Mathematics in Industry 35

Hans Georg Bock · Karl-Heinz Küfer ·
Peter Maass · Anja Milde ·
Volker Schulz *Editors*

German Success Stories in Industrial Mathematics

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Mathematics in Industry

Volume 35

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ISSN 1612-3956 ISSN 2198-3283 (electronic)
Mathematics in Industry
ISBN 978-3-030-81454-0 ISBN 978-3-030-81455-7 (eBook)
https://doi.org/10.1007/978-3-030-81455-7

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PREFACE

Over twenty years ago, the slogan "Mathematics: Key technology of the future" became the vision and driving force for applied mathematicians working on real life industrial applications. Since then, mathematics has proved to deliver groundbreaking contributions for a wide range of applications; however, this is still only the tip of the iceberg. The huge technological potential of mathematics for problem-solving and algorithmic development is still just beginning to show its ability to produce industrial innovation. This book is a collection of success stories of industrial mathematics with the goal of giving inspiration to industrial and academic research units as well as decision-makers in industry and politics.

The contributions in this book demonstrate the power of mathematics as a technology. We show that mathematics can decisively contribute to the solutions of present and future economic, environmental, and societal changes. In selecting which stories to feature, we used the following criteria:

+ The industrial problems needed to be both relevant for the core business of the industrial partners and also ones which couldn't be solved using standard methods.
+ There had to be sufficient documentation of the domain-specific expertise of the industrial partners, including existing models, experimental data and evaluation criteria.
+ The use of novel mathematics was essential in solving the problem – for analyzing models, designing and optimizing algorithms, or efficiently implementing solutions beyond the present state of the art.

The selected contributions span different industrial sectors and methodologies but all involve two unique, underlying factors of mathematics. First of all, mathematics is the ultimate scientific discipline of rigor and precision. The concept of a mathematical proof is the basis for a reliable analysis of algorithms, for the correctness of physical-engineering models or for the statistical evaluation in scientific computing and data analysis. As a result, algorithms based on novel mathematical theory have shown a development similar to that of Moore's Law. And in all cases, such math-based algorithmic improvements outperform machine improvement, sometimes by significant factors.

Second, mathematics is a discipline of abstraction with the power to reduce any physical or engineering model to its essential core. This allows for an analysis of a model's properties in theoretical terms and a translation of the results back into their physical-engineering context. The analysis of a single abstract model typically covers the essential features of a variety of applications; hence, the path back from one new mathematical insight to applications is useful for additional physical/engineering models. As a consequence, mathematics is highly specialized in its own field but highly diverse and transdisciplinary in its applications.

In particular, those two factors play a decisive role when analyzing novel AI (artificial intelligence) concepts or general machine learning algorithms for data analysis. These approaches can be seen as implicit model adaptations allowing for modelling, simulation and optimization of highly non-linear, high-dimensional problems. Mathematics is the basis for merging the best of both worlds, i.e. for integrating model-based and domain-specific expert knowledge into such data-driven concepts. Moreover, it allows for determining the potential as well as the limitations of AI algorithms and it leads to novel network architectures. Mathematics is indispensable for obtaining optimal simulation results.

Before proceeding with the main content of this book, we want to acknowledge and emphasize that most of the following contributions have benefitted at least partially from the unique funding program 'Mathematics for Innovations' of the German Federal Ministry of Education and Research (BMBF). This funding program has existed for more than 25 years, and has created powerful collaborations between industry and mathematical research. It has allowed us to train several generations of industrial mathematicians and most importantly, it has led to substantial and sustainable industrial innovations.

MATHEMATICS MAKES THE IMPOSSIBLE POSSIBLE

Digitalization is the megatrend of the 21st century. Due to the exponential growth of computing power (Moore's law) and the miniaturization of chips, digitalization is now penetrating all areas of life and all industries. At the core of digitalization are algorithms and especially mathematical algorithms. In the last decades, their performance has also increased exponentially, in many cases even outpacing the growth in computing power. Without mathematics this incredible increase in performance would not have been possible.

Many industrial products, systems, and infrastructures – from electric motors to computer tomographs or traffic networks – rely on corresponding algorithms. Life without algorithms is hard to imagine. Today, they enable us to predict and test the properties and performance of products using virtual models long before they are built. For example, this allows early optimization of products and systems to realize continuously increasingly sophisticated, efficient and ecologically compatible products. Without appropriate simulation methods, the speed of today's innovation cycles could not be realized. Many technologies would not have been mastered. At the same time, corresponding virtual models can also be used during operation, e.g. to realize highly efficient control systems. Mathematics enables highly complex models to be run parallel to operation by means of sophisticated pre-calculations. Combined with continuous streams of sensor data and machine learning allows to optimize operation and service to a level not seen before.

The continuous prediction and optimization of characteristics, behavior, and performance, from early design to end-of-life, using digital information, data, and models is reflected in the vision of the digital twin. The digital twin and corresponding software solutions are also central technologies at Siemens AG. For example, the corresponding research and predevelopment is well funded, with investments in the high doubledigit millions. Examples include mathematical innovations[1] enabling the realization of industrial milling robots[2] or increasing the availability of motors [3].

Without mathematics, many products would be unthinkable, as the examples in this book impressively show. Mathematics is the key technology for digital twins and probably even the key technology for the 21st century itself.

Dirk Hartmann
Senior Principal Scientist Simulation &
Digital Twin, Siemens AG
Siemens Top Innovator
1st Deputy Chairman KoMSO

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[1] https://new.siemens.com/global/en/company/stories/research-technologies/digitaltwin/passion-for-digital- twins.html

[2] https://youtu.be/2iIN-9Kno3o

[3] https://youtu.be/86vkjykbHRM

KEYNOTES

We live in the age of mathematics. Its influence pervades economic and social activity and its influence and impact are intense. Our economy increasingly relies on innovation to provide a significant proportion of the productivity gains required to support rising standards of living. Mathematics is playing an ever-expanding role in generating innovation and impact and, via knowledge exchange, is adding substantial social and economic value to our economy. This has been quantified in a number of reports published in several European countries, demonstrating that the economic contribution of mathematics represents around 25 – 30 % of a country's national income. In addition to the evidence from the reports on the economic impact, recent data may be used to show that mathematical research produces an outstanding rate of return on investment as compared to other disciplines like engineering, chemistry and physics[1].

Every day the mathematical sciences are used to solve otherwise intractable problems. We rely on cryptography securing our transactions over the internet and the optimal allocation of scarce resources, such as the radio spectrum which allows our mobile phones to work in crowded areas. Mathematics underpins numerous scientific, technical and social advances that improve health and raise living standards. Genetic analysis relies on statistical methodologies, allowing improvements in human, animal and plant health. Machine learning, artificial intelligence (AI) and data science are dependent on mathematics to find patterns in complex datasets and to explain the behaviour of deep neural networks. The risk of pension and investment funds is managed and minimised using mathematical models and actuarial science. Many more examples can be given here.

This booklet provides a number of impressive success stories setting out a very powerful and well-argued case for extra investment and new institutional initiatives that can accompany it. Taken together, they could be fundamental elements of the drive for productivity growth, innovation and a redefinition of the role of mathematics in a world which is seeing very rapid changes in international and technological structures. New mathematical understanding does not come out of the ether. It requires investment in the pure mathematics that underlies all the rest, in the applications working with partners and other disciplines, in the people, particularly the young who will take it forward, and in understanding of mathematics from the top CEOs and ministers to those in the more technical areas who will do the 'hard graft.'

The success stories in this booklet make a very powerful case for investing in mathematics. This is the age of mathematics and its influence will become still more intense. It is a discipline in which Europe can shine and lead. Now is the time to invest in its future.

Wil Schilders
President of EU-MATHS-IN (European Service Network of Mathematics for Industry and Innovation)
Officer at large, ICIAM (The International Council for Industrial and Applied Mathematics)
Director of Dutch National Platform for Mathematics
Professor of Scientific Computing for Industry, Eindhoven University of Technology

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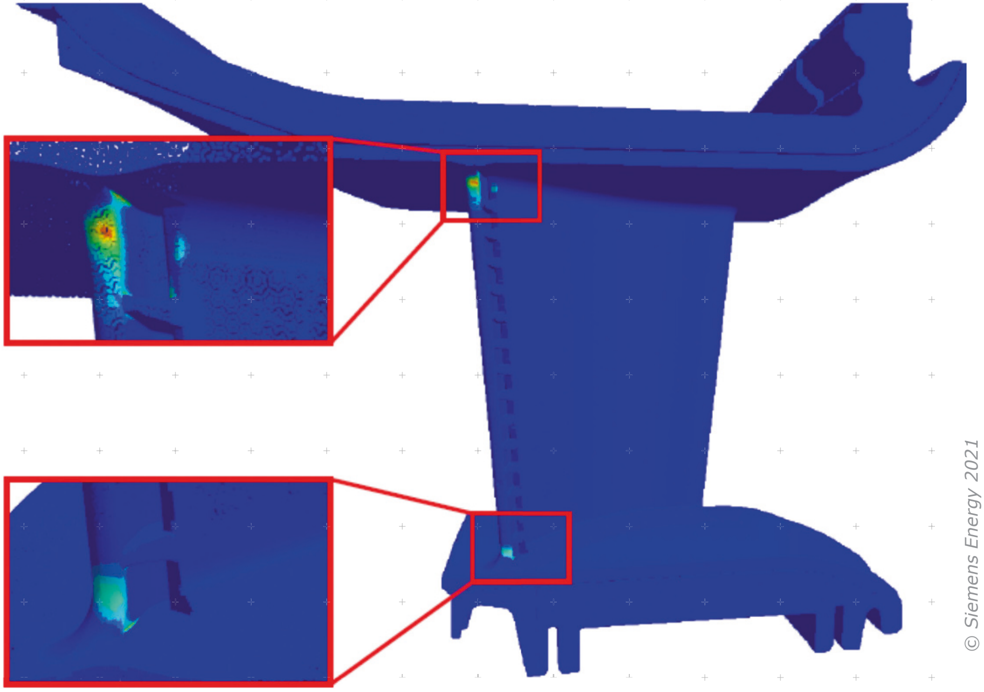
[1] "The era of mathematics", page 6



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Hazard density for a turbine vane calculated with a poisson point process

H. G. Bock et al. (eds.), *German Success Stories in Industrial Mathematics*,
Mathematics in Industry 35, https://doi.org/10.1007/978-3-030-81455-7_1

FROM PROBABILISTIC PREDICTION OF FATIGUE LIFE TO A NEW DESIGN APPROACH FOR GAS TURBINES

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HANNO GOTTSCHALK
University of Wuppertal

ROLF KRAUSE
Universita della Svizzera Italiana

Gas turbines are used in aviation and energy production. As efficiency of gas turbines increases with firing temperatures, the hot gas components of a gas turbine are subject to extreme termo-mechanical load. Activation and deactivation cycles from start to landing of an aircraft or during the temporal activation of a gas power plant to stabilize an energy grid drive mechanical fatigue, which therefore has to be taken into account in design procedures and operation and service plans. Fatigue life however is not predictable in a deterministic fashion. Even under lab conditions, material test specimens show a scatter of fatigue life by a factor 10 of the average life. The probabilistic assessment of risk during operation therefore is of highest importance. In almost 10 years of continuous collaboration, new design procedures for the probabilistic calculation of risks for low cycle fatigue (LCF) have been developed by Siemens. The mathematical modeling, based on the theory of point processes, provided a sound theoretical foundation that was complemented with intense research and testing in materials science. The continuous confrontation of modeling approaches with the requirements of industrial applicability and experimental data triggered innovation in materials science, mathematics and gas turbine design and operation.

PARTNERS

GEORG ROLLMANN, SEBASTIAN SCHMITZ and **LUCAS MÄDE,** Siemens

Industrial challenge and motivation

Gas turbines are used for jet propulsion and power production. In aviation, gas turbine technology provides compact, lightweight and efficient engines. In power production, the specific C0$_2$ output per produced energy unit is $1/3$ rd of that of lignite power plants, if the gas turbine is run in a combined cycle with a steam turbine that uses the gas turbines' exhaust gas. Due to their quick start capabilities, gas fired power plants also play a role in stabilizing the energy grid in times of high influx of volatile renewable energy. At the same time, the demand for top efficiency remains an important driver for gas turbine development. Apart from GE, Mitsubishi Heavy Industries and Siemens offer technology for power plants operating at over 60% efficiency. As such efficiencies can only be achieved with firing temperatures way above the melting point of the engineering materials, sophisticated cooling technology is needed. Nevertheless, extreme thermal and mechanical loads during activation, deactivation and operation limit the life of the components which has to be thoroughly considered in design and and maintanancs. Quick start operation regimes lead to low cycle fatigue, in particular. The time to the initiation of a fatigue crack however is highly stochastic and the component safe life time rather is a random number than a deterministic value. Even under lab conditions, the maximum scatter band in lifetime is up to a factor 10 larger than the median life under the same nominal test conditions. Therefore, probabilistic design procedures and a proper calculation of probabilities of crack initiation is not only much more adequate given the experimental findings, but also provides more qualified information for risk assessment in design and maintenance The challenge in setting up a probabilistic design approach towards fatigue life has been taken up by Siemens (L. Mäde, S. Schmitz and G. Rollmann) in a joint effort with materials scientists from TU Kaiserslautern (T. Beck and B. Engel) and Jülich Research Center (T. Seibel) and Mathematicians from the University Lugano (R. Krause) and University of Wuppertal (H. Gottschalk, N. Moch and M. Saadi) in a series of research projects under the auspices of the 'AG Turbo' research collaboration co-funded by the Federal Ministry of Economics and Energy (BMWi) and industry partners within the AG Turbo. The scope of the first research period between 2011 – 2013 was an effective probabilistic model that is capable to provide probabilistic calculations of the risk of crack initiation over time for turbo-machinery components with complex geometry. In a second period 2012 – 2015, some consequences of probabilistic life prediction were exploited, namely the fact that shape sensitivities can be calculated for probabilistic – but not deterministic – component life. Application areas lie in design and the setting of geometric tolerances in production. This research and development (RnD) direction is further elaborated by the ongoing BMBF-funded GIVEN project (www.given-project.de).

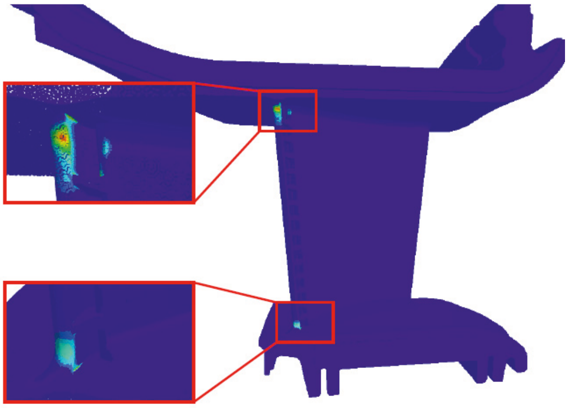

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Figure 1: Hazard density for a turbine vane calculated with a poisson point process involving notch support factors

In the third period with projects from 2014 – 2017 and 2019 – 2022 a better understanding of the impact of materials' heterogeneous micro structures as a root cause of the scatter of LCF life time is investigated and included in multi-scale approaches to probabilistic fatigue life calculation. This also gives interesting insight in the impact of parameters in production, as e.g. cooling and solidification rates in the casting process influence the micro-structure, to the safe life of a heavily loaded turbine component.

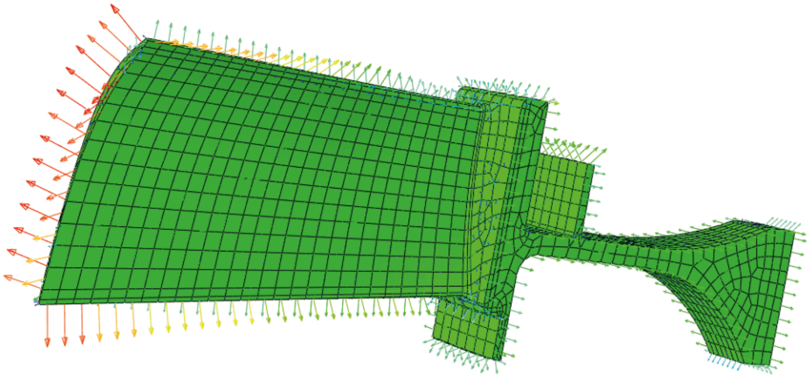

Figure 2: Shape sensitivities for failure probability calculated by the adjoint method

Mathematical and interdisciplinary research

The probabilistic models that have been proposed in the joint research effort are based on the theory of spatio-temporal point processes[14][7]. Indentifying a crack initiation event with a point on the component's surface x and a time t, we parameterize all configurations of crack initiations as (x, t) – pairs. A random crack initiation history then is given by a random configuration η that consists of collections of such pairs. Defining $\eta(A \times I)$ as the number of crack initiation events in a surface region A that happened in a time interval I, we obtain as the probability of survival without cracks

$$\begin{aligned} S(t) &= P\left(\eta\left(\partial\Omega \times [0,t]\right) = 0\right) \\ &= \exp\left(-\int_{\partial\Omega}\left(\frac{t}{N(\sigma)}\right)^{m} dA\right) \end{aligned}$$

where is the entire surface of the component. In the second equation we already used a special Poisson point process that is based on the deterministic cycles to crack initiation as a scale parameter and a Weibull probability distribution with shape parameter $m > 1$. Here is the stress field that is calculated in practice as the numerical solution of the elasticity equation using finite elements. This basic model has been calibrated with data, tested experimentally and has been implemented a finite element post processor for the numerical evaluation of survival or failure probabilities[12, 13], see Figure 1. Further extensions concern thermo-mechanical loads [13]and the modeling of notch support factors[10][9]. Interestingly, taking the probability of survival as an objective in shape optimization fosters new theoretical developments on the mathematical side: The probability of failure is a more singular objective functional as e.g. the compliance functional or tracking type objectives that are often used in shape optimization. This insight has lead to the development of theoretical foundations for shape optimization in connection with elliptic regularity theory[2, 7]. Mathematical results cover the existence of optimal shapes and detailed studies of the regularity of shape derivatives[1]. A crucial observation with survival probabilities is that they are essentially given as a surface integral, as opposed to a deterministic life given by a minimum life over all points on the component's surface. It therefore is possible to compute shape sensitivities using the adjoint method, see Figure 2. This program has been pursued in [6, 8] for complex 3d geometries. It is also shown that gradient based methods of mono and multi-criteria optimization can be effectively based on this approach, opening up new prospectives in multi criteria shape optimization [3].

The ongoing research on probablistic life calculation for low cycle fatigue does not satisfy itself with an empirical approach to the probability of failure like using the Weibull distribution. Instead, the

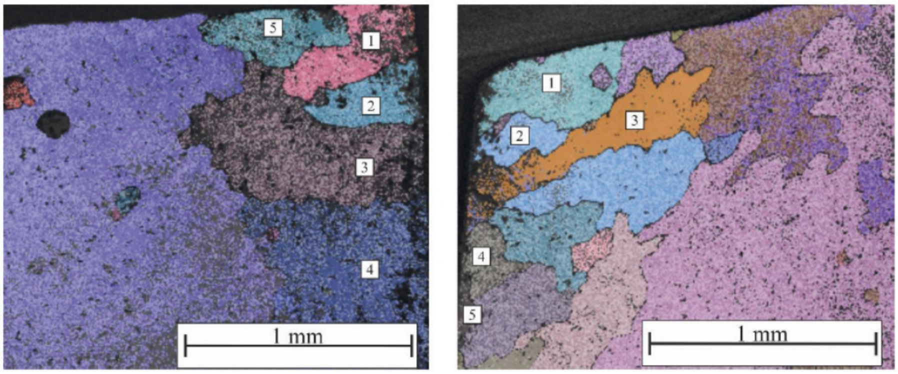

Figure 3: EBSD analysis of grains along a crack path

scatter in lifetime is derived from the random microstructure in the nickel based superalloys using multi scale modeling. These models are based on detailed experimental investigations using electon backscatter diffraction to measure the orientation of crystallographic planes in the neighborhood of locations of crack initiation, see figure 3. Several models have been compared and benchmarked, obtaining theoretical predictions of scatter bands of the size that is actually observed[4, 5, 11].

Implementation

The way forward for the RnD on the probabilistic modeling of low cycle fatigue has been characterized by the close integration of mathematical modeling and software prototyping, experimental work and the careful evaluation and review processes in industry, before tool development and new design procedures in industry could be based on the foundations laid in research. Test campaigns had to prove the validity of the mathematical models, going beyond the mathematical verification of their interior logical consistency. Based on this rigorous verification and validation, the probabilistic fatigue life methodology that has been developed in the first research phase has been implemented within Siemens to support decision-making in design and service of power plant components. In order to assess corresponding shape sensitivities in an efficient manner, the adjoint approach from the second collaboration period has been incorporated in an in-house finite element tool suite as well. The current third phase of joint R&D focuses, on the one hand, on adjoint methods in multi criteria shape optimization, and on the other hand on refined multiscale models for the scatter in fatigue life.

Industrial relevance and summary

Within Siemens, the joint R&D effort has significantly contributed to the field of probabilistic life assessment. The resulting, more realistic service life assessments have allowed for additional customer value through increased sustainability by better utilization of power plant components. In addition, the use of probabilistic target functionals in design optimizations have led to improved component geometry definitions resulting in higher durability. Also because of this success-story, probabilistic design was presented as one of four key development areas during the Zurich forum of the Global Power and Propulsion Society in 2018.

Patents

- Procedure for the integrated prediction of failure probabilities for mechanical components due to material scatter and and manufacturing tolerances (with S. Schmitz and M. Saadi) submitted to EP office, file 102016221928.6 09.11.16.

Acknowledgements

The authors acknowledge Funding by the Federal Ministry for Education and Research via the GIVEN project under the grant no. 05M18PXA. This work has also profited form direct funding by Siemens and the Federal Ministry of Economic Affairs and Energy via grants 03ET2013I and 03ET7041J.

References

[1] L. Bittner. On shape calculus with elliptic pde constraints in classical function spaces, 2020.

[2] L. Bittner and H. Gottschalk. Optimal reliability for components under thermomechanical cyclic loading. *Control and Cybernetics*, 45, 2016.

[3] M. Bolten, H. Gottschalk, C. Hahn, and M. Saadi. Numerical shape optimization to decrease failure probability of ceramic structures. *Computing and Visualization in Science*, 21(1-6):1–10, July 2019.

[4] Engel, Mäde, Lion, Moch, Gottschalk, and Beck. Probabilistic modeling of slip system-based shear stresses and fatigue behavior of coarse-grained ni-base superalloy considering local grain anisotropy and grain orientation. *Metals*, 9(8):813, July 2019.

[5] B. Engel, T. Beck, N. Moch, H. Gottschalk, and S. Schmitz. Effect of local anisotropy on fatigue crack initiation in a coarse grained nickel-base superalloy. *MATEC Web of Conferences*, 165:04004, 2018.

[6] H. Gottschalk and M. Saadi. Shape gradients for the failure probability of a mechanic component under cyclic loading: a discrete adjoint approach. *Computational Mechanics*, 64(4):895–915, 2019.

[7] H. Gottschalk and S. Schmitz. Optimal reliability in design for fatigue life. *SIAM Journal on Control and Optimization*, 52(5):2727–2752, 2014.

[8] H. Gottschalk, S. Schmitz, T. Seibel, G. Rollmann, R. Krause, and T. Beck. Probabilistic schmid factors and scatter of low cycle fatigue (LCF) life. *Materialwissenschaft und Werkstofftechnik*, 46(2):156–164, Feb. 2015.

[9] L. Mäde, H. Gottschalk, S. Schmitz, T. Beck, and G. Rollmann. Probabilistic lcf risk evaluation of a turbine vane by combined size effect and notch support modeling. In *Turbo Expo: Power for Land, Sea, and Air*, volume 50923, page V07AT32A004. American Society of Mechanical Engineers, 2017.

[10] L. Mäde, S. Schmitz, H. Gottschalk, and T. Beck. Combined notch and size effect modeling in a local probabilistic approach for LCF. *Computational Materials Science*, 142:377–388, Feb. 2018.

[11] N. Moch. From microscopic models of damage accumulation to the probability of failure of gas turbines. 2019.

[12] S. Schmitz. *A Local, probabilistic Model for LCF*. Hartung-Gorre Verlag, 2014.

[13] S. Schmitz, H. Gottschalk, G. Rollmann, and R. Krause. Risk estimation for lcf crack initiation. In *Turbo Expo: Power for Land, Sea, and Air*, volume 55263, page V07AT27A007. American Society of Mechanical Engineers, 2013.

[14] S. Schmitz, T. Seibel, T. Beck, G. Rollmann, R. Krause, and H. Gottschalk. A probabilistic model for lcf. *Computational Materials Science*, 79:584–590, 2013.

Optimizing torque control for a multi-megawatt compressor.

H. G. Bock et al. (eds.), *German Success Stories in Industrial Mathematics*,
Mathematics in Industry 35, https://doi.org/10.1007/978-3-030-81455-7_2