} G(t, u(t), \cdot) \\ & \dot{u}(t) = v(t), \quad u(0) = u_0 \end{aligned}\right\}$$

Classical rate variational problems

- Classical rate problems only determine the rate of the system at a particular instant in time for given state of the system
- State *u*, force field *DE(u),* may not be defined for energies lacking differentiability, lower semicontinuity.
- Need: Minimum principles defined in terms of $\Psi(v)$ and $E(u)$ directly
- One approach: Time discretization

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

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

- Incremental problem: For $t_0, \dots, t_n, t_{n+1}, \dots,$ $u(t_0) = u_0$,

$$\inf_{u_{n+1} \in Y} F(u_{n+1}; u_n)$$

Rate problems – Time discretization

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

$$\inf_{u_1 \in Y} F(u_1; u_0) \to u_1$$

$$\inf_{u_2 \in Y} F(u_2; u_1) \to u_2$$

$$\cdots$$

- But incremental problems may lack attainment!
- Initial conditions for next minimum problem may be ill-defined → '***restart problem***'
- Instead: Form a single minimum principle for entire trajectories by combining all incremental problems in the sense of Pareto optimality

Energy-dissipation functionals

- Energy-dissipation functional: $\lambda_n > 0$, $u \in Y^N$,

$$F(u) \equiv \sum_{n=0}^{N-1} \lambda_{n+1} F(u_{n+1}; u_n) \to \text{inf!}$$

with *causal* weights: $\lambda_1 \gg \lambda_2 \gg \dots$

- Choose: $\lambda_n = \mathrm{e}^{-t_n/\epsilon}$, $\epsilon \to 0$ (*causal limit*).
- Formally, taking the limit of $\Delta t \to 0$,

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

- Minimum principle: $\mathbb{Y} = \{u : [0,T] \to Y\}$,

$$\inf_{u \in \mathbb{Y}} F_\epsilon(u)$$

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Energy-dissipation functionals

- Euler-Lagrange equations

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

- 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 ε

$$F_\epsilon(u) = \int_0^T \underbrace{\mathrm{e}^{-t/\epsilon}}_{\text{“Arrow of time”}} [\underbrace{\Psi(\dot{u})}_{\text{Dissipation}} + \underbrace{\frac{1}{\epsilon} E(t,u)}_{\text{Energy}}]\, dt + [\mathrm{e}^{-t/\epsilon} E]_0^T$$

Energy

Dissipation

“Arrow of time”

Example – Viscous bi-stable bar

Kohn & Müller, *Phil. Mag. A*, **66** (1992) 697.

- Energy: $$E(u) = \begin{cases} \int_0^1 |u_{xx}|\, dx, & \text{if } |u_x| = 1 \text{ a. e.,} \\ +\infty, & \text{otherwise.} \end{cases}$$
- Dissipation potential: $$\Psi(\dot{u}) = \int_0^1 u_t^2 dx$$
- Energy-dissipation functional: $F_\epsilon(u) =$

$$\begin{cases} \int_0^T \int_0^1 e^{-t/\epsilon} \left[u_t^2 + \frac{1}{\epsilon} |u_{xx}| \right] dx dt, & \text{if } |u_x| = 1 \text{ a. e.,} \\ +\infty, & \text{otherwise.} \end{cases}$$

- IBC: $u(x, 0) = 0;\ u(0, t) = u(1, t) = 0.$

Viscous bi-stable bar − Relaxation

- Neglect interfacial energy:

$$F_\epsilon(u) = \begin{cases} \int_0^T \int_0^1 e^{-t/\epsilon} u_t^2 \, dx dt, & \text{if } |u_x| = 1 \text{ a. e.,} \\ +\infty, & \text{otherwise.} \end{cases}$$

Theorem (S. Conti & MO). *The functional F_ϵ is coercive with respect to the weak topology of $W^{1,2}$. Its relaxation is*

$$sc^- F_\epsilon(u) = \begin{cases} \int_0^T \int_0^1 e^{-t/\epsilon} u_t^2 dx dt & \textit{if } |u_x| \leq 1 \textit{ a. e.} \\ +\infty & \textit{otherwise.} \end{cases}$$

Viscous bi-stable bar − Relaxation

- By inspection of *sc⁻F*$_\varepsilon$*(u)*:

$$\Psi^{\text{eff}}(\dot{u}) = \int_0^1 u_t^2 dx$$

$$E^{\text{eff}}(u) = \begin{cases} 0, & \text{if } |u_x| \leq 1 \text{ a. e.} \\ +\infty, & \text{otherwise.} \end{cases}$$

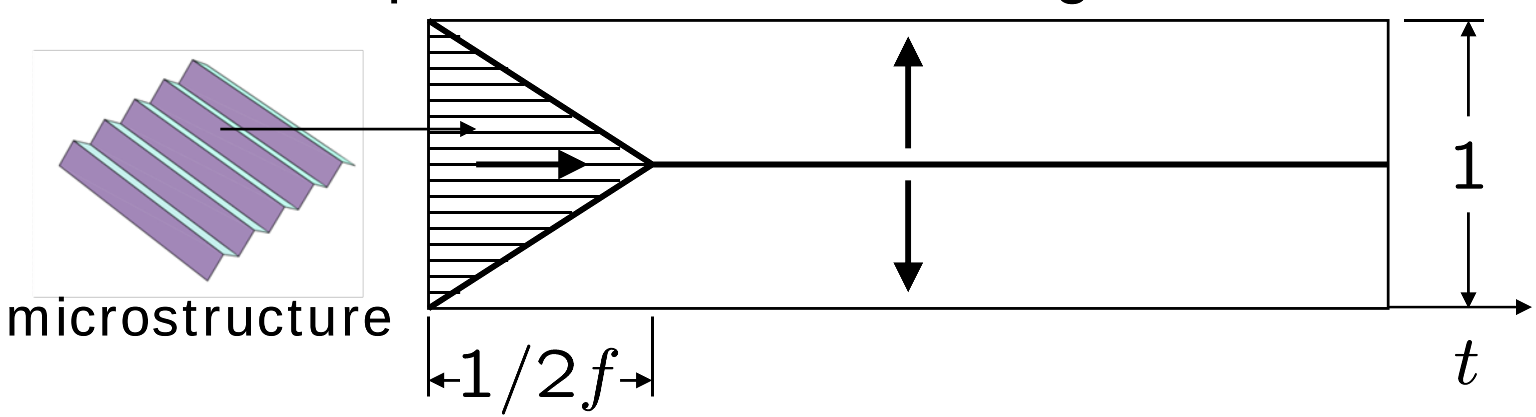
- *sc⁻F*$_\varepsilon$*(u)* is the energy-dissipation functional defined by $\Psi^{eff}(v)$ and $E^{eff}(u)$ for all ε.
- Can regard $\Psi^{eff}(v)$ and $E^{eff}(u)$ as an effective dissipation potential and an effective energy of the system, respectively.

Viscous bi-stable bar − Relaxation

- The relaxed energy-dissipation functional:

$$sc^{-}F_{\epsilon}(u) = \begin{cases} \int_0^T \int_0^1 e^{-t/\epsilon} u_t^2 \, dx dt & \text{if } |u_x| \leq 1 \text{ a. e.} \\ +\infty & \text{otherwise.} \end{cases}$$

  describes the 'macroscopic trajectories' of system
- Macroscopic trajectories *u* with $|u_x| \leq 1$ can be attained as weak limits of microscopic trajectories v^k with $|v^k_x| = 1$ a. e.
- Example: Add constant forcing *f*,



Viscous bi-stable bar – Scaling

- Include interface energy: $F_\epsilon(u) =$

$$\begin{cases} \int_0^T \int_0^1 e^{-t/\epsilon} \left[u_t^2 + \frac{1}{\epsilon} |u_{xx}| \right] dx dt, & \text{if } |u_x| = 1 \text{ a. e.,} \\ +\infty, & \text{otherwise.} \end{cases}$$

- Heuristic one-dimensional model: $d : [0, T] \to [0, \infty) \equiv$ typical length scale, $d(0) = 0$,

$$F_\epsilon(u) \sim F_\epsilon(d) = \int_0^T e^{-t/\epsilon} \left(d_t^2 + \frac{1}{\epsilon}\frac{1}{d} \right) dt$$

- Explicit solution: $\inf F_\epsilon \sim \epsilon^{-1/3}$,

$$d \sim \begin{cases} t^{2/3}\epsilon^{-1/3}, & \text{if } t < \epsilon \\ t^{1/3}, & \text{if } t > \epsilon \end{cases}$$

Viscous bi-stable bar − Scaling

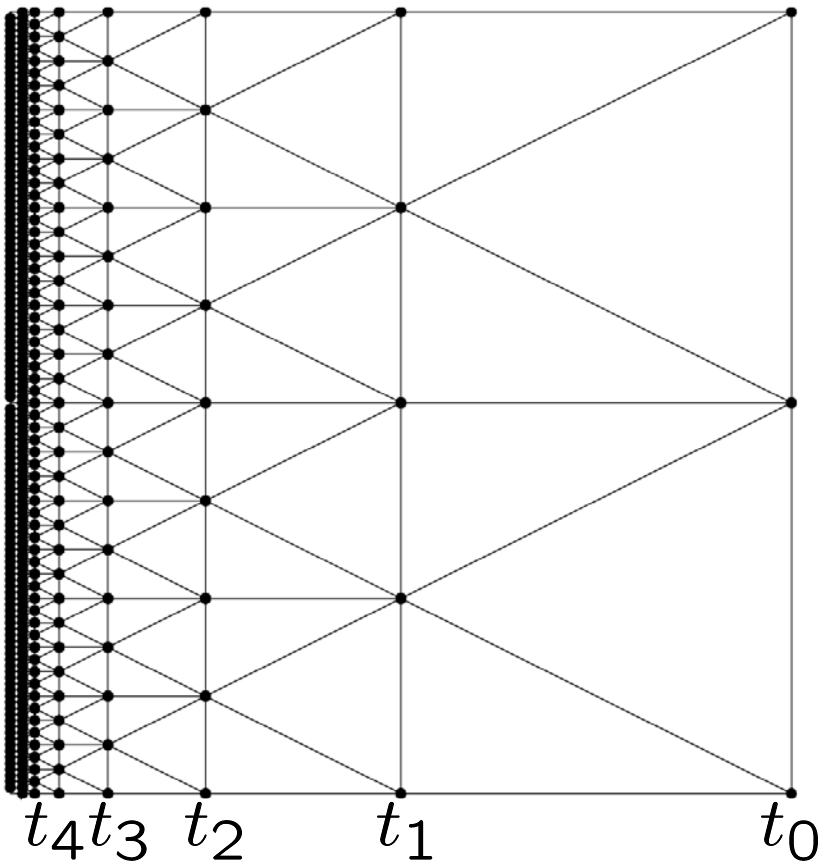
Theorem (S. Conti & MO). *There is* $c > 0$ *such that for any* $\epsilon \in (0,1)$, *and any* $T > \epsilon$,

$$\frac{c}{\epsilon^{1/3}} \leq \inf F_\epsilon(u) \leq \frac{1}{c\epsilon^{1/3}}.$$

- Proof of the upper bound follows the original ideas of Kohn and Müller ’94.
- Proof of the lower bound follows Conti, *Cont. Mech. Thermod.*, **17** (2006) 469.

Viscous bi-stable bar – Scaling

Sketch of upper bound.



- From construction, $d_i = 2^{-i}$:

$$E \leq c \sum_i e^{-t_i/\epsilon} \left(\frac{d_i^2}{t_i} + \frac{1}{\epsilon} \frac{t_i}{d_i} \right)$$

- From heuristics:

$$t_i = \begin{cases} d_i^{3/2} \epsilon^{1/2}, & \text{if } d_i < \epsilon^{1/3} \\ d_i^3, & \text{if } d_i \geq \epsilon^{1/3} \end{cases}$$

- Estimating: $E \leq \dfrac{1}{c\epsilon^{1/3}}$

- Causal limit $\epsilon \to 0$: $d \sim t^{1/3}$ for $t > 0$.

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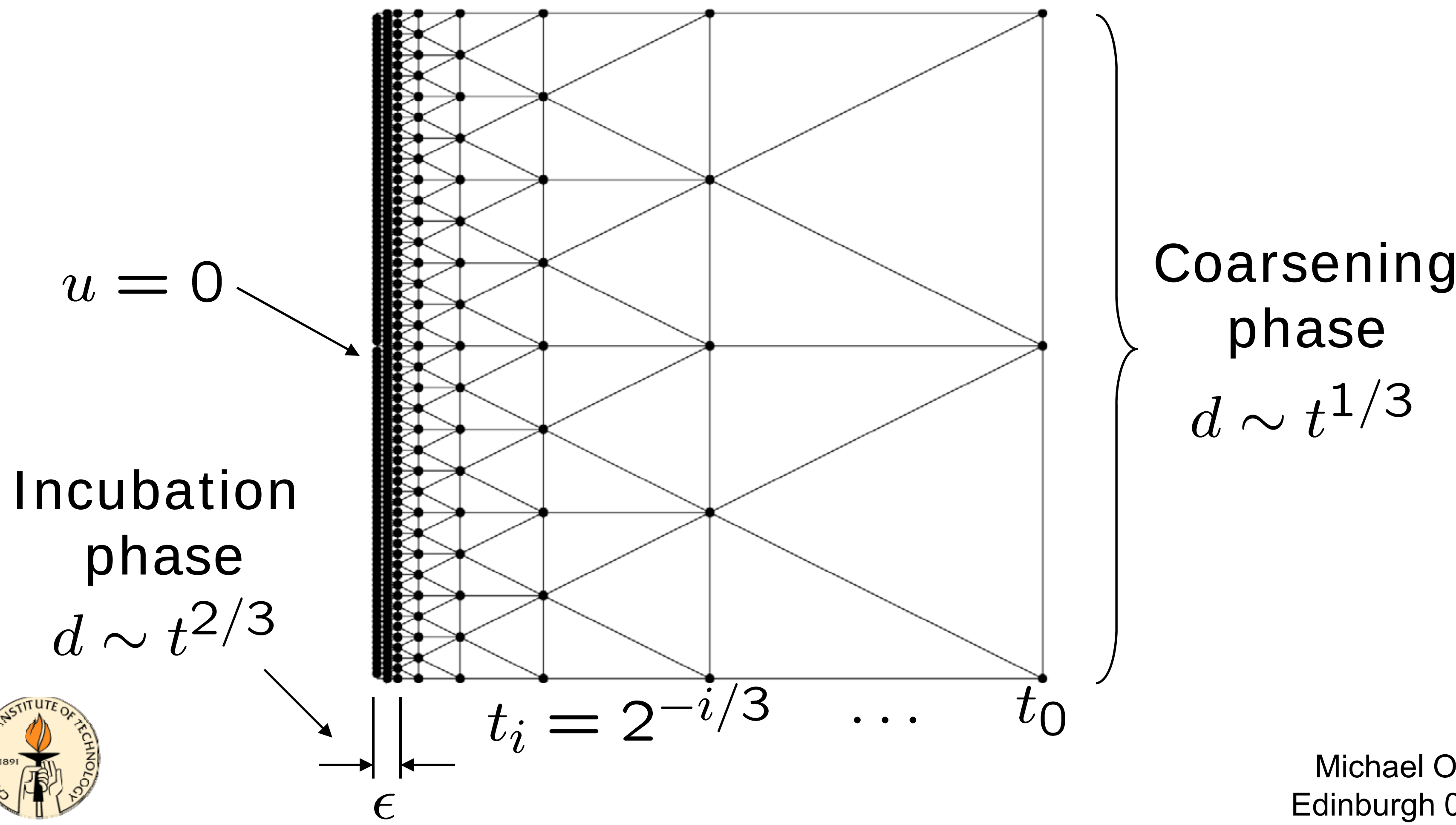
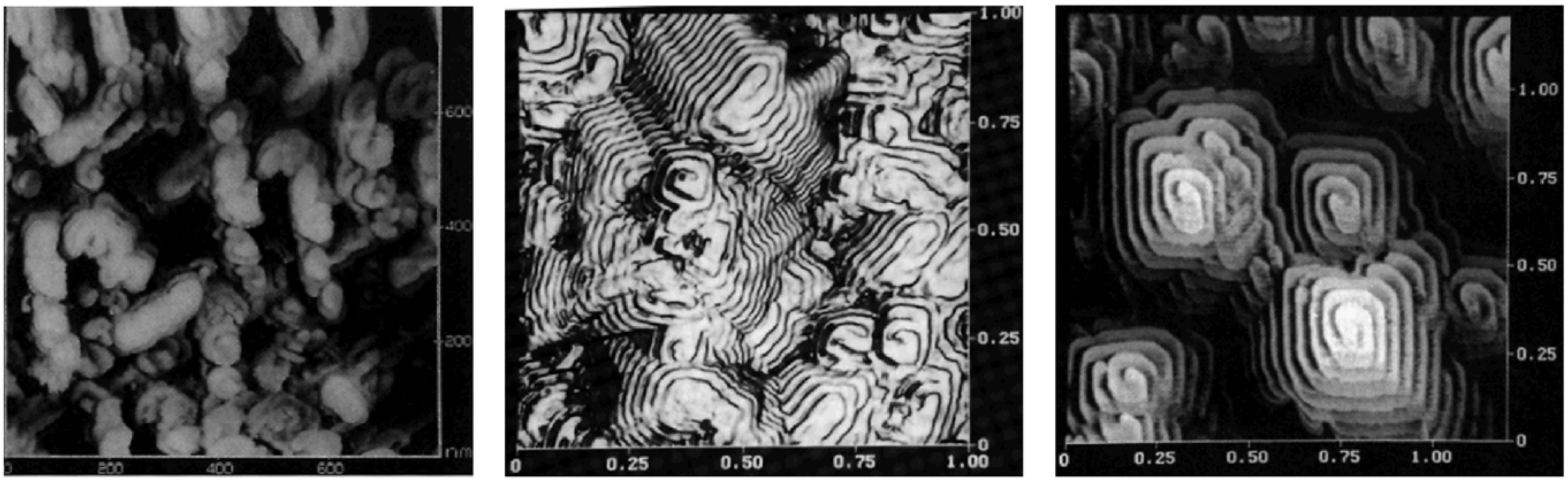
Viscous bi-stable bar − Relaxation

- Upper bound construction provides ‘insight’ into the likely evolution of microstructure.



Example − Epitaxial thin-film growth



(a) $h = 10nm$ (b) $h = 160nm$ (c) $h = 500nm$

Sputtered YBCO Film on MgO substrate

I.D. Raistrick and H. Hawley, in: S.L. Shinde and D.A. Rudman (eds.) Interfaces in High T_c Superconducting Systems, Springer-Verlag, 1994.

Example – Epitaxial thin-film growth

MO, Repetto & Si, *JMPS*, **47** (1999) 697.

- Energy: $K = \{(0,\pm 1),(\pm 1,0)\}$,

$$E(u) = \begin{cases} \int_{(0,1)^2} |\nabla^2 u| dx dt, & \nabla u \in K \text{ a. e.} \\ +\infty, & \text{otherwise} \end{cases}$$

- Dissipation potential: $\Psi(\dot{u}) = \int_{(0,1)^2} u_t^2 dx$

- Energy-dissipation functional: $F_\epsilon(u) =$

$$\begin{cases} \int_0^T \int_{(0,1)^2} e^{-t/\epsilon} \left[u_t^2 + \frac{1}{\epsilon}|\nabla^2 u| \right] dx dt, & \nabla u \in K \text{ a. e.} \\ +\infty, & \text{otherwise} \end{cases}$$

- IBC: $u(x,0) = 0$; $u(x,t) = 0$ on $\partial(0,1)^2$.

Epitaxial thin-film growth − Relaxation

- Neglect interfacial energy:

$$F_\epsilon(u) = \begin{cases} \int_0^T \int_{(0,1)^2} e^{-t/\epsilon} u_t^2 \, dx dt, & \nabla u \in K \text{ a. e.} \\ +\infty, & \text{otherwise} \end{cases}$$

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Epitaxial thin-film growth − Relaxation

- By inspection of *sc⁻F*$_\varepsilon$*(u)*:

$$\Psi^{\text{eff}}(\dot{u}) = \int_{(0,1)^2} u_t^2 \, dx$$

$$E^{\text{eff}}(u) = \begin{cases} 0, & \text{if } |\partial_1 u| + |\partial_2 u| \leq 1 \text{ a. e.} \\ +\infty, & \text{otherwise} \end{cases}$$

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Epitaxial thin-film growth − Relaxation

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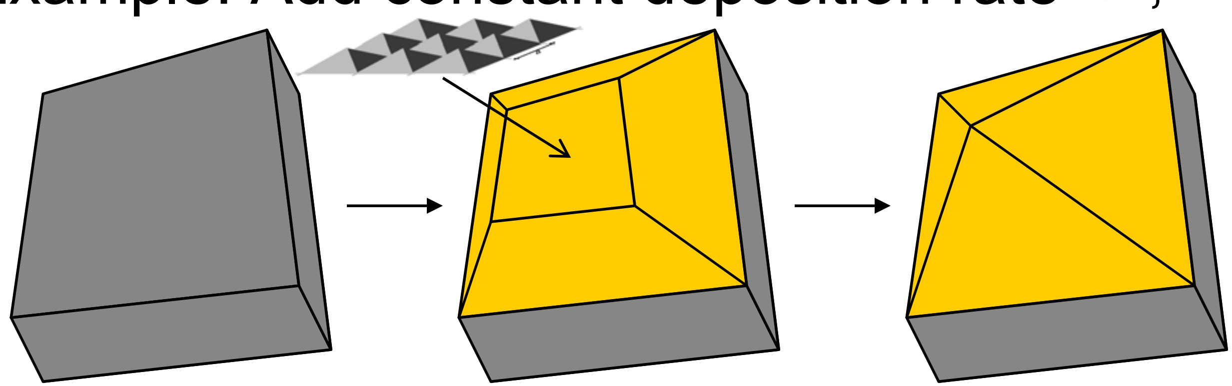
describes the 'macroscopic trajectories' of system
- Macroscopic trajectories u with $\nabla u \notin K$ can be attained as weak limits of microscopic trajectories v^k with $\nabla v^k \in K$ a. e.
- Example: Add constant deposition rate V,



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Epitaxial thin-film growth − Scaling

- Include interface energy: $F_\epsilon(u) =$

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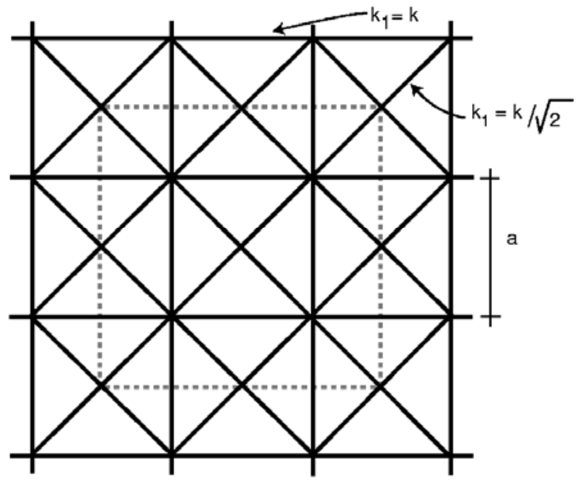
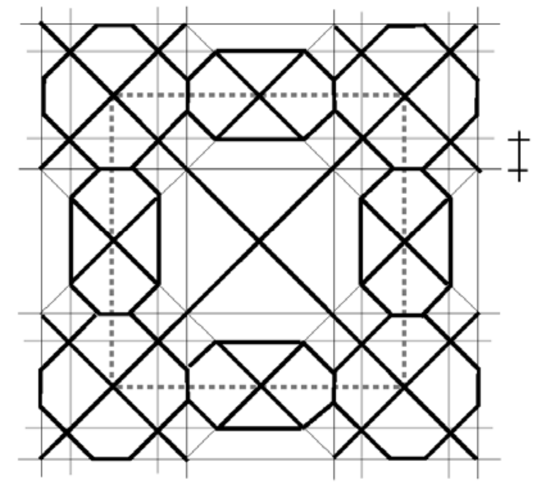
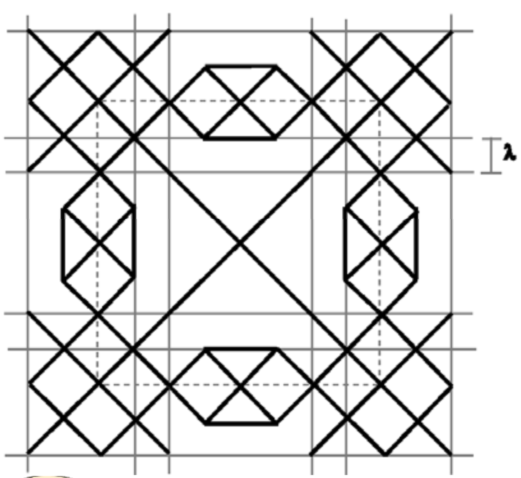
$$\frac{c}{\epsilon^{1/3}} \leq \inf F_\epsilon(u) \leq \frac{1}{c\epsilon^{1/3}} .$$

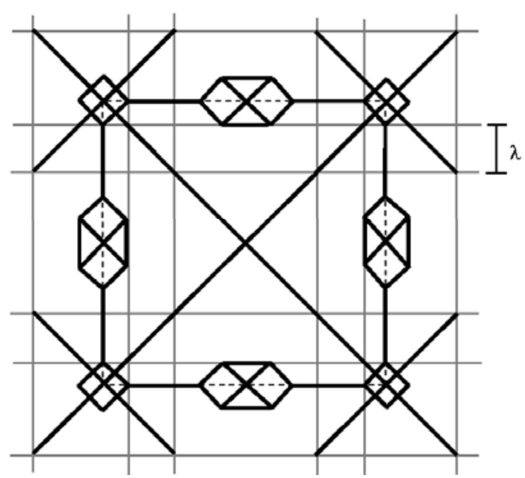
Epitaxial thin-film growth − Scaling

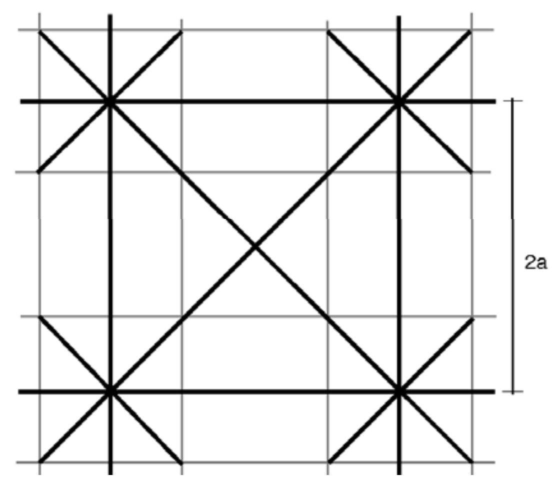
Upper bound construction:



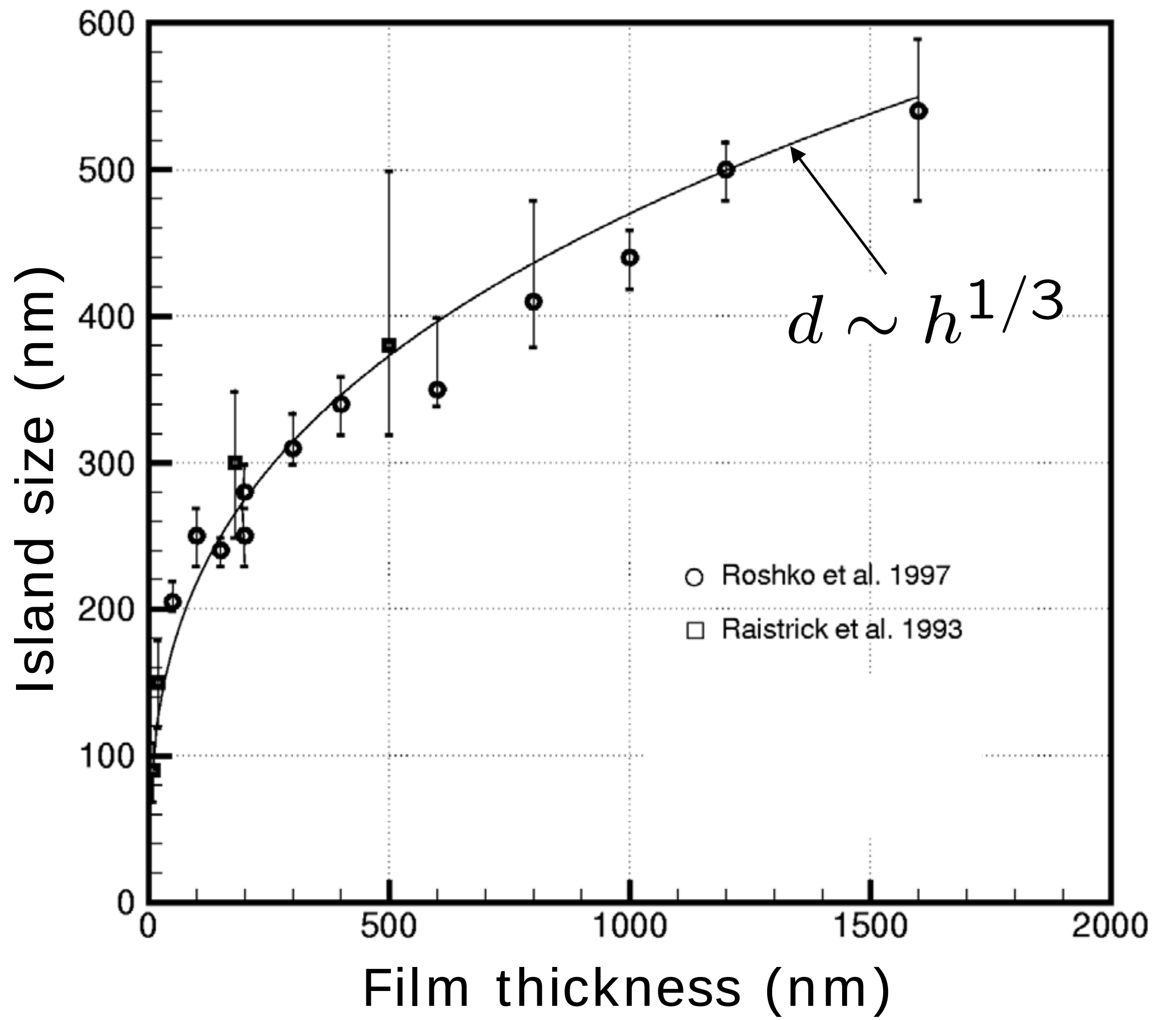








Epitaxial thin-film growth − Scaling



Island size vs average film thickness.
Data by Raistrick and Hawley (1993)
And Roshko et al. (1997)

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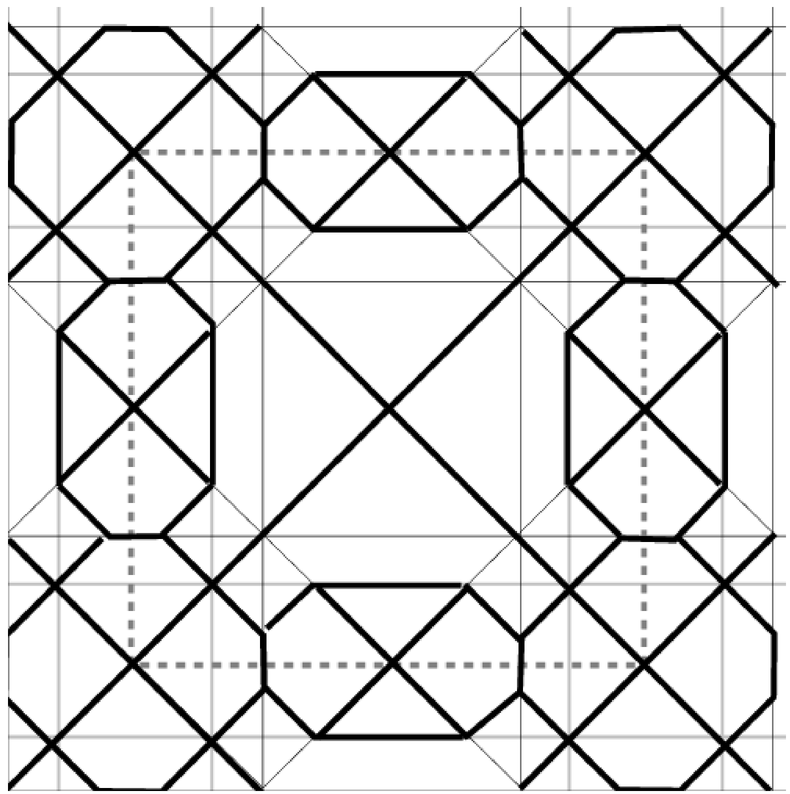
Epitaxial thin-film growth − Scaling

- Approach can predict key features of microstructure evolution such as scaling relations, time exponents
- Upper bound construction provides ‘insight’ into the likely evolution of microstructure.



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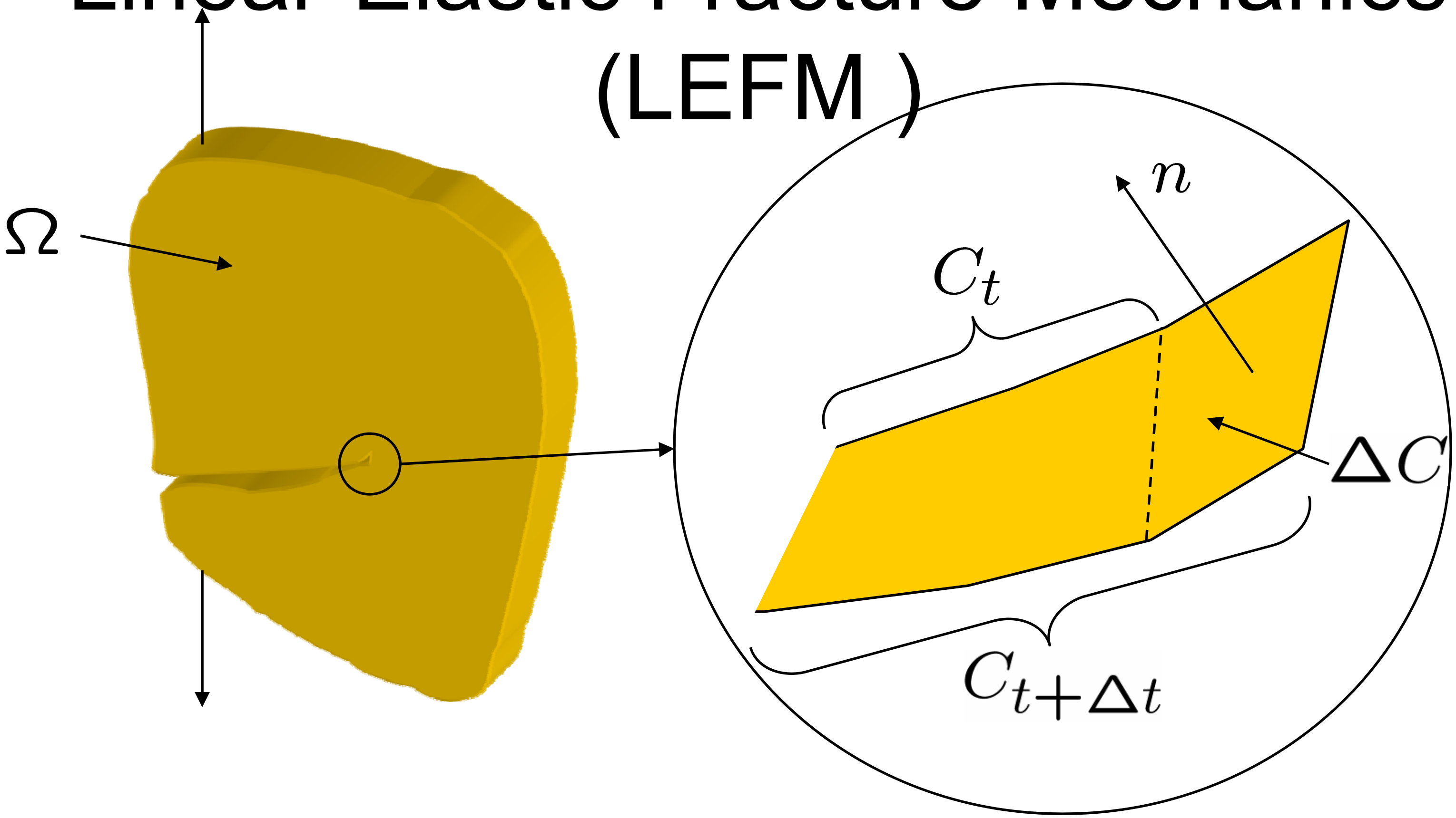
Linear-Elastic Fracture Mechanics (LEFM)



- Assume regularity, smoothness . . .
- Load increment, crack extension:

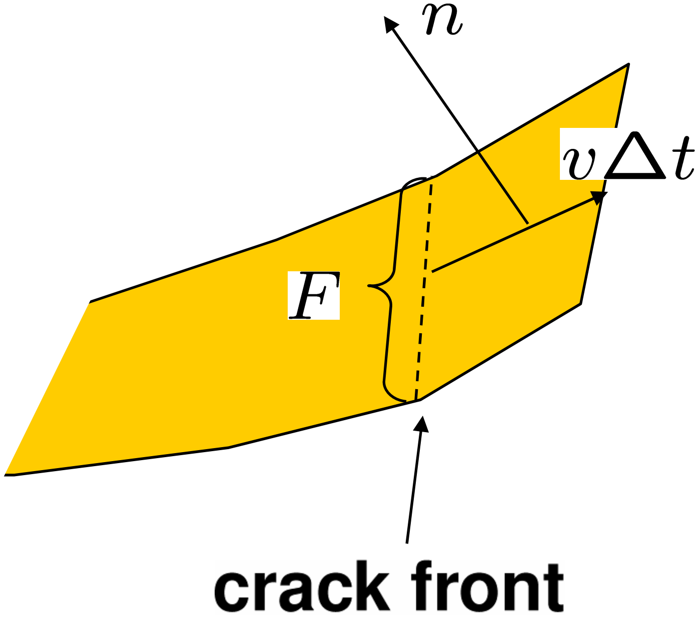
$$-\Delta E = \int_{\Delta C} [DW(\nabla u_t)\, n] \cdot [\![u_{t+\Delta t}]\!] \, d\mathcal{H}^2 + h.o.t.$$

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:

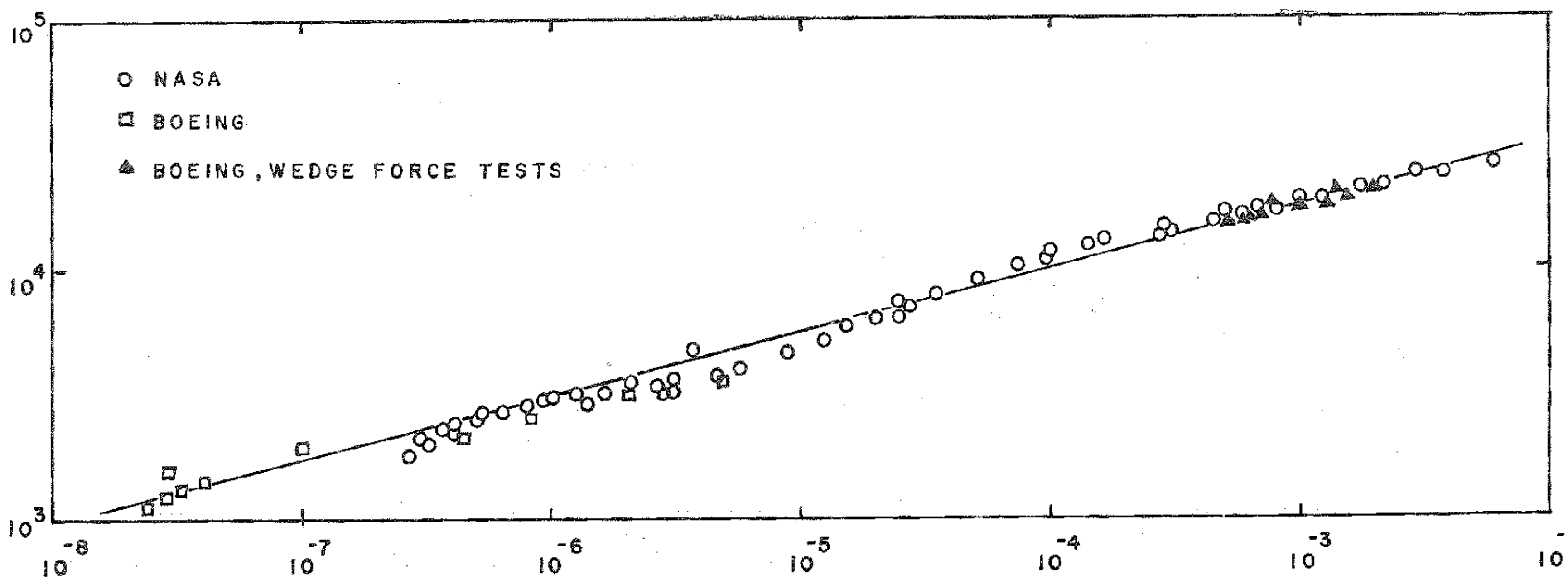
$$f(n) = \lim_{\Delta t \to 0} \frac{1}{\Delta t} [DW(\nabla u_t)\, n] \cdot [\![u_{t+\Delta t}]\!]$$

- 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



stress-intensity factor (lbs/in$^{3/2}$)

da/dN (in/cycle)

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

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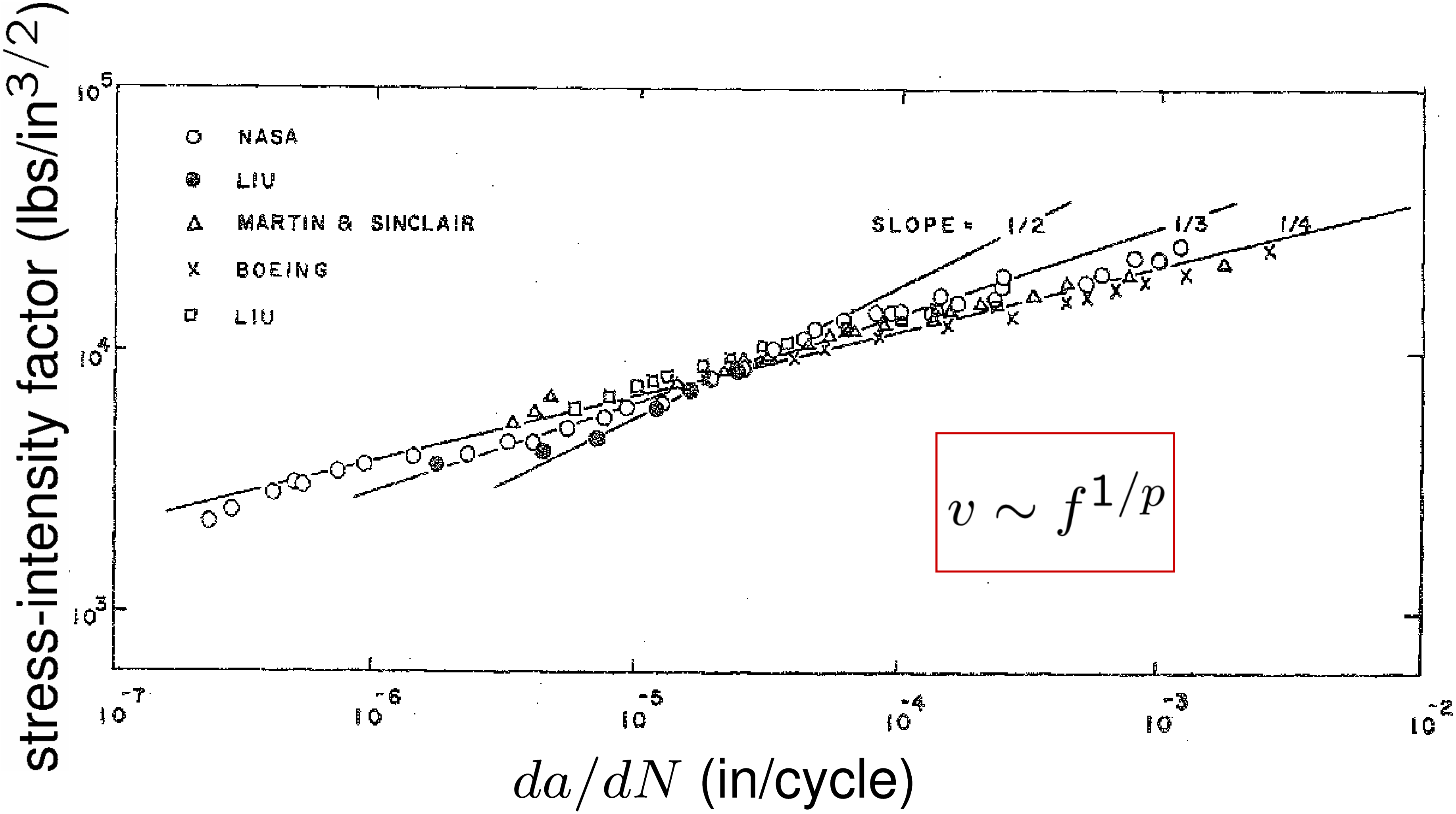
The rate problem of LEFM



Crack-growth data for 2024-T3 aluminum alloy
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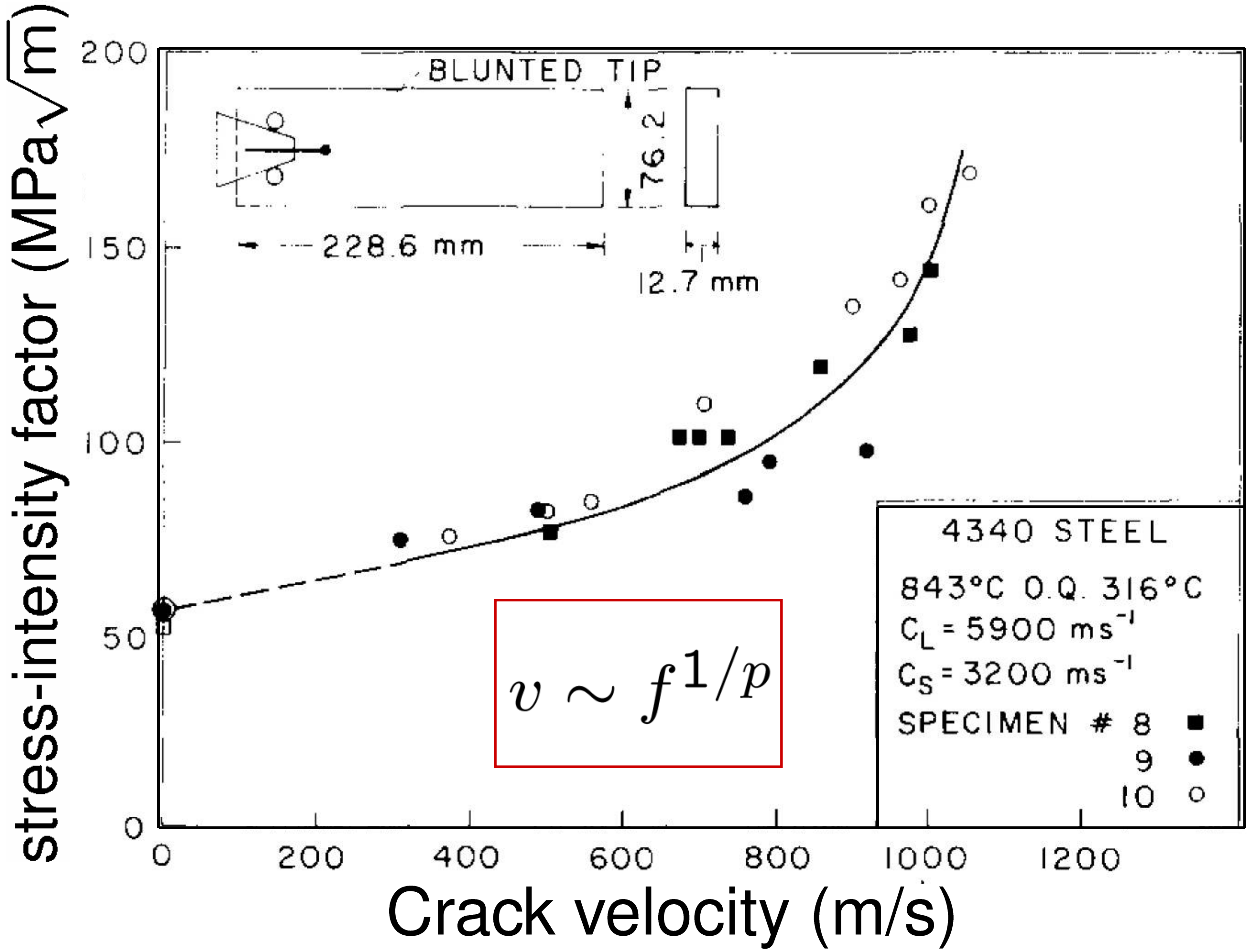
The rate problem of LEFM

Dynamic crack-tip equation of motion



$$v \sim f^{1/p}$$

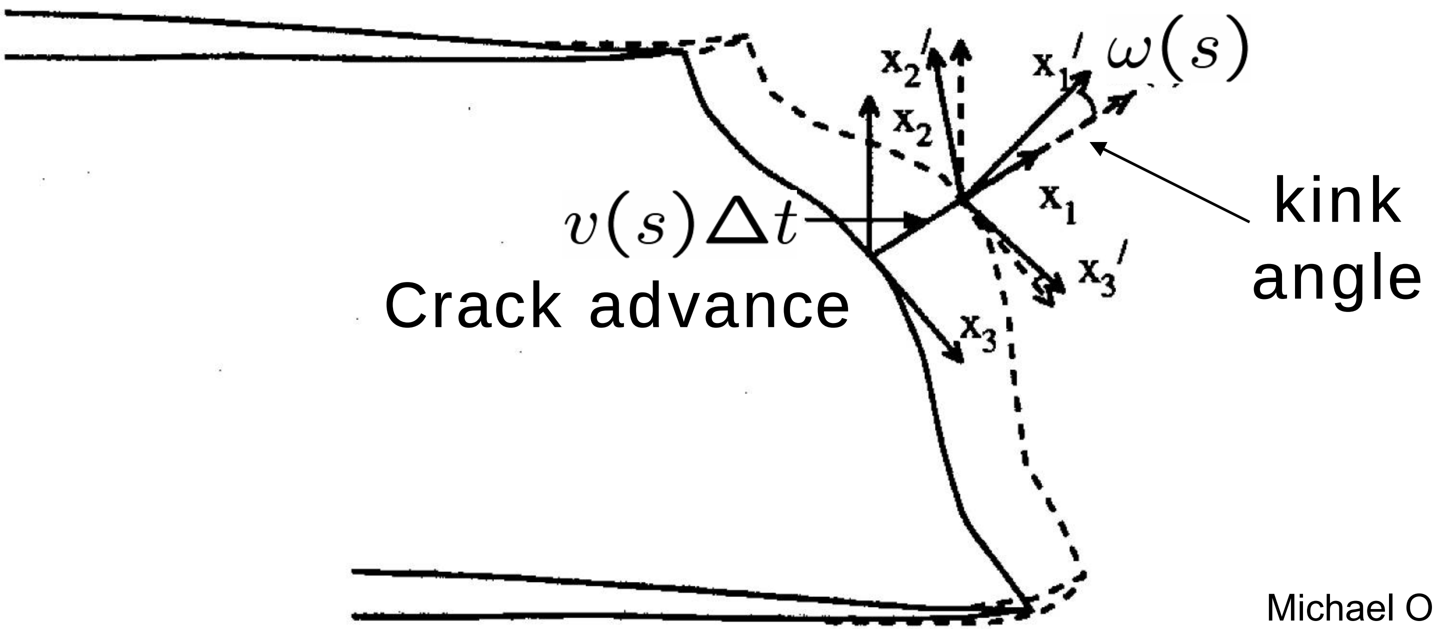
Rosakis, Duffy and Freund, *JMPS* (1984)

The rate problem of LEFM

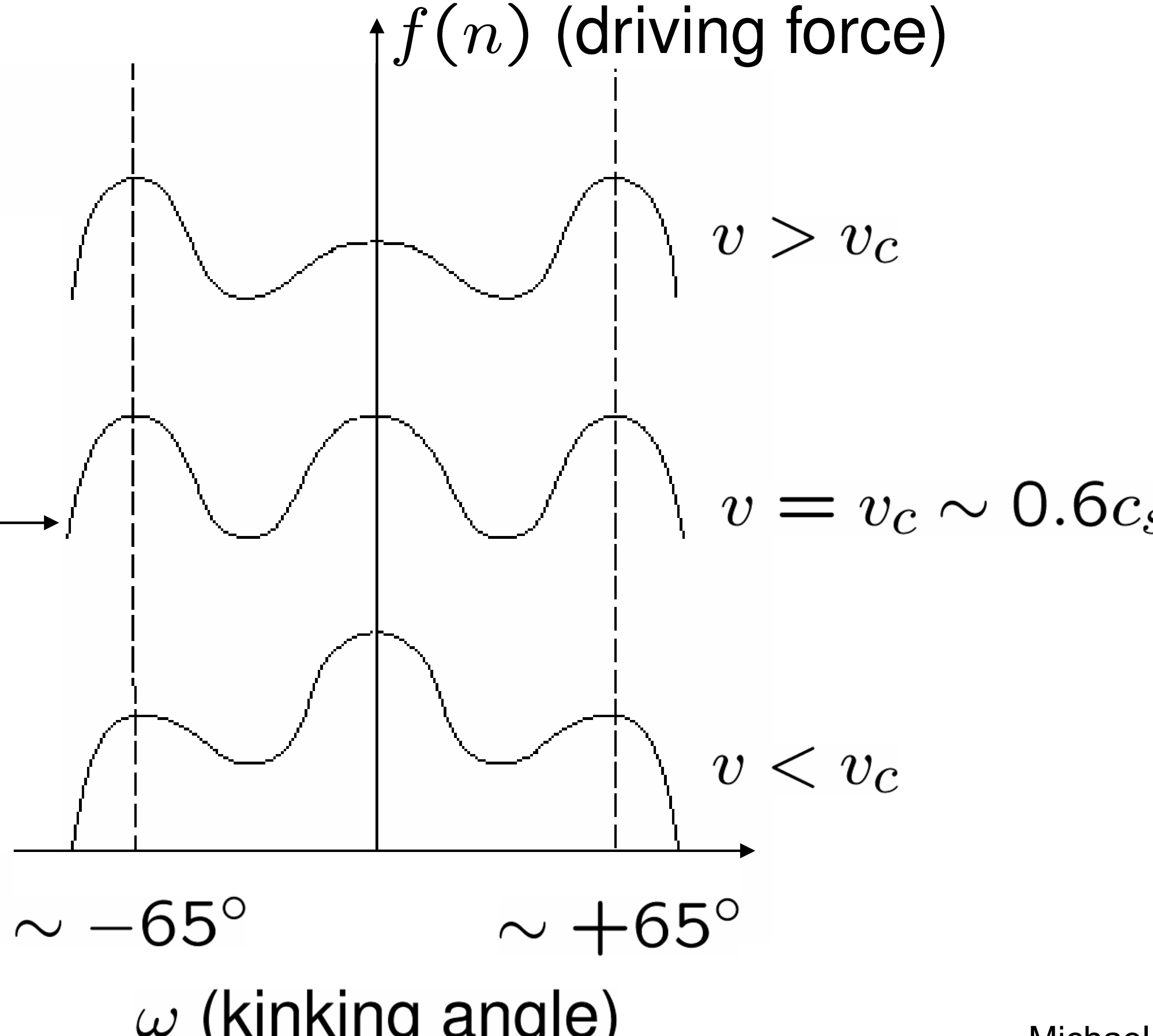
- Rate problem: $\inf_{v,n} \int_F [\psi(v) - f(n)\, v] \, d\mathcal{H}^1$

$$\Rightarrow \left\{ \begin{array}{l} \partial\psi(v) = f(n) \\ \partial\psi^*(f(n)) = 0 \end{array} \right\} \longrightarrow (v, n)$$

(maximum driving force)



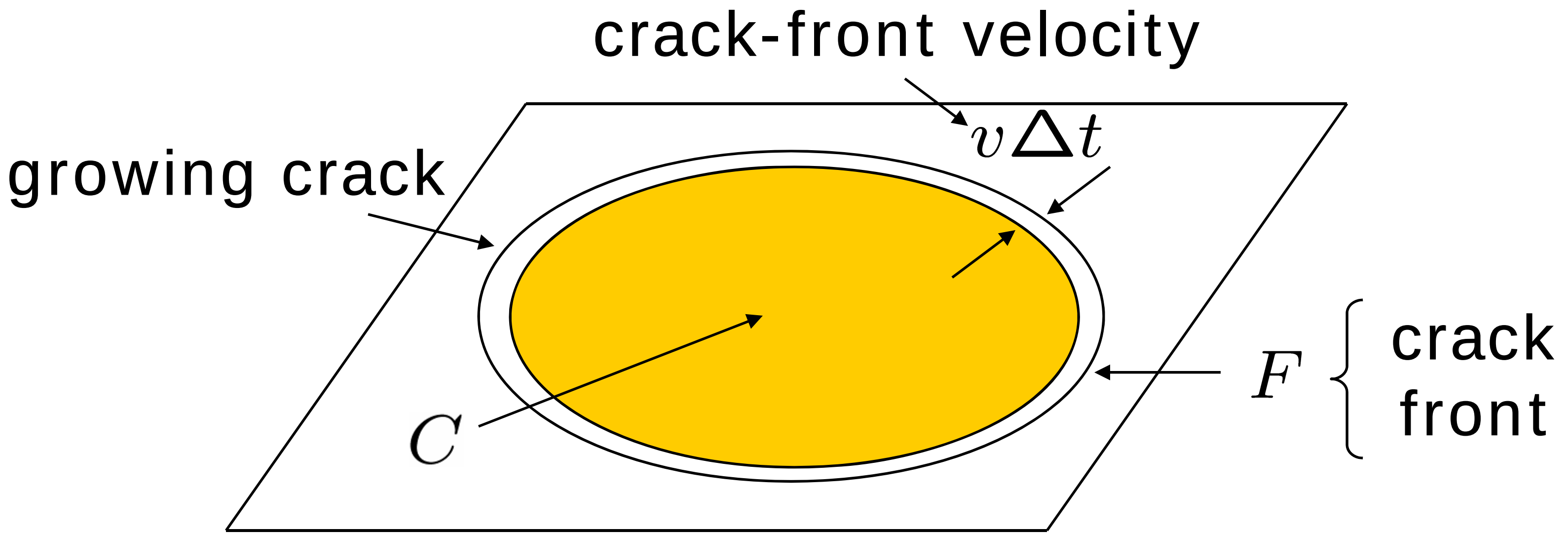
LEFM rate problem — Dynamics



branching instability

E.H. Yoffe, *Phil. Mag.* (1951)

LEFM energy-dissipation functionals



- Crack set: C, $0 < \mathcal{H}^{n-1}(C) < +\infty$.
- Crack-front measure: $\forall \varphi \in C_0^1([0,T])$, $\forall f \in C_0(\Omega)$,

$$\int_0^T \dot{\varphi} \int_{C(t)} f \, d\mathcal{H}^{n-1} dt = -\int_0^T \varphi \int_\Omega f \, d\mu_t(x) dt$$

- Crack front, velocity: $d\mu_t = v_t d\mathcal{H}^{n-2} \lfloor F(t)$.

LEFM energy-dissipation functionals

- Trajectories: $\mathbb{Y} \sim \{u(t) \in SBV_p(\Omega), J_u$ increasing$\}$.
- Energy-dissipation functional:

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

- Energy: $E(u) = \int_\Omega W(\nabla u)\, dx$
- Dissipation: $\Psi(v) = \int_{F(t)} (\alpha + v^p)\, d\mathcal{H}^{n-2}$

nucleation energy (→ α)

rate-dependent crack-tip equation of motion (→ v^p)

LEFM energy-dissipation functionals

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

$$sc^- F_\epsilon(p) =$$

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

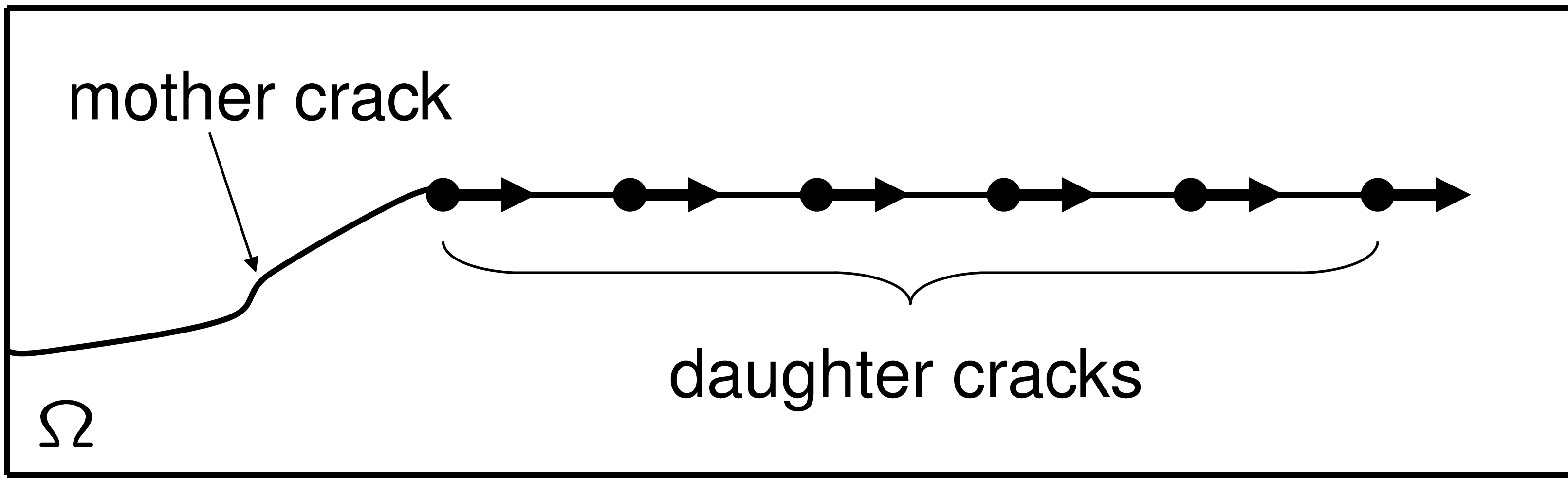
where: $\gamma = p \left(\frac{\alpha}{p-1} \right)^{\frac{p-1}{p}}$

- Relaxed energy-dissipation functional is **rate-independent**!

Michael Ortiz
Edinburgh 06/08

LEFM energy-dissipation functionals

Sketch of proof: Mother-daughter mechanism:



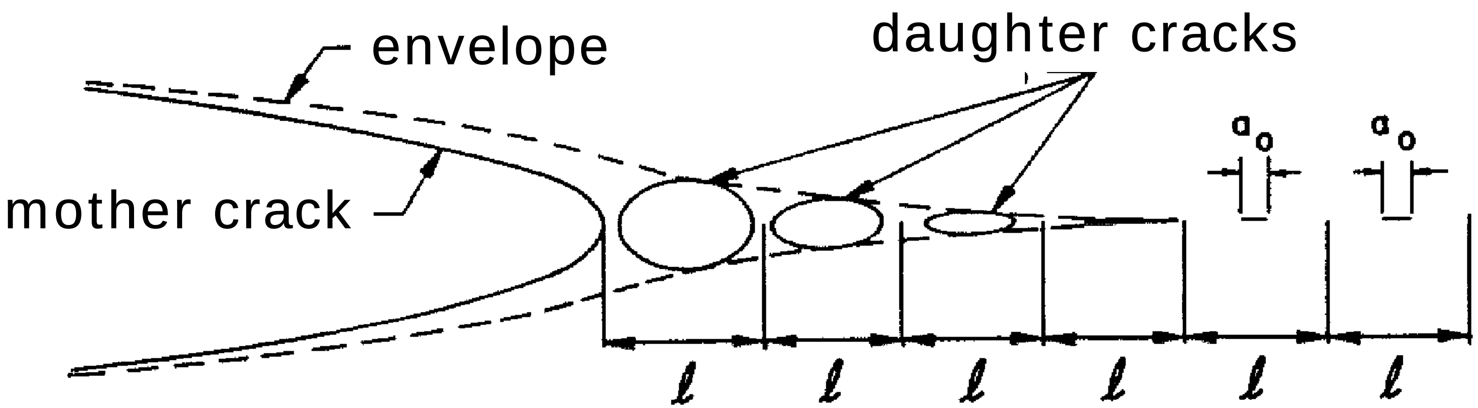
- Twin daughters (optimal by Jensen's inequality):

$$\Psi = n\alpha + n\left(\frac{v}{n}\right)^{p} \to \text{min} \Rightarrow$$

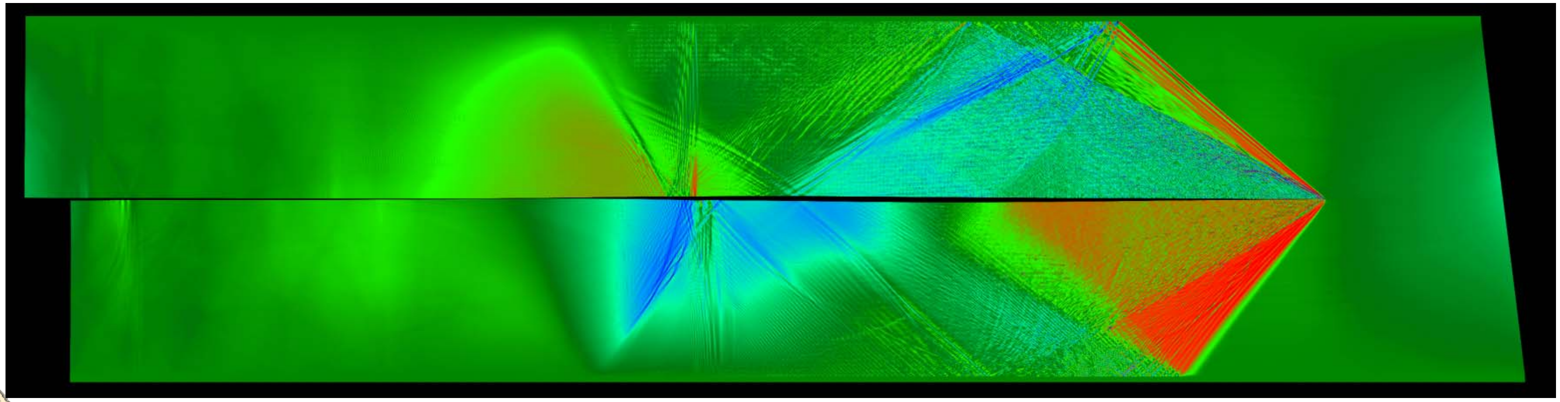
$$n_{\text{min}} = \left(\frac{p-1}{\alpha}\right)^{(1/p)} v, \quad \Psi_{\text{min}} = p\left(\frac{\alpha}{p-1}\right)^{(1-1/p)} v$$

LEFM energy-dissipation functionals

- The mother-daughter crack mechanism:



(Ortiz, *IJSS*, 1988)



(F. Abraham, M. Buehler, H. Gao...)

Concluding remarks

- Energy-dissipation functionals provide a useful tool for understanding microstructure evolution within the framework of the calculus of variations.
- They help to identify the ‘effective’ kinetics and energetics of systems that exhibit evolving microstructure
- Recovery sequences yield insight into microstructural evolution mechanisms
- Causal limit?
- Inertia?