Probabilistic failure mechanisms in fatigue life and optimal reliability via shape control

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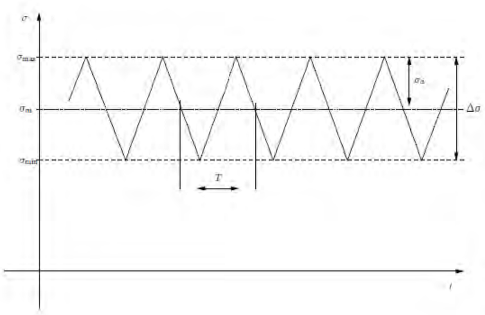
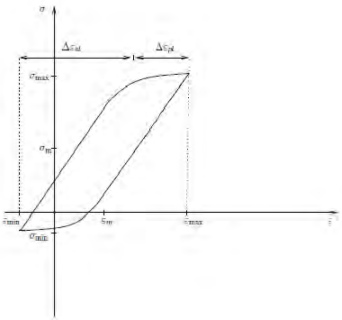
The Irsching Gas Turbine Accident 1987

- Catastrophic accidents are caused by microscopic flaws in the material
- Need material science input to develop service concepts
- These models should be probabilistic - however often they aren't

Elastic-Plastic Material Behaviour



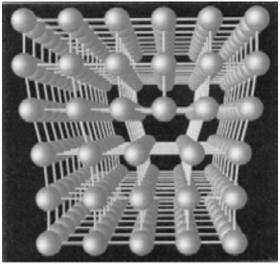


- Under cyclic loading, the material undergoes a elasto-plastic deformation
- The non linear plastic behaviour in the strain-stress hysteresis is a consequence of microscopic motion of 1D lattice defects

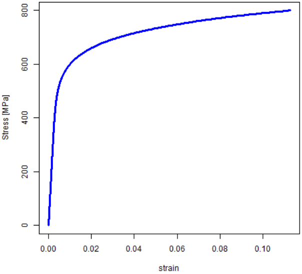
Motion of Linear Displacements

- Linear displacements (1D lattice defects) ’travel’ along slip systems . . .
- . . . and create intrusions and extrusions at the surface . . .
- . . . . . . which initiates a fatigue crack!

(Image from Gottstein – Physical Foundations of Material Science)



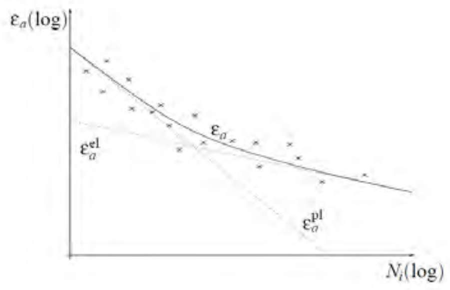
Deterministic Life Prediction



$$\varepsilon = \frac{\sigma}{E} + \left(\frac{\sigma}{K}\right)^{1/n'}$$

- σ stress (uniaxial), ε strain
- E Young's modulus, K scale for onsetting plasticity, n' hardening exponent

Low Cycle Fatigue – Strain Life Relation



$$\varepsilon_a = \frac{\sigma_f'}{E}(2\mathrm{N}_{\mathrm{det}})^b + \varepsilon_f'(2\mathrm{N}_{\mathrm{det}})^c$$

- Coffin-Manson Basquin Equation ($b, c < 0$, $\sigma_f', \varepsilon_f' > 0$ CMB parameters)

Elasticity PDE

- $\Omega \subseteq \mathbb{R}^3$ area filled with material – 'shape' of the design
- $u : \Omega \to \mathbb{R}^3$ displacement field – under given loads
- $\varepsilon(u) = \frac{1}{2}(Du + Du^T)$ linearised strain tensor in the material
- $\sigma(u) = \lambda \mathrm{tr}(\varepsilon(u))I + 2\mu\varepsilon(u)$, elastic stress field (linearised)
- Elasticity - PDE (Newton's 2nd law)

$$-\mathrm{div}\sigma(u) = f$$

- Boundary conditions $\sigma(u)n = g$, n unit normal vector field on $\partial\Omega_N$ and $u = 0$ on $\partial\Omega_D$. $\partial\Omega = \partial\Omega_D \cup \partial\Omega_N$ (displacement-traction problem).
- Convert $\sigma(u)$ in elastic-plastic equivalent stress and determine the deterministic LCF life $N_{\mathrm{det}}(\Omega) = \inf_{x\in\partial\Omega} N_{\mathrm{det}}(\sigma(u(x)))$.

Crack Initiation Histories

- $\mathcal{C} = [0, \infty) \times \partial\Omega$ configuration space for crack initiation.
- $\gamma : \mathcal{B}(\mathcal{C}) \to \mathbb{N} \cup \{\infty\}$ simple Radon counting measure $(\mathcal{C}, \mathcal{B}(\mathcal{C}))$

$$\gamma \restriction_{(0,T]\times\partial\Omega} = \sum_{j=1}^{N(T)} \delta_{c_j}, \; c_j = (t_j, x_j) \in \mathcal{C}$$

  Interpretation: A possible history of crack initiations.
- Time of first crack initiation, given history γ:

$$T_i(\gamma) = \inf\{t \geq 0 : \gamma((0,t] \times \partial\Omega) > 0\}.$$

Crack Initiation Processes

- $(\mathcal{R}, \mathcal{B}) =$ space of all simple Radon counting measures with σ-algebra $\mathcal{B} = \sigma\left(\gamma \to \gamma(A) : A \in \mathcal{B}(\mathcal{C})\right)$.
- **Def.:** A non atomic simple point process is a measurable mapping

$$\Gamma : (\mathscr{X}, \mathcal{A}, P) \to (\mathcal{R}, \mathcal{B}), \quad P(\Gamma(\{c\}) > 0) = 0.$$

- **Theorem (Kallenberg):** Every non atomic simple point process with independent increments is a Poisson Point Process (PPP)

$$\Gamma(A_1), \ldots, \Gamma(A_j) \text{ u.h. for } A_i \cap A_j = \emptyset \; i \neq j \;\Rightarrow\; \Gamma \text{ is PPP.}$$

- $\exists \rho$ Radon measure on $(\mathcal{C}, \mathcal{B}(\mathcal{C}))$ – 'intensity measure'– such that

$$P(\Gamma(A) = n) = e^{-\rho(A)} \frac{\rho(A)^n}{n!}$$

- $\forall\, \rho$ Radon $\exists!$ PPP Γ with intensity measure ρ.

A Local Probabilistic Model for LCF

- For every shape Ω and every load f, g we require a crack initiation process $\Gamma(\Omega, f, g)$.
- If crack initiations do not influence each other, it suffices to define a Radon measure $\rho(\Omega, f, g)$ auf $\mathcal{C}(\Omega) = \mathbb{R}_+ \times \partial\Omega$.
- **Def.:** The local Weibull model for LCF is the PPP given by the crack initiation intensity ρ

$$\rho(da, dt) = \frac{m}{N_{\det}(\sigma(u))} \left(\frac{t}{N_{\det}(\sigma(u))} \right)^{m-1} dadt, \quad m \geq 0$$

with da the induced surface measure on $\partial\Omega$ and with the state equation

$$-\mathrm{div}\sigma(u) = f \text{ auf } \Omega \text{ und } \sigma(u) \cdot n = g \text{ on } \partial\Omega_N,$$

and $u = 0$ on $\partial\Omega_D$.

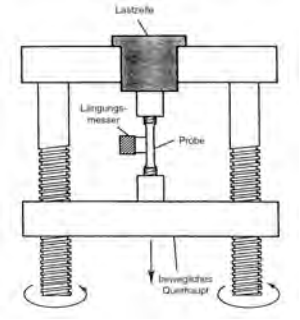
Crack Initiation Probability

- Consider the random time $T_i = T_i(\Gamma)$ of the initiation of the first crack.
- For the entire component, one obtains the survival probability

$$\begin{aligned} S_{T_i}(t) &= P(T_i > t) = P(\Gamma([0,t] \times \partial\Omega) = 0) \\ &= \exp\left\{ -\int_0^t \int_{\partial\Omega} \frac{m}{N_{\det}(\sigma(u))} \left(\frac{s}{N_{\det}(\sigma(u))} \right)^{m-1} dads \right\} \\ &= \exp\left\{ -\left\| \frac{t}{N_{\det}(\sigma(u))} \right\|^m_{L^m(\partial\Omega,da)} \right\}. \end{aligned}$$

- $\Rightarrow T_i \sim$Weibull with scale parameter $\left\| \frac{1}{N_{\det}} \right\|^{-1}_{L^m(\partial\Omega,da)}$ and shape parameter m.

Calibration and Validation



(Gottstein)

- In tensile experiments one counts for given stress level σ_j and specimen surface $|\partial\Omega_j|$ the time to crack initiation t_j (or termination of the experiment t_j^+, right censoring).

Calibration and Validation II

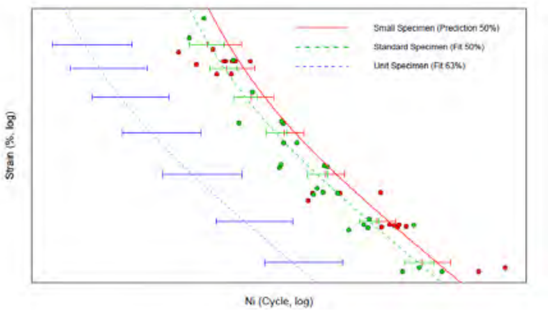
- Setting up the log-Likelihood functional:

$$
\begin{aligned}
\log \mathcal{L}(\{t_j,\sigma_j,\Omega_j\}|\theta,m) &= \sum_{j=1}^{n}\Bigg[\log\left(\frac{m}{N_{\text{det}}(\sigma_j|\theta)}\right) \\
&+ (m-1)\log\left(\frac{t_j}{N_{\text{det}}(\sigma_j|\theta)}\right) \\
&+ \log(|\partial\Omega_j|) - |\partial\Omega_j|\left(\frac{t_j}{N_{\text{det}}(\sigma_j|\theta)}\right)^{m}\Bigg] \\
&- \sum_{j=n+1}^{n+n^+}|\partial\Omega_j|\left(\frac{t_j^+}{N_{\text{det}}(\sigma_j|\theta)}\right)^{m}.
\end{aligned}
$$

- Estimate $\hat{\theta},\hat{m}$ using the Maximum Likelihood Principle via numerical optimization

$$(\hat{\theta},\hat{m}) = \text{argmax}_{(\theta,m)}\log\mathcal{L}(\{t_j,\sigma_j,\Omega_j\}|\theta,m)$$

Validation – Experiment

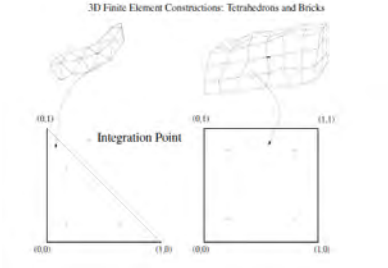


(with S. Schmitz, T. Seibold, R. Krause, G. Rollman und T. Beck, Material Ni-Basis Super-Alloy Rene80 bei 850°C, J. Comput. Mat. Sci. 2013)

- Green Points: Original-specimen geometry, red points: small geometry, red line prediction from model
- Good prediction for small strain amplitude
  High strain amplitudes show problems
  with multiple crack initiations at one specimen

Numerical Implementation

- To calculate the survival probabilities of complex components, we need a FEA postprocessor compatible to professional FEA tool suites (ABAQUS and CalculiX)



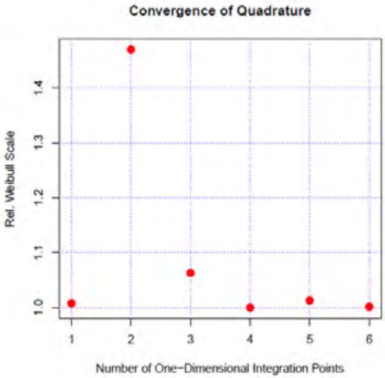
$$S_{T_i}(t) \approx \exp\left(-t^m \sum_{i=1}^{N_{el}} \sum_{j=1}^{N_F} \delta_{\mathcal{F}_{ij},\partial\Omega} \sum_{l=1}^{l_q} \frac{\omega_l \sqrt{g(\xi_l)}}{\left(N_{\det}(\sigma(\sum_{j=1}^{N_F} u_{i,j}\gamma_{ij}))(\xi_l)\right)^m}\right)$$

Numerical Implementation – Quadrature

- By the non linearity of $\frac{1}{\mathrm{N}_{\mathrm{det}}}$, quadratures are not exact

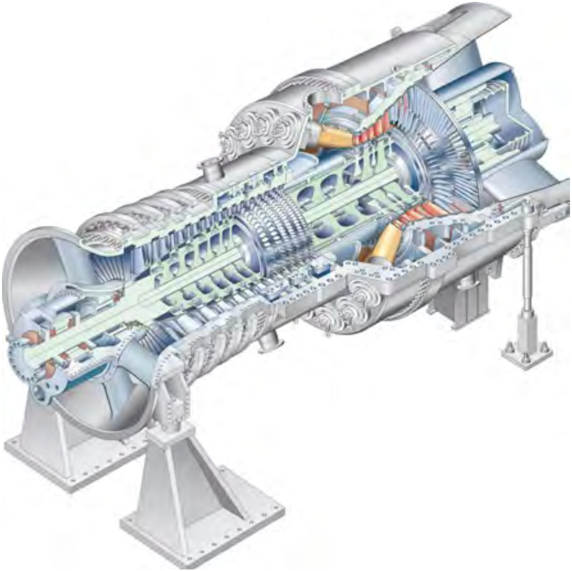
TABLE 1. QUADRATURE ON THE INTERVAL $K = [a,b]$ WIT $\tilde{m} = (a+b)/2$ AND $\tilde{\delta} = b-a$.

k_q	l_q	Int. Points ξ_l	Weights ω_l
1	1	$\tilde{m}$	$\tilde{\delta}$
3	2	$\tilde{m} \pm \frac{\tilde{\delta}}{2\sqrt{3}}$	$\frac{1}{2}\tilde{\delta}$
5	3	$\tilde{m} \pm \frac{\tilde{\delta}}{2}\sqrt{\frac{3}{5}}$	$\frac{5}{18}\tilde{\delta}$
		$\tilde{m}$	$\frac{8}{18}\tilde{\delta}$
7	4	$\tilde{m} \pm \frac{\tilde{\delta}}{2}\left(\sqrt{(15+2\sqrt{30})/35}\right)$	$\left(\frac{1}{4} - \frac{1}{12}\sqrt{\frac{5}{6}}\right)\tilde{\delta}$
		$\tilde{m} \pm \frac{\tilde{\delta}}{2}\left(\sqrt{(15-2\sqrt{30})/35}\right)$	$\left(\frac{1}{4} + \frac{1}{12}\sqrt{\frac{5}{6}}\right)\tilde{\delta}$



(mit S. Schmitz, G. Rollmann und R. Krause, Proc. ASME Turbo Expo 2013)

Design Study: Cooled Turbine Blade



Optimal Reliability

- **Def.:** A design $\Omega^* \in \mathscr{O}_{\text{ad}}$ is **optimally reliable** w.r.t. the local Weibull model with given loads f, g, if

$$S_{T_i(\Omega^*)}(t) \geq S_{T_i(\Omega)}(t), \quad \forall t \in \mathbb{R}_+,\ \Omega \in \mathscr{O}_{\text{ad}}.$$

- Since

$$S_{T_i(\Omega)}(t) = \exp\{-t^m J(\Omega, u(\Omega))$$

this is equivalent to

$$J(u(\Omega^*), \Omega^*) = \inf_{\Omega \in \mathscr{O}_{\text{ad}}} J(u(\Omega), \Omega)$$

with $u(\Omega)$ solves the elasticity PDE on Ω and

$$J(u(\Omega), \Omega) = \int_{\partial\Omega} \left(\frac{1}{N_{\text{det}}(\sigma(u(\Omega)))} \right)^m da.$$

- The problem of optimal reliability has thus been transferred to a shape optimization (SO) problem.

Strategy for Existence in SO

- Choose a minimizing sequence $\Omega_k \in \mathscr{O}_{\rm ad}$:

$$J(\Omega_k, u(\Omega_k)) \to \inf_{\Omega \in \mathscr{O}_{\rm ad}} J(\Omega, u(\Omega)).$$

- Choose a relatively compact topology on $\mathscr{O}_{\rm ad}$ such that

$$\Omega_{k_l} \to \Omega^*.$$

- Show that in a suitable topology

$$u(\Omega_{k_l}) \rightsquigarrow u(\Omega^*) \quad \text{(graph compactness of state eqn.)}$$

- Show lower semicontinuity of the objective functional in the graph topology

$$q \leq J(\Omega^*, u(\Omega^*)) \leq \liminf_l J(\Omega_{k_l}, u(\Omega_{k_l})) = q$$

The $C^{3,\phi}$-Regularity Approach to Optimal Shapes

- **Problem:** $J(u,\Omega)$ is not well defined $u \in H^1(\Omega,\mathbb{R}^3)$.
- We can not expect lower semicontinuity of $J(u,\Omega)$ within the weak (H^1) solution theory.
- We need $\mathscr{O}^{\mathrm{ad}}$-shapes with $C^{4,\phi}$-with uniform Hölder constant, ans sufficiently smooth solutions (cf. Chiarlet, Mathematical Elasticity, 1988).
- We therefore use $C^{3,\phi}$-solutions and strong elliptic regularity results.
- We also need boundary regularity (Schauder estimates for elliptic PDE systems).
- We need to prove uniform estimates in $\mathscr{O}^{\mathrm{ad}} \Rightarrow$ to obtain compactness of the solution space in suitable topologies that render $(\Omega,u) \to J(\Omega,u(\Omega))$ lower semicontinuous.

Uniform Schauder Estimates

- **Theorem:** f, g sufficiently regular. Let $0 < \varphi < \phi < 1$, then there exits C uniform in $\mathscr{O}_{\mathrm{ad}}$ such that

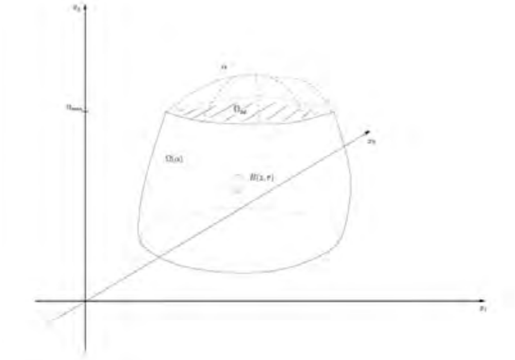
$$\|u(\Omega)\|_{C^{3,\varphi}(\Omega,\mathbb{R}^3)} \leq C \left(\|f\|_{C^{1,\phi}(\Omega,\mathbb{R}^3)} + \|g\|_{C^{2,\phi}(\Omega,\mathbb{R}^3)} + \underbrace{\|u(\Omega)\|_{H^1(\Omega,\mathbb{R}^3)}}_{\substack{\text{unnif. bounded} \\ \text{Korn's ineq.}}} \right)$$

  (S. Schmitz and G.)

- **Theorem:** Analogous estimates for thermo-mechanical PDE systems (L. Bittner and G., 2013)

Parametrization of the Boundary

- We obtain $\mathscr{O}^{\text{ad}}$ be parametrizing pieces of the boundary by $C^{4,\phi}$-functions $\alpha : \partial\Omega_{2d} \to \mathbb{R}$ with uniformly bounded norm.



- We equip $\mathscr{O}_{\text{ad}}$ with the $C^{4,\varphi}$-topology, $\varphi < \phi$, then $\mathscr{O}_{\text{ad}}$ is compact by the Theorem of **Arzelà-Ascoli**.

Konvergence of Solutions of the PDE

- **Problem:** Need the convergence of solutions that live on different domains Ω.
- We thus need a continuation operator $p_\Omega : C^{3,\varphi}(\bar{\Omega}) \to C_0^{3,\varphi}(\hat{\Omega})$, $\Omega \subseteq \hat{\Omega}$ for all $\Omega \in \mathscr{O}_{\text{ad}}$.
- These continuation operators have to be uniformly bounded in Ω.

Theorem: (Schmitz, G. 2012) Since $\exists$ convergent, minimizing sequence $\alpha_l \to \alpha^*$ in $C^{4,\varphi}$ and $\alpha^* \in C^{(4,\phi)}$, thus exists a sub sequence α_{k_l} such that for $\tilde{\varphi} < \varphi$

$$\hat{u}(\Omega(\alpha_{k_l})) \to \hat{u}(\Omega(\alpha^*)), \quad \text{in } C^{3,\tilde{\varphi}}(\hat{\Omega}, \mathbb{R}^3), \quad \hat{u}(\Omega) = p_\Omega u(\Omega)$$

Idea of Proof: Use relative compactness of $C_0^{3,\varphi}(\hat{\Omega})$ in $C_0^{3,\tilde{\varphi}}(\hat{\Omega})$ (Arzelà-Ascoli) and show convergence of a sub sequence in $C_0^{3,\tilde{\varphi}}(\hat{\Omega}, \mathbb{R}^3)$. C^3-convergence $\Rightarrow$
Restriction of limit to $\Omega(\alpha^*)$ solves the PDE.

Existence of Shapes with Optimal Reliability

Theorem: (Schmitz, G. 2012, arXiv:1210.4954) $\exists\ \Omega^*$ in $\mathscr{O}_{\text{ad}}$, such that

$$S_{T_i(\Omega^*)}(t) = \sup_{\Omega \in \mathscr{O}_{\text{ad}}} S_{T_i(\Omega)}(t) \quad \forall t \in \mathbb{R}_+.$$

Analogous result for thermo-mechanics (L. Bittner, G., MA-Thesis 2013)

Idea of proof:

$$J(u(\Omega(\alpha_{l_k})), \Omega(\alpha_{l_k})) \to \inf_{\Omega \in \mathscr{O}_{\text{ad}}} J(u(\Omega), \Omega) = q$$

and we have graph compactness for the state equation in the C^3-topology

$$(\hat{u}(\Omega(\alpha_{l_k}), \alpha_{l,k}) \to (\hat{u}(\Omega(\alpha^*)), \alpha^*).$$

We can apply Lebesgue's theorem to show even continuity in the C^3-graph-topology:

$$q = \liminf J(u(\Omega(\alpha_{k_l})), \Omega(\alpha_{k_l}) = J(u(\Omega(\alpha^*), \Omega(\alpha^*)). \quad \square$$

Outlook

- Use the calculus of shapes to actually minimize failure probabilities

  $dJ(\Omega, u(\Omega))[V] =$ change of J under infinitisimal deformation by V

- Combine with adjoint method to calculate shape gradients (ongoing project with first discretize, then adjoin approach)
- Do the same as above, but the other way round. . .
- Different failure modes (e.g. for brittle material, [arXiv:1311.6779v1] with M. Bolten and S. Schmitz)