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14. ABSTRACT
Fragmentation is a key damage mechanism determining ballistic impact performance of ceramic armors as well as reliability of gun barrels. This program, which was sponsored by the Army Research Office, focuses on the relation between defect populations and fragment-size distributions via robust physics-based numerical simulations. The originality of the present simulations lies in the capability of dealing with fragmentation of large and heterogeneous structures. The understanding of how the microstructure acts on the global macroscopic response is our main

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FINAL TECHNICAL REPORT

Controlled dynamic fragmentation of ceramics

PI: JF Molinari (Johns Hopkins University, Ecole Polytechnique Fédérale of Lausanne)

Attention: Dr. D. Stepp, Army Research Office

Fragmentation is a key damage mechanism determining ballistic impact performance of ceramic armors as well as reliability of gun barrels. This program, which was sponsored by the Army Research Office, focuses on the relation between defect populations and fragment-size distributions via robust physics-based numerical simulations. The originality of the present simulations lies in the capability of dealing with fragmentation of large and heterogeneous structures. The understanding of how the microstructure acts on the global macroscopic response is our main concern. Defects are strategically placed during the design of a material or a structure in order to optimize the geometrical (shape and size) or velocity characteristics of fragments.

Key simulation features:

- Comprehensive physics to capture dynamic crack propagation
- Presence of material defects
- Novel modeling strategies: Discontinuous Galerkin fragmentation
- Massively parallel simulations

Below, we detail a few salient scientific results of the program. The complete list of publications is given at the end of the document.

Part 1: Fragment sizes resulting from brittle fragmentation.

The average fragment mass is perhaps the most studied physical property resulting from dynamic fragmentation. This is no surprise, as fragment masses find applications in several engineering and scientific fields (including ballistic impact performance). Starting from the pioneering analytical work of Mott [1], up to the seminal energy model of Grady [2], several models have sought to understand the link between material properties, strain rate, and fragment mass. Recent work has focused on resorting to numerical simulations to address the limitations of analytical work. Our contribution follows this trend. Our originality lies in coupling the best practices in mechanical modelling of rupture with a rigorous analysis of the physics at play. In our approach, material rupture is captured by having recourse to cohesive elements [3], which are dynamically inserted in a previously continuous finite-element mesh. The influence of material defects having been seldom studied, we conducted parametric studies of fracture parameters distributions to capture statistical heterogeneity.

Our results reveal that, despite statistical heterogeneity at the small scale, and complex dynamics, the output of fragmentation is not random but displays universal features, see figure 1. The normalisation procedure that we used to obtain the remarkably simple law is the subject of a publication [4]. It involves three parameters, which characterize the distribution of defects. They are the largest defects (also known as the weakest links), the average defect size, and the left slope of the defect distribution. We have demonstrated that this slope controls the rate of crack initiation at a given strain rate. These parameters being known, we are able to **predict the average fragment** mass obtained from brittle fragmentation events. The inverse problem is perhaps even more interesting: our theoretical model opens the door, from inspecting the average fragment mass at various strain rates, to characterizing the defect distribution in a given material.

In a follow up study [5], we have analyzed the fragment size distributions. The end result of a brittle fragmentation event is a diverse population of fragment sizes. We are for instance well acquainted with the breakage of kitchen plates, resulting in large pieces, which are easily cleaned, and finer wreckage, which may go unnoticed for weeks. Several semi-empirical models describing this diversity in fragment masses have been derived in the last century. We compared our numerical predictions to these models, and discovered a surprising feature. If we normalize the fragment sizes with the average fragment size (which we can now reliably predict, see above), all our distributions fall under a unique mixed-power-exponential form (fig. 2a). The end result of

this numerical investigation is that we are not only in position to predict an average fragment mass, but also the statistics of the entire defect distribution.
Interestingly, the largest fragments do not seem to obey such a simple scaling, as we see in fig. 2b. The influence of defects on the emergence of large fragments remains a mystery that we are currently studying through extreme value statistics analysis.

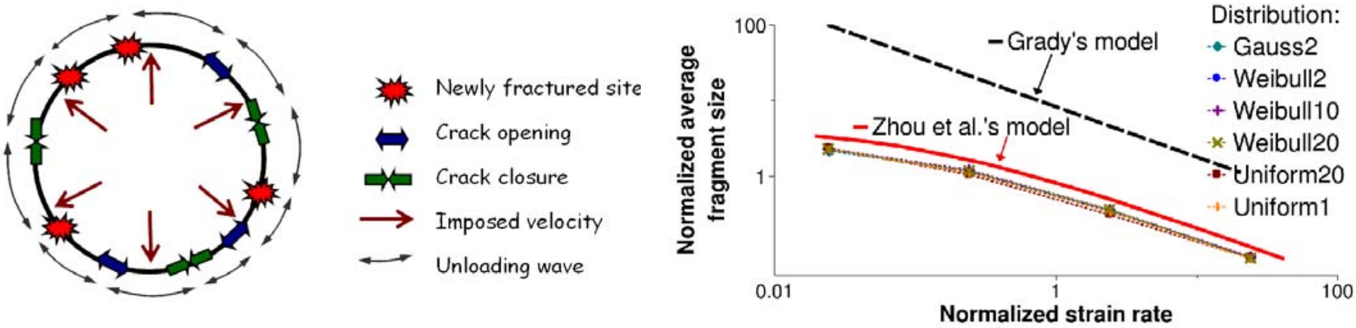
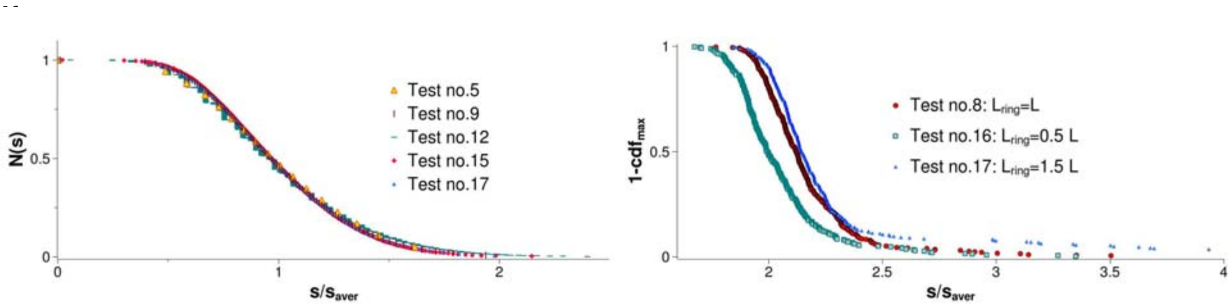


Fig 1: Schematic of ceramic ring expansion test showing the initiation of multiple fracture sites and the development of a complex network of stress waves interactions. On the right, our results show the surprising robustness of the average fragment size prediction as a function of strain rate for a ceramic material. The normalization procedure of the axes is subject of a publication, and involves an explicit dependence on materials properties (elastic and fracture) and defect population statistics. It is noteworthy that all the defect distributions that were considered (Weibull, Gauss and Uniform) fall on a single universal curve.



a) *b)*

Fig 2 : a) Inverse cumulative density function of fragment size (s). Each test involves different material properties, defect distribution, and strain rates. Yet, the normalisation by the average fragment size yields a unique master curve. b) Extreme value statistics reveal that the same simple scaling law does not hold true for the largest fragments. The link between defect population and the largest fragments remains a mystery.

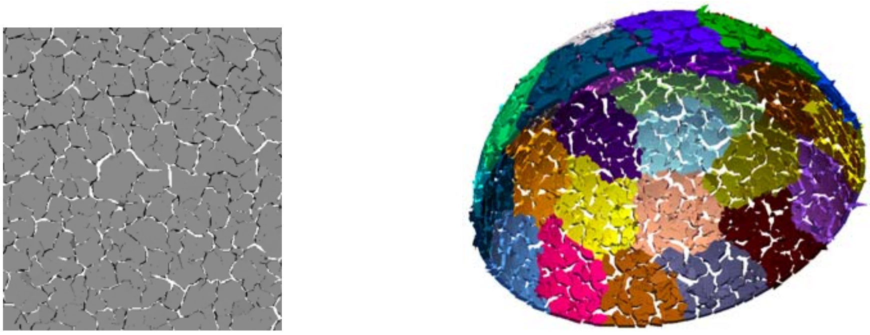
Part 2: Discontinuous Galerkin fragmentation and massively parallel simulations

In collaboration with Prof. R. Radovitzky and A. Seagraves (MIT) we have conducted parallel simulations of 3D fragmentation (see figure 3) using a Discontinuous Galerkin (DG) approach [7], which was developed at MIT [6,8].

The DG approach is finding an increasingly broader appeal in the mechanics community, due to a more accurate description of shock fronts, than what is achieved with regular continuous Galerkin approaches (regular finite element codes). In DG, all element boundaries are initially separated, and flux terms are added to satisfy equilibrium weakly. This initial splitting of all mesh elements fixes the mesh topology. In standard cohesive elements codes, insertion of cracks must be done dynamically, which implies that the mesh topology is constantly changing. This is easily achieved on single processor machines, but is a much harder endeavour on multiple processor machines, in which cracks may propagate from a processor to another.

DG methods open the door to massively (and scalable) fragmentation simulations of 3D structures.

Therefore, the method shows excellent potential for scaling on HPC machines. The PI has purchased significant computing power and DG is currently tested to generated fragment size statistics in simulations involving hundreds of processors (see figure 3). We are currently evaluating how defects influence fragment shapes. Simulations reveal, as fragmentation damage unfolds, a complex yet “organized” percolation network of cracks. Strategically placed defects influence the organization of this network and can effectively control the sharpness of fragments in impacted ceramics.



Fi*gure 3: a) 3D ceramic plate under rapid biaxial tension (10^4/s); a random Weibull distribution of initial defects yields heterogeneous fragment sizes or roughly equi-axed shapes. b) Parallel simulations of a fragmenting concrete dome due to an internal explosion. Each colour represents a different processor. Notice how cracks propagate from one processor to another.*

Key achievements:

Robust, yet simple, numerical and analytical predictors of fragments sizes, which are function of material parameters and defect distributions.

Ability to conduct massively parallel fragmentation simulations.

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[8] A. Seagraves, R. Radovitzky, "Advances in cohesive zone modeling of dynamic fracture", book chapter in "Dynamic Failure of Materials and Structures" (Shulka, Arun, Ravichandran, Guruswami, Rajapakse, Yapa), 2010.

Scientific output

Ph.D. theses

Defended thesis: Reuben Kraft, Ph.D. 2008, The Johns Hopkins University (USA); Dr. Kraft is now an Army Research Laboratory scientist.

One thesis under way at Ecole Polytechnique Fédérale de Lausanne (Switzerland): Ms Sarah Levy, "Fragmentation the signature of defects", expected defense summer 2010. Ms Levy is currently in her third year of her Ph.D.

Publications (international journals)

S. Levy, J.F Molinari, "Dynamic fragmentation of ceramics, signature of defects, and scaling of fragment sizes", *Journal of the Mechanics and Physics of Solids,* **58**(1), pp. 12-26, 2010

S. Levy, J.F Molinari, A. Davison, "Fragmentation of a ring: on the universality of the fragment size distribution", *in preparation for submission to Phys. Rev. Let*

R.H. Kraft, J.F. Molinari, K.T. Ramesh, and D.H. Warner, "Computational micromechanics of dynamic compressive loading of a brittle polycrystalline material using a distribution of grain boundary properties", *Journal of the Mechanics and Physics of Solids, **56**(8)*, pp. 2618-2641, 2008

R.H. Kraft, J.F. Molinari, "A statistical investigation of the effects of grain boundary properties on transgranular fracture", *Acta Materialia, **56**(17)*, pp. 4739-4749, 2008

Presentations/seminars:

J.F. Molinari, "Structures under extreme loading", Leçon inaugurale, EPFL, November 24, 2009. (planery lecture)

S. Levy (speaker), A. Seagraves, J.F. Molinari, R. Radovitzky, "The Discontinuous Galerkin method, a tool for parallel simulations in the context of dynamic fragmentation", Scientific event on High Accuracy Numerical Methods and their Application to Complex Physics Problems, Toulouse, France, December 7-8, 2009.

S. Levy (speaker), J.F. Molinari, "Statistical fragmentation of a heterogeneous expanding ring", 9^{th} World Congress in Computational Mechanics & ECCOMAS, Venice, Italy. July 2008.

S. Levy (speaker), J.F Molinari, "Describing the dynamique response of a ceramic: The search for universality in fragment statistics." 12th International Conference on Fracture (ICF), Ottawa, Canada, 2009

J.F. Molinari, "Dynamic failure of materials under extreme loading conditions: the case of brittle fragmentation", LAMCOS seminar, INSA Lyon, France, March 6, 2008. (invited seminar)

J.F. Molinari, "Convergence of cohesive-element approach in fragmentation problems", LMA CNRS, Marseille, France, February 25, 2008. (invited seminar)

J.F. Molinari (speaker), R. Kraft, "A micro-mechanical study of dynamic failure in a polycrystalline ceramic", Advances in heterogeneous material mechanics, International Conference on Heterogeneous Materials Mechanics (ICHMM), Huangshan, China, pp. 1240-1241, June 3-8, 2008. (invited)

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Proceedings

S. Levy, J.F Molinari, "Statistical fragmentation of heterogeneous ceramics", 8th. World Congress on Computational Mechanics (WCCM8), 5th. European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS), Venice, Italy, (2 pages), 2008

S. Levy, A. Seagraves, J.F. Molinari, R. Radovitzky, "Discontinuous Galerkin method applied to fragmentation of heterogeneous materials", proceedings 9e Colloque National en Calcul des Structures, Giens, France, Vol. 2, pp. 145-151, 2009

S. Levy, J.F Molinari, "Describing the dynamique response of a ceramic: The search for universality in fragment statistics." 12th International Conference on Fracture (ICF), Ottawa, Canada (9 pages), 2009