PhD proposal (2023)

Modeling and numerical simulation of the fluid dynamics at the neighbourhood of critical point

keywords: continuum mechanics, hyperbolic systems, scientific computing.

Context and objective

The liquid-vapor critical point is the end point of the pressure-temperature curve that designates conditions under which a liquid and its vapor can coexist (figure 1, left). Around this point, parts of isotherms yield regions of negative compressibility (figure 1, right). Simulating the liquid-vapor phase transition at the neighborhood of the critical point is of major interest in many applications, such as transport of cryogenic fluids in turbopumps, polymer solvent-mixture and expansion during pipe breaks under pressure for CO2, etc.

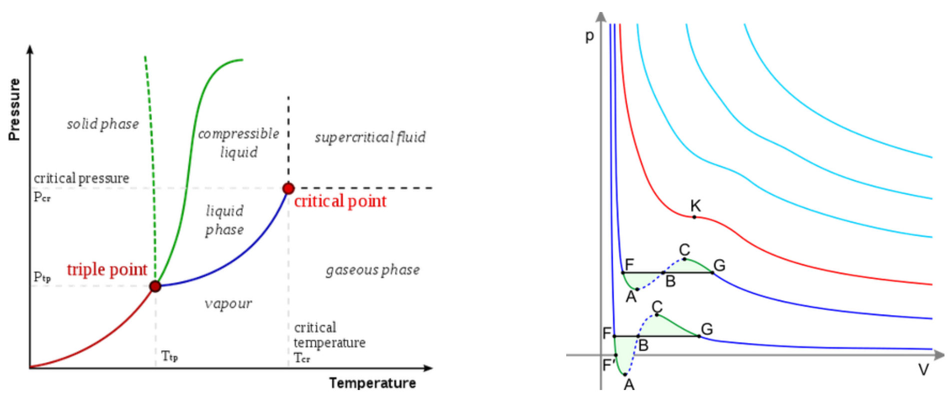

Figure 1: illustration of a critical point. Left: liquid-vapor critical point in a pressure-temperature phase diagram. Right: the red line is the critical isotherm, with critical point K. The dashed lines represent parts of isotherms which are forbidden since the gradient would be positive, giving the gas in this region a negative compressibility. Issued from Wikipedia.

There is only few models able to deal with phase transition. These ones are based on a system of partial differential equation s(PDE) closed by two convex equations of state, and they need a multiphase approach. On the contrary, the quasi-static behavior of the fluid near the critical point is based on one non-convex equation of state (EOS) and cannot be solved with classical Navier Stockes solvers because of the loss of hyperbolicity in the spinodal zone. This is the case e.g. for Van der Waals EOS.

The aim of this PhD proposal is to get rid of the nature of the EOS to solve the dynamic of a fluid near the critical point. Moreover, the tools developed should be extended to various other configurations, such as the dynamic of bistable structure, phase transition in solids, etc. The novelty of the approach is to describe the flow dynamics by a set of van der Waals-Euler-Korteweg equations (vdWEK) [1], with a non-convex hydrodynamic energy EOS for the hydrodynamic part and a density gradient dependance.

The fundamental notion of hyperbolicity will be recovered thanks to the *hyperbolization* of the resulting dispersive equations and that will be described later). The flow description is then the same as in one-phase flow and the phase transition model is included in the EOS without concavification of the EOS. Doing so enables to consider also metastable states which is almost impossible with the classical multiphase flow approach.

Methodology

The final objective of the PhD thesis is to develop a numerical code for the full Navier Stokes Korteweg equation for general $K(\rho)$ in the one and multi D case. Then a numerical studies of the influence of the $K(\rho)$ will be done depending the impact of viscosity will be also studied. For this purpose, the work can be divided into two parts:

Extended Lagrangian for Navier-Stokes-Korteweg equation. To obtain the numerical scheme, a new hyperbolization technique developed by the team member [2, 3]) will be considered and will be extended to this model. Using a well-chosen c-order parameter, the energy can be written as:

$$E = \rho\frac{|u|^2}{2} + E^h(\rho,\eta) + 1/2K|\bigtriangledown c|^2 + \lambda\frac{|c-\rho|^2}{2} + \frac{\beta}{2}\left(\frac{Dc}{Dt}\right)^2, \tag{1}$$

where λ is a large penalization parameter and β is a small one. The variation of the associated Lagrangian allows to obtain a hyperbolic system (even in the case of non convex EOS) with source terms and mathematical constraints. Such a system can be solved using classical finite-volume methods. The regularization technique based on the extended Lagrangian method have already been used in the 1D isothermal case for convex EOS [4] and non-convex EOS in [3]. In addition, whatever the nature of the equation of state, the hyperbolicity of the equations will be guaranteed: one will be able to use non-convex and/or tabulated EOS, etc. The variational approach will also allow to obtain a hyperbolic equation for the description of thermal and viscous effects.

Choice of the hydrodynamic energy. When considering compressible flows, one cannot ignore the propagation of shock waves, i.e. the discontinuity of thermodynamic quantities, in pure fluids. They highly depend on the terms $E^h(\rho,\eta) + \frac{K(\rho)}{2}|\bigtriangledown c|^2$ in (1). Choosing these terms is an open question. Indeed, the terms $\bigtriangledown\rho$ are only useful in the vicinity of the phase transition. How can the fluid be considered far from this zone in order to allow the propagation of shocks? More generally, how to account for a discontinuity in a fluid when its energy depends on the gradient of a state function or an order parameter? The choice of the function $K(\rho)$ will be paramount.

Supervision

The PhD will be located at IUSTI (Marseille). The supervision will be ensured by:

- Nicolas Favrie, Assistant Professor HDR, IUSTI, Marseille
  `nicolas.favrie@univ-amu.fr`

- Bruno Lombard, Senior Researcher, LMA, Marseille
  `lombard@lma.cnrs-mrs.fr`
  http://www.lma.cnrs-mrs.fr/spip.php?auteur30&lang=fr

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