Combining traditional modelling, model order reduction and big data

Wil Schilders, TU Eindhoven (Netherlands)

4TU.AMI symposium, June 8, 2018

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Where innovation starts

Aim of talk

- Sketch a global picture
  - Relations between physical modeling, model order reduction and the use of data
- Start with a specific example from the electronics industry, owing to the work that was done at Philips and NXP Semiconductors
- Discuss some major challenges and developments
- Present the way forward

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GOING BACK IN TIME
30 YEARS

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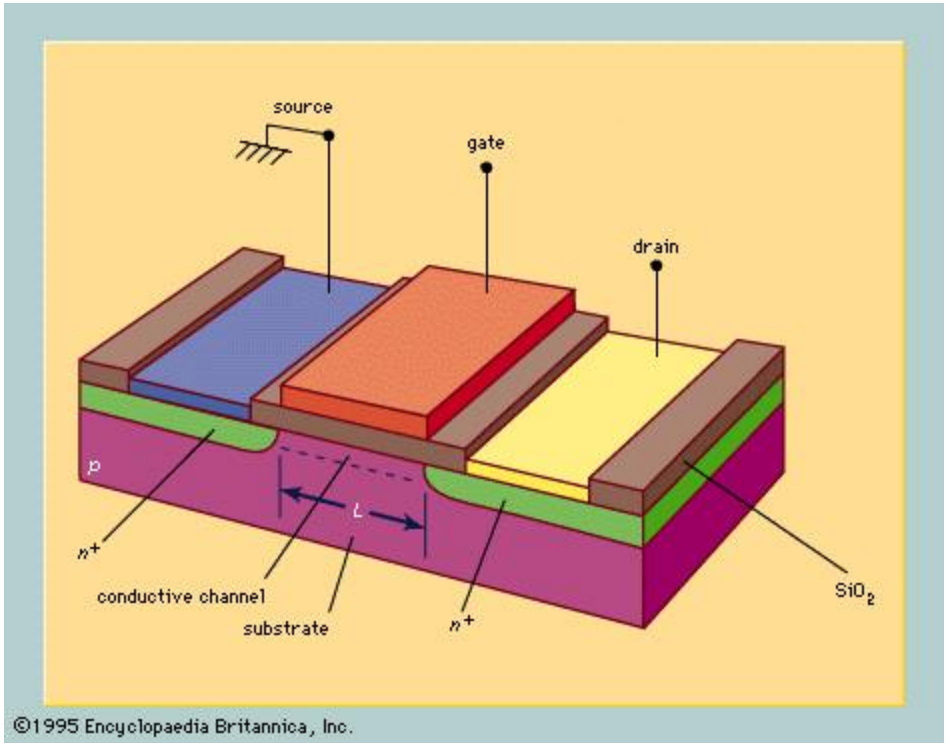
Semiconductor devices

- Semiconductor devices are the building blocks of all electronics products
  - Resistors, Capacitors, Inductors, Diodes
  - Bipolar transistors
  - MOS transistors (metal oxide semiconductor)



Semiconductor device simulation at Philips Research

- Semiconductor devices are described by using 2 types of particles: electrons and holes (="absence of electron")
- Starting point for the modelling is the Boltzmann Transport Equation (BTE), for both particles ("n" referring to electrons, "p" to holes):

$$\frac{\partial f_p}{\partial t} + \frac{1}{\hbar}\nabla_{\mathbf{k}} E_p \cdot \nabla_{\mathbf{x}} f_p + \frac{1}{\hbar}\mathbf{F}_{\text{eff,p}}(\mathbf{x},t) \cdot \nabla_{\mathbf{k}} f_p = Q_p(f_p, f_p) + R_p(f_p, f_n),$$

$$\frac{\partial f_n}{\partial t} + \frac{1}{\hbar}\nabla_{\mathbf{k}} E_n \cdot \nabla_{\mathbf{x}} f_n + \frac{1}{\hbar}\mathbf{F}_{\text{eff,n}}(\mathbf{x},t) \cdot \nabla_{\mathbf{k}} f_n = Q_n(f_n, f_n) + R_n(f_p, f_n).$$

The BTE need to be solved, in 6-dimensional phase space, for the density functions f

→very time consuming…alternative?

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The method of moments

- Moments of the BTE have a physical meaning: the zero order moment relates to the concentration of particles

$$M^0(x,t) = \int f(x,k,t)\mathrm{d}k_1\mathrm{d}k_2\mathrm{d}k_3,$$

- The first order moment relates to the current density:

$$M^1(x,t) = \int \mathbf{k} f(x,k,t)\mathrm{d}k_1\mathrm{d}k_2\mathrm{d}k_3,$$

$$\mathbf{J}(x,t) = -\frac{q\hbar}{m}M^1(x,t),$$

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Using the method of moments up to order 1, we arrive at the drift-diffusion model

- The drift-diffusion model consists of the Poisson equation for the electric potential:

$$-\nabla \cdot (\varepsilon \nabla \psi) = q(p - n + D),$$

- Plus the continuity equations for holes and electrons:

$$q\frac{\partial p}{\partial t} = -\nabla \cdot \mathbf{J}_p - qR, \qquad q\frac{\partial n}{\partial t} = \nabla \cdot \mathbf{J}_n - qR.$$

- And constitutive relations for the current densities:

$$\mathbf{J}_p = -kT\mu_p \nabla p + q\mu_p p \mathbf{E}_p, \qquad \mathbf{J}_n = kT\mu_n \nabla n + q\mu_n n \mathbf{E}_n.$$

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D is the doping profile, specific for the device

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The recombination R and the mobilities μ are parameters to be determined/given

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Models for mobility and recombination

- At Philips Research, there was a group of physicists and electronic engineers working constantly on **new models for mobility and recombination**
- Also at other companies, such groups existed, and they were **competing on a world wide scale**

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How were these models constructed?

- The Philips group performed many experiments and many simulations
- Then used physical/electronic insight, curve-fitting, interpolation and other methods to come up with a model that
  - Had increased functionality
  - Improved the accuracy of simulations
  - Brought experimental results and simulations closer together in the process of on-going miniaturization of semiconductor devices

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Hierarchy of models for mobility

- Simple initial simulations using constant mobilities
- Models describing lattice scattering (particles interact with the atoms in the semiconductor lattice)
- Ionized impurity scattering (interactions with the ionized impurities → doping)
- Carrier-carrier scattering (electrons and holes with each other and with the different species)
- Effects of ultra-high concentration
- Velocity saturation, field dependence, …

Similar story for the recombination R

Electronic circuits

- Semiconductor devices may be the basic building blocks, a level higher we find the electronic circuits that consist of hundreds, thousands and often millions of semiconductor devices

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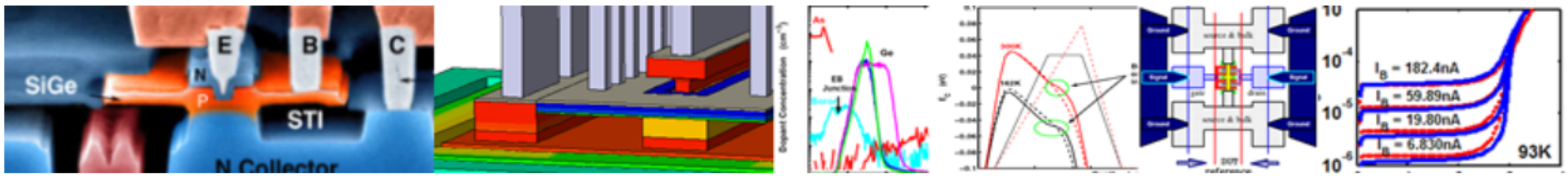
Electronic circuit simulation

- Simulating the behavior of an electronic circuit by using (coupled) semiconductor device simulation for all devices in the circuit is an impossible task
- Fortunately, not all devices are different, often only a few types of transistors are used
- For these devices, so-called **compact device models** are constructed, in a way that is very similar to constructing models for mobility and recombination:
  - Perform many measurements and simulations
  - Use physical/electronic insight, discard certain phenomena
- Big difference/complication:
  - The model must be parameterized!
  - Models like MEXTRAM contain 50 parameters



Mextram – Most EXquisite TRAnsistor Model

Welcome to the official web page of Mextram, one of the Compact Model Coalition (CMC) industry standard transistor compact models that power circuit simulations that power the electronics world. Mextram stands for Most EXquisite TRAnsistor Model. Mextram is excellent for Si and SiGe processes, including high speed RF as well as high voltage high current devices. It accounts for high injection effects with a dedicated epi-layer model, self heating, avalanche, low-frequency and high frequency noises in physical manners, and is formulated with minimal interactions between DC and AC characteristics that simplifies parameter extraction.

Mextram is currently developed and supported by the SiGe group at Alabama Micro/Nano Electronics Science and Technology Center, Electrical and Computer Engineering Department, Auburn University. It was previously developed by NXP Semiconductors (–2006), Delft University of Technology (2006–2014 Q2), and Silvaco (2014 Q3–2015 Q1).

Model improvements are charted by the Compact Model Coalition (CMC), a consortium of semiconductor companies and EDA vendors world-wide promoting industry-standard compact model development. The council is affiliated with Si2. For more information on CMC and a list of its member companies, please visit CMC site.

- Documentation
- Mextram Verilog-A Codes and Documentation
    - Current CMC Release Including QA Suite (Members only)
    - Current Public Release
    - Previous Releases

Developments in last 15 years

- Besides the transistor models developed in the major semiconductor companies, the so-called **BSIM models** were developed at Berkeley
- These models are constructed in an **automatic way**, by using also many experimental results as well as results from simulations
- <u>Major questions:</u>
  - can the work done by the specialized groups be replaced by automatic procedures generating advanced mobility and recombination models, or even complete device models?
  - Can “insight” be incorporated in some way?

Delphi4LED Task 2.5 – Model Calibration

Robin Bornoff

Market Development Manager

Mechanical Analysis Division

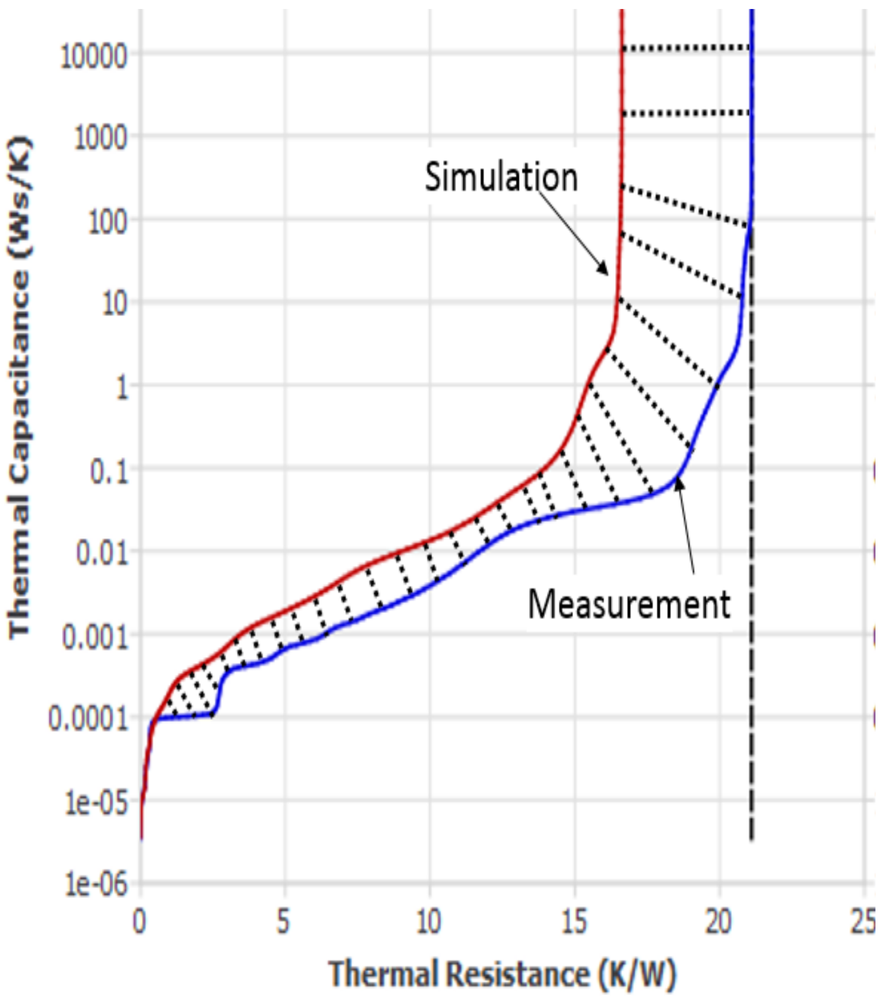
January, 2018

Mentor®

A Siemens Business

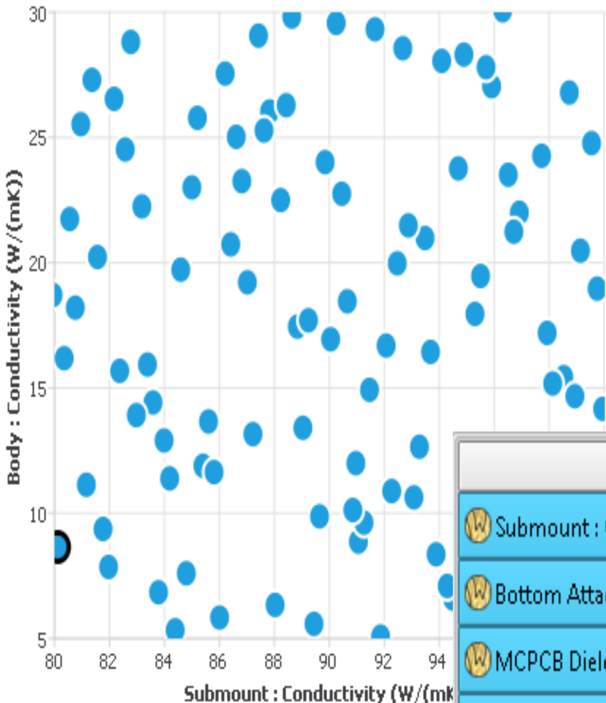
Summary of Calibration Studies – Royal Blue

- Cost Function a quantification of the difference between measured and simulated SFs



Summary of Calibration Studies – Royal Blue

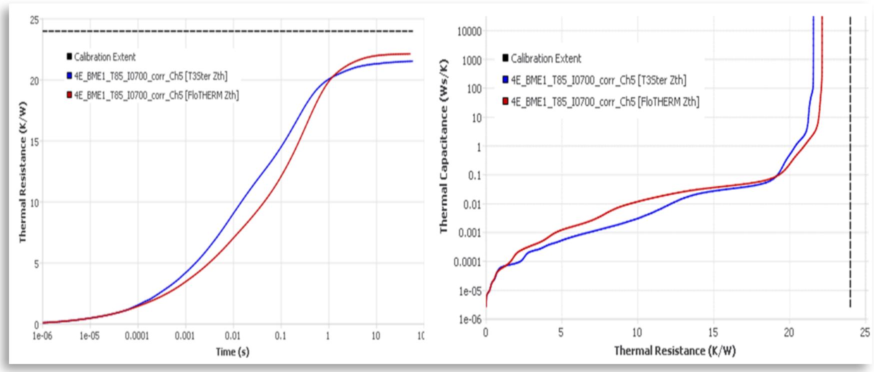
- 100 (Computational) Design of Experiments set and solved

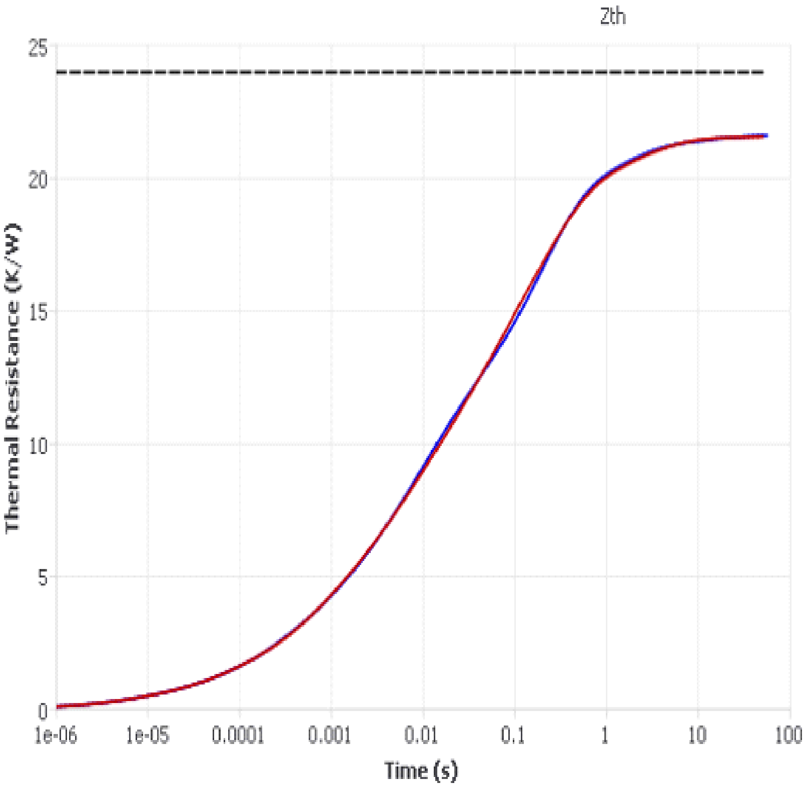


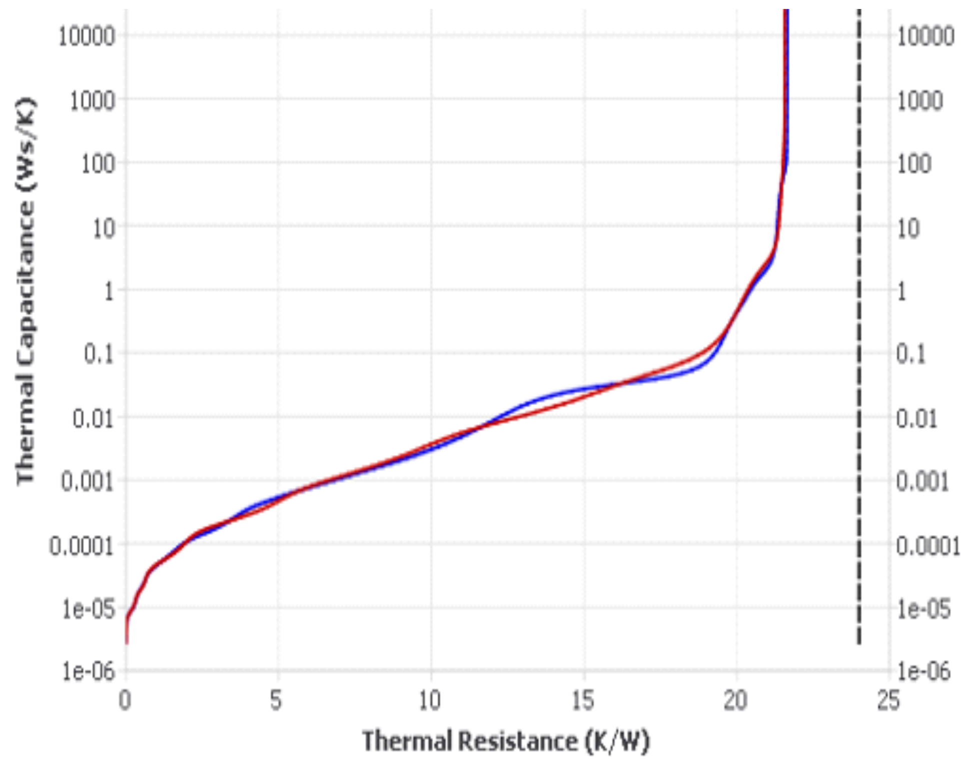
	Design 1	Design 2	Design 3	Design 4	Design 5
Submount : Conductivity (W/(mK))	80.40404	91.11111	80.80808	84.44444	96.9697
Bottom Attach : Conductivity (W/(mK))	6.323232	5.828283	7.454545	5.191919	3.989899
MCPCB Dielectric : Conductivity (W/(mK))	2.090909	1.080808	2.717172	2.59596	1.383838
MCPCB-Coldplate Interface : Conductivity (W/(mK))	0.3373737	0.2929293	0.2585859	0.3252525	0.3737374
Body : Conductivity (W/(mK))	16.11111	8.787879	18.13131	5.252525	21.91919

Summary of Calibration Studies – Royal Blue

- Global minima identified from the cost function response surface







Lessons learned in the electronics industry

- Modelling of semiconductor devices and electronic circuits is done in a mixed way:
  - Using physical/electronic insight, several effects are described by partial and ordinary differential equations, as well as by algebraic relations that mimic the physical effects
  - Many measurements and simulations are performed in order to produce tables of values for parameters in the models
  - Compact device models are needed to perform electronic circuit simulation in an efficient way – these models are also constructed as a combination of physical effects and parameter extraction
- Physical insight must be used to reduce the complexity of models, but data are necessary to make such models accurate descriptions of reality

Automatic via MOR?

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RECENT DEVELOPMENTS

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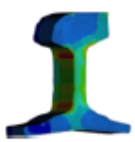
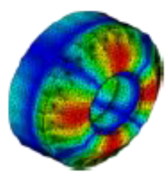
Modelling, Simulation & Optimization in a Data rich Environment

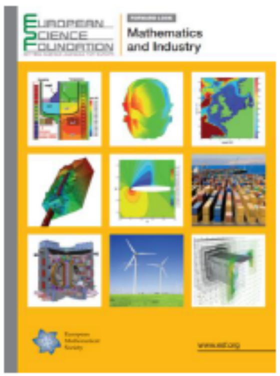
A window of opportunity to boost innovations in Europe

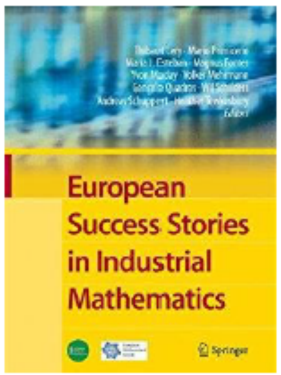
Modeling, Simulation and Optimization is evolving from a trouble shooting tool to key business drivers e in the form of digital twins

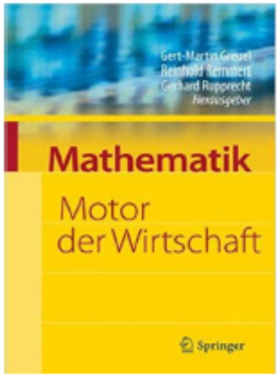
Product Lifecycle Management

Model Pioneers	CAx Sunrise	PLM Pervasion	Digital Twin Era
			
Timeline	**~1985**	**~2000**	**~2015**
Scientific experts use models	Computer aid in product design and engineering	Key for communication in across departments & companies	Nexus of data and executable models accessible to everyone
▪ Understanding of phenomena ▪ Failure Analysis	▪ Design Validation and Design ▪ Decision Support	▪ Design Driver ▪ Model-based Systems engineering	▪ Business Driver bridging different value chains ▪ Generative Design

Modeling, Simulation and Optimization is a Key Enabling Technology for Europe







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The Value of MSO in Europe

Automotive industry: **1000 bn €/year**
- Ecological and digital challenges

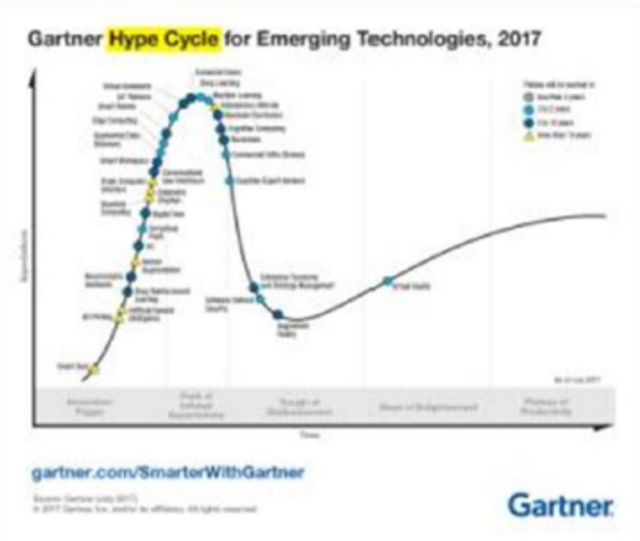
Aeronautics: **200 bn €/year**
- Test saving

Energy **priceless**
- Green transition

Impact studies of Mathematics in Europe

France	15% GNP,	9% of employments
Netherlands	30% GNP*,	11% of employments
UK	16% GNP,	10% of employments
Germany	"Mathematik: Motor der Wirtschaft"	

The digital twin concept has developed from a NASA[1] concept to one of the hottest technical trends in 2018 [2,3,4]



Digital Twins [2,3]

A digital twin is a digital representation of a real-world entity or system. Digital twins are linked to real-world objects and offer information on the state of the counterparts, respond to changes, improve operations and add value.

The concept of digital twins is not new.

Several factors have now converged to bring the concept of the digital twin to the forefront as a disruptive trend.

1) E. Glaessgen, D. Stargel(2012): *The digital twin paradigm for future NASA and U.S. air force vehicles*. 53rd AIAA/ASME/ASCE/AHS/ASC
2) L. Panetta (2017): Gartner Top 10 Strategic Technology Trends for 2018, Gartner
3) K. Panetta (2017): *Top Trends in the Gartner Hype Cycle for Emerging Technologies 2017*, Gartner
4) C. Pettey (2017): *Prepare for the Impact of Digital Twins*, Gartner

Digital Twins will have a major impact

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Digital Twins will make **Modeling, Simulation and Optimization widely available** & appropriate to drive **improved decision making** to a level not seen before throughout the **entire life-cycle** of engineered products and processes

ASSESS
ANALYSIS, SIMULATION AND SYSTEMS ENGINEERING SOFTWARE STRATEGIES

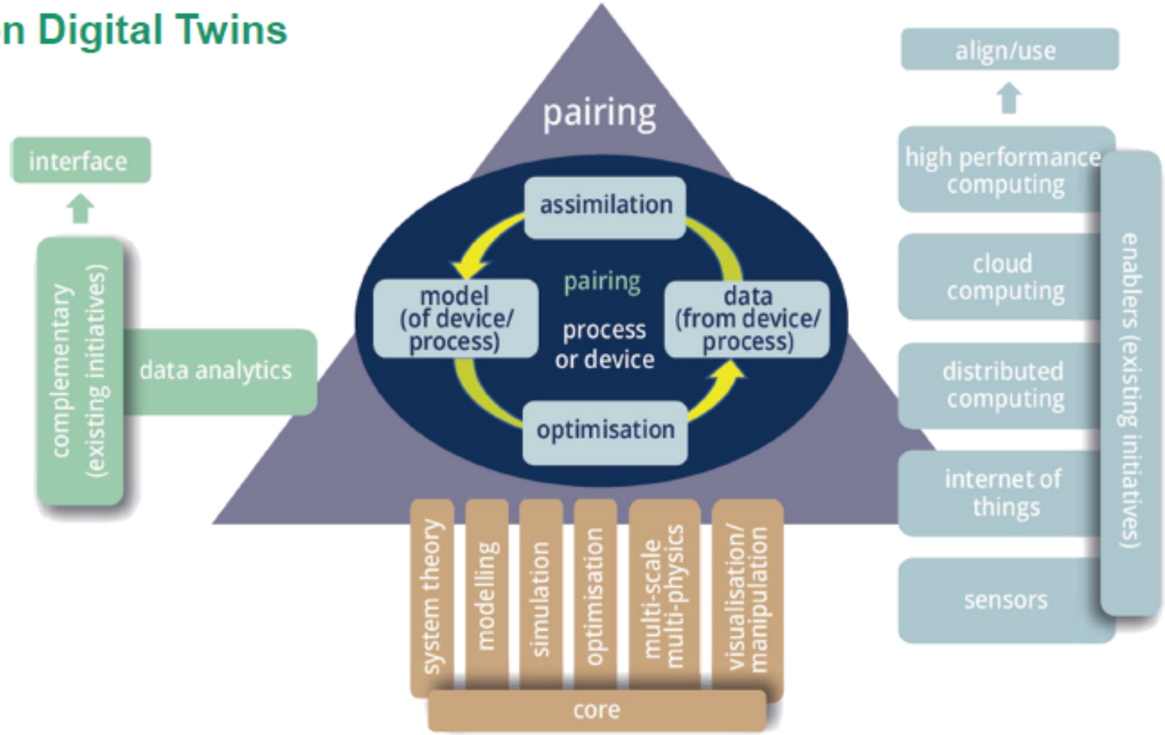
- The "Digital Twin" approach will dramatically increase the **demand, amount, breadth, and complexity of Engineering Simulation**
- Digital Twins will generate a **significant amount of data** in addition to sensor data
- **Machine Learning** can play a role in managing the data and **working with Systems Engineering** to determine what simulations are needed

Today's road blockers have to be resolved by the Next Generation of Digital Twins

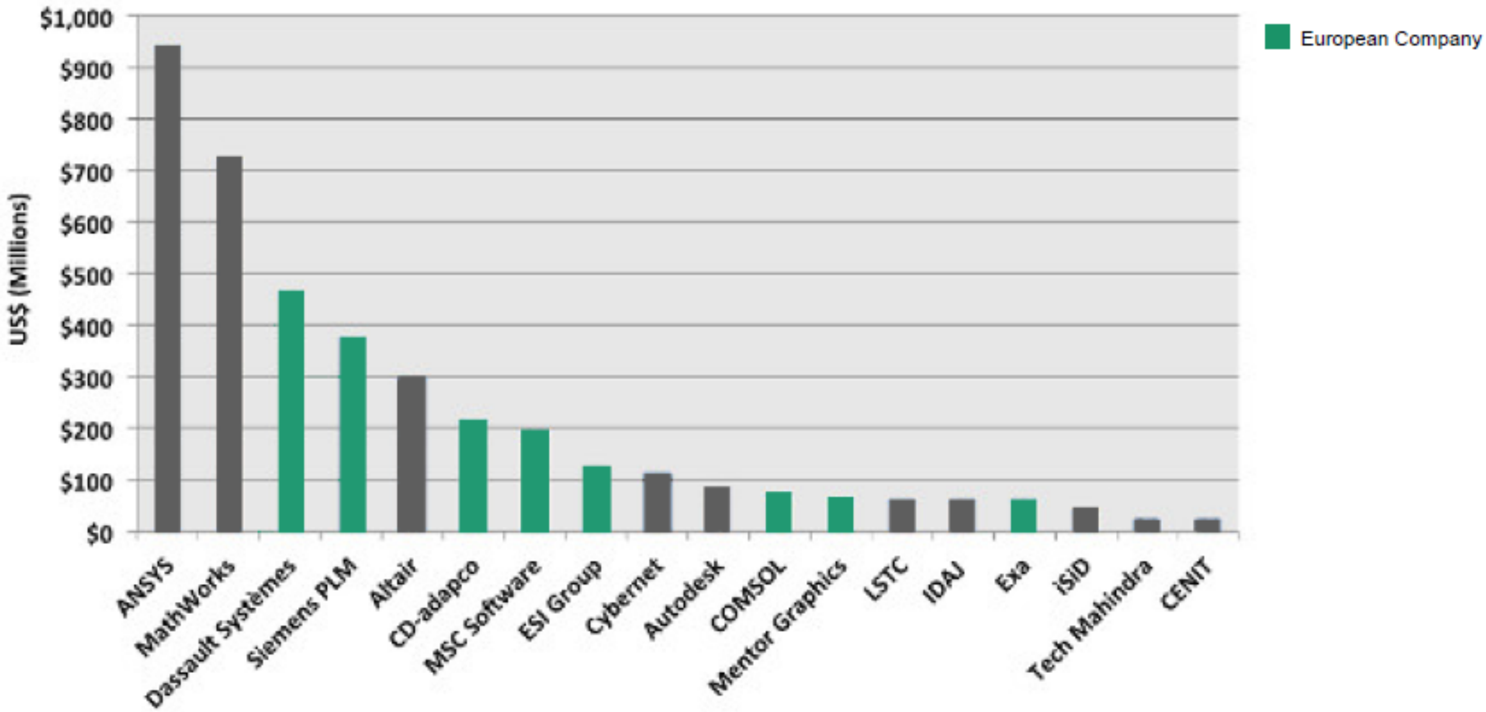
- **Transition** from powerful, but energy and time consuming computing **to intelligent edge computing** close to end-users and operations *(Proximity)*
- **Make current algorithmic capabilities accessible** to close the gap between state-of-the-art science and intelligent industrial use *(Accessibility)*
- **Provide a large well-trained workforce** covering the gap in human capital to maintain and accelerate the current economic development
- **Enhance the productivity engineers** who are a limited resource and cannot cover today's demands *(Usability)*
- **Address further identified opportunities** are not technologically covered with existing paradigms *(Interactivity, Reliability, Security)*

Multi-disciplinary efforts are required to drive new MSO paradigms closely linking with data analytics to leverage the vision of digital twins

Next Generation Digital Twins



Europe possesses a worldwide asset as it concentrates major simulation companies



1) CIMdata (2017) 2017 Simulation & Analysis Market Analysis Report

Digital twins are a key enabling technology to accelerate the development a optimization of industrial processes and devices

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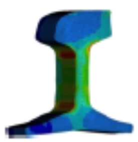
Next-generation digital twin

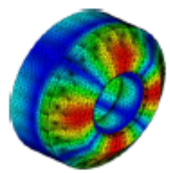
Digital Twin Era

PLM Pervasion

CAx Sunrise

Model Pioneers





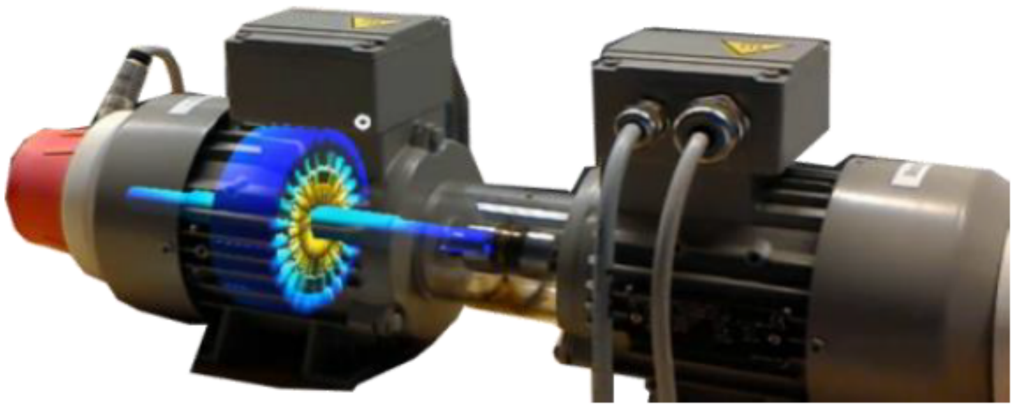
Timeline	~1985	~2000	~2015
Scientific experts use models	Computer aid in product design and engineering	Key for communication in across departments & companies	Nexus of data and executable models accessible to everyone

Key challenges

- Proximity
- Accessibility
- Usability
- Interactivity
- Reliability
- Security
- …

Digital Twins in Operation: *Measure the impossible by virtual soft sensors leading to higher availabilities up to 20%*

SIEMENS
Ingenuity for life



Model reduction

Reuse of engineering models speed up by a factor of > 1000

\+

Online simulation

Continuous calibration and UQ to go to the limit

\+

Novel Interaction

Intuitively grasp complex situations via Augmented Reality

Benefits

- Temperature **soft sensor** where no real sensor can be positioned
- **Reduced time** for restart and maintenance by **~20%**
- **An hour** could costs as much as **200k€ in the O&G industry**

Abbreviation: QU – Uncertainty Quantification

Executive Summary

- Accelerating the development and optimization of industrial processes and devices
- Extending current MBSE concepts to model-based assistance along the complete lifecycle

Needed:

- High powered multi-disciplinary effort to bring mathematical MSO methods together with techniques for the treatment of big data and AI methods
- To make these methods efficient on modern hardware envirionments

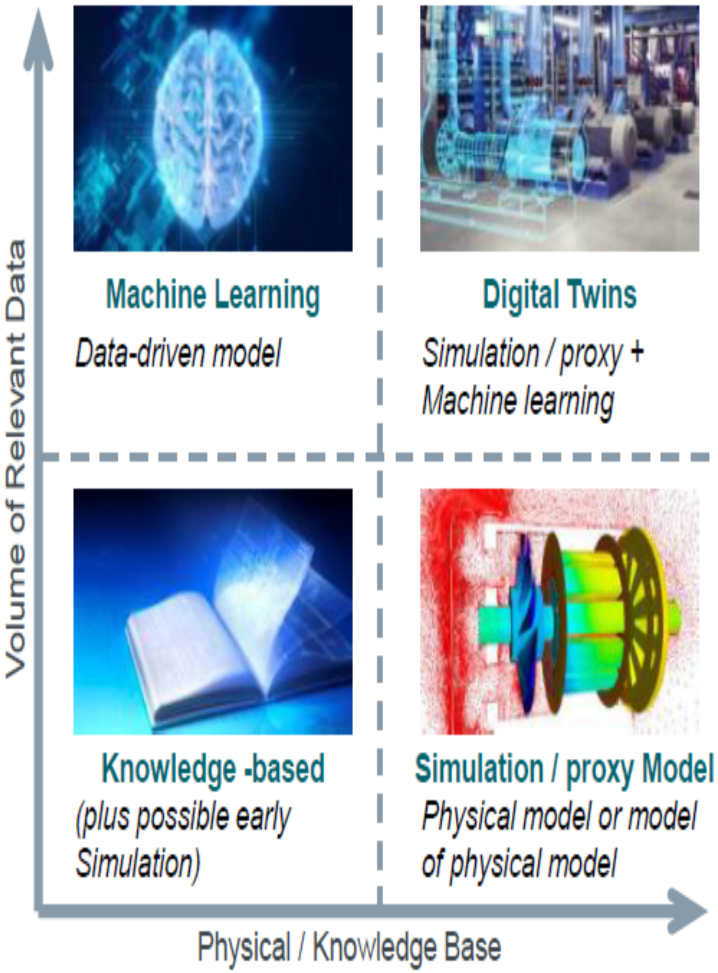
- Europe is traditionally very strong in mathematics (initially, more than in HPC & Exascale)
- MSO industry is focussing more and more in Europe (Siemens, ESI, Dassault Systemes, SAP)

Opportunities:

- Much more is possible when a major and concerted effort is developed to truly bridge the gap, and unite the strengths of European mathematicians with Industry 4.0 (…) to bring European Industry to the forefront
- Develop new business interactions

CONCLUSION

The particular approach depends upon the existing state of simulation and / or proxy model implementation



	Physical Models	Data Driven Models
Data Reliance	**Small Data**	Big Data
Domain Reliance	Deep Domain Expertise	**Little domain knowledge**
Fidelity & Robustness	**Highly non-linear and complex relations**	Limited to data and model complexity
Adaptability & Deployability	Complex and time consuming setup	**Rapidly adapt to a specific problem**
Interpretability	**Consistent physical meaningful**	Physics agnostics surrogate

Important to start/join new initiatives

- We recently got our MSCA EID proposal BIGMATH funded: "**Big** Data Challenges for **Math**ematics" (4 years, 7 PhD students, 8 academic/industry partners)
- NWA (Nationale Wetenschaps Agenda): call was published by NWO on May 24
  - 2-step procedure, 1st proposal in September
- NWO Cross-Over: call to be published soon
- We proposed a topic for FET Proactive: "Digital Twins for Industry and Innovation", outcome expected soon
  - If successful, ~20 Meuro available for calls in 2020