

Three-dimensional fracture and fragmentation of artificial kidney stones

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Abstract

The brittle fracture of a gypsum cylinder, which is used as an artificial kidney stone in lithotripsy research, is simulated by the use of the finite element method. The cylinder is submerged in water and is subjected to a pressure front parallel to one of its planar faces. The stresses induced by the pressure wave lead to fracture in the interior of the cylinder, with the formation of a spall plane located about 2/3 of the length from the face on which the pressure is applied. We show that the simulation reproduces the salient features of experimental observations.

1 Introduction

We simulate the brittle fracture of a gypsum cylinder subjected to a pressure pulse. The cylinder is submerged in water, and the pressure pulse is applied as a front parallel to one of the planar faces of the cylinder. This configuration is commonly used to study the effects that pressure waves generated by lithotripters have on kidney stones.

Lithotripsy is the technique of applying pressure pulses to the exterior of the body to induce high stresses in renal calculi. A lithotripter is a machine which is used to generate and apply these pressure waves. The waves are designed with the purpose to induce stresses that lead to the fracture and fragmentation of the kidney stones. The fragments are then expected to naturally exit the body through the urethra.

To study the effects that lithotripter have on kidney stones, experiments are conducted which employ gypsum cylinder as artificial kidney stones. The cylinders are submerged in water, which plays the role of the tissue in which the pressure waves propagate. The geometry of the artificial stone is simple to better understand the effects of the pressure waves on it.

Successive pressure pulses are applied to the stones. All the pulses have the same duration and have the same shape. Fracture occurs in the stones depending on the peak pressure of the pulse and the number of applied pulses. The salient feature of the fracture of the stones is that a spall plane forms about 2/3 of the length from the face which is reached first by the wave.

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2 Graph fracture

Fracture and fragmentation are simulated by the use of cohesive interface elements, which assume that fracture occurs at the interface between bulk elements [4]. It is assumed that the cohesive surface has a stored energy function of the form

$$\phi = \phi(\boldsymbol{\delta}, \mathbf{q}; \mathbf{N}) \quad (1)$$

in which $\boldsymbol{\delta}$ is the displacement jump at the interface or opening displacement, \mathbf{q} is a vector of internal variables dependent on the chosen cohesive law, and \mathbf{N} is the normal at the interface. Thus, the relationship between traction and opening displacement is

$$\mathbf{t} = \frac{\partial \phi(\boldsymbol{\delta}, \mathbf{q}; \mathbf{N})}{\partial \boldsymbol{\delta}}. \quad (2)$$

Define the effective opening displacement as

$$\delta = \sqrt{\beta^2 \delta_S^2 + \delta_n^2}, \quad (3)$$

in which

$$\delta_n = \boldsymbol{\delta} \cdot \mathbf{n} \quad (4)$$

is the normal opening displacement and

$$\delta_S = |\boldsymbol{\delta}_S| = |\boldsymbol{\delta} - \delta_n \mathbf{n}| \quad (5)$$

is the perpendicular displacement (sliding). The parameter β is used to assign different weights to these displacement components. Thus, the cohesive constitutive law can be written as

$$\mathbf{t} = \frac{t}{\delta} (\beta^2 \boldsymbol{\delta}_S + \delta_n \mathbf{n}) \quad (6)$$

in which

$$t = \frac{\partial \phi}{\partial \delta}(\delta, \mathbf{q}) \quad (7)$$

or

$$t = \sqrt{\beta^{-2} |\mathbf{t}_S|^2 + t_n^2}. \quad (8)$$

Fracture occurs when the failure criterion $t \geq \sigma_c$ is satisfied, where σ_c is the fracture critical stress [5, 6].

Using this method, the finite element mesh is initially coherent. As the simulation advances, the failure criterion is computed at bulk-element interfaces each time a specified number of computational steps have been performed. When the failure criterion is satisfied at a particular interface, a cohesive element is introduced into the mesh. This element in turn governs the mechanics of the fracture process at the interface.

The introduction of a cohesive element in an interface, however, changes the topology of the mesh. Repeated introduction of these elements effects the propagation of fracture, which may lead to more complex changes in topology due to crack branching and fragmentation.

The topology of the mesh is commonly represented by a connectivity table, in which each row lists the nodes of a particular element according to an ordering convention. The connectivity table, although simple in its implementation, has proved to be cumbersome for complex topological manipulations of finite element meshes, in particular for the changes introduced by fracture and fragmentation.

As an alternative, we introduce an approach for the topological representation of simplicial finite element meshes as graphs [3]. By using a graph, the original n -dimensional simplicial complex that is the finite element mesh is represented by means of a uni-dimensional simplicial complex, thus greatly reducing the complexity of topological manipulations.

A finite element mesh in the context of the graph representation is a simplicial complex in which an extra graph vertex is introduced, as shown in Fig. 1. This *root* vertex, shown as a white oval in the figure, guarantees that the graph is *weakly connected*, regardless of whether the mesh is intact or in a highly fragmented state. This greatly simplifies the manipulation of the graph. For the tetrahedron in Fig. 1, the colors of the edges define an ordering of the vertices that is considered canonical, and any deviations from it are recorded within the graph.

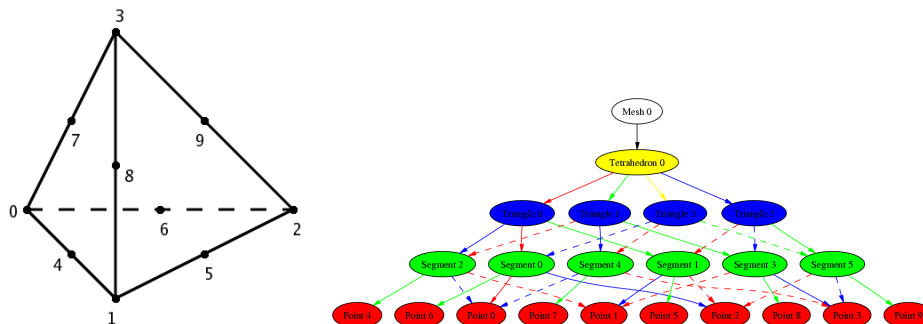


Figure 1: Single-tetrahedron mesh and its corresponding graph.

3 Gypsum experiment

Lithotripsy is the technique of administering focused shock waves to induce renal calculi fracture and fragmentation. Although shock wave lithotripsy has become the primary technique for the treatment of renal calculi, there remains much controversy as to the mechanisms that lead to stone comminution. It appears, however, that one of the main mechanisms of stone fragmentation is that the stress waves induced by the shocks lead to brittle fracture [1]. In view of the difficulties associated with observing and controlling stone fragmentation in live tissue, and also to study lithotripter performance separately, artificial stones are used in the research of the mechanisms of fracture and fragmentation. The Ultracal-30 gypsum is adopted as a model for a stone, as it is suitable for lithotripsy studies in vitro, acute animal experiments in which the stones are implanted in the kidney, and as a target to compare in vitro performance of intra-corporeal lithotripters [2].

A schematic representation of the experiment is shown in Fig. 2a, and a plot of the pressure profile applied to the gypsum sample is shown in Fig. 2b.

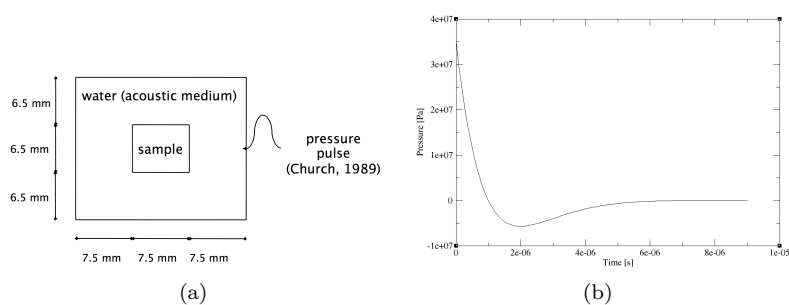


Figure 2: Gypsum stone experiment setup with pressure pulse applied to the gypsum sample.

The salient feature of shock wave experiments conducted on cylindrical gypsum stones submerged in water is the formation of a spall plane approximately at 2/3 of the length from the face on which the shocks arrive, as shown in Fig. 3.

4 Finite element simulation

The finite element simulation of the fracture of the gypsum stone uses a mesh of approximately 300,000 elements. A finer stone mesh is used to provide as many paths as possible for the propagation of cracks.

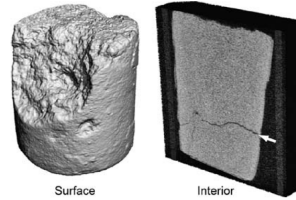


Figure 3: 3D surface reconstruction (left) shows damage from cavitation, and cross-section (right) shows the characteristic spallation plane [2].

The water is simulated by using acoustic elements that allow for the propagation of pressure waves only. The finite-deformation acoustic formulation is displacement-based, thus it simplifies the interaction of fluid and solid. Gypsum is a brittle material, and therefore it is modeled as a neo-hookean finite-deformation elastic solid. Composite tetrahedral finite elements are used to avoid locking and numerical problems [7]. The material properties used are shown in Table 1, in which E , ν , ρ_g , σ_c and G_c are the Young's modulus, Poisson's ratio, mass density, fracture critical stress and fracture energy of the gypsum, respectively, and K and ρ_w are the bulk modulus and mass density of water, respectively.

E [GPa]	ν	ρ_g [kg m ⁻³]	σ_c [MPa]	G_c [J m ⁻²]	K [GPa]	ρ_w [kg m ⁻³]
10.8	0.3461	1700	6.0	21.88	2.25	1000

Table 1: Material parameters used in the simulation

The finite element simulation ran on Linux alpha cluster on 16 nodes and its results are shown in Fig. 4. The sub-figures show different perspectives of the gypsum sample, with cracks represented by solid color and the sample itself as a translucent cylinder. The color represents the value is the component of the normal stress along the axis of the cylinder, with blue for lower values and green for higher values. Frontal cracks where the pulse first reached the sample are observed in Fig. 4a. A failure cone typical of fracture in compression is clearly observed in Figs. 4b, 4c, 4d. The spall plane at 2/3 of the length observed in experiments is reproduced by the simulation and is clearly observed in all figures, in particular Fig. 4c. Exfoliation can be observed in Fig. 4e.

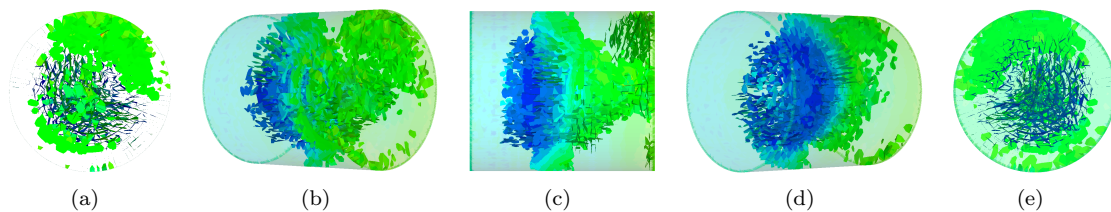


Figure 4: Gypsum fracture simulation results: (a) Frontal cracks. (b) Surface and internal cracks. (c) Spall at 2/3 of length. (d) Spall and failure cone. (e) Exfoliation and spall.

5 Conclusions

We presented the finite-element simulation of the brittle fracture of a gypsum cylinder subjected to pressure waves. The methods used for the simulation, namely cohesive fracture by means of cohesive interface elements and the graph representation of the mesh to track its changes in topology are specially well suited for this kind of computation, as the comparison of the results with the experimental observations show.

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References

- [1] M. Lokhandwalla and B. Sturtevant. Fracture mechanics model of stone comminution in eswl and implications for tissue damage. *Physics in Medicine and Biology*, 45:1923–1940, 2000.
- [2] J.A. McAteer, J.C. Williams, R.O. Cleveland, J van Cauwelaert, M.R. Bailey, D.A. Lifshitz, and A.P. Evan. Ultracal-30 gypsum artificial stones for research on the mechanisms of stone breakage in shock wave lithotripsy. *Urological Research*, 33(6):429–434, 2005.
- [3] A. Mota, J. Knap, and M. Ortiz. Fracture and fragmentation of simplicial finite elements meshes using graphs. *Internat. J. Numer. Meths. Engrg.*, 2006. in preparation.
- [4] M. Ortiz and A. Pandolfi. Finite-deformation irreversible cohesive elements for three-dimensional crack-propagation analysis. *Internat. J. Numer. Meths. Engrg.*, 44:1267–1282, 1999.
- [5] A. Pandolfi and M. Ortiz. Solid modeling aspects of three-dimensional fragmentation. *Eng. Comput.*, 14(4):287–308, 1998.
- [6] A. Pandolfi and M. Ortiz. An efficient adaptive procedure for three-dimensional fragmentation simulations. *Eng. Comput.*, 18(2):148–159, 2002.
- [7] P Thoutireddy, J.F. Molinari, E.A. Repetto, and M. Ortiz. Tetrahedral composite finite elements. *Internat. J. Numer. Meths. Engrg.*, 53:1337–1351, 2002.