Model order reduction

POD and Homogenisation

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Ways to reduce the models

- Homogenisation (FE^2, etc.) - Hierarchical
- Concurrent and hybrid (bridging domain, ARLEQUIN, etc.)
- Enrichment (PUFEM, XFEM, GFEM)
- Model reduction (algebraic)
Reduction methods based on homogenisation
Coupling of macroscopic and microscopic levels

The volume averaging theorem is postulated for:

1) Strain tensor:

\[
\epsilon^c = \frac{1}{|\Omega(x^c)|} \int_{\partial \Omega(x^c)} \mathbf{u}^f \otimes_s \mathbf{n} \, d\Gamma
\]

2) Virtual work (Hill-Mandel condition):

\[
\sigma^c : \delta \epsilon^c = \frac{1}{|\Omega(x^c)|} \int_{\partial \Omega(x^c)} \mathbf{t}^f \cdot \delta \mathbf{u}^f \, d\Gamma
\]

3) Stress tensor:

\[
\sigma^c = \frac{1}{|\Omega(x^c)|} \int_{\partial \Omega(x^c)} \mathbf{t}^f \otimes \mathbf{x}^f \, d\Gamma
\]
Hierarchical multi-scale approaches (FE^2)

Advantages and abilities:
The macroscopic constitutive law is not required
Non-linear material behaviour can be simulated
Microscale behaviour of material is monitored at each load step

Drawbacks:
In softening regime:
• Lack of scale separation
• Macroscale mesh dependence
RealTcut
Details in Phil. Magazine, 2015, Akbari, Kerfriden, Bordas
a) DNS

b) The adaptive multiscale method
The distribution of strain-gradient sensitivity $L_Y \| \nabla \nabla u^c \|_e$
Reduction methods based on algebraic reduction
Illustration of the method of separated representation

\[ C^1 = \sin(0.01\,x) \]
\[ \alpha^1 = e^{-0.02\,t} \]
\[ C^2 = (x - 500)^3 \]
\[ \alpha^2 = \cos(\sqrt{t}) \]
Illustration of the method of separated representation

\[ C^1 = \sin(0.01x) \]

\[ \alpha^1 = e^{-0.02t} \]

\[ C^2 = (x - 500)^3 \]

\[ \alpha^2 = \cos(\sqrt{t}) \]
Illustration of the method of separated representation

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Very rich approximations!
Data compression: get the nose with the POD!

\[ \bar{u}(x_i, y_i) = \sum_{i=1}^{n_c} C^i_x(x_i) C^i_y(y_i) \]

\[ (C^i_x, C^i_y)_{i \in [1, n_c]} = \text{argmin} \sum_{x_i} \sum_{y_j} (u(x_i, y_j) - \bar{u}(x_i, y_j))^2 \]

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Data compression: get the nose with the POD!

$\bar{u}(x_i, y_i) = \sum_{i=1}^{n_c} C^i_x(x_i) C^i_y(y_i)$

$(C^i_x, C^i_y)_{i \in [1, n_c]} = \arg\min \sum_{x_i} \sum_{y_j} (u(x_i, y_j) - \bar{u}(x_i, y_j))^2$

Got the nose (rectangle, approximation of order 2 is enough)
Data compression: get the nose with the POD!

\[
\bar{u}(x_i, y_i) = \sum_{i=1}^{n_c} C^i_x(x_i) C^i_y(y_i)
\]

\[
(C^i_x, C^i_y)_{i\in[1,n_c]} = \arg\min \sum_{x_i} \sum_{y_j} (u(x_i, y_j) - \bar{u}(x_i, y_j))^2
\]

n_c = 1

n_c = 2

n_c = 5

n_c = 10

Got the nose (rectangle, approximation of order 2 is enough)

Converges slowly locally (idem fracture)

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a posteriori model order reduction. **Idea:** search for the solution as a linear combination of a set of pre-calculated representative solutions.

\[ S = (S^1 \ S^2 \ ... \ S^{n_S}) \]

(1) Solve FINE for \( n_S \) parameters (EXPENSIVE!)

(2) Singular value decomposition

\[ S = U \Sigma V^T = \sum_{k=1}^{n_S} \Sigma^k U^k V^k^T \]

\( n_S \) solutions, sorted by relevance

where \((\Sigma^k)_{k\in[1\ n_S]}\)

(3) Truncation

**Initial set of equations**

\[ \mathbf{F}_{\text{Int}}(\mathbf{U}) + \mathbf{F}_{\text{Ext}} = 0 \]

(4) Galerkin orthogonality

\[ \mathbf{C}^T \mathbf{F}_{\text{Int}}(\mathbf{C} \alpha) + \mathbf{C}^T \mathbf{F}_{\text{ext}} = 0 \]

Approximation of the solution in a space of small dimension \((n_c)\)

**Reduced basis:** family of representative solutions

\[ \mathbf{C} = (U^1 \ U^2 \ ... \ U^{n_C}) \]
Limitations: case of highly non-linear fracture mechanics pbs


This solution is not in the snapshot!

error graph

Reduced Ritz basis

- $C^1$
- $C^2$
- $C^3$

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Application to a parametric fracture problem

Initial crack

\[ \theta \in [15^\circ, 45^\circ] \]
Application to a parametric fracture problem

- The POD solution is not able to reproduce the solution in the cracked area.
- Due to lack of correlation introduced by crack growth.
- Leads to a local projection error.
Parametric / stochastic multiscale fracture mechanics

Highly correlated solution fields

First realisation

Second realisation

Localisation of fracture, uncorrelated

Direct numerical simulation: efficient preconditioner?

Reduced order modelling?

Adaptive coupling?
THE RETURN OF THE MONKEY!
What can we do to address this lack of separation of scales/reducibility?
How we got to this point...


http://www.ncbi.nlm.nih.gov/pmc/articles/PMC3672853/
http://orbilu.uni.lu/bitstream/10993/12454/2/presentationUSNCCM
Data compression: fracture

Snapshot POD (snapshot space is spanned by the ensemble of solutions at all time steps)

“Exact” solution

POD order 1

POD order 3
Reduced DDM-POD

- Decompose the structure into subdomains
- Perform a reduction in the highly correlated region
- Couple the reduced to the non-reduced region by a primal Schur complement
Choice of the reduced subdomains: local error estimation by “leave one out cross-validation” (LOOCV)

- Reduced subspaces are independent and we assume a snapshot is \textit{a priori} available
  - (1) Dimension of the local space for each subdomain?
  - (2) Is a given subdomain is reducible?

- (1) and (2) will be treated by cross-validation (e.g. W. J. Krzanowski. Cross-validation in principal component analysis. Biometrics, 43(3):575-584, 1987.)
  - \textbf{Training set}: snapshot
  - \textbf{Validation set}: set of additional finescale solutions
  - Independent training/validation avoids overfitting
  - Cross validation \textit{emulates independence}. Error calculated using the local reduced basis obtained by a snapshot POD transform of all the available snapshot solutions except the one corresponding to the value of the summation variable.

- \textbf{NOTE}: If the snapshot is not assumed \textit{a priori} then
  - Assess whether the snapshot contains sufficient information, and generate additional, suitable, data if required
Domain Partitioning

Order of the POD transforms

Cross-validation error estimate
Performance: load angle 40 | 27 - 121 nodes

Relative error

\[ \nu^{\text{app}}(\mu)(U^{\text{app}})^2 = \frac{\sum_{t_n \in T^h} \|U^{\text{app}}(t_n, \mu) - U^{\text{ex}}(t_n, \mu)\|^2_2}{\sum_{t_n \in T^h} \|U^{\text{ex}}(t_n, \mu)\|^2_2} \]

\(40^\circ\) \hspace{1cm} \(27^\circ\)

(a) Relative error for the different models using 121 nodes per subdomain

(b) Relative error for the different models using 121 nodes per subdomain
Relative error

\[
\nu^{\text{app},(\mu)}(U^{\text{app}})^2 = \frac{\sum_{t_n \in \mathcal{T}^h} \|U^{\text{app}}(t_n, \mu) - U^{\text{ex}}(t_n, \mu)\|_2^2}{\sum_{t_n \in \mathcal{T}^h} \|U^{\text{ex}}(t_n, \mu)\|_2^2}
\]

40°

(b) Relative error for the different models using 256 nodes per subdomain

27°

(b) Relative error for the different models using 256 nodes per subdomain
Performance: load angle 40 | 27 - 441 nodes

Relative error

\[ \nu_{\text{app}}(\mu) \left( \frac{\sum_{t_n \in T^h} \| U_{\text{app}}(t_n, \mu) - U_{\text{ex}}(t_n, \mu) \|^2}{\sum_{t_n \in T^h} \| U_{\text{ex}}(t_n, \mu) \|^2} \right)^2 \]

40°

27°

(c) Relative error for the different models using 441 nodes per subdomain
Performance: load angle 40° | 27° - 961 nodes

Relative error

\[
\nu_{\text{app},(\mu)} \left( \mathbf{U}_{\text{app}} \right)^2 = \frac{\sum_{t_n \in \mathcal{T}^h} \left\| \mathbf{U}_{\text{app}}(t_n, \mu) - \mathbf{U}_{\text{ex}}(t_n, \mu) \right\|_2^2}{\sum_{t_n \in \mathcal{T}^h} \left\| \mathbf{U}_{\text{ex}}(t_n, \mu) \right\|_2^2}
\]

(d) Relative error for the different models using 961 nodes per subdomain
Applications to surgical simulation

with INRIA, France; Karol Miller, UWA.
Surgical simulation (real time/interactivity)

- Reduce the problem size while controlling error in solving very large multiscale mechanics problems

Courtecuisse et al. PBMB 2011
Interactive simulation of cutting in soft tissue

Real-time/interactivity for non-linear problems involving topological changes

- reduce the problem size but preserve relevant mechanical information, control the error
Concrete objective: compute the response of organs during surgical procedures (including cuts) in real time (50-500 solutions per second)

Two schools of thought
- constant time
  - accuracy often controlled visually only
- model reduction or “learning”
  - scarce development for biomedical problems
  - no results available for cutting

Proposed approach: maximize accuracy for given computational time. Error control

First implicit, interactive method for cutting with contact

[Courtecuisse et al., MICCAI, 2013]
Collaboration INRIA
Four main difficulties

- Complex geometries from medical images
- Topological changes & contact
- Region of interest (RoI)
- Model reduction
- Error control
  - Interactivity
  - Space-time discretization?
  - Optimize use of compute resources
- Verification & Validation
calculs offline

génération solutions particulières

calcul champs asymptotiques

action de l’instrument

30^6 snapshots

tri pré-opératoire

“mapping” spécifique patient

~10^3 snapshots

POD

O(10) fonctions

espace réduit de petite dimension

enrichissement “pointe de coupe”

calculs online: interactivité

répresentation locale

approximation POD globale
A semi-implicit method for real-time deformation, topological changes, and contact of soft tissues
There's a fine line between wrong and visionary.

Unfortunately, you have to be a visionary to see it.

Sheldon Cooper,
*The Big Bang Theory: The Pirate Solution*
GEOMETRICAL MODEL

DISCRETISATION

MATERIAL MODELS
Phenomenological
  Elasticity/Plasticity
  Crack growth law (Paris...)
  Fracture energy
  Maximum tensile strength
  Multi-scale
  Debonding, fibre pull-out
  Fibre breakage, interface fracture, grains, dislocations, MD, quantum...

NUMERICAL SOLUTION

EXPERIMENTS

A POSTERIORI ERROR CONTROL

CONVENTIONAL APPROACH

Validation & parameter identification
DIGITAL TWIN OF THE SYSTEM

GEOMETRICAL MODEL

DISCRETISATION

LEARN MATERIAL MODELS

which scales?
what models?
what parameters?
what scale transition?
what data is missing?

NUMERICAL SOLUTION

A POSTERIORI ERROR

REAL SYSTEM

Crack growth rate
Scales of interest
Worst load combination

INFORMATION

Mission?

DATA

Strain
Environment Conditions
Structural Health
Cracks

Worst load combination
Inspection interval

Scales of interest

Mission?
General approach
No predefined model

a-priori knowledge

upscaling techniques

automatic model selection

data & measurements

Machine Learning

Algorithm

Models $f_k[p](x)$

Probability

Updates

Scales++

VISION

Machine Learning data

Models

50

No predefined model

a-priori knowledge

General approach

upscaling techniques

automatic model selection

data & measurements

fracture patterns in a composite panel
Digital Twins...

Characterisation

Monitoring

Multiscale models are unreliable

Learn better models

Quantitative predictions ?

Fracture/lack of scale separation

Measure

Analyse & Learn from data

Improved model

Identify missing data

Validate
• Experience every event that its flying twin experiences

• Will revolutionise certification, fleet management and support (mirrors life of the “as-built” state)

• Will decrease weight
  • no reliance on statistical distribution of material properties
  • no reliance on heuristic design methods
  • less reliance on physical testing (environment?)
  • no assumed similitude between testing and operational conditions
NUMERICAL SOLUTION

DISCRETISATION

GEOMETRICAL MODEL

MATERIAL MODELS
- Phenomenological
  - Elasticity/Plasticity
  - Crack growth law (Paris...)
  - Fracture energy
  - Maximum tensile strength
- Multi-scale
  - Debonding, Fibre pull-out
  - Fibre breakage, interface fracture, grains, dislocations, MD, quantum...

EXPERIMENTS

A POSTERIORI ERROR CONTROL

CONVENTIONAL APPROACH
NUMERICAL SOLUTION

IMAGE/MODEL

DISCRETISATION

MATERIAL MODELS

Phenomenological
Neo-Hookean, Ogden, ...
Multi-scale
cutting, fracture,

Patient specific

NUMERICAL SOLUTION

A POSTERIORI
ERROR CONTROL

Verification

EXPERIMENTS

Validation & parameter identification

Alex Bilger
DIGITAL TWIN OF THE PATIENT

REAL PATIENT

DATA

INFORMATION

Treatment simulation
Scales of interest
“Inspection” interval
Fitness

Disease evolution

Disease
Environment Conditions
Organ state
Health
Global single scale model selection

Model

Data

Global error

\( \geq E_g \)

\( \leq E_g \)

Local errors

Multi-physics

Multi-scale

Data-enriched

- atomistics
  - meso-scopic
    - continuum

- h, p refinement
- analytical enrichment

- experimental enrichment
  - a priori
  - a posteriori
  - real-time
Papers on fracture

http://orbilu.uni.lu/handle/10993/26421
http://orbilu.uni.lu/handle/10993/22289
http://orbilu.uni.lu/handle/10993/20721
http://orbilu.uni.lu/handle/10993/24170
http://orbilu.uni.lu/handle/10993/21427
http://orbilu.uni.lu/handle/10993/21295
http://orbilu.uni.lu/handle/10993/16323
http://orbilu.uni.lu/handle/10993/22420
http://orbilu.uni.lu/handle/10993/19535
http://orbilu.uni.lu/handle/10993/21330
http://orbilu.uni.lu/handle/10993/18262
http://orbilu.uni.lu/handle/10993/19509
http://orbilu.uni.lu/handle/10993/19371
http://orbilu.uni.lu/handle/10993/17536
http://orbilu.uni.lu/handle/10993/17647
http://orbilu.uni.lu/handle/10993/14135
http://orbilu.uni.lu/handle/10993/16842
Papers on fracture

https://orbilu.uni.lu/bitstream/10993/22331/2/paper.pdf

http://orbilu.uni.lu/handle/10993/25048
http://orbilu.uni.lu/handle/10993/20721
http://orbilu.uni.lu/handle/10993/22420
http://orbilu.uni.lu/handle/10993/19960
http://orbilu.uni.lu/handle/10993/12316
http://orbilu.uni.lu/handle/10993/15109
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http://orbilu.uni.lu/handle/10993/12113
http://orbilu.uni.lu/handle/10993/12116
http://orbilu.uni.lu/handle/10993/21337
http://orbilu.uni.lu/handle/10993/15234
http://orbilu.uni.lu/handle/10993/19960
Other related documents

http://orbilu.uni.lu/handle/10993/15387

Plenary talk at XDMS2017
http://orbilu.uni.lu/handle/10993/31487

What makes Data Science different?
http://hdl.handle.net/10993/30235

Energy-minimal crack growth
http://hdl.handle.net/10993/29414

Uncertainty quantification for soft tissue biomechanics
http://orbilu.uni.lu/handle/10993/28618
http://orbilu.uni.lu/handle/10993/30946

Needle insertion real-time simulation and error control
http://orbilu.uni.lu/handle/10993/29846
http://orbilu.uni.lu/handle/10993/30937

Bayesian parameter identification in mechanics
http://orbilu.uni.lu/bitstream/10993/28631/1/1606.02422v4.pdf