Discontinuous Galerkin method applied to fragmentation of heterogeneous materials

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Abstract — Since it generates a multitude of interacting cracks, the computational modeling of fragmentation requires special attention. The discontinuous Galerkin formulation provides an efficient scalable framework to simulate non-linear dynamics of spatially discontinuous structures. Cracks can initiate at any element boundary and evolve driven by a cohesive law. A DG-cohesive weak formulation is derived, implemented into a parallel finite element code, and applied to the fragmentation of a three-dimensional plate submitted to biaxial tension.

Keywords — Discontinuous Galerkin method, explicit time integration, cohesive elements, fragmentation, heterogeneous materials.

1 Introduction

In the recent years, discontinuous Galerkin (DG) methods have received considerable attention both for problems in which advection and diffusion terms are present, and more recently for problems allowing physical discontinuities. They are the result of a century work during which mathematicians and physicians have improved their formulations [12]. The name of Discontinuous Galerkin (DG) seems to appear first in a paper by Lesaint and Raviart [5] who defined a method to link separate domains in a weak manner. An approximation is computed independently in each domain, weakly connected to the others afterwards. Other theories have been derived to link such separate domains, among which the method of domain decomposition [3]. It adds Lagrange multiplier functions at contiguous interfaces of the various domains in such a manner that the number of unknown variables increases. The essence of the DG method lies in the elimination of the Lagrange multiplier functions so that the total number of unknown variables does not depend on the interfaces. An obvious way to accomplish this elimination is the direct substitution. Nitsche derived a mathematical theory of elimination in the variational principle [7]. He also discovered that his process could lead to numerical singularities. Hence, he added a further constraint of least-square type, to avoid numerical indefiniteness. The parameter that he introduced can be seen as a stabilization term.

Practical applications of the DG method range several fields. It has been classically employed for the computation of fluid flow [1] and more recently in solid mechanics. For instance, approximate solutions of problems involving cracks [6], beams and plates [2], shells [4], and constitutive models that include spatial gradients [11], have been computed in quasi statics. A recent effort

has also been made to use the DG method in dynamic problems involving large deformation and plasticity [8, 9]. In the present paper, as exposed in [8, 9], we apply the DG method to dynamic fragmentation of brittle materials. Fragmentation is the breakage of a structure into several pieces. In dynamics, an explosive loading generates many fragments. During the process, multiple micro-cracks appear simultaneously at seemingly random locations, interact through stress waves, propagate, coalesce and eventually form macro-cracks. A complex network of stress waves takes place within the structure, which makes the dynamics highly non-linear. An efficient parallelizable numerical framework is thus required. The DG method has been shown to be accurate and scalable for such problems [9]. It deals with the bulk solution while cohesive interfaces address the problem of crack opening and crack closure [10]. In addition, we include microstructural heterogeneities in the numerical framework to account for the effect of bulk defects. Defects are known to determine the initiation of the cracks and a fortiori the evolution of the dynamic behavior. In practice, they are included by setting a distribution of cohesive properties.

The paper is organized as follows. In the first section, we derive the discontinuous Galerkin (DG) framework in the elasto-dynamic context for large deformations. Then, we allow for cracks to initiate and propagate using the cohesive methodology, which leads to a natural hybrid DG-cohesive formulation. In the last section, we present preliminary results of the fragmentation of a heterogeneous plate, submitted to biaxial tension.

2 Formulation of the boundary value problem

This section is a summary of the rigorous derivation of the DG theory detailed in [8]. We first review the strong form of the boundary value problem of large dynamic deformations of an elastic body Ω_0. Then, we divide the initial body into two subbodies Ω_0^1 and Ω_0^2 such that $\Omega_0 = \Omega_0^1 \cup \Omega_0^2$ and $\partial_I\Omega_0 = \Omega_0^1 \cap \Omega_0^2$ (fig.1). Stresses and displacements can be discontinuous across the surface $\partial_I\Omega_0$, which can either model a physical boundary or be a fictitious numerical interface. The weak DG formulation provides an efficient mean to handle this discontinuous interface. Finally, we generalize the one-interface equation to a finite number of interfaces and couple the method to a dynamic finite element framework.

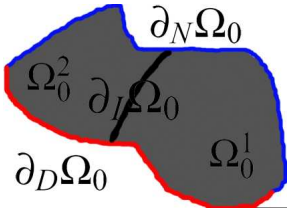


Figure 1: Partition of the initial body and boundary surfaces

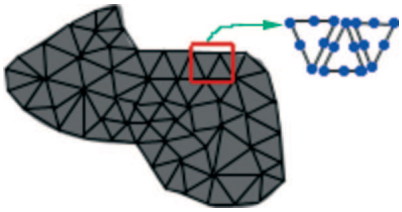


Figure 2: Duplication of all the nodes from the original mesh

2.1 Strong formulation of the continuous problem

Let us consider the dynamic motion of a body which reference configuration is Ω_0 at time t_0. At any time t in $T = [t_0, t_f]$, the position $\mathbf{x}$ of the material point $\mathbf{X}$ is described by the deformation mapping:

$$\mathbf{x} = \varphi(\mathbf{X}, t) \quad \forall \mathbf{X} \in \Omega_0, \forall t \in T \tag{1}$$

Its boundary surface $\partial\Omega_0$ is partitioned into a Dirichlet part $\partial_D\Omega_0$ and a Neumann part $\partial_N\Omega_0$ such that $\partial\Omega_0 = \partial_D\Omega_0 \cup \partial_N\Omega_0$ and $\partial_D\Omega_0 \cap \partial_N\Omega_0 = \emptyset$. Considering that no body force applies, the

continuum equations are:

$$\rho_0 \ddot{\varphi} = \nabla_0 \mathbf{P} \quad \forall \mathbf{X} \in \Omega_0, \forall t \in T \tag{2}$$

$$\varphi = \bar{\varphi} \quad \forall \mathbf{X} \in \partial_D \Omega_0, \forall t \in T \tag{3}$$

$$\mathbf{P} \cdot \mathbf{N} = \bar{\mathbf{T}} \quad \forall \mathbf{X} \in \partial_N \Omega_0, \forall t \in T \tag{4}$$

where ρ_0 is the initial density function, $\dot{\bullet}$ refers to the partial differentiation with respect to time, $\mathbf{P}$ is the first Piola-Kirchhoff stress tensor, and $\mathbf{N}$ is the unit normal to the reference configuration. The system of equations has a solution if initial conditions are provided. We consider the case of hyperelastic materials for which a strain density function W exists and is such that:

$$\mathbf{P} = \frac{\partial W}{\partial (\nabla_0 \varphi)} \tag{5}$$

2.2 Insertion of an interface and DG formulation

Integration over the body in the reference configuration, multiplied by a suitable test function, leads to the usual weak Galerkin formulation. Let us add an inside boundary $\partial_I \Omega_0$. Equations 1 to 5 are independently valid in Ω_0^1 and Ω_0^2. The interface allows for jumps between Ω_0^1 and Ω_0^2. The *jump* $[\bullet]$ and the *average* $\langle \bullet \rangle$ operators are respectively defined by:

$$[\bullet] = \bullet_2 - \bullet_1 \qquad \langle \bullet \rangle = \frac{\bullet_2 + \bullet_1}{2} \tag{6}$$

We note $\mathbf{N}$ the normal vector to $\partial_I \Omega_0$ pointing from 2 to 1 ($\mathbf{N} = \mathbf{N}_{21} = -\mathbf{N}_{12}$). The DG method relaxes the equilibrium conditions of the interface $\partial_I \Omega_0$ and enforces weakly the compatibility equation:

$$[\varphi] = 0 \quad \forall \varphi \in \partial_I \Omega_0 \tag{7}$$

Besides the usual terms of the Galerkin continuous equation, the DG formulation involves an interface term which fields are discontinuous across $\partial_I \Omega_0$. The DG problem consists in defining the suitable spaces B_X, B_P, B_X^0 (one may refer to [8] for more details), and in finding $\varphi \in \mathrm{B}_X$ and $\mathbf{P} \in \mathrm{B}_P$ such that:

$$\int_{\Omega_0} (\rho_0 \ddot{\varphi}\, \delta\varphi + \mathbf{P} : \nabla_0 \delta\varphi)\, dV - \int_{\partial_I \Omega_0} [\mathbf{P}\, \delta\varphi]\, \mathbf{N}\, dS = \int_{\partial_N \Omega_0} \bar{\mathbf{T}}\, \delta\varphi\, dS \quad \forall \delta\varphi \in \mathrm{B}_X^0, \forall t \in T \tag{8}$$

We simplify the equation 8 by using the relation $[\mathbf{P}\, \delta\varphi] = [\mathbf{P}]\, \langle \delta\varphi \rangle + \langle \mathbf{P} \rangle\, [\delta\varphi]$, and by considering that only the compatibility of the displacements needs to be enforced. Finally, in addition to its weak enforcement, the equation of compatibility must be ensured quadratically by adding a stabilization term, proportional to $[\varphi] \otimes \mathbf{N} : \mathbb{C} : [\delta\varphi] \otimes \mathbf{N}$, where $\mathbb{C}$ is the tangent material moduli. This term stabilizes the jump in displacements and the influence of the material relations for large displacements is properly included. The final formulation of the DG method is:

$$\begin{aligned} &\int_{\Omega_0} (\rho_0 \ddot{\varphi}\, \delta\varphi + \mathbf{P} : \nabla_0 \delta\varphi)\, dV - \int_{\partial_I \Omega_0} \langle \mathbf{P} \rangle\, [\delta\varphi]\, \mathbf{N}\, dS \\ &+ \int_{\partial_I \Omega_0} [\varphi] \otimes \mathbf{N} : \langle \frac{\beta}{h_s} \mathbb{C} \rangle : [\delta\varphi] \otimes \mathbf{N}\, dS = \int_{\partial_N \Omega_0} \bar{\mathbf{T}}\, \delta\varphi\, dS \quad \forall \delta\varphi \in \mathrm{B}_X^0, \forall t \in T \end{aligned} \tag{9}$$

$\beta > 0$ is the stabilization parameter and h_s is a suitable characteristic length.

2.3 Generalization: Finite Element implementation

In the case of finite elements, the previous formulation is still valid. The initial domain is partitioned into elements $\Omega_0 \approx \Omega_{0h} = \bigcup_{e=1}^{E} \Omega_0^e$. One possible way to define the interior boundary $\partial_I \Omega_0$ is to refer to all the boundaries between elements (fig. 2):

$$\partial_I \Omega_0 = \left(\bigcup_{e=1}^{E} \partial \Omega_0^e \right) \Big\backslash \partial \Omega_{0h} \tag{10}$$

The characteristic length h_s is the mesh size. Equation 9 is still valid for any finite number of interfaces. The only difference is the definition of the spaces in which the unknown displacements and stresses are defined. Furthermore, the discretization in time is a conventional explicit integration. A second-order central difference scheme with mass lumping is adopted. The space-DG formulation imposes a condition on the time step:

$$\Delta t \leq \Delta t_{critic} = \frac{h_s}{\sqrt{\beta} c} \tag{11}$$

3 Handling fracture with the DG methodology

3.1 Hybrid formulation

Failure occurs when a threshold criterion is satisfied. Before fracture, the DG law governs the evolution of the interface. Once the average local stress along the interface reaches a given threshold called the cohesive strength σ_c, the interface follows the Camacho and Ortiz linear cohesive law [10]. The weak formulation becomes:

$$\begin{aligned} &\int_{\Omega_0} (\rho_0 \ddot{\varphi}\, \delta\varphi + \mathbf{P} : \nabla_0 \delta\varphi)\, dV + \alpha \left(\int_{\partial_I \Omega_0} \mathbf{T}([\varphi])\, [\delta\varphi]\, dS \right) \\ &+ (1-\alpha) \left(- \int_{\partial_I \Omega_0} \langle \mathbf{P} \rangle\, [\delta\varphi]\, \mathbf{N}\, dS + \int_{\partial_I \Omega_0} [\varphi] \otimes \mathbf{N} : \langle \frac{\beta}{h_s} \mathbb{C} \rangle : [\delta\varphi] \otimes \mathbf{N}\, dS \right) \\ &= \int_{\partial_N \Omega_0} \bar{\mathbf{T}}\, \delta\varphi\, dS \qquad \forall \delta\varphi \in \mathrm{B}_X^0, \forall t \in T \end{aligned} \tag{12}$$

$\alpha = 0$ at each element boundary before fracture initiation. When the fracture criterion is satisfied, α is 1. $\mathbf{T}$ is the cohesive traction, and is function of the jump in displacements across the interface. Its behavior can follow any cohesive law. In the present study, the law is linear [10].

3.2 Linear cohesive law definition

First, let us respectively denote by T, δ_{norm} and δ_{tang} the norms of $\mathbf{T}$, of the normal and of the tangential parts of $[\varphi]$. The interface effective opening is a combination of δ_{norm} and δ_{tang}.

$$\delta_{coh} = \sqrt{\delta_{norma}^2 + \gamma \delta_{tang}^2} \tag{13}$$

The parameter γ balances the tension and shear contributions. Denoting the cohesive strength σ_c and the critical opening δ_c, the traction T behaves by following the cohesive law:

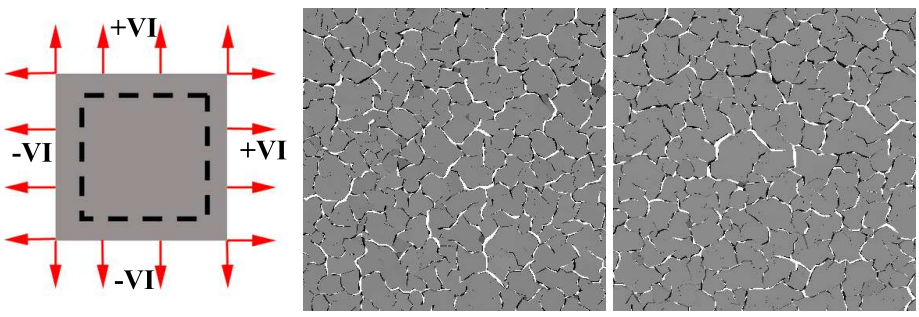
$$\frac{T}{\sigma_c} = 1 - \frac{\delta_{coh}}{\delta_c} \text{ , for } \dot{\delta}_{coh} > 0 \text{ , } \delta_{coh} = \delta_{max} \text{ and } D < 1 \tag{14}$$

$$\frac{T}{\sigma_c} = 1 - \frac{\delta_{max}}{\delta_c} \text{ , for } \delta_{coh} < \delta_{max} \text{ and } D < 1 \tag{15}$$

The element opening is governed by the first equation while the second equation accounts for the closing. D is the local damage, and is comprised between 0 (initiation of the cohesive crack) and 1 (the cohesive crack is fully broken). Consequently, only two parameters are necessary to define this law: the cohesive strength σ_c and the critical opening δ_c. One can either choose these values equal for every cohesive element (homogeneous material), or different (heterogeneous material). In this study, the critical opening δ_c is kept constant and the cohesive strengths σ_c follow a uniform or a Weibull distribution. In this way, the DG method and the cohesive approach can easily be inserted into a conventional finite element code to simulate the fragmentation of heterogeneous structures.

4 Fragmentation of a heterogeneous plate

A ceramic plate of area 1cm by 1cm and of thickness 0.015mm, is submitted to biaxial tension. The velocity is imposed on the four sides and drives the plate expansion at a strain rate of $10^5 s^{-1}$. Before fracture, the behavior is elastic (Young modulus equal to $260 GPa$, Poisson ratio of 0.21 and volumetric mass set to $3690 kg.m^{-3}$). When the stress is high enough, the plate begins to damage locally, cracks are propagating and eventually coalesce. Figure 3 represents the applied boundary conditions and the resulting fragments for two initial distributions of defects. In the first case, we consider a nearly homogeneous material with a uniform distribution in which cohesive strengths vary in a 1% range around the mean ($\sigma_c = 300 MPa$). In the second case, the cohesive strengths follow a Weibull distribution of modulus of two and around the same mean as before. This second distribution has a larger standard deviation and represents a more heterogeneous material. The results reveal a larger spread in fragment sizes for the heterogeneous plate, and a smaller final number of fragments. These findings are in accordance with prior results obtained with classical continuous Galerkin methods coupled with cohesive zone modeling. This confirms the potential of using DG for robust scalable fragmentation simulations. Statistics on fragment sizes, shapes and how they can be impacted by defects will be computed in future work.



(a) ***Boundary conditions and region of interest*** **(b)** ***Fragmented region of interest for a uniform distribution of defects*** **(c)** ***Fragmented region of interest for a Weibull distribution of defects***

Figure 3: Plate under rapid biaxial tension

5 Conclusion

DG methods are efficient to simulate the fragmentation of heterogeneous materials. In this paper, we have briefly derived the DG equations and applied them to a usual finite element code. While the DG methodology handles the bulk behavior, the failure process is governed by a linear cohesive law which allows numerous cracks to open, interact and coalesce simultaneously. The last section focuses on the fragmentation of a heterogeneous plate submitted to biaxial tension.

Two distributions of cohesive stresses model the material heterogeneity: a uniform with low standard deviation and a Weibull distribution with Weibull modulus 2 (larger standard derivation). In both cases, the DG methodology resolves well the intense loading applied as boundary conditions. At the end of the process, the uniform distribution (more homogeneous material) leads to smaller and more numerous fragments than the Weibull distribution (more heterogeneous material), which confirms prior experimental and numerical observations.

References

[1] B. Cockburn. An introduction to the discontinuous Galerkin method for convection-dominated problems. *Advanced Numerical Approximation of Nonlinear Hyperbolic equations*, Springer: Berlin, 151-268, 1998.

[2] G. Engel, K. Garikipati, T-J-R. Hughes, M-G. Larson, L. Mazzei, R-L. Taylor. Continuous/discontinuous finite element approximations of fourth-order elliptic problems in structural and continuum mechanics with applications to thin beams and plates. *Computer Methods in Applied Mechonics and Engineering*, 191: 36669-3750, 2002.

[3] P. Gosselet, C. Rey. Non-overlapping domain decomposition methods in structural mechanics. *Archives of computational methods in engineering*, 13: 515-572, 2006.

[4] S. Guzey, H-K. Kuhl, B. Cockburn, K-K. Tamma. Design and development of a discontinuous Galerkin method for shells. *Computer Methods in Applied Mechanics and Engineering*, 195: 3528-3548, 2006.

[5] P. Lesaint, P-A. Raviart. On a finite element method for solving neutron transport equation. *Mathematical aspects of Finite Elements in Partial Differential Equations* , de Boor, Academic Press: New York, 1974.

[6] J. Mergheim, E. Kuhl, P. Steinmann. A hybrid discontinuous Galerkin/interface method for the computational modeling of failure. *Communications in Numerical Methods in Engineering*, 20: 511-519, 2004;

[7] J-A. Nitsche. Uber ein Variationsprinzip zur Losung Dirichlet-Problemen bei Verwendung von Teilraumen, die keinen Randbedingungen uneworfen sind. *Abh. Math. Sem. Univ. Hamburg*, 36: 9-15, 1971.

[8] L. Noels, R. Radovitzky. A general discontinuous Galerkin method for finite hyperelasticity. Formulation and numerical applications. *International Journal for numerical methods in engineering*, 68: 64-97, 2006.

[9] L. Noels, R. Radovitzky. An explicit discontinuous Galerkin method for non-linear solid mechanics: Formulation, parallel implementation and scalability properties. *International Journal for numerical methods in engineering*, 74: 1393–1420, 2008.

[10] G-T. Camacho, M. Ortiz. Computational modelling of impact damage in brittle materials; *International Journal of solids and structures*, 33: 2899-2938, 1996.

[11] G-N. Wells, K. Garikipati, L. Molari. A discontinuous Galerkin formulation for a strain gradient-dependent damage model. *Computer Methods in Applied Mechanics and Engineering*, 193: 3633-3645, 2004.

[12] O-C. Zienkiewicz, R-L. Taylor, S-J. Sherwin, J. Peiró. On discontinuous Galerkin methods. *International journal for numerical methods in engineering*, 58: 1119-1148, 2003.