RESEARCH CENTRE

Sophia Antipolis - Méditerranée

IN PARTNERSHIP WITH:

CNRS, Université Côte d'Azur

2021

ACTIVITY REPORT

Project-Team

COFFEE

COmplex Flows For Energy and Environment

IN COLLABORATION WITH: Laboratoire Jean-Alexandre Dieudonné (JAD)

DOMAIN

Digital Health, Biology and Earth

THEME

Earth, Environmental and Energy Sciences

Contents

Project-Team COFFEE

Creation of the Project-Team: 2013 January 01

Keywords

Computer sciences and digital sciences

A6.1.1. – Continuous Modeling (PDE, ODE)

A6.1.4. – Multiscale modeling

A6.1.5. – Multiphysics modeling

A6.2.1. – Numerical analysis of PDE and ODE

A6.2.7. – High performance computing

A6.5. – Mathematical modeling for physical sciences

A6.5.2. – Fluid mechanics

A6.5.3. – Transport

A6.5.4. – Waves

Other research topics and application domains

B1.1.5. – Immunology

B1.1.8. – Mathematical biology

B3.3.1. – Earth and subsoil

B4.1. – Fossile energy production (oil, gas)

B4.2. – Nuclear Energy Production

B7.1. – Traffic management

1 Team members, visitors, external collaborators

Research Scientists

- Thierry Goudon [Team leader, Inria, Senior Researcher, HDR]
- Laurent Monasse [Inria, Researcher]

Faculty Members

- Florent Berthelin [Univ Côte d'Azur, Professor, HDR]
- Konstantin Brenner [Univ Côte d'Azur, Associate Professor]
- Remi Catellier [Univ Côte d'Azur, until Feb 2021]
- Stéphane Junca [Univ Côte d'Azur, Associate Professor, HDR]
- Stella Krell [Univ Côte d'Azur, Associate Professor]
- Roland Masson [Univ Côte d'Azur, Professor, HDR]

Post-Doctoral Fellows

- Francesco Bonaldi [Inria, until Aug 2021]
- Daniel Castanon-Quiroz [Univ Côte d'Azur]
- Florent Chave [CNRS]
- Sean Mc Govern [Inria, until May 2021]

PhD Students

- Nadine Dirani [Inria, until Oct 2021]
- Paul Paragot [Univ Côte d'Azur]
- Christian Tayou Fotso [CNRS, from Oct 2021]

Interns and Apprentices

- Amele Ahraoui [Inria, from Jul 2021 until Aug 2021]
- Celia Mazzucotelli-Bertrand [Inria, from Sep 2021]

Administrative Assistant

- Marie-Cecile Lafont [Inria]

2 Overall objectives

The project aims at studying mathematical models issued from environmental and energy management questions. We consider systems of PDEs of hydrodynamic type or hybrid fluid/kinetic systems. The problems we have in mind involve unusual coupling, which in turn leads to challenging difficulties for mathematical analysis and the need of original numerical solutions. By nature many different scales arise in the problems, which allows to seek hierarchies of reduced models based on asymptotic arguments. The topics require a deep understanding of the modeling issues and, as far as possible boosted by the mathematical analysis of the equations and the identification of key structure properties, we wish to propose innovative and performing numerical schemes. To this end, the development of innovative Finite Volumes schemes with unstructured meshes on complex geometries will be a leading topic of the team activity.

3 Research program

Mathematical modeling and computer simulation are among the main research tools for environmental management, risks evaluation and sustainable development policy. Many aspects of the computer codes as well as the PDEs systems on which these codes are based can be considered as questionable regarding the established standards of applied mathematical modeling and numerical analysis. This is due to the intricate multiscale nature and tremendous complexity of those phenomena that require to set up new and appropriate tools. Our research group aims to contribute to bridging the gap by developing advanced abstract mathematical models as well as related computational techniques.

The scientific basis of the proposal is two–fold. On the one hand, the project is "technically–driven": it has a strong content of mathematical analysis and design of general methodology tools. On the other hand, the project is also "application–driven": we have identified a set of relevant problems motivated by environmental issues, which share, sometimes in a unexpected fashion, many common features. The proposal is precisely based on the conviction that these subjects can mutually cross-fertilize and that they will both be a source of general technical developments, and a relevant way to demonstrate the skills of the methods we wish to design.

To be more specific:

- We consider evolution problems describing highly heterogeneous flows (with different phases or with high density ratio). In turn, we are led to deal with non linear systems of PDEs of convection and/or convection–diffusion type.

- The nature of the coupling between the equations can be two–fold, which leads to different difficulties, both in terms of analysis and conception of numerical methods. For instance, the system can couple several equations of different types (elliptic/parabolic, parabolic/hyperbolic, parabolic or elliptic with algebraic constraints, parabolic with degenerate coefficients....). Furthermore, the unknowns can depend on different sets of variables, a typical example being the fluid/kinetic models for particulate flows. In turn, the simulation cannot use a single numerical approach to treat all the equations. Instead, hybrid methods have to be designed which raise the question of fitting them in an appropriate way, both in terms of consistency of the discretization and in terms of stability of the whole computation. For the problems under consideration, the coupling can also arises through interface conditions. It naturally occurs when the physical conditions are highly different in subdomains of the physical domain in which the flows takes place. Hence interface conditions are intended to describe the exchange (of mass, energy...) between the domains. Again it gives rise to rather unexplored mathematical questions, and for numerics it yields the question of defining a suitable matching at the discrete level, that is requested to preserve the properties of the continuous model.

- By nature the problems we wish to consider involve many different scales (of time or length basically). It raises two families of mathematical questions. In terms of numerical schemes, the multiscale feature induces the presence of stiff terms within the equations, which naturally leads to stability issues. A clear understanding of scale separation helps in designing efficient methods, based on suitable splitting techniques for instance. On the other hand asymptotic arguments can be used to derive hierarchy of models and to identify physical regimes in which a reduced set of equations can be used.

We can distinguish the following fields of expertise

- Numerical Analysis: Finite Volume Schemes, Well-Balanced and Asymptotic-Preserving Methods
  - Finite Volume Schemes for Diffusion Equations and Viscous Flows
  - Finite Volume Schemes for Conservation Laws

- Well-Balanced and Asymptotic-Preserving Methods
- Domain Decomposition Methods

- Modeling and Analysis of PDEs
  - Kinetic equations and hyperbolic systems
  - PDEs in random media
  - Interface problems

4 Application domains

4.1 Multiphase porous media flows and multi-physics coupling

Our research focuses on the numerical modeling of multiphase porous media flows accounting for complex geology and for nonlinear and multi-physics couplings. It is applied to various problems in the field of energy such as the simulation of geothermal systems in collaboration with BRGM, of nuclear waste repositories in collaboration with Andra, and of oil and gas recovery in collaboration with Total. Our research directions include the development of advanced numerical schemes adapted to polyhedral meshes and highly heterogeneous media in order to represent more accurately complex geologies. A special focus is made on the modeling of multiphase flows in network of faults or fractures represented as interfaces of co-dimension one coupled to the surrounding matrix. We also investigate nonlinear solvers adapted to the nonlinear couplings between gravity, capillary and viscous forces in highly heterogeneous porous media. In the same line, we study new domain decomposition algorithms to couple non-isothermal compositional liquid gas flows in a porous medium with free gas flows occurring at the interface between the ventilation gallery and the nuclear waste repository or between a geothermal reservoir and the atmosphere. We have begun exploring the coupling between the multiphase flow in the porous matrix and the solid mechanics involved in opening fractures.

4.2 Particulate and mixture flows

We investigate fluid mechanics models referred to as “multi–fluids” flows. A large part of our activity is more specifically concerned with the case where a disperse phase interacts with a dense phase. Such flows arise in numerous applications, like for pollutant transport and dispersion, the combustion of fuel particles in air, the modelling of fluidized beds, the dynamic of sprays and in particular biosprays with medical applications, engine fine particles emission... There are many possible modelings of such flows: microscopic models where the two phases occupy distinct domains and where the coupling arises through intricate interface conditions; macroscopic models which are of hydrodynamic (multiphase) type, involving non standard state laws, possibly with non conservative terms, and the so–called mesoscopic models. The latter are based on Eulerian–Lagrangian description where the disperse phase is described by a particle distribution function in phase space. Following this path we are led to a Vlasov-like equation coupled to a system describing the evolution of the dense phase that is either the Euler or the Navier-Stokes equations. It turns out that the leading effect in such models is the drag force. However, the role of other terms, of more or less phenomenological nature, deserves to be discussed (close packing terms, lift term, Basset force...). Of course the fluid/kinetic model is interesting in itself and needs further analysis and dedicated numerical schemes. In particular, in collaboration with the Atomic Energy Commission (CEA), we have proposed a semi-Lagrangian scheme for the simulation of particulate flows, extending the framework established in plasma physics to such flows.

We also think it is worthwhile to identify hydrodynamic regimes: it leads to discuss hierarchies of coupled hydrodynamic systems, the nature of which could be quite intriguing and original, while they share some common features of the porous media problems. We are particularly interested in revisiting the modeling of mixture flows through the viewpoint of kinetic models and hydrodynamic regimes. We propose to revisit the derivation of new mixture models, generalizing Kazhikov-Smagulov equations, through hydrodynamic asymptotics. The model is of “hybrid” type in the sense that the constraint reduces to the standard incompressibility condition when the disperse phase is absent, while it involves derivatives of the particle volume fraction when the disperse phase is present.

4.3 Fungal network growth

Members of the team have started an original research program devoted to fungal network growth. We started working on this subject through a collaboration with biologists and physicists at LIED (Université Paris Diderot) and probabilists in CMAP (Ecole Polytechnique) and Université Paris Sud, involving Rémi Catellier and Yves D'Angelo in LJAD in Nice. The motivation is to understand branching networks as an efficient space exploration strategy, with fungus *Podospora Anserina* being the biological model considered. This research is submitted as an ANR-project and has been supported by various local fundings.

4.4 Tumor growth and immune response

We have developed a size and space structured model describing interaction of tumor cells with immune cells based on a system of partial differential equations. This model is intended to describe the earliest stages of this interaction and takes into account the migration of the tumor antigen-specific cytotoxic effectors cells towards the tumor microenvironment by a chemotactic mechanism. This study reveals cancer persistent equilibrium states as expected by biologists, as well as escape phases when protumoral immune responses are activated. This effect which leads to persistent tumors at a controlled level was inferred from clinical observations and demonstrations using mouse model. Therefore, the maintenance of cancer in a viable equilibrium state represents a relevant goal of cancer immunotherapy. The mathematical interpretation of the equilibrium state by means of eigenvalue problems and constrained equations, has permitted us to develop new numerical algorithms in order to predict at low numerical cost the main features of the equilibrium and to discriminate, in biologically relevant cases, the parameters that are the most influential on the equilibrium.

4.5 Self organization in population dynamics

This topic is addressed mainly with Paulo Amorim (Univ. Federal Rio de Janeiro) and Fernando Peruani (Lab. de Physique Théorique et Modélisation, Cergy Paris Université).

We are interested in the mathematical modeling of physico-biological phenomena that drive towards a self-organization of a population of individuals reacting to external signals. It might lead to the formation of remarkable patterns or the following of traveling external signal. We develop microscopic and hydrodynamic models for such phenomena, with a specific interest in the modeling of ant foraging.

5 Social and environmental responsibility

T. Goudon is Scientific officer for Mathematics, General Directorate for Research and Innovation, Ministry of Higher Education and Research, since 2016. As such he also contributes to the national design of the AI policy.

6 New results

New results are concerned with

- Analysis and development of Finite Volume Methods for polyphasic flows in porous media with fractures
- Analysis and development of Finite Volume Methos for complex flows
- Domain decomposition methods for DDFV schemes
- Analysis of PDEs describing the behavior of particles interacting with their environment: Landau damping and dissipation mechanisms
- Simulation of fluid-structure interactions

- Modeling of tumors-immune system interactions
- Fractional BV framework for hyperbolic systems

7 Bilateral contracts and grants with industry

- Contract with Andra financing the two year postdoctoral position of Joubine Aghili and Florent Chave and dealing with the simulation of compositional liquid gas Darcy flows in highly heterogeneous porous medium with network of fractures using Discrete Fracture Matrix models (DFM). It is applied to the simulation of the desaturation of the nuclear waste storage in the neighbourhood of the galleries. Supervision Roland Masson and Konstantin Brenner from LJAD-Inria, Jean-Raynald de Dreuzy from Geosciences Rennes, Laurent Trenty and Marc Leconte from Andra.
- The team has also on-going collaboration with Storengy (post-doc of Daniel Constantin-Quiroz).

8 Partnerships and cooperations

8.1 International initiatives

8.1.1 Inria associate team not involved in an IIL or an international program

HDTHM

Title: Mathematical and numerical methods for thermo-hydro-mechanical models in porous media with discontinuities

Duration: 2019 ->

Coordinator: Jérome Droniou (jerome.droniou@monash.edu)

Partners:

- Monash University

Inria contact: Roland Masson

Summary:

8.2 National initiatives

8.2.1 ANR

- ANR CHARMS (Quantitative Reservoir Models for Complex Hydrothermal Systems), Roland Masson and Konstantin Brenner: december 2016 - december 2020, partners BRGM (leader), LJAD-Inria, Storengy, MdS, LJLL.
- ANR JCJC PRECIS (Effect of a shock wave on a structure with contact using mesh refinement and parallelism), Laurent Monasse: april 2018 - april 2021, partners Inria (leader), Ecole des Ponts, CEA, Université Paris-Est.
- ANR TOP-UP, Konstantin Brenner, Roland Masson: LJLL CNRS-Sorbonne Univ., Ecole des Ponts, LNCC Brazil. The project is devoted to the numerical modeling of urban floods, helping to size and position protective systems including dams, dikes or rainwater drainage network.

8.2.2 National and European networks

- GdR MANU.

  The research group MANU has activities centered around scientific computing, design of new numerical schemes and mathematical modelling (upscaling, homogenization, sensitivity studies, inverse problems,...). Its goal is to coordinate research in this area, as well as to promote the emergence of focused groups around specific projects

- GdR Mamovi

  The team is involved in the activities of the research group dedicqted to applications to life sciences.

- S. Junca is involved in GdR 3437 DYNOLIN “Dynamique non linéaire” and GdR MecaWave.

- LJAD-Inria and BRGM are the French partners of the Norvergian, German French project InSPiRE "International Open Source Simulation Software Partnership in Research and Education” which has just been accepted by the Research Council of Norway with the code ComPASS as one of the softwares of this project together with Dune, Dumux and OPM.

8.3 Regional initiatives

- T. Goudon is involved in the UCAncer pluridisplinary network, which involves mathematics, biology and medicine for cancer modeling and improvement of cures.

9 Dissemination

9.1 Promoting scientific activities

9.1.1 Scientific events: organisation

We do not keep track of such data.

9.1.2 Scientific events: selection

We do not keep track of such data.

Chair of conference program committees We do not keep track of such data.

Member of the conference program committees We do not keep track of such data.

Reviewer We do not keep track of such data; members of the team regularly serve as reviewers in the journals in applied math. or scientific computing: Archiv. Rat. Mec. Anal., SIAM J. Math. Anal., SIAM J. Geosc., SIAM J. Math. Anal., Numerische, Math of Comp. M3AS, IMAJNA, M2AN, etc

9.1.3 Journal

Member of the editorial boards

- T. Goudon is Editor in chief of SMAI Journal of Computational Mathematics.

- T. Goudon is academic editor for PlosOne.

Reviewer - reviewing activities The team members are involved in numerous reviewing activities, which we do not record.

9.1.4 Invited talks

We do not keep track of such data.

9.1.5 Scientific expertise

T. Goudon is expert at the Ministry for Reserach, Higher Education and Innovation. He is involved in any expertise concerning mathematics: PEPR, AI, Equipex...

9.1.6 Research administration

- T. Goudon is a member of the steering committee of IHES, CIMPA, IHP and CIRM.

9.2 Teaching - Supervision - Juries

9.2.1 Teaching

- Florent Berthelin, Master 2 Mathématiques fondamentales, Univ Côte d'Azur, 120h.
- Florent Berthelin, Chair of the Master 2 Mathématiques fondamentales, Univ Côte d'Azur.
- Florent Berthelin, Analysis, L2, Univ Côte d'Azur, 72h.
- Laurent Monasse, Introduction to continuum mechanics, M1, 30h., Univ Côte d'Azur
- Thierry Goudon is a member of the jury of the national competition to hire teachers (agregation de mathematiques).
- Thierry Goudon: CliMaths program. Lecture on traffic flows modeling, Ecole Centrale de Marseille
- Thierry Goudon: Master, lectures on signal processing, Univ Côte d'Azur
- Thierry Goudon: Master, lecture on PDEs, Univ. Côte d'Azur
- Stella Krell: Master, Finite Volume methods, Univ Côte d'Azur

9.2.2 Supervision

F. Berthelin is chair of the preparation to agregation at Univ Côte d'Azur in math.

9.3 Popularization

9.3.1 Interventions

- L. Monasse was involved in the popularization programmes "Regard de géomètre" and "Cordées de la réussite".
- T. Goudon attends the Academy of Nice award ceremony of the Olympiades of Mathematics.

10 Scientific production

10.1 Publications of the year

International journals

[1] J. Aghili, J.-R. De Dreuzy, L. Trenty and R. Masson. 'A hybrid-dimensional compositional two-phase flow model in fractured porous media with phase transitions and Fickian diffusion'. In: *Journal of Computational Physics* 441 (2021), p. 110452. DOI: 10.1016/j.jcp.2021.110452. URL: https://hal.archives-ouvertes.fr/hal-02994152.

[2] P. Amorim and T. Goudon. 'Analysis of a model of self-propelled agents interacting through pheromone'. In: *Nonlinearity* 34.9 (29th July 2021), pp. 6301–6330. DOI: 10.1088/1361-6544/ac149d. URL: https://hal.archives-ouvertes.fr/hal-03577497.

[3] K. Atsou, F. Anjuère, V. M. Braud and T. Goudon. 'A size and space structured model of tumor growth describes a key role for protumor immune cells in breaking equilibrium states in tumorigenesis'. In: *PLoS ONE* 16.11 (22nd Nov. 2021), e0259291. DOI: 10.1371/journal.pone.0259291. URL: https://hal.archives-ouvertes.fr/hal-03452282.

[4] F. Bonaldi, K. Brenner, J. Droniou and R. Masson. 'Gradient discretization of two-phase flows coupled with mechanical deformation in fractured porous media'. In: *Computers & Mathematics with Applications* (2021). DOI: 10.1016/j.camwa.2021.06.017. URL: https://hal.archives-ouvertes.fr/hal-02549111.

[5] F. Bonaldi, K. Brenner, J. Droniou, R. Masson, A. Pasteau and L. Trenty. 'Gradient discretization of two-phase poro-mechanical models with discontinuous pressures at matrix fracture interfaces'. In: *ESAIM: Mathematical Modelling and Numerical Analysis* 55.5 (Sept. 2021), pp. 1741–1777. DOI: 10.1051/m2an/2021036. URL: https://hal.archives-ouvertes.fr/hal-03348216.

[6] F. Bonaldi, J. Droniou, R. Masson and A. Pasteau. 'Energy-stable discretization of two-phase flows in deformable porous media with frictional contact at matrix–fracture interfaces'. In: *Journal of Computational Physics* 455 (2022). DOI: 10.1016/j.jcp.2022.110984. URL: https://hal.archives-ouvertes.fr/hal-03349229.

[7] C. Bourdarias, A. P. Choudhury, B. Guelmame and S. Junca. 'Entropy solutions in BV^s for a class of triangular systems involving a transport equation'. In: *SIAM Journal on Mathematical Analysis* 54.1 (2022), pp. 791–817. DOI: 10.1137/20M1351783. URL: https://hal.archives-ouvertes.fr/hal-02895603.

[8] K. Brenner, J. Droniou, R. Masson and E. H. H. Quenjel. 'Total-velocity-based finite volume discretization of two-phase Darcy flow in highly heterogeneous media with discontinuous capillary pressure'. In: *IMA Journal of Numerical Analysis* (27th Apr. 2021). DOI: 10.1093/imanum/drab018. URL: https://hal.archives-ouvertes.fr/hal-02957054.

[9] M. Gander, L. Halpern, F. Hubert and S. Krell. 'Optimized Schwarz methods with general Ventcell transmission conditions for fully anisotropic diffusion with discrete duality finite volume discretizations'. In: *Moroccan Journal of Pure and Applied Analysis* 7.2 (1st July 2021), pp. 182–213. DOI: 10.2478/mjpaa-2021-0014. URL: https://hal.archives-ouvertes.fr/hal-03352652.

[10] M. J. Gander, L. Halpern, F. Hubert and S. Krell. 'Discrete Optimization of Robin Transmission Conditions for Anisotropic Diffusion with Discrete Duality Finite Volume Methods'. In: *Vietnam Journal of Mathematics* (2nd Sept. 2021). DOI: 10.1007/s10013-021-00518-3. URL: https://hal.archives-ouvertes.fr/hal-02539124.

[11] M. J. Gander, J. Hennicker and R. Masson. 'Modeling and Analysis of the Coupling in Discrete Fracture Matrix models'. In: *SIAM Journal on Numerical Analysis* 59.1 (13th Jan. 2021), pp. 195–218. DOI: 10.1137/20M1312125. URL: https://hal.archives-ouvertes.fr/hal-02437030.

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[13] T. Goudon, S. Krell and G. Lissoni. 'Non-overlapping Schwarz algorithms for the incompressible Navier–Stokes equations with DDFV discretizations'. In: *ESAIM: Mathematical Modelling and Numerical Analysis* 55.4 (July 2021), pp. 1271–1321. DOI: 10.1051/m2an/2021024. URL: https://hal.archives-ouvertes.fr/hal-03350932.

[14] T. Goudon, J. Llobell and S. Minjeaud. 'An explicit finite volume scheme on staggered grids for the Euler equations: Unstructured meshes, stability analysis, and energy conservation'. In: *International Journal for Numerical Methods in Fluids* (2021). DOI: 10.1002/fld.5048. URL: https://hal.archives-ouvertes.fr/hal-03428367.

[15] T. Goudon and L. Vivion. 'Numerical investigation of solitary wave stability for quantum dissipative systems'. In: *Journal of Mathematical Physics* 62.1 (1st Jan. 2021), p. 011509. DOI: 10.1063/5.0021246. URL: https://hal.archives-ouvertes.fr/hal-03577474.

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[20] B. Al-Taki, K. Atsou, J.-J. Casanova, T. Goudon, P. Lafitte, F. Lagoutière and S. Minjeaud. 'Numerical investigations of the compressible Navier-Stokes system'. In: *ESAIM: Proceedings and Surveys*. CEMRACS 2019 - Geophysical Fluids, Gravity Flows 70 (2021), pp. 1–13. DOI: 10.1051/proc/202107001. URL: https://hal.archives-ouvertes.fr/hal-03314984.

[21] F. Xing. 'New optimized Schwarz algorithms for one dimensional Schrödinger equation with general potential'. In: *Journal of Computational and Applied Mathematics* 383 (28th Feb. 2021), pp. 113018–. DOI: 10.1016/j.cam.2020.113018. URL: https://hal.archives-ouvertes.fr/hal-03492509.

Doctoral dissertations and habilitation theses

[22] S. Krell. 'Développement et analyse de schémas Volumes Finis en mécanique des fluides complexes'. Université Côte D'Azur, 17th June 2021. URL: https://tel.archives-ouvertes.fr/tel-03265697.

Reports & preprints

[23] K. Atsou, S. Khou, F. Anjuère, V. Braud and T. Goudon. *Analysis of the equilibrium phase in immune-controlled tumors predicts best strategies for cancer treatment*. 19th Jan. 2021. URL: https://hal.archives-ouvertes.fr/hal-03115518.

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[26] C. Cancès, V. Ehrlacher and L. Monasse. *Finite Volumes for the Stefan-Maxwell Cross-Diffusion System*. 2021. URL: https://hal.archives-ouvertes.fr/hal-02902672.

[27] T. Goudon and L. Vivion. *On quantum dissipative systems: ground states and orbital stability*. 19th Jan. 2021. URL: https://hal.archives-ouvertes.fr/hal-03115521.

[28] B. Guelmame. *Global weak solutions of the Serre–Green–Naghdi equations with surface tension*. 23rd Feb. 2022. URL: https://hal.archives-ouvertes.fr/hal-03585433.

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[30] F. Marazzato, A. Ern and L. Monasse. *Quasi-static crack propagation with a Griffith criterion using a variational discrete element method*. 21st Oct. 2021. URL: https://hal.archives-ouvertes.fr/hal-03102982.