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► To cite this version:

Lecointre Luc, Kudriakov Sergey, Studer Etienne, Vicquelin Ronan, Tenaud Christian. Hydrogen/Air flame acceleration: advanced numerical modeling and criteria for detonation. Journée Thématique Combustion Hydrogène, Laboratoire PRISME, Orléans, Oct 2023, Orléans, France. hal-04322114

HAL Id: hal-04322114

<https://hal.science/hal-04322114>

Submitted on 4 Dec 2023

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Hydrogen/Air flame acceleration: advanced numerical modeling and criteria for detonation.

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The acceleration and transition from deflagration to detonation of hydrogen/air flames are critical for hydrogen safety in chemical and nuclear industries. It is, therefore, important to define criteria for flame acceleration and transition to detonation (DDT). This study investigates the relevance of existing criteria for the transition in the configuration of reflected shock detonation.

A high-order numerical solver has been developed to predict such configurations based on splitting methods, using numerical schemes adapted to each operator. In particular, the resolution of the compressible Euler equations is performed with a high-resolution Lax-Wendroff scheme built from the Roe approximate Riemann solver, with a shock-capturing method satisfying monotonicity preservation constraints. As a wide range of spatial scales is involved, multiresolution tools are applied to adapt the mesh locally. Immersed boundary methods have also been integrated to allow non-trivial geometric configurations while maintaining a structured mesh.

We illustrate the numerical approach on several configurations that deal with phenomena occurring in hydrogen flame acceleration and detonation. We mainly focus on reflected shock detonation in shock tubes and analyze adequate criteria for DDT prediction.