NUMERICAL MODELING OF IMPACT CRATERING

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ABSTRACT

Numerical modelling is a fundamental tool for understanding the dynamics of impact cratering, in particular at planetary scales. Impacts have influenced the formation and evolution of nearly every planetary surface in the solar system, yet we can only observe the scars left by past events. Detailed computer modeling of the physics of the impact process provide the possibility of studying the dynamics of impact cratering at all scales, becoming an invaluable tool that connects and complements geologic and remote sensing observations, and small scale laboratory experiments. The main requirements for computer modelling are a good understanding of the physics and chemistry of the process and enough computer power to model the part of the impact process we are interested in.

1.   INTRODUCTION

Impacts of asteroid and comets have affected the formation and evolution of nearly every solid planetary surface of the solar system. They produce impact craters of all sizes, which are easily observed both remotely (on various planetary surfaces) and in-situ (on Earth). Experimentally, laboratory tests can produce small-scale analogues of large impacts; the largest man-made experiments, high explosive/nuclear tests and the most recent Deep Impact cratering mission, can only create structures that are comparable to the smallest observed planetary impact craters. In particular, processes like shock melting and vaporization in large impacts, which involve extreme pressures and temperatures, cannot be easily reproduced in the laboratory, while the influence of planetary gravity in the late stages of crater formation makes it difficult to extrapolate small-scale laboratory collapse experiments to planetary impact cratering.

Computer simulations provide the only feasible method for studying the physics of the impact cratering process connecting and complementing planetary-scale geologic and remote sensing observations to small-scale laboratory experiments. Moreover, they provide detailed temporal and spatial information of various variables of interest, in a controlled environment, in a sense making them the best instrumented experiment [1]. The main requirements for computer models are a good understanding of the physics of the process and enough computer power to model the part of the impact process we are interested in.

This paper will provide a brief overview of the most important aspects of numerical modelling of impact cratering, including recent progress made in the field and future developments. For more information see also [2].

2.   THE THEORY BEHIND MODELING

The continuum dynamics of impact cratering and relative hydrodynamics and solid state deformations are well understood and implemented in the computer programs used to model impacts, usually referred to as hydrocodes. A high speed impact causes a sudden compression of projectile and target materials at the impact point, generating a shock wave that propagates through both projectile and target. As the shock passes, the material's initial thermodynamic state changes rapidly and irreversibly to a shocked state. As the shock wave reaches the projectile's rear end, or the target surface, it is reflected back as a rarefaction wave that adiabatically releases the material from the shock state. The speed of the rarefaction wave is usually higher than that of the shock wave and ultimately the shock wave becomes a thin shell sandwiched between the shock front and the rarefaction wave. Behind the shell, some residual particle velocity remains in the target with a tangential component (due to the presence of the target's free surface) that initiate the excavation of the crater.

The physics required to describe large meteorite impacts consists essentially of the classical Newtonian mechanics (F=ma plus conservation equations) supplemented by classical thermodynamics [3].

Newton's Laws of motion are implemented in hydrocodes as a set of differential equations, first derived by P.H. Hugoniot from the principles of conservation of mass, momentum and energy across the shock discontinuity. The Hugoniot equations are entirely general, regardless of the phase of medium through which the shock wave propagates.

The thermodynamics of impacts is not as straightforward as Newtonian mechanics. Thermodynamics is implemented through the response of materials to the shock, and it is represented in the model by material equations of state. The combination
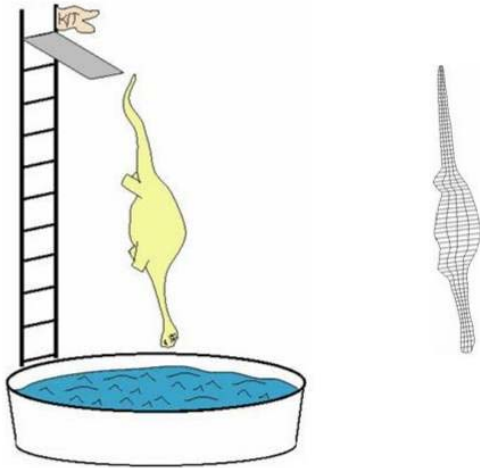
Fig. 1: Numerical modeling of any impact event begins with a discretization process. Projectile and target are divided into discrete blocks, or cells, each with associated individual sets of physical parameters. (Image courtesy of Gareth Collins).

of the Hugoniot equations and the equation of state completely specify the conditions on either side of the shock. In addition, material strength is crucial in the late stages of an impact event. To date, few good equations of state and strength models exist for geologic materials, such as rock and ice.

Material modelling is further complicated by porosity that can affect the partition of energy in the impact process and the overall response of material to an impact event. Finally, it must be kept in mind that the composition of planetary crusts is rarely homogeneous, both microscopically and macroscopically. The mixing of materials of different impedances in the target affects the distribution of the shock wave, causes shock reverberations at material boundaries, and overall modifies the final thermodynamic state of the various materials. In turn, this affects material melting, vaporization and ejection, and the final crater morphology.

3. FROM THE THEORY TO THE NUMERIC CODE

The implementation of the continuum dynamics of impact cratering into a numerical code occurs through a discretization process that consists of dividing space and time into discrete blocks, or cells. The total number of cells, i.e., the mesh of the simulation, can vary and is ultimately limited by the computer's physical memory and the amount of time available for the computation. The combination of the total number of cells possible and the total mesh required for the simulation determines the spatial and temporal resolution of the simulation. The choice of resolution in space and time is important when modelling impact

events. On one hand, any simulation's resolution should be high enough to resolve all the important flow variations in space and time. On the other hand, we are limited by the available computer power and time allowed to complete the simulation. For example, a spatial resolution of 100m in the modelling of a 100 km diameter impact crater requires around 10^{10} cells in a 3D simulation, yet 100m resolution is too coarse to distinguish small, meter scale features, that can be observed in the field by a geologist. Modelling the entire impact process to the final 100 km crater may require a timescale around 500s that corresponds to around 500,000 time steps if the temporal resolution is around 10^{-3}s. However, 10^{-3}s may not be good enough to clearly distinguish the early development and propagation of the shock wave in the target and projectile and that may introduce instabilities in the integration process. This is usually avoided by introducing a stability condition (Courant-Friedrichs-Lewy stability condition), which requires that no signal (e.g., the shock wave) can propagate across the shortest dimension of a cell in a single time-step [1]. Resolution problems can be mitigated somewhat by better solution algorithms, such as those employing smooth particle hydrodynamics (SPH; [4]) or adaptive mesh refinement (AMS; [5]). Finally, the total computer storage needed to record the important parameters in an impact simulation depends on the total number of parameters recorded, the total number of cells in the simulation and the total number of time steps required to complete the simulations. Thus computer hardware can severely limit the comprehensiveness of a simulation.

3.1 Resolution Effects

Computer power may limit the maximum number of cells that can be used to cover the spatial mesh required for any particular impact simulation. This is particularly true in the case of 3D simulations. However, much care must be exerted to make sure that the desired results of impact simulations (e.g., mass of rock melted, maximum shock pressure, mass and speed
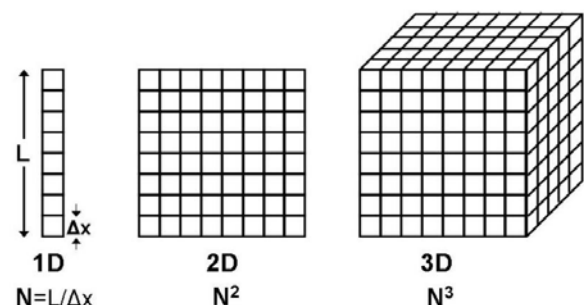
Fig. 2: Schematic of the number of cells involved in a numeric simulations for 1- 2- and 3-dimensions. L is the spatial scale of the simulation, Δx is the desired spatial resolution and N is the number of cell in any direction.

of ejecta, etc.) do not depend on the simulation resolution and mesh chosen.

The danger of using inadequate mesh resolutions can be illustrated by two simple examples (Fig. 3), dealing with a) the determination of target melt/vapour volumes in 2D simulations and b) the estimate of maximum shock pressure in 3D simulations.

Melt/vapour volumes from impacts into a crystalline rock target were estimated for several 2D simulations at different resolutions [6]. The upper panel of Fig. 3 shows the results of planetary-scale simulations for four different resolutions: 5, 10, 20 and 40 cells-per-projectile-radius, or cppr. The lowest resolutions, 5 and 10 cppr, are similar to resolutions used in early modelling work, while the higher resolution, 40 cppr, is rather typical of today's 2D simulations. The figure shows the clear deterioration of melt/vapour estimates with decreasing resolution. The resolution effects are strongest (low melt production) for simulations with impact velocities that are typical of asteroidal impacts on Earth (v≤30 km/s), resulting in artificially small estimates of melt/vapour production by as much as a factor of 2.

Estimates of maximum shock pressure in a crystalline rock target were obtained for a series of 3D hydrocode


simulations at different resolutions. The simulations indicate that low resolution affects the results of the simulations by reducing the intensity of the recorded shock (recorded shock parameters are averaged over the volume of the cell: the smaller the cell the sharper the shock), as shown in the lower panel of Fig. 3. This affects the final estimates of melting/vaporization volumes. In particular, even at typical resolutions currently used in 3D runs (given computer availability), i.e., 18-20 cppr, the volumes associated with high shock pressures may still be underestimated. Overall, in the simulations with CTH there is a loss of about 20% in melt-volume when the mesh resolution is degraded from 18 to 8 cppr. This result is similar to studies done with similar 3D hydrocodes [7].

## 3.2 Eulerian versus Lagrangian Treatment

The solution of the equations describing the shock event can be approached in two ways: using a coordinate system moving with the material, known as the Lagrangian approach, or fixed in space, known as the Eulerian approach. [1].

In the Lagrangian approach the mesh is fixed with the material. The mesh is generated by assigning a single material to each cell. No material flows in or out of a cell, so mass in the cell is a constant and it is possible to record the evolution of material in each individual cell. Any variation of density inside the cell is dues to changes in the cell's volume during the simulation. With this approach, free surfaces and contact surfaces between different materials are easily determined and remain distinct throughout the calculation. This is an important advantage over the Eulerian approach, in which the mesh is fixed in space and material flows through it. In this case it is the cell's volume that stays constant and any change in density within the cell is due to variation in the cell's mass during the simulation. In this approach material interfaces are quickly blurred with the introduction of "mixed cells", thus making boundaries less sharp. This problem can be partly obviated by using high resolutions, but at the price of a longer simulation run.

The major limitation of the Lagrangian approach is the inaccuracy in the solution of the shock equations when the cells are significantly distorted; an extreme case is a computed negative cell volume occurring when a cell folds over itself. A way to overcome the extreme grid distortion problem is to stop the simulation, carefully rezone the computational grid by overlaying a new, undistorted grid, on the old distorted mesh and restart the run. This process may have to be repeated many times when strong distortions are involved, making it a highly unfeasible approach for modeling the early stages of impact cratering. The problem does not exist or Eulerian codes, which can easily handle flows with large distortion, and are thus ideal to simulate the early
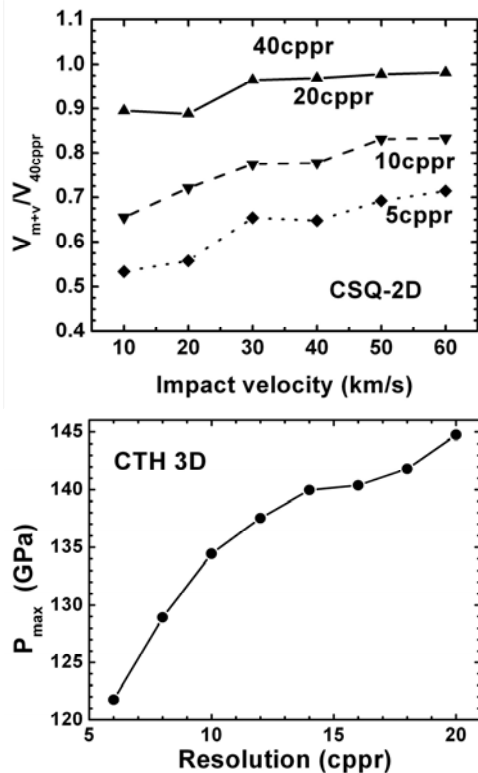
Fig. 3: _Upper_: Resolution effects in estimates of melt volumes for 2D simulations (using the hydrocode CSQ). From [6]. _Lower_: resolution effects in estimates of target's maximum shock pressures for 3D simulations (using the hydrocode CTH) [7].
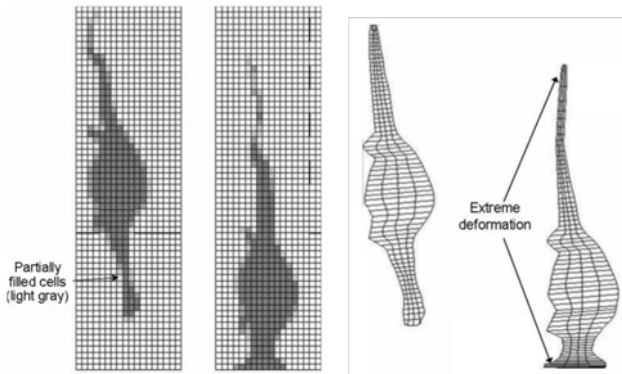
Fig. 4: Eulerian (*left*) versus Lagrangian (*right*) approach
For numerical modeling. (Image courtesy of Gareth Collins).

stages of the impact process and the evolution of the expansion plume.

An alternative approach to typical Eulerian and Lagrangian "cell-codes" is the Smoothed Particle Hydrodynamics (SPH) approach, routinely used in the study of astrophysical fluid dynamics [4]. In the SPH approach material is represented by individual nodes with mass associated with them so that they can be considered and treated as physical fluid particles. Each node represents an average of its immediate area and its characteristics are determined as weighted sums over its neighboring node's values. One advantage of the SPH approach is that it is not subject to boundary conditions because it is not bound to a fixed grid, typical of "cell-codes". Among the main limitations of the SPH approach are resolution problems (it is intrinsically a low-resolution approach when compared to typical cell-based hydrocodes) and problems with material models, in particular with the implementation of strength models.

3.2 Material Models

Specific material properties govern the response of materials to stress, resulting in different behaviours of different materials for nominally the same impact conditions. The changes in a material's density and internal energy with pressure are described by the *equation of state* (EOS). This relation is critical in the early stages of an impact event, when material strength is negligible compared to the pressure involved. The relation between stress and the strain (distortion) that produced it is given by the *constitutive equation*. This relation is fundamental for modelling the late stages of impact cratering, when material strength determines the final shape and characteristics of the crater.

The EOS is a necessary complement to the Hugoniot equations as to completely describe the conditions on either side of the shock. Thanks to the EOS it is then possible to specify the final thermodynamic state of shocked materials, usually represented graphically in pressure-volume, or in shock velocity-particle velocity plots.

Equations of state depend on the complexities of a material's atomic, molecular and crystalline structure and are unique for each material. In impact modeling studies they must describe the material's thermodynamic behavior over a wide range of pressures, temperatures and specific volumes (or densities). The famous Tillotson EOS [8], specifically built for and widely used in impact modeling, is an analytical EOS which can describe the material below or above vaporization. However, it provides an incomplete description of a material's thermodynamic properties as it cannot model two-phase regions nor it provides any information on how to compute the temperature or entropy of the material.

More complete equations of state consist in sophisticated computer codes that use different physical approximations in different thermodynamic regions. A widely used example of such codes is ANEOS [9], which uses Helmholtz free energy to obtain thermodynamically consistent estimates of properties like pressure, temperature, density, entropy. Material specific properties are provided through a series of parameters. ANEOS offers a (limited) treatment of phase changes, which is especially important when they interfere with the shock state. An updated version of ANEOS [10] expands the vapor phase treatment from simply monoatomic to biatomic species, improving the treatment of the vapor phase.

An important limitation of ANEOS is that it does not allow us to simultaneously treat solid-solid and solid-liquid phase changes. As a result, for complex materials, such as many minerals of geologic interest, a choice must be made between the two types of phase changes, depending on their influence on the material's Hugoniot shock curve. A proper reproduction of the Hugoniot shock state has been the main drive to treat the solid-solid phase transition (in compression) in the development of ANEOS EOSs for geologic materials [e.g., 6]. The price for this capability, however, is an oversimplified description of the solid-liquid (melting) transition and unrealistic values of the heat expansion coefficients (too large for low-pressure solid phases). This generally does not affect strongly the early stages of impact cratering, especially when the determinations of average melt/vapor volumes are based on experimentally determined estimates of shock pressures for incipient and complete melting (assuming that the material always reaches ambient pressure after release from the shock state). On the other hand, the lack of an explicit treatment of melting as a gradual transition from a solid to a liquid state may cause severe errors in estimating the energy balance in the impact, especially when the latent heat of fusion may affect the P-T path of the material's thermodynamic evolution. For example, in very large impacts (>300

km in diameter; [11,12]) large amounts of material may be compressed above incipient melting shock pressures at some depth below the surface, unloading to non-ambient pressure where they could be strongly heated but not completely melted.

Failing to correctly account the utilization of impact energy for (partial) melting, and the correct status of the material upon unloading from the shock state will strongly affect the subsequent modeling of important impact processes such as material ejection and crater collapse.

4. ADVANTAGES OF IMPACT MODELS

Hydrocode modeling is the only approach that can describe the dynamic of the impact process, including crater excavation, material ejection, melting/vaporization, crater collapse, ejecta launch and deposition. Throughout the simulation it can provide detailed information regarding all variables of interest which can ultimately be tested against observations. In this respect, numerical modeling is a crucial and unique approach in the study of impact cratering.

Historically, there has been a separation between early and late stage modeling of impact cratering. Each stage is modeled separately from the other, and often using different codes. This approach allows us to maximize the scientific return of numerical simulations. Early stage studies, usually carried out using Eulerian codes, focus on evaluating shock states in the target and projectile and require simulations with high temporal resolution and high spatial resolution near the impact point. Late stage studies focus on the process of crater collapse and the formation of the final impact structure. They require long integration times, not necessarily with high temporal resolutions, and a large spatial mesh that can be accompanied by a lower spatial resolution. Reasonable deformations in the cells during the late stage of impact cratering permits the use of Lagrangian codes, which in turn have the advantage of a better control over the material boundaries and material properties. Detailed studies of both impact stages in a single, continuous numerical simulation are becoming a possibility today with the aid of increasingly more powerful computers.

5. LIMITATIONS OF IMPACT MODELS

The colorful and spectacular images and animations generated by impact models may instill the notion that impact models can tell us anything about the impact process from microscopic (e.g., fragment sizes in impact melt breccia) to macroscopic levels (e.g., final ejection and deposition of materials in different shock states around the crater). However, spatial and temporal resolutions combined with computer

hardware limitations place severe constraints on what can be investigated in any individual simulation. In particular, numerical simulations cannot model processes that fall below the resolution limit of the model used. As described in section 3.1, accurate testing must be done before and after numerical studies, to ensure that the results are not affected by numerical limitations.

Furthermore, numerical simulations can only model processes that have been (correctly) implemented in the numeric code. Thus, limitations in material models, described in section 3.2 will limit the usefulness of the simulations. Other processes of interest may not be described in the code. For example, at this time no current hydrocode can model the chemistry that occurs inside the expansion plume. This does not mean that such process is untreatable, only that the correct implementation of the process of interest in the numeric code has not been developed yet. In some instances, the implementation cannot be carried out until we have a better understanding of the process, i.e., the physics and thermodynamics that govern it.

6. UNDERSTANDING IMPACT CRATERING THROUGH MODELING

Hydrocodes offer a means for studying various aspects of the impact process that cannot be investigated by other methods. Two obvious examples are the role of hydrocode simulations in constraining the amount and distribution of impact melt and vapor production and in characterizing the evolution of complex morphologies observed in large craters.

### 6.1 Melt Production and Ejecta

The amount of melt and vapor produced in an impact
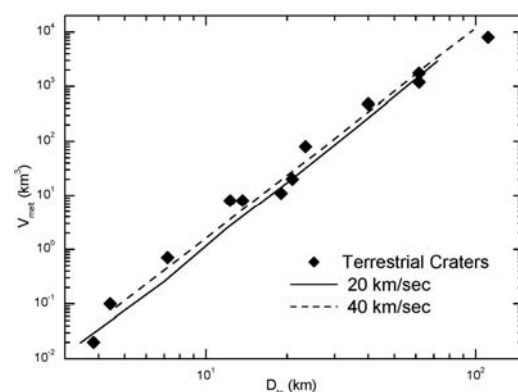
Fig. 5: Numerically estimated impact melt volumes versus transient crater diameter (solid and dashed lines) compared with terrestrial data on crystalline targets (diamonds) compiled by [12]. Simulations are for dunite projectiles on dunite targets at 20 and 40 km/s in 2D. From [6].

influences various aspects of the impact cratering event and its effects, from heat deposition to the development and composition of the vapor plume, to crater shape and impact lithology. In an impact event, melting and vaporization is an early stage phenomenon, governed by the thermodynamics of shock compression and release. Melt production cannot be reproduced in laboratory experiments (due to limitations in impact energy associated with experiments). Numerical modeling is thus the only approach that provides a handle on estimating melt/vapor production in impact events. This requires, however, accurate material equations of state, as well as realistic target compositions, where material mixing can occur at all spatial scales.

Numerical estimates of melt production in crystalline targets suggest that melt volumes increase linearly with increasing impact energy [6,13]. This result, holds for
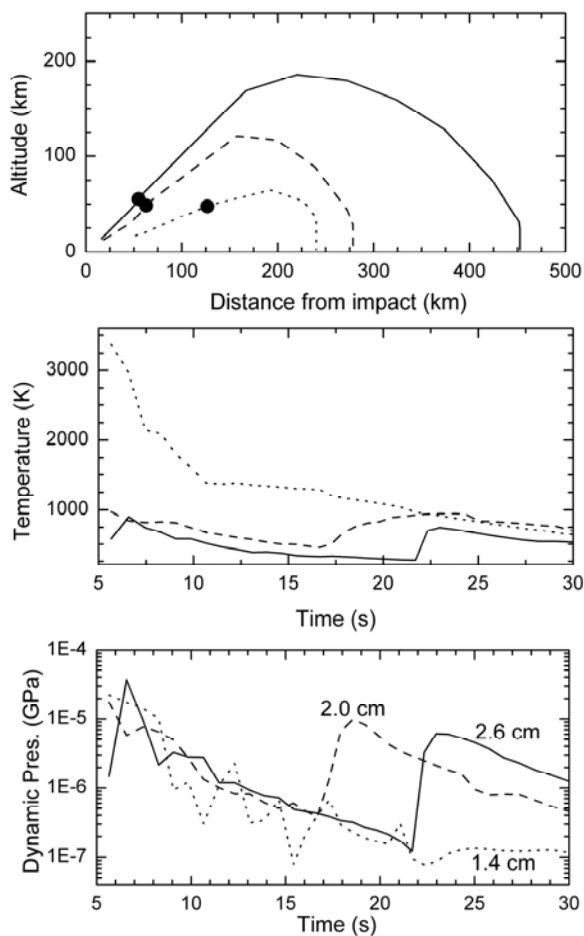

Fig. 6: Trajectories (**upper**), temperatures (**intermediate**), and dynamic pressure (**lower**) versus time for a few tektite-type particle of different sizes. The solid line represents a tektite 1.3 cm in diameter, dashed line a tektite 1.0 cm in diameter, and dotted line a tektite 0.7 cm in diameter. Solid circles in the upper panel mark the end of the hydrodynamic simulations (~30 seconds after the impact). From that point on the trajectories represent the motion of particles in an undisturbed atmosphere. From [16].

all but the lowermost impact angles (≤15°, measured from the impact surface). Fig. 5 from [6] shows that numerical estimates of melt volumes appear to be in good agreement with available observational data from terrestrial structures [14]. For oblique impacts a rough direct relationship seems to hold between melt production and transient crater volumes for all but the lowermost impact angles [15].

Accurate numerical studies of melt production in impact events have helped in understanding the production of a unique kind of impact ejecta that has fascinated and puzzled scientists for many years: tektites. As recently as the 1960s, O'Keefe argued strenuously that tektites originated on the Moon; however, geochemical comparison between tektites and lunar rocks returned by the Apollo program made it clear that they are in fact of terrestrial origin. Tektites are naturally occurring glasses, usually not more than few centimeters in diameter. Today they are grouped into four distinct strewn fields: central European, Ivory Coast, North American and Australasian, all but one (Australasian) associated by spatial and geochemical characteristics to an impact crater (European: Ries, Ivory Coast: Bosumtwi, North American: Chesapeake Bay). Tektites have very low extraterrestrial component, with a maximum of about 0.06 wt% in Ivory Coast tektites. Water content, cosmogenic nuclides and chemical and physical homogeneity indicate that tektites originate from high-temperature melting of the uppermost few tens of meters of terrestrial rocks during impact cratering. Numerical modeling of the formation moldavites [16], Ivory Coast tektites [17] and Popigai distal ejecta [18] has indicated that tektites arise from a restricted area inside the growing crater in the very uppermost layer of the target rocks. During their flight in a post-impact plume they are not subjected to high pressures and cool slowly, as shown in Fig. 6, thus allowing for the time necessary to loose water/volatiles and obtain their hydrodynamic shape [16]. No special conditions are required to produce tektites: the study presented in [16-19] shows that the deficiency of tektite strewn fields (4 against ~180 impact structures) can be easily explained by the need of relatively large impact events (final crater diameter >10 km) and by the quick degradation of natural glasses under weathering (natural glasses are normally <50 Myr old).

3.2 Crater Collapse

Impact crater collapse is controlled by the competition between the gravitational forces tending to close the excavated cavity and the inherent material strength properties of the post-shock target. Thus, accurate simulations of crater collapse require a realistic constitutive model to represent the target material, and a good understanding of the fundamentals of dynamic
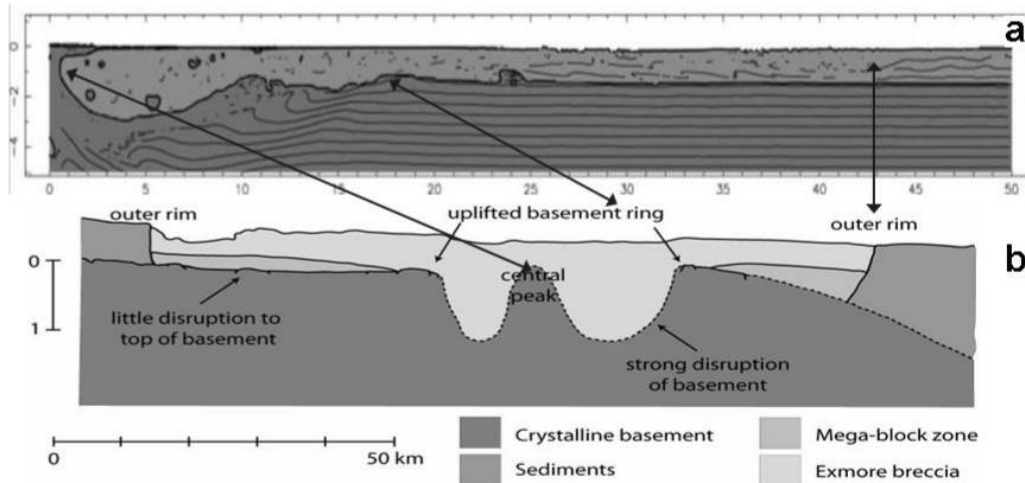
Fig. 7: Comparison between **a**) the crater collapse model result of Chesapeake Bay crater [24] and **b**) the schematic cross-section of the structure based on interpretations of seismic data and drill cores [22,23]. Double-arrowed lines show the correspondence in central peak uplift, inner rim, and outer deformation zone. From [24].

rock failure. It has been found that to reproduce the observed morphologies of complex crater collapse requires significant, but temporary, weakening of the target material beneath the crater floor. Suggested mechanisms for such a temporary strength-weakening effect include acoustic fluidization [20] and strain localization and thermal softening [21]. Both mechanisms seem to significantly improve the hydrocodes' ability to model crater collapse (i.e., the collapse of a geometrically simple, bowl-shaped "transient crater" during the late phase of crater formation); however, the relative importance of each mechanism is still poorly constrained.

A good example of the usefulness of crater collapse modelling is shown by the investigation of the Chesapeake Bay structure [22] in Virginia, United States. Late Eocene in age (35.2-36.0 Ma), the Chesapeake Bay impact occurred in a shallow marine environment, with a crystalline basement overlain by close to 1km of sediments and few hundred meters of water. Schematically, the crater has the morphology of an inverted sombrero, with a deep inner basin surrounded by a shallower brim (Fig. 7b), typical of marine impacts on Earth. Its surface morphology, however, is almost entirely flat, due to the presence of an unusually thick crater fill deposit, the Exmore breccia. The morphology of the Chesapeake Bay structure is quite different from similar-sized subaerial structures on Earth, or large craters on other planets, making it difficult to estimate the size of the impacting object, comet or asteroid, that formed it. This causes problems in evaluating the energy involved in the impact event and consequently the overall environmental consequences of the impact event. Early investigations suggested the edge of the shallow brim as the outer rim of the crater, analogous to the outer rim of complex craters while the inner basin edge was

compared to the peak ring of complex extraterrestrial craters [23].

Recent numerical studies of the Chesapeake Bay impact event [24] provide a different interpretation. The model results, Fig. 7a, indicate that the morphology of the crater was strongly affected by the particularities of the target rocks. The water-saturated sedimentary layer of low density and strength (modelled as wet tuff) was strongly mobilized during crater collapse. The water column also played an important role in aiding the mobilization of the underlying sediments. As a result, the initial opening cavity process which excavated the crystalline basement and created the inner basin was followed by a prolonged collapse phase in which impact ejecta landing outside the opening cavity disrupt the sedimentary unit to a radius of about 40 km. The final distribution includes a large fraction of the disrupted sediments moving back into the inner basin, filling it up (Exmore breccia). The resulting picture, shown in Fig. 7, is that of a flat crater, with a sombrero-like shape, just as observed at Chesapeake,.

While current impact simulations have produced a consistent paradigm for how large craters might collapse to form the final complex form, they still do not provide a complete explanation for why large impact craters collapse in this manner. A full mechanical understanding of large impact crater formation requires further testing and refining of numerical crater collapse models, supported by geological observation, geophysical data and drill cores.

7. SUMMARY AND FUTURE TASKS

There are still many important and difficult problems that computer modeling can help investigate. At this

time, material models are still the weakest component of impact modelling and require further improvement so that other important open questions can be addressed. Some of these questions deal with the role of complex targets in the cratering process, from porous (i.e. sediments) to mixed targets, such as ice/rock mixing in the Martian crust that may be responsible for the formation of rampart craters. The evolution of the expansion plume is another important area of impact studies, from target/projectile degassing to the themodynamic evolution of ejecta (i.e., tektites and or ejecta blankets), to the chemical evolution of expansion plumes.

8. ACKNOWLEDGMENTS

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