Modelling & Simulation

*from mechanics to medicine*

Elias Aifantis
Pierre Kerfriden
Stéphane P.A. Bordas *

stephane.bordas@alum.northwestern.edu  +352 621 131 048
Wilbur and Orville Wright

Wright Flyer

10:35am Dec 17, 1903
Wilbur and Orville Wright

On Dec 14 Wilbur won the coin toss, made the first attempt and stalled. Orville made the first flight on Dec. 17, 12 seconds & 120 ft.
Aircraft safety

20,000 years
Worldwide statistics

[1959-2001] 1,307 commercial jet aircraft losses

Today:
1 accident per 1,000,000 departures
Accident rates and fatalities/year
Accident rates and fatalities/year

Source: Flight Safety Foundation/Boeing Commercial Airplane Group
Learning from intuition & theory

Franklin Institute Science Museum. Wilbur Wright's handwriting
Learning from experience

Increased practical understanding of mechanics — in particular fracture and fatigue

Aloha airlines accident - fatigue cracks at corners

Bird strikes

Novel convertible aircraft
Learning from experience

The Liberty Ships
Learning from experience

At low temperatures, steel becomes more brittle

Welds are not good crack arrestors
WELDED CONSTRUCTION

RIVETED CONSTRUCTION

CRACK

PLATE EDGES & RIVET HOLES STOP CRACK PROGRESSION
Learning from experience

The liberty bell
(Philadelphia)
Learning from experience

The liberty bell
(Philadelphia)
Learning from experiments

World’s largest wind tunnel (2014)

Replica of the 1901 Wright Wind Tunnel (constructed with assistance from Orville Wright)
teaching...
New materials for more payload

Introduction of composite materials have reduced the weight of structures by 20%

Over 1,000km saving of 8,660kg of fuel [A340-300]
Material complexity
Material complexity

- Heterogeneous & multi-functional
- Experiments required to attain sufficient confidence in their behavior are increasingly costly
Material complexity

- Heterogeneous & multi-functional
- Experiments required to attain sufficient confidence in their behavior are increasingly costly
- Factor-of-Safety or probabilistic based methods cannot handle unknown unknowns
- Lack of similitude between testing (experimental) and operating conditions — also encountered in geophysics...
Material complexity

- Heterogeneous & multi-functional
- Experiments required to attain sufficient confidence in their behavior are increasingly costly
- Factor-of-Safety or probabilistic based methods cannot handle unknown unknowns - lack of similitude

- Move **away from heuristics** and experience-based engineering
- Develop **fundamental understanding** of physical processes (degradation, ...)
- Reduce weight
Increase product durability?

Virtual testing & Simulation

Analysis of the results

Virtual model of the device

product-specific
Buy or sell?

\[
\frac{\partial V}{\partial t} + \frac{1}{2}\sigma^2 S^2 \frac{\partial^2 V}{\partial S^2} + rS \frac{\partial V}{\partial S} - rV = 0
\]

Mathematical model + initial conditions

Identify behaviour

Real-time future option pricing
Devise effective deep brain stimulation
- reach the target area
- maintain contact with the electrode

Electrode separates from target

Model of the brain material

Predict electrode behaviour

Patient-specific
New kinds of experiments for new kinds of models

A bolted joint
A380 giant

Large structures
Small features
Very large problems
Model reduction - physics-based (1)

- Multilevel methods to reduce CPU time by orders of magnitude and devise robust, efficient code/model coupling

- HPC Adaptive multiscale models/solvers with controlled accuracy

Open problem: adaptive error controlled algorithms for model and discretization error. Use the right model at the right place/time.
Model reduction - algebraic (2)

- Multilevel methods to reduce CPU time by orders of magnitude and devise robust, efficient code/model coupling

- Virtual chart with controlled accuracy via ROM for multiscale modelling and real-time optimisation

Open problem: algebraic model reduction for non-linear problems with localisation - fracture, moving interfaces
NASA’s digital twin

Actual aircraft

- Life prediction and extension
- High fidelity modeling and simulation

Digital aircraft model

- Situation awareness
- Certification and design methods
**Medicine**

The average drug developed by a major pharmaceutical company costs at least $4 billion, and it can be as much as $11 billion.

**Mechanics**

The development cost of the A380 11 billion euros...

of the dreamliner...

32 billion US$
Mechanics

Macro (wing) - Micro (carbon fibres)

Environmental effects (Temperature, irradiation...)

Medical

Macro (Body, Physiology) to micro (microbes, needle/scalpel...)

Patient’s environment, living conditions, habits...

Organ properties depend strongly on age, gender, ...
**Medicine**

Clean hands before assisting childbirth to avoid infections

*In 1847 in Vienna, Ignaz Semmelweis (1818–1865) marginalized and attacked by professional peers*

**Mechanics**

Use rivets to arrest cracks

Avoid sharp angles

*Liberty ships, Aloha airlines accident...*

---

“Digital Twin” (Medic)

“Digital Twin” (NASA)

**Personalisation**
Patient/plane-specific simulation

Practical early-stage design simulations (interactive)

- Reduce the problem size while controlling the error (in QoI) when solving very large (multiscale) mechanics problems

Discretise

Discretise

Surgical simulation

[Allix, Kerfriden, Gosselet 2010]

courtesy: EADS
Surgical simulation

RealTcut

Learning → Planning → Assistance

Precision

Cataract Surgery

Abdominal minimally invasive surgery simulation (Inria, Shacra)

First implicit, interactive method for cutting with contact

[Courtecuisse et al., MICCAI, 2013 and Medical Image Analysis, 2014]
Interactive simulations

- Interactive simulations:
  - Fast computation
  - Human interaction

Several steps:
- Computation of the deformation
- Collision detection
- Contact resolution
- Rendering of the simulation

All must be done 25 times per second

Human interaction:
- Use stable algorithms
- Unpredictable motion
- Haptic device
Difficult to increase the frequency of processors

Heat dissipation

Electric consumption

Parallelization of algorithms
Surgical simulation

RealTcut

Learning  Planning  Assistance

Precision

Cataract Surgery

Abdominal minimally invasive surgery simulation (Inria, Shacra)

First implicit, interactive method for cutting with contact

[Courtecuisse et al., MICCAI, 2013 and Medical Image Analysis, 2014]
Surgical simulation

RealTcut

Learning  Planning  Assistance

Precision

Cataract Surgery

Abdominal minimally invasive surgery simulation (Inria, Shacra)

First implicit, interactive method for cutting with contact

[Courtecuisse et al., MICCAI, 2013 and Medical Image Analysis, 2014]
Abdominal minimally invasive surgery simulation (Inria, Shacra)
...not exactly brain surgery

Deep-brain stimulation

Cotin et al., 2013, 2014

Brain tumor resection

[Courtecuisse et al., MICCAI, 2013 and Medical Image Analysis, 2014]
...not exactly brain surgery

Deep-brain stimulation
…not exactly brain surgery

Deep-brain stimulation

Brain tumor resection

Cotin et al., 2013, 2014

[Courtecuisse et al., MICCAI, 2013 and Medical Image Analysis, 2014]
Tumour resection

Our goal is to simulate a brain tumor removal similar to this video
Source: http://www.youtube.com/watch?v=yhORvX-4Bx4
offline calculations

- generate particular solutions
- sort the solutions (surgeon)
- POD

online calculations

- compute asymptotic fields
- patient-specific mapping
- enrichment for tip of the cut
- small reduced order space
- local representation
- Global POD approximation

~10^6 snapshots

~10^3 snapshots

O(10) functions

~10^6 snapshots

instrument actions

patient-specific mapping

enrichment for tip of the cut

local representation

Global POD approximation
A few other directions for mechanics in medicine
Grand Challenge: Organs-on-a-chip
A Digital-Human-Twin
Multi-disciplinary modelling

- Multi-disciplinary modelling
- bio-compatible materials
- micro-fluidics/cell interaction modelling
- software controllers
- organ coupling and control
- manufacturing scale
- surface functionalisation
- influx
- sensing
- bio-compatible materials

adapted from Wyss institute, Harvard
Other directions for mechanics in medicine

Optimal anatomy
mathematical, multi-
scale homogenization
type to predict the
characteristics of
body parts, as they
are most likely to
emerge in the course
of evolutionary
selection.
Optimal anatomy mathematical, multi-scale homogenization theory to predict the characteristics of body parts, as they are most likely to emerge in the course of evolutionary selection.
Other directions for mechanics in medicine

Optimal anatomy
mathematical, multi-
scale homogenization
type to predict the
characteristics of
body parts, as they
are most likely to
emerge in the course
of evolutionary
selection.

not exactly brain surgery...

- Medicine will rely increasingly on modeling and simulation
  - understanding of physiological mechanisms and evolution
  - patient-specific drug design
  - patient-specific surgical operations

... medical twinning
Mechanics will rely increasingly on modeling and simulation to design, control, certify increasingly complex systems.

- multiscale and multiphysics phenomena - fracture, ...
- self-aware self-healing/monitoring structures
- simulations will have to be able to deal with the actual environment and operating conditions
- real-time simulations will help gain insight into non-intuitive phenomena (composites, nano-scale...)
... but will require

- Predictive models
  - multiscale and multiphysics
  - adaptive - focusing effort only where required
  - model reduction - algebraic and physics-based
  - able to learn from real-time data

... mechanical twinning
Gracias por su atención
Merci de votre attention
Thank you for your attention
Danke für Ihre Aufmerksamkeit
Gracie per la vostra attenzione

stephane.bordas@alum.northwestern.edu +352 621 131 048
Summary of our lab’s work (1)

- Efficient numerical prediction of material and structural failure

  [Kerfriden et al., 2010]

  L. Beex  S.P.-A. Bordas  P. Kerfriden

- Characterisation and optimisation of composites

  [Sutula et al., 2013]

  [Silani et al., 2013]
Summary of our lab’s work (2)

- Interactive simulations of biological structures

- Simplified Link between CAD/CT scans and analysis

[Scott et al., 2013]

[Courteguissee et al., 2013]

[Nguyen et al., 2013]
Summary of our lab’s work (3)

- Advanced discretization techniques for complex PDEs

  - XFEM/meshfree

  - Isogeometric analysis

  - Taylor bar problem (dynamic fragmentation)

  - Model simplification (CAD)

  - IGA

[Sources: Bordas et al., 2008; Tornincasa et al., 2013]
• Multilevel methods to reduce CPU time by orders of magnitude and devise robust, efficient code/model coupling

- HPC Adaptive multiscale models/solvers with controlled accuracy

[Image: Diagram showing cohesive interfaces, bolt (steel), laminate (carbon/epoxy), orthotropic linear piles.

[Reference: Kerfriden et al., 2010]

[Reference: Akbari et al., 2013]
Summary of our lab’s work (5)

- Multilevel methods to reduce CPU time by orders of magnitude and devise robust, efficient code/model coupling

- Virtual chart with controlled accuracy via ROM for multiscale modelling and real-time optimisation

[Hoang et al., 2013]

[Kerfriden et al., 2013]
New Research Directions

- Organ model and simulation
- Sensitivity and stochastic analysis
- Model order reduction and machine learning
- Multi-scale/physics modelling

Luxembourg Centre for Computational Modelling and Simulation

New Markets
- Self-diagnostics
- Immunology
- Toxicology
- Pharma
- Research groups
- Biochips

Existing Luxembourg Industry
- Control
- Micro-fluidics
- Micro-fabrication
- Organ-on-chips
- Disease and treatment modelling
- Optimal design of experiments
- Increase reliability of experiments
- Decrease amount of animal experiments
- 3D printing
- Rapid prototyping
- IEE
- Delphi
- Advanced functional materials
- HPC
- Sensing
- 3D printing
- Rapid prototyping
- Dupont

Training and Education
- Self-diagnosics
- Immunology
- Toxicology
- Pharma
- Research groups
- Biochips

Pilot Unit
Other approach to ERA
Chairs based on reinforcing
Core Competencies

Computer Science
- Data Mining
- Imaging
- Machine Learning
- Mathematics

Mathematics
- Financial Mathematics
- Statistical Physics
- Quantum Physics

Computer Graphics
- Geometry
- Interactive Simulation
- Modelling & Simulation

Materials
- Solid State Physics
- Stochastic PDEs

Quantum Computing
- Uncertainty
- Soft-matter Physics

Complex systems
- Multi-Physics
- Multi-scale
- Model reduction

Life Sciences
- Genetics
- Geophysics
- Physics

Health
- Multi-scale
- Model reduction

Engineering
- Civil Engineering
- Mechanics

Physics
- Quantum Physics
- Soft-matter Physics

Life Sciences
- Genetics
- Geophysics
- Physics

Health
- Multi-scale
- Model reduction

Engineering
- Civil Engineering
- Mechanics

Other approach to ERA
Chairs based on reinforcing
Core Competencies
Other approach to ERA
Chairs based on reinforcing
Core Competencies

Mathematics

Financial Mathematics

Stochastic
PDEs

Statistical
Physics

Soft-matter
Physics

Physics

Geophysics

Multi-Physics
Genetics

ERA

Model reduction

Interactive Simulation

Modelling & Simulation

Multi-scale

Engineering

Life Sciences

Computer Graphics

Computer Science

Data Mining

Imaging

Machine Learning

Geometry

Solid State Physics

Mathematics

Physics

Interactive Simulation

Multi-Physics

ERA

ERA

ERA

ERA

ERA
Scientific challenges

- micro-fluidics
- software controllers
- real-time (big) data analysis
- functional surfaces
- multi-scale/physics simulation
- optimal design of experiments
- manufacturing
- uncertainty
- cell differentiation
- active biocompatible materials
- 3D cell culture
- disease

- Biomedicine
- Computer Science
- Engineering
- Mathematics
- Physics

- micro-fluidics
- durability
- interfaces