# Abstract

This PhD thesis presents the development, implementation, and validation of advanced computational models for the thermodynamic simulation of highly energetic materials. Detonation, like combustion, can be defined as a path where the initial compound evolves into a mixture of multiphase products in thermodynamic equilibrium. In recent years, there has been a growing interest within the European community in developing software capable of simulating such phenomena. This is driven by the wide range of potential applications, from the military and civilian explosives sectors to mining and aerospace propulsion. The aerospace field, in particular, is increasingly focused on identifying innovative solutions to enhance the performance of existing technologies, and on simulation tools that can support the development of emerging systems.

This thesis provides a detailed description of the equations of state, physical models, and numerical algorithms implemented in the developed simulation code. One specific category of energetic materials that has attracted significant attention in the scientific community is aluminized explosives. These materials have been modeled by introducing suitable corrections to well-established detonation theories, and by developing a computational tool that strikes a balance between experimental accuracy and computational efficiency, allowing the software to run even on a standard laptop. Finally, for each physical model implemented, the results have been thoroughly compared against published experimental data and well-established simulation codes, in order to ensure comprehensive validation of the various components.