Computational Techniques for Moving Interfaces

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1 Introduction

Currently some of the most difficult problems in computational science involve moving interfaces between flowing or deforming media. Typically partial differential equations must be satisfied on each side of the interface (often different equations on each side) and these solutions coupled through relationships or jump conditions that must hold at the interface. These conditions may be in the form of differential equations on the lower-dimensional interface. Often the movement of the interface is unknown in advance and must be determined as part of the solution. The interface shape may be geometrically complex and may change topology with time. Particularly in three space dimensions, the ability to solve such problems accurately is limited. Exciting research is currently underway in the development of better algorithms, the analysis of the accuracy and stability of such algorithms, and the application of these techniques to specific scientific and engineering problems.

The primary goal of this Workshop was to bring together a number of researchers (mostly applied mathematicians) who are working on such methods, to foster interaction and the exchange of ideas. The focus was primarily on three broad classes of methods and the workshop started with introductory talks on these basic methodologies — *Moving Grid Methods* by **Mike Baines**, *Level Set Methods* by **Hong-Kai Zhao**, and *Fixed Grid / Moving Interface Methods* by **Randy LeVeque**. These overview talks were fleshed out over the course of the 5-day workshop in 24 additional talks on various mathematical aspects and applications. Several informal evening sessions were held to discuss technical details, recent progress, and directions for future research.

There was consensus that the Banff setting and informal workshop format created an ideal environment to foster openness and the surprisingly frank discussions. The organizers are extremely grateful to BIRS for having had the opportunity to hold this exciting workshop. Participants discussed the shortcomings as well as the successes of each approach and cross-fertilization between the groups led to interesting discussions and some new directions for research.

2 Moving Grid Methods

There are 3 types of methods to perform grid, or mesh, adaption — the so-called $h-$, $p-$, and $r-$ methods. The first two do static (fixed time) regridding, where the $h-$ method does coarsening or refining as needed and the $p-$ method takes higher or lower order approximations locally as needed. In contrast, the $r-$ methods, or *moving grid methods*, are designed in principle to move the grid in conjunction with the solutions to the time-dependent PDEs or corresponding interfaces.

These $r-$ methods have received considerably less attention than the others; nevertheless, there have been some recent developments which clearly demonstrate their potential for problems such as those having moving interfaces. The intention at this workshop was to discuss implementation techniques and success at solving physical problems as well as progress in deriving an underlying theory for these methods.

2.1 Some general issues

The excellent overview of moving grid methods by **Mike Baines** set the stage for the talks to follow in this area. The grid generation problem can be equated to constructing a mapping $x(\xi, t)$ from computational space (with coordinate ξ) to physical space (with coordinate x). The two basic types of methods, location based and velocity based, generally involve respectively computing x by minimizing a variational form or computing the mesh velocity $v = x_t$ using a Lagrangian like formulation.

For the location based methods, several variational forms were reviewed. One common type of method involves solving the variational problem using a steepest descent method to introduce the time derivative for grid movement. Another is the classical moving finite element method of Miller. There is frequently no clear consensus on the relative merits of one of these approaches over another.

Several velocity based methods designed for general problems were then discussed. The ALE methods were described in a general framework, and then related to the Geometric Conservation Law, or GCL, method. The GCL method [1], which has undergone renewed interest and spawned investigation of related methods, was discussed in several talks.

Near the end of the workshop, a moving grid breakout session was held. It was attended by those working in the field as well as interested participants with expertise in the other workshop areas. Since moving grid methods are generally less developed and less well-known than the other adaptive techniques, there was felt to be a need to discuss what attempts should be made to see that recent advances make their way into the repertoire of more scientists and engineers. It was agreed that there were three key challenges (and partial solutions): (1) providing better reviews of the literature (e.g., through a SIAM Review article), (2) having more accessible software (aided by developing modular codes on a web site and compiling a list of test problems), and (3) developing a firmer theoretical foundation.

2.2 Overview of work presented

There was a diversity of talks varying from very theoretical talks to ones about the concrete solution of specific physical problems.

An underlying question with any adaptive method is how to interpret the various factors arising in anisotropic grid generation. **Weizhang Huang** discussed a general steady state error analysis for such grids. The three key grid features or qualities which play a role in determing the interpolation error (e.g., in a finite element analysis setting) are (1) geometric quality in physical space, (2) alignment quality in physical space or isotropy in computational space, and (3) adaptive quality or level of equidistribution. From the way that terms representing these three features arise in the interpolation error bound, it was shown how these terms tend to compensate for one another, but argued that generally the latter two are the most important. **Weiming Cao** performed a related analysis for anisotropic triangular grids. One additional feature was the role of two different types of stretched triangles – those with small and large angles – in the alignment. It was demonstrated why care must be taken to choose the former over the latter.

Chris Budd considered the class of PDEs for which scaling invariance and self similar solutions play a primary role. For them, moving grid methods are used which have the same scaling invariance built into the expanded physical PDE/moving grid PDE system. Numerical results for the resulting methods were shown for a number of challenging blowup problems in one space dimension. The argument was made that these moving grid methods are ideally suited for blowup problems because the grid naturally evolves on the proper space and time scales.

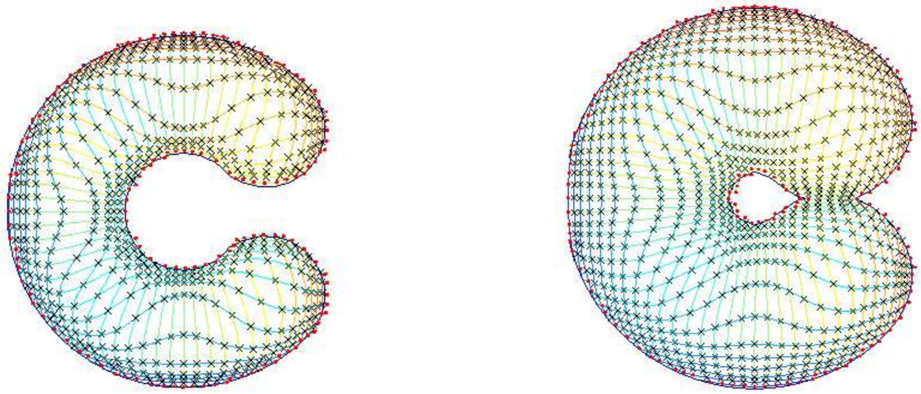

Figure 1: Starting from a uniform mesh, the mesh is adapted to put more grid points near the domain boundary (left). As the domain grows outwards with some constant normal velocity, a change in topology is automatically handled (right) [4].

Jeff Williams discussed a method for doing adaptivity for time-dependent PDES based upon the Monge-Ampere equation. Specifically, relating the coordinate mapping $x(\xi, t)$ for mesh adaptivity to the mapping used for solving the classical Mass Transfer Problem (recast as a dynamic framework), the Monge-Ampere equation is solved for the gradient of $v = x_t$, allowing straightforward computation of x. The relation was given between this and the GCL method, another velocity based. Advantages and disadvantages of this promising method were presented, as well as computational results for two and three dimensional problems.

John Mackenzie discussed a number of features of his numerical implementation of a moving grid method for solving PDEs. An analysis of several choices of monitor functions was given and the importance of using a conservative form for the PDE in computational (quasi-Lagrangian) space discussed. Numerical examples of the method, including on a Stefan problem with grid moving with the interface, were given.

Ben Ong gave a talk bridging moving grid methods and level set methods. In his preliminary computational experiments, he demonstrated how the change in topology of a physical region, while captured well by level set methods when the boundary is fairly smooth, can lose resolution around areas of high curvature. Using a GCL approach, he was able to demonstrate the clear potential of combining these two areas. See Figure 1 for an illustration of his approach on an evolving domain with topological change.

3 Level Set Methods

Level set methods are numerical techniques introduced by Osher and Sethian in 1988 to track the motion of interfaces. Rather than evolving marker cells placed along the interface, these methods represent the interface as the zero contour of a function, ϕ, defined over the computational domain. The evolution of the interface is carried out according to the level set PDE,

$$\phi_t + v \cdot |\nabla \phi| = 0$$

where v is the normal velocity of the evolving interface. This interface velocity can depend on the geometry of the interface or on external physics defined by equations off the interface. It is commonplace to discretize level set equations on fixed, uniform grids, leading to relatively simple methods with good stability properties. These methods have the powerful advantage of automatically handling topological merger and breakage.

The generality and robustness of level set techniques have made them natural choices for a wide range of applications, including problems in fluid mechanics, computer graphics, manufacturing of computer chips, combustion and image processing.

3.1 A general issue

A particularly lively debate arose in the discussion following Hong-Kai Zhao's introductory talk. It was noted that while level set methods automatically handle topological shape changes, there will be situations where the corresponding evolutions are not physically correct. While the theory of viscosity solutions may provide some answers, it is clear that detailed modelling of the underlying physics will be needed in certain problems. No universal solution to this interesting problem was found during the workshop, however, discussions illuminated the need for careful design of level set algorithms in physical problems.

3.2 Overview of work presented

A broad spectrum of level set talks were given over the course of the workshop.

David Adalsteinsson gave a talk on his recent work on transport and diffusion of material quantities on propagating interfaces using level set methods. Material quantities defined on an interface are not easily handled by traditional level set methods. Adalsteinsson described an approach for extending the level set method to these problems.

Anne Bourlioux gave a talk on her research into multi-scale strategies for turbulent burning fronts. In many practical applications (for instance, engines), flame fronts are thin and can be viewed at the large scale as a zero-thickness interface that separates burnt and unburnt gases. Her talk described research on how the effective dynamics of the front at the large scales of interest are influenced by the small scale stirring by the turbulent flow.

Li-Tien Cheng discussed work that combines the level set method and the heterogeneous multiscale method for interface problems in multi-scale settings. Examples that were considered included flows related to the homogenization of Hamilton-Jacobi equations and to the phase-field model, all in the presence of highly oscillating or random data that introduce a small scale. His approach incorporated the advantages of both methods to produce a fast algorithm that handles the multiscale and topological aspects of the interface dynamics.

Oliver Dorn reported on his recent work on identifying, localizing and tracking penetrable objects. In this problem, an array of electromagnetic or acoustic sources is located at a certain position and emits waves which propagate through the environment and are scattered by objects. Dorn described approach for finding information on the location, trajectory, orientation and the shape of the moving object in a stable way using a variety of techniques including level set methods.

Isaac Klapper described recent work in the study of biofilm response to mechanical stress. Biofilms are dense ubiquitous aggregates of microorganisms. Klapper and collaborators are interested in characterizing physical properties of biofilm with the longterm aim of understanding phenomena such as mechanical failure. He described work on methods to treat these problems efficiently and accurately.

Ian Mitchell reported on some of his recent work on level set methods for control and verification. His talk described a recent method for warning air traffic controllers of of potential collisions. Drawing on results from optimal control, differential games and level set methods, he described methods for calculating the reachable sets corresponding to aircraft collisions. High dimensional systems are still difficult; however, one possible counter to Bellman's curse of dimensionality that was given is to compute an overapproximation of a high dimensional reachable set as a collision of lower dimensional projections. See Figure 2. Recent related work on particle level set methods for increasing the accuracy of level set methods near high curvature regions was also described.

Jamie Sethian reported on a variety of recent work including the industrial simulation of evolving droplets in ink jet printers. His work on ink jet printers made use of recent level set techniques to robustly treat the evolving drops. He discussed how mass conservation is particularly relevant to the treatment of such problems and showed how practical methods can be designed by combining a 2nd order Godunov method, a finite element projection method and fast marching algorithms.

Peter Smereka described a Monte-Carlo method for surface growth simulations. His approach combined aspects of continuum mechanics and kinetic Monte-Carlo to achieve an efficient way to approximate models arising in epitaxial growth. The methods give a more realistic account of

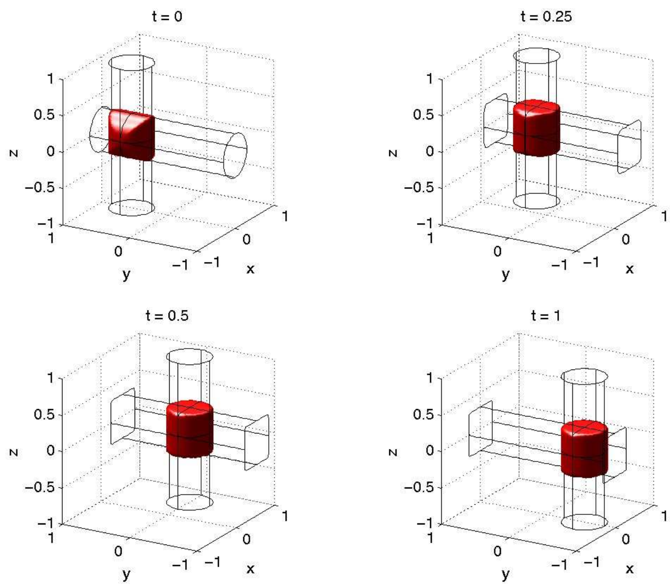

Figure 2: Overapproximating Reachable Sets by Hamilton-Jacobi Projections. From [3].

fluctuations in island shape than deterministic methods while still maintaining efficiency in problems where kinetic Monte-Carlo is impractically slow.

4 Fixed Grid / Moving Interface Methods

With this class of methods, a fixed computational grid is used over the global spatial domain that typically does not align with any internal interfaces. The interfaces are then represented as codimension 1 surfaces moving relative to the fixed grid. An advantage of this approach is that expensive grid generation and regridding is avoided each time step. Fast and accurate methods can often be used on the fixd grid, at least away from the interface, and special methods are needed only near the lower dimensional surface.

4.1 Some general issues

A number of issues arise that can each be addressed in many ways, leading to a multitude of methods of this type. Some of these issues will be broadly described and then some some specific methods and discussion points from the workshop will be mentioned.

What sort of global grid should be used and what is the underlying discretization method away from the interfaces? For example, a finite difference method might be applied to obtain pointwise approximations to the solution at discrete points as illustrated in Figure 3(a), or a finite volume method might be applied over grid cells as indicated in Figure 3(b). In each case an interface is also shown that cuts between grid points or through grid cells. A finite element method might be used with elements consisting of the distinct cells shown in Figure 3(b) or of the full rectangular cells with special basis functions that incorporate jump conditions at the interface.

How are the equations discretized near the interface? Typically a PDE must be solved on each side with some coupling or jump conditions imposed at the interface. Depending on the application, it may be the same equation on each side or two very different equations. If the equation has the same form then it may be possible to difference across the interface with additional terms included from the interface, or it may be ncessary to use one-sided approximations on each side with appropriate coupling.

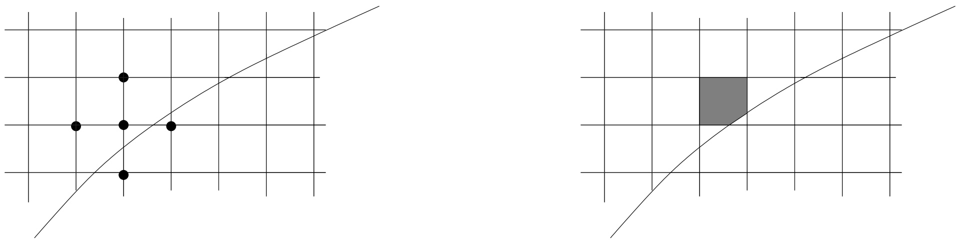

Figure 3: (a) A finite difference grid (b) A finite volume grid.

How is the interface represented and moved? The interface might be specified by a set of marker points that are densely distributed on the interface (with spacing comparable to the mesh spacing) and the interface determined solely by these points. Alternatively, marker points may be spaced more widely and a curve or surface fit through these points at each time to determine the interface. For some problems it is better to have an entire spatial domain covered by marker points. In any case the marker points must be moved in an appropriate manner each time step. Another approach is to represent the interface location implicitly via a level set function. Then an evolution equation for this function must be developed that is compatible with the desired interface motion, and this equation coupled with the equations being solved.

4.2 Overview of work presented

A number of participants work on *immersed boundary methods*, an approach pioneered by Charles Peskin originally for modeling blood flow in the heart that has since been applied to many other problems, particularly in biofluid dynamics. See [5] for a recent review. In recent years a great deal of progress has been made in applying this method to full three dimensional simulations in biofluid dynamics. Figure 4 shows a sample computation of a swimming organaism, from [2].

Robert Dillon reported on recent work modeling the movement of eucaryotic flagella and cilia. A three-dimensional model has been developed that represents the physiology of the axoneme in a detailed manner and links the elastic properties of this structure to the fluid dynamics via the immersed boundary method.

Gretar Tryggvason described recent work on simulating bubbly flow, where full three dimensional simulations are being performed with hundreds of bubbles in some cases. Figure 5 shows a portion of such a simulation. Recent work has focused on the use of methods for simulations of multifluid flows to understand the dynamics of large disperse systems and on the development of methods for systems where it is necessary to deal with complex physics, such as phase change in boiling processes.

Ricardo Cortez reported on *regularized Stokeslets*, a method for Stokes flow with immersed boundaries or obstacles that is based on smoothing a point force and explicitly calculating the resulting pressure and velocity. These can be superposed to determine the response to forces distributed along an interface. The velocity expression can be inverted to find the forces that impose a given velocity boundary condition. This allows the solution of flow problems past fixed obstacles as well as flexible boundaries.

Anna-Karin Tornberg described some recent research on the accuracy that can be achieved when using discrete delta functions distributed along an interface. This is an issue both in immersed boundary methods, where a tensor product of one-dimensional delta approximations is frequently used for a multidimensional delta function at a point, and in level set methods where a one-dimensional delta function based on the distance function comes into play.

John Stockie gave a talk on the stability of fluid flows containing immersed elastic boundaries, where the fluid-structure interaction is driven by periodic variations in the elastic properties of the solid material. This leads to parametric resonances that can be studied with Floquet theory and compared to direct numerical simulations of the fluid-structure interaction problem using the immersed boundary method.

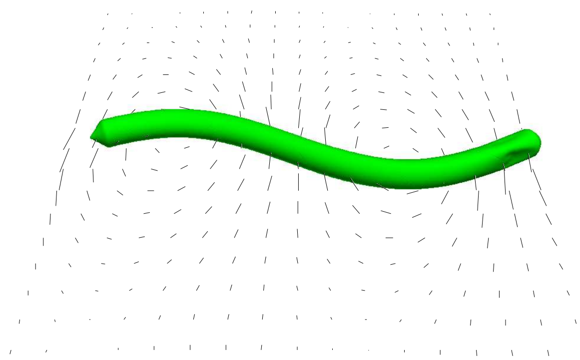

Figure 4: An immersed boundary computation of the motion of a nematode, depicting the fluid velocity field on the plane coinciding with the organism's centerline. From [2].

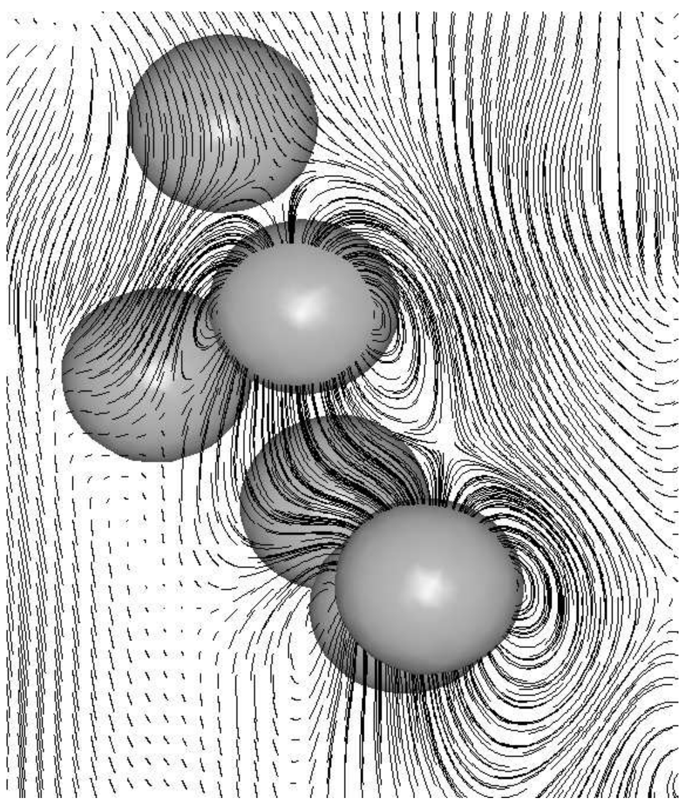

Figure 5: Flow field near rising bubbles. From [6].

Zhilin Li gave an overview talk on the *immersed interface method* and recent applications. This approach is based on the immersed boundary method, but instead of using a discretized version of a delta function or a dipole at an interface, the appropriate jump conditions for the partial differential equations are built into the discretization of the equations directly. When this can be done it typically results in sharper approximations of the the solution near the interface and perhaps higher order of accuracy overall. This has been applied to a number of moving interface problems in fluid dynamics, solidification, and elasticity. Some recent progress on finite element formulations was also described.

Xudong Liu described joint work with Songming Hou on a numerical method for solving variable coefficient elliptic equation with interfaces. In his talk a new 2nd order accurate numerical method on non-body-fitting grids was given for solving the variable coefficient elliptic equation. His method allowed the presence of interfaces where the variable coefficients, the source term, and hence the solution itself and its derivatives may be discontinuous.

Deborah Sulsky presented work on the material-point method, an extension of the particle-in-cell approach in fluid dynamics to problems in solid mechanics. Rather than tracking only the interfaces, particles within the solid are tracked. By tracking particles and their stress tensors during the deformation of the body, it is possible to represent large deformations without the problems of mesh tangling that could arise in other Lagrangian descriptions. Information from the particles is transferred to a background computational grid to solve the momentum equations and efficiently compute interactions. The method can be used to solve problems where elastic bodies come in contact, such as the problem shown in Figure 6.

Xiaolin Li discussed a front tracking approach to solving interface problems that is an integration of the original front tracking approach of Glimm and McBryan, the Eulerian level-set method by Osher and Sethian, and the marching cube method for computer graphics by Lorenson and Cline. The interface is described as a set of topologically connected marker points which follow the Lagrangian propagation based on the solution of Riemann problem (in fluid dynamics), and the use of the Riemann solution along an oblique boundary in space-time to compute the interface fluxes, making the method conservative.

Petri Fast talked about the use of moving overset grids to track interface dynamics. The key idea is to use thin, body-fitted grids that move and deform with moving boundaries, while using fixed Cartesian grids to cover most of the computational domain. This has the advantage of using a grid that conforms to the interface locally but without the need for global regridding. Fast discussed the Overture code developed at LLNL and applications to viscous fingering and to simulations of elastic boundaries in a flow.

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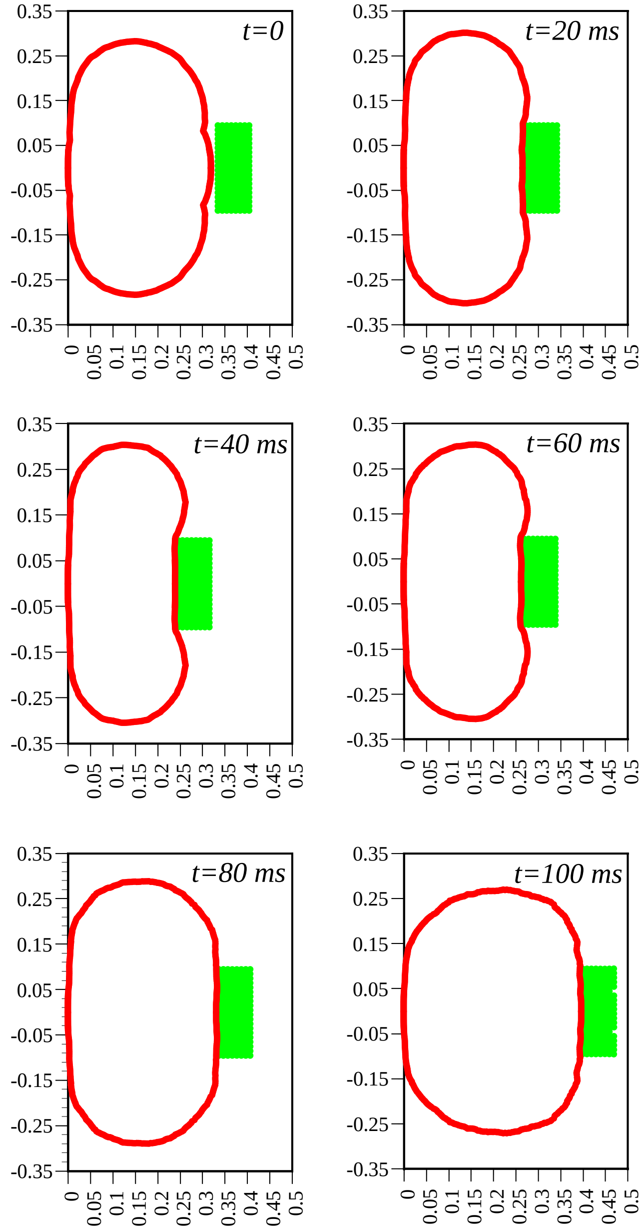

Figure 6: Axisymmetric calculation of a pre-inflated airbag being impacted by a solid, cylindrical probe, the deformation of the airbag as it is compressed and the subsequent rebound of the probe. From [7].