

## **Laboratory for Scientific Computing**

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### Multi-phase flows in inhomogeneous liquid explosives

#### **Motivation**

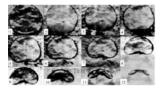
It has been observed that for insensitive explosives, bulk heating is not sufficient to cause ignition. Thus, in order to sensitize the explosive, micro-bubbles of air are artificially injected into the explosive matrix to sensitize it.

Micro-

Micro-bubbles in a liquid explosive produced by ORICA

This research is related with the numerical simulations of shock-induced collapse of voids in heterogeneous explosives and is funded by ORICA Mining Services. Upon the collapse of the bubble, formation of hotspots is observed, as well as subsequent generation of ignition sites. The ignition of reaction in an explosive matrix is a subject of great discussion, as the causes of local ignition are not universally agreed, mainly due to the presence of several contributing mechanisms. The purpose of this research is to investigate this mechanisms , examine the bubble collapse and the subsequent ignition in the ambient liquid explosive, to lead to the understanding of the heterogeneous explosive behaviour.

The numerical simulations are motivated by experiments on shock-induced collapse that have been carried out in the Cavendish laboratory and elsewhere.



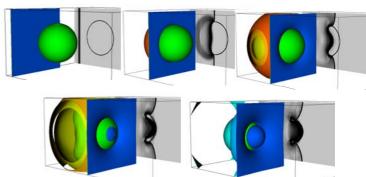
Single bubble collapse in gelatine by N.K. Bourne and J. E. Field. Explosive ignition by the collapse of cavities. Proc. R. Soc. Lond. A (1999) 455, 2411-2426

In the picture on the left, the collapse process of a 12-mm diameter bubble in gelatine is seen, which collapses under the effect of a 0.26GPa shock wave, travelling from the bottom of the cavity to the top.

When the shock wave encounters the bubble wall, it is partly transmitted into the cavity as a weaker shock wave and partly reflected as a release wave. For slow collapses, like this one, i.e. when the

incident shock wave is of low Mach number, the transmitted wave travels back and forth in the cavity and forms an instability at the back face, which eventually develops into a jet.

#### Results



The 3D bubble pictured above represents the volume fraction contour of value 0.5 and the 3D contours pictured are contours of the pressure field that help visualize the waves. The mock-schlieren technique is also employed to aid in the visualization of the waves.

When the incident shock wave encounters the bubble boundary, it is partly reflected and partly transmitted. The instability that is formed on the back face of the cavity due to baroclinic vorticity forms an intrusive jet, which upon reaching the upstream cavity wall generates a new shock wave and the cavity collapses. After the collapse, two distinct lobes



are formed an sustained by the linear vortices that were generated at the back of the cavity. A good qualitative match between the experiments and the simulations is observed.

# Mathematical Formulation and Numerical Method

One of the challenges of numerical simulations is the huge density ratio across material interfaces. For this work, and augmented Euler formulation (N=3) was used to mathematically describe the problem.

$$\begin{split} \frac{\partial \rho}{\partial t} + \sum_{j=1}^{N} \frac{\partial}{\partial x_{j}} (\rho u_{j}) &= 0 \\ \frac{\partial}{\partial t} \left( \frac{1}{\Gamma} \right) + \sum_{j=1}^{N} \left[ u_{j} \frac{\partial}{\partial x_{j}} \left( \frac{1}{\Gamma} \right) - \rho \left( \frac{\Gamma'}{\Gamma^{2}} \right) \frac{\partial u_{j}}{\partial x_{j}} \right] &= 0 \\ \frac{\partial}{\partial t} (\rho u_{i}) + \sum_{j=1}^{N} \frac{\partial}{\partial x_{j}} (\rho u_{i} u_{j} + \delta^{ij} \rho) &= 0 \quad \text{for } i = 1, 2, \dots, N \\ \frac{\partial}{\partial t} \left( \rho \varepsilon_{ref} \right) + \sum_{j=1}^{N} \left[ u_{j} \frac{\partial}{\partial x_{j}} \left( \frac{1}{\Gamma} \right) - \rho \left( \frac{\Gamma'}{\Gamma^{2}} \right) \frac{\partial u_{j}}{\partial x_{j}} \right] &= 0 \\ \frac{\partial}{\partial t} \left( \rho \varepsilon_{ref} \right) + \sum_{j=1}^{N} \left[ u_{j} \frac{\partial}{\partial x_{j}} \left( \rho \varepsilon_{ref} \right) - \rho \left( \frac{\Gamma'}{\Gamma^{2}} \right) \frac{\partial u_{j}}{\partial x_{j}} \right] &= 0 \\ \frac{\partial}{\partial t} \left( \rho \varepsilon_{ref} \right) + \sum_{j=1}^{N} \left[ u_{j} \frac{\partial}{\partial x_{j}} \left( \rho \varepsilon_{ref} \right) + \rho \left( \varepsilon_{ref} + \rho \varepsilon_{ref}' \right) \frac{\partial u_{j}}{\partial x_{j}} \right] &= 0 \\ \frac{\partial}{\partial t} \left( \rho \varepsilon_{ref} \right) + \sum_{j=1}^{N} \left[ u_{j} \frac{\partial}{\partial x_{j}} \left( \rho \varepsilon_{ref} \right) + \rho \left( \varepsilon_{ref} + \rho \varepsilon_{ref}' \right) \frac{\partial u_{j}}{\partial x_{j}} \right] &= 0 \\ \frac{\partial}{\partial t} \left( \rho \varepsilon_{ref} \right) + \sum_{j=1}^{N} \left[ u_{j} \frac{\partial}{\partial x_{j}} \left( \rho \varepsilon_{ref} \right) + \rho \left( \varepsilon_{ref} + \rho \varepsilon_{ref}' \right) \frac{\partial u_{j}}{\partial x_{j}} \right] &= 0 \\ \frac{\partial}{\partial t} \left( \rho \varepsilon_{ref} \right) + \sum_{j=1}^{N} \left[ u_{j} \frac{\partial}{\partial x_{j}} \left( \rho \varepsilon_{ref} \right) + \rho \left( \varepsilon_{ref} + \rho \varepsilon_{ref}' \right) \frac{\partial u_{j}}{\partial x_{j}} \right] &= 0 \\ \frac{\partial}{\partial t} \left( \rho \varepsilon_{ref} \right) + \sum_{j=1}^{N} \left[ u_{j} \frac{\partial}{\partial x_{j}} \left( \rho \varepsilon_{ref} \right) + \rho \left( \varepsilon_{ref} + \rho \varepsilon_{ref}' \right) \frac{\partial u_{j}}{\partial x_{j}} \right] &= 0 \\ \frac{\partial}{\partial t} \left( \rho \varepsilon_{ref} \right) + \sum_{j=1}^{N} \left[ u_{j} \frac{\partial}{\partial x_{j}} \left( \rho \varepsilon_{ref} \right) + \rho \left( \varepsilon_{ref} + \rho \varepsilon_{ref}' \right) \frac{\partial u_{j}}{\partial x_{j}} \right] &= 0 \\ \frac{\partial}{\partial t} \left( \rho \varepsilon_{ref} \right) + \sum_{j=1}^{N} \left[ u_{j} \frac{\partial}{\partial x_{j}} \left( \rho \varepsilon_{ref} \right) + \rho \left( \varepsilon_{ref} + \rho \varepsilon_{ref}' \right) \frac{\partial u_{j}}{\partial x_{j}} \right] &= 0 \\ \frac{\partial}{\partial t} \left( \rho \varepsilon_{ref} \right) + \sum_{j=1}^{N} \left[ u_{j} \frac{\partial}{\partial x_{j}} \left( \rho \varepsilon_{ref} \right) + \rho \left( \varepsilon_{ref} + \rho \varepsilon_{ref}' \right) \frac{\partial u_{j}}{\partial x_{j}} \right] &= 0 \\ \frac{\partial}{\partial t} \left( \rho \varepsilon_{ref} \right) + \sum_{j=1}^{N} \left[ u_{j} \frac{\partial}{\partial x_{j}} \left( \rho \varepsilon_{ref} \right) + \rho \left( \varepsilon_{ref} \right) \frac{\partial u_{j}}{\partial x_{j}} \right] &= 0 \\ \frac{\partial}{\partial t} \left( \rho \varepsilon_{ref} \right) + \sum_{j=1}^{N} \left[ u_{j} \frac{\partial u_{j}}{\partial x_{j}} \left( \rho \varepsilon_{ref} \right) + \rho \left( \varepsilon_{ref} \right) \right] \\ &= 0 \\ \frac{\partial}{\partial t} \left( \rho \varepsilon_{ref} \right) + \sum_{j=1}^{N} \left[ u_{j} \frac{\partial u_{j}}{\partial x_{j}} \left( \rho \varepsilon_{ref} \right) + \rho \left( \varepsilon_{ref} \right) \right] \\ &= 0 \\ \frac{\partial}{\partial t} \left$$

The system consists of the compressible, unsteady Euler equations (left) along with three extra partial differential equations (PDEs) that evolve variables found in the Mie-Grüneisen equation of state. Another PDE which evolves volume fraction is used to distinguish between the different fluids in the computational domain.

A high-resolution, shock capturing numerical scheme, namely the Wave Propagation method, is used to integrate the system numerically, coping successfully with the high density ratio.

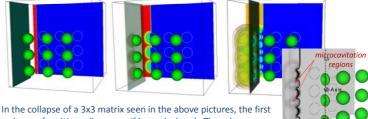


Hierarchical Adaptive Mesh Refinement (HAMR) is used to increase the resolution at regions of great importance (e.g. where the density gradient is large) by placing 'patches' of higher resolution over the coarser grid.

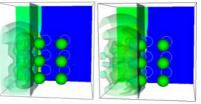
The use of HAMR results in great computational speed-ups, which are vital, especially in 3D simulations.

In real explosives, the bubbles don't appear spread and isolated. They form clusters of cavities, which could be ordered if the bubbles are artificially and carefully placed into the body of the explosive matrix or in randomly placed arrays.

Several features present in multiple cavities collapse, like the superposition of shock waves or rarefaction waves and microcavitation, bring extra effects into play, effects that are not of course present in the collapse of isolated cavities.



column of cavities collapses as if it was isolated. The release waves generated at the interaction of the incident shock wave with the bubble boundary, overlap and produce regions of low pressure and microcavitation. Upon the collapse



of the top and bottom cavities. This results in the asymmetric collapse of these bubbles as indicated by the arrows. The investigation of this phenomenon is of great importance as it is absent from existing bulk explosive models and it is believed that the implementation of these effects will lead to a more accurate model of real explosives.

of the first column, 3 new shock waves are born, and these are the waves that initiate the collapse of the second column, as it is shielded from the incident shock wave by the presence of the first column. These new shock waves overlap in pairs in the regions between the cavities and form a non-symmetric pressure field at the back





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