Thèse d'habilitation à diriger des recherches

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Towards the next generation of high-fidelity simulators for online computing: adaptive modelling through the scales

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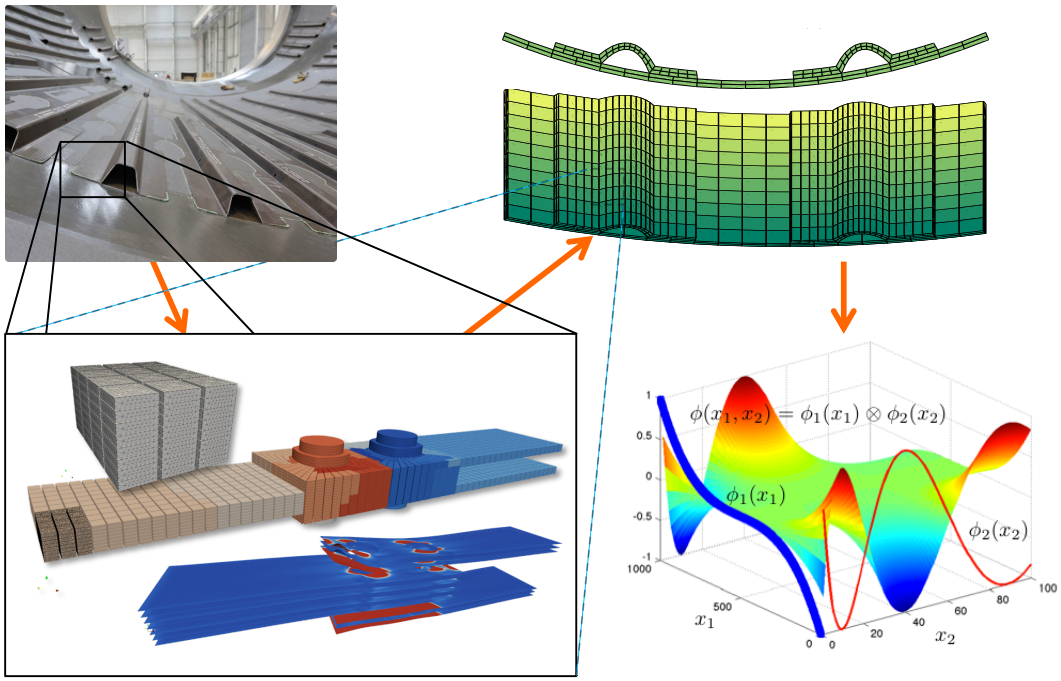


Abstract

High-fidelity modelling and simulation have profoundly transformed the area of material and structural design. Through advances in computer hardware and software, material failure can be reliably predicted using multiscale high-fidelity models coupled with appropriately designed discretisation strategies. Yet, such heavy numerical tasks are restricted to "one-shot" virtual experiments. Emerging applications such as real-time control or interactive design require performing thousands of repeated analyses, with potentially limited computational facilities. Models used for such applications require extreme robustness and swiftness of execution. To unleash the full potential of high-fidelity computational mechanics, we need to develop a new generation of numerical tools that will bridge the gap between, on the one hand, heavy numerical solvers and, on the other hand, computationally demanding "online" engineering tasks. This thesis introduces and summarises research contributions that aim to help bridge this gap, through the development of robust model reduction approaches to control the cost associated with multiscale and physically detailed numerical simulations, with a particular emphasis on reliability assessment for composite materials and fracture.

L'ingénierie des matériaux et des structures a été transformée en profondeur par la généralisation de simulation numérique. Grâce à l'avancée des outils de calcul scientifique, la rupture des matériaux peut être prédite de manière fiable par des modèles multi-échelles, en conjonction avec des méthodes de résolution numérique haute-performance. Cependant, ces simulations coûteuses restent limitées à l'expérience virtuelle unitaire. Les applications modernes comme le contrôle en temps réel ou la conception interactive requièrent des vitesses d'exécution et des niveaux de stabilité des modèles qui restent hors de portée. Le potentiel des simulations mécaniques haute-fidélité ne pourra être réalisé que par le développement d'une nouvelle génération d'outils numériques chargés de réduire les coûts de calculs afin de permettre l'utilisation de modèles numériques fins dans des applications impliquant des calculs "à-la-volée". Cette thèse présente quelques contributions de recherche visant à combler ce fossé technologique. L'accent est porté sur le développement de méthodes de réduction de modèle pour le contrôle des coûts de calcul associés aux simulations haute-fidélité, avec un intérêt particulier pour la mécanique des composites et la prédiction multi-échelles de la rupture.

Acknowledgments

Contents

CHAPTER 1

Présentation synthétique des activités d'enseignement et de recherche

1.1 Parcours professionnel et formation universitaire

Je suis enseignant-chercheur au Centre des matériaux de l'Ecole Mines ParisTech. De 2009 à 2018, j'ai travaillé à l'Université de Cardiff, au Royaume-Uni, dans le département de Génie Civil. J'ai soutenu ma thèse à l'ENS de Cachan en 2008. Une présentation détaillée de mon parcours professionnel est donnée Figure 1.1.

1.2 Thématiques de recherche

Ma recherche a pour but ultime le développement de méthodes de calcul pour la prédiction du comportement des matériaux et des structures complexes, ceci afin de réduire le besoin de recourir à l'expérimentation physique. Afin de contribuer à ce vaste projet scientifique, je développe des approches numériques innovantes pour rendre possible ou faciliter les applications suivantes :

- Les simulations multi-échelle, c'est-à-dire les simulations à l'échelle de l'ingénieur qui prennent en comptes une connaissance partielle de la physique à une ou des échelles sous-jacentes;
- L'optimisation et le contrôle basés sur la simulation numérique, pour lesquelles des simulateurs lourds doivent être appelées de nombreuses fois au sein d'une boucle d'optimisation, avec peu ou pas de possibilité pour l'utilisateur de vérifier la qualité des calculs, ceci en vue d'optimiser, de contrôler un système et/ou d'identifier certains de ses paramètres.

Les applications principales de mes travaux concernent la prédiction de la rupture des matériaux composites (stratifiés et bétons principalement) et les vibrations des structures, avec quelques travaux issus des collaborations en mécanique des fluides [1], électrostatique [2], biomécanique [3] et procédés de fabrication [4].

2019 -	**Chargé de recherche, Centre des matériaux, MINES ParisTech**, France
2013 -	**Senior Lecturer**, Cardiff University, School of Engineering, Royaume-Uni, Department of Civil Engineering / Advanced Materials and Computational Mechanics group
2009-2012	**Lecturer**, Cardiff University, School of Engineering
2008-2009	**Attaché temporaire d´éducation et de recherche** (ATER) à l'Ecole Normale Supérieure (ENS) de Cachan, Laboratoire de Mécanique et Technologie (LMT), France
2005-2008	**Etudiant de thèse à l'ENS de Cachan** (LMT), Thèse obtenue en November 2008 avec mention très honorable. Jury : Alberto Corigliano (rapporteur), Nicolas Moës (rapporteur), Jean-Louis Chaboche (Président), Serge Maison-le-Poëc (examinateur), Olivier Allix (Directeur de thèse), Pierre Gosselet (co-encadrant) **Moniteur** à l'Ecole Normale Supérieure des Arts et Métiers (ENSAM)
2005-2008	**Master TACS** (Techniques Avancées en Calcul des Structures) au LMT Cachan / Université Paris 6 **Projet de recherche** à TU Delft, Pays-Bas
2004	**Agrégation de Mécanique**
2001-2005	**Licence et Maitrise de Génie mécanique**, ENS Cachan **Stage de maitrise** à EADS Innovation Works
1999-2001	**Classes préparatoires aux grandes écoles**, Lycée J.B. Say, Paris
1999	**Baccalauraurréat scientifique**

Figure 1.1: Parcours professionnel et formation universitaire

1.3 Vue d'ensemble des activités de recherche en mécanique numérique

Simulations multi-échelles adaptatives.

J'ai débuté ma carrière académique sur une thématique de prédiction de l'évolution du délaminage dans les composites stratifiés [5, 6, 7]. Ce type de problèmes est typiquement multi-échelle, car l'initiation et la propagation des fissures à l'échelle des hétérogénéités a des conséquences importantes à l'échelle de l'ingénieur, en termes de résistance structurelle par exemple (*i.e.* coalescence de microfissures et propagation macroscopique, conduisant potentiellement à la rupture ultime). De tels phénomènes ne peuvent pas être directement prédits par des modèles à l'échelle fine, car les modèles structuraux résultants sont (et seront toujours) trop lourds pour être résolus par des ordinateurs. C'est un problème d'une importance croissante, car les ingénieurs du XXIème siècle veulent être capables de maîtriser des systèmes conçus sur plusieurs échelles couplées de façon à maximiser leur efficacité (compos-

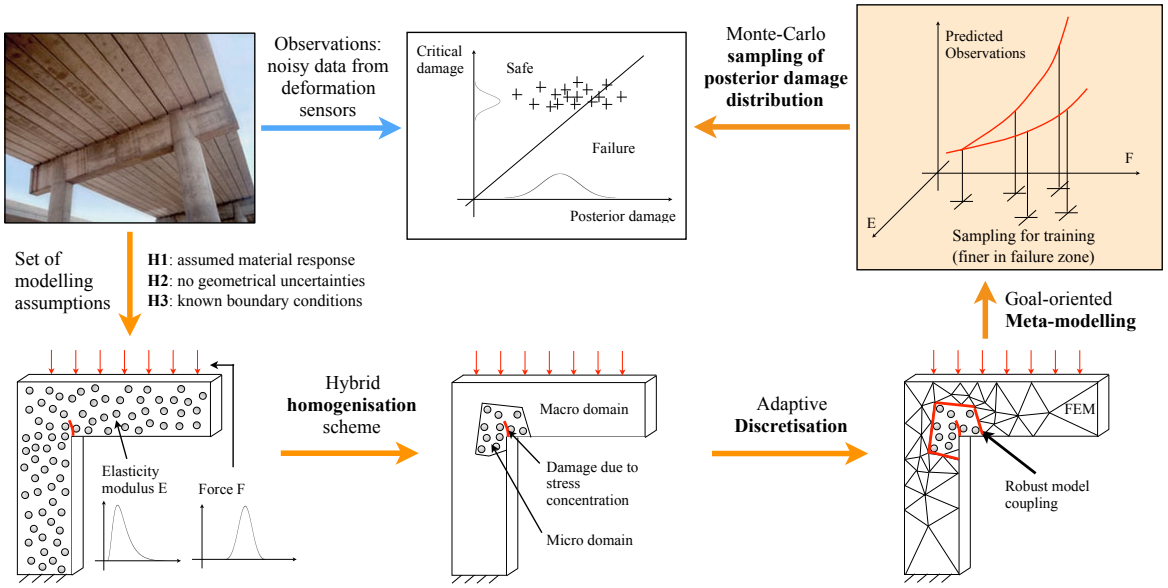


Figure 1.2: Principe du jumelage numérique (inexistant à l'heure actuelle). Une modèle numérique fin de la structure est recalé en temps réel, et peut être résolu pour prédire l'issu de différents cas de charge ou cycles d'utilisation.

ites, matériaux architecturés, fabrication additive, ...).

Il n'y a pas, hélas, de méthode générique pour prendre en compte les aspects multi-échelle lors de la simulation de systèmes complexes. Je développe donc des approches dédiées, en utilisant la nature du problème multi-échelle à résoudre pour rendre de tels calculs possibles. Par exemple, dans le cadre de la mécanique nonlinéaire de la rupture, j'ai tiré parti du fait que les fissures localisent en espace et en temps pour proposer une méthode de zoom dans laquelle le modèle fin n'est utilisé de manière directe que dans les zones fissurées [8]. Dans le cadre de la diffusion thermique dans les matériaux composites, j'ai développé une méthode d'homogénéisation stochastique qui propage grossièrement les incertitudes de données microscopiques et ne fait appel au modèle fin qu'au besoin. L'adaptation de modèle est alors réalisée de manière gloutonne, avec un critère d'erreur basée sur la dualité [9]. J'ai également contribué au développement d'approches de couplages entre méthodes particulaires utilisées localement pour représenter des physiques à des échelles très fines, et des approches continues permettant de transmettre les conditions aux limites au modèle particulaire tout en limitant les coûts de calculs [10, 11]. Finalement, j'ai développé des approches de defeaturing, dans lesquelles des formes locales décrites en CAO sont automatiquement ignorées si leur effet sur la solution globale est peu significatif [2].

Réduction de modèle pour l'optimisation et le contrôle.

Les applications modernes émergentes telles que l'optimisation virtuelle, le jumelage numérique (Figure 1.2) ou le contrôle en temps réel, requièrent la résolution de centaines, de milliers voire de dizaines de milliers de problèmes numériques directs, sujets à variations paramétriques. En conséquence, les modèles utilisés sont ultra-simplifiés *a priori* (0D par exemple avec en-

richissement par la donnée). Pour réconcilier l'utilisation de modèles physiques fiables et les applications utilisant des boucles d'optimisation numériques, je développe des méthodes de réduction de modèle intelligentes, basées sur la science des données. Dans une phase hors-ligne, un algorithme glouton permet d'amasser des données relatives à la solution du problème paramétrique que l'on souhaite réduire. Dans un second temps, on projette le problème initial dans un espace de petite taille générer par compression optimale des données accumulées. Les coûts de calcul associés à la résolution des problèmes réduits sont de 10 à 100 fois inférieurs à ceux engendrés par la résolution du problème d'origine [12, 13]. Je suis un des premiers à avoir travaillé sur la réduction du modèle par projection pour la mécanique de l'endommagement. J'ai effectué un travail important sur l'exclusion des zones où les fissures s'initient et se propagent, qui ne se réduisent pas ou se réduisent mal [14, 15]. J'ai également contribué au développement de méthodes de rédction de modèle dans le cadre des calculs numériques multi-échelles de type FE^2 [16, 17]. Finalement, j'ai proposé des développements innovants en termes de réduction de modèle à-la-volée, pour lequel le modèle réduit est construit ou enrichi au besoin lors du calcul de structure, et réutilisé pour accélérer les calculs suivants [18, 19].

Activité transversale 1 : méthodes de discrétisation avancées.

Mes recherches sur la réduction des coûts de calculs associés aux problèmes multi-échelle et aux problèmes "en ligne" sont facilitées par l'utilisation de méthodes de résolutions numériques avancées telles que la XFEM, qui permet la représentation de l'évolution de fissures sans remaillage, ou la méthode CutFEM, qui permet de s'affranchir en partie de l'étape de maillage lors de la virtualisation de systèmes à géométries complexes. Je participe au développement de ces méthodes, dans le cadre de mes recherches et au travers de collaborations [20, 21, 22, **?**, 4]. Finalement, j'ai contribué au développement de méthodes de type analyse isogéométrique, notamment en vue de leurs utilisations pour la simulation de la propagation de fissures [23, 24].

Activité transversale 2 : contrôle automatisé de la qualité des calculs.

La vérification des calculs intervient à tous les niveaux dans ma recherche, et en particulier pour guider les algorithmes multi-échelles adaptatifs et les algorithmes d'apprentissage des modèles réduits. Je développe dans ce cadre des estimateurs d'erreur *a posteriori* basés sur les techniques de lissage et de résidus implicites [25, 21, 26]. Je développe également des indicateurs basés sur la dualité pour les problèmes convexes [27, 13, 9, 2].

1.4 Groupe de recherche et financements

Je suis (Senior) Lecturer à l'université de Cardiff depuis fin 2009. J'ai supervisé le travail de 14 doctorants, dont 6 en tant que directeur de thèse (voir Figure 1.3). Mon groupe est couramment composé de 4 thésards. J'ai été financé de manière continue par des sources extérieures, et en particulier par EPSRC (agence de financement britannique pour les sciences), l'équivalent gallois NRN, et l'UE (FP7 puis H2020). La liste des financements de recherche qui m'ont été accordés est donnée ci-dessous :

- P. Kerfriden, Rapid Biomechanics and Simulation for Personalised Clinical Design (RAINBOW) MCSA European Training Network H2020 (Investigateur principal : Dr Erleben – University Copenhagen), valeur pour Cardiff : £300,000, 09/2018-09/2021;

- S. Claus, P. Kerfriden, D. Barrow, A.D. Jefferson, T. Phillips, Virtual Design of Microencapsulation processes, National Research Network in Advanced Engineering and Materials, valeur : £150,000, 03/2015-08/2018;

- P. Kerfriden, L.A.A. Beex, An adaptive multiscale method for sandwich-structured panels, National Research Network in Advanced Engineering and Materials, valeur : £59,349, 01/2015-01/2018;

- S. Adhikari, E.A. de Souza Neto, P. Kerfriden, D. Kennedy, A multiscale approach for uncertainty quantification in composite structures (Investigateur principal : Prof. Adhikari, Swansea University), valeur : £81,952, National Research Network in Advanced Engineering and Materials, 01/2015-01/2018;

- P. Kerfriden, Towards rationalised computational expense for simulating fracture over multiple scales (RationalMSFrac) EPSRC First Grant EP/J01947X/1, valeur : £124,630, 01/2013-12/2014;

- P. Kerfriden, 9th World Congress in Computational Mechanics and 4th asian pacific congress on computational mechanics and 4th asian pacific congress on computational mechanics, Royal Society Travel Grant, valeur : £3,123, 07/2010-07/2010;

- S.P.A. Bordas, P. Kerfriden, R. Simpson, S. Kulasegaram, R. Martin, F. Langbein, Integrating numerical simulation and geometric design technology (INSIST), European Commission FP7 - Marie Curie Action (Investigateur principal : Prof. Rabczuk – Bauhaus-Universität), valeur pour Cardiff : £1,201,338, 01/2012-12/2016.

1.5 Activités d'encadrement scientifique

Au cours des 10 dernières années, j'ai dirigé ou co-encadré les thèses et post-doctorats listés dans la table donnée Figure 1.3. Le code couleur est expliqué sous le tableau.

1.6 Participation à la vie de la communauté scientifique

J'ai co-organisé deux conférences à Cardiff. La première est la conférence thématique ECCOMAS XFEM 2011 (co-chair : S.P.A. Bordas), une conférence internationale centrée sur la méthode des éléments finis étendus, et qui a attirée environ 150 participants. La seconde est la conférence ACME 2016, une conférence nationale britannique annuelle attirant environ 100 participants autour des thèmes de mécanique numérique (co-chair : A.D. Jefferson).

Je suis depuis début 2018 éditeur associé pour le journal Computer Modeling in Engineering and Sciences (CMES). Je fais également partie du comité de relecture d'un certain nombre de journaux, donc International Journal for Numerical Methods in Engineering, Computational Mechanics, Computer Methods in Applied Mechanics and Engineering, Computers and Structures, Finite Elements in Analysis and Design, Thin-Walled Structures, Engineering Failure Analysis, International Journal for Computational Methods in Engineering Science and Mechanics, et Mathematical Problems in Engineering and Computational Mechanics.

Au cours des 10 dernières années, j'ai également fait partie de plusieurs de jurys de thèse, dont la liste est donnée ci-dessous :

Période	*Chercheur*	*Type*	*Rôle*	*Sujet d'étude*
2019-22	Mr Hilal	PhD	**Dir. thèse**	Hybrid data-driven modelling for 3D printing
2019-22	Mr Krokos	PhD	**Dir. thèse**	Fracture directly from CAD through stat. learning
2018-21	Mr Mikaeili	PhD	**Dir. thèse**	Self-learning multiscale fracture models
2015-18	Mr P. Bonilla	PhD	**Dir. thèse**	Adaptive, Data-driven Modelling of Damage
2015-18	Mr P. Yu	PhD	**Dir. thèse**	Adaptive Solution for the Wave Equation
2014-17	Mr X. Du	PhD	**Dir. thèse**	Non-intrusive Reduced Order Modelling
2013-17	Mr N. Rahimi	PhD	Encadrant	Defeaturing Error Estimation by Machine Learning
2013-15	Dr. C. Heaney	Post-doc	**Encadrant principal**	Reliable quality control in Homogenization
2013-16	Mr. A. Surleaux	PhD	Encadrant	Data-driven Modelling of Micro-EDM processes
2013-17	Mr K. Bronik	PhD	Encadrant	Modelling of skin deformations
2012-16	Mr. D. A. Paladim	PhD	**Dir. thèse**	Error control in Stochastic Homogenisation
2012-15	Dr. C. Hoang	Post-doc	**Encadrant principal**	Goal-oriented Reduced Order modelling
2012-14	Dr. V.P. Nguyen	Post-doc	**Encadrant principal**	Weakly intrusive modelling of composites from CAD
2012-13	Dr .H. Courtecuisse	PDRA	Encadrant	Real-time simulation of surgical cuts
2011-15	Mr. C.K.Lee	PhD	Encadrant	Smoothed FEM in nonlinear elasticity
2011-15	Mr. D. Sutula	PhD	Encadrant	Extended Element Method for multiple cracks
2011-15	Mr X. Peng	PhD	Encadrant	Extended Isogeometric Boundary Elements
2010-14	Dr. O. Goury	PhD	**Dir. thèse**	Reliable Model Order Reduction for Fracture
2010-14	Dr. A. Akbari	PhD	**Dir. thèse**	Adaptive Multiscale Modelling of Fracture
2010-14	Dr. H. Lian	PhD	Encadrant	Isogeometric Boundary Elements in Optimisation
2010-13	Dr. O. G. Estrada	PDRA	Encadrant	Error Estimation and Adaptivity for X-FEM
2009-11	Dr. S. Natarajan	PhD	Encadrant	Reliable and efficient Smoothed X-FEM

Terminé avec succés | Supervision en cours | Compétences principales

Figure 1.3: Liste des thèses encadrées.

- Examinateur interne pour 3 thèses à Cardiff University entre 2010 et 2018;
- Rapporteur pour une thèse à l'école des Mines de Paris en 2018;
- Examinateur pour une thèse à l'INSA de Lyon en 2014, rapporteur pour la même institution en 2018;
- Examinateur externe pour une thèse de MPhil à l'université de Manchester en 2017;
- Rapporteur pour une thèse à Politecnico di Milano en 2015;
- Examinateur externe pour deux thèses à University of Western Australia en 2012 et 2013.

1.7 Prix et autres indicateurs de reconnaissance scientifique

J'ai reçu les prix et indicateurs de reconnaissance suivants :

- Invité au "stage 2" d'une demande de financement ERC Starting Grant, Bruxelles, 2016;
- Prix de la meilleure thèse décerné par UK Association for Computational Mechanics in Engineering pour la thèse d'Olivier Goury, 2015;
- Nomination pour le prix Celebrating Excellence "Rising Star" Awards à Cardiff University, 2013;
- Placé second au concours d'entrée CNRS CR1, 2013;
- Prix de la meilleure thèse décerné par UK Association for Computational Mechanics in Engineering pour la thèse de Sundarajan Natarajan, 2011;
- Prix Emerald LiteratiNetwork "Outstanding Paper Award", Engineering Computations, 2013
- Reçu au concours de l'agrégation de mécanique, 2004.

1.8 Conférences, séminaires et invitations à participer à des collaborations scientifiques

J'ai été invité à travailler dans plusieurs centres de recherche pour initier ou poursuivre des collaborations scientifiques. Voici la liste de ces activités.

- **University of Copenhagen, 2017**. J'ai été invité à passer deux semaines dans la School of Computer Science par Kenny Erleben. Nous travaillons sur un projet de recalage d'images médicales avec prise en compte du contact entre organes. Un premier article est en préparation. Cette collaboration est un projet de longue haleine menée dans le cadre du projet H2020 ITN RAINBOW (voir la liste des financements).
- **Stanford University, 2014**. J'ai été invité par Charbel Farhat à passer trois semaines dans leur laboratoire. Nous avons travaillé sur la réduction de modèle au sein des algorithmes de Markov-Chain Monte-Carlo, et également sur les thématiques de réduction de modèle dans un cadre multi-échelles. Les résultats de cette dernière activité sont publiés dans [17] et dans [28].
- **Universitat de València, 2013**. J'ai été invité à travailler avec Juan José Rodenas à Valence, Catalogne. Cette collaboration a été fructueuse, comme le montre la série d'articles joints entre nos deux équipes sur le thème de l'estimation d'erreur *a posteriori* [25, 21, 27].
- **Bauhaus-Universität Weimar, 2011**. J'ai été invité à travailler pendant une semaine avec le groupe de recherche de Timon Rabczuk en 2011. Cet échange scientifique est un des aspects d'une collaboration soutenue sur plusieurs années [10, 11, 16], au travers notamment du projet ITN FP7 INSIST.

J'ai également été invité à donner un certain nombre de présentations scientifiques. Elles sont listées ci-après.

Présentations sur invitation lors de conférences et dans le cadre de des groupes de travail internationaux :

- Présentation invitée à ECCOMAS XDMS'17, Umea, 2017;
- Présentation invitée à Workshop on Computational Sciences for Medicine, University of Luxembourg, 2016;
- Présentation invitée à EU-MORNET meeting (COST action European Network for Model Reduction), Eindhoven, 2014;
- Présentation invitée à 5th International Conference on Computational Methods (ICCM2014), Cambridge, 2014;
- Présentation invitée à WIMCS 2010 (Wales Institute of Mathematics and Computational Sciences).

Cours doctoraux invités :

- Cours invité (1h) à "Bridging the scales: from simulation to structural assessment", short-course on Multiscale damage modelling, University of Nottingham, 2018;
- Cours invité (2h) à ACME 2016 School, 24th UK Conference of the Association for Computational Mechanics in Engineering, Cardiff University, 2016;
- Cours invité (6h) à CISM-ECCOMAS International Summer School, Modelling, Simulation and Characterisation of Multi-Scale Heterogeneous Materials, Udine, 2015;
- Cours invité (3h) à 4th Workshop on Advanced Numerical Analysis Techniques, Universitat Politècnica de València, 2013.

Liste des séminaires invités :

- Mines ParisTech, 2018;
- University of Copenhagen, 2017;
- Cardiff University, School of Mathematics, 2016;
- Politecnico di Milano, 2015;
- Durham University, 2014;
- University of Sheffield, June 2014;
- Stanford University, November 2014.

1.9 Activités d'enseignement

Une description succincte de mes activités d'enseignement est présentée dans le tableau de la figure 1.4. Les activités au niveau Master of Science sont soulignées car elles sont liées à mes activités de recherche. En particulier, la plupart des 25+ projets de Master que j'ai supervisé concernent les méthodes numériques pour la mécanique des structures et la rupture des composites (utilisation de codes de calcul commerciaux pour réaliser des études avancées, ou développement d'outils numériques spécialisés pour préparer des activités de recherche).

Période	***Matière***	***Type***	***Niveau***	***Rôle***	***Taux horaire***
2015-18	Mathématiques appliquées	TD	1ere année CU*	Enseignant	48h p.a.
2011-18	Vibrations des structures	Cours magistral	3eme année CU	Responsable de module	36h p.a.
2018	**Méthode scientifique**	Divers	**Master CU**	Responsable de module	36h p.a.
2009-10 et 2015-18	Relevés topographiques	TP	1ere année CU	Enseignant	35h p.a.
2010-18	*Bachelor projects*	Projet	3eme année CU	Encadrant	Environ 100h p.a. (5 élèves par an)
2010-18	***MSc projects***	Projet	**Master CU**	Encadrant	Environ 60h p.a. (3 élèves par an)
2010-12	Résistance des matériaux	TP	1ere et 2eme année CU	Enseignant	36h p.a.
2011-11	Conception en Génie Civil	Cours magistral + TD	1ere année CU	Responsable de module	48h p.a.
2009	Méthodes numériques pour la mécanique	TD+TP	1ere et 2eme année ENS	Enseignant	80h eq. TD
2009	Conception/CAO	TP	1ere année ENS	Enseignant	20h eq. TD
2005-08	Conception Mécanique	Divers	2eme année ENSAM	Responsable de module	64h eq. TD p.a.

*Cardiff University

Figure 1.4: Liste des enseignements dispensés

1.10 Responsabilités administratives

J'ai effectué un certain nombre de tâches administratives au cours des années pendant lesquelles j'ai travaillé à Cardiff. Les plus importantes d'entre elles sont listées et expliquées ci-dessous.

- **Year Tutor.** Le cursus scolaire dans les universités britanniques est de trois (Bachelor)

à quatre années (Master of Engineering ou Master of Science). Un membre du corps académique est responsable du suivi de l'ensemble des élèves d'une année particulaire, dans sa discipline d'enseignement (Génie Civil dans mon cas). L'objectif est d'aider les élèves ayant des difficultés personnelles, de s'assurer que l'ensemble des cours soient correctement dispensés, et coordonnés de manière appropriée. J'ai fait ce travail pour les élèves de première année de 2010 à 2012, et pour les élèves de deuxième année en 2017 et 2018. Il s'agissait de promotions d'environ 150 élèves.

- **Health and Safety commitee representative.** J'ai été responsable sécurité pour les laboratoires de Génie Civil de 2015 à 2018, mon rôle était de faire le lien entre le comité de sécurité charge d'émettre et de faire appliquer les lois et règles en termes de sécurité du travail, et les membres du corps académique dans les laboratoires et les départements d'enseignement relevant de ma discipline.

- **Post-graduate tutor.** En 2018, J'ai été responsable du suivi de l'ensemble des étudiants de thèse inscrits au programme doctoral de Génie Civil.

- **Department management board.** En 2017 et 2018, j'ai fait partie du comité de présidence du département de Génie Civil, chargé de faire appliquer les règles imposées par l'université, et de prendre les décisions nécessaires au bon déroulement et à l'amélioration du cursus académique dans son ensemble.

Articles de revues internationales avec comité de relecture

[1] Susanne Claus and Pierre Kerfriden. A CutFEM method for two-phase flow problems. *Computer Methods in Applied Mechanics and Engineering*, 348:185–206, 2019.

[2] Pierre Kerfriden, Abhishek Kundu, and Susanne Claus. Adaptivity in Bayesian Inverse Finite Element Problems: Learning and Simultaneous Control of Discretisation and Sampling Errors. *Materials*, 12(4):642, 2019.

[3] Navid Rahimi, Pierre Kerfriden, Frank C Langbein, and Ralph R Martin. CAD model simplification error estimation for electrostatics problems. *SIAM Journal on Scientific Computing*, 40(1):B196–B227, 2018.

[4] Susanne Claus, Samuel Bigot, and Pierre Kerfriden. CutFEM Method for Stefan–Signorini Problems with Application in Pulsed Laser Ablation. *SIAM Journal on Scientific Computing*, 40(5):B1444–B1469, 2018.

[5] Danas Sutula, Pierre Kerfriden, Tonie Van Dam, and Stéphane PA Bordas. Minimum energy multiple crack propagation. Part I: Theory and state of the art review. *Engineering Fracture Mechanics*, 191:205–224, 2018.

[6] Danas Sutula, Pierre Kerfriden, Tonie Van Dam, and Stéphane PA Bordas. Minimum energy multiple crack propagation. Part-II: Discrete solution with XFEM. *Engineering Fracture Mechanics*, 191:225–256, 2018.

[7] Danas Sutula, Pierre Kerfriden, Tonie van Dam, and Stéphane P.A. Bordas. Minimum energy multiple crack propagation. Part III: XFEM computer implementation and applications. *Engineering Fracture Mechanics*, 191:257–276, 2018.

[8] Peng Yu, Cosmin Anitescu, Satyendra Tomar, Stéphane Pierre Alain Bordas, and Pierre Kerfriden. Adaptive Isogeometric analysis for plate vibrations: An efficient approach of local refinement based on hierarchical a posteriori error estimation. *Computer Methods in Applied Mechanics and Engineering*, 342:251–286, 2018.

[9] Susanne Claus and Pierre Kerfriden. A stable and optimally convergent LaTIn-CutFEM algorithm for multiple unilateral contact problems. *International Journal for Numerical Methods in Engineering*, 113(6):938–966, 2018.

[10] D. A. Paladim, J. P. Moitinho de Almeida, S. P. A. Bordas, and P. Kerfriden. Guaranteed error bounds in homogenisation: An optimum stochastic approach to preserve the numerical separation of scales. *International Journal for Numerical Methods in Engineering*, 110:103–132, 2017.

[11] X. Peng, E. Atroshchenko, P. Kerfriden, and S.P.A. Bordas. Isogeometric boundary element methods for three dimensional static fracture and fatigue crack growth. *Computer Methods in Applied Mechanics and Engineering*, 316:151–185, 2017. Special Issue on Isogeometric Analysis: Progress and Challenges.

[12] Xuan Peng, Elena Atroshchenko, Pierre Kerfriden, and S. P. A. Bordas. Linear elastic fracture simulation directly from CAD: 2D NURBS-based implementation and role of tip enrichment. *International Journal of Fracture*, 204(1):55–78, 2017.

[13] Haojie Lian, P. Kerfriden, and S. P. A. Bordas. Shape optimization directly from CAD: An isogeometric boundary element approach using T-splines. *Computer Methods in Applied Mechanics and Engineering*, 317:1–41, 2017.

[14] Chang-Kye Lee, L. Angela Mihai, Jack S. Hale, Pierre Kerfriden, and Stéphane PA Bordas. Strain smoothing for compressible and nearly-incompressible finite elasticity. *Computers & Structures*, 182:540–555, 2017.

[15] Olivier Goury, David Amsallem, Stéphane Pierre Alain Bordas, Wing Kam Liu, and Pierre Kerfriden. Automatised selection of load paths to construct reduced-order models in computational damage micromechanics: From dissipation-driven random selection to Bayesian optimization. *Computational Mechanics*, 58(2):213–234, 2016.

[16] K.C. Hoang, P. Kerfriden, and S.P.A. Bordas. A fast, certified and "tuning free" two-field reduced basis method for the metamodelling of affinely-parametrised elasticity problems. *Computer Methods in Applied Mechanics and Engineering*, 298:121–158, 2016.

[17] Haojie Lian, Pierre Kerfriden, and Stéphane PA Bordas. Implementation of regularized isogeometric boundary element methods for gradient-based shape optimization in two-dimensional linear elasticity. *International Journal for Numerical Methods in Engineering*, 106(12):972–1017, 2016.

[18] Ahmad Akbari Rahimabadi, Pierre Kerfriden, and Stéphane Bordas. Scale selection in nonlinear fracture mechanics of heterogeneous materials. *Philosophical Magazine*, 95:3328–3347, 2015.

[19] O.A. González-Estrada, J.J. Ródenas, S.P.A. Bordas, E. Nadal, P. Kerfriden, and F.J. Fuenmayor. Locally equilibrated stress recovery for goal oriented error estimation in the extended finite element method. *Computers & Structures*, 152:1–10, 2015.

[20] Khac Chi Hoang, Pierre Kerfriden, B. C. Khoo, and S. P. A. Bordas. An efficient goal-oriented sampling strategy using reduced basis method for parametrized elastodynamic problems. *Numerical Methods for Partial Differential Equations*, 31(2):575–608, 2015.

[21] S. Dey, T. Mukhopadhyay, H. Haddad Khodaparast, Pierre Kerfriden, and S. Adhikari. Rotational and ply-level uncertainty in response of composite shallow conical shells. *Composite Structures*, 131:594–605, 2015.

[22] Hamid Ghasemi, Pierre Kerfriden, Stéphane PA Bordas, Jacob Muthu, Goangseup Zi, and Timon Rabczuk. Probabilistic multiconstraints optimization of cooling channels in ceramic matrix composites. *Composites Part B: Engineering*, 81:107–119, 2015.

[23] Hamid Ghasemi, Pierre Kerfriden, Stéphane PA Bordas, Jacob Muthu, Goangseup Zi, and Timon Rabczuk. Interfacial shear stress optimization in sandwich beams with polymeric core using non-uniform distribution of reinforcing ingredients. *Composite Structures*, 120:221–230, 2015.

[24] Mohammad Silani, Hossein Talebi, Saeed Ziaei-Rad, Pierre Kerfriden, Stéphane PA Bordas, and Timon Rabczuk. Stochastic modelling of clay/epoxy nanocomposites. *Composite Structures*, 118:241–249, 2014.

[25] Vinh Phu Nguyen, Pierre Kerfriden, Marco Brino, Stéphane PA Bordas, and Elvio Bonisoli. Nitsche's method for two and three dimensional NURBS patch coupling. *Computational Mechanics*, 53(6):1163–1182, 2014.

[26] Hadrien Courtecuisse, Jérémie Allard, Pierre Kerfriden, Stéphane PA Bordas, Stéphane Cotin, and Christian Duriez. Real-time simulation of contact and cutting of heterogeneous soft-tissues. *Medical image analysis*, 18(2):394–410, 2014.

[27] P. Kerfriden, J. J. Ródenas, and S. P.-A. Bordas. Certification of projection-based reduced order modelling in computational homogenisation by the constitutive relation error. *International Journal for Numerical Methods in Engineering*, 97(6):395–422, 2014.

[28] Vinh Phu Nguyen, Pierre Kerfriden, and Stéphane PA Bordas. Two-and three-dimensional isogeometric cohesive elements for composite delamination analysis. *Composites Part B: Engineering*, 60:193–212, 2014.

[29] Hossein Talebi, Mohammad Silani, Stéphane PA Bordas, Pierre Kerfriden, and Timon Rabczuk. A computational library for multiscale modeling of material failure. *Computational Mechanics*, 53(5):1047–1071, 2014.

[30] L. A. A. Beex, Pierre Kerfriden, Timon Rabczuk, and Stéphane Pierre Alain Bordas. Quasicontinuum-based multiscale approaches for plate-like beam lattices experiencing in-plane and out-of-plane deformation. *Computer Methods in Applied Mechanics and Engineering*, 279:348–378, 2014.

[31] Sundararajan Natarajan, Pierre Kerfriden, D. Roy Mahapatra, and Stéphane Pierre Alain Bordas. Numerical analysis of the inclusion-crack interaction by the extended finite element method. *International Journal for Computational Methods in Engineering Science and Mechanics*, 15(1):26–32, 2014.

[32] Vinh Phu Nguyen, Pierre Kerfriden, Stéphane PA Bordas, and Timon Rabczuk. Isogeometric analysis suitable trivariate NURBS representation of composite panels with a new offset algorithm. *Computer-Aided Design*, 55:49–63, 2014.

[33] O.A. González-Estrada, E. Nadal, J.J. Ródenas, P. Kerfriden, S.P.-A. Bordas, and F.J. Fuenmayor. Mesh adaptivity driven by goal-oriented locally equilibrated superconvergent patch recovery. *Computational Mechanics*, 53:957–976, 2013.

[34] P. Kerfriden, K. M. Schmidt, T. Rabczuk, and S. P.-A. Bordas. Statistical extraction of process zones and representative subspaces in fracture of random composites. *International Journal for Multiscale Computational Engineering*, 11(3):271–292, 2013.

[35] Hossein Talebi, Mohammad Silani, Stéphane PA Bordas, Pierre Kerfriden, and Timon Rabczuk. Molecular dynamics/XFEM coupling by a three-dimensional extended bridging domain with applications to dynamic brittle fracture. *International Journal for Multiscale Computational Engineering*, 11(6), 2013.

[36] Olivier Allix, Pierre Gosselet, Pierre Kerfriden, and Karin Saavedra. Virtual delamination testing through non-linear multi-scale computational methods: Some recent progress. *Computers, Materials & Continua*, 32(2):107–132, 2013.

[37] Pedro Baiz, Sundararajan Natarajan, Stéphane Bordas, Pierre Kerfriden, and Timon Rabczuk. Linear buckling analysis of cracked plates by SFEM and XFEM. *Journal of Mechanics of Materials and Structures*, 6(9):1213–1238, 2012.

[38] Lei Chen, Timon Rabczuk, Stephane Pierre Alain Bordas, G. R. Liu, K. Y. Zeng, and Pierre Kerfriden. Extended finite element method with edge-based strain smoothing (ESm-XFEM) for linear elastic crack growth. *Computer Methods in Applied Mechanics and Engineering*, 209:250–265, 2012.

[39] O.A. González-Estrada, J.J. Ródenas, S.P.-A. Bordas, M. Duflot, P. Kerfriden, and E. Giner. On the role of enrichment and statical admissibility of recovered fields in a posteriori error estimation for enriched finite element methods. *Engineering Computations*, 29(8), 2012.

[40] P. Kerfriden, O. Goury, T. Rabczuk, and S.P.-A. Bordas. A partitioned model order reduction approach to rationalise computational expenses in nonlinear fracture mechanics. *Computer Methods in Applied Mechanics and Engineering*, 200(5):850–866, 2012.

[41] Olivier Allix, Pierre Gosselet, and Pierre Kerfriden. Improved multiscale computational strategies for delamination. In *Multiscale Methods in Computational Mechanics*, pages 261–279. Springer, 2011.

[42] S. Natarajan, Pedro M. Baiz, Stéphane Bordas, Timon Rabczuk, and P. Kerfriden. Natural frequencies of cracked functionally graded material plates by the extended finite element method. *Composite structures*, 93(11):3082–3092, 2011.

[43] Stéphane PA Bordas, Sundararajan Natarajan, Pierre Kerfriden, Charles Edward Augarde, D. Roy Mahapatra, Timon Rabczuk, and Stefano Dal Pont. On the performance of strain smoothing for quadratic and enriched finite element approximations (XFEM/GFEM/PUFEM). *International Journal for Numerical Methods in Engineering*, 86(4-5):637–666, 2011.

[44] P. Kerfriden, J.-C. Passieux, and S.P.-A. Bordas. Local/global model order reduction strategy for the simulation of quasi-brittle fracture. *International Journal for Numerical Methods in Engineering*, 89(2):154–179, 2011.

[45] S. Natarajan, P. M. Baiz, M. Ganapathi, P. Kerfriden, and Stéphane Bordas. Linear free flexural vibration of cracked functionally graded plates in thermal environment. *Computers & Structures*, 89(15-16):1535–1546, 2011.

[46] N. Vu-Bac, H. B. Nguyen-Xuan, L. Chen, Stéphane Bordas, P. Kerfriden, R. N. Simpson, G. R. Liu, and Timon Rabczuk. A node-based smoothed extended finite element method (NS-XFEM) for fracture analysis. *Computer Modeling in Engineering and Sciences*, 73(4):331, 2011.

[47] Cyrille F. Dunant, Stéphane PA Bordas, Pierre Kerfriden, Karen L. Scrivener, and Timon Rabczuk. An algorithm to compute damage from load in composites. *Frontiers of Architecture and Civil Engineering in China*, 5(2):180–193, 2011.

[48] Stephane Pierre Alain Bordas, T. Rabczuk, J. J. Rodenas, Pierre Kerfriden, M. Moumnassi, and S. Belouettar. Recent advances towards reducing the meshing and re-meshing burden in computational sciences. 2010.

[49] P. Kerfriden, P. Gosselet, S. Adhikari, and S.P.-A. Bordas. Bridging proper orthogonal decomposition methods and augmented Newton-Krylov algorithms: An adaptive model order reduction for highly nonlinear mechanical problems. *Computer Methods in Applied Mechanics and Engineering*, 200(5-8):850–866, 2011.

[50] O. Allix, P. Kerfriden, and P. Gosselet. On the control of the load increments for a proper description of multiple delamination in a domain decomposition framework. *International Journal for Numerical Methods in Engineering*, 83:1518–1540, 2010.

[51] O. Allix, P. Kerfriden, and P. Gosselet. A relocalization technique for the multiscale computation of delamination in composite structures. *Computer Modeling in Engineering and Sciences*, 55(3):271–291, 2010.

[52] P. Kerfriden, O. Allix, and P. Gosselet. A three-scale domain decomposition method for the 3D analysis of debonding in laminates. *Computational Mechanics*, 44(3):343–362, 2009.

CHAPTER 2

Introduction

High-fidelity simulations: from understanding hidden physics to controlling smart systems.

During the last 40 years, we have witnessed the tremendous increase of the predicting power of computer simulations. This transformation has been brought by major computing hardware and software improvement, and in particular by the development of parallel computing capabilities. Over the years, the area of finite element modelling and simulation has adapted to this new landscape. Today, the models used to predict the evolution of complex engineering systems are extremely detailed. Numerical composite material models, for instance, may explicitly represent hundreds of microscopic material phases explicitly, with complex, nonlinear evolution laws for every one of these interacting bodies. A large aerospace structure of complex geometry may be certified virtually by assembling its components, and simulating the time evolution of this assembly using distributed computing capabilities.

Of course, it is a natural engineering desire to make use of such simulation capabilities to control engineering systems, using the virtualised systems to provide feedback to their physical counterpart. For instance, non-destructive condition monitoring could be augmented with detailed physical simulations to identify structural defects, and predict their potential evolution in the future. Simulation of manufacturing processes could be used to automatically help calibrate machines, through the progressive minimisation of the deviation of manufactured goods to design specifications. However, the advent of such modern applications of finite element modelling is obstructed by a doubly intractable computational cost issue Firstly, simulators needs to be called repeatedly, thousands of time, within optimisation loops. These loops may be required to calibrate design parameters in order to increase the efficiency of the physical system, or to identify unknown system parameters from data, or to generate optimal experimental design strategies. Secondly, integrated simulators may not have access to large computing resources, and may be required to produce results in real or quasi-real time. Finally, high-fidelity numerical models come with a certain level of complexity which does not allow for unsupervised computing.

In order to unleash the full potential of physics-based numerical predictions, there is a

need for a new generation of numerical tools that are lightweight yet reliable, and numerically stable over possibly wide ranges of model parameters.

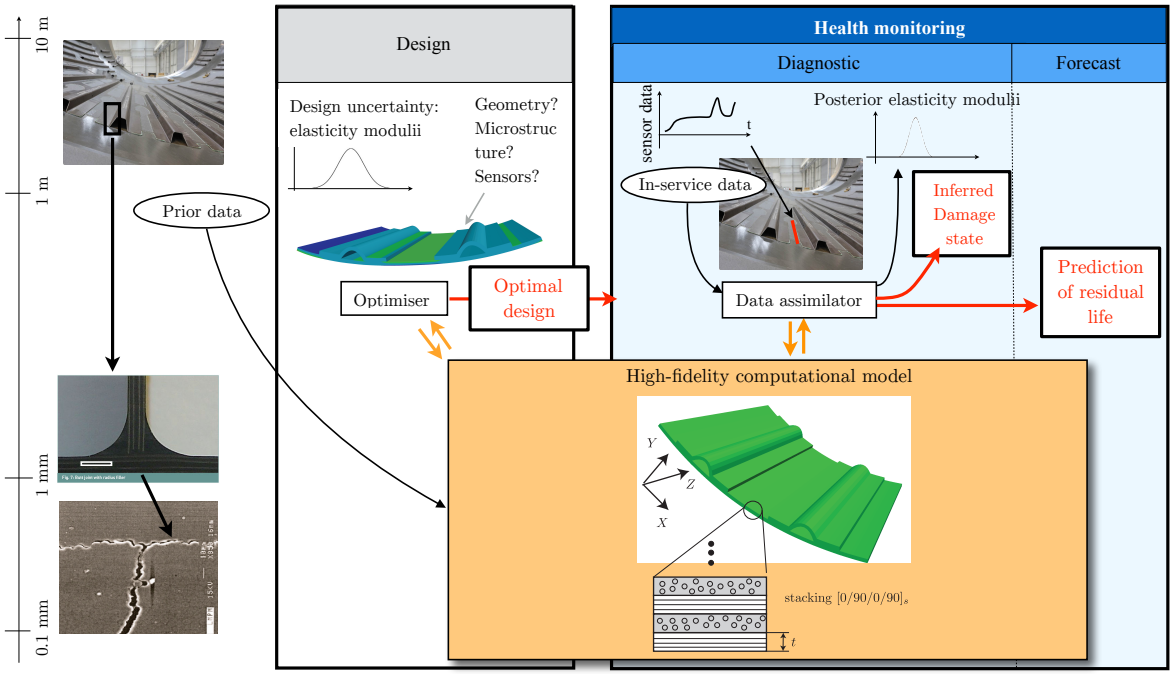


Figure 2.1: The digital twinning concept. A computer model of a physical engineering systems accompanies its physical couterpart and mimics its behaviour. At any time, the virtual twin may be interrogated to predict unobservable quantities, such as the development of hidden defects or the prediction of the evolution of identified defects in the future.

Routes to the advent of online high-fidelity simulations

The continuous improvement in computer hardware efficiencies will not solve the aforementioned issue. This is because the resolution of high-fidelity computer models does not increase linearly with computing power. To illustrate this, let us assume that Moore' law[1] and Dennard scaling[2] both hold. Through this empirical modelling, one can roughly estimate that the number of flops per second and per Watt doubles every 2 years. Yet, the error for the classical low order discretisation scheme finite element in space / finite difference in time decreases with the fourth root of the number of degrees of freedom (if the system of PDEs is solved over space and time using a solver with optimal $\mathcal{O}(N)$ numerical complexity). Hence, for a given amount of energy, hardware improvement may only help decrease the error by a factor 2 every 16 years. Such a time scale seems to be incompatible with the prospect of integrating high-fidelity computer simulators within smart engineering systems.

One potential way forward, however, is to decrease the computational cost associated with heavy simulations by improving the generic algebraic solvers upon which Computational Mechanics relies. This can be done by decreasing the operation count at the mathematical

[1] the number of transistors in a dense integrated circuit doubles about every two years
[2] Transistor power requirements are proportional to area

level and by taking better advantage of available hardware, so as to avoid computational bottlenecks (*e.g.* better libraries and compilers for linear algebra, minimisation of MPI communications in parallel computing, GPU programming).

The alternative and complementary route is to eliminate unnecessary or redundant degrees of freedom, by only using detailed physics where and when it matters *i.e.* where and when using inexpensive modelling alternatives may negatively affect the output of the simulation. Over the last decade, my research has focussed on developing tools that will allow engineers to coarsen models automatically, efficiently, robustly and with as much level of genericity as possible. To be more precise about the later qualification, the numerical reduction methods that will be introduced next are, in general, dedicated to specific classes of engineering problem, which is key to generating significant reduction, but core algorithmic ideas may be more general and reusable in wider contexts.

Towards automatised, adaptive model reduction

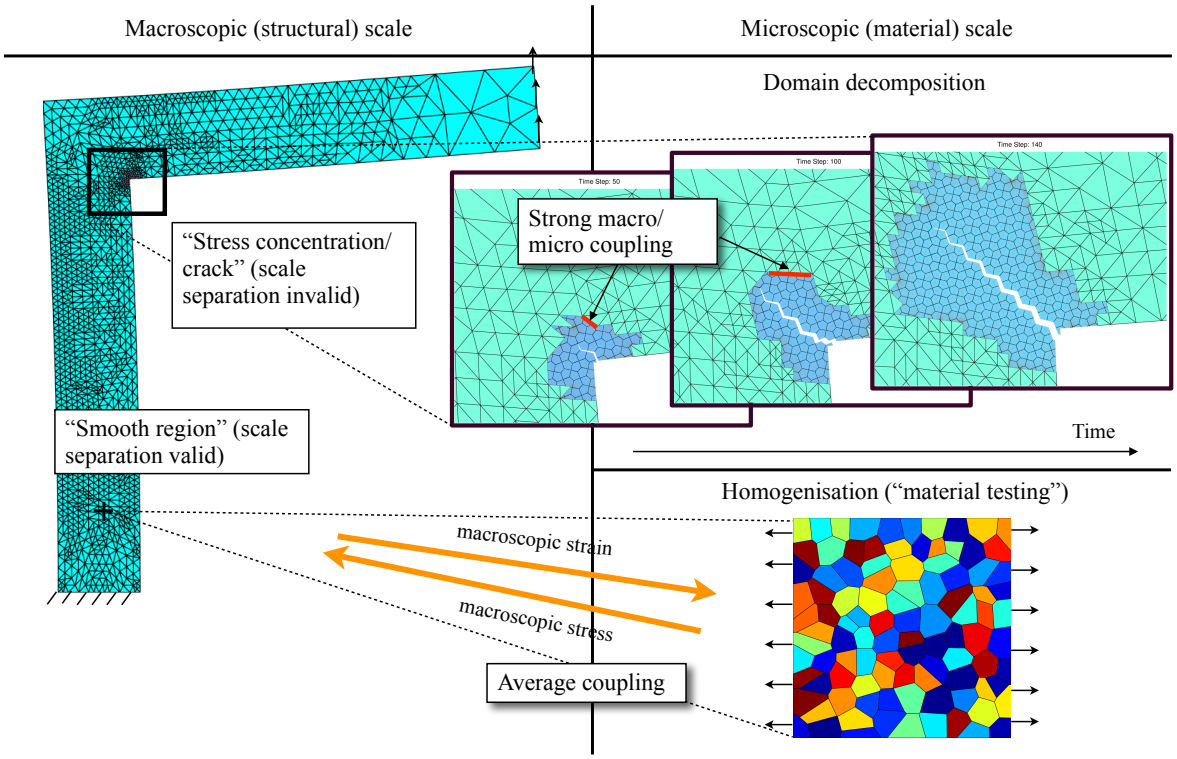


Figure 2.2: Adaptive multiscale fracture modelling, from [8]. Nonlinear computational homogenisation (FE^2) is used away from the crack. Explicit microscale modelling is used in the damaged regions. The model adaptation is driven by an estimate of the modelling error due to the homogenisation process.

Model reduction may be performed by taking advantage of characteristics of the high-fidelity problem to be solved, and make relevant use of surrogates to compute approximate

solutions at a fraction of the original cost. For instance, one may (and should) take advantage of the existence of distinct scales and apply some form of homogenisation. One may take advantage of the symmetries and repeated patterns in the geometry and/or external conditions in order to restrict the analyse to unit cells. One may also search for and use hidden patterns in parametric high-fidelity solutions in order to derive meta-models based on subspace projections. Crucially, high level of complexity reduction can be obtained by simplifying model features whose detailed description do not contribute to the accuracy of *what is actually being observed* (*i.e.* the quantity of interest).

Categorisation of the model reduction approaches explored in this thesis. This thesis presents several innovative contributions that can be classified within the following two families of model reduction approaches.

- **Algebraic *a posteriori* model reduction.** Such techniques are typically developed to reduce the costs associated with repeated calls to parametrised PDE solvers. In this case, the high-fidelity model is tractable. The computational burden that we aim to alleviate is that of repeated calls to this model, which may arise in the context of optimisation, inverse problems and stochastic modelling approaches. The basic cost reduction idea is to sample the parameter domain, deploy machine learning tools to extract the hidden structures that these samples exhibit, and use these structures to fasten subsequent calls, through replacing the high-fidelity model by a reduced order surrogate. The snapshot POD is probably the most well-known of these methods. In a nutshell, when may see Model Order Reduction (MOR) as a meta-modelling approach, whereby the interpolation in the parameter domain is performed via a numerically compressed physical model rather than via *a priori* defined polynomial or radial bases functions. In this thesis, I will present original developments in this area, with particular emphasis on the reduction of parametrised fracture mechanics problem.

- **Adaptive model reduction based on asymptotics or heuristic *a priori* simplifications.** These approaches reduce PDEs whose solutions are simply out-of-reach. As an example, the discrete system of equations arising when modelling a large composite structure at the scale of its micro constituents cannot be solved (see Figure 2.1). In such cases, model simplification needs to be done *a priori*, and we may consider enriching the simplified mode adaptively, by performing *local* model enrichment incrementally, in a greedy fashion (see Figure 2.2). In this thesis, I will look in particular at the construction of homogenisation models with adaptive local zooms, and the adaptive, error-controlled removal of small features from CAD (Computer Assisted Design) models.

The central role of error estimation. Fundamentally, the adaptive model reduction approaches that will be presented hereafter are built upon reliable indicator of errors. Error estimation is required (i) to identify the regions of space/time/parameter domains where the accuracy of a surrogate model is too low, thereby triggering local model refinement and (ii) to quantify the overall level of accuracy of the model, thereby providing a stopping criterion for the adaptive algorithm. Ideally, the error estimates should be sharp. More importantly though, they should aim to quantify errors in engineering quantities of interest. It should be noted that developing robust *a posteriori* error estimates is a difficult endeavour in general, and the field of *modelling* error estimation is relatively imature.

Driving adaptive modelling by error estimation principals implicitly requires the availability of a trusted, reference, model, at every stage of the analysis. In simple words, we may not know the right model (which is, of course, a nonsensical notion), but given a working model, we may construct a "truth" model that we believe would yield better results if it could be solved *i.e.* that would deliver results that are closer to the physical observations. This is the approach that will be systematically pursued in this thesis.

Advanced discretisation methods for PDEs and robust model coupling. Adaptive modelling approaches challenge the robustness of numerical methods. This can be seen in figure 2.2, where the interface between the fully resolved region, which is microscopically remeshed as it expands, needs to be explicitly coupled to the macroscopically meshed smooth region. As a consequence, research in adaptive modelling cannot be done without state-of-the-art robust and relatively generic approaches to handle moving interfaces and nonconforming model coupling. Over the years, I have built an expertise in immersed boundary methods for PDEs, and in particular in eXtended Finite Element (XFEM) technologies. Such frameworks facilitate the development of research in adaptive modelling by providing building block to reduce the dependency of modelling techniques to meshing and to control the overall stability of heterogeneously coupled problems.

Outlines of the thesis

This document is organised in three chapters. In chapter 1, I will introduce *offline-online*, projection-based model reduction approaches for parametrised nonlinear PDEs. I focus in particular on the basic building blocks that have to be assembled for a MOR methodology to be successful: an efficient sampling and compression algorithm for the parametrised solution of the reference problem and a hyper-reduction component. I will then present MOR algorithms developed specifically for the reduction of parametrised fracture mechanics problem, which are locally non-reducible. In this context, I will expose two novel local/global MOR strategies, whereby fracture zones is tracked adaptively and solved without reduction. Finally, I will explore the application of MOR to multiscale fracture modelling. In particular, I propose a novel approach to sample and reduce the material point problem in FE^2.

Chapter 2 focusses on adaptive, *a priori* model reduction, and in particular on the development of robust error estimates to guide the refinement process and guarantee the quality of numerical predictions. The developments are restricted to linear elliptic PDEs, where error bounding techniques by duality is relatively well-established. After introducing these fundamental concepts, I will show how one may apply them to develop novel strategies of adaptive homogenisation and model defeaturing, with accuracy certification. In these contributions, the reference solution is out-of-reach. Local/global model adaptivity must be performed in a "blind" way, which is made possible by using of the Constitutive Relation Error. Finally, I present a novel, certified and highly efficient Reduced Basis sampling method for parametrised PDEs, whereby reduced order models for the primal problem and for the dual problem are constructed jointly.

The last chapter presents some of my recent work regarding the CutFEM implicit boundary finite element technology. After showing the potential of this approach to help develop robust adaptive modelling strategies, I will introduce two original contributions to the field: the stabilisation of a primal/dual CutFEM formulation of unilateral contact for composite

materials, and further development of this idea to treat moving interface problems arising when modelling manufacturing by thermal ablation.

CHAPTER 3

Model Order Reduction in nonlinear solid mechanics

Introduction

The direct application of state-of-the-art numerical solvers for partial differential equations (PDE) is unaffordable in the context of virtual design and feedback-loop control. High-fidelity, potentially 3D and time-dependent PDE-based numerical simulators cannot possibly be called within optimisation loop. The area of Model Order Reduction (MOR) consists of a series of tools and methodologies that aim to address this fundamental shortcoming in today's available digital technology. This is done through a relatively unified development framework: that of separation of variables combined with error-minimising solution algorithms.

MOR provides methodological guidance and numerical toolboxes in order to take advantage of the similarities that appear in most (parametrised) PDE solutions, such as (i) similarities between solution fields corresponding to different instants of a time-dependent PDE, (ii) similarities between solution fields corresponding to different values of a parameter of interest (see Figure 3.1), (iii) repeated patterns that may appear in the space/time domain due to the existence of cycles and symmetries. Through capturing these similarities and eliminating the redundancies associated with computing similar features multiple times, one may be able to reduce the computational cost associated with the solution of the PDE by a large factor.

In this chapter, I will first propose an overview of the key elements of MOR applied to nonlinear solid mechanics problems. Then, I will introduce three original contributions in the area of MOR for nonlinear fracture mechanics: two journal articles on adaptive local/global MOR strategies for parametrised fracture problem, and a third article on the reduction of the material point problem in FE^2.

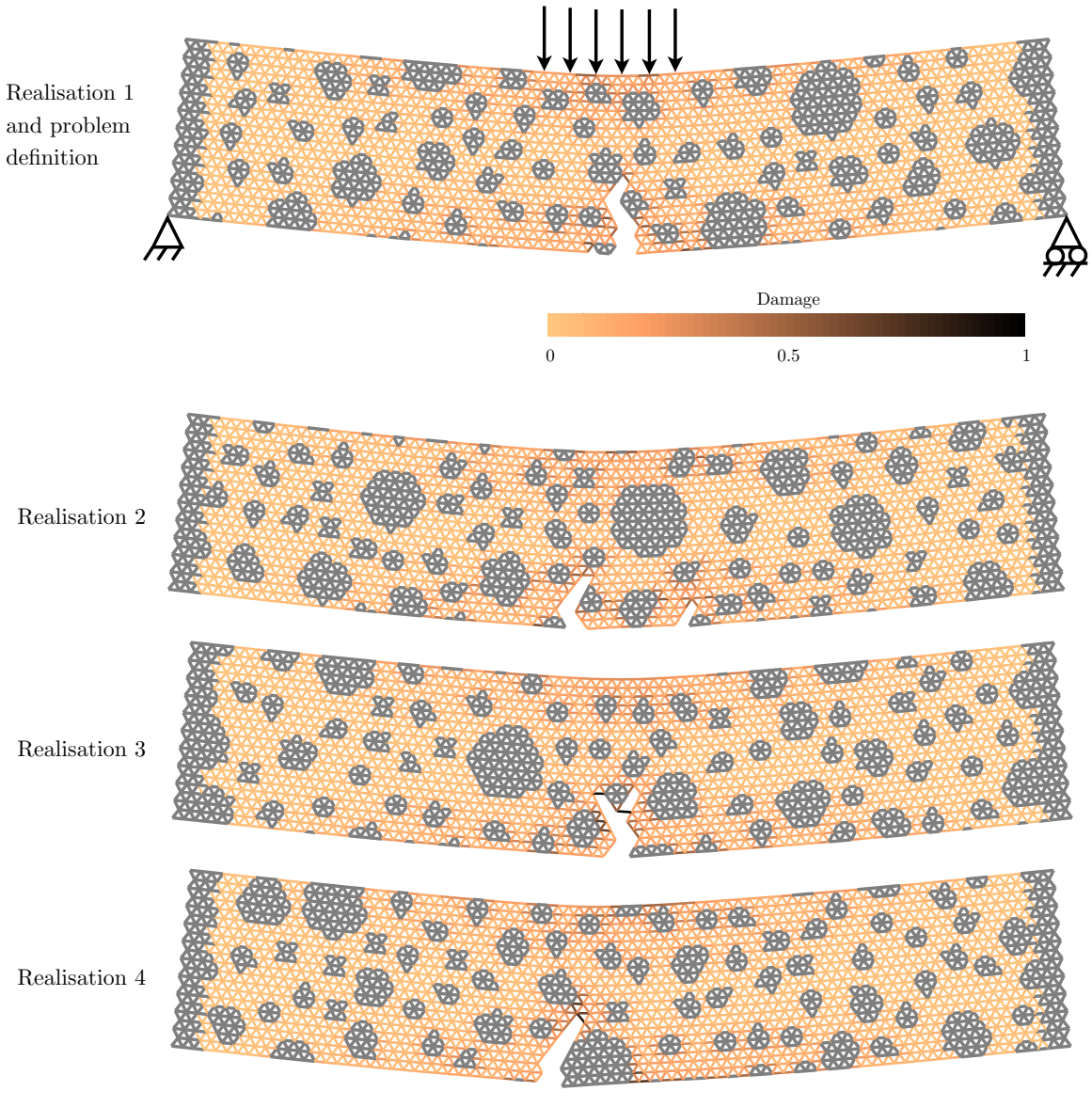


Figure 3.1: Crack patterns in a three-point bending problem with randomised microstructures, from [15]. Clearly, away from the crack, the four solutions are similar. MOR can automatically detect and exploit such features.

3.1 Reduced basis methods in nonlinear mechanics

3.1.1 Reduced modelling surrogate

The finite element discretisation of a generic elastic damageable structural model results in the semi-discrete system of equations

$$\forall\, \mathbf{v}, \quad \mathbf{v}^T \mathbf{M}\left(\boldsymbol{\mu}\right) \ddot{\mathbf{u}}(t;\boldsymbol{\mu}) + \mathbf{v}^T \mathbf{t}\left(\left\{\mathbf{u}(\tau;\boldsymbol{\mu})\right\}_{\tau\leq t}; \boldsymbol{\mu}\right) = \mathbf{v}^T \mathbf{f}\left(t;\boldsymbol{\mu}\right) \tag{3.1}$$

where we have used symbol $\boldsymbol{\mu}$ to denote a vector of scalar parameters, and the other symbols are assumed to be self-explanatory. Arbitrary test vector $\mathbf{v}$ should satisfy the homogeneous kinematic conditions at time $t \in [0\ T] =: \mathcal{T}$. The system is closed by initial conditions for degrees of freedom $\mathbf{u}$ and their time-derivative. The vector of internal forces $\mathbf{t}$ is a nonlinear vector-valued function of the time history of the displacement $\mathbf{u}$ (which includes potential dependency to the $\dot{\mathbf{u}}$). This dependency is a consequence of the non-conservative nature of the damage processes.

Basic ROM surrogate

The reduced-modelling surrogate takes the following separation-of-variables form

$$\boxed{\bar{\mathbf{u}}(t;\boldsymbol{\mu}) = \sum_{i=1}^{n_\phi} \boldsymbol{\phi}_i \alpha_i(t;\boldsymbol{\mu}) + \mathbf{u}_d(t;\boldsymbol{\mu}) =: \boldsymbol{\Phi}\boldsymbol{\alpha}(t;\boldsymbol{\mu}) + \mathbf{u}_d(t;\boldsymbol{\mu}) \approx \mathbf{u}(t;\boldsymbol{\mu})} \tag{3.2}$$

where n_ϕ is very small compared to the size of $\mathbf{u}$, and $\mathbf{u}_d$ satisfies the kinematic constraints and the elements of $\boldsymbol{\Phi}$ satisfy the homogeneous kinematic constraints. To simplify the presentation, we will assume in the following that $\mathbf{u}_d = 0$.

3.1.2 Reduced Order Model

We now need to define how the components of (3.2) are to be estimated, starting from the generalised variables. The computation of the reduced basis will be discussed later on. For now, we assume that $\boldsymbol{\Phi}$ is given.

A Galerkin ROM is obtained by choosing $\mathbf{v}$ in the span of $(\boldsymbol{\phi}_i)_{i\in[\![1,n_\phi]\!]}$: $\forall\, i \in [\![1, n_\phi]\!]$,

$$\boxed{\boldsymbol{\phi}_i^T \mathbf{M}\left(\boldsymbol{\mu}\right) \boldsymbol{\Phi}\ddot{\boldsymbol{\alpha}}(t;\boldsymbol{\mu}) + \boldsymbol{\phi}_i^T \mathbf{t}\left(\left\{\boldsymbol{\Phi}\boldsymbol{\alpha}(\tau;\boldsymbol{\mu})\right\}_{\tau\leq t}; \boldsymbol{\mu}\right) = \boldsymbol{\phi}_i^T \mathbf{f}\left(t;\boldsymbol{\mu}\right)} \tag{3.3}$$

At any time t, this is a system of n_ϕ equations with n_ϕ reduced (or generalised) variables.

The Galerkin Reduced Order problem may be solved by employing a standard time integrator, which yields a sequence of nonlinear problems for the generalised variables. For every $t_n \in \{t_1 = \Delta t, t_2 = 2\,\Delta t, \ldots, t_{n_t} = n_t\,\Delta t =: T\} =: \bar{\mathcal{T}}$.

$$\boldsymbol{\Phi}^T \mathbf{r}_{n+1}\left(\boldsymbol{\Phi}\boldsymbol{\alpha}(t_{n+1};\boldsymbol{\mu});\boldsymbol{\mu}\right) = \boldsymbol{\Phi}^T\left(\mathbf{b}_{n+1}(\boldsymbol{\mu}) - \mathbf{a}_{n+1}\left(\boldsymbol{\Phi}\boldsymbol{\alpha}(t_{n+1};\boldsymbol{\mu});\boldsymbol{\mu}\right)\right) = 0 \tag{3.4}$$

If the Newmark time integration method is used for instance, we have

$$\begin{aligned}\mathbf{b}_{n+1}(\boldsymbol{\mu}) &= \mathbf{f}(t_{n+1};\boldsymbol{\mu}) + \mathbf{M}(\boldsymbol{\mu})\boldsymbol{\Phi}\left(\xi_1\boldsymbol{\alpha}(t_n;\boldsymbol{\mu}) + \xi_2\dot{\boldsymbol{\alpha}}(t_n;\boldsymbol{\mu}) + \xi_3\ddot{\boldsymbol{\alpha}}(t_n;\boldsymbol{\mu})\right)\\ \mathbf{a}_{n+1}\left(\boldsymbol{\Phi}\boldsymbol{\alpha}(t_{n+1};\boldsymbol{\mu});\boldsymbol{\mu}\right) &= \xi_1\mathbf{M}(\boldsymbol{\mu})\boldsymbol{\Phi}\boldsymbol{\alpha}(t_{n+1};\boldsymbol{\mu})\\ &\quad +\hat{\mathbf{t}}\left(\boldsymbol{\Phi}\boldsymbol{\alpha}(t_{n+1};\boldsymbol{\mu}), \boldsymbol{\Phi}\dot{\boldsymbol{\alpha}}(t_{n+1};\boldsymbol{\mu}), \{\boldsymbol{\Phi}\boldsymbol{\alpha}(\tau;\boldsymbol{\mu})\}_{\tau\leq t_n}\right)\end{aligned} \tag{3.5}$$

and the Newmark integration formulas may be expressed as

$$\begin{aligned}\ddot{\boldsymbol{\alpha}}(t_{n+1};\boldsymbol{\mu}) &= \xi_1\left(\boldsymbol{\alpha}(t_{n+1};\boldsymbol{\mu}) - \boldsymbol{\alpha}(t_n;\boldsymbol{\mu})\right) - \xi_2\dot{\boldsymbol{\alpha}}(t_n;\boldsymbol{\mu}) - \xi_3\ddot{\boldsymbol{\alpha}}(t_n;\boldsymbol{\mu})\\ \dot{\boldsymbol{\alpha}}(t_{n+1};\boldsymbol{\mu}) &= \xi_4\left(\boldsymbol{\alpha}(t_{n+1};\boldsymbol{\mu}) - \boldsymbol{\alpha}(t_n;\boldsymbol{\mu})\right) + \xi_5\dot{\boldsymbol{\alpha}}(t_n;\boldsymbol{\mu}) + \xi_6\ddot{\boldsymbol{\alpha}}(t_n;\boldsymbol{\mu})\end{aligned} \tag{3.6}$$

The expression of the coefficients $\{\xi_i\}_{i\in[\![1,6]\!]}$, which depend on the Newmark parameters and time step Δt, can be found in [**?**]. We have also replaced $\mathbf{t}$ by $\hat{\mathbf{t}}$ to make the potential dependency of the vector of internal forces upon the instantaneous velocity explicit. The initial acceleration is calculated by solving (3.3) at time $t = 0$, given the initial conditions ($\mathbf{u}(0)$ and $\dot{\mathbf{u}}(0)$ are supposed to be zero for simplicity of presentation).

Procedure (3.3) is sequentially optimal when the vector of internal forces is linear with the displacement and velocity vectors. Indeed, in this case, the Galerkin procedure becomes

$$\boldsymbol{\Phi}^T\mathbf{r}_{n+1}\left(\boldsymbol{\Phi}\boldsymbol{\alpha}(t_{n+1};\boldsymbol{\mu});\boldsymbol{\mu}\right) = \boldsymbol{\Phi}^T\left(\mathbf{b}^l_{n+1}(\boldsymbol{\mu}) - \mathbf{A}(\boldsymbol{\mu})\boldsymbol{\Phi}\boldsymbol{\alpha}(t_{n+1};\boldsymbol{\mu})\right) = 0 \tag{3.7}$$

where

$$\begin{aligned}\mathbf{b}^l_{n+1}(\boldsymbol{\mu}) &= \mathbf{b}_{n+1}(\boldsymbol{\mu}) + \mathbf{C}(\boldsymbol{\mu})\boldsymbol{\Phi}\left(\xi_4\boldsymbol{\alpha}(t_n;\boldsymbol{\mu}) - \xi_5\dot{\boldsymbol{\alpha}}(t_n;\boldsymbol{\mu}) - \xi_6\ddot{\boldsymbol{\alpha}}(t_n;\boldsymbol{\mu})\right)\\ \mathbf{A}(\boldsymbol{\mu}) &= \left(\xi_1\mathbf{M}(\boldsymbol{\mu}) + \xi_4\mathbf{C}(\boldsymbol{\mu}) + \mathbf{K}(\boldsymbol{\mu})\right)\end{aligned} \tag{3.8}$$

which, if $\mathbf{A}$ is symmetric positive definite, is equivalent to minimising functional

$$J(\boldsymbol{\alpha}^\star) = \left\|\mathbf{A}(\boldsymbol{\mu})^{-1}\mathbf{b}^l_{n+1}(\boldsymbol{\mu}) - \boldsymbol{\Phi}\boldsymbol{\alpha}^\star\right\|^2_{\mathbf{A}(\boldsymbol{\mu})} \tag{3.9}$$

In the previous expression, the first term in the A-norm symbol is the full-order solution at time $n+1$, given the *reduced* trajectory up to time t_n, and the second term is its approximation in the reduced space. In this entire document, and unless otherwise specified, we use notation $\|\,.\,\|_{\mathbf{X}} = \sqrt{.\,^T\mathbf{X}\,.}$.

In the nonlinear and/or nonsymmetric case, the sequential optimality delivered by the Galerkin procedure is lost. Some researchers recommend employing an incremental residual-minimising approach (see [29]), which consists in minimising

$$J(\boldsymbol{\alpha}^\star) = \left\|\mathbf{r}_{n+1}\left(\boldsymbol{\Phi}\boldsymbol{\alpha}^\star;\boldsymbol{\mu}\right)\right\|^2_{\mathbf{X}(\boldsymbol{\mu})^{-1}} \tag{3.10}$$

where pre-conditioner $\mathbf{X}(\boldsymbol{\mu})^{-1}$ is SPD, which yields the reduced Euler-Lagrange system of equations

$$\boldsymbol{\Phi}^T\mathbf{A}^T_{T,n+1}(\boldsymbol{\mu})\mathbf{X}(\boldsymbol{\mu})^{-1}\mathbf{r}_{n+1}\left(\boldsymbol{\Phi}\boldsymbol{\alpha}(t_{n+1};\boldsymbol{\mu});\boldsymbol{\mu}\right) = 0 \tag{3.11}$$

$$\mathbf{A}_{T,n+1}(\boldsymbol{\mu}) = -\left.\frac{\partial\mathbf{r}_{n+1}\left(\mathbf{u};\boldsymbol{\mu}\right)}{\partial\mathbf{u}}\right|_{\mathbf{u}=\boldsymbol{\Phi}\boldsymbol{\alpha}(t_{n+1};\boldsymbol{\mu})} \tag{3.12}$$

which may be solved by using the Gauss-Newton algorithm. The optimality is only sequential. Enforcing space-time optimality breaks the unidirectional flow of information in time which is, arguably, not desirable.

The Galerkin optimisation or quasi-optimisation is performed for any parameter $\boldsymbol{\mu}$, locally in the parameter domain. This is in contrast with response surface methods, whereby one restricts the functional shape (*e.g* polynomials, splines) *a priori* or at least assume some smoothness (*e.g* Gaussian process) of the meta-model in the parameter domain. The Galerkin projection may be interpreted as an *implicit* and quasi-optimal data smoothing in the parameter domain. Noticeably, if the vector of internal forces is linear, the Galerkin-ROM procedure is not only residual minimising, but also *error* minimising (in the sense of the norm or semi-norm associated with the linear elliptic differential operator).

3.1.3 Offline-online procedures

In practice, the reduced modelling approach is an offline-online procedure. The "offline" phase consists in performing expensive computations, typically full-order simulations at well-chosen points of the parameter domain, known as *snapshot* computations. Additionally, the expensive part of the assembly of the various operators appearing in (3.3) must be done in advance, during this "offline" stage. In a second stage, the reduced model can be used as an inexpensive surrogate for the full order model to perform a variety of engineering tasks requiring to call the finite element model repeatedly, as a "black-box" input-output relationship.

Online efficiency. As a general rule, we must ensure that the complexity of all the operations performed online is independent of the size of the finite element space (and that the numerical complexity remains linear with the number of time steps). The efficiency can be measured in terms of speedup: the ratio between the CPU time required to solve the full problem and the CPU time required to solve the ROM. Similar measures can also be defined for the reduction in terms of memory usage, and are particularly relevant when considering reduced integration domains.

The "many-query" setting. It should be clear that Model Order Reduction as exposed in this section is only of interest in the "many-query" setting, whereby the gain done "online" outweigh the initial "offline" cost.

3.1.4 Hyper-reduction

In the context of nonlinear models, solving the Galerkin ROM by the Newton algorithm remains expensive owing to the cost of evaluating inner products $\boldsymbol{\phi}_i^T \mathbf{t}$.

To illustrate this computational bottleneck, consider alternatively the first term of (3.3), and its right-hand side. In a relatively unrestrictive manner, we can assume that both terms admit an affine decomposition of the form

$$\boldsymbol{\phi}_i^T \mathbf{M}(\boldsymbol{\mu}) \boldsymbol{\Phi} = \sum_{j=1}^{n_m} \left(\boldsymbol{\phi}_i^T \mathbf{M}_j \boldsymbol{\Phi} \right) \gamma_{m,j}(\boldsymbol{\mu}) \tag{3.13}$$

$$\boldsymbol{\phi}_i^T \mathbf{f}\left(t; \boldsymbol{\mu}\right) = \sum_{j=1}^{n_f} \left(\boldsymbol{\phi}_i^T \mathbf{f}_j \right) \gamma_j(t; \boldsymbol{\mu}) \tag{3.14}$$

where the γ symbols denote scalar-valued functions. The matrix/vector and inner products appearing in the sum can be preassembled online, and weighted by the γ coefficients online.

In this case, online computations do no depend on the size of the finite element space, and are therefore efficient in the "offline-online" sense.

However, the nonlinear term does not, in general, admit such a decomposition. This decomposition needs to be hypothesised and built numerically [30]. One of the most successful approaches is the DEIM [31, 32], which supposes that the following expansion is valid

$$\mathbf{t}\left(\{\boldsymbol{\Phi}\boldsymbol{\alpha}(t;\boldsymbol{\mu})\}_{\tau\leq t}\,;\boldsymbol{\mu}\right)\approx\sum_{i=1}^{n_\xi}\boldsymbol{\xi}_i\beta_i=:\boldsymbol{\Xi}\boldsymbol{\beta}\tag{3.15}$$

where $\boldsymbol{\alpha}$ is to be understood as the solution to the unaffordable Galerkin ROM described by equation (3.3). The $\boldsymbol{\beta}$ coefficient may be found optimally by performing a "gappy" reconstruction with respect to *some* of the components of $\mathbf{t}$. This reads

$$\boldsymbol{\beta}=\arg\min_{\boldsymbol{\beta}^\star}\|\mathbf{t}-\boldsymbol{\Xi}\boldsymbol{\beta}^\star\|_{\mathbf{G}}^2\tag{3.16}$$

where $\mathbf{G}$ is a diagonal, Boolean matrix that possesses very few ones. The minimisation yields the gappy approximation

$$\boxed{\bar{\mathbf{t}}\left(\{\boldsymbol{\Phi}\boldsymbol{\alpha}(t;\boldsymbol{\mu})\}_{\tau\leq t}\,;\boldsymbol{\mu}\right):=\boldsymbol{\Xi}\left(\boldsymbol{\Xi}^T\mathbf{G}\boldsymbol{\Xi}\right)^{-1}\boldsymbol{\Xi}^T\mathbf{G}\mathbf{t}\left(\{\boldsymbol{\Phi}\boldsymbol{\alpha}(t;\boldsymbol{\mu})\}_{\tau\leq t}\,;\boldsymbol{\mu}\right)}\tag{3.17}$$

$\bar{\mathbf{t}}$ is now affine in $\boldsymbol{\Xi}^T\mathbf{G}\mathbf{t}$, which can be computed using standard numerical integration over a reduced integration domain: the set of all finite elements that are connected to one of the nodes whose corresponding degree-of-freedom index is non zero in $\mathbf{G}$. In practice, reduced basis matrix $\boldsymbol{\Xi}$ is obtained by performing a snapshot-POD of the vector of internal forces. Operator $\mathbf{G}$ can be constructed by an aliasing-minimising procedure, as proposed in [32] and recalled in Paper 1.1.

3.1.5 Computation of the reduced basis

The Snaphsot POD

The classical way to obtain reduced basis $(\phi_i)_{i\in[\![1,n_\phi]\!]}$ is the snapshot Proper Orthogonal Decomposition (POD) (see *e.g.* [33]. Typically, the parameter space is sampled at n_s points, and the corresponding full order computation is performed at these points. The reduced basis is then defined as the columns of operator $\boldsymbol{\Phi}$, which is the solution of

$$\boldsymbol{\Phi}=\arg\min_{\boldsymbol{\Phi}^\star}\left(\min_{\boldsymbol{\alpha}^\star}\sum_{\boldsymbol{\mu}\in\boldsymbol{\mathcal{M}}_s}\sum_{t\in\bar{\mathcal{T}}}\|\boldsymbol{\Phi}^\star\boldsymbol{\alpha}^\star(t;\boldsymbol{\mu})-\mathbf{u}(t;\boldsymbol{\mu})\|_2^2\right)\tag{3.18}$$

where the n_ϕ columns of $\boldsymbol{\Phi}$ form an orthonormal basis, and $\boldsymbol{\alpha}^\star$ is to be understood as a vector-valued function that is defined over the set of sample points only. $\bar{\mathcal{T}}$ denotes the set of nodes of the computational time grid. This problem can be solved by performing a Singular Value Decomposition (SVD) of the so-called snapshot matrix. This is a well-known result, which is recalled in Paper 1.1. The evaluation of the convergence of the snapshot-POD procedure must be done with great care. Indeed, it overfits the data, and particularly so when the snapshot is poor. This means that the error measure minimised in (3.18) to construct the reduced basis

is generally smaller that the generalisation error, which is averaged over all the points of the parameter domain (the metric defined in (3.18) needs to be normalised by the cardinal of the snapshot for this statement to be correct).

Performing the SVD may become prohibitively expensive when the number of time steps and sample points increase, in which case one may use methods that build $\mathbf{\Phi}$ incrementally.

The major shortcoming of the snapshot POD is the absence of guidance to sample the parameter space. Some form of adaptivity must be performed in order to control the efficiency of the sampling strategy. At the very least, an early-stopping approach should be associated with uniform sampling methods such as the full factorial sampling (in low dimensions) or the quasi-Monte Carlo sampling strategy. In this case, a randomised Cross-Validation (CV) technique may be employed to evaluate whether the prediction error[1] decreases when further increasing the cardinal of the sample set. This strategy is adopted in Paper 1.1. and in [15].

However, the uniform sampling strategy may be far from efficient. Several approaches have been proposed in the literature to locally adapt the sampling density to the problem at hand [34]. This can be done, for instance, by making use of tree structures, which are refined Greedily towards regions where prediction errors remain large. Alternative, optimisation-based approaches may be found in [35].

The Reduced Basis Method

Principle. The desire to sample parameter spaces efficiently in order to build Reduced Order Models is at the heart of the fundamental ideas underlying the Reduced Basis Method. Whilst the POD searches for an optimum basis in norm 2 over the parameter domain, the Reduced Basis Method [36, 37, 38] is designed as an infinity norm approach. Typically, we search for

$$\mathbf{\Phi} = \arg\min_{\mathbf{\Phi}^\star} \left(\max_{\boldsymbol{\mu}^\star} \min_{\boldsymbol{\alpha}^\star} \sum_{t \in \bar{\mathcal{T}}} \| \mathbf{\Phi}^\star \boldsymbol{\alpha}^\star(t;\boldsymbol{\mu}^\star) - \mathbf{u}(t;\boldsymbol{\mu}^\star) \|_{\mathbf{X}}^2 \right) \tag{3.20}$$

where the n_ϕ columns of $\mathbf{\Phi}$ form an orthonormal basis. As there is no direct algebraic solution to the above minimisation problem, it is approximately solved in a Greedy manner. Given a reduced basis of cardinal $k \geq 1$, the k^{th} Greedy step reads as:

- Find point $\boldsymbol{\mu}_k$ such that

$$\boldsymbol{\mu}_k = \arg\max_{\boldsymbol{\mu}^\star} \left(\min_{\boldsymbol{\alpha}^\star} \sum_{t \in \bar{\mathcal{T}}} \| \mathbf{\Phi}^k \boldsymbol{\alpha}^\star(t;\boldsymbol{\mu}^\star) - \mathbf{u}(t;\boldsymbol{\mu}^\star) \|_{\mathbf{X}}^2 \right) \tag{3.21}$$

  i.e. find the point where the current ROM error is maximum.

- Compute the full order model at point $\boldsymbol{\mu}_k$.

[1] Here, prediction is to be understood in the statistical sense, as the value of the functional defined in (3.18) when evaluated at a set of sample points that have not necessarily been used to perform the SVD:

$$\epsilon = \frac{1}{\mathrm{Card}(\tilde{\mathcal{M}}_s)} \min_{\boldsymbol{\alpha}^\star} \sum_{\boldsymbol{\mu} \in \tilde{\boldsymbol{\mathcal{M}}}_s} \sum_{t \in \bar{\mathcal{T}}} \| \mathbf{\Phi} \boldsymbol{\alpha}^\star(t;\boldsymbol{\mu}) - \mathbf{u}(t;\boldsymbol{\mu}) \|_2^2 \tag{3.19}$$

This to avoid quality measures to be affected by overfitting.

- Compute the snapshot-POD vector of the error in the time-dependent solution computed at $\boldsymbol{\mu}_k$:
$$\mathbf{e}(t;\boldsymbol{\mu}_k) = \mathbf{u}(t;\boldsymbol{\mu}_k) - \boldsymbol{\Phi}^k \boldsymbol{\alpha}^k(t;\boldsymbol{\mu}_k) \tag{3.22}$$
where $\boldsymbol{\alpha}^k$ is computed using the Galerkin procedure (3.3), possibly with Hyper-Reduction.
- Add this vector to the current reduced basis, after orthonormalisation.
- $k \leftarrow k+1$ and go back to the first step of the Greedy procedure.

Identification of $\boldsymbol{\mu}_k$. One of the most important steps of the Reduced Basis Method is the identification of the point where the error of prediction is maximum. This is a difficult, problem-dependent task that must be approached with great care. This can be done in one of two ways:

- sample the parameter space "exhaustively" and replace the exact error measure in (3.21) by a cheap but reliable error estimate, ideally an upper bound for the exact error measure;
- make use of a gradient-based optimisation algorithm to solve (3.21) approximately.

The first approach is scientifically satisfying. However, it is mathematically involved, and usually limited to well-behaved PDEs. Such an approach is developed in Paper 2.1. Recently, there has been a growth in the application of machine learning techniques that construct error-estimates semi-automatically [39, 40, 17, 41]. In paper 1.2, this idea is utilised as part of the developments. Notice that the error estimation element only *reduces* the cost of evaluating the error locally. It does not fully eliminate the difficulties associated with *a priori* uniformly sampled parameter spaces, as discussed in the section dedicated to the snapshot-POD.

The second approach listed previously is attractive but the computation of the first and possibly second gradients may become prohibitively expensive in large parameter dimensions. An interesting way forward is to make use of the adjoint method [42, 43, 44] to calculate the gradient of error measures at reduced numerical cost[45]. The success of such strategies relies on tailoring initialisation strategies. In paper 1.2, a gradient-free Bayesian optimisation technique is proposed to locate regions that exhibit large ROM errors. The curse of dimensionality kicks-in for dimensions larger than 3, owing to the generally poor performances of gaussian processes in such settings.

3.2 A note on Meta-Modelling approaches

A polynomial meta-model approximates the displacement field as

$$\mathbf{u}(t;\boldsymbol{\mu}) = \sum_{i=1}^{n_\phi} \boldsymbol{\phi}_i(t)\alpha_i(\boldsymbol{\mu}) \tag{3.23}$$

where $((\alpha)_i)_{i\in[\![1,n_\phi]\!]}$ are *known* functions of the parameter, with global support. Then, an optimal meta-model with respect to norm $\sqrt{\int_{\boldsymbol{\mu}\in\mathcal{P}} \|\,.\,\|^2\, d\boldsymbol{\mu}}$ (here, $\boldsymbol{\mu}$ is assumed to be integrated

over a parameter space $\mathcal{P}$ of finite size) is as follows:

$$\forall\, j \in [\![1, n_\phi]\!], \qquad \sum_{i=1}^{n_\phi} \left(\int_{\boldsymbol{\mu}\in\mathcal{P}} \alpha_i(\boldsymbol{\mu})\alpha_j(\boldsymbol{\mu})\, d\boldsymbol{\mu} \right) \boldsymbol{\phi}_i(t) = \int_{\boldsymbol{\mu}\in\mathcal{P}} \alpha_j(\boldsymbol{\mu})\mathbf{u}(t;\boldsymbol{\mu})\, d\boldsymbol{\mu} \tag{3.24}$$

which is a set of n_ϕ coupled, linear equations for coefficients $(\boldsymbol{\phi}_i(t))_{i\in[\![1,n_\phi]\!]}$ [2]. Standard quadrature rules may be applied to evaluate (3.24) numerically. Of course, this formula is simply that of polynomial regression applied independently to every spatial degree of freedom. Notice that the amplitude of the vector of coefficients is an outcome of the procedure (the functions of the parameters are of fixed amplitudes here).

This approach is limited by several factors: (i) the coefficient vectors vary with time, which may be a problem if we want to store the entire time history, (ii) the functions of the parameters are predefined, and the polynomial expansion may have to be of high order to capture local features in the parameter space, and (iii) the reference solution needs to be computed at every quadrature point, which may be prohibitively expensive for large n_ϕ. However, this approach is non-intrusive, which makes it appealing.

In order to address point (iii), we may replace the previous procedure by a Galerkin approach. For a time-independent, linear problem of the form,

$$\mathbf{A}(\boldsymbol{\mu})\mathbf{u}(\boldsymbol{\mu}) = \mathbf{f}(\boldsymbol{\mu}) \tag{3.26}$$

such procedure consists in solving the set of coupled equations

$$\forall\, j \in [\![1, n_\phi]\!], \qquad \sum_{i=1}^{n_\phi} \left(\int_{\boldsymbol{\mu}\in\mathcal{P}} \alpha_j(\boldsymbol{\mu})\mathbf{A}\left(\boldsymbol{\mu}\right)\boldsymbol{\alpha}_i(\boldsymbol{\mu})\, d\boldsymbol{\mu} \right) \boldsymbol{\phi}_i = \int_{\boldsymbol{\mu}\in\mathcal{P}} \alpha_j(\boldsymbol{\mu})\mathbf{f}\left(\boldsymbol{\mu}\right)\, d\boldsymbol{\mu} \tag{3.27}$$

This type of Galerkin approximations is typically used in stochastic FEM, with Hermite polynomials and integrals weighted by the probability measure. Similarly to MOR, and as opposed to classical meta-modelling, Galerkin meta-modelling is intrusive.

Points (ii) and points (iii) may be alleviated by making use of more advanced meta-modelling topics such as Higher-Order SVDs and the Galerkin Proper Generalised Decomposition [46, 47, 48].

3.3 "On-the-fly" Reduced Order Modelling

The reduced basis technology is not limited to purely "offline-online" procedures or to the many-query setting. For some heavy engineering applications, the snapshot may be out-of-reach in terms of computational resources. In this cases, we would like to build ROMs "on-the-fly" (or *a priori* [49, 50, 18, 51]), utilising information generated during the previous past time steps and/or previously computed full order solutions to fasten subsequent simulations.

[2] In particular, if the polynomials are orthogonal (*e.g.* Legendre polynomials),

$$\forall\, j \in [\![1, n_\phi]\!], \qquad \boldsymbol{\phi}_j(t) = \frac{1}{\left(\int_{\boldsymbol{\mu}\in\mathcal{P}} \alpha_j^2(\boldsymbol{\mu})\, d\boldsymbol{\mu}\right)} \int_{\boldsymbol{\mu}\in\mathcal{P}} \alpha_j(\boldsymbol{\mu})\mathbf{u}(t;\boldsymbol{\mu})\, d\boldsymbol{\mu} \tag{3.25}$$

which is used to define the classical Polynomial Chaos Expansion, with $\alpha_i(\boldsymbol{\mu})$ the Hermite polynomials and where the integral need to be weighted by a Gaussian Kernel.

Such approaches have been developed in various context, for instance in [49], [51], [52] [53]. In [18] it is shown that ROMs can be used as preconditioners for iterative solvers applied to full order systems. Conversely, incomplete MOR-preconditioned solutions may be utilised as efficient "on-the-fly" corrections to the Reduced Order Model.

The control of the accuracy of Reduced Order Models built "On-the-fly" is challenging. Whilst duality-based error bounds may still apply in the context of linear elliptic and linear parabolic PDEs [36, 54, 55, 56, 27], significant challenges arise in the general case. This is because there is no "offline" exploration phase of the parameter domain, and therefore no opportunity to construct reliability indicators through interpolation in the parameter domain (see the above discussion about the Reduced Basis Method). There may be opportunities to build such reliability indicators using auxiliary, cheaper problems or coarsened numerical solvers, but, as far as we know, this avenue of research remains virtually unexplored.

3.4 Summary of papers

Paper 1.1: Partitioned Reduced Order Modelling [14]

Fracture localises. Localisation is an unstable phenomenon that is very sensitive to small variations in the parameters of the problem. As a result, classical Model Order Reduction methods such as the Galerkin-POD fail to capture crack propagations correctly. However, in the context of quasi-static analyses, the absence of correlation in parametrised solutions is a local phenomenon that can be shown to decrease fast with the distance to the damaged regions [15]. Therefore, we may be able to apply MOR away from cracks, whilst fully resolving fracture regions.

This is the topic of Paper 1.1, which presents an automatised manner to identify fracture regions, and apply MOR in the complementary part of space. This is done through the development of a partitioned MOR approach. The domain of interest is split into non-overlapping subdomains *a priori*. Snapshot simulations are performed using the primal Schur Complement method -BDD [57]- as linear solver. SVDs of the local snapshot correlation operators are computed locally for each subdomain, and local prediction errors are evaluated by cross-validation. Those domains for which the SVD fails to deliver adequately small prediction errors (see Figure 6 of the paper), will not be considered for reduction by projection. Last, the Galerkin POD is deployed subdomain-by-subdomain, using the DEIM to ensure that the approach is numerically efficient. One of the main shortcomings of the paper, namely that interface degrees of freedom where treated without reduction, thereby hampering the observed speed-up, was addressed shortly after publication of the paper. Closely related work is reported in [58, 59].

In paper [15], we propose an alternative approach whereby the reduced domain is not defined as an assembly or pre-defined block, but rather looked for in a quasi-optimal manner via a tailored weighted POD algorithm. Broadly speaking, we look for both the reduced basis and the region of space to which it should be applied so that this pair of arguments minimise the standard POD error measure, under constraint that the excluded fracture zone should be of given size. A greedy algorithm is proposed to solve this problem, and a sophisticated cross-validation process is deployed to ensure that the "fracture zone", which is treated without reduction is optimally sized (see Figure 3.2).

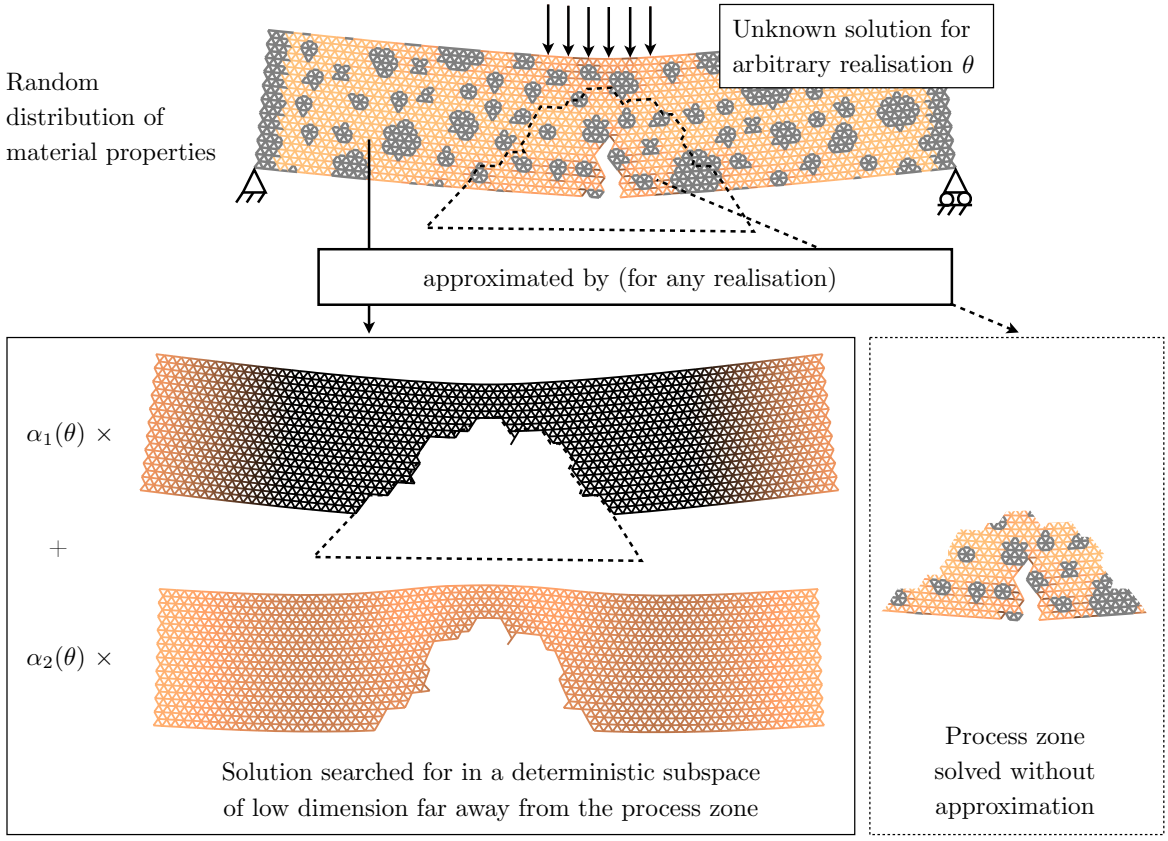


Figure 3.2: Restricted projection-based Reduced Order Model (from [15]). Subspace projection is only performed away from cracks. The damaged regions are found algebraically, using a measure of correlation between snapshot vectors, together with a dedicated greedy methodology, to progressively "eat-way" zones that should not be reduced.

Related research findings from other authors include those reported in [60] [61] [62] [63] [6] [46], where authors make use of domain decomposition to automatically channel the computational effort where it has the most impact, through either local linearisations, nonlinear subiterations, upscaling, or subspace projections. Another approach to MOR for damage models is detailed in [64], where the authors map the physical space to a feature space where some level of reducibility is recovered, even in the fractured region.

Partitioned reduced base approaches have been developed in a different context in [65]. In these references, the aim is not to address the problem of local irreducibility. Instead, the authors propose to use local reduced bases for the simulation of large structures that exhibit repeated patterns in space *e.g. assembly of pipes or beams*.

Paper 1.2: Local/Global "on-the-fly" Model Order Reduction [19]

With Paper 1.2, we continue exploring the potential for Reduced Bases approaches to help fasten the solution of high-fidelity fracture mechanics problems. The localisation phenomenon,

and its detrimental effect on the reducibility of the fracture problem, is here circumvented by treating the regions where internal damage variables are significantly larger than 0 without reduction. This is in contrast with the more elaborate approaches presented previously, whereby "fracture regions" were extracted algebraically.

However, the innovative aspects of the paper lie elsewhere. Here, the model order reduction is performed "on-the-fly", starting from an initial guess (*e.g.* snapshot-POD with very spare sampling, coarse time stepping and/or early termination of the time integrator). The solver used to solve the linearised Galerkin local/global ROM is a Krylov algorithm, which is ran orthogonally to the space spanned by the extension of the reduced basis into the fully resolved region (*i.e.:* projected conjugate gradient algorithm). This is done so that reduced basis information available in the fracture zone may also be used to reduce the overall computational expense, via the construction of a pre-conditioner. Following or previous work published in [18], we perform global corrections to the reduced basis if a measure of the residual of the discrete governing equations becomes too large at the current time step. In this case, the correction is performed by running a Krylov algorithm for the non-reduced problem, using the current reduced basis to construct a good pre-conditioner. The corrections are subsequently used to enrich the reduced basis and update the reduced integration domain associated with the hyper-reduction.

Unsurprisingly, we find that, when the damaged region is solved without reduction, the "on-the-fly" ROM requires very few corrections during the time integration process. Conversely, projecting the entire problem into the reduced space, without exclusion of the fracture zone, yields an adaptive strategy that performs corrections so often that the overall ROM strategy is more expensive than the direct solver.

Paper 1.3: Bayesian optimisation-based ROM for the material point problem [17]

Computational homogenisation is a modern and appealing manner to simulate the mechanics of structures when detailed information about the behaviour of their micro-constituents is available. The material point is described as a computational representative Volume Element (RVE), every phase being represented explicitly and modelled using an adequately fine discretise in space. In particular, the computational homogenisation premise circumvents the need to introduce mean-field assumptions, which are often difficult to justify and may lead to erroneous homogenisation results.

However, if attempted naively, this approach is computationally intractable. We illustrate the case of nested scale computations, whereby the computational RVE replaces an heuristically and explicitly defined constitutive law, in Figure 3.3. In this context, the RVE needs to be solved at every quadrature point of the macroscopic mesh, with the corresponding macroscopic strain applied as boundary condition, which leads to prohibitive CPU times. Moreover, fields of internal variables defined over the entire RVE must be stored at every quadrature point, leading to memory requirements that cannot possibly be met.

Fortunately, the microscopic problem is highly reducible. Solution fields corresponding to different load-cases, which may be seen as parameters of the RVE problem, can be accurately represented in a space of low dimension. This is, of course, not a new finding. For instance, a considerable amount of research effort has led to a dense family of approaches that seamlessly bridge the gap between mean-field analytical methods and "vanilla" FE^2

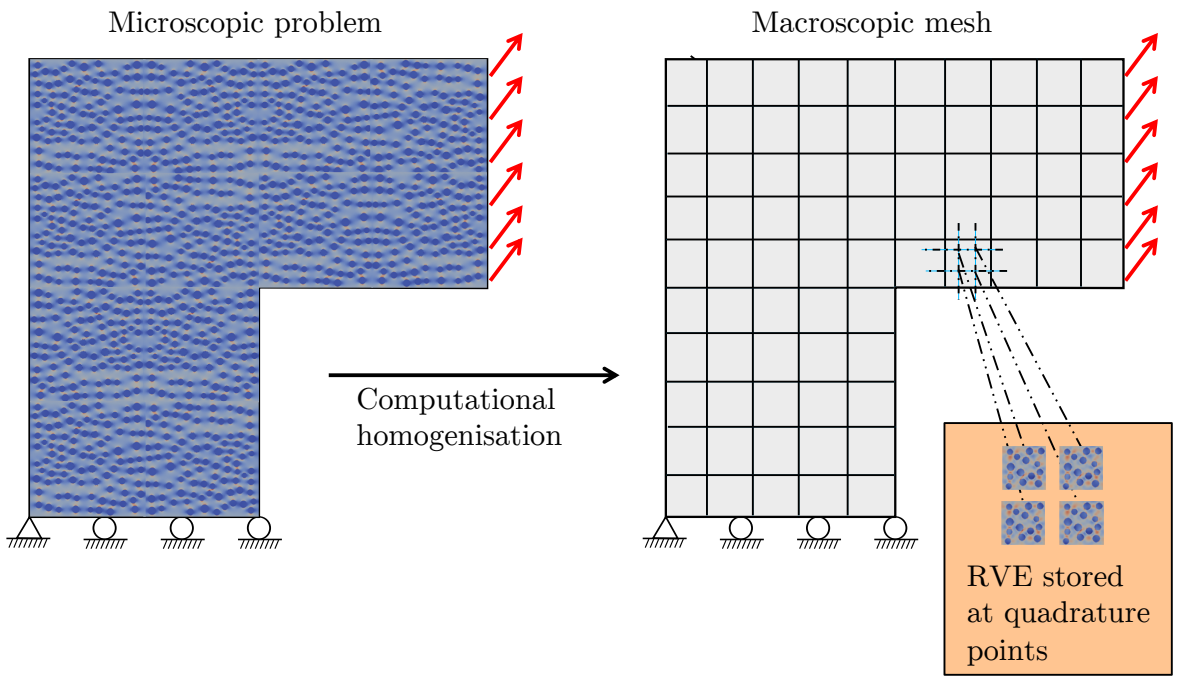
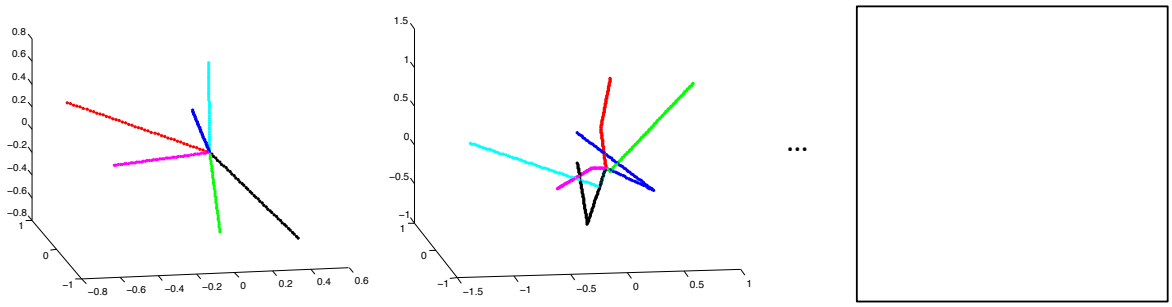


Figure 3.3: The FE^2 approach. High-fidelity numerical material point models are used in stead of macroscopic material laws. The time evolution of these material point problems needs to be calculated at every quadrature point of macroscopic meshes, leading to tremendous computational cost. Fortunately, material point problems can be algebraically reduced.

[66, 67, 68, 69, 70, 71, 72, 73, 74, 75, 76]. In this paper, we propose an approach based on the Reduced Basis Method paradigm, with the standard DEIM as additional hyper-reduction component. This idea amounts to selecting the snapshot simulations, *i.e.* RVE solutions under particular macroscopic strain histories, so as to minimise the error of prediction over all admissible macroscopic strain trajectories. This is in contrast to existing work on snapshot-based multiscale ROM, where sampling is performed uniformly in the subspace of proportional macroscopic strain trajectories (*e.g* [76]), or designed in an heuristic manner, following mechanistic principles similar to those used to test a solid material in a lab (*e.g.* [73]).

Although the proposed *optimal snapshot location* approach is appealing, it is very challenging, due to the infinite dimension of the parameter space. Indeed, the parameters of the RVE problem are 3 *functions* of time in 2D, and 6 *functions* of time in 3D. In order to circumvent this difficulty, we proposed a greedy process that successively selects optimal strain histories in hierarchically enriched discrete spaces, as represented in figure 3.4. The training phase is automatically stopped when enriching the space of load histories stops improving the accuracy of the Galerkin ROM. The optimisation algorithm is a global, gradient-free approach called Bayesian optimisation, which relies heavily on Gaussian processes. As part of the development, we built upon the work described in [39] to progressively construct a reliability indicator, in a data-driven fashion (we use a second Gaussian process regression to calibrate a -noisy- relationship between a measure of the residual that is relatively inexpensive to compute and the true error in the quantity of interest). The results provided in



Proportional loading:
2 parameters (2 angles)

Sequence of 2 piecewise linear trajectories:
5 parameters (4 angles and dissipated energy at kink)

...

Sequence of piecewise trajectories:
(add 3 parameters per level)

Figure 3.4: Hierarchical snapshot generation for the computational material point problem (from [17]). Optimisation is performed in spaces of increasing dimensions so as to maximally decrease the error of ROM projection.

the paper are encouraging. The optimal snapshot location strategy allows us to construct appropriate ROMs very fast for elastic damageable materials. The extension of this work to the homogenisation of (visco)-plastic behaviour would be very interesting, as the overall stress-strain evolution of such materials is potentially more complex.

CHAPTER 4

Adaptive multiscale modelling with guarantees of accuracy

Introduction

Model adaptation needs to be triggered and subsequently driven by appropriate indicators of error levels. More precisely, within the context of this thesis, we wish to replace high-fidelity models by surrogates. This model approximation process generates so-called modelling errors (this terminology may be confusing, and will be justified later on), which we are required to measure in order to drive the surrogate construction and adaptation. Of course, we do not have access to the high-fidelity solution, which means that measures of errors have to be *estimated*. Unfortunately, surrogate modelling errors are notoriously difficult to estimate.

In this section, I will present several contributions that aim to bridge the area of error estimation for FE discretisation errors, which is well-developed, and the area of modelling error estimation, which is less mature. The focus is on the development of duality-based error estimates for linear elliptic PDEs. I will show how such techniques can be used to adapt one-shot multiscale models, where the fine scale solution is intractable, and to construct parametric ROM, where the solution is tractable but cannot be computed over the entirety of the design space. The duality-based approach will deliver error bounds that will be used to certify the quality of the surrogate modelling process, using notably the usual adjoint problem framework.

The chapter is organised as follows. I will first introduce key elements of verification and validation, and clarify the type of modelling error that I refer to in this thesis. Then, I propose to introduce duality-based error bounding, using linear algebra to simplify the derivations. Finally, I will introduce three contributions in the field: the first related to the homogenisation of random media, the second about defeaturing CAD models, and the third one concerning the optimal construction of ROM surrogates for parametrised PDEs.

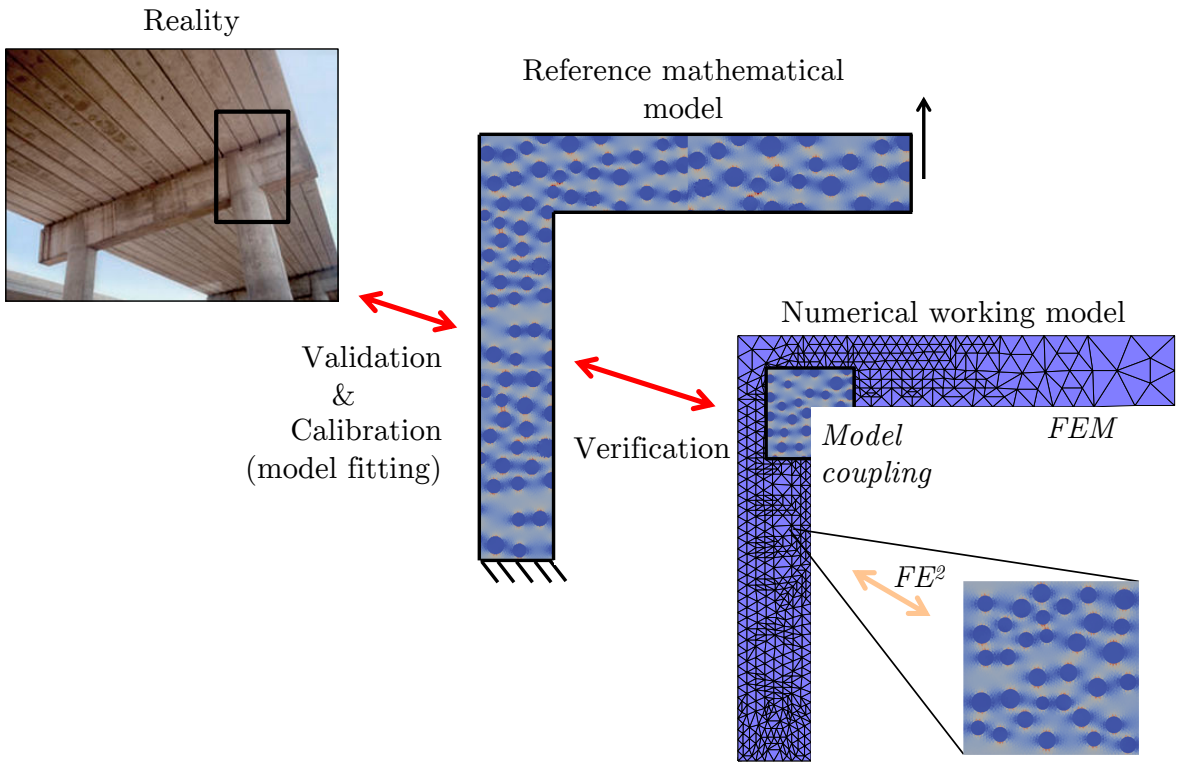


Figure 4.1: Verification and validation of numerical models.

4.1 Validation and verification

In the context of error estimation, the term validation is usually associated with the task of assessing the ability of a mathematical model to predict observations from the real-world. It answers the question: *Am I solving the right equations?* Verification is usually understood as the task of assessing the impact of simplifying assumptions and/or numerical approximations on the numerical output. Verification is about answering the question: *Am I solving the equations right?*. Within the scope of this thesis, model verification is a purely mathematical task that has nothing to do with the real-world. Model verification implies the availability of a high-fidelity mathematical model (which may be a probabilistic mixture of models) that is intractable but, if solved, would generate the ideal numerical predictions desired by the engineer. This high-fidelity mathematical model may be called reference model, "truth" model, "fine-scale" model, high-fidelity model or full-order model depending on the context of application.

At the most basic level, model verification needs to ensure that numerical computations are performed with an appropriate level of accuracy. For instance, a finite element analyst needs to refine the computational mesh and time grid to check that the numerical method has reached a sufficient level of convergence. Similarly, one-at-a-time analyses of sensibility may be performed to provide *some level of confidence* that simplifying assumptions such as linearisations, asymptotics or term-neglecting are not significantly altering the computed outputs.

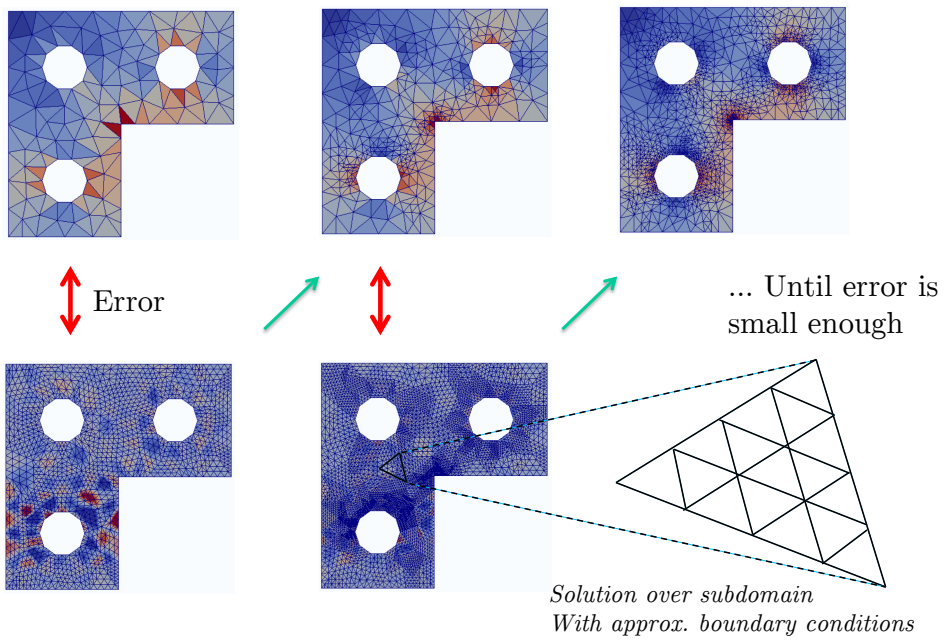


Figure 4.2: Finite element mesh adaptivity driven by an implicit residual error estimate. The estimate is obtained by solving the residual equation over elements independently, using the coarse finite element solution to generate element-wise boundary conditions.

At the next level however, verification is the key enabler to performing automatised model reduction. Indeed, if one knows *how much* error is made, one can choose to refine the computational strategy *i.e.* inject more CPU resources into the simulation. If, in addition to this, one knows *where* the error comes from, one may target the source of large errors and (i) eliminate the corresponding model simplification, or (ii) refine the corresponding computational grid locally. Starting from a coarse approximation of the reference model, one may develop a Greedy process to progressively release the computational effort where it has the most impact on the measure of accuracy. The Reduced Basis Method [36, 55], which we have described in the first chapter, is a perfect example of such a modern approach. As another example, adaptive finite element methods [77, 78, 79] are often based on a Greedy algorithm that progressively refine the mesh in regions of high gradients (see Figure 4.2).

4.2 Modelling errors

In the context of model validation, the term "model error" may be used in an unusual way. Outsiders to the field may understand this term as some form of distance between results given by a particular model, and real-world observations. However, here, we use model error to denote a *verification task* that is applied beyond the traditional context of quality control for discretisation schemes. Modelling errors may refer to the effect of various model simplifications that are designed to make approximate solutions tractable, such as

- mutiscale approximations (see figure 4.1);

- simplification of boundary conditions;
- *a priori* linearisation of the governing equations (small perturbations in solid mechanics, Kalman filter in optimal control);
- *a priori* elimination of terms: inertia, viscous forces;
- replacement of a stochastic model by a deterministic surrogate, ...

Evaluating the impact of such simplifications onto the quality of numerical results, without computing the corresponding unaffordable reference solution, is particularly challenging. Available techniques to estimate error levels in the context of spatial and temporal discretisation of PDEs rely heavily on the convergence properties of these schemes. For instance, in the context of linear elliptic PDEs, the convergence rate of the finite element method of polynomial order p may be *a priori* shown to be such that

$$|||T - T^h||| \leq Ch^p \tag{4.1}$$

which implies in particular, using the triangle inequality, that

$$|||T - T^h||| \leq |||T^{\frac{h}{\alpha}} - T^h||| + |||T - T^{\frac{h}{\alpha}}||| \leq |||T^{\frac{h}{\alpha}} - T^h||| + C\left(\frac{h}{\alpha}\right)^p \tag{4.2}$$

and the last term on the right-hand side can be made small enough by choosing α large enough. This expression suggests that we can estimate the total error by *computing* the solution corresponding to a finer discretisation. Of course, this may be numerically expensive, and appropriate multilevel approximation methods should be used to cap the numerical cost of estimating this error. But essentially, error estimation by refinement *can* be done. However, modelling approximations may not possess such refinement characteristics. In the context of mutiscale modelling for example, we may use a multiscale surrogate locally and solve the problem at the scale of the heterogeneities elsewhere (see figure 4.2). But there is no obvious progressive ladder of models of increasing accuracy and numerical cost to bridge the gap between these two extrema[1].

In this challenging context, duality-based error estimates are particularly appealing. Indeed, they provide ways to directly *bound* the distance to the intractable reference solution, without the need to solve a "finer problem". Instead, an auxiliary dual problem is created and solved approximately, and standard results of convex analysis are invoked to prove the desired bounding properties.

In the following, the principle underlying duality-based error estimation is recalled, using generic algebraic notations and Lagrangian duality. We then briefly outline how this principle has been used over the last decades to bound the discretising errors arising in FE procedures. Finally, we introduce three papers where this setting is extended to the estimation and control of modelling errors.

[1]Perturbation methods can, in general, be used to continuously morph the approximate surrogate to the reference model. This is a valid framework for estimating modelling errors, and its is used in many areas of engineering to solve intractable reference problems approximately (*e.g.* asymptotic homogenisation, stochastic perturbation). But developing a sound perturbation approach to modelling error estimation is dificult and largely problem-dependent. Solving the perturbed homotopy model at zero may be as expensive as solving the reference model, rendering the approach impractical. Importantly, convergence with the homotopy parameter may be extremely slow, leading to widely underestimated levels of errors.

4.3 Duality-based error bounds: an algebraic introduction

4.3.1 Primal problem and lower bounding

Let us consider the algebraic system of linear equation

$$\mathbf{A}\mathbf{x} = \mathbf{b} \tag{4.3}$$

where we require matrix $\mathbf{A}$ to be symmetric definite positive. We assume that $\mathbf{x}$ is intractable, because $\mathbf{A}$ is very large. We may, however, compute an approximation $\bar{\mathbf{x}}$ of $\mathbf{x}$. This approximation may, or may not, be obtained by Galerkin projection

$$\boldsymbol{\phi}^T \mathbf{A} \underbrace{\boldsymbol{\phi}\,\boldsymbol{\alpha}}_{=\bar{\mathbf{x}}} = \boldsymbol{\phi}^T \mathbf{b} \tag{4.4}$$

Now, defining quadratic functional $\mathcal{J}(\mathbf{x}^\star) = \frac{1}{2}\mathbf{x}^{\star T}\mathbf{A}\mathbf{x}^\star - \mathbf{x}^{\star T}\mathbf{b}$, (4.3) is equivalent to the minimisation principle:

$$\boxed{\mathbf{x} = \arg\min_{\mathbf{x}^\star} \mathcal{J}(\mathbf{x}^\star)} \tag{4.5}$$

Let us further recall that identity

$$\|\mathbf{x} - \mathbf{x}^\star\|_{\mathbf{A}}^2 = 2\left(\mathcal{J}(\mathbf{x}^\star) - \mathcal{J}(\mathbf{x})\right) \tag{4.6}$$

holds for all $\mathbf{x}^\star$. Although computing error $\mathbf{e} := \mathbf{x} - \bar{\mathbf{x}}$ is as difficult as computing the reference solution itself, computing a lower bound for error measure $\|\mathbf{x} - \bar{\mathbf{x}}\|_{\mathbf{A}}^2 = (\mathbf{x} - \bar{\mathbf{x}})^T \mathbf{A} (\mathbf{x} - \bar{\mathbf{x}})$ is easy (the $\mathbf{A}$ norm is called energy norm when the algebraic problem corresponds to the finite element discretisation of a linear elliptic PDE). We substitute any "better" solution $\tilde{\mathbf{x}} = \mathbf{x} + \bar{\mathbf{e}}$ for the exact $\mathbf{x}$ in (4.6). Owing to the minimisation principle (4.5), we have that $\mathcal{J}(\mathbf{x}) \leq \mathcal{J}(\tilde{\mathbf{x}})$, and therefore

$$\boxed{\|\mathbf{x} - \bar{\mathbf{x}}\|_{\mathbf{A}}^2 \geq \max(2\left(\mathcal{J}(\bar{\mathbf{x}}) - \mathcal{J}(\tilde{\mathbf{x}})\right), 0)} \tag{4.7}$$

or, after some algebraic manipulations, [23]

$$\|\mathbf{e}\|_{\mathbf{A}}^2 \geq \|\bar{\mathbf{e}}\|_{\mathbf{A}}^2 + 2\,\bar{\mathbf{e}}^T(\mathbf{b} - \mathbf{A}\tilde{\mathbf{x}}) \tag{4.9}$$

where the residual $\mathbf{r}$ is defined by $\mathbf{r} = \mathbf{b} - \mathbf{A}\bar{\mathbf{x}}$ and satisfies the error equation $\mathbf{A}\mathbf{e} = \mathbf{r}$.

4.3.2 Disassembling the primal problem - Lagrangian duality

Unfortunately, the primal minimisation principle can only yield one-sided error bounds as we can only compute majorants of $\mathcal{J}(\mathbf{x})$. This particular side is arguably the least interesting

[2] When enhanced solution vector $\tilde{\mathbf{x}}$ is obtained by a Galerkin procedure, the second term vanishes.

[3] Another bound may be obtained by applying the Cauchy-Schwartz identity to inner product $\bar{\mathbf{e}}^T\mathbf{A}\mathbf{e}$:

$$\|\mathbf{e}\|_{\mathbf{A}}^2 \geq \frac{|\bar{\mathbf{e}}^T\mathbf{r}|}{\|\bar{\mathbf{e}}\|_{\mathbf{A}}^2} \tag{4.8}$$

of the two: we would like to make sure that *the error is less than x*, rather than *the error is more than y*[4].

To obtain upper bounds for the error, one needs to derive a computable minorant for $\mathcal{J}(\mathbf{x})$ (remember equation (4.7)). In duality-based error estimation, upper bounds are obtained by looking for approximate solutions in spaces that are "richer" than the initial search space. To understand this, let us consider a system with constraints. We assume that the solution is obtained by solving the minimisation problem

$$\mathbf{x} = \arg \min_{\mathbf{x}^\star | \mathbf{C}\mathbf{x}^\star = 0} \mathcal{J}(\mathbf{x}^\star) \tag{4.10}$$

where operator $\mathbf{A}$ is now positive *semi*-definite. We further assume that $\mathbf{C}$ has full row rank (the constraints are linearly independent), and that $\mathbf{A}$ is strictly positive on the nullspace of $\mathbf{C}$[5]. Such a system can be obtained, for instance, if the mechanical problem leading the discrete system studied in the previous section is divided into subproblems. The solution is then obtained by minimising the sum of the potential energies, under constraint of continuity at the interface (see figure 4.2 and *e.g.* [80])[6]. Lower error bounds in the norm associated with $\mathbf{A}$ can still be obtained using the derivations of the previous sections, using the nullspace of $\mathbf{C}$ as search space, without enrichment.

For the upper bound, we reformulate problem (4.10) as the extremisation of the Lagrangian

$$\mathcal{L}(\mathbf{x}^\star, \boldsymbol{\lambda}^\star) = \mathcal{J}(\mathbf{x}^\star) + \boldsymbol{\lambda}^T (\mathbf{C}\mathbf{x}^\star) \tag{4.11}$$

which corresponds to the Karush–Kuhn–Tucker equations

$$\begin{pmatrix} \mathbf{A} & \mathbf{C}^T \\ \mathbf{C} & 0 \end{pmatrix} \begin{pmatrix} \mathbf{x} \\ \boldsymbol{\lambda} \end{pmatrix} = \begin{pmatrix} \mathbf{b} \\ 0 \end{pmatrix} \tag{4.12}$$

Due to the previously stated assumptions, the solution of the KKT system is unique [81].

We may now minimise the Lagrangian with respect to the primal variable, for an arbitrary vector of Lagrange multipliers, and use the result to eliminate $\mathbf{x}$ (*i.e.* solve the first equation and substitute the result in the expression of the Lagrangian), which yields the dual maximisation problem:

$$\boldsymbol{\lambda} = \arg \max_{\boldsymbol{\lambda}^\star | \mathbf{N}^T(\mathbf{b} - \mathbf{C}^T\boldsymbol{\lambda}^\star) = 0} \mathcal{Q}(\boldsymbol{\lambda}^\star) \tag{4.13}$$

$$\mathcal{Q}(\boldsymbol{\lambda}^\star) = -\frac{1}{2}(\boldsymbol{\lambda}^\star)^T \mathbf{C}\mathbf{A}^+\mathbf{C}^T\boldsymbol{\lambda}^\star + (\boldsymbol{\lambda}^\star)^T \mathbf{C}\mathbf{A}^+\mathbf{b} \tag{4.14}$$

where $\mathbf{A}^+$ is the Moore-Penrose inverse of $\mathbf{A}$. The minimisation with respect to the primal variable can only be performed if the right-hand side is in the range of $\mathbf{A}$, *i.e.* satisfying $\mathbf{N}^T \left(\mathbf{b} - \mathbf{C}^T\boldsymbol{\lambda}^\star\right) = 0$, where the columns of $\mathbf{N}$ form a basis of the nullspace of $\mathbf{A}$.

[4] In goal-oriented settings, the two sides of the frame are of equal importance. The effectivity of the method depends on the distance between the two bounds. For more details, see the parallelogram identity bounding techniques developed in [42], and also reported and used in Paper 2.1.

[5] If $\mathbf{Z}$ denotes a basis of this nullspace, then $\mathbf{Z}^T\mathbf{A}\mathbf{Z}$ is positive definite)

[6] By not enforcing interface continuity *a priori*, we have made the search space richer. At the discrete level, $\mathbf{x}$ now possesses more degrees of freedom, as the nodes at the interface are doubled. The increase in the number of degrees of freedom is equal to the dimension of the nullspace of $\mathbf{A}$.

4.3.3 Duality-based upper bound

Due to the concavity of $\mathcal{L}^\star$, any surrogate vector $\bar{\boldsymbol{\lambda}}$ will yield an upper bound for $\mathcal{J}(\mathbf{x})$:

$$\mathcal{Q}(\bar{\boldsymbol{\lambda}}) \leq \mathcal{Q}(\boldsymbol{\lambda}) = \mathcal{L}(\mathbf{x}, \boldsymbol{\lambda}) = \mathcal{J}(\mathbf{x}) \leq \mathcal{J}(\bar{\mathbf{x}}) \tag{4.15}$$

where $\mathbf{C}\mathbf{x} = 0$ by property of the exact solution, and $\mathbf{C}\bar{\mathbf{x}} = 0$ by choice of the approximate primal solution. We therefore obtain the error upper bound

$$\boxed{\|\mathbf{x} - \bar{\mathbf{x}}\|^2_{\mathbf{A}} \leq 2\left(\mathcal{J}(\bar{\mathbf{x}}) - \mathcal{Q}(\bar{\boldsymbol{\lambda}})\right)} \tag{4.16}$$

Of course, a good surrogate should approximately minimise the complementary energy $-\mathcal{Q}$. On the other hand, the approximate dual solution should not be more expensive to compute than the primal one, so that the error estimation procedure remains computationally efficient. Deriving adequate duality-based a posteriori estimates means balancing these two conflicting requirements.

4.3.4 Hyper-circle theorem

Let us assume that we have an approximate primal solution $\bar{\mathbf{x}}$ satisfying the primal constraints, $\mathbf{C}\bar{\mathbf{x}} = 0$, an approximation $\bar{\boldsymbol{\lambda}}$ of the Lagrange multiplier vector satisfying admissibility condition $\mathbf{N}^T\left(\mathbf{b} - \mathbf{C}^T\bar{\boldsymbol{\lambda}}\right) = 0$, and the corresponding dual approximate solution $\bar{\mathbf{x}}_d = \mathbf{A}^+\left(\mathbf{b} - \mathbf{C}^T\bar{\boldsymbol{\lambda}}\right)$. If $\mathbf{e} = \mathbf{x} - \bar{\mathbf{x}}$ denotes the primal error and $\mathbf{e}_d = \mathbf{x} - \bar{\mathbf{x}}_d$ denotes the dual error, the fundamental property below holds:

$$\boxed{\begin{array}{rcl} \|\bar{\mathbf{x}} - \bar{\mathbf{x}}_d\|^2_{\mathbf{A}} & = & \|\bar{\mathbf{x}} - \mathbf{x} + \mathbf{x} - \bar{\mathbf{x}}_d\|^2_{\mathbf{A}} = \|\mathbf{e} + \mathbf{e}_d\|^2_{\mathbf{A}} \\ & = & \|\mathbf{e}\|^2_{\mathbf{A}} + \|\mathbf{e}_d\|^2_{\mathbf{A}} + 2\mathbf{e}_d^T\mathbf{A}\mathbf{e} \\ & = & \|\mathbf{e}\|^2_{\mathbf{A}} + \|\mathbf{e}_d\|^2_{\mathbf{A}} \end{array}} \tag{4.17}$$

The last equality can be shown by observing that $\mathbf{e}$ is primarily admissible, *i.e.* it satisfies the constraints, $\mathbf{C}\mathbf{e} = 0$, $\mathbf{e}_d = \mathbf{A}^+\mathbf{C}^T(\boldsymbol{\lambda} - \bar{\boldsymbol{\lambda}})$, and $\mathbf{A}^+\mathbf{A} = \mathbf{I}$. The result is remarkable. Although both *exact* error measure on the right-hand side of the equation are not computable, their sum, which is shown on the right-hand side, is available without any knowledge of the exact solution. In particular, the following upper bound property holds: $\|\mathbf{e}\|_{\mathbf{A}} \leq \|\bar{\mathbf{x}} - \bar{\mathbf{x}}_d\|_{\mathbf{A}}$. This result can also be derived from previous results (4.16)[7][8].

[7] The more general duality formalism may be extended to the minimisation of non-quadratic convex functionals

[8] This can be shown by writing that

$$\begin{array}{rcl} \|\bar{\mathbf{x}} - \bar{\mathbf{x}}_d\|^2_{\mathbf{A}} & = & 2\left(\mathcal{J}(\bar{\mathbf{x}}) - \mathcal{Q}(\bar{\boldsymbol{\lambda}})\right) \\ & = & 2\left(\mathcal{J}(\bar{\mathbf{x}}) - \mathcal{J}(\mathbf{x}) + \mathcal{J}(\mathbf{x}) - \mathcal{Q}(\bar{\boldsymbol{\lambda}})\right) \\ & = & 2\left(\mathcal{J}(\bar{\mathbf{x}}) - \mathcal{J}(\mathbf{x})\right) + 2\left(\mathcal{Q}(\boldsymbol{\lambda}) - \mathcal{Q}(\bar{\boldsymbol{\lambda}})\right) \\ & = & \|\mathbf{x} - \bar{\mathbf{x}}\|^2_{\mathbf{A}} + 2\left(\mathcal{Q}(\boldsymbol{\lambda}) - \mathcal{Q}(\bar{\boldsymbol{\lambda}})\right) \\ & = & \|\mathbf{x} - \bar{\mathbf{x}}\|^2_{\mathbf{A}} + \|\boldsymbol{\lambda} - \bar{\boldsymbol{\lambda}}\|^2_{\mathbf{C}\mathbf{A}^+\mathbf{C}^T} \\ & = & \|\mathbf{e}\|^2_{\mathbf{A}} + \|\mathbf{e}_d\|^2_{\mathbf{A}} \end{array} \tag{4.18}$$

The duality-based bound is obtained from the right-hand side of the first line and fourth, noticing that the second term of the fourth line is always positive.

4.4 Duality-based error bounds for the finite element method

Duality-based bounds have been used for several decades to certify the accuracy of the finite element method. One way to do this, as outlined in the previous section, is to decompose the domain into individual elements and solve the PDE of interest over these domains, using a hierarchically refined mesh and reconstructed flux boundary conditions. The admissibility constraints for the reconstructed element fluxes is rather technical to enforce when the restriction of the elliptic forms to individual subdomain has a non-vanishing nullspace, but so-called flux equilibration techniques are now well-established [82, 77, 83, 84, 85, 86]. Alternatively, the patch-based approaches proposed in [87, 88] do not require any flux equilibration. These methods are usually coined "equilibrated residual" error estimation approaches.

As an alternative to breaking the inter-element continuity, equilibrated finite element methods relax kinematic compatibility conditions within the bulk of the domain [**?**, 89, 77, 90, 91]. These approaches largely inspired the modelling error estimates that will be presented later on in this thesis. To illustrate this idea, let us consider a scalar linear elliptic partial differential equation (*i.e* steady-state temperature diffusion or electrostatics)

$$\begin{array}{rcll} \nabla \cdot q & = & f & \text{in } \Omega \\ q & = & -k\nabla T & \text{in } \Omega \\ T & = & T_d & \text{in } \partial\Omega_T \\ q \cdot n & = & q_d & \text{in } \partial\Omega_q \end{array} \tag{4.19}$$

This problem is equivalent the the extremisation of Lagrangian

$$\mathcal{L}\left((T^\star, \epsilon^\star), q^\star\right) = \mathcal{J}(T^\star, \epsilon^\star) + \int_\Omega q^\star \cdot (\epsilon^\star - \nabla T^\star)\, dx \tag{4.20}$$

where

$$\mathcal{J}(T^\star, \epsilon^\star) = \frac{1}{2}\int_\Omega k\, \epsilon^\star \cdot \epsilon^\star\, dx - \int_\Omega f\, T^\star\, dx + \int_{\partial\Omega_q} (q_d \cdot n)\, T^\star\, dx \tag{4.21}$$

with respect to primal pair (T, ϵ) and dual field q (*i.e.* a Lagrange multiplier for the relaxed condition that ϵ must be the gradient of T).

Minimising the Lagrangian with respect to the primal fields, we obtain the following relationships

$$\nabla T^\star = -k^{-1} q^\star \tag{4.22}$$

and

$$\forall \delta T \in \mathcal{U}_0, \qquad -\int_\Omega q^\star \cdot \nabla \delta T\, dx - \int_\Omega f\, \delta T\, dx + \int_{\partial\Omega_q} q_d\, \delta T\, dx = 0 \tag{4.23}$$

where $\mathcal{U}_0$ contains fields that vanish over $\partial\Omega_T$. We will denote by $\mathcal{S}$ the set of Lagrange multipliers q that satisfy the previous equation, which is that of flux equilibrium.

We can now use these two conditions to expression the Lagrangian as a function of q only, which reads as

$$\mathcal{Q}(q^\star) = -\frac{1}{2}\int_\Omega k^{-1}\, q^\star \cdot q^\star\, dx - \int_{\partial\Omega_T} (q^\star \cdot n)\, T_d\, dx \tag{4.24}$$

which is maximised when $q^\star = q$.

For any $\bar{q} \in \mathcal{S}$, *i.e.* satisfying the flux balance (4.23), and for any approximations $\bar{T}$ and $\tilde{T}$ ($\tilde{T}$ "better" than $\bar{T}$ for the resulting bound to be non-trivial) satisfying the Dirichlet boundary conditions,

$$2\left(\mathcal{J}(\bar{T},\nabla\bar{T})-\mathcal{J}(\tilde{T},\nabla\tilde{T})\right) \leq \|\bar{T}-T\|_k^2 \leq 2\left(\mathcal{J}(\bar{T},\nabla\bar{T})-\mathcal{Q}(\bar{q})\right) \tag{4.25}$$

and the upper bound may be also be written as

$$\|\bar{T}-T\|_k^2 = \|\bar{q}+k\nabla\bar{T}\|_{k^{-1}}^2 - \|q-\bar{q}\|_{k^{-1}}^2 \leq \|\bar{q}-(-k\nabla\bar{T})\|_{k^{-1}}^2 \tag{4.26}$$

where we have used norms $\|\,.\,\|_k = \sqrt{\int_\Omega k\,.\,.\,dx}$ and $\|\,.\,\|_{k^{-1}} = \sqrt{\int_\Omega k^{-1}\,.\,.\,dx}$. When written in this form, the upper bound is clearly the Constitutive Relation Error [77], a measure of the residual of the only equation that is not satisfied by pair $(\bar{T},\bar{q})$.

Equilibrium finite element methods [91] look for fields $\bar{q} \in \mathcal{S}$ that satisfy the balance equations *a priori* over polygonal domain (*i.e.* elements), using specially derived polynomial bases, and ensure the normal continuity of these fields through a constrained minimisation of the complementary energy $-\mathcal{Q}$.

4.5 Quantity of interest, adjoint method and model adaptivity

Estimating errors in "energy norms" is interesting for adaptivity, and even more so if strict bounds for these error measures can be derived. In the context of linear elliptic PDEs for instance, energy norms are computed by summation of positive terms over space and time. Reducing energy error estimates may be done by eliminating the sources of errors (refine the mesh) where and when the corresponding summand is large, and in a greedy manner.

However, a quantitative criterion needs to be provided in order to stop the adaptivity process. The only meaningful way to do this is to provide a stopping criterion fot the output of the simulation: the quantity of interest (QoI). Ideally, we would like *the error in the QoI to be less than X%*. This is similar to requiring for the exact and intractable QoI to be contained within a small uncertainty interval, the length of which is less than $2X$ times the QoI.

Over the last two decades, a significant amount of research effort has been dedicated to linking the error in QoI to the error in energy norm, for which good estimates and bounds have been developed in the 20^{th} century. The result of this research is the adjoint theory. Simply put, the variation of the linear QoI $Q = \mathbf{\Sigma u} \in \mathbb{R}$, where $\mathbf{\Sigma}$ is an extractor, is

$$\delta Q = \mathbf{\Sigma}^T \delta\mathbf{e} = \underbrace{\mathbf{\Sigma}^T\mathbf{A}^{-T}}_{\mathbf{z}^T}\delta\mathbf{R} = \tag{4.27}$$

where we have used the residual equation $\mathbf{Ae} = \mathbf{R}$. The adjoint problem is

$$\mathbf{A}^T\mathbf{z} = \mathbf{\Sigma} \tag{4.28}$$

and $\mathbf{z}$, the adjoint solution, can be interpreted as *the sensitivity of the QoI with respect to a variation in the quality of the satisfaction of the governing equations* $\mathbf{R} = \mathbf{b} - \mathbf{A}\bar{\mathbf{u}} \underset{\text{want}}{=} 0$ [9].

[9] The ^{T} symbol is important. For self-adjoint problems, it has no effect. However, time-dependent problem that are discretised by finite difference in time and finite element in space result in block-lower bidiagonal algebraic systems, when fully assembled in space and time, due to the direction of the flow of information from the past to the future. For the adjoint problem, the system to solve is block-*upper* bidiagonal: the flow of information is reversed in time.

Now, the sensitivity field may be used in a first-order Taylor expansion, which is an exact identity in the case of a linear algebraic problem, to express the error in QoI as a function of the residual:

$$Q - \mathbf{\Sigma}\bar{\mathbf{u}} = \mathbf{z}^T\mathbf{R} = \bar{\mathbf{z}}^T\mathbf{R} + (\mathbf{z} - \bar{\mathbf{z}}^T)\mathbf{A}\mathbf{e} \tag{4.29}$$

where $\mathbf{z}$ is a computable approximation of the adjoint solution, which is as expensive to compute as the "reference" adjoint. The first term is computable. If $\mathbf{A}$ is SPD, the second term is the inner product between the adjoint and forward errors. They can be separated using either Cauchy-Schwarz identity or the parallelogram identity, yielding exact errors in energy norm, which in turn may be bounded by duality.

These techniques are standard [42, 43, 44, 92], and are used in all the papers on modelling error estimation and adaptivity presented below. In these papers, the challenge lies in the definition and bounding of energy-norm error terms that arise when deploying the classical adjoint method.

4.6 Summary of papers

Paper 2.1: Error-controlled stochastic homogenisation [9]

Assessing and controlling the quality of homogenised results is a tremendously difficult task. The introduction of Paper 2.1 summarises the recent developments that researchers have proposed to extend the tools of *a posteriori* error estimation and control to the context of multiscale modelling (see *e.g.* [93, 94, 95] and further references in [8] and Paper 2.1). In particular, in the last decade, significant effort has led to the development of bounding approaches for multiscale errors [96, 97, 92, 98, 99, 100].

The approach that we follow here is that of Oden's team [92], which relies on (i) applying duality principles to obtain bounds for the error measured in the norm associated with the heterogeneous diffusion operator, and (ii) using the adjoint method to establish a relationship between the bound and the accuracy of the engineering quantity of interest. Subsequently, spatially localised error contributions are evaluated and used as indicators for model refinement: the macroscopic model is locally replaced by the high-fidelity model, in a spatially-greedy manner.

Duality-based bound for the surrogate models of heterogeneous structures. To illustrate the error estimation approach, let us consider a problem of linear diffusion in a composite medium, described by rapidly varying conductivity $k(x)$. We assume that we have at our disposal an homogenised solution $\bar{T}$, computed by solving the diffusion problem with *constant* surrogate conductivity $\bar{k}$ using the finite element method. The direct application of duality, using the finite element field as approximate dual, which is valid if the finite element

error is small compared to the homogenisation error, leads to upper bounding property[10]

$$\begin{aligned} \|T-\bar{T}\|_k^2 &= \|\bar{q}-(-k\nabla\bar{T})\|_{k^{-1}}^2 - \|q-\bar{q}\|_{k^{-1}}^2 \\ &\lesssim \|\bar{q}-(-k\nabla\bar{T})\|_{k^{-1}}^2 \\ &\lesssim \|-\bar{k}\nabla\bar{T}+\nabla\bar{T})\|_{k^{-1}}^2 \\ &\lesssim \int_\Omega \frac{(k(x)-\bar{k})^2}{k(x)}\,\nabla\bar{T}\cdot\nabla\bar{T}\,dx \end{aligned} \tag{4.30}$$

However, the bound is not computable. This is because $\frac{(k(x)-\bar{k})^2}{k(x)}$ may vary arbitrarily fast. Even if surrogate $\bar{T}$ is smooth and described using a macroscopic mesh, the integration of the upper bound requires meshing the heterogeneity explicitly. In our view, this approach breaks the numerical separation of scales, as microscale operations, meshing and performing the corresponding quadrature, would be performed over the entire macroscopic domain.

Duality-based bound for random composites. The solution that we have proposed is quite simple: randomise the spatial distribution of heterogeneities, through the definition of a random diffusion field k. For large domains, this is not restrictive as we are unlikely to know the exact distribution of heterogeneities. Moreover, we are often interested in ensemble predictions. In this case, we will make use of energy measures $\sqrt{E\left(\int_\Omega k\,\ldots dx\right)}$ and $\sqrt{E\left(\int_\Omega k^{-1}\,\ldots dx\right)}$, where the expectation symbol denotes an averaging over all possible outcomes of a random field generator, weighted by the associated probability measure (see also [**?**]). The duality-based bounding approach holds in these extended norms, assuming for now that $\bar{T}$ and $\bar{q}=-\bar{k}\nabla\bar{T}\in\mathcal{S}$ are constructed such that they are independent of the realisation of the random field. Taking the expectation on both side of (4.30), we arrive at

$$\begin{aligned} E\left(\|T-\bar{T}\|_k^2\right) &= E\left(\|\bar{q}-(-k\nabla\bar{T})\|_{k^{-1}}^2\right) - E\left(\|q-\bar{q}\|_{k^{-1}}^2\right) \\ &\lesssim E\left(\int_\Omega \frac{(k(x)-\bar{k})^2}{k(x)}\,\nabla\bar{T}\cdot\nabla\bar{T}\,dx\right) \\ &\lesssim \int_\Omega E\left(\frac{(k(x)-\bar{k})^2}{k(x)}\right)\,\nabla\bar{T}\cdot\nabla\bar{T}\,dx \end{aligned} \tag{4.31}$$

The term appearing in the expectation operator, which is now slow in space, can be precomputed by hand, or numerically using microstructural samples.

This randomisation strategy is the fundamental idea upon which the methodology described in Paper 2.1 is constructed. In addition to delivering truly tractable error bounds for homogenisation, the proposed approach allow us to clearly show the link between structure-scale bounds obtained by duality, and the classical material point bounds of Reuss and Voigt (a first effort in this direction was proposed in [96]). This is done through the strict optimisation of the error bound over the set of homogenised tensors used to compute the primal and dual solutions, which, as opposed to what was exposed previously for the sake of simplicity, should be allowed to differ.

[10] The point being made hereafter extends to the lower bound. However, homogenisation lower bounds obtained by the methods described in the previous sections are of poor quality: finding a primal field $\tilde{T}$ that is better than $\bar{T}$ in the sense of the potential energy, but remains numerically computable is very hard. Unlike what is usually done in the FEM context, there is here no possibility to "just refine the mesh".

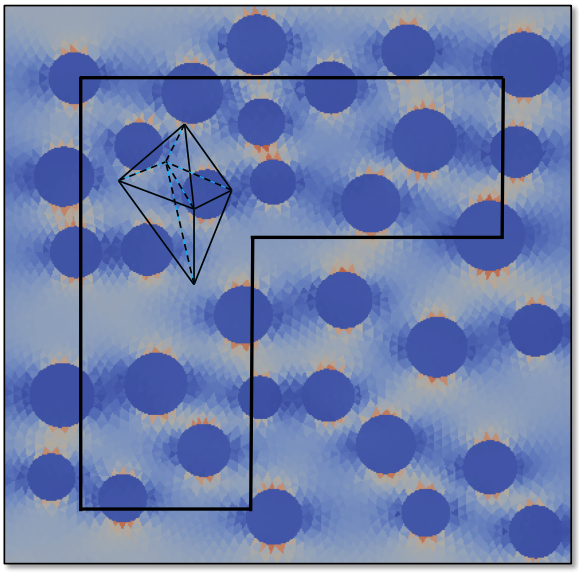


Figure 4.3: Mutiscale XFEM strategy. Fine-scale, stochastic solutions fields are formally defined over a large domain encompassing the entire structure. The application of the partition-of-unity enrichment strategy for the fine-scale problem yields a fully compatible, equation-free homogenisation scheme.

Stochastic micro/macro primal surrogates: towards duality in FE^2 The error bounds described previously lose their sharpness when the contrast between the diffusion constant of the micro-constituents increases. This is because the primal and dual surrogates used in our approach are not allowed to vary with the realisation of the random field (similar to Reuss/Voigt approaches, where the trial fields are assumed to be constant over the RVE). Classical micromechanics for random media delivers micro corrections that do vary in the RVE but violate the primal constraints at the structural scale, and therefore do not easily lend themselves to duality-based error estimation. In the PhD thesis of D. Alves Paladim [101], we developed an approach that allows us to compute compatible primal solutions that may vary in the stochastic direction. This is done by a novel Extended Finite Element (XFEM [102, 103]) strategy, whereby stochastic solutions are *formally* used to enrich the structural scale field, using the Partition-of-Unity method [102]:

$$\bar{T}(x) = \bar{T}^h(x) + \sum_{j=1}^{n_\psi} \sum_{i=1}^{n_\phi} \psi_j(x)\phi_i(x)\alpha_{i,j} \tag{4.32}$$

In the previous expression, the ψ_j's are the standard finite element "hat" functions, whilst the ϕ_i's are enrichment functions that *formally* solve the stochastic, heterogeneous temperature diffusion problem defined over a polygonal domain that strictly encompasses the structural domain, and that is subjected to uniform boundary conditions. We emphasise that the enrichment functions are random.

Writing a Galerkin formulation for the previous stochastic surrogate, we obtain the XFEM

formulation

$$\begin{array}{lrcl} \forall j \in [\![1, n_\psi]\!], & E\left(a(\psi_j, \bar{T}^h)\right) & = & E\left(l(\psi_j)\right) \\ \forall (j,i) \in [\![1, n_\psi]\!] \times \in [\![1, n_\phi]\!], & E\left(a(\psi_j\phi_i, \bar{T} - \bar{T}^h)\right) & = & E\left(l(\psi_j\phi_i)\right) \end{array} \tag{4.33}$$

where a and l are the standard bilinear and linear forms associated with realisations of the thermal diffusion problem. The key observation is that the exact RVE solutions do not need to be computed, but only appear in the Galerkin formulation as "material constants" that can be pre-computed by a combination of Monte-Carlo procedures and calculations over SVEs.

We have shown that this primal, compatible multiscale formulation can be used in the duality framework presented previously. Doing so reduces the contribution of the primal error to the total Constitutive Relation Error by a significant amount. This is encouraging and, in our opinion, is an important step towards constant-free and sharp error bounding for FE^2 schemes. More research is required to derive a similar enrichment strategy for the dual problem, and evaluate the impact of the boundary layer, where, for instance, the stochastic enrichment in the vicinity of the Dirichlet boundary vanishes at a speed that depends on the size of the macro elements.

Paper 2.2: Defeaturing with accuracy certification [2]

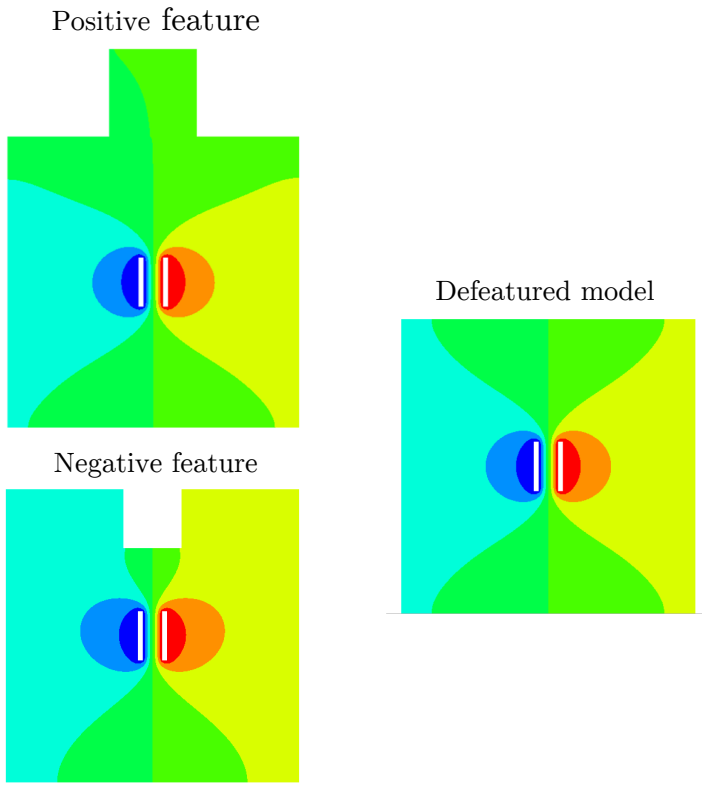


Figure 4.4: Defeaturing approach. We are to estimate whether ignoring negative or positive geometrical features impacts the quality of the output of the numerical analysis or not, without computing the fully featured solution.

The methodology of paper 2.1 may be interpreted as an approach to estimating the loss of accuracy due to model defeaturing: we effectively "removed" the heterogeneities from the medium. This type of idea is of prime interest in stress analysis, and design in general, when a CAD representation of a system is too detailed for the finite element analysis to be tractable. Subsequently, analysts would like to assess whether ignoring small CAD features when performing the finite element simulation has a significant impact on the quantity of interest or not (see figure 4.4 and [104, 105] for pioneering work on deriving energy-based criteria for estimating the impact of feature removal). Paper 2.2 addresses precisely this problem, in the context of elastostatics, the governing equations being similar to those of steady-state temperature diffusion.

The approach is systematic and relies on recasting the geometrical error as an error induced by a modification of the local stiffness, in a penalty-like manner. For instance, a negative feature with Neumann (resp. Dirichlet) boundary conditions may be asymptotically described by removing (resp. adding) a large amount of local stiffness to the defeatured model. In this sense, the proposed approach is related to the work proposed in [106], where a modelling error estimation approach, without certification, was developed based on the work of [92][11]. A similar operation may be performed for positive feature, the key idea for the systematisation of the approach being to reformulate the reference *and* the defeatured problem as two problems defined over the same (positively-featured) domain: the union of (i) the defeatured domain and (ii) the domains occupied by all individual features.

This penalty-based defeaturing interpretation is coupled with the Constitutive Relation Error, so as to provide a systematic basis for the derivation of approximate primal and dual solutions corresponding to the unaffordable, reference featured model. These solutions need to be appropriately localised in negatively featured domains, extended in positively featured domains, and evaluated through the various integral terms that appear in the uncertainty interval for the exact quantity of interest. Our proposed strategy only requires the defeatured solutions, and additional local computations corresponding to individual features. This is well adapted to a CAD-to-simulation pipeline, where features may be analysed independently from their CAD description.

In Paper 2.1, we limited ourselves to local computations over the domains of individual features, which limits the efficiency of the energy bounds. However, the framework does accommodate extended reconstructions that are computed over domains that strictly encompass individual features (see [105] for related concepts). The key for such an approach to be successful would be to ensure its non-intrusivity, as integrals may need to be calculated over domains and interfaces that are not directly described by the CAD geometry.

Paper 2.3: Model Order Reduction with controlled accuracy [13]

Paper 2.3 presents a New Greedy algorithm to construct the Reduced Basis Galerkin ROM [36] for parametrised linear elliptic partial differential equations, as presented in Chapter 1.

[11] Another approach for the estimation of the impact of feature removal is developed in [107, 108]. In these publications, featuring is seen as a perturbation of the defeatured problem, using homotopy mappings and Taylor expansions. In this context, approximate error estimate may be obtained using the shape/topology derivative concepts traditionally used in structural optimisation. However, the approach cannot provide any *guarantee* of accuracy.

The traditional way of constructing the Reduced Basis ROM is to greedily minimise the error in the primal field or QoI by sequentially computing the solutions corresponding to the points of the parameter domain where the error estimate is maximum, and using these solutions to enrich the Reduced Basis. The error bound, which should be sufficiently sharp for this approach to be successful, is usually constructed and calibrated as a preliminary step of the learning process [54, 55, 109, 110]. We are going to proceed differently. The main idea of our approach comes from the observation of the Hypercircle theorem, now written in the context of a temperature diffusion problem with affinely parametrised conductivity field $k(x, \boldsymbol{\mu})$.

$$\forall \boldsymbol{\mu} \in \mathcal{P}, \qquad \|T(\boldsymbol{\mu}) - \bar{T}(\boldsymbol{\mu})\|^2_{k(\boldsymbol{\mu})} + \|q(\boldsymbol{\mu}) - \bar{q}(\boldsymbol{\mu})\|^2_{k(\boldsymbol{\mu})^{-1}} = \|\bar{q}(\boldsymbol{\mu}) + k\nabla\bar{T}(\boldsymbol{\mu})\|^2_{k(\boldsymbol{\mu})^{-1}} \tag{4.34}$$

where $\bar{T}(\boldsymbol{\mu})$ is the reduced basis surrogate and we require that approximate dual field $\bar{q}(\boldsymbol{\mu}) \in \mathcal{S}$ be equilibrated[12]. In the second-term, the error in the dual field, can be seen as the sharpness of the error bound for the primal field. However, we see the hypercircle as symmetric in the dual and primal surrogate, and propose to construct a Galerkin ROM for

$$T(\boldsymbol{\mu}) \approx \bar{T}(\boldsymbol{\mu}) = \sum_{i=1}^{n_\phi} \phi_i \alpha_i(\boldsymbol{\mu}) + T_l(\boldsymbol{\mu}) \tag{4.35}$$

and a Galerkin ROM for

$$q(\boldsymbol{\mu}) = -k(\boldsymbol{\mu})\nabla T(\boldsymbol{\mu}) \approx \bar{q}(\boldsymbol{\mu}) = \sum_{i=1}^{n_\phi} \psi_i \beta_i(\boldsymbol{\mu}) + q_l(\boldsymbol{\mu}) \tag{4.36}$$

In these models, individual bases vectors ϕ_i satisfy the homogeneous Dirichlet conditions, while the ψ_i's satisfy the homogeneous flux admissibility conditions (set $f = 0$ and $q_d = 0$ in (4.23)). Liftings T_l and q_l satisfy, respectively, the Dirichlet constraints and the flux admissibility condition. They can be constructed easily by solving the reference finite element problem at a particular point $\boldsymbol{\mu}_0 \in \mathcal{P}$ with multiple right-hand sides corresponding to the affine terms of the inhomogeneous primal and dual admissibility conditions. Consequently, we can find the optimal reduced solutions by minimising, without constraint, the potential energy and the complementary energy. Notice that this idea is closely related to that proposed in [56] in the context of the Proper Generalised Decomposition and is detailed in [27] for Galerkin-POD ROMs.

We then seek to construct the primal and dual reduced bases by successive minimisation of the Constitutive Relation Error *as a whole*, which will seamlessly take care of the trade-off between the accuracy in the primal surrogate and the sharpness of the error bound. One step of the corresponding Greedy algorithm is as follows:

- Locate the point of the parameter domain where the Constitutive Relation Error is maximum
- Compute the exact solution *i.e.* solve for the primal field and post-process the corresponding flux

[12] In the finite element sense only, as our reference is a finely discretised finite element mode. See Paper 2.3 for more details.

- Determine whether it is preferable to enrich the primal or dual reduced basis, and enrich accordingly, after performing the usual orthonormalisation step.

We also extended the methodology to the construction of goal-oriented ROM, through the greedy minimisation of the uncertainty interval in which the quantity of interest is found, and guaranteed, to lie. In this case, the proposed algorithm jointly constructs four Galerkin ROM, two for the primal and dual surrogates associated with the forward parametrised problem and two for the primal and dual surrogates associated with the adjoint problem (see *e.g.* [42, 43, 44, 111, 110, 25]).

The approach is conceptually simple, and it is shown to be computationally advantageous compared to competing methodologies, notably in terms of computational time required to explore the parameter domain and build the Galerkin ROM offline.

CHAPTER 5

Towards seamless model adaptivity: the role of implicit boundary finite element solvers

Introduction

Integrated computational paradigms that blend together geometrical descriptions and finite element analyses are emerging. This is in response to aa strong engineering need to facilitate data flows from geometrical design and image processing tools to PDE solvers.

Technological bottlenecks in this area are complex and varied. For instance, aircraft manufacturing is heading towards digital twining. However, performing detailed finite elements simulations of entire aircraft is simply out-of-the question. Hotspots need to be identified and analysed in a global-to-local manner, for instance to predict the growth of local defects from global stress levels. This suggests a need to generate computational models at different scales, starting from a coarse, shell-based geometrical model of the entire aircraft, zooming-in to 3D models of joints and critical parts, and finally going down to the micro/meso-scale where the composite failure may initiate. Such complex digital pipelining needs to be highly automatised in order to minimise the need for engineers to manipulate heavy geometrical models by hand.

The model adaptivity framework advocated in this thesis, whereby the level of fidelity of computational models is adapted based to solution features, makes the need for seamless geometry-to-analysis pipelines even more stringent. Indeed, within this framework, model enrichment may be done "on-the-fly", which requires a level of robustness and automatism that is still not delivered by today's meshing technology.

Simplifying and robustifying geometry-to-analyses pipelines is a multi-disciplinary challenge in which the Computational Mechanics community is playing an important role. Innovative developments include the Isogeometric Analysis methodology proposed in [112], which proposes to use the shape descriptors of CAD softwares (*e.g.* NURBS) to approximate PDE unknowns. In this way, the complexity of the operations that are required to produce an analysis-ready model from CAD data is considerably reduced [113, 114]. Another approach to enable data-to-simulation seamless pipelining is the family of implicit boundary solvers,

which include the XFEM [103, 115, 116] and the CutFEM [117, 118] methods. In this case, the requirement for the computational mesh to conform to the geometry is dropped, which eventually leads to reduced meshing complexity. In the version of CutFEM that will be briefly discussed in this section, the geometry is described by the level-set method, which treats geometrical data like any other finite element field, allowing us to perform automatised, simulation-controlled geometrical modifications in an agile and robust manner. As it stands, this technology is a very promising tool for model adaptivity. This section exemplifies this idea, and introduces my research contributions in this area, which concerns the development of primal/dual CutFEM solvers for the simulation of composite materials and manufacturing by thermal ablation.

5.1 Towards seamless model adaptivity: a flexible implicit boundary "Cut" finite element solver.

5.1.1 The CutFEM / level-set technology

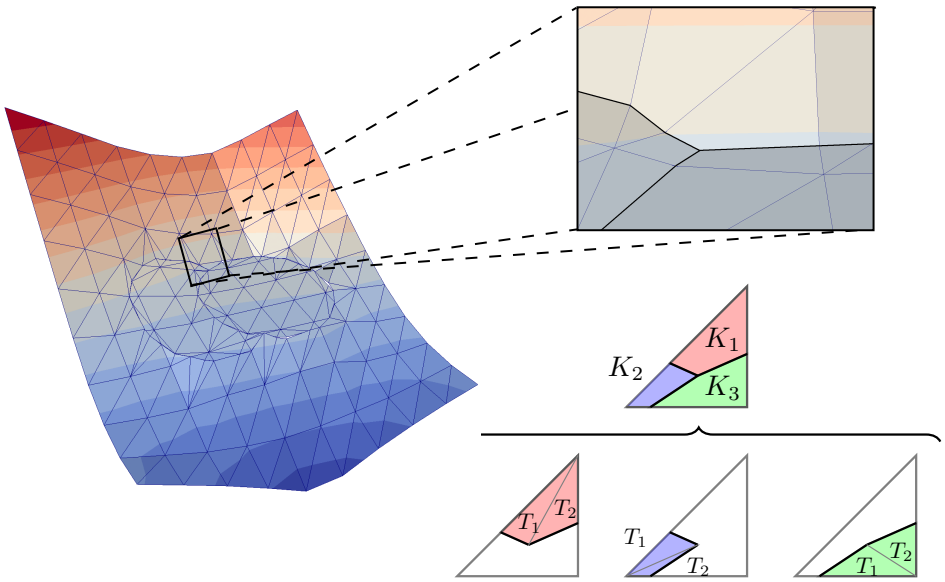


Figure 5.1: CutFEM technology. The primal field is described by the finite element space associated with the background finite element mesh, independently for the two inclusions and for the embedding matrix. This domain decomposition approach naturally introduces jumps and kinks in solution fields at the interface between components.

The CutFEM method is an overlapping domain decomposition approach. The geometries of interacting bodies, material phases or embedded manifolds, are described independently of the computational mesh. The mesh is regular and allowed to be cut by the boundary of the geometrical entities. Each body, phase or embedded manifold is independently described by the kinematics of all the elements of the regular background mesh that are either strictly contained within the domain occupied by the body, or that are cut by the boundary of the body. The PDE is only integrated over the physical part of this union of elements, which

requires dedicated integration schemes. Noticeably, elements that are intersected by the interface between two interacting bodies are naturally doubled. This overlapping domain decomposition strategy generates the same element kinematics than that provided by XFEM through partition-of-unity enrichments of Heavisde type [102, 103, 94, 21, **?**].

The overlapping domains may be coupled by the user's method of choice. Traditionally, Nitsche's method has been used to enforce perfect bonding conditions between heterogeneous bodies [117, 118]. The work presented in this thesis focusses on Signorini conditions, for which LaTIn-based primal/dual formulations [119, 5, 120, 22], and Nitsche, purely primal nonlinear solvers [121, 122, 4] have been developed.

A critical aspect of CutFEM solvers is the regularisation strategy, which must be performed in order to circumvent the conditioning issues associated with "bad cuts". These difficulties may be worsen in the context of high-contrast and non-conforming interface coupling, which is particularly relevant to the context of model adaptivity. In most cases, the Ghost-Penalty regularisation technique [123] is employed.

5.1.2 Examples of numerical capabilities

The CutFEM strategies that are discussed in this thesis have been implemented in the finite element package FEniCS [124, 125, 126, 118]. One of the strong points of this computational library is that finite element operator are generated automatically from a dedicated python interface where problems are described in a form "a(u,v)=l(v)" *i.e.* very close to the mathematical formalism of PDEs. To do this, the FEniCS library relies on an exhaustive collection of finite elements, a full integration of PETSc solvers for parallel computing, and automatic differentiation capabilities. Coupled with the "no-meshing" capabilities of CutFEM, this is a very strong starting point to develop frictionless digital pipelines such as those illustrated below.

Digital pipelining from CAD and voxel maps to analysis. Avoiding meshing and remeshing is one of the traditional uses of implicit boundary FE methods. Figure 5.2 illustrates a digital pipeline whereby STL (stereolithography CAD) descriptions of surfaces, which may not be of sufficient quality for analyses purposes (*e.g.* gaps, distorted elements) are first converted into a level-set, which is described as a finite element field over on regular grid, before deploying the CutFEM technology over the "repaired" geometry described by the zero isoline of the finite element level-set.

Flexible model coupling. An example of model coupling that the CutFEM technology simplifies is the case of PDEs over embedded manifold. This is exemplified in Figure 5.3. The embedded 1D elements are bars with zero bending energy. These bars transmit forces to the matrix phase of the composite through friction. Damage is captured by making use of the phase-field method proposed in [127], and iterations between the three material phases are performed by a LaTIn primal/dual domain decomposition algorithm. Interestingly, the 1D fibrous elements are not meshed. Instead, the PDE of the bar is solved by making use of the kinematic space defined by the trace of the intersected elements.

Another example of model coupling that is relevant to the model adaptivity approaches that were presented in Chapter 2 is illustrated in figure 5.4. Two hierarchical background grids are used to allow for model unrefinement. The geometry is described by two level sets,

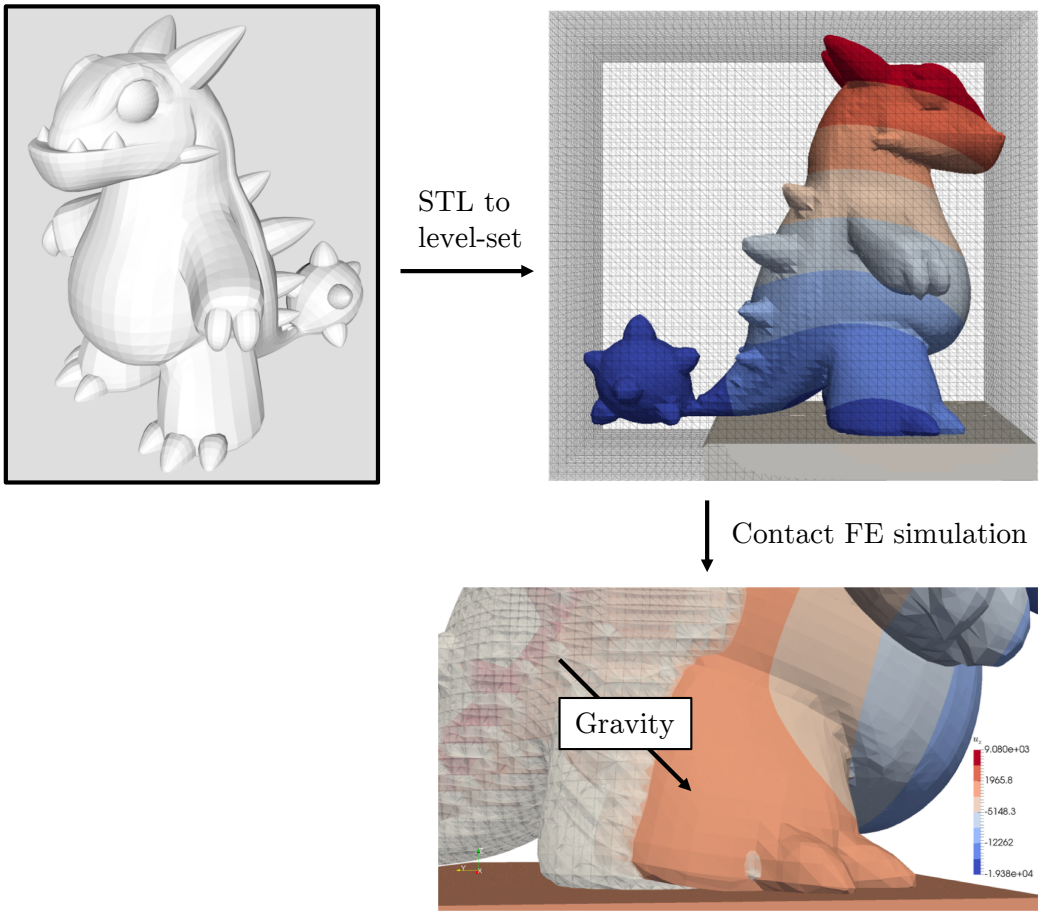


Figure 5.2: Digitial pipeline from geometrical data to FE analysis. The 3D STL Model was created by ThinkerThing to be 3D printed. Only the surface mesh of the component is avaliable. The quality of this mesh is insufficient for analysis purposes. An analysis-ready geometrical description is recovered through the construction of a finite element level-set, which constitutes the starting point of a "Cut" FE analysis.

a fine-scale for the micro-inclusions, and a coarse-scale level set for the coarse model. All interactions are handled by Nitsche's (weighted) method. With such a technology, model adaptivity can be done almost seamlessly by simply modifying the nodal values of the coarse level set. Of course, finite element operators have to be reconstructed, at least locally, but there is no remeshing operation involved. This feature ensures that the scheme is robust, which cannot be expected of a traditional mesh-conforming concurrent multiscale solver.

5.2 Summary of papers

The last part of my thesis introduces two original contributions in the area of CutFEM solvers. The developments are dedicated to the treatment and stabilisation of Signorini problems written in mixed forms, with applications in contact mechanics and precision manufacturing

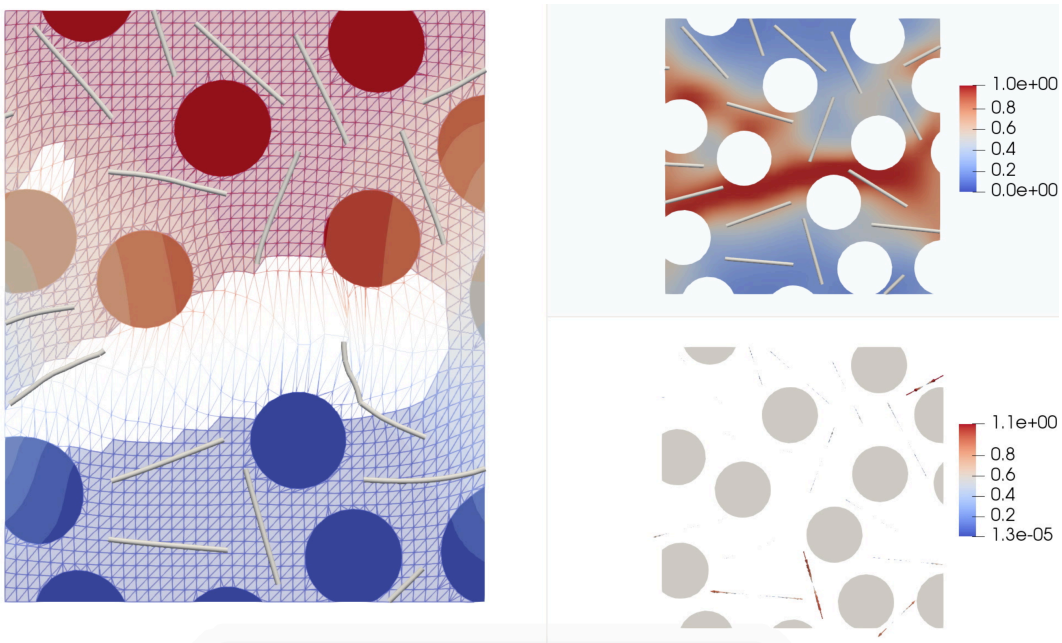


Figure 5.3: Unidirectional elastic fiber elements embedded in a damageable matrix. The bond between the fibers and the matrix is inelastic, and yields above a certain level of axial force. A dedictaed LaTIn algorithm is deployed to solve the coupled problem in primal/dual form.

by laser ablation.

Paper 3.1: Primal dual CutFEM method for unilateral contact [22]

This paper is one of the first applications of CutFEM for the simulation of composite structures with imperfect contact conditions. The general strategy is the LaTIn domain decomposition approach, as presented for instance in [128, 119, 5]. This solver is both a primal-dual domain decomposition strategy (see [129, 130] for different but closely related solvers), and an Uzawa-type solution algorithm when applied to the Karush-Kuhn-Tucker systems that arises in the simulation of unilateral contact. Noticeably, the method is algorithmically similar to the augmented Lagrangian method proposed in [131].

Primal-dual methods are notoriously difficult to develop due to the fact that the Lagrange multipliers need to be chosen in Inf-Sup stable spaces. A wide range of papers have been published on the topic. In the LaTIn method, authors have used P0/P2 discretisation techniques (piecewise constant Lagrange multiplier fields and piecewise quadratic finite element fields for the displacement in the bulk) and they have reported stabilising effects.

This difficulty is even more stringent in the context of the proposed implicit boundary method [132, 133, 134, 135], where the contact interface is non-conforming and may lead to "bad cut" cases. The paper describes an algorithmic stabilisation approach based on the Ghost Penalty method. At the end of the usual local stage of the LaTIn algorithm, the

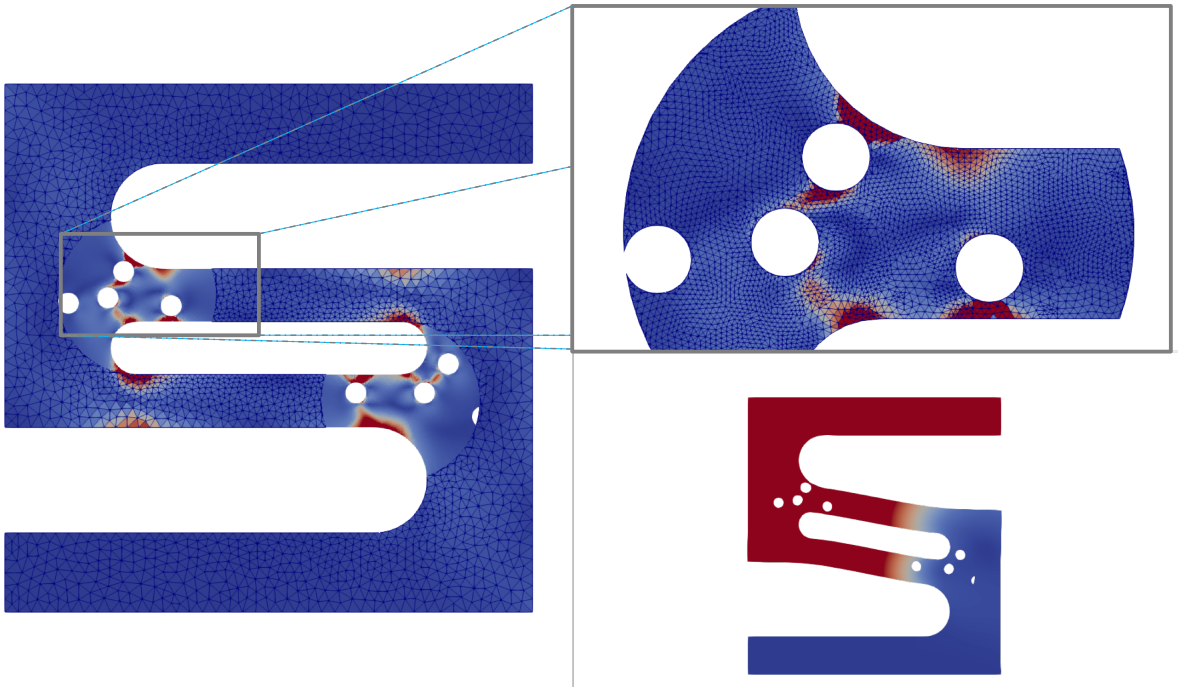


Figure 5.4: The "Zoom" FEM multi-resolution methodology. A fine regular finite element mesh is easily obained by hierarchical refinement of a coarse grid. One may adapt the level of local resolution by simply evolving the (coarse) level-set that desribes the interface between micro and macro regions.

Lagrange multiplier field is "smoothed" by using a stabilised projection operation, which only involves the solution of a linear system of equations for the band of intersected elements.

The proposed stabilised LaTIn-CutFEM method can be shown to be related to the Ghost-Penalty stabilisation of the augmented Lagrangian approach proposed in [120] (our approach is a non-symmetric variant of it). However, our approach can be applied to more complex interface conditions. For example, the STL dinosaur represented in Figure 5.2 is sliding on an inclined plane (gravity is titled), which is simulated using Coulomb friction. This solver is also the core of the embedded manifold modelling formulation that was discussed in the previous section (Figure 5.3).

Paper 3.2: CutFEM method for Stefan-Signorini problems [4]

The second paper of this section focusses on the development of a CutFEM solver for Stefan-Signorini problems, whereby phase changes are represented using a unilateral latent heat condition (see for instance [136], which has inspired our work). This is the area of moving interface problems, where implicit boundary approaches are appealing alternatives to mesh moving solvers and smoothed interface methods [137].

Although we could have used the primal-dual approach described in the previous section, we developed here a nonlinear primal Nitsche approach similar to that described in [121, 138]. The key point of the paper is the extension and smoothing of the velocity (*i.e.* dual interface variables in the Stefan-Signorini problem) using a Ghost-Penalty stabilised projection. To-

gether with a higher-order solution of the advection problem corresponding to the sequential update of the level-set, this operation ensures that the convergence rate of the CutFEM solver is optimal in the space-time domain.

CHAPTER 6

Conclusion and perspectives

6.1 Concluding statement

There is a growing interest in integrating high-fidelity digital twins into engineering systems. Indeed, this technology is expected to constitute the computational core of the next generation of smart digital systems. For instance, digital twinning would allow engineers to accurately predict the risk of failure of ageing aircrafts, through continuous data assimilation and high-fidelity-model-based forecasting. Complex manufacturing technologies could be controlled in real-time using reliable model predictions of product deviations to design specifications. However, the rise of computational-mechanics-based digital twinning is obstructed by the cost of the computations associated with finite element models, and by a certain lack of robustness of associated digital pipelines. In this thesis, I have introduced and summarised my contributions towards the development of high-fidelity digital twinning paradigms in computational mechanics. In particular, I have proposed a range of innovative numerical algorithms that automatically redirect the numerical effort to where it is needed most, using specificities of classes of PDE-based problems to fasten their solutions by several order of magnitude. I have organised the thesis in three chapters, each of them dedicated to one family of reduced modelling approaches: (i) projection-based model reduction techniques for nonlinear fracture (ii) error-driven adaptive multiscale modelling and (iii) no-meshing implicit boundary finite element solvers. The conclusions below will be given chapter-by-chapter.

To fasten online high-fidelity simulations, one of the most attractive technological avenues is that of Reduced Order Modelling. Over the last ten years, a significant research effort has made these advanced meta-modelling techniques applicable to a wide range of problems. In the first chapter of this thesis, I have presented innovative developments in the area of ROM for damage mechanics. In this context, regions of materials and structures exhibiting high levels of propagating damage must be treated without reduction for projection-based ROM to deliver significant speed-up. I have also shown the importance of acquiring the right "offline" data (snapshot). This should be done through an appropriate combination of uncertainty minimisation and greedy-based training algorithms, I have applied this concept for

the efficient ROM of time-dependent computational material point problems, where sample material responses may be generated "offline" in a quasi-optimal manner. The future of ROM lies in combining offline/online decomposition with "on-the-fly" adaptivity. Weakly reducible problems in large parameter dimensions cannot be expected to be treated in a pure offline/online fashion. Instead, offline computations must be used to segregate regions of spatial and parameters domains, allowing for the construction and selection of local reduced models. The reduced models must be adaptive to correctly capture structural behaviour that has not been correctly identified offline. This is especially important in the context of reliability assessment where the tail of distributions (outliers) is the quantity of interest. Further research is needed in this area. In particular, error estimates for reduced bases approaches are insufficiently developed and should be strengthened to guide the adaptive construction of reduced models in high-dimensional spaces.

Multiscale modelling is and will continue to be central to the development of high-fidelity computational mechanics models. Indeed, incorporating smaller scales knowledge allows scientists to go beyond phenomenological approaches for complex multiscale phenomena such as material damage and fracture. However, the accurate representation of complex microscopic evolutions incurs a tremendous computational cost. This is an important bottleneck for online high-fidelity computing. In the second chapter of this thesis, I have presented methods aimed to control the amount of energy used to upscale microscopic information. Only the information that has an effect on the micro or macro quantities of interest should be upscaled, the information flow being treated by averaging or in a phenomenological manner everywhere else. The key here is to be able to locate and quantify errors due to upscaling and/or other model approximations. I have presented several contributions that estimate such errors, using duality principles to certify the quality of adaptively refined two-scale models. The extension of such techniques to nonlinear problems is difficult but should be pursued. For instance, model error estimation may benefit from current developments in machine learning technologies. In this context, we may wish to develop general strategies to build or correct error models using elements of statistical learning.

With the prominence of the "big data" premise and machine learning technologies, there is a growing appetite for the development of data-driven computational mechanics approaches. For instance, 3D imaging offers access to new sources of information to calibrate and correct high-fidelity PDE-based models. However, the digital flow to and from finite element models remains far from seamless, and must be facilitated. In the third scientific chapter of this thesis, I have presented my contributions to the development of unfitted finite element solvers for computational micromechanics and advanced manufacturing simulations. This technology diminishes engineers' reliance upon meshing tools, and may be used to perform simulations from 3D images and CAD models directly. The robustness of this technology is key as it will allow testing scenarios within optimisation loops, and may eventually be used to construct simulation-based machine learning methodologies, where the prior knowledge about engineering materials and structures is faithfully encoded in a finite element model.

6.2 Quelques perspectives de recherche

L'ingénierie digitale est à une croisée des chemins. En effet, les méthodes de résolution des équations aux dérivées partielles sont aujourd'hui relativement matures. Cependant, l'impact

de ces méthodes reste limité lorsque l'on considère leur intégration dans des systèmes industriels (contrôle en temps réel, certification virtuelle et automatisée, lien avec le Big Data). Fort de ce constat, je souhaite continuer mes recherches en méthodes numériques avancées, avec comme direction générale le développement d'une nouvelle génération de cerveaux numériques pour les systèmes intelligents. Ces algorithmes seront basés sur une représentation fine de la partie bien comprise des phénomènes physiques impliqués, et seront complétés par des approches de type machine learning et assimilation de données pour, respectivement, pallier le manque de compréhension du reste de ces phénomènes et (ii) recaler les modèles, avec la possibilité d'acquérir des donnés de qualité de manière automatisée (minimisation des méconnaissances, ...). De telles approches seront extrêmement lourdes en ressources de calculs, et demanderont (i) un contrôle rationalisé du rapport coût/qualité des différents outils numériques impliqués dans ces systèmes intelligents et (ii) une stabilité accrue des outils numériques pour leur utilisation dans des systèmes numériques fermés.

Dans la suite de ce chapitre, je présente brièvement les thèmes de recherche que je souhaite approfondir. J'aborde deux sujets en particulier: le jumelage numérique pour les procédés de fabrication de l'industrie 4.0 et l'apprentissage des modèles multi-échelles par la donnée.

6.2.1 Jumelage numérique pour l'usinage laser de précision et la fabrication additive.

Je travaille depuis quelques années sur les thématiques d'usinage laser avec mon collègue Samuel Bigot à Cardiff, et c'est une discipline dans laquelle je compte investir de plus en plus de temps. Un des verrous scientifiques liés à cette discipline concerne le manque de stratégie fiable pour le contrôle de qualité par boucles de rétroaction, que ce soit au niveau des tolérances de forme, ou des propriétés matériaux constituant les pièces usinées. Aujourd'hui encore, la calibration empirique des paramètres d'usinage, comme le trajet d'outil ou les caractéristiques du signal d'entrée du laser, sont invalides en dehors du champ des configurations testées, ce qui limite grandement les possibilités d'optimisation du procédé. Une approche de type jumelage numérique, avec comme cœur un simulateur fiable du procédé d'ablation thermique, permettrait de pallier cette limitation technologique, en explorant l'espace des paramètres d'usinage de manière virtuelle (Figure 6.1). En outre, les données géométriques sont aujourd'hui faciles à générer grâce l'imagerie 3D, ouvrant des portes pour effectuer le recalage de nombreux paramètres, voire de laisser libres des parties entières du modèle (modèle mixte entre équations aux dérivées partielles et réseaux de neurones par exemple).

Il s'agit d'un thème scientifique passionnant pour lequel des compétences interdisciplinaires complémentaire sont nécessaires. Mon expertise en réduction des coûts de calculs sera particulièrement mise à profit dans le cadre du développement de simulateurs multi-échelle pour l'usinage laser et la fabrication additive, le but ultime est de pouvoir réaliser des séries d'usinages virtuels de taille réaliste avec des ressources numériques limitées.

6.2.2 Optimisation robuste et caractérisation de l'endommagement dans les structures composites.

Les calculs de rupture des matériaux composites et architecturés, notamment ceux réalisés sur plusieurs échelles couplées, sont trop lourds pour ne serait-ce qu'envisager leur utilisation dans des systèmes avec boucles de rétroaction, ou dans le cadre de l'assimilation de données.

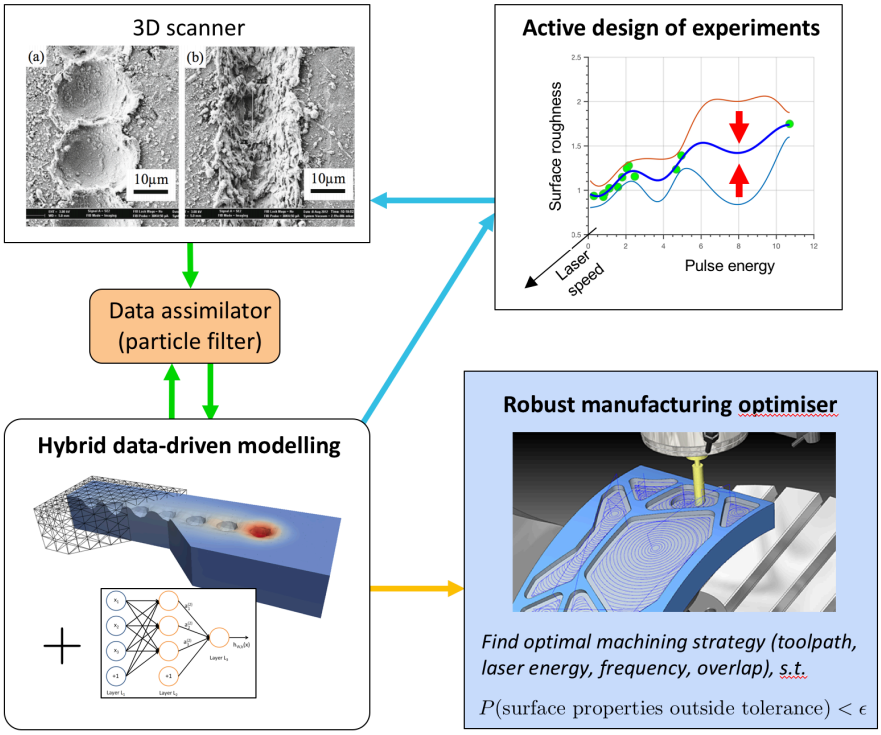


Figure 6.1: Jumeau numérique pour l'usinage laser de précision

Je propose donc de continuer mon travail sur la rationalisation des coûts de calcul associés aux simulations multi-échelle haute-fidélité. Dans ce cadre j'envisage plusieurs directions de recherche complémentaires :

- **Prédiction de la durée de vie résiduelle de structures mécaniques en service.** Bien qu'on soit aujourd'hui capable de détecter la propagation de défauts dans les structures (par suivi des émissions acoustiques par exemple), il est aujourd'hui difficile de diagnostiquer l'état de la structure, et donc de prévoir l'évolution de l'endommagement. Je souhaite utiliser des modèles multi-échelle d'endommagement, associé à une représentation probabiliste du chargement à l'échelle macroscopique, pour calculer une distribution des états d'endommagements possibles, et la durée de vie résiduelle associée.

- **Contrôles des chaines d'approximations.** Depuis quelques années, je m'intéresse au problème de quantification de l'effet combiné de différentes sources d'erreurs dans les chaines d'approximation numériques. Des travaux préliminaires ont montré qu'il est possible de réduire la taille des modèles éléments finis de manière à adapter le niveau d'erreur au niveau d'incertitudes existant sur les données, et à la précision des algorithmes de Monte-Carlo [28]. Je compte poursuivre ces travaux importants, que je vois comme une passerelle déterminante entre la mécanique numérique haute-fidélité d'une part, et les approches de recalage reposant sur des modélisation simplifiées d'autre part.

- **Apprentissage des modèles multi-échelle par la donnée numérique.** Une nou-

velle utilisation des outils de la science des données est aujourd'hui en train de voir le jour. Dans ce cadre, la donnée est numérique, générée en utilisant un modèle fin de la physique, peut-être local, et l'on cherche à calibrer un modèle plus grossier, utilisable à coût réduit. Bien sûr, cette idée est au cœur de la démarche de réduction de modèle par projection sur lesquelles j'ai travaillé dans le passé, et elle semble être généralisable à la construction d'autres types d'approximations numériques. Dans ce cadre, je souhaite développer des méthodes permettant d'apprendre des corrections numériques pour les modèles multi-échelle (apprentissage d'un terme d'erreur par exemple, comme proposé dans [17, 28]). Ces corrections seront utilisées pour accroitre le pouvoir de prédiction des modèles micro/macro dans les zones d'amorçage des défauts, là où la séparation des échelles sur laquelle les méthodes d'homogénéisation sont fondées est généralement perdue.

References

[1] Susanne Claus and Pierre Kerfriden. A CutFEM method for two-phase flow problems. *Computer Methods in Applied Mechanics and Engineering*, 348:185–206, 2019.

[2] Navid Rahimi, Pierre Kerfriden, Frank C Langbein, and Ralph R Martin. CAD model simplification error estimation for electrostatics problems. *SIAM Journal on Scientific Computing*, 40(1):B196–B227, 2018.

[3] Hadrien Courtecuisse, Jérémie Allard, Pierre Kerfriden, Stéphane PA Bordas, Stéphane Cotin, and Christian Duriez. Real-time simulation of contact and cutting of heterogeneous soft-tissues. *Medical image analysis*, 18(2):394–410, 2014.

[4] Susanne Claus, Samuel Bigot, and Pierre Kerfriden. CutFEM Method for Stefan–Signorini Problems with Application in Pulsed Laser Ablation. *SIAM Journal on Scientific Computing*, 40(5):B1444–B1469, 2018.

[5] P. Kerfriden, O. Allix, and P. Gosselet. A three-scale domain decomposition method for the 3D analysis of debonding in laminates. *Computational Mechanics*, 44(3):343–362, 2009.

[6] O. Allix, P. Kerfriden, and P. Gosselet. A relocalization technique for the multiscale computation of delamination in composite structures. *Computer Modeling in Engineering and Sciences*, 55(3):271–291, 2010.

[7] O. Allix, P. Kerfriden, and P. Gosselet. On the control of the load increments for a proper description of multiple delamination in a domain decomposition framework. *International Journal for Numerical Methods in Engineering*, 83:1518–1540, 2010.

[8] Ahmad Akbari Rahimabadi, Pierre Kerfriden, and Stéphane Bordas. Scale selection in nonlinear fracture mechanics of heterogeneous materials. *Philosophical Magazine*, 95:3328–3347, 2015.

[9] D. A. Paladim, J. P. Moitinho de Almeida, S. P. A. Bordas, and P. Kerfriden. Guaranteed error bounds in homogenisation: An optimum stochastic approach to preserve

the numerical separation of scales. *International Journal for Numerical Methods in Engineering*, 110:103–132, 2017.

[10] Hossein Talebi, Mohammad Silani, Stéphane PA Bordas, Pierre Kerfriden, and Timon Rabczuk. Molecular dynamics/XFEM coupling by a three-dimensional extended bridging domain with applications to dynamic brittle fracture. *International Journal for Multiscale Computational Engineering*, 11(6), 2013.

[11] Hossein Talebi, Mohammad Silani, Stéphane PA Bordas, Pierre Kerfriden, and Timon Rabczuk. A computational library for multiscale modeling of material failure. *Computational Mechanics*, 53(5):1047–1071, 2014.

[12] Khac Chi Hoang, Pierre Kerfriden, B. C. Khoo, and S. P. A. Bordas. An efficient goal-oriented sampling strategy using reduced basis method for parametrized elastodynamic problems. *Numerical Methods for Partial Differential Equations*, 31(2):575–608, 2015.

[13] K.C. Hoang, P. Kerfriden, and S.P.A. Bordas. A fast, certified and "tuning free" two-field reduced basis method for the metamodelling of affinely-parametrised elasticity problems. *Computer Methods in Applied Mechanics and Engineering*, 298:121–158, 2016.

[14] P. Kerfriden, O. Goury, T. Rabczuk, and S.P.-A. Bordas. A partitioned model order reduction approach to rationalise computational expenses in nonlinear fracture mechanics. *Computer Methods in Applied Mechanics and Engineering*, 200(5):850–866, 2012.

[15] P. Kerfriden, K. M. Schmidt, T. Rabczuk, and S. P.-A. Bordas. Statistical extraction of process zones and representative subspaces in fracture of random composites. *International Journal for Multiscale Computational Engineering*, 11(3):271–292, 2013.

[16] Mohammad Silani, Hossein Talebi, Saeed Ziaei-Rad, Pierre Kerfriden, Stéphane PA Bordas, and Timon Rabczuk. Stochastic modelling of clay/epoxy nanocomposites. *Composite Structures*, 118:241–249, 2014.

[17] Olivier Goury, David Amsallem, Stéphane Pierre Alain Bordas, Wing Kam Liu, and Pierre Kerfriden. Automatised selection of load paths to construct reduced-order models in computational damage micromechanics: From dissipation-driven random selection to Bayesian optimization. *Computational Mechanics*, 58(2):213–234, 2016.

[18] P. Kerfriden, P. Gosselet, S. Adhikari, and S.P.-A. Bordas. Bridging proper orthogonal decomposition methods and augmented Newton-Krylov algorithms: An adaptive model order reduction for highly nonlinear mechanical problems. *Computer Methods in Applied Mechanics and Engineering*, 200(5-8):850–866, 2011.

[19] P. Kerfriden, J.-C. Passieux, and S.P.-A. Bordas. Local/global model order reduction strategy for the simulation of quasi-brittle fracture. *International Journal for Numerical Methods in Engineering*, 89(2):154–179, 2011.

[20] Stéphane PA Bordas, Sundararajan Natarajan, Pierre Kerfriden, Charles Edward Augarde, D. Roy Mahapatra, Timon Rabczuk, and Stefano Dal Pont. On the performance of strain smoothing for quadratic and enriched finite element approximations (XFEM/GFEM/PUFEM). *International Journal for Numerical Methods in Engineering*, 86(4-5):637–666, 2011.

[21] O.A. González-Estrada, J.J. Ródenas, S.P.A. Bordas, E. Nadal, P. Kerfriden, and F.J. Fuenmayor. Locally equilibrated stress recovery for goal oriented error estimation in the extended finite element method. *Computers & Structures*, 152:1–10, 2015.

[22] Susanne Claus and Pierre Kerfriden. A stable and optimally convergent LaTIn-CutFEM algorithm for multiple unilateral contact problems. *International Journal for Numerical Methods in Engineering*, 113(6):938–966, 2018.

[23] Vinh Phu Nguyen, Pierre Kerfriden, and Stéphane PA Bordas. Two-and three-dimensional isogeometric cohesive elements for composite delamination analysis. *Composites Part B: Engineering*, 60:193–212, 2014.

[24] Vinh Phu Nguyen, Pierre Kerfriden, Marco Brino, Stéphane PA Bordas, and Elvio Bonisoli. Nitsche's method for two and three dimensional NURBS patch coupling. *Computational Mechanics*, 53(6):1163–1182, 2014.

[25] O.A. González-Estrada, E. Nadal, J.J. Ródenas, P. Kerfriden, S.P.-A. Bordas, and F.J. Fuenmayor. Mesh adaptivity driven by goal-oriented locally equilibrated superconvergent patch recovery. *Computational Mechanics*, 53:957–976, 2013.

[26] Peng Yu, Cosmin Anitescu, Satyendra Tomar, Stéphane Pierre Alain Bordas, and Pierre Kerfriden. Adaptive Isogeometric analysis for plate vibrations: An efficient approach of local refinement based on hierarchical a posteriori error estimation. *Computer Methods in Applied Mechanics and Engineering*, 342:251–286, 2018.

[27] P. Kerfriden, J. J. Ródenas, and S. P.-A. Bordas. Certification of projection-based reduced order modelling in computational homogenisation by the constitutive relation error. *International Journal for Numerical Methods in Engineering*, 97(6):395–422, 2014.

[28] Pierre Kerfriden, Abhishek Kundu, and Susanne Claus. Adaptivity in Bayesian Inverse Finite Element Problems: Learning and Simultaneous Control of Discretisation and Sampling Errors. *Materials*, 12(4):642, 2019.

[29] Kevin Carlberg, Charbel Farhat, Julien Cortial, and David Amsallem. The GNAT method for nonlinear model reduction: Effective implementation and application to computational fluid dynamics and turbulent flows. *Journal of Computational Physics*, 242:623–647, 2013.

[30] D Ryckelynck and D M Benziane. Multi-level a priori hyper-reduction of mechanical models involving internal variables. *Computer Methods in Applied Mechanics and Engineering*, 199(17-20):1134–1142, 2010.

[31] M. Barrault, Y. Maday, N.C. Nguyen, and A.T. Patera. An 'empirical interpolation' method: Application to efficient reduced-basis discretization of partial differential equations. *Comptes Rendus de Mathématiques*, 339(9):667–672, 2004.

[32] S. Chaturantabut and D.C. Sorensen. Nonlinear Model Reduction via Discrete Empirical Interpolation. *SIAM Journal on Scientific Computing*, 32:2737–2764, 2010.

[33] K. Kunisch and S. Volkwein. Galerkin Proper Orthogonal Decomposition Methods for a General Equation in Fluid Dynamics. *SIAM Journal on Numerical analysis*, 40(2):492–515, 2003.

[34] T. Braconnier, M. Ferrier, J.-C. Jouhaud, and P. Sagaut. Towards an Adaptive POD/SVD Surrogate Model for Aeronautic Design. *Computers and Fluids*, 40(1):195–209, 2011.

[35] K. Kunisch and S. Volkwein. Optimal snapshot location for computing POD basis functions. *ESAIM: Mathematical Modelling and Numerical Analysis*, 44(3):509–529, 2010.

[36] C. Prud'homme, D. V. Rovas, K. Veroy, L. Machiels, Y. Maday, A. T. Patera, and G. Turinici. Reliable Real-Time Solution of Parametrized Partial Differential Equations: Reduced-Basis Output Bound Methods. *Journal of Fluids Engineering*, 124(1):70–80, 2002.

[37] D.B.P. Huynh G. Rozza and A.T. Patera. Reduced basis approximation and a posteriori error estimation for affinely parametrized elliptic coercive partial differential equations: Application to transport and continuum mechanics. *Archives of Computational Methods in Engineering*, 15(3):229–275, 2008.

[38] Bernard Haasdonk and Mario Ohlberger. Reduced basis method for finite volume approximations of parametrized linear evolution equations. *ESAIM: Mathematical Modelling and Numerical Analysis*, 42:277–302, 2008.

[39] A. Paul-Dubois-Taine and D. Amsallem. An adaptive and efficient greedy procedure for the optimal training of parametric reduced-order models. *International Journal for Numerical Methods in Engineering*, 2014.

[40] Martin Drohmann and Kevin Carlberg. The ROMES method for statistical modeling of reduced-order-model error. *SIAM/ASA Journal on Uncertainty Quantification*, 3(1):116–145, 2015.

[41] Sumeet Trehan, Kevin T. Carlberg, and Louis J. Durlofsky. Error modeling for surrogates of dynamical systems using machine learning. *International Journal for Numerical Methods in Engineering*, 112(12):1801–1827, 2017.

[42] J. Tinsley Oden, Serge Prudhomme, J. T. Oden, and S. Prudhomme. Goal-Oriented Error Estimation and Adaptivity for the Finite Element Method. *Compututer Methods in Applied Mechanics and Engineering*, 41:735–756, 1999.

[43] F. Cirak and E. Ramm. A posteriori error estimation and adaptivity for elastoplasticity using the reciprocal theorem. *International Journal for Numerical Methods in Engineering*, 47:379–393, January 2000.

[44] Roland Becker and Rolf Rannacher. An optimal control approach to a posteriori error estimation in finite element methods. *Acta Numerica 2001*, 10:1–102, 2001.

[45] T. Bui-Thanh, K. Willcox, O. Ghattas, and B. van Bloemen Waanders. Goal-oriented, model-constrained optimization for reduction of large-scale systems. *Journal of Computational Physics*, 224(2):880–896, 2007.

[46] P. Ladevèze, J.C. Passieux, and D. Néron. The LaTIn multiscale computational method and the Proper Generalized Decomposition. *Computer Methods in Applied Mechanics and Engineering*, 199(21):1287–1296, 2009.

[47] F. Chinesta, A. Ammar, and E. Cueto. Recent Advances and New Challenges in the Use of the Proper Generalized Decomposition for Solving Multidimensional Models. *Archives of Computational Methods in Engineering - State of the Art Reviews*, 17(4):327–350, 2010.

[48] A. Nouy. A priori model reduction through Proper Generalized Decomposition for solving time-dependent partial differential equations. *Computer Methods in Applied Mechanics and Engineering*, 199(23-24):1603–1626, 2010.

[49] D. Ryckelynck. A priori hyperreduction method: An adaptive approach. *Journal of Computational Physics*, 202(1):346–366, 2005.

[50] D. Ryckelynck, F. Chinesta, E. Cueto, and A. Ammar. On the a priori model reduction: Overview and recent developments. *Archives of Computational Methods in Engineering, State of the Art Reviews*, 13(1):91–128, 2006.

[51] Alberto Corigliano, Martino Dossi, and Stefano Mariani. Domain decomposition and model order reduction methods applied to the simulation of multi-physics problems in MEMS. *Computers & Structures*, 122:113–127, 2013.

[52] Matthew J. Zahr and Charbel Farhat. Progressive construction of a parametric reduced-order model for PDE-constrained optimization. *International Journal for Numerical Methods in Engineering*, 102(5):1111–1135, 2015.

[53] Tiangang Cui, Youssef M. Marzouk, and Karen E. Willcox. Data-driven model reduction for the Bayesian solution of inverse problems. *International Journal for Numerical Methods in Engineering*, 102(5):966–990, 2015.

[54] S. Sen, K. Veroy, D.B.P. Huynh, S. Deparis, N.C. Nguyen, and A.T. Patera. "Natural norm" a posteriori error estimators for reduced basis approximations. *Journal of Computational Physics*, 217(1):37–62, 2006.

[55] D.B.P. Huynh, G. Rozza, S. Sen, and A.T. Patera. A successive constraint linear optimization method for lower bounds of parametric coercivity and inf–sup stability constants. *Comptes Rendus Mathematique*, 345(8):473–478, 2007.

[56] P. Ladevèze and L. Chamoin. On the verification of model reduction methods based on the proper generalized decomposition. *Computer Methods in Applied Mechanics and Engineering*, 200(23-24):2032–2047, 2011.

[57] J. Mandel. Balancing domain decomposition. *Communications in Numerical Methods in Engineering*, 9(3):233–241, 1993.

[58] A. A. Radermacher and S. Reese. Model reduction in elastoplasticity: Proper orthogonal decomposition combined with adaptive sub-structuring. *Computational Mechanics*, 54(3):677–687, 2014.

[59] Alberto Corigliano, Federica Confalonieri, Martino Dossi, and Stefano Mariani. Coupled domain decomposition–proper orthogonal decomposition methods for the simulation of quasi-brittle fracture processes. *Advanced Modeling and Simulation in Engineering Sciences*, 3(1):28, November 2016.

[60] D. Rixen. A dual Craig-Bampton method for dynamic substructuring. *Journal of Computational and Applied Mathematics*, 168:383–391, 2004.

[61] P. Cresta, O. Allix, C. Rey, and S. Guinard. Nonlinear localization strategies for domain decomposition methods in structural mechanics. *Computer Methods in Applied Mechanics and Engineering*, 196:1436–1446, 2007.

[62] O. Lloberas-Valls, D.J. Rixen, Simone A., and L.J. Sluys. Domain decomposition techniques for the efficient modeling of brittle heterogeneous materials. *Computer Methods in Applied Mechanics and Engineering*, 200:1577–1590, 2011.

[63] P.-A. Guidault, O. Allix, L. Champaney, and S. Cornuault. A multiscale extended finite element method for crack propagation. *Computer Methods in Applied Mechanics and Engineering*, 197(5):381–399, 2008.

[64] F. Galland, A. Gravouil, E. Malvesin, and M. Rochette. A global model reduction approach for 3D fatigue crack growth with confined plasticity. *Computer Methods in Applied Mechanics and Engineering*, doi:10.1016/j.cma.2010.08.018, 2010.

[65] Dinh Bao Phuong Huynh, David J Knezevic, and Anthony T Patera. A static condensation reduced basis element method: Approximation and a posteriori error estimation. *ESAIM: Mathematical Modelling and Numerical Analysis*, 47(1):213–251, 2013.

[66] George J Dvorak. Transformation field analysis of inelastic composite materials. *Proc. R. Soc. Lond. A*, 437(1900):311–327, 1992.

[67] S. Ghosh, K. Lee, and P. Raghavan. A multi-level computational model for multi-scale damage analysis in composite and porous materials. *International Journal of Solids and Structures*, 38:2335–2385, 2001.

[68] J. Michel and P. Suquet. Computational analysis of nonlinear composite structures using the nonuniform transformation field analysis. *Computer Methods in Applied Mechanics and Engineering*, 193:5477–5502, December 2004.

[69] Caglar Oskay and Jacob Fish. Eigendeformation-based reduced order homogenization for failure analysis of heterogeneous materials. *Computer Methods in Applied Mechanics and Engineering*, 196(7):1216–1243, 2007.

[70] J. Yvonnet and Q.C. He. The reduced model multiscale method (R3M) for the nonlinear homogenization of hyperelastic media at finite strains. *Journal of Computational Physics*, 223(1):341–368, 2007.

[71] E. Monteiro, J. Yvonnet, and Q.C. He. Computational homogenization for nonlinear conduction in heterogeneous materials using model reduction. *Computational Materials Science*, 42(4):704–712, 2008.

[72] F. Fritzen and T. Böhlke. Three-dimensional finite element implementation of the nonuniform transformation field analysis. *International Journal for Numerical Methods in Engineering*, 84:803–829, November 2010.

[73] J.A. Hernández, J. Oliver, A.E. Huespe, M.A. Caicedo, and J.C. Cante. High-performance model reduction techniques in computational multiscale homogenization. *Computer Methods in Applied Mechanics and Engineering*, 276:149–189, 2014.

[74] A. Abdulle, Y. Bai, and G. Vilmart. Reduced basis finite element heterogeneous multiscale method for quasilinear elliptic homogenization problems. *Journal of Computational Physics*, (231):7014–7036, 2012.

[75] P. Breitkopf L. Xia. A reduced multiscale model for nonlinear structural topology optimization. *Computer Methods in Applied Mechanics and Engineering*, 280:117–134, 2014.

[76] Felix Fritzen and Matthias Leuschner. Nonlinear reduced order homogenization of materials including cohesive interfaces. *Computational Mechanics*, 56(1):131, July 2015.

[77] P. Ladevèze and J.-P. Pelle. *Mastering Calculations in Linear and Non Linear Mechanics*. Springer Verlag, New York, 2004.

[78] Erwin Stein and Marcus Rüter. Encyclopedia of Computational Mechanics. chapter Finite Element Methods for Elasticity with Error-controlled Discretization and Model Adaptivity. John Wiley & Sons, Ltd, 2004.

[79] P. Díez, N. Parés, and A. Huerta. Encyclopedia of Aerospace Engineering. chapter Error Estimation and Quality Control. Wiley Online Library, 2010.

[80] P. Gosselet and C. Rey. Non-overlapping domain decomposition methods in structural mechanics. *Archives of Computational Methods in Engineering*, 13:515–572, 2006.

[81] Jorge Nocedal and Stephen J. Wright. *Numerical Optimization*. Springer series in operation research and financial engineering. Springer, New York, NY, second edition edition, 2006.

[82] M. Ainsworth and J.T. Oden. *A Posteriori Error Estimation in Finite Element Analysis*. Wiley, Chichester, 2000.

[83] Pekka Neittaanmäki and Sergey R Repin. *Reliable Methods for Computer Simulation: Error Control and Posteriori Estimates*, volume 33. Elsevier, 2004.

[84] Thomas Grätsch and Klaus-Jürgen Bathe. A posteriori error estimation techniques in practical finite element analysis. *Computers and Structures*, 83:235–265, 2005.

[85] F. Pled, L. Chamoin, and P. Ladevèze. On the techniques for constructing admissible stress fields in model verification: Performances on engineering examples. *International Journal for Numerical Methods in Engineering*, 88(5):409–441, 2011.

[86] Rüdiger Verfürth. *A Posteriori Error Estimation Techniques for Finite Element Methods*. OUP Oxford, 2013.

[87] N. Pares, P. Diez, and A. Huerta. Subdomain-based flux-free a posteriori error estimators. *Computer Methods in Applied Mechanics and Engineering*, 195(4-6), 2006.

[88] L Gallimard. A constitutive relation error estimator based on traction-free recovery of the equilibrated stress. *International Journal for Numerical Methods in Engineering*, 78(4):460–482, 2009.

[89] P. Ladevèze and Leguillon D. Error estimate procedure in the finite element method and applications. *SIAM Journal on Numerical analysis*, 20(3):485–509, 1983.

[90] JP Moitinho De Almeida and JA Teixeira De Freitas. Alternative approach to the formulation of hybrid equilibrium finite elements. *Computers & Structures*, 40(4):1043–1047, 1991.

[91] JP Moitinho De Almeida and Edward A Maunder. *Equilibrium Finite Element Formulations*. John Wiley & Sons, 2017.

[92] J.Tinsley Oden and Serge Prudhomme. Estimation of Modeling Error in Computational Mechanics. *Journal of Computational Physics*, 182(2):496–515, 2002.

[93] I. Temizer and P. Wriggers. An adaptive multiscale resolution strategy for the finite deformation analysis of microheterogeneous structures. *Computer Methods in Applied Mechanics and Engineering*, 200:2639–2661, 2011.

[94] Stefan Loehnert, Corinna Prange, and Peter Wriggers. Error controlled adaptive multiscale XFEM simulation of cracks. *International journal of fracture*, 178(1-2):147–156, 2012.

[95] Franck J. Vernerey and Mirmohammadreza Kabiri. An adaptive concurrent multiscale method for microstructured elastic solids. *Computer Methods in Applied Mechanics and Engineering*, 241-244:52–64, 2012.

[96] T.I. Zohdi, J.T. Oden, and G.J. Rodin. Hierarchical modeling of heterogeneous bodies. *Computer Methods in Applied Mechanics and Engineering*, 138(1-4):273–298, 1996.

[97] Kumar S. Vemaganti and J. Tinsley Oden. Estimation of local modeling error and goal-oriented adaptive modeling of heterogeneous materials. *Computer Methods in Applied Mechanics and Engineering*, 190:6089–6124, 2001.

[98] Albert Romkes, J Tinsley Oden, and Kumar Vemaganti. Multi-scale goal-oriented adaptive modeling of random heterogeneous materials. *Mechanics of materials*, 38(8-10):859–872, 2006.

[99] Assyr Abdulle and Achim Nonnenmacher. Adaptive finite element heterogeneous multiscale method for homogenization problems. *Computer Methods in Applied Mechanics and Engineering*, 200(37-40):2710–2726, 2011.

[100] Ludovic Chamoin and Frédéric Legoll. A posteriori error estimation and adaptive strategy for the control of MsFEM computations. *Computer Methods in Applied Mechanics and Engineering*, 336:1–38, 2018.

[101] D. A. Paladim. *Multiscale Numerical Methods for the Simulation of Diffusion Processes in Random Heterogeneous Media with Guaranteed Accuracy*. PhD thesis, Cardiff University, 2016.

[102] J. Melenk and I. Babŭska. The partition of unity finite element method: Basic theory and applications. *Computer Methods in Applied Mechanics and Engineering*, 39:289–314, 1996.

[103] N. Moës, J. Dolbow, and T. Belytschko. A finite element method for crack growth without remeshing. *International Journal of Engineering Science*, 46:131–150, 1999.

[104] R. Ferrandes, P.M. Marin, J.-C. Léon, and F. Giannini. A posteriori evaluation of simplification details for finite element model preparation. *Computers & Structures*, 87(1):73–80, 2009.

[105] Sankara Hari Gopalakrishnan and Krishnan Suresh. A formal theory for estimating defeaturing-induced engineering analysis errors. *Computer-Aided Design*, 39(1):60–68, 2007.

[106] Ming Li and Shuming Gao. Estimating defeaturing-induced engineering analysis errors for arbitrary 3D features. *Computer-Aided Design*, 43(12):1587–1597, 2011.

[107] Sankara Hari Gopalakrishnan and Krishnan Suresh. Feature sensitivity: A generalization of topological sensitivity. *Finite Elements in Analysis and Design*, 44(11):696–704, 2008.

[108] Ming Li, Bo Zhang, and Ralph R. Martin. Second-order defeaturing error estimation for multiple boundary features. *International Journal for Numerical Methods in Engineering*, 100(5):321–346, 2014.

[109] D. B. P. Huynh, D. J. Knezevic, Y. Chen, J. S. Hesthaven, and A. T. Patera. A natural-norm Successive Constraint Method for inf-sup lower bounds. *Computer Methods in Applied Mechanics and Engineering*, 199:1963–1975, June 2010.

[110] A Quarteroni, G Rozza, and A Manzoni. Certified reduced basis approximation for parametrized partial differential equations and applications. *Journal of Mathematics in Industry*, 1(3):1–44, 2011.

[111] M. Meyer and H.G. Matthies. Efficient model reduction in non-linear dynamics using the Karhunen-Loeve expansion and dual-weighted-residual methods. *Computational Mechanics*, 31(1):179–191, 2003.

[112] T.J.R. Hughes, J.A. Cottrell, and Y. Bazilevs. Isogeometric analysis: CAD, finite elements, NURBS, exact geometry and mesh refinement. *Computer Methods in Applied Mechanics and Engineering*, 194(39):4135–4195, 2005.

[113] X. Peng, E. Atroshchenko, P. Kerfriden, and S.P.A. Bordas. Isogeometric boundary element methods for three dimensional static fracture and fatigue crack growth. *Computer Methods in Applied Mechanics and Engineering*, 316:151–185, 2017. Special Issue on Isogeometric Analysis: Progress and Challenges.

[114] Haojie Lian, Pierre Kerfriden, and Stéphane PA Bordas. Implementation of regularized isogeometric boundary element methods for gradient-based shape optimization in two-dimensional linear elasticity. *International Journal for Numerical Methods in Engineering*, 106(12):972–1017, 2016.

[115] S. Bordas and B. Moran. Enriched finite elements and level sets for damage tolerance assessment of complex structures. *Engineering Fracture Mechanics*, 73(9):1176–1201, 2006.

[116] Thomas-Peter Fries. A corrected XFEM approximation without problems in blending elements. *International Journal for Numerical Methods in Engineering*, 75(5):503–532, 2008.

[117] Anita Hansbo and Peter Hansbo. A finite element method for the simulation of strong and weak discontinuities in solid mechanics. *Computer methods in applied mechanics and engineering*, 193(33-35):3523–3540, 2004.

[118] Erik Burman, Susanne Claus, Peter Hansbo, Mats G. Larson, and André Massing. CutFEM: Discretizing geometry and partial differential equations. *International Journal for Numerical Methods in Engineering*, 104(7):472–501, 2015.

[119] Pierre-Alain Boucard and Laurent Champaney. A suitable computational strategy for the parametric analysis of problems with multiple contact. *International Journal for Numerical Methods in Engineering*, 57(9):1259–1281, 2003.

[120] Erik Burman, Peter Hansbo, and Mats Larson. Augmented Lagrangian finite element methods for contact problems. *arXiv preprint arXiv:1609.03326*, 2016.

[121] Franz Chouly and Patrick Hild. A Nitsche-based method for unilateral contact problems: Numerical analysis. *SIAM Journal on Numerical Analysis*, 51(2):1295–1307, 2013.

[122] Franz Chouly, Patrick Hild, and Yves Renard. Symmetric and non-symmetric variants of Nitsche's method for contact problems in elasticity: Theory and numerical experiments. *Mathematics of Computation*, 84(293):1089–1112, 2015.

[123] Erik Burman. Ghost penalty. *Comptes Rendus Mathematique*, 348(21-22):1217–1220, 2010.

[124] Claes Johnson. *Numerical Solution of Partial Differential Equations by the Finite Element Method*. Courier Corporation, 2012.

[125] Martin S. Alnæs, Jan Blechta, Johan Hake, August Johansson, Benjamin Kehlet, Anders Logg, Chris Richardson, Johannes Ring, Marie E. Rognes, and Garth N. Wells. The FEniCS project version 1.5. *Archive of Numerical Software*, 3(100):9–23, 2015.

[126] Jack S. Hale, Lizao Li, Christopher N. Richardson, and Garth N. Wells. Containers for Portable, Productive, and Performant Scientific Computing. *Computing in Science & Engineering*, 19(6):40–50, 2017.

[127] Christian Miehe, Fabian Welschinger, and Martina Hofacker. Thermodynamically consistent phase-field models of fracture: Variational principles and multi-field FE implementations. *International Journal for Numerical Methods in Engineering*, 83(10):1273–1311, 2010.

[128] P. Ladevèze, A. Nouy, and O. Loiseau. A multiscale computational approach for contact problems. *Computer Methods in Applied Mechanics and Engineering*, 191:4869–4891, 2002.

[129] M. Barboteu, P. Alart, and M. Vidrascu. A domain decomposition strategy for nonclassical frictional multi-contact problems. *Computer Methods in Applied Mechanics and Engineering*, 190:4785–4803, August 2001.

[130] P. Avery, G. Rebel, M. Lesoinne, and C. Farhat. A numerically scalable dual-primal substructuring method for the solution of contact problems—part I: The frictionaless case. *Computer Methods in Applied Mechanics and Engineering*, 193:2403–2426, 2004.

[131] Pierre Alart and Alain Curnier. A mixed formulation for frictional contact problems prone to Newton like solution methods. *Computer methods in applied mechanics and engineering*, 92(3):353–375, 1991.

[132] John Dolbow, Nicolas Moës, and Ted Belytschko. An extended finite element method for modeling crack growth with frictional contact. *Computer methods in applied Mechanics and engineering*, 190(51-52):6825–6846, 2001.

[133] Thomas Elguedj, Anthony Gravouil, and Alain Combescure. A mixed augmented Lagrangian-extended finite element method for modelling elastic–plastic fatigue crack growth with unilateral contact. *International Journal for Numerical Methods in Engineering*, 71(13):1569–1597, 2007.

[134] E. Pierrès, M.C. Baietto, and A. Gravouil. A two-scale extended finite element method for modelling 3D crack growth with interfacial contact. *Computer Methods in Applied Mechanics and Engineering*, 199(17):1165–1177, 2010.

[135] Erik Burman, Peter Hansbo, and Mats G. Larson. The penalty-free Nitsche method and nonconforming finite elements for the Signorini problem. *SIAM Journal on Numerical Analysis*, 55(6):2523–2539, 2017.

[136] Arsen Narimanyan. Unilateral conditions modelling the cut front during plasma cutting: FEM solution. *Applied mathematical modelling*, 33(1):176–197, 2009.

[137] Junuthula Narasimha Reddy and David K. Gartling. *The Finite Element Method in Heat Transfer and Fluid Dynamics*. CRC press, 2010.

[138] Franz Chouly, Mathieu Fabre, Patrick Hild, Rabii Mlika, Jérôme Pousin, and Yves Renard. An overview of recent results on Nitsche's method for contact problems. In *Geometrically Unfitted Finite Element Methods and Applications*, pages 93–141. Springer, 2017.

Selected journal articles

A partitioned model order reduction approach to rationalise computational expenses in nonlinear fracture mechanics

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Abstract

We propose in this paper a reduced order modelling technique based on domain partitioning for parametric problems of fracture. We show that coupling domain decomposition and projection-based model order reduction permits to focus the numerical effort where it is most needed: around the zones where damage propagates. No *a priori* knowledge of the damage pattern is required, the extraction of the corresponding spatial regions being based solely on algebra. The efficiency of the proposed approach is demonstrated numerically with an example relevant to engineering fracture.

Keywords: model order reduction, proper orthogonal decomposition (POD), domain decomposition, nonlinear fracture mechanics, system approximation, parametric time-dependent problems

1 Introduction

Engineering problems are very often characterised by a large ratio between the scale of the structure and the scale at which the phenomena of interest need to be described. In fracture mechanics, the initiation and propagation of cracks is the result of localised microscopic phenomena. These phenomena are usually represented in a homogenised manner at a scale which is suitable for the simulation: the scale of the coarser material heterogeneities (meso-scale), or the engineering scale when such a coarse representation allows for predictive results. In any case, the local nature of fracture leads to large numerical models because sharp local gradients need to be correctly represented or because the meso-structure needs to be described in an explicit manner. To some extent, the availability of super-computing facilities alleviate this difficulty. However, in engineering design processes, a prohibitively high number of solutions might be of interest, for a range of values of design parameters, or to take into account the effect of randomness in the model for instance. Therefore, one needs to devise efficient strategies for the solution to parametric multiscale problems. In doing so, the availability of a range of efficient numerical methods for the solution to one particular realisation of the parametric problem (homogenisation techniques, advanced discretisation tools, domain decomposition and multiscale-based preconditioners for parallel computing) should not be ignored.

Model order reduction techniques that are based on the projection of fine scale problems in reduced spaces are a potential solution to this issue. Such strategies rely on the fact that the solutions to the fine-scale problem obtained for different values of the input parameters can be often represented accurately in low-dimensional subspaces spanned by well-chosen basis functions at the fine scale. Applying this idea, the numerous unknowns that arise from the discretisation of the fine-scale problem are reduced to a few state variables (i.e. the amplitude associated to each of the basis functions). Of course, obtaining the aforementioned global basis functions still requires heavy computations at the fine scale.

Local/global model order reduction strategy for the simulation of quasi-brittle fracture

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Abstract

This paper proposes a novel technique to reduce the computational burden associated with the simulation of localised failure. The proposed methodology affords the simulation of damage initiation and propagation whilst concentrating the computational effort where it is most needed, i.e. in the localisation zones. To do so, a local/global technique is devised where the global (slave) problem (far from the zones undergoing severe damage and cracking) is solved for in a reduced space computed by the classical Proper Orthogonal Decomposition, while the local (master) degrees of freedom (associated with the part of the structure where most of the damage is taking place) are fully resolved. Both domains are coupled through a local/global technique. This method circumvents the difficulties associated with model order reduction for the simulation of highly non-linear mechanical failure and offers an alternative or complementary approach to the development of multiscale fracture simulators.

Keywords: Adaptive Model Order Reduction (MOR); Local/global Approach, Nonlinear Fracture Mechanics; Proper Orthogonal Decomposition (POD); Newton/Krylov Solver;

1 Introduction

Simulating damage initiation and subsequent global structural failure is one of the most active topics in computational mechanics. Several mathematical models and numerical methods have been developed over the years to assess various limit states such as failure due to permanent deformations, cracks or decohesion/delamination, e.g. in composite materials. Yet, these models, be they damage based or relying on discrete cracks are generally computationally expensive, as they require a fine scale description of the structural and material properties. Therefore, today's engineers are not able to use these state-of-the-art models for routine design. For important recent advances in the treatment of material failure (e.g. discontinuous fracture [1], advanced damage models [2, 3], damage plasticity models [4, 5] or their combination [6], etc.) to become useful in practice, it is thus important to devise techniques which are able to significantly reduce the computational effort required without sacrificing accuracy.

Historically, reducing the computational time associated with solving nonlinear problems in solid mechanics has mainly been addressed by developing homogenisation techniques [7, 8]. In this case, the material properties associated with a material point in a coarse representation of the structure is obtained by averaging of the fine scale material behaviour over a "representative volume element"

Automatised selection of load paths to construct reduced-order models in computational damage micromechanics: from dissipation-driven random selection to Bayesian optimization.

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Abstract

In this paper, we present new reliable model order reduction strategies for computational micromechanics. The difficulties rely mainly upon the high dimensionality of the parameter space represented by any load path applied onto the representative volume element (RVE). We take special care of the challenge of selecting an exhaustive snapshot set. This is treated by first using a random sampling of energy dissipating load paths and then in a more advanced way using Bayesian optimization associated with an interlocked division of the parameter space. Results show that we can insure the selection of an exhaustive snapshot set from which a reliable reduced-order model (ROM) can be built.

Keywords: model order reduction, computational homogenisation, reduced basis, Hyperreduction, damage mechanics, multiscale

1 Introduction

Multiscale modelling permits to take into account partial microscopic data when deriving engineering-scale working models. In solid mechanics, homogenisation is routinely used to obtain coarse-scale stress/strain relationships that are consistent with some statistical knowledge of the microstructure [1, 2, 3, 4]. This is particularly useful when modelling complex phenomena that would require cumbersome heuristic inference if the subscale physics was ignored. In more advanced applications of upscaling concepts, the conservation laws of the coarse-scale medium themselves may be obtained from lower-scale data [5, 6]. Homogenisation can be seen as one particular class of upscaling technique, whereby coarse-scale models approximate the limit of the underlying microscale model when

Guaranteed error bounds in homogenisation: an optimum stochastic approach to preserve the numerical separation of scales

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Abstract

This paper proposes a new methodology to guarantee the accuracy of the homogenisation schemes that are traditionally employed to approximate the solution of PDEs with random, fast evolving diffusion coefficients. We typically consider linear elliptic diffusion problems in randomly packed particulate composites. Our work extends the pioneering work presented in [27, 33] in order to bound the error in the expectation and second moment of quantities of interest, without ever solving the fine-scale, intractable stochastic problem. The most attractive feature of our approach is that the error bounds are computed without any integration of the fine-scale features. Our computations are purely macroscopic, deterministic, and remain tractable even for small scale ratios. The second contribution of the paper is an alternative derivation of modelling error bounds through the Prager-Synge hypercircle theorem. We show that this approach allows us to fully characterise and optimally tighten the interval in which predicted quantities of interest are guaranteed to lie. We interpret our optimum result as an extension of Reuss-Voigt approaches, which are classically used to estimate the homogenised diffusion coefficients of composites, to the estimation of macroscopic engineering quantities of interest. Finally, we make use of these derivations to obtain an efficient procedure for multiscale model verification and adaptation.

1 Introduction

Composites play an increasing role in modern mechanical systems. This raises tremendous challenges for computational mechanics. Indeed, the direct modelling of such systems results in intractable problems due to the fast spatial variations of material properties. The analysis of realistic composite systems requires an additional modelling step, whereby the microscopic constituents are substituted by a single material in such a way that this resulting model captures the global behaviour of the system. This process is known as homogenisation (see for example [23, 39]). The theory of homogenisation is well established for linear elliptic operators. In particular, homogenisation can be seen as the limit of heterogeneous problems when the scale ratio tends to zero [35]. However, most composite systems used in engineering exhibit a weak scale separation. Worse still, the most interesting features of mechanical problems are located in regions where the scale separation is lost altogether, typically in regions of steep gradients (*e.g.* stress concentration in solid mechanics, localised limit-states such as damage, sharp geometrical irregularities, *etc.*). In such cases, the results provided by homogenised schemes may differ

CAD Model simplification error estimation for electrostatics problems

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Abstract

Simplifying the geometry of a CAD model using defeaturing techniques enables more efficient discretisation and subsequent simulation for engineering analysis problems. Understanding the effect this simplification has on the solution helps to decide whether the simplification is suitable for a specific simulation problem. It can also help to understand the functional effect of a geometry feature. The effect of the simplification is quantified by a user-defined quantity of interest which is assumed to be (approximately) linear in the solution. A bound on the difference between the quantity of interest of the original and simplified solutions based on the energy norm is derived. The approach is presented in the context of electrostatics problems, but can be applied in general to a range of elliptic partial differential equations. Numerical results on the efficiency of the bound are provided for electrostatics problems with simplifications involving changes inside the problem domain as well as changes to the boundaries.

Keywords: geometry simplification error, defeaturing, finite-element analysis, goal-oriented error estimation, electrostatics.

1 Introduction

Computational engineering analysis requires discretization of a continuous boundary value problem. The discretization quality strongly influences the solution accuracy, which depends mainly on (i) how well the properties of the continuous solution space are preserved in the discretized functional solution space and (ii) how well the discrete geometry (typically a 2D or 3D mesh) represents the continuous geometry. It is well known that generating mesh models from CAD models for engineering analysis is time-consuming and expensive, taking 60% to 70% of the total analysis time, because of the algorithms failing to produce a suitable mesh and so manual intervention is required [4]. A common approach therefore, is to simplify or idealize the CAD model geometry, removing small or insignificant features which have little effect on the analysis results. This has two advantages: firstly the simpler geometry means that it can be represented by a simpler mesh with fewer, larger elements, making meshing both quicker, and more robust. Secondly, as the resulting mesh is simpler, analysis is also quicker. Fig. 1 illustrates an example of simplifying a geometric model of a shielded coil prior to magnetostatic analysis. The model is an example for shielding the magnetic field of a coil. The grey box is the outer boundary which is usually made of metal. The internal components are the coil and shield. The red and orange parts are features on the coil and shield that may be simplified. Much of the geometry has little effect on the solution, and can be removed before meshing.

A fast, certified and "tuning free" two-field reduced basis method for the metamodelling of affinely-parametrised elasticity problems

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Abstract

This paper proposes a new reduced basis algorithm for the metamodelling of parametrised elliptic problems. The developments rely on the Constitutive Relation Error (CRE), and the construction of separate reduced order models for the primal variable (displacement) and flux (stress) fields. A two-field greedy sampling strategy is proposed to construct these two fields simultaneously and in an efficient manner: at each iteration, one of the two fields is enriched by increasing the dimension of its reduced space in such a way that the CRE is minimised. This sampling strategy is then used as a basis to construct goal-oriented reduced order modelling. The resulting algorithm is certified and "tuning-free": the only requirement from the engineer is the level of accuracy that is desired for each of the outputs of the surrogate. It is also shown to be significantly more efficient in terms of computational expense than competing methodologies.

Keywords: two-field reduced basis method (TF-RBM); model order reduction; constitutive relation error; goal-oriented greedy sampling; *a posteriori* error estimation

1 Introduction

Model order reduction is an increasingly popular family of metamodelling techniques for parametrised boundary value problems (BVP) solved using numerical methods. As opposed to response surface methodologies, the output of the computation is not interpolated directly over the parameter domain. Instead, one constructs an approximation of the BVP that can be solved efficiently, and from which the quantities of interest can be post-processed. The applicability of reduced order modelling requires a certain smoothness of the solution to the original BVP over the parameter domain.

Reduced order modelling (ROM) can be performed in various ways (*e.g. a priori* reduction approach [1], Proper Generalised Decomposition [2, 3, 4], operator interpolation in attractive manifolds [5], machine-learning-based interpolations in attractive manifolds [6], classical mode synthesis, ...), but we will focus our discussion on the popular case of projection-based ROM (*e.g.* [7, 8, 9]). In this context, the reduced model is obtained by the projection of the original boundary value problem in a space of small dimension. Three ingredients are required for the metamodel to be efficient: (i) a reliable way to construct the projection space, (ii) an efficient (if possible optimum) projection of the solution to the BVP in this space and (iii) a method to decompose the numerical complexity of tasks (i) and (ii) in an "offline/online" manner. The latter point means that the expensive operations should be performed in advanced ("offline"), whilst the solution of the reduced model itself ("online") should remain computationally inexpensive.

A stable and optimally convergent LaTIn-CutFEM algorithm for multiple unilateral contact problems

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Abstract

In this paper, we propose a novel unfitted finite element method for the simulation of multiple body contact. The computational mesh is generated independently of the geometry of the interacting solids, which can be arbitrarily complex. The key novelty of the approach is the combination of elements of the CutFEM technology, namely the enrichment of the solution field via the definition of overlapping fictitious domains with a dedicated penalty-type regularisation of discrete operators, and the LaTIn hybrid-mixed formulation of complex interface conditions. Furthermore, the novel P1-P1 discretisation scheme that we propose for the unfitted LaTIn solver is shown to be stable, robust and optimally convergent with mesh refinement. Finally, the paper introduces a high-performance 3D level-set/CutFEM framework for the versatile and robust solution of contact problems involving multiple bodies of complex geometries, with more than two bodies interacting at a single point.

Keywords: unilateral contact, LaTIn, nonconforming finite element, CutFEM, ghost penalty, multiple level sets, composite materials

1 Introduction

Unfitted or non-conforming finite element methods uncouple the description of the geometry from the representation of the solution field itself. Typically, the geometry of the computational domain is projected over a regular background grid. In this setting, boundaries or interfaces between objects cut through elements of the corresponding mesh. Non-conforming methods are attractive for applications where coupling analysis codes and third party meshing libraries is either impractical, numerically expensive and/or prone to errors. In particular, contact problems in engineering applications often involve a large assembly of interacting solids of complex geometry. These assemblies can be extremely challenging to mesh due to sharp angles or small gaps between assembly parts. Here, the decoupling of the geometry from the finite element mesh, as featured within non-conforming finite element frameworks, can help alleviate this meshing burden. Nonetheless, a number of specific challenges needs to be addressed for unfitted numerical solutions to be computable. Firstly, integrals need to be calculated over cut elements, which requires specialised numerical quadratures. Secondly, unfitted approaches require stabilisation. This is because combinations of degrees of freedom may be poorly controlled in regions where contributions from cut elements to integral forms are small. Finally, in the context of multiple interacting materials, enrichment of the finite element solution space is required in order to allow for numerical jumps or kinks to develop over embedded interfaces. Failure to do so may severely impair the convergence rate of the unfitted finite element solver.

Over the last two decades, several encompassing frameworks have been developed to provide guidance for the development of unfitted finite element solvers. The eXtended Finite Element Method (XFEM) [36, 18, 7, 21] relies on the Partition of Unity Method [34] to enrich the approximation space.

A CutFEM method for Stefan-Signorini problems with application in pulsed laser ablation

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Abstract

In this article, we develop a cut finite element method for one-phase Stefan problems with applications in laser manufacturing. The geometry of the workpiece is represented implicitly via a level set function. Material above the melting/vaporisation temperature is represented by a fictitious gas phase. The moving interface between the workpiece and the fictitious gas phase may cut arbitrarily through the elements of the finite element mesh, which remains fixed throughout the simulation, thereby circumventing the need for cumbersome re-meshing operations. The primal/dual formulation of the linear one-phase Stefan problem is recast into a primal non-linear formulation using a Nitsche-type approach, which avoids the difficulty of constructing inf-sup stable primal/dual pairs. Through the careful derivation of stabilisation terms, we show that the proposed Stefan-Signorini-Nitsche CutFEM method remains stable independently of the cut location. In addition, we obtain optimal convergence with respect to space and time refinement. Several 2D and 3D examples are proposed, highlighting the robustness and flexibility of the algorithm, together with its relevance to the field of micro-manufacturing.

Keywords: CutFEM, Stefan problem, Stefan-Signorini-Nitsche formulation, pulsed laser ablation.

1 Introduction

The simulation of phase changes requires tracking the evolution of solid/liquid and liquid/gas interfaces, which is numerically challenging. In the context of the finite element method (FEM), two main approaches for interface tracking can be distinguished. The first family of approaches smooths the transition between phases, allowing for the existence of a mushy region in space where both phases coexist (*i.e.* enthalpy method [62, 25, 3, 24], phase field method [57, 64]). The width of this region may be thought of as a trade-off between computational cost, which is lower for fatter transition zones, and modelling accuracy, whereby the"true" model corresponds to an infinitely thin transition zone. The second approach describes the interface between phases as a sharp surface in 3D or a line in 2D. Although this may seem to be the "natural" approach to interface tracking, the sharp interface approach is difficult to handle within a finite element context. Indeed, the mesh either needs to conform to this interface, leading to a class of moving mesh algorithms such as ALE, or special finite element methods need to be developed so as to allow the interface to *cut through* the element. The latter family of methods are the so-called implicit boundary methods (see for instance [47, 6, 7, 31, 37, 12]), which are of prime interest in this paper.

The XFEM method was proposed in [47], and relies on a partition-of-unity enrichment to represent embedded kinks and discontinuities. The XFEM method has been applied to the simulation of two-phase Stefan problems in *e.g.* [45, 15, 63, 28, 53, 4, 22, 44, 39]. In this case, the interface between solid and liquid moves through a regular background mesh, which may be refined around the