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Advanced modeling of detonation dynamics in energetic materials and explosive systems

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Explosives are energetic materials that support a supersonic detonation wave; a shock followed by an exothermic reaction zone. Because the explosive products expand rapidly behind the shock, the flow can choke. A sonic (characteristic) surface forms that propagates at about the same velocity as the lead shock, sealing the reaction zone from the trailing flow. Since detonation propagates in autonomous and robust way and induces large pressure changes (hundreds of Kilo bars for condensed explosives), they are useful for engineering purposes. The explosive system is detonation in the explosive and its interaction with its environment. Explosive systems include material processing, for example. Extreme miniaturized explosive systems have many alternative applications that include prospects for bio-medical uses. Since the detonation reaction zone is extremely thin compared to the domain in which it propagates, the calculation of detonation dynamics is a difficult multi-scale problem. Direct numerical simulation of the behavior of detonation dynamics is usually not an option. Fortunately, the scale disparity allows asymptotic treatments of the detonation front, and these have led to a rich and interesting theory of detonation shock dynamics where one obtains evolution equations for the front that are geometric in character and that relate the normal detonation shock velocity to the shock front curvature and higher intrinsic derivatives. Detonations exhibit generic instabilities that include pulsations and cellular instabilities; some of these can be described by the asymptotic theory. The theory of detonation shock dynamics has provided new way to interpret experiments and measure the properties of condensed explosives. Validation of theory with experiments requires multi-material (fluid) simulation of the interaction of the explosive with inert materials. The use of modern high-resolution numerical methods and modern material interface treatments, such as level-set methods is required. The talk will summarize some key advances in this subject.