# Understanding the Physics of the Deflagration-to-Detonation Transition

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**Computer Resources: Cray XE6 *(Raptor)*, AFRL DSRC; Cray XE6 *(Garnet)*, ERDC DSRC**

On the morning of December 11, 2005, a violent explosion shook the London suburb of Hemel Hempstead. The incident occurred at the Hertfordshire Oil Storage Terminal, also known as the Buncefield complex, when the spill from one of the storage tanks led to the formation of a large fuel-vapor cloud. Subsequent ignition resulted in an exceptionally powerful explosion, considered by many accounts to be the largest in Europe since the end of the World War II. Thirty five years earlier, almost to the day, on December 9, 1970, a similar explosion of an open-air vapor cloud, which formed as a result of a propane pipeline break, occurred in Port Hudson, Missouri. In both cases, the magnitude of the devastation was unprecedented for this type of industrial accidents.

Unlike these two examples, which are devastating but, fortunately, relatively rare, a very different and incredibly more powerful kind of explosions is observed on a daily basis. These explosions, however, occur on cosmological distances and are an astronomical phenomenon known as the Type Ia supernovae (SN Ia). They result from the thermonuclear incineration of compact, degenerate, white dwarf stars. These stars are the end product of the evolution of normal stars such as the Sun. When formed in isolation, they lead a fairly peaceful existence slowly cooling after their nuclear fuel has been exhausted. However, in binary systems when a close-by stellar companion is present, white dwarfs can end their life in an extremely powerful and bright explosion, which fully disrupts the star in a matter of seconds and is capable of outshining the entire galaxy for the period of several days. Such brightness, along with the remarkable similarity of the majority of the explosions, has turned SN Ia in the last fifteen years into an indispensible tool for measuring cosmological distances. This, in turn, led to the discovery of the accelerating expansion of the Universe and of the existence of dark energy.

These are the examples of some of the most powerful explosions on Earth (aside from nuclear ones) and in the Universe. While they might seem very different from each other, there is, in fact, a fundamental similarity of the key physical processes that power these events. In both cases, the explosion starts when a subsonic flame is ignited in the system. In an industrial explosion, this could occur due to some external factor, e.g., a spark. In a SN Ia, ignition would be caused by the increase in density and temperature in the stellar core as the white dwarf siphons matter from its stellar companion and grows in mass approaching the Chandrasekhar mass limit. Resulting energy release, and the associated fluid expansion, produces turbulent motions, which wrinkle and fold the flame, thus, accelerating burning significantly. An example of a turbulent thermonuclear flame inside the white dwarf during the later stages of a SN Ia explosion is shown in Fig. 1. Figure 2 gives an example of a turbulent chemical flame formed in a methane-air mixture initially under atmospheric conditions.

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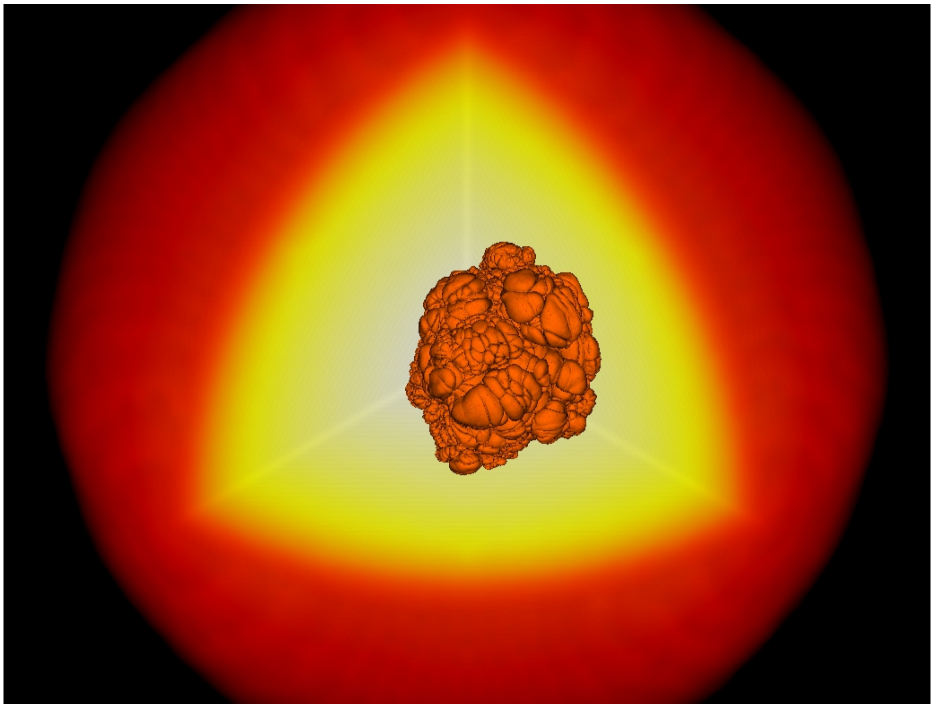

**Figure 1.** Complex structure of the turbulent thermonuclear flame propagating through the interior of a white dwarf star during a SN Ia explosion prior to the transition to a detonation. Computation is performed on an adaptive mesh with the highest resolution of ~600 m. Diameter of the star is ~4,000 km. The turbulent flame dynamics is captured using a subgrid-scale model intended to reproduce the correct burning rate on small unresolved scales. Shown is the isosurface of the flame progress variable representing the surface of the turbulent flame surrounded by the volume rendering of the density distribution representing the structure of the white dwarf.

Turbulent flame acceleration alone, however, is often not sufficient to explain the observed properties of these explosions, primarily their power. The possible missing piece of the puzzle is the deflagration-to-detonation transition (or DDT), in which a subsonic flame develops into a detonation, a supersonic shock-driven reaction wave. The rate of energy release in a detonation is significantly higher resulting in a much more powerful explosion. It must be emphasized, however, that it is far from certain whether DDT can indeed occur in the interior of a star or in an open-air vapor cloud. The reason for that is our lack of understanding of the DDT process in such unconfined systems. In fact, it is not even clear whether truly unconfined DDT is possible at all. For SN Ia, for instance, this prompted a search for alternative explosion models, which, however, are currently not as successful in explaining the observations as the model based on DDT. Therefore, elucidating the physics of DDT, as well as the conditions that can lead to it, is important for problems ranging from the safety of fuel storage and chemical processing facilities to the nature of the SN Ia phenomenon and of the enigmatic dark energy. Furthermore, better insight into the process of detonation formation is crucial for the development of the next generation of propulsion systems. This primarily concerns detonation-based engines, which hold promise to provide up to 25% increase in fuel efficiency.

Over the past 50 years, significant experimental and theoretical progress has been made in understanding the mechanism of DDT in confined systems, such as closed channels. In this case,

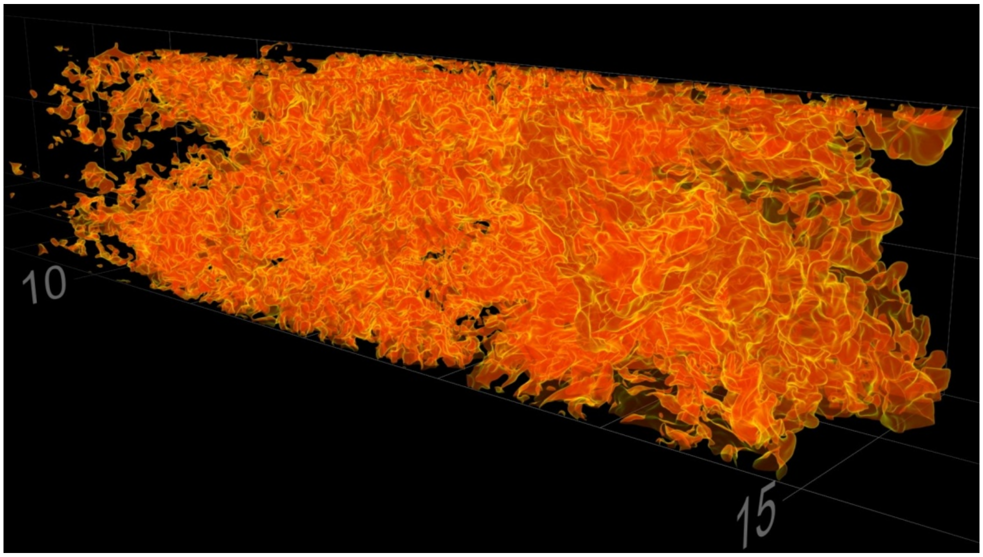

**Figure 2.** Complex structure of the turbulent chemical flame in a stoichiometric methane-air mixture. Uniform computational grid has dimensions 1.33 × 1.33 × 42.5 cm and resolution of ~50 μm. Shown is the isosurface of the fuel mass fraction corresponding to the boundary between the preheat and the reaction zone. In this simulation, burning is fully resolved on all scales. Axis scale along the direction of flame propagation gives the distance from the left boundary of the domain in cm. Full evolution of the flame from the laminar state through the highly turbulent state (seen in this figure) to the transition to a detonation is shown in the video that accompanies this paper. Image rendering was performed by the HPCMP Data Analysis and Assessment Center.

however, there is a significant simplification. Burning in a closed space naturally leads to pressure increase and the formation of shock waves, which are driven by hot expanding burning products. These shock waves can eventually become strong enough to ignite a detonation. In contrast, in an unconfined system, there is no obvious way to form shock waves of sufficient strength. Furthermore, turbulence that can develop in the course of the explosion in the interior of a white dwarf or in the fuel-vapor cloud is subsonic and, thus, it cannot itself form shocks or accelerate the flame to supersonic speeds. *The question then arises: Can a highly subsonic flame interacting with the highly subsonic turbulence spontaneously develop a supersonic detonation without any assistance from the confining effect of external walls, boundaries, or obstacles?*

Answering this question using numerical modeling presents a number of challenges. The main difficulty is associated with a very broad dynamical range of scales involved in the problem. For instance, an open-air vapor cloud can reach hundreds of meters in size, while the characteristic burning scale (flame width) can be less than a millimeter (Fig. 2). The dissipative (Kolmogorov) scale of the fast turbulence that develops in the explosion can be even smaller. This disparity of scales is further exacerbated in SN Ia. While the thermonuclear burning scale is similar to that of chemical flames (fractions of a millimeter to centimeters), the overall size of a star is thousands of kilometers (Fig. 1). Thus, modeling the full system from the first principles, while resolving all relevant scales, is not feasible.

In addition to the multi-scale nature of the problem, there is also a wide variety of physical processes involved. These include complex nuclear or chemical reactions, thermal conduction and species diffusion, complex equation of state, radiation transport, etc. An attempt to include a detailed description of all these processes would typically make the cost of any three-dimensional (3D) computation prohibitive.

Therefore, in our approach, we attempted to find the simplest yet realistic setting that would exhibit a spontaneous transition to a detonation. Most importantly, this requires fully resolving the flame width in a 3D computation in order to avoid using any model descriptions of burning that could introduce significant uncertainties into the end result. The resolution requirement, associated with this, constrains the maximum practical physical dimensions of the computational domain. Since the acceleration of the flame through its interaction with turbulence is an essential part of the overall process, accurate generation of the turbulent flow field is also important. Turbulence is typically stirred on large scales, which cannot be captured in the simulation. Therefore, in our calculations, homogeneous, isotropic, Kolmogorov-type turbulence is generated on the computational grid using a spectral method. Finally, we use a simplified, single-step, Arrhenius-type reaction kinetics calibrated to represent stoichiometric hydrogen-air and methane-air mixtures. In particular, this reaction mechanism produces realistic speeds and widths of both flames and detonations and is much more efficient computationally than complex reaction networks.

The primary numerical tool for this work was the code *Athena-RFX*, developed in collaboration with Dr. T. Gardiner (Sandia National Laboratories). This is the reactive flow extension of the astrophysical magnetohydrodynamic code *Athena*, initially developed by Drs. T. Gardiner and J. Stone (Princeton University). The code is fixed grid, finite volume, higher order, Godunov-type and is massively parallel with excellent scalability demonstrated up to 50,000 CPU cores. It was successfully deployed both at the Air Force Research Laboratory DoD Supercomputing Resource Center (DSRC) on *Raptor* and at the U.S. Army Engineer Research and Development Center (ERDC) DSRC on *Garnet,* where most of the results discussed here were obtained.

Since the conditions required for the onset of DDT were not known *a priori*, a survey of a large parameter space was required. This involved varying the type of the reactive mixture, which primarily affected the characteristic burning speed, as well as the system size and turbulence intensity. The largest calculations had the computational grid size in the range from 256×256×8096 cells (0.5 billion cells) to 256×256×16384 cells (1 billion cells). Since we use a fully compressible, explicit numerical solver and prior to the development of a detonation the flow in the system is highly subsonic, the overall number of time steps per calculation was substantial exceeding 100,000 or, equivalently, ~$10^{14}$ cell-steps. The total CPU cost of each calculation ranged from 100,000 to 500,000 CPU hours. Overall, several dozen calculations were required to fully sample the parameter space.

The key conclusion that emerged from these models was that subsonic turbulent flames are inherently susceptible to the formation of a detonation even in the absence of any confining factors, such as walls or boundaries.[5] Upon reaching a critical burning velocity, the flame develops a catastrophic runaway process illustrated in Fig. 3, which shows DDT in a stoichiometric methane-air mixture interacting with fast turbulence. The characteristic turbulent velocity at the scale of the domain width is ~36 m/s, or ~10% of the sound speed. Shortly after ignition, once the turbulent flame becomes fully developed, pressure begins to rise throughout

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the volume of the flame accelerating it and forming the leading planar global shock. Shock waves, repeatedly generated within the flame, coalesce at the leading shock front amplifying it until the detonation is ignited (panels e-i).

The underlying physical cause of the spontaneous pressure increase is the development of the supersonic flow of burning products downstream of the flame. In the reference frame co-moving with the flame, fuel enters the flame with the speed equal to the flame burning velocity. Products leave the flame with a much higher velocity due to the overall fluid expansion caused by heating. This means that at a certain subsonic flame speed, the product velocity will become equal to the speed of sound. At this point, any pressure increase as a result of burning cannot be propagated upstream by pressure waves, which will cause an overpressure to form within the flame volume. Such overpressure compresses and heats up the fuel, which, in turn, accelerates burning and further increases the outflow velocity of the burning products. This promotes pressure confinement and sets off the runaway process, which ultimately leads to a detonation.

The critical threshold, at which this process begins, is known as the Chapman-Jouguet (CJ) deflagration speed, the theoretical maximum speed for the steady flame propagation. Laminar flames, both chemical and thermonuclear, never reach such high speeds. Turbulent flames, in contrast, can become sufficiently fast. When they exceed this threshold, their steady-state propagation is indeed no longer possible.

These results are, by no means, the end of the story but rather a promising starting point. They show that spontaneous DDT is indeed possible in unconfined systems, such as open-air fuel-vapor clouds or the interior of a star. Furthermore, they specify a precise condition for the flame speed required for DDT to occur.

One of the major outstanding problems is that it is not known how to predict reliably the speed of a turbulent flame formed by the turbulent flow field, which may exist in a given practical situation. This is particularly true for highly unsteady flows encountered in the course of DDT. Turbulent flame models can be developed on the basis of *ab initio* 3D simulations, such as the ones discussed here. However, their validity has to be verified through calculations that use much larger ratios of the domain size to the characteristic burning scale along with more realistic turbulent flow fields. In particular, calculations must allow for the turbulence (possibly, inhomogeneous and anisotropic) to form self-consistently, rather than through the artificially imposed mechanisms. It is also crucial to relax some of the simplifications that made this study possible. This primarily concerns more detailed descriptions of the reaction kinetics, which can properly account for the complexity of real chemical and thermonuclear flames. Such next generation of calculations will not be possible without the next generation of petascale supercomputing platforms in the 100,000-core class.

## Acknowledgments

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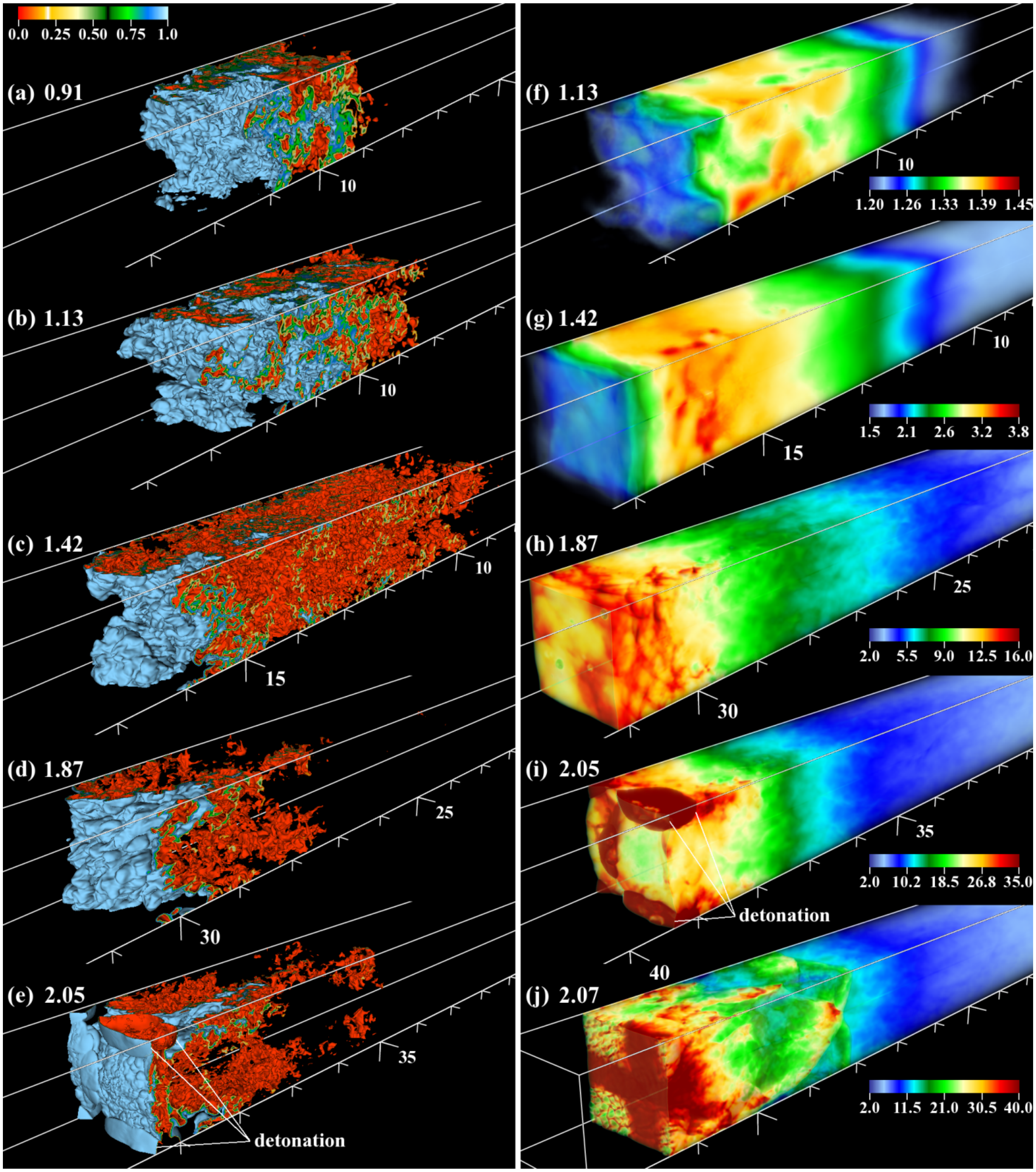

**Figure 3.** Structure of the turbulent flame and the corresponding pressure distribution during DDT in a stoichiometric methane-air mixture. **(a) – (e):** Isovolume of the fuel mass fraction with the bounding isosurfaces corresponding to 0.95 (blue, almost pure fuel) and 0.05 (red, almost pure product), which approximately mark the outer flame extents. **(f) – (j):** Volume rendering of pressure with the linearly increasing opacity. Colormap legend is given in units of atmospheres. Note a different colormap range in each panel. In all panels, horizontal axis scale gives the distance from the right boundary of the domain in cm. The time from the start of the simulation is indicated in each panel in units of the large-scale turbulent eddy turnover time. Note that panels (b)-(f), (c)-(g), (d)-(h), (e)-(i) correspond to the same time instants.