Modelling and Simulating Complex Systems

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Speak up

DataAndComput:
Number: 73334
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2 messages,
0 comments,
2 votes

23/01/2019 14:21 by me
This room will remain open during the whole course and allows you to ask questions without being shy, or interrupting the flow. You can also vote for a question if you find it relevant. All this can be done online. Enjoy! Stéphane BORDAS

+1
1 vote

23/01/2019 14:20 by me
Dear course participants, welcome! I am opening this room so that you can start asking questions you’re interested in hearing about tomorrow for the “upskilling” course you will be participating in.

+1
1 vote
Speak up
Acknowledgements

The University of Luxembourg

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The legato-team
legato-team.eu
What is Truth?

• Sciences are plural, they have validity domains, hence truth has multiple faces;

• Knowledge is never complete and Research never finished;

• Knowledge itself is less important than the method used to acquire it;

• What we discover through research is the BEST we can discover at a given instant in time;

• Investing in Research indicates trust in the scientific method.
Data

• 90% of the data available today was generated in the last two years;

• Developing new scientific methodologies to optimise the acquisition of new understanding from data;

• Develop methodological core based on the language of mathematics and common to various application areas;

• These new methodologies will fuel science and technology by creating multi-disciplinary interactions in two fields: personalised medicine and advanced materials.
Access to TRUTH(S)

Access to Reality(ies)

Trust in Institutions, Methods, Human discourse
\[ \frac{\partial V}{\partial t} + \frac{1}{2} \sigma^2 S^2 \frac{\partial^2 V}{\partial S^2} + rS \frac{\partial V}{\partial S} - rV = 0 \]

MATHEMATICS

\[ \hat{\mathcal{H}} \Psi = E \Psi \]
Outline

• Scientific method, experiments, analytical methods and models

• What is a complex system?

• What models are available to understand and predict?

• What are agent-based models?

• Equation-based (mathematical) models

• How to choose the “best” model?
The scientific method and the 3 pillars of science
(or should we say 4?)
How do we think about the world?
Aristotle
384-322 BC
Geocentrism
Copernicus
1473-1543
Heliocentrism
Galileo Galilei
1564-1642
innovative combination of experiments and mathematics
Isaac Newton
1643-1727

Universality of gravitation...
Our lack of knowledge is uncertainty
How do we think about the world?
Inductive thinking
Observations -> conclusions on governing laws
Write mathematical models from observations
Experiments to
- Formulate hypotheses and laws about the world
- Identify parameters of mathematical models
Conduct numerical experiments to
- Formulate hypotheses and laws about the world
- Identify parameters of mathematical models
Conduct numerical experiments to
- Formulate hypotheses and laws about the world
- Identify parameters of mathematical models
Computational Sciences: the discipline concerned with the use of computational methods and devices to enable scientific discovery and engineering applications of science.
Simulation based science
Simulation based science

RISING ABOVE THE GATHERING STORM
Energizing and Employing America for a Brighter Economic Future

National Academy of Sciences
National Academy of Engineering
Institute of Medicine
Simulation based science

Report to the President

Computational Science: Ensuring America’s Competitiveness

President’s Information Technology Advisory Committee

June 2005
Simulation based science

US National Science Foundation (NSF)

2006
Research and Education in Computational Science and Engineering
September 2016

Report from a workshop sponsored by the Society for Industrial and Applied Mathematics (SIAM) and the European Exascale Software Initiative (EESI-2), August 4-6, 2014, Breckenridge, Colorado

Workshop Organizers:
Officers of the SIAM Activity Group on Computational Science and Engineering (SIAG/CSE), 2012-2014:
Ulrich Rüde, Universität Erlangen-Nürnberg, Chair
Karen Willcox, Massachusetts Institute of Technology, Vice Chair
Lois Curfman McInnes, Argonne National Laboratory, Program Director
Hans De Sterck, Monash University, Secretary

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Additional Contributors:

What computational & data sciences enable that traditional science doesn’t

LOOK INTO THE PAST
- Earthquakes, climate, oil discovery, archeology, seismology, law, economics, finance

PROBE THE FUTURE
- Explore the effects of thousands of scenarios
- Drug design, space exploration, climate change, natural disasters, …

CHOOSE MODELS
- Explore consequences of breakdown of models and theory…

OPTIMISE
- Optimize procedures, designs, products, systems, etc.
Most Grand Challenge problems today involve complex phenomena and systems that lie on **disciplinary boundaries**.

**Interdisciplinary research** moves beyond simple collaboration and teaming to integrate **data**, methodologies, perspectives, and concepts from multiple disciplines in order to advance fundamental understanding and to solve **real world problems**.

Interdisciplinary research holds the promise of pushing fields forward and accelerating scientific **discovery**.

Interdisciplinary study and training **prepares a workforce** that undertakes scientific challenges in new and innovative ways.
Mission for Computational and Data Sciences in Luxembourg

Mission

To provide the infrastructure and intellectual leadership for developing outstanding interdisciplinary research programs in computational and data sciences.

To enable world-leading education in computational and data sciences in Luxembourg.

To promote and facilitate digital literacy and provide the fundamental building blocks necessary to the development of Industry 4.0 in Luxembourg.
Outline

- Scientific method, experiments, analytical methods and models
- What is a complex system?
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- What are agent-based models?
- Equation-based (mathematical) models
- How to choose the “best” model?
Complex systems

- Large number of interacting components
- Evolving over time
- Decentralised decisions vs. Centralised control
- **Local** interactions $\rightarrow$ **emergence** of **global** patterns
Examples

• Biological systems (brain, cancer, bacteria…)
• Policy and government
• Environment (weather, ice sheet, pollution…)
• Economy, stock market
• Ecosystems (bats, fish…)
• Functional/sensing materials (graphene…)
Emergence

- Micro (local) level leads to patterns at the macro level
  - Ant/bee colonies
  - Housing patterns, traffic jams
  - Populations in ecosystems
  - Pressure of gases
  - Pricing
  - Effect of individual behaviours in societies
Two questions about emergence

- You know the micro, you want to understand the macro
- You observe the macro, you want to deduce the micro rules

THIS IS HARD
Outline

• Scientific method, experiments, analytical methods and models

• What is a complex system?

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• What are agent-based models?

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• How to choose the “best” model?
What is a model?

When we were kids ;-) or grownup kids…
What is a model?

Biologists
What is a model?

If you are in fashion...
What is a model?

• An abstract description of a process, object, system, event which exaggerates certain aspects compared to others

• “Essentially, all models are wrong, but some are useful” George Box, 1987

• The choice of the model depends on the quantities of interest (QoI)
What is a model?

If you are into geography or geophysics
What is a model?

Physical model

Mathematical model

J.F. Remacle
Quantity of Interest: neuro-transmission

Tissue phantoms/mimics
(Dini, Imperial College London)
Quantity of Interest: stiffness
Types of models

- Mental Model
  - Statistical
  - Mechanistic/Dynamic
    - Mathematical
      - ODE
      - PDE
      - Eulerian-Lagrangian
    - Algorithmic
      - Artificial Neural Networks
      - Cellular Automata
      - Agent-based
      - Mixed (e.g. SSM)
What is a “good” dynamic model?

• “All models are wrong. Some of them are useful.” -- George E.P. Box (1979)
How to build dynamic models?

The modelling process

1. Define a new problem
2. Define the system
3. Decide on boundaries & scale
4. Isolate state variables & processes
5. Express system in modelling terms
6. Run simulations and get results
7. Compare with real patterns/data
8. Answer the question

OK

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COMPUTATIONAL & DATA SCIENCES

Industrial/clinical Valorisation

Identification of Phenomena

Model Evaluation & Comprehension

Model Genesis & Evolution

Local economy

Data Analysis

Model Properties

Model Analysis

MODELLING
Stirling murmuration (Rome)
Flocking of Stirlings

• Is there a leader?

• Are the global patterns attributable to local rules? Can we derive global equations governing their behaviour? Is the process deterministic?

• What is their acceleration, maximum velocity, reaction time, minimum distance with other birds, line of sight, manoeuvrability?

Made using NetLogo
Outline

• Scientific method, experiments, analytical methods and models
• What is a complex system?
• What models are available to understand and predict?
  • What are agent-based models?
  • Equation-based (mathematical) models
• How to choose the “best” model?
Boids flocking local rules for global behaviour

Made using NetLogo

Separation: steer to avoid crowding local flockmates
Alignment: steer towards the average heading of local flockmates
Cohesion: steer to move toward the average position of local flockmates
Applications of ABM/IBM

• A growing, unified community

(Vincenot, 2018)
Applications of ABM/IBM

• Over 12,000 publications
• Everywhere in science!

(Vincenot, 2018)
Mathematical models

59% is a threshold (50/50 probability)

Self-Organised Criticality

Fire spreading through a forest for various tree densities by NetLogo
Self-Organised Criticality

The Forest-Fire model belongs to the class of Self-Organized-Critical (SOC) systems, which are governed by a slow driving energy input and burst (avalanches) of dissipative outputs resulting often in fractal structures. These systems were introduced by P. Bak et al. [2] in 1987 using the example of a sandpile model. These SOC models can be applied to many different fields, famous applications are for instance: earthquakes, solar flares, co-evolution, forest fires, hydraulic fracture and more. In addition they show scaling laws and are related to critical phenomena.

https://pdfs.semanticscholar.org/ec58/3f6f99f1d15a1d1ae2de1d243b648efd2ba8.pdf
https://www.sciencedirect.com/science/article/pii/B9780128001301000047
Algorithmic Languages

• ABMs are always coded as algorithms
• Most often, simple deductive behavior:
  e.g. “if hungry, search food”
    \[condition \quad action\]
• Implementations require coding skills, but simplified languages exist
Netlogo

- Most used by ecologists
- Simplified language
- Slow, but good for relatively simple models
- Simple random movement model →

```
to setup
  clear-all
  create-turtles 10
  reset-ticks
end

to go
  ask turtles [ fd 1 ;; forward 1 step
              rt random 10 ;; turn right
              lt random 10 ;; turn left
            ]
  tick
end
```
Netlogo
Gama

- Computer scientists
- More complex language
- Powerful, but difficult
Gama
• “Keep it Simple, Stupid” (KISS) principle
• Try to make models as simple as possible
• Many processes/parameters does NOT mean better accuracy!!
Pattern-oriented Modelling

• Use patterns instead of numerical fitting to validate model (Grimm et al. 2005)
Pattern-oriented Modelling

1. Define a new problem
2. Define the system
3. Decide on boundaries & scale
4. Isolate state variables & processes
5. Express system in modelling terms
6. Run simulations and get results
7. Compare with real patterns/data

Patterns
ODD: Describing ABM Models

• The ODD Protocol
  – Overview, Design concepts, and Details (ODD)
  – A strict set of guidelines to describe and publish ABMs
  – Guarantees the replicability of models and studies
  – More than 2000 citations
  – 2\textsuperscript{nd} version already; 3\textsuperscript{rd} version in preparation
  – See Grimm et al. (2006 and 2010)

• Please \textit{always} use when developing ABMs!
Useful Reads

Agent-based Modelling


Vegetation model

Outline

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Mathematical models

59% is a threshold (50/50 probability)

Self-Organised Criticality

Fire spreading through a forest for various tree densities by NetLogo
Physics-based or mathematical models
Physics-based model

$T (K)$ is the temperature of the fire layer,
$S \in [0, 1]$ is the fuel supply mass fraction (the relative amount of fuel remaining),
k $(m^2 s^{-1})$ is the thermal diffusivity,
$A (K s^{-1})$ is the temperature rise per second at the maximum burning rate with full initial fuel load and no cooling present,
$B (K)$ is the proportionality coefficient in the modified Arrhenius law,
$C (K^{-1})$ is the scaled coefficient of the heat transfer to the environment,
$C_S (s^{-1})$ is the fuel relative disappearance rate,
$T_a (K)$ is the ambient temperature, and
$\vec{v} (ms^{-1})$ is the wind speed given by atmospheric data or model.

The model is derived from the conservation of energy, balance of fuel supply, and the fuel reaction rate:

\[
\frac{dT}{dt} = \nabla \cdot (k \nabla T) - \vec{v} \cdot \nabla T + A \left( S e^{-B/(T-T_a)} - C (T-T_a) \right), \quad (1)
\]

\[
\frac{dS}{dt} = -C_S S e^{-B/(T-T_a)}, \quad T > T_a, \quad (2)
\]

https://arxiv.org/pdf/0709.0086
\[
\frac{dT}{dt} = \nabla \cdot (k \nabla T) - \vec{v} \cdot \nabla T + A \left( S e^{-B/(T-T_0)} - C (T - T_a) \right), \quad (1)
\]

\[
\frac{dS}{dt} = -C_S S e^{-B/(T-T_0)}, \quad T > T_a, \quad (2)
\]

with the initial values

\[
S(t_{\text{init}}) = 1 \text{ and } T(t_{\text{init}}) = T_{\text{init}}. \quad (3)
\]

The diffusion term \( \nabla \cdot (k \nabla T) \) models short-range heat transfer by radiation in a semi-permeable medium, \( \vec{v} \cdot \nabla T \) models heat advected by the wind, \( S e^{-B/(T-T_0)} \) is the rate fuel is consumed due to burning, and \( A C (T - T_a) \) models the convective heat lost to the atmosphere. The reaction rate \( e^{-B/(T-T_0)} \) is obtained by modifying the reaction rate \( e^{-B/T} \) from the Arrhenius law by an offset to force zero reaction at ambient temperature, with the resulting reaction rate smoothly dependent on temperature.

**Questions:** Identification of parameters?
Outline

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- What is a complex system?
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When use agent-based models

- Not too few, nor too many - medium numbers of entities
- Heterogeneous systems
- Local interactions
- Rich environments
Not too many, not too few

- Casti, 1996
  - Too few agents, the system is too simple: game theory and ethnography are sufficient
  - Too many agents, averages work well, statistical descriptions
Richness of the environments

- Social networks
- Geographical systems
- The environment can itself be an agent
Compare agent-based models (ABM), mathematical models (MM), statistical models (SM)

• MM are often continuous: Nano-wolf problem (Wilson 1998), but if you can write equations, do it

• ABM and MM approaches need parameters which are difficult to measure (agents need local parameters and rules)

• SM need large data sets of high quality

• ABM can be coupled to MM

• Both ABM and MM can learn from SM and Machine Learning and become adaptive
Some future prospects

- Lab experiments are costly, they are sometimes impossible, dangerous... they can help generate theories.

- ABM or MM can be created from lab experiments.

- Models can help scale up from experiments.

- Experiments are done within a laboratory setting, far removed from real-life, where the models would be used.

- Digital twins can avoid such issues, but are still illusory in practice.

- Models can help provide insights into sensitivities and uncertainties.
Use of models

- Describe systems
- Explain behaviour
- Experiment and test systems
- Measure sensitivities
- Create analogies
- Educate
- Predict

Mathematical models

Agents
Thank you to COMPLEXITY EXPLORER, SANTA FE INSTITUTE.
A focus on equation-based models

• How can we control the quality of simulations, verification and validation?

• Why are set-in-stone-models limited?

• How can we leverage statistical models to improve our models?
Porous media models

**Microscale (pore scale)**
*Interfaces identifiable*

- Solid phase
- Liquid water
- Gaseous phase (mostly air)

**Macroscale (Darcy scale)**
*At each point more phases coexist*

**RVE**

**Microscale Conservation EQS**

**Macroscale Conservation EQS**

**TCAT**
*Thermodynamically Constrained Averaging Theory (Gray & Miller, 2005)*

*From Ms. Stanton – Science (http://www.oconee.k12.sc.us/)*
Can also help model tumours

Avascular

Vascular

Metastatic

...angiogenesis
MANY PROBLEMS
SHARE THE SAME FORMALISM

Option Pricing


\[
\frac{\partial V}{\partial t} + \frac{1}{2} \sigma^2 S^2 \frac{\partial^2 V}{\partial S^2} + rS \frac{\partial V}{\partial S} - rV = 0
\]
MANY PROBLEMS
HAVE THE SAME FORMALISM

Option Pricing


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

Transport in Porous Media

Mathematical Modelling

Continuous Problem
Continuous Problem

Bijar, Rohan, Perrier & Payan 2015
Mathematical Modelling

Continuous Problem

Mathematical Model
Mathematical Modelling

Continuous Problem

Mathematical Model

\[
\min_{u \in V} \frac{1}{2} \int_{\Omega} \sigma(u, \beta) : \varepsilon(u) \, dx - \int_{\Omega} g \cdot u \, dx
\]

with

\[
\sigma(u, \beta) = \sigma_P(u) + \sigma_A(\beta)
\]

\[
\sigma_A(\beta) = \beta T e_A \otimes e_A
\]

- \(e_A\): fiber direction
- \(T\): tension
- \(\beta\): activation

- passive material
- muscular activation
Mathematical Modelling

Continuous Problem

Mathematical Model

IVUS – Plaque # 1

B

Real contours

Necrotic core

Fibrosis

Region of interest

Fixed
Mathematical Modelling

Continuous Problem

Mathematical Model

Discrete Problem
Mathematical Modelling

Continuous Problem

Mathematical Model

Discrete Problem

Finite element mesh of a tongue with F. Chouly et al.

Hexahedral mesh of a brain with Bruno Lévy, Inria

Meshless brain discretization with Bruno Lévy, Inria
Mathematical Modelling

Continuous Problem

Mathematical Model

Discrete Problem

Numerical Solution

$u$
Mathematical Modelling

- Continuous Problem
- Mathematical Model
- Discrete Problem
- Numerical Solution
Mathematical Modelling

Continuous Problem

Mathematical Model

Discrete Problem

Numerical Solution

Bijar, Rohan, Perrier & Payan 2015

\[ \min_{u \in V} \frac{1}{2} \int_{\Omega} \sigma(u, \beta) : \varepsilon(u) \, dx - \int_{\Omega} g \cdot u \, dx \]
Mathematical Modelling

Continuous Problem

Mathematical Model

Discrete Problem

Numerical Solution

Model Error

Bijar, Rohan, Perrier & Payan 2015

\[
\min_{u \in V} \frac{1}{2} \int_{\Omega} \sigma(u, \beta) : \varepsilon(u) \, dx - \int_{\Omega} g \cdot u \, dx
\]

Physical Problem
Constitutive Model
Material Parameters
Mathematical Modelling

Continuous Problem

Mathematical Model

Discrete Problem

Numerical Solution

Model Error

Geometry
Boundary conditions

IVUS – Plaque # 1

Region of interest

Fixed
Mathematical Modelling

Continuous Problem

Mathematical Model

Discrete Problem

Model Error

Discretization Error

Numerical Solution

vs.
Mathematical Modelling

Continuous Problem

Mathematical Model

Discrete Problem

Model Error

Discretization Error

Numerical Solution
Mathematical Modelling

Continuous Problem

Mathematical Model

Discrete Problem

Numerical Solution

Model Error

Discretization Error

Numerical Error

32 bit?

64 bit?
Mathematical Modelling

Continuous Problem

Mathematical Model

Discrete Problem

Numerical Solution

Model Error

Discretization Error

Numerical Error

Total Error

Reality vs. Simulation

Our goal is to simulate a brain tumor removal similar to this video.
Source: https://www.youtube.com/watch?v=yhORVx4I8e4

Cannula insertion
Mathematical Modelling

- Continuous Problem
- Mathematical Model
- Discrete Problem
- Numerical Solution

- Model Error
- Total Error
- Discretization Error
- Numerical Error

Are we solving the right problem?

Numerical Solution
Mathematical Modelling

Continuous Problem

Mathematical Model

Discrete Problem

Numerical Solution

Model Error

Discretization Error

Numerical Error

Total Error

Are we solving the right problem?
Mathematical Modelling

Continuous Problem

Mathematical Model

Discrete Problem

Numerical Solution

Model Error

Discretization Error

Numerical Error

Total Error

Are we solving the right problem?

Are we solving the problem right?
Mathematical Modelling

- Continuous Problem
- Mathematical Model
- Discrete Problem
- Numerical Solution

- Model Error
- Discretization Error
- Numerical Error
- Total Error

- VALIDATION
- VERIFICATION

Are we solving the right problem?
Are we solving the problem fast enough?
Mathematical Modelling

Continuous Problem → Mathematical Model → Discrete Problem → Numerical Solution

Model Error
Discretization Error
Numerical Error
Total Error

Exact solution is not known

Are we solving the right problem?
Are we solving the problem fast enough?
Are we solving the problem right?

VALIDATION
VERIFICATION
Outline

A focus on equation-based models

- How can we control the quality of simulations, verification and validation?
- Why are set-in-stone-models limited?
- How can we leverage statistical models to improve our models?
Outline

• Data-driven modelling: Beyond setting models in stone
  • Data assimilation
    • How can we learn from observations “on-the-fly”.
    • The power of digital twins.
  • Future challenges
Introduction to data assimilation

- Bayesian inference
- Kalman filtering
Model and parameter identification through Bayesian inference in solid mechanics

Hussein Rappel

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September 07, 2018
Bayesian inference

Primer
Where the ball “usually” lands based on experience
Where the ball “usually” lands based on experience
Where it looks “likely” that the ball will land given the position of the opponent and the orientation of the racket and our internal model of ball motion
Plausible position of the ball given the combined prior knowledge, observations and our model of ball motion
What you know a priori

Prior

Likelihood

Posterior

Combined knowledge

What you guess based on your model and observations
What you know a priori

\[ \pi(x), \pi(y|x) \]

Combined knowledge

\[ \pi(x, y) \]

What you guess based on your model and observations

\[ \pi(x, y) = \pi(y|x)\pi(x) \]
posterior = \frac{\text{prior} \times \text{likelihood}}{\text{evidence}}

\pi(x, y) = \pi(y|x)\pi(x)

What you know a priori

\pi(x)

\pi(y|x)

What you guess based on your model and observations

\pi(x, y)

Combined knowledge
Bayes’ theorem

$$\text{posterior} = \frac{\text{prior} \times \text{likelihood}}{\text{evidence}}$$

$$\pi(x|y) = \frac{\pi(x)\pi(y|x)}{\int \pi(x)\pi(y|x)dx}$$

prior $\pi(x)$  
likelihood $\pi(y|x)$  
posterior $\propto \pi(x|y)$
Bayes’ theorem

\[ \pi(x|y) = \frac{\pi(x)\pi(y|x)}{\int \pi(x)\pi(y|x)dx} \]

\(\pi(.)\) : probability distribution function

\(\pi(.|.)\) : conditional probability distribution function

\(x\) : material parameter

\(y\) : observations
Parameter identification: Bayesian approach

**Bayes’ theorem**

\[
\pi(x|y) = \frac{\pi(x)\pi(y|x)}{\int \pi(x)\pi(y|x)dx}
\]

**Descriptive formula**

\[
\text{Posterior} = \frac{\text{Prior} \times \text{Likelihood}}{\text{Evidence}}
\]
A discrete example of Bayes’ theorem
This is our prior information for the probability of each face: 1/6
$P = \frac{1}{6}$
Assume that after throwing the dice, you see the above evidence
Goal: determine the probability of this evidence for each face of the dice
One would never see a dot at the star positions for this face.

The probability of the evidence is zero.
Two possibilities (a,c) and (b,d)
Also two possibilities (a,c) and (b,d)
Four possibilities
Four possibilities
Four possibilities
\[
\pi(y) = \frac{0 + 2 + 2 + 4 + 4 + 4}{6 \times 4} = \frac{16}{24}
\]
\[ \pi(x|y) = \frac{\text{Prior} \times \text{Likelihood}}{\text{Evidence}} = \frac{\frac{1}{6} \times \frac{1}{2}}{\frac{16}{24}} = 0.125 \]
Stress-strain data
Identify the parameters
Construct the likelihood function

Model

\[ Y = f(X, \Omega) \]
\[ \Omega : \text{Error} \]
\[ X : \text{Material parameter} \]

observations = f(parameters, error)
Additive noise model

\[ Y = f(X) + \Omega \]
Likelihood function for additive model

\[ \pi(y|x) = \pi(\omega) = \pi(y - f(x)) \]

\[ Y = f(X) + \Omega \]
Constitutive law: linear elasticity

Constitutive model

\[ \sigma = E \varepsilon \quad \text{or} \quad \sigma = x \varepsilon \]

Observed data

\[ Y = X \varepsilon + \Omega \]
Prior information on Young’s modulus

\[ \pi_{\text{prior}}(x) = N(210, 900) \]
Error model (noise)

\[ \pi(e)_{error} = \mathcal{N}(0, 0.0001) \]
Likelihood function

\[ \pi(y|x) = N(y - x\varepsilon, 0.0001) \]

\[ \pi(y|x) = \pi(\omega) = \pi(y - f(x)) \]
Bayes’ theorem: calculate the posterior

\[
\text{posterior} = \frac{\text{prior} \times \text{likelihood}}{\text{evidence}}
\]

\[
\pi(x|y) = \frac{\pi(x)\pi(y|x)}{\int \pi(x)\pi(y|x)dx}
\]
Bayes’ theorem: calculate the posterior

\[
\text{posterior} = \frac{\text{prior} \times \text{likelihood}}{\text{evidence}}
\]

\[
\pi(x|y) = \frac{\pi(x)\pi(y|x)}{\int \pi(x)\pi(y|x)dx}
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Bayes’ theorem: calculate the posterior

\[
\text{posterior} = \frac{\text{prior} \times \text{likelihood}}{\text{evidence}}
\]

\[
\pi(x|y) = \frac{\pi(x)\pi(y|x)}{\int \pi(x)\pi(y|x) \, dx}
\]

prior \hspace{1cm} \pi(x)

likelihood \hspace{1cm} \pi(y|x)

\[
\pi(y|x) = N(y - x\epsilon, 0.0001)
\]

\[
\pi(y|x) = \pi(\omega) = \pi(y - f(x))
\]
Bayes’ theorem: calculate the posterior

\[ \text{posterior} = \frac{\text{prior} \times \text{likelihood}}{\text{evidence}} \]

\[ \pi(x|y) = \frac{\pi(x)\pi(y|x)}{\int \pi(x)\pi(y|x)\,dx} \]

prior \( \pi(x) \)

likelihood \( \pi(y|x) \)

\[ \pi(y|x) = N(y - x\epsilon, 0.0001) \]

\[ \pi(y|x) = \pi(\omega) = \pi(y - f(x)) \]

posterior \( \propto \pi(x|y) \)

\[ \text{prior probability} \]

\[ \text{Error(Gpa)} \]
Posterior probability

\[ \pi(x|y) = \frac{\pi(x) \pi(y|x)}{\int_{\Omega} \pi(x) \pi(y|x) \, dx} \]

\[ \pi_{\text{prior}}(x) = N(210, 900) \]

\[ \pi(e_{\text{error}}) = N(0, 0.0001) \]

\[ \pi_{\text{posterior}} = N(215.1533, 19.6168) \]

\[ N_{\text{sample}} = 10 \]

inCERT - Computer-assisted surgery with confidence - Stéphane BORDAS
A focus on equation-based models

- How can we control the quality of simulations, verification and validation?
- Why are set-in-stone-models limited?
- How can we leverage statistical models to improve our models?
Outline

• Data-driven modelling: Beyond setting models in stone
  • Data assimilation
    • How can we learn from observations “on-the-fly”.
    • The power of digital twins.
  • Future challenges
Data-driven Modelling

The structure of $f$ is known but its parameters are not.

There is no a priori knowledge about the function $f$ available.

model calibration

model identification

Embrace the conceptual shift from "model through data abstraction" to "data is the model".
Data-driven Modelling

The structure of $f$ is known but its parameters are not.

Hypothesis-based Models

There is no a priori knowledge about the function $f$ available.

Data-Driven Models

$f : x \rightarrow y$
Data-driven Modelling

The structure of \( f \) is known but its parameters are not.

Hypothesis-based Models

There is no a priori knowledge about the function \( f \) available.

Data-Driven Models

Small data
Data-driven Modelling

The structure of $f$ is known but its parameters are not.

Hypothesis-based Models

There is no a priori knowledge about the function $f$ available.

Data-Driven Models

Small data

$f : x \rightarrow y$
Data-driven Modelling

The structure of $f$ is known but its parameters are not.

Hypothesis-based Models

There is no a priori knowledge about the function $f$ available.

Data-Driven Models

Small data
Data-driven Modelling

The structure of $f$ is known but its parameters are not.

Hypothesis-based Models

There is no a priori knowledge about the function $f$ available.

Data-Driven Models

$f : x \rightarrow y$
Model Discovery

The structure of $f$ is known but its parameters are not.

Hypothesis-based Models

Adaptive Models

Data-Driven Models

There is no a priori knowledge about the function $f$ available.

Small Data

Big Data

Input

Model

Output

$f : x \rightarrow y$

Sliding cursor

less data

more data
Model Discovery

The structure of $f$ is known but its parameters are not.

Hypothesis-based Models

Adaptive Models

Data-Driven Models

There is no a priori knowledge about the function $f$ available.

$\begin{align*}
  f : x & \rightarrow y \\
  \text{input} & \xrightarrow{\text{model}} \text{output} 
\end{align*}$

Small Data

Big Data

Computational Engineering Sciences

Computational Physics

Mathematics
GEOMETRY & BCs

MODELS

- Elasticity/Plasticity
- Crack growth law
- Fracture energy
- Maximum tensile strength
- Multi-scale
- Debonding
- Fibre pull-out
- Fibre breakage
- Interface fracture
- Grains
- Dislocations
- MD
- Quantum...

NUMERICAL SOLUTION

EXPERIMENTS

Parameter identification

Validation

DISCRETISATION

VERIFICATION QUALITY CONTROL
Phenomenological
Neo-Hookean, Ogden, ...

Multi-scale
cutting, fracture,

???

Patient specific ???

Validation
Parameter identification

EXPERIMENTS
DIGITAL TWIN

- GEOMETRY/BCs
- DISCRETISATION

LEARN MATERIAL MODELS
which scales? what models? what parameters? what scale transition? what data is missing?

QUALITY CONTROL

- REAL-TIME INFORMATION
- QUALITY CONTROL

REAL SYSTEM

- Worst load combination
- Crack growth rate
- Inspection interval
- Mission?

DATA
- Strain
- Environment Conditions
- Structural Health
- Cracks

Scales of interest

Worst load combination

CRACK GROWTH RATE

INSPECTION INTERVAL

MISSION?
DIGITAL TWIN OF THE PATIENT

Scales of interest

Disease evolution

“Inspection” interval

Fitness

REAL PATIENT

Treatment simulation

QUALITY CONTROL
REAL-TIME INFORMATION

DATA

Environement Conditions

Organ state

Disease

Health

Alex Garland, *Ex Machina*, 2015

DRIVEN
VISION

General approach
No predefined model

fracture patterns in a composite panel

a-priori knowledge
upscaling techniques
automatic model selection
data & measurements

Machine Learning
Algorithm

data

Models

Probability

Scales++

VISION Scales++

ifψ=Ψ

Models $f_k[p](x)$

Airbus A350

Machine Learning data

Models

probability

Algorithm
Digital Twins...

Characterisation

Monitoring

Multiscale models are unreliable

Quantitative predictions?

Fracture/lack of scale separation

Learn better models

Measure

Analyse & Learn from data

Improved model

Identify missing data

Validate
CONTROL INFORMATION

DATA/SENSING
Prior Knowledge
Prior Knowledge

Hypothesis

Domain expert
Prior Knowledge

(Big) Data

Hypothesis

Domain expert
Prior Knowledge

Data-driven modelling

Computed in Luxembourg

Hypothesis
Domain expert

(Big) Data

Conclusions
Patient-specific material models

1. Prior

Prior knowledge
Material parameters inc. distribution from general population

Noise
- Model (e.g. additive)
- Distribution (Gauss)
- Characterisation

Constitutive model

\[ \psi_{\text{eq}}(F) = \frac{\mu}{2} \left( \frac{\text{tr}B}{J^{2/3}} - 3 \right) + \frac{1}{2} K (J - 1)^2 \]
Patient-specific material models

1. **Prior**

   **Prior knowledge**
   Material parameters including distribution from general population

   **Noise**
   - Model (e.g. additive)
   - Distribution (Gauss)
   - Characterisation

**Constitutive model**

\[
\psi^{\text{eq}}(F) = \frac{\mu}{2} \left( \frac{\text{tr} \mathbf{B}}{J^{2/3}} - 3 \right) + \frac{1}{2} K (J - 1)^2
\]

**Data assimilator**

Bayesian inference

\[
\Pr(M|D) = \frac{\Pr(D|M) \Pr(M)}{\Pr(D)}
\]
Patient-specific material models

1. Prior
   Prior knowledge
   Material parameters inc. distribution from general population
   Noise
   ‣ Model (e.g. additive)
   ‣ Distribution (Gauss)
   ‣ Characterisation
   Constitutive model
   \[ \psi^{\text{eq}}(F) = \frac{\mu}{2} \left( \frac{\text{tr} B}{J^{2/3}} - 3 \right) + \frac{1}{2} K (J - 1)^2 \]

2. Posterior data
   Data assimilator
   Bayesian inference
   \[ \Pr(M|D) = \frac{\Pr(D|M) \Pr(M)}{\Pr(D)} \]

MRI
Stereo-cameras
CT
Ultrasound
Patient-specific material models

1. Prior
   - Prior knowledge
     - Material parameters inc. distribution from general population
   - Noise
     - Model (e.g. additive)
     - Distribution (Gauss)
     - Characterisation
   - Constitutive model

\[ \psi^{eq}(F) = \frac{\mu}{2} \left( \frac{(\text{tr} B)}{J^{2/3}} - 3 \right) + \frac{1}{2} K (J - 1)^2 \]

2. Posterior data
   - CT
   - Ultrasound

3. Simulator
   - Model selector
     - Model updates
     - Probability
     - Selected Model
     - Model 1 Models
     - Model 2

\[ \Pr(M|D) = \frac{\Pr(D|M) \Pr(M)}{\Pr(D)} \]

CT scans
MRI
Stereo-cameras
Mechanical solver

Data assimilator
Bayesian inference

Posterior data
Simulator
Mechanical solver

Prior
Model selector
Mechanical solver
Patient-specific material models

1. Prior
   - Prior knowledge
     - Material parameters inc. distribution from general population
   - Noise
     - Model (e.g. additive)
     - Distribution (Gauss)
     - Characterisation
   - Constitutive model
     \[ \psi^{eq}(F) = \frac{\mu}{2} \left( \frac{\text{tr} B}{J^{2/3}} - 3 \right) + \frac{1}{2} K (J - 1)^2 \]

2. Posterior data
   - CT
   - Ultrasound
   - MRI
   - Stereo-cameras

3. Simulator
   - Model selector
     - Model updates (P>P1>P2)
     - Model selector
     - Selected Model
     - Models

4. Feedback
   - Mechanical solver

Data assimilator
Bayesian inference

Pr(M|D) = \frac{Pr(D|M) Pr(M)}{Pr(D)}
Patient-specific material models

1. Prior
   - Prior knowledge
     - Material parameters inc. distribution from general population
   - Noise
     - Model (e.g. additive)
     - Distribution (Gauss)
     - Characterisation
   - Constitutive model
     \[ \psi^{\text{eq}}(F) = \frac{\mu}{2} \left( \frac{\text{tr} B}{J^{2/3}} - 3 \right) + \frac{1}{2} K(J - 1)^2 \]

2. Posterior data
   - CT
   - Ultrasound

3. Model selector
   - Probability
   - Model updates
   - Selected Model
   - Model 1
   - Model 2
   - Models

4. Feedback
   - Action

5. Mechanical solver

Data assimilator
Bayesian inference

\[ \Pr(M|D) = \frac{\Pr(D|M) \Pr(M)}{\Pr(D)} \]
Prior Knowledge
Prior Knowledge

Data

Hypothesis
Bayesian Inference

Prior Knowledge

Posterior Distribution

Data

Hypothesis

Updates
Bayesian Inference

Prior Knowledge

Feedback

Posterior Distribution

Data

Hypothesis

Updates
Bayesian Inference

Prior Knowledge

Feedback

Posterior Distribution

Data

Hypothesis

Updates

206
Bayesian Inference

Prior Knowledge

Feedback

Posterior Distribution

Data

Hypothesis

Updates
Bayesian Inference

Prior Knowledge

Feedback

Posterior Distribution

Data

Hypothesis

Updates
Bayesian Inference

Prior Knowledge

Feedback

Posterior Distribution

Data

Hypothesis

Updates
Some applications

- Focus on the finite element method
- Applications in materials science
- Applications in fluid dynamics
- Applications in manufacturing
- Applications in biomechanics
- Applications in real-time simulation for surgical training and surgical guidance
Cut Finite Element Methods for Contact Problems

Susanne Claus

Department of Computer Science, University of Copenhagen, Denmark.

AI Seminar Series, Copenhagen, Jan 2019
Geometry is meshed

Geometry is embedded in fixed background grid and described by a function (e.g. level set function)
Consider the following diffusion partial differential equation (PDE)

\[-\Delta u = f \text{ in } \Omega\]

\[u = 0 \text{ on } \Gamma\]

Find \( u \in V \) such that

\[\int_{\Omega} \nabla u \cdot \nabla v \, dx = \int_{\Omega} f v \, dx \quad \forall v \in V\]
Convergence with mesh refinement

The error decreases with mesh refinement. However, how fast the error decreases with mesh refinement (convergence order) depends on multiple factors.
Convergence strongly depends on

**Accuracy**

- **Numerical error**: error from piecewise polynomial approximation of the solution and of the geometry.
- **Mesh Quality**: The quality and size of the mesh has a significant impact on the accuracy of the solution

**Stability**

- **Instabilities**: frequently occur in simulations as numerical errors can grow in the solution process. Numerical error growth needs to be controlled and stabilised carefully. Too much stabilisation leads to inaccuracies.

\[
\text{Convergence} = \text{Accuracy} + \text{Stability}
\]
Difficulty of maintaining a high quality mesh

Advantages of Mesh Independent Geometry Descriptions

1. reduces the computational cost for preprocessing or transformation of acquired geometry descriptions
2. efficient and robust for problems involving evolving geometries undergoing large deformations
Important aspects of implicit geometry/cut finite element methods

Geometry Algorithms
Discretisation of the geometry based on implicit interface description

Accuracy and Stabilisation
Construction of stable and accurate finite element methods independent of how the interface intersects the mesh.
FEniCS

Open Source Finite Element Library for the Automated Solution of PDEs

- high level mathematical input language
- generates efficient C++ code from these mathematical inputs
- supports a wide range of different finite element types
- supports simulations in 2D and 3D
- fully parallelised
- active world wide developer community, e.g. Simula Research Laboratory, University of Cambridge, University of Chicago, University of Texas at Austin, KTH Royal Institute of Technology, Chalmers University of Technology.

http://fenicsproject.org
Consider the elliptic problem

\[-\Delta u = f \text{ in } \Omega,\]
\[u = 0 \text{ on } \Gamma.\]

Find \( u \in V \) such that

\[\int_{\Omega} \nabla u \cdot \nabla v \, dx = \int_{\Omega} f v \, dx \quad \forall v \in V\]

from dolfin import *

# Create mesh and define function space
mesh = UnitSquareMesh(32, 32)
V = FunctionSpace(mesh, "CG", 1)

# Define boundary condition
bc = DirichletBC(V, 0.0, DomainBoundary())

# Define variational problem
u = TrialFunction(V)
v = TestFunction(V)
f = Expression("x[0]*x[1]")

a = inner(grad(u), grad(v))*dx
L = f*v*dx

# Compute solution
u = Function(V)
solve(a == L, u, bc)
Input: File in Python and Unified Form Language

Unified Form Language (UFL)
Interprets expressions close to mathematical notation

\[ a(u, v) = \int \nabla u \nabla v \, dx \]

\[ a = \text{inner}(\text{grad}(u), \text{grad}(v)) \times dx \]
**FEniCS: Under The Hood**

**Input:** File in Python and Unified From Language

\[ a = \text{inner}(\text{grad}(u), \text{grad}(v)) \ast dx \]

\[ a(u, v) = \int \nabla u \nabla v \, dx \]

**Unified Form Language (UFL)**
Interprets expressions close to mathematical notation

**FEniCS Form Compiler (FFC)**
Generates Header file with information about
Elemental matrices (form)
Degrees of Freedom Map (element)

**DOLFIN**
(Mesh, Communicator and Assembler)

```cpp
/// Evaluate basis function i at given point x in cell
_evaluate_basis(std::size_t i, double* values, const double* x, const double* coordinate_dofs)
```

```cpp
/// Tabulate the tensor for the contribution from a local cell
virtual void tabulate_tensor(double* A, const double* x, const double* coordinate_dofs)
```
Implementation Aspects of Unfitted FEM

1. Description of domain boundary location independent of background mesh.
   
   - Level-set method.

2. Evaluation of integrals over arbitrarily shaped elements.
   
   - Sub-triangulation.

3. Element matrix assembly involving contributions from element parts.
   
   - Generated tabulate tensor function which takes arbitrary quadrature points and weights.

Signed Distance Function

Level Set Function

Finite Element Approximation

Mesh/Levelset intersection for integration
Describe geometry using Level-Set Function

Normal
\[ \mathbf{n}_\Gamma = \frac{\nabla \phi}{||\nabla \phi||_0} \]

Curvature
\[ \kappa = \nabla \cdot \mathbf{n} \]

Sense of Vicinity
\[ |\phi(x)| < \delta \]
Fictitious Domain Poisson Problem

Find $u_h \in V_h$ such that for all $v_h \in V_h$

$$A(u_h, v_h) = a(u_h, v_h) + j(u_h, v_h) = L(v_h)$$

$$a(u_h, v_h) = \int_\Omega \nabla u_h \cdot \nabla v_h \, dx + \int_\Gamma (-\nabla u_h \cdot n v_h - \nabla v_h \cdot n u_h + \frac{\gamma}{h} u_h v_h) \, ds$$

$$L(v_h) = \int_\Omega f v_h \, dx + \int_\Gamma (-g \nabla v_h \cdot n + \frac{\gamma}{h} g v_h) \, ds$$

$$j(u_h, v_h) = \gamma_1 \sum_{F \in \mathcal{F}_{\Gamma^*}} h_F([\partial_n u_h], [\partial_n v_h])_F$$
Poisson with contrast in diffusivities

\[-\nabla \cdot (\alpha \nabla u) = f \quad \text{in} \quad \Omega_1 \cup \Omega_2,\]
\[u = 0 \quad \text{on} \quad \partial \Omega,\]
\[\left[ u \right] = 0 \quad \text{on} \quad \Gamma,\]
\[\left[ -\alpha_i \nabla u_i \cdot n \right] = 0 \quad \text{on} \quad \Gamma.\]

Choose \(\alpha_1 = 1, \alpha_2 = 10, f_1 = f_2 = 1.\)

Without Enrichment

With Enrichment
**Implementational Aspects of Unfitted FEM**

1. Description of domain boundary location independent of background mesh.
   - **Level-set method.**

2. Evaluation of integrals over arbitrarily shaped elements.
   - **Sub-triangulation.**

3. Element matrix assembly involving contributions from element parts.
   - **Generated tabulate tensor function which takes arbitrary quadrature points and weights.**

\[ \phi(x) = x^2 + y^2 - 1 \]

\[ \phi(x) = x^2 + y^2 + z^2 - 1 \]

\[ \phi(x) = (R - \sqrt{x^2 + y^2})^2 + z^2 - r^2 \]

**Examples: Level-Set Function**

- **Circle**
  \[ \phi(x) = x^2 + y^2 - 1 \]

- **Sphere**
  \[ \phi(x) = x^2 + y^2 + z^2 - 1 \]

- **Torus**
  \[ \phi(x) = (R - \sqrt{x^2 + y^2})^2 + z^2 - r^2 \]

**Constructing Complex Geometries using Level-Set Functions**

- **Union:**
  \[ \phi(x) = \min(\phi_1(x), \phi_2(x)) \]

- **Intersection:**
  \[ \phi(x) = \max(\phi_1(x), \phi_2(x)) \]
Limitations with single level set function

Partitions the domain into one inside and one outside domain (max. 2 different materials)

Zero level set surface contour is a closed surface, i.e it is not possible to describe geometries with open boundaries such as cracks
Use multiple level set functions for complex geometries

N-1 level set functions can described N different subdomains

\[ \Omega^1 \]
\[ \Omega^2 \]
\[ \Omega^3 \]

\[ \phi_1 < 0 \]
\[ \phi_2 > 0 \]

\[ \phi_1 > 0 \]
\[ \phi_2 < 0 \]

\[ \phi_1 > 0, \phi_2 > 0 \]
Enrichment for jump and kink representation

Triple Poisson Problem
Contact Problems
Contact Problem in linear Elasticity

### Bulk Problem

For all \( \Omega_i \), find the displacement fields \( u^i : \Omega_i \rightarrow \mathbb{R} \), such that

\[
-\nabla \cdot \sigma(u^i) = f \\
\sigma(u^i) = \lambda^i \text{tr}(\varepsilon(u^i)) I + 2\mu^i \varepsilon(u^i) \\
u^i = g \text{ on } \partial \Omega_D, \quad \sigma(u^i) \cdot n = F_N \text{ on } \partial \Omega_N
\]

Here, \( \varepsilon(u) = \frac{1}{2} (\nabla u + \nabla u^T) \) is the strain tensor, \( f \) is the body force, \( F_N \) is the surface load, \( g \) the Dirichlet boundary condition, \( \lambda^i \) and \( \mu^i \) are the two Lamé coefficients (\( E^i \) is the Young’s modulus, \( \nu = 0.3 \) is the Poisson’s ratio)

\[
\mu^i = \frac{E^i}{2(1 + \nu)}, \quad \lambda^i = \frac{E^i \nu}{(1 + \nu)(1 - 2\nu)}.
\]
Unilateral contact for isotropic linear elasticity

Contact Conditions

For any displacement field $u_i$, we decompose the surface traction $F^i = \sigma(u_i) \cdot n^{ij}$ on the interface $\Gamma^{ij}$ into its normal and tangential components

$$F^i = F_n^i + F_t^i.$$ 

Then, the conditions of contact with Coulomb friction reads

$$(u^i - u^i) \cdot n^{ij} \geq 0,$$

$$F^i \cdot n^{ij} \leq 0,$$

$$(u^i - u^i) \cdot n^{ij} \cdot (F^i \cdot n^{ij}) = 0,$$

$$\|F_t^i\| \leq c F^i \cdot n^{ij} \quad \text{if } \|\hat{g}_t^i\|_2 = 0$$

$$F_t^i = -c F^i \cdot n^{ij} \frac{\hat{g}_t^i}{\|\hat{g}_t^i\|_2} \quad \text{if } \|\hat{g}_t^i\|_2 > 0$$

Here, $n^{ij}$ is the normal pointing from $\Omega_i$ to $\Omega_j$, $c$ is the Coulomb friction coefficient, and $\hat{g}_t := (I - n^{ij} \otimes n^{ij}) \cdot (\dot{u}^i - \dot{u}^i)$ is the relative tangential velocity.
LaTIn Algorithm

\[ \Gamma^{i,j} \]

Linear Elasticity

Contact

Linear Elasticity

Local Stage

Contact Law

\[ \hat{F}^i - k^+ \hat{w}^i = F^i - k^+ w^i \]

where \( \hat{F}^i \) and \( \hat{w}^i \) satisfy contact

Linear Stage

Robin BC

\[ \sigma(u^i) \cdot n = F^i \text{ on } \Gamma^{i,j} \]

\[ u^i = w^i \text{ on } \Gamma^{i,j} \]

\[ F^i + k^- w^i = \hat{F}^i + k^- \hat{w}^i \]
LaTIn Algorithm: Stability

\[ u = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \]

\[ u = 0 \]

\[ \sigma \cdot n = 0 \]

\[ \sigma \cdot n \parallel \]

\[ \Sigma \]

P1/P0 scheme polluted \( \mathbf{F}^i \)

\[ \begin{array}{ccc}
\text{Normal Traction} & \text{Normal Traction} \\
\text{Normal Traction} & \text{Normal Traction}
\end{array} \]

\[ \begin{array}{ccc}
\text{it}=5 & \text{it}=27 & \text{it}=210
\end{array} \]

\[ \begin{array}{ccc}
\text{Normal Traction} & \text{Normal Traction} & \text{Normal Traction}
\end{array} \]

\[ \begin{array}{ccc}
\text{Normal Traction} & \text{Normal Traction} & \text{Normal Traction}
\end{array} \]

\[ \begin{array}{ccc}
\text{Normal Traction} & \text{Normal Traction} & \text{Normal Traction}
\end{array} \]
For all interfaces $\Gamma_{i,j}$, we couple the interface and bulk quantities through approximate compatibility conditions:

$$W_{i,j}^h = u_{\cdot i}^\cdot, W_{j,i}^h = u_{\cdot j}^\cdot$$

on $\Omega_{i,j}$:

$$F_{i,j}^h \cdot u_d^\cdot = \int_{\Omega_{i,j}} F_{i,j}^h \cdot n_{\cdot i}^\cdot \cdot \cdot$$

These are standard conditions whereby the kinematic continuity is enforced exactly, whilst the continuity of dual quantities is only enforced on average, i.e. in a finite element sense.

When solving our problem using the LaTIn algorithm, these two conditions will be introduced in (29) to yield our working expression of the linear stage.

Compatibility between interface and heart:

We project the heart quantities onto the continuous piecewise linear approximation space $V_{i,j}$ (28) for each using a stabilised $L^2-P_1/P_1$ Stabilised Projection.
LaTIn Algorithm: Stability

\[ u = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \]

\[ \sigma \cdot n = 0 \]

\[ u = 0 \]

P1/P0 scheme polluted

(a) P1/P0  
(b) P1/P0  
(c) P1/P0

Proposed Solution: P1/P1 scheme with stabilisation

(d) P1/P1  
(e) P1/P1  
(f) P1/P1
Two Inclusions Frictionless Contact

\[ u = (0, -1) \]

\[ E_1 = E_2 = E_3 = 1 \]

\[ u = 0 \]

\[ \sigma_{yy} \]

\[ \log(||u_h - u_h||_{\Omega_h}) \]
Applications in Engineering
Braided Composite

\[ \phi_1(x) \]

\[ \phi_2(x) \]
Braided Composite
Braided Composite
Damage in Concrete: Parallelisation

Linear Stage

Local Stage
Damage in Concrete
Pulsed Thermal Ablation
Pulsed Thermal Ablation
3D Machining Path
Applications in Biomechanics
Cut Finite Element Hip Modelling Motivation

Treatment options for hip malformations: (left) untreated hip deformity of a 4-year-old child, (middle) well-formed hip 8 years post guided growth surgery¹, i.e. insertion of one screw through the growth plate of the femur bones, (right) well-formed hip after an invasive femur and hip osteotomy, i.e. cutting through the bones and insertion of screws and plates.

Study stress in hip joint using FE Modelling to enhance understanding of bone growth and bone shape changes

Figure 10.3. A-E: RSA radiographs at postoperative time 0 weeks, 5 weeks, 3 months, 6 months and 12 months, respectively. In figure D and E the VDRO is considered radiographic stable. F: Shows the orientation of the 6 degrees of freedom with positive values of a right distal femur distal. Hence, translations $x^+$ = medial, $y^+$ = superior and $z^+$ = anterior and rotations $Rx^+$ = anterior tilt, $Ry^+$ = internal rotation and $Rz^+$ = varisation.

Segmented Img. Configuration, Loading Cond. Simulated Grown Bone Finite Deformation Contact Growth
Surface Triangulation to CutFEM pipeline

Segmentation with 3D Slicer (Faezeh Moshfeghifar) of CT-image from the cancer imaging archive (TCIA)
Create Regular Background mesh

Hip bone surface triangulation embedded in regular background mesh

Femur bone surface triangulation embedded in regular background mesh
Determine inside, outside and intersected cells
Compute signed distance function for each bone

\[ \phi_1 \]  

\[ \phi_2 \]
Geometrical Error (Linear Approximation)
Refine elements that are intersected by surface triangulation.
Extract elements and set boundary conditions

\[ \mathbf{u} = (0, -1, 0)^T \]

\[ \mathbf{u} = 0 \]
Stress Profile $\sigma_{yy}$
Patient-Specific Data

Expert Knowledge

https://rainbow.ku.dk
Brain shift and electrode implantation

Error estimation and adaptivity


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Controlling the Error on Target Motion through Real-time Mesh Adaptation: Application to Deep Brain Stimulation

Goal-oriented error estimate

\[ Q(u) = \frac{1}{|\omega|} \int_{\omega} \nabla u d\omega \]

\[ Q(u) - Q(u_h) \]

\[ |Q(u) - Q(u_h)| \leq \varepsilon \]

**Figure 1:** If we are interested in some quantity of interest defined on a subdomain \( \omega \), what is the optimal mesh?


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Goal-oriented error estimate

Primal problem: \[ a(u, v) = l(v) \quad \forall v \in V \]

Solve by FEM: \[ a(u_h, v_h) = l(v_h) \quad \forall v_h \in V_h \]

Weak residual: \[ r(v) = l(v) - a(u_h, v) \quad \forall v \in V \]

If we define a dual problem:

Find \( z \in V \) such that \[ a(v, z) = Q(v) \quad \forall v \in V \]

We observe:

\[ Q(u) - Q(u_h) = a(u, z) - a(u_h, z) = l(z) - a(u_h, z) = r(z) \]

Hyperelasticity

Equilibrium equations in initial configuration:

\[-\text{div} \Pi = B \quad \text{in} \quad \Omega^0\]
\[u = 0 \quad \text{on} \quad \Gamma_D^0\]
\[\Pi \cdot N = T \quad \text{on} \quad \Gamma_N^0\]

- \(\Pi = \Pi(u)\) is the first Piola-Kirchhoff stress tensor
- \(B\) is a given body force per unit volume
- \(u\) is the displacement
- \(T\) is a given boundary traction

Cantilever beam

Parameters
Saint Venant-Kirchhoff material: $E = 1000, \nu = 0.4$

Cantilever beam (2)
Cantilever beam (3)

Adaptivity using quadrilaterals

Human artery

\[ \sum \eta_K, \text{ uniform} \]
\[ \sum \eta_K, \text{ adaptive} \]
\[ Q(u) - Q(u_h), \text{ uniform} \]
\[ Q(u) - Q(u_h), \text{ adaptive} \]
Human heel

Conclusions

Cut FEM/XFEM for surgical simulations with complex geometries

Making the discretization as independent as possible from geometric description

Verification of convergences with optimal rates

Cut FEM is suitable for real-time and patient specific simulations

Perspectives

Higher order cut elements

Alexei Lozinski and Franz Chouly: avoid integration on cut elements

References


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AMIES
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Real-time needle steering

Brain shift occurs prior to cannula insertion