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Mini-Workshop: Hyperbolic Aspects of Phase Transition Dynamics

Organised by
Rinaldo M. Colombo, Brescia
Dietmar Kröner, Freiburg
Philippe G. LeFloch, Paris

February 24th – March 1st, 2008

Abstract. The subject of this mini-workshop concerned the analysis and numerical investigations of mathematical models for phase transitions. In particular recent results about the dynamics of liquid-vapor flows and the relevance of traveling wave solutions, properties of kinetic relations associated with phase dynamics and nonclassical shocks, the justification of the vanishing viscosity-capillarity limits, numerical approximation of the kinetic relation associated with finite difference schemes and applications have been discussed.

Mathematics Subject Classification (2000): 35Lxx.

Introduction by the Organisers

The workshop "Hyperbolic aspects of phase-transition dynamics", organized by Rinaldo M. Colombo (Brescia), Dietmar Kröner (Freiburg) and Philippe G. LeFloch (Paris) was held February 24th – March 1st, 2008. We had 15 participants from five different countries. The atmosphere in the Oberwolfach Research Institute was very stimulating and has initiated many fruitful discussions and exchange of ideas. The participants of the mini-workshop thank the administration of the institute for the possibility for organize this meeting.

The Navier-Stokes equations for van der Waals fluids with viscosity and capillarity effects included form a challenging model of partial differential equations describing important physical phenomena. The associated set of first-order conservation laws is of hyperbolic or hyperbolic-elliptic type, and admits propagating discontinuities (shock waves). Understanding the singular limit when the viscosity and capillarity coefficients vanish is particularly challenging and is required

to single out physically admissible, discontinuous solutions to the first-order conservation laws. These solutions turn out to contain both compressive shocks and undercompressive shocks which violate standard entropy criteria and must be characterized via the so-called kinetic relations.

There were two talks (N. Bedjaoui, P.G. LeFloch) on conservation laws with non-convex flux functions which are supplemented by nonlinear, possibly singular, diffusive and dispersive terms. Such systems of equations arise in the dynamics of complex materials undergoing phase transitions and in the dynamics of van der Waals fluids, viscosity and capillarity effects included. Questions which are related to existence, uniqueness and the properties of the viscosity or dispersion limits were discussed. In particular the kinetic relations associated with phase dynamics and nonclassical shocks have been considered. Closely related was a contribution of W. Dreyer about the derivation of the kinetic relations from global entropy inequalities.

Three other talks (D. Diehl, D. Kröner, C. Rohde) were dealing with the Navier-Stokes-Korteweg model including non-local formulations, the numerical approximation and the special structure of the interface conditions for the pressure fields respectively.

In two talks R.M. Colombo and P. Goatin reported on recent results about analytical and numerical techniques for hyperbolic phase transitions/non-classical shocks in models for vehicular or pedestrian traffic. In this model for high speeds (low densities) the flow is free and described by scalar conservation law and for low speeds (high densities) the flow is congested and is described by a 2×2 system.

A different model for the phase transition in fluids is used by S. Müller. In order to take into account two different fluids he introduced a new function, the fraction of gas. This is controlled by an additional transport equation. Mass transfer across the interface is neglected.

Other models have been considered in the talk of F. Coquel. He has examined the links between a model consisting of two distinct partial differential momentum equations and a single momentum equation for the mixture plus an algebraic closure for governing the relative velocity.

H. Fan considered in his contribution a nonlinear system with viscosity terms for the specific volume, the velocity of the fluid and the weight portion of vapour in the liquid/vapour mixture. The simplified version of this model with zero viscosity has been considered in the talk of A. Corli. A global existence result for large data has been obtained.

S. Benzoni-Gavage gave a report on the stability analysis for planar subsonic phase boundaries and the existence of linear surface waves.

M. Shearer considered the surfactants of a free surface which is transported by the local speed of the free surface but also by diffusion of surfactant molecules on the surface.

Mini-Workshop: Hyperbolic Aspects of Phase Transition Dynamics

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Abstracts

A Review on Kinetic Relations Generated by Traveling Waves

Nabil Bedjaoui
(joint work with P.G. LeFloch)

We present a review on kinetic relations generated by traveling wave solutions of perturbed conservation laws.

We consider first the case of scalar conservation laws with concave-convex flux which are supplemented with *nonlinear, possibly singular,* diffusive and dispersive terms. The model takes the following form:

$$\partial_t u + \partial_x f(u) = \beta^{p+1} \big(b(u, \beta u_x)\, |u_x|^p u_x\big)_x + \delta \left(c_1(u)\, (c_2(u)\, u_x)_x\right)_x.$$

The case $p = 0$, i.e, *regular and linear* diffusion, was treated in [1]. We prove existence, uniqueness, and several properties of *classical and nonclassical traveling waves,* the latter being characterized by the so-called *kinetic function.*. We generalize these results in [2], for the case of singular diffusion ($p > 0$). The behavior of the kinetic function near the origin is carefully investigated. We discover that $p = 1/3$ is a somewhat unexpected critical value. For $p \leq 1/3$ we obtain properties that are similar to the linear diffusion case. However, for $p > 1/3$, non-classical shocks can have arbitrary small strength. The behaviour of the kinetic function near the origin depends on whether $p < 1/2$, $p = 1/2$ or $p > 1/2$. In particular, in the special case of the cubic flux-function, with $p = 0, 1/2$, or 1, the kinetic function can be computed *explicitly*. When $p = 1/2$ the kinetic function is simply a *linear function.*

In the second part, we present a system of two conservation laws arising in elastodynamics and fluid dynamics in the case of concave-convex flux, with linear viscosity and capillarity terms, i.e, of the form:

$$\begin{aligned} &\partial_t v - \partial_x u = 0, \\ &\partial_t u + \partial_x \sigma(v) = \beta\, \partial_x (b(v)\ \partial_x u) - \delta\, \partial_x (a(v) \partial_x (a(v) \partial_x v)). \end{aligned}$$

The kinetic relation obtained in the hyperbolic case is similar to the scalar case, at least near the origin (for small shocks)(see [3]). In the hyperbolic-elliptic case, the kinetic relation for the $2 - Shock$ wave is uniquely defined but fails to be monotone near the Maxwell-line. This means that the kinetic relation for the $1 - Shock$ wave is multivaluated in this region (see [4]).

Finally, we treat the previous hyperbolic-elliptic model where the fluid is governed by van der Waals pressure law. In addition, the model includes now, more general nonlinear viscosity and capillarity terms and writes:

$$\partial_t \tau - \partial_x u = 0,$$
$$\partial_t u + \partial_x p(\tau) = \alpha\, \partial_x (\beta(\tau)\, |\partial_x \tau|^q\, \partial_x u) - \partial_{xxx} \tau.$$

The global description of traveling waves seems to be a novelty for functions admitting *two inflexion points*. For a fixed right-hand state and a fixed propagation speed, we prove the existence of a nonclassical traveling wave for a sequence of parameter values representing the ratio of viscosity and capillarity. Our analysis exhibits a surprising lack of monotonicity of traveling waves. The behavior of these nonclassical trajectories is also investigated numerically. In addition we prove that the kinetic function for the $2-Shock$ wave, contrairely to the case of one inflexion point, is not uniquely defined near the Maxwell line (see [5]).

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Surface Waves at Phase Boundaries?

Sylvie Benzoni-Gavage
(joint work with M.D. Rosini)

In the sharp interface theory of compressible fluids exhibiting phase changes, the bulk equations (in the phases) are merely the (hyperbolic) Euler equations, given by the conservation of mass, momentum and energy, together with a (monotone) pressure law. It is jump conditions across interfaces that may incorporate physical phenomena such as surface tension or/and dissipation. In the absence of dissipation, the stability analysis of planar subsonic phase boundaries – undercompressive shocks in the hyperbolic terminology – shows the existence of linear surface waves, which are special solutions of the linearized bulk and jump equations, in the form of 'normal modes' propagating along perturbed interfaces [1, 2]. Surface waves are neutral modes of finite energy, like Rayleigh waves in Elasticity, in that they oscillate along the boundary and decay exponentially fast in the transverse direction. As regards the well-posedness theory of initial-boundary value problems, neutral modes are in general responsible for a loss of derivatives in the energy estimates

[5] (see however [2] for a case without loss of derivatives), which makes more difficult to prove, but does not preclude the existence of nearby solutions [6]. Anyway, this is a local-in-time theory, since even the Cauchy problem for multi-dimensional Euler equations is still wide open. To gain insight in multi-dimensional problems, another approach has been developed by Hunter [7], focusing on the weakly nonlinear behavior of surface waves on larger time scales, for 'standard' scale-invariant initial-boundary value problems. From an abstract point of view, it is possible to extend his approach and derive an asymptotic equation for the amplitude of weakly nonlinear surface waves associated with neutrally stable undercompressive shocks [4]. This amplitude equation is a nonlocal generalization of Burgers' equation – its time variable being a 'slow' time – which turns out to admit energy estimates without loss of derivatives if the involved kernel satisfies a suitable (explicit) stability condition [3, 7]. Unlike what happens for Rayleigh waves, this condition is violated by the kernel associated with to subsonic phase boundaries [4]. This may give an interpretation of why surface waves have hardly ever been observed at phase boundaries.

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Phase Transitions in Car Traffic & Pedestrian Flow Modeling

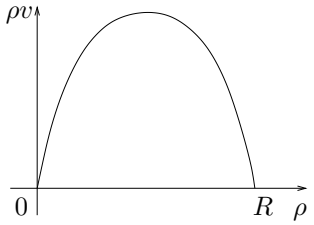
Rinaldo M. Colombo

This talk overviews recent results in which analytical techniques related to hyperbolic phase transitions / non-classical shocks are used in models for vehicular or pedestrian traffic.

1. Car Traffic

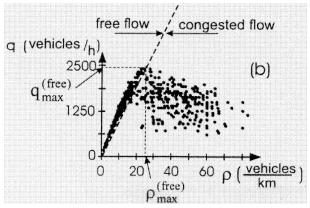
The starting point in the continuum modeling of vehicular traffic is the Lighthill–Whitham [15] and Richards [19] (LWR) model

$$\partial_t \rho + \partial_x \left(\rho\, v(\rho)\right) = 0 \tag{1}$$

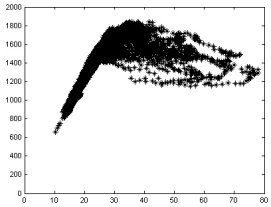


x	space variable, $x \in \mathbb{R}$
t	times, $t \in [0, +\infty[$
ρ	vehicular density, $\rho \in [0, R]$
R	maximal density
$v(\rho)$	vehicular speed

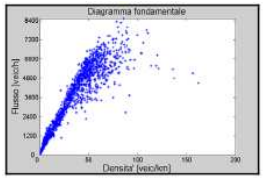
The LWR model relies on only two assumptions: the total number of cars is conserved and speed is a function of the density. The latter postulate is only very approximately satisfied. More precisely, at high speeds, experimental measures support a functional dependence of v (and, hence, of the flow ρv) on ρ. But at lower speeds, this dependence is questionable, as the following pictures show:



Data from Germany [12].



Data from Italy [17].



Data from Italy [16].

Recently, the following model was presented in [3] and its analytical properties were studied in [6]:

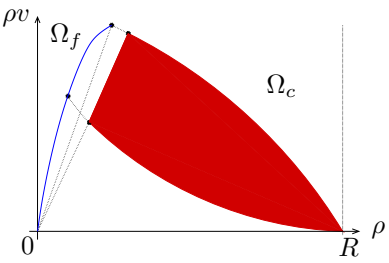
$$\begin{array}{ll} \text{Free flow: } (\rho, q) \in \Omega_f, & \text{Congested flow: } (\rho, q) \in \Omega_c, \\ \partial_t \rho + \partial_x (\rho\, v) = 0, & \begin{cases} \partial_t \rho + \partial_x (\rho\, v) = 0, \\ \partial_t q + \partial_x \left[(q - q_*)\, v\right] = 0, \end{cases} \\ v = \left(1 - \frac{\rho}{R}\right) \cdot V\,, & v = \left(1 - \frac{\rho}{R}\right) \cdot \frac{q}{\rho}\,. \end{array} \tag{2}$$

where Ω_f and Ω_c denote the *free* and the *congested* phases, respectively. In Ω_f the only variable is the car density ρ and the car speed v is assumed to be a known function of the car density. In Ω_c the variables are the car density ρ and the car speed v or, equivalently, ρ and the weighted flow q; see [2]. Thus, at a fixed density, different speeds are admissible, as raw data observations require. Note that there may well be car densities at which the flow may be either free or congested. R is the maximal possible car density and V is the maximal possible

speed. More general expressions can be considered, but we limit ourselves to the expressions above in order to keep the formal analytical difficulties at a minimum, while keeping all the more interesting qualitative features.

As shown in [3], a global *Riemann Solver* for (2) is uniquely defined by:
(1) the conservation of the total number of cars;
(2) if the initial data attains values in Ω_f, respectively Ω_c, then the solution attains values in Ω_f, respectively Ω_c, for all times;
(3) the Riemann Solver is consistent, see [3, I and II] or [7, Definition II.3]

Condition (2) also defines the possible free phase Ω_f and congested phase Ω_c as invariant sets for (2). The qualitative properties of the solutions to (2) are compatible with real data: density and speed are non negative and bounded, information propagates at the speed of vehicles and persistent *wide jams* are possible, see [13] for a benchmark of different 2×2 traffic models.



The Cauchy problem for (2) turns out to be well posed in $\mathbf{L^1}$, for all initial data having bounded, not necessarily small, total variation, see [4, 6]. A numerical algorithm to integrate (2) is proposed in [1].

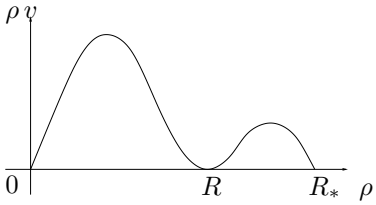
2. Pedestrian Flow

Our target is the description of the following phenomena: when a crowd has to pass through a relatively narrow exit, the rise of panic may result in the crowd being overcompressed and in a dramatic fall of the outflow.

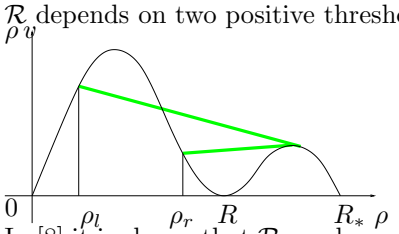
We aim at capturing the essential features of this fact through a 1D macroscopic model, see [11, 20] for other continuum models for pedestrian flow. Hence, again, the starting point is the LWR model (1), with ρ, v being the pedestrian density and speed. Fix $\rho_{\min}, \rho_{\max} \in [0, R]$. A well known property of scalar conservation laws is the *maximum principle*, i.e. if the initial datum ρ_o satisfies the bounds $\rho_o(x) \in [\rho_{\min}, \rho_{\max}]$ for all $x \in \mathbb{R}$, then the corresponding solution ρ to (1) keeps satisfying to the same bounds, i.e. $\rho(t,x) \in [\rho_{\min}, \rho_{\max}]$ for all $x \in \mathbb{R}$ and $t \in [0, +\infty[$. Hence, a standard Cauchy problem for a scalar conservation law may not describe the desired phenomena.

A possible attempt, then, is to consider an initial – boundary value problem for (1), the exit being described by a suitable unilateral constraint on the outflow. However, the analytical properties of the solution to this kind of problem may not describe the fall in the outflow, see [5].

We are thus lead to reconsider (1) and modify it, first inserting the states $[R, R_*]$ to account for the *overcompressed* states. The result is (1) with a fundamental diagram as that on the right. For the precise qualitative features necessary for the construction below, see [8, 9].



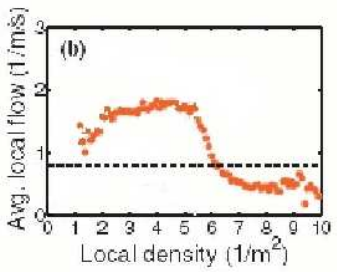
Now, we modify the evolution of (1) to avoid the maximum principle. To this aim, we introduce *nonclassical shocks* in the solution to Riemann problems for (1). For the precise definition of this nonclassical Riemann solver $\mathcal{R}$, see [8, **(R1)**, **(R2)** and **(R3)**]. This lengthy definition requires, as usual in this context [14], the introduction of functions related to the fundamental diagram above. Essentially, $\mathcal{R}$ depends on two positive threshold parameters, s and Δs as follows.

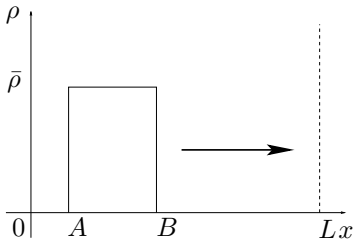


Let ρ^l, ρ^r be initial states in the Riemann problem for (1). Then, $\mathcal{R}(u^l, u^r)$ is the standard Lax solution unless $\rho^l > s$ and $\rho^l - \rho^r > \Delta s$. In this case, the solution consists of a nonclassical shock followed by classical waves, as here on the right.

In [8] it is shown that $\mathcal{R}$ can be uniquely extended to all pairs of states. Moreover, suitable interaction estimates in [9, 18] ensure the existence of solutions to the nonclassical Cauchy problem for (1).

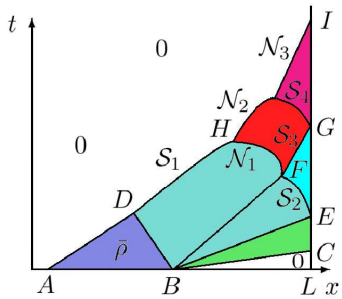
Recently, the above analytical construction was experimentally confirmed in [10]. Indeed, a fundamental diagram with 2 different points of maxima was measured, with a set of (dramatically) *overcompressed* densities corresponding to panic states. The diagram on the right is taken from [10]. Remark that the analytical assumptions in [8, 9, 18] do not require that the flow vanishes at R, R being the maximal density of non-panic states.





Finally, consider a crowd distributed on the segment AB with uniform density $\bar\rho$. At time 0, all pedestrians start moving towards an exit sited at L whose maximal outflow is q, a value below the maximal flow in the standard states and above the (local) maximum in the panic states, see the fundamental diagram above. The resulting nonclassical Cauchy problem is solved gluing solutions to Riemann problems.

Indeed, a shock arises from A and a rarefaction from B. When the latter wave first hits the door at C, people start exiting with and the outflow through the door increases. At E the outflow q is reached and a classical shock $\mathcal{S}_2$ is reflected. In the time interval between E and G, the outflow is maximal, according to the door capacity. The shock $\mathcal{S}_2$ interacts with the rarefaction and at F the jump between the two sides of $\mathcal{S}_2$ exceeds Δs.



A nonclassical shock $\mathcal{N}_1$ is formed and the crowd enters the panic states. At G,

these overcompressed states reach the door and the outflow fall below q, remaining below that value up to I, when the last individual exits the door.

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The Drift-Flux Time Asymptotic of Two-Phase Two-Pressure PDE Models

Frédéric Coquel
(joint work with A. Ambroso, C. Chalons, E. Godlewski, P.A. Raviart, N. Seguin)

A full hierarchy of PDE systems for modeling two-phase flows does exist in the literature [6] and may be formally arranged through a cascade of relaxation mechanisms with finite rate. Motivated by the mathematical coupling of two given models (see [1] for instance), we wish to clarify their potential time asymptotic relationships. In the present work, we specifically examine the possible links between the two-phase models and the drift-flux ones. Roughly speaking, the formers make use of two distinct PDE momentum equations while the latters involve a single momentum equation for the mixture, plus an algebraic closure law for governing the relative velocity: the so-called drift law. We point out the precise conditions according to which a drift-flux model stands as a good candidate for governing the long-time behavior of the solutions of a given two-phase two-pressure model. The main tools are Chapman-Enskog expansions and long-time rescaling, an essential intermediate step being the introduction of a drift-flux like model with a Darcy closure law, *i.e.* depending not only on the unknown but also on its gradient.

Within the barotropic two-phase two-pressure setting, the PDE equations in d space variables read for some small parameter $\epsilon > 0$ (omitting the subscript ϵ for simplicity) :

$$
\begin{aligned}
&\partial_t \alpha_2 + V_i(\mathbf{u}) \cdot \nabla_x \alpha_2 = \frac{\theta(\mathbf{u})}{\epsilon^2}(p_2 - p_1), \qquad t > 0,\ x \in I\!R^d,\\
&\partial_t(\alpha_1\rho_1) + \nabla_x \cdot (\alpha_1\rho_1 u_1) = 0,\\
&\partial_t(\alpha_2\rho_2) + \nabla_x \cdot (\alpha_2\rho_2 u_2) = 0,\\
&\partial_t(\alpha_1\rho_1 u_1) + \nabla_x \cdot (\alpha_1\rho_1 u_1 \otimes u_1 + \alpha_1 p_1 I\!I) - P_i(\mathbf{u})\nabla_x \alpha_1\\
&\qquad\qquad = \alpha_1\rho_1 \mathbf{g} + \frac{\lambda(\mathbf{u})}{\epsilon}(u_2 - u_1),\\
&\partial_t(\alpha_2\rho_2 u_2) + \nabla_x \cdot (\alpha_2\rho_2 u_2 \otimes u_2 + \alpha_2 p_2 I\!I) - P_i(\mathbf{u})\nabla_x \alpha_2\\
&\qquad\qquad = \alpha_2\rho_2 \mathbf{g} + \frac{\lambda(\mathbf{u})}{\epsilon}(u_1 - u_2),
\end{aligned}
\tag{1}
$$

where $\mathbf{u}$ denotes the unknown $(\alpha_2, \alpha_1\rho_1, \alpha_2\rho_2, \alpha_1\rho_1 u_1, \alpha_2\rho_2 u_2)^T$. Here α_k, ρ_k, u_k are the void fraction, the density and the velocity of the phase k with $\alpha_1 + \alpha_2 = 1$. We asume that each pressure law $p_k = \mathcal{P}_k(\rho_k)$, $k = 1, 2$, is given by a smooth function $\mathcal{P}_k$ satisfying :

$$
\mathcal{P}_k'(\rho) > 0, \quad \text{for all } \rho > 0, \qquad \lim_{\rho \to 0^+} \mathcal{P}_k(\rho) = 0, \qquad \lim_{\rho \to +\infty} \mathcal{P}_k(\rho) = +\infty. \tag{2}
$$

The so-called interfacial velocity and pressure, namely $V_i(\mathbf{u})$ and $P_i(\mathbf{u})$, are chosen under the general form :

$$
V_i(\mathbf{u}) = \beta(\mathbf{u})u_1 + (1 - \beta(\mathbf{u}))u_2, \quad P_i(\mathbf{u}) = (1 - \beta(\mathbf{u}))p_1 + \beta(\mathbf{u})p_2, \tag{3}
$$

for some given smooth function $\beta(\mathbf{u})$ (see [4] for the existence of an additional non-trivial law). At last, θ and λ denote two positive functions of the unknown $\mathbf{u}$ respectively accounting for the pressure and velocity relaxation mechanisms, the pressure relaxation being much stiffer than the velocity one as indicated by its ϵ^2-scaling. Denoting by p_r (or rather p_r^ϵ) the relative pressure $p_r = p_2 - p_1$ and by $u_r = u_2 - u_1$ the relative velocity, the relaxation procedures formally yield the following limits:

$$\lim_{t\to+\infty} p_r^\epsilon(t,x) = 0, \quad \lim_{t\to+\infty} u_r^\epsilon(t,x) = 0, \qquad \text{a.e. } (t,x) \in I\!R_+ \times I\!R^d.$$

A vanishing relative pressure p_r indeed yields the expected closure equation for α_2 in the frame of a generic drift-flux model, *i.e.* we can define α_2^e as the unique solution (see assumptions (2)) of:

$$\mathcal{P}_1(\rho(1-Y)/(1-\alpha_2^e)) = \mathcal{P}_2(\rho Y/\alpha_2^e), \text{ being given } \rho = \alpha_1\rho_1 + \alpha_2\rho_2,\ \rho Y = \alpha_2\rho_2.$$

However, a vanishing relative velocity u_r does not fit with the general setting. We are thus led to study the long but finite time behavior of the relative pressure and velocity when analyzing their first order correctors. This is the matter of the next statement:

Proposition *Let us introduce the unknown* $\mathbf{v} = (\rho, \rho Y, \rho u)^T$ *with* $\rho u = \alpha_1\rho_1 u_1 + \alpha_2\rho_2 u_2$. *Assume that* λ *and* θ *in (1) only depend on* $\mathbf{v}$. *Then the first order asymptotic model for (1) reads:*

$$\begin{aligned} &\partial_t\rho^\epsilon + \nabla_x\cdot(\rho^\epsilon u^\epsilon) = 0,\\ &\partial_t(\rho^\epsilon Y^\epsilon) + \nabla_x\cdot(\rho^\epsilon u^\epsilon Y^\epsilon + \rho^\epsilon Y^\epsilon(1-Y^\epsilon)u_r^\epsilon) = 0,\\ &\partial_t(\rho^\epsilon u^\epsilon) + \nabla_x\cdot(\rho^\epsilon u^\epsilon\otimes u^\epsilon + p^\epsilon I\!I) = \rho^\epsilon\mathbf{g}, \end{aligned} \tag{4}$$

where at the first order in ϵ, *the relative velocity* u_r^ϵ *is given from a Darcy like closure law :*

$$u_r^\epsilon = \epsilon\frac{\rho^\epsilon Y^\epsilon(1-Y^\epsilon)}{\lambda(\mathbf{v}^\epsilon)}\left(\frac{1}{\rho_1(\mathbf{v}^\epsilon)} - \frac{1}{\rho_2(\mathbf{v}^\epsilon)}\right)\nabla_x p^\epsilon, \tag{5}$$

while $p_r^\epsilon = 0$, *i.e. the pressure law* $p = \mathcal{P}(\mathbf{v})$ *follows from the solution* (p, α_2^e) *of the* 2×2 *nonlinear system*

$$p = \mathcal{P}_1(\rho(1-Y)/(1-\alpha_2^e)), \quad \mathcal{P}_1(\rho(1-Y)/(1-\alpha_2^e)) = \mathcal{P}_2(\rho Y/\alpha_2^e). \tag{6}$$

The proposed first order corrector (5) for the relative velocity follows from a Chapman-Enskog expansion (see also [5]) and thus naturally involves the gradient of the unknown $\mathbf{v}$, in strong opposition with the existing literature [6]. In order to derive the required zeroth order hydrodynamic closure law, we propose to tackle the long-time behavior of the solutions of (4) along the characteristics of the flow, *i.e.* when expressing (4) in the Lagrangian coordinates instead of the Eulerian setting. Indeed, being given the solution of the following differential system, the so-called characteristics of the mixture flow,

$$d_t x(t,\xi) = u^\epsilon(x(t,\xi),t), \quad t>0, \quad x(0,\xi) = \xi, \tag{7}$$

for any given initial data $\xi \in I\!R^d$, we introduce the associated change of Lagrangian coordinates $\overline{\phi}(\xi,t) = \phi(x(\xi,t),t)$ for any arbitrary function $\phi(x,t)$ expressed in Eulerian coordinates. Observing the easy chain rule $\partial_t\overline{\phi} = \overline{\partial_t\phi + u^\epsilon\cdot\nabla_x\phi}$, we have the following formal result :

Lemma *Consider the time-scaling $s=\epsilon t$ and the rescaled relative velocity v_r^ϵ defined by $u_r^\epsilon = \epsilon v_r^\epsilon$. Then the solutions of (4)–(6) expressed in the Lagrangian coordinates (7), solve :*

$$
\begin{aligned}
&\epsilon\partial_s\overline{\rho}^\epsilon + \overline{\rho^\epsilon\nabla_x\cdot u^\epsilon} = 0,\\
&\epsilon\partial_s\overline{\rho^\epsilon Y^\epsilon} + \overline{\rho^\epsilon Y^\epsilon\nabla_x\cdot u^\epsilon} + \epsilon\overline{\nabla_x\cdot(\rho^\epsilon Y^\epsilon(1-Y^\epsilon)v_r^\epsilon)} = 0,\\
&\epsilon\partial_s\overline{\rho^\epsilon u^\epsilon} + \overline{(\rho^\epsilon\nabla_x\cdot u^\epsilon)u^\epsilon} + \overline{\nabla_x p^\epsilon} = \overline{\rho^\epsilon\mathbf{g}}.
\end{aligned}
\tag{8}
$$

Denoting by $(\rho,\ Y,\ u)$ the formal limits of $(\rho^\epsilon,\ Y^\epsilon,\ u^\epsilon)$ as ϵ goes to zero, we have

$$\overline{\rho\nabla_x\cdot u} = 0, \tag{9}$$

$$\partial_s\overline{\rho Y} + \overline{\nabla_x\cdot(\rho Y(1-Y)v_r)} = 0, \tag{10}$$

$$\overline{\nabla_x p} = \overline{\rho\mathbf{g}}. \tag{11}$$

Hence the rescaled relative velocity v_r takes the form of a zeroth order closure law

$$v_r = \frac{\rho Y(1-Y)}{\lambda(\mathbf{v})}\left(\frac{1}{\rho_1(\mathbf{v})} - \frac{1}{\rho_2(\mathbf{v})}\right)\rho\mathbf{g}. \tag{12}$$

The drift law (12) actually reflects the Archimedes principle and provides a simple example of hydrodynamic closure. A more general framework is discussed in [2] when addressing, in place of the gravity $\mathbf{g}$, general external forces $f_k(\mathbf{u})$, $k=1,2$, in the momentum equations of (1). The derivation of numerical schemes for (1) capable of capturing the time asymptotic behavior described by (9)–(11) is addressed in [3] in the simpler setting of the Euler-Darcy equations for a single phase.

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Hyperbolic Phase-Mixing Flows: a Global Existence Result for Large Data

Andrea Corli
(joint work with D. Amadori)

We present a recent result about a model of one-dimensional isothermal flow for an inviscid compressible fluid where the liquid and the vapor phase coexist and are mixed together. In Lagrangian coordinates the model writes

$$\begin{cases} v_t - u_x & = 0 \\ u_t + p(v,\lambda)_x & = 0 \\ \lambda_t & = 0\,. \end{cases} \tag{1}$$

Here $t > 0$, $x \in \mathbb{R}$, $v > 0$ is the specific volume, u the velocity, λ the mass density fraction of vapor in the fluid. The pressure is defined by $p(v,\lambda) = a^2(\lambda)/v$ where a is a smooth function satisfying $a(\lambda) > 0$ and $a'(\lambda) > 0$ for every $\lambda \in [0,1]$. As a consequence, the system (1) is strictly hyperbolic with eigenvalues $e_1 = -c$, $e_2 = 0$, $e_3 = c$ for $c = \sqrt{-p_v} = a(\lambda)/v$. The eigenvalues e_1 and e_3 are genuinely nonlinear, while e_2 is linearly degenerate.

This model is a simplified version of a model proposed by Fan [6], which includes viscosity and relaxation terms, see also [5]. The focus here is on the global existence of solutions to the Cauchy problem for (1) with initial data

$$(v,u,\lambda)(0,x) = \big(v_o(x), u_o(x), \lambda_o(x)\big)\,, \qquad v_o(x) \geq \underline{v} > 0,\ 0 \leq \lambda_o(x) \leq 1, \tag{2}$$

for some constant $\underline{v}$, in the case $\big(v_o, u_o, \lambda_o\big)$ have finite (not necessarily small) total variation. We denote for short $a_o(x) \doteq a\left(\lambda_o(x)\right)$, $p_o(x) \doteq p\left(v_o(x), \lambda_o(x)\right)$.

On one hand this problem is a first step toward the study of more complex models, where (1) is supplemented by source terms; on the other hand, from a merely analytical point of view, our result can be seen as a contribution to the still widely unknown field of global solution to conservation laws in presence of data with large variation. We also refer to the recent paper [7] for a similar model of fluid flow where the equation of state is a γ-pressure law with varying $\gamma > 1$.

We denote by $\mathrm{TV}(f)$ the total variation of a function f. In order to obtain precise bounds on the variation of the initial data we introduce in the case $f : \mathbb{R} \to (0,+\infty)$ the *weighted total variation* of f by

$$\mathrm{WTV}(f) = 2 \sup \sum_{j=1}^{n} \frac{|f(x_j) - f(x_{j-1})|}{f(x_j) + f(x_{j-1})}\,,$$

where the supremum is taken over all $n \geq 1$ and $(n+1)$-tuples of points x_j with $x_o < x_1 < \ldots < x_n$. One can prove that $\mathrm{WTV}(f) \leq \mathrm{TV}\left(\log(f)\right)$, with $\mathrm{WTV}(f) = \mathrm{TV}\left(\log(f)\right)$ if f is continuous.

The Riemann problem for system (1) and the wave interactions were studied in [1]; our main result is the following, [2].

Theorem. *Consider the initial data (2). For every $m > 0$ and a suitable function $k(m) \in (0, 1/2)$, if*

$$\mathrm{TV}\left(\log(p_o)\right) + \frac{1}{\inf a_o}\mathrm{TV}(u_o) \quad < \quad 2\Big(1 - 2\mathrm{WTV}(a_o)\Big)m \tag{3}$$

$$\mathrm{WTV}(a_o) \quad < \quad k(m) \tag{4}$$

then the Cauchy problem (1), (2) has a weak entropic solution (v, u, λ) defined for $t \geq 0$. The solution is valued in a compact set of $(0, +\infty) \times \mathbb{R} \times [0, 1]$ and there is a constant $C(m)$ such that for every $t \geq 0$

$$\mathrm{TV}\left(v(t, \cdot), u(t, \cdot)\right) \quad \leq \quad C(m)\,.$$

The function $k(m)$ above, that can be explicitly computed, depends on the damping of reflected waves in interaction of waves of the same family 1 or 3; it is a positive function decreasing to 0 as $m \to +\infty$, with $k(0) = 1/2$. In particular $\mathrm{WTV}(a_o) < 1/2$, which makes positive the right-hand side term in (3). The assumptions (3), (4) are then analogous to those in [8]: the larger m, the smaller $k(m)$.

The proof of the theorem above makes use of a wave-front tracking scheme inspired by [4, 3], where we exploit the special structure of the system (1). In particular we do not introduce a simplified Riemann solver for interactions between 1 and 3 waves but only for interactions involving the 2-contact discontinuities. As in [3] we consider a linear functional that accounts for the strengths of all 1 and 3 waves, with a weight $\xi > 1$ assigned to shock waves; a crucial point in the proof is the choice of ξ as a function of m. The interaction potential considers then uniquely interactions of 2 waves with 1 or 3 waves approaching to it.

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Higher Order Schemes for Simulation of Liquid-Vapor Flows with Phase Change

Dennis Diehl

Liquid-Vapor flows that can undergo phase transition arise in many technical, medical and chemical applications. For instance, it is well known that the collapse of small vapor bubbles that arise due to the operation of a ship propeller can dramatically reduce the lifetime of the blades of a ship propeller. This type of cavitation damage was first studied by Lord Rayleigh at the end of the 19th century. From the mathematical point of view Two-Phase-Flow models can be separated into two classes: sharp interface models, characterized by a discontinuous jump between the phases and diffuse interface models that are characterized by a smooth (but rapid) change between the phases. The model considered in this work, the Navier-Stokes-Korteweg model, belongs to the class of diffuse interface models. It is an extension of the compressible Navier-Stokes equations and introduces an additional contribution to the stress tensor that includes (at least at the static equilibrium, see [4]) the effect of surface tension implicitly. For the sake of simplicity we consider only the isothermal version of the model, i.e., the temperature is fixed to some constant below the critical temperature and the energy balance equation is neglected. The equation that has to be satisfied in some domain $\Omega \subset \mathbb{R}^n$ then reads

$$\begin{array}{rcrcl} \rho_t & + & \nabla \cdot (\rho \mathbf{u}) & = & 0, \\ (\rho \mathbf{u})_t & + & \nabla \cdot (\rho \mathbf{u}\mathbf{u}^T) + \nabla p(\rho) & = & \nabla \cdot (\tau + \mathbf{K}) \,. \end{array} \tag{1}$$

Here τ denotes the usual viscous part of the stress tensor, p is given by a van der Waals equation of state and the tensor $\mathbf{K}$ is the Korteweg part of the stress tensor that is given by the relation

$$K = \lambda \left[\left(\rho \Delta \rho + \frac{1}{2} |\nabla \rho|^2 \right) \mathbf{I} - \nabla \rho \nabla \rho^T \right], \quad \lambda > 0.$$

The unknowns are the density $\rho > 0$ and the velocity $\mathbf{u} \in \mathbb{R}^n$ that have to be initialized at $t = 0$ with some meaningful values. On a bounded domain we introduce the boundary conditions

$$\mathbf{u} = \mathbf{0} \quad \text{and} \quad \nabla \rho \cdot \mathbf{n} = 0 \quad \text{on } \partial\Omega. \tag{2}$$

The first boundary condition is the usual condition on a solid wall as it arises in the framework of the compressible Navier-Stokes equations. The introduction of the second one becomes necessary due to the introduction of the Korteweg part of the stress tensor. This condition enforces a ninety degree contact angle of an interface at the wall. It can be generalized to enforce arbitrary contact angles, see [3].

On a bounded domain the total physical energy $E[\rho, \mathbf{u}]$ of smooth solutions of (1), (2) given by

$$E[\rho, \mathbf{u}](t) = \int_\Omega W(\rho(\mathbf{x}, t)) + \frac{\lambda}{2} |\nabla \rho(\mathbf{x}, t)|^2 + \frac{1}{2} \rho(\mathbf{x}, t) |\mathbf{u}(\mathbf{x}, t)|^2 \, d\mathbf{x}$$

satisfies

$$\frac{d}{dt}E[\rho,\mathbf{u}](t) \leq 0. \tag{3}$$

Furthermore, static equilibrium solutions, i.e., solutions with $\rho_t = 0$ and $\mathbf{u} = \mathbf{0}$ satisfy the nonlinear elliptic equation

$$-\lambda\Delta\rho + W'(\rho) = \text{const in } \Omega, \tag{4}$$

where the constant on the right hand side is in general unknown and the energy function W is associated with the pressure p by the relation $W(\rho) = \rho W'(\rho) - p(\rho)$. The aim of this work is the construction of a family of reliable higher order schemes that have corresponding properties as (3) and (4) on the discrete level. In order to achieve this it turned out to be of advantage to discretize the equivalent nonconservative reformulation

$$\begin{array}{rcrcl} \rho_t & + & \nabla\cdot(\rho\mathbf{u}) & = & 0, \\ (\rho\mathbf{u})_t & + & \nabla\cdot(\rho\mathbf{u}\mathbf{u}^T) + \rho\nabla\left(W'(\rho) - \lambda\Delta\rho\right) & = & \nabla\cdot\tau, \end{array} \tag{5}$$

instead of equation (1) directly. Using this reformulation a first order well-balanced scheme can be constructed in a natural and straightforward way, see [3] for details.

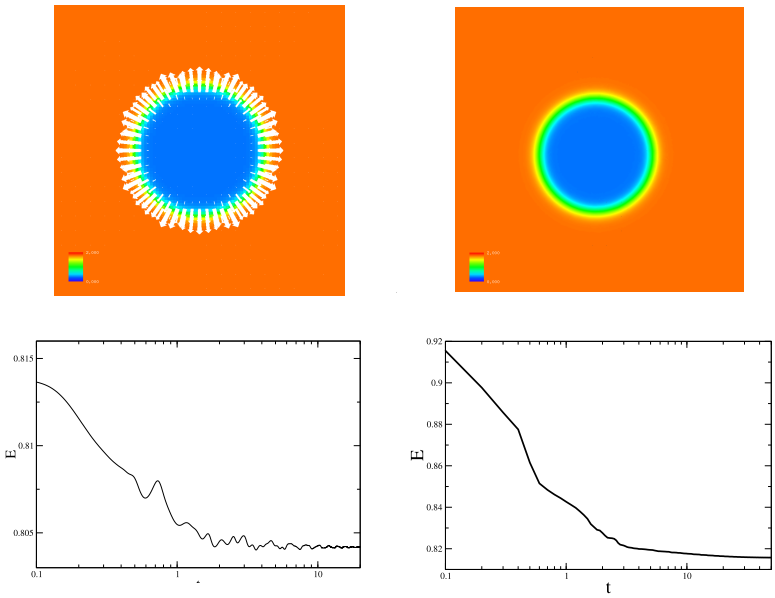

FIGURE 1. Standard scheme (left) versus nonconservative well-balanced scheme (right).

Figure 1 shows the difference between a standard discretization (left) of equation (1) and the nonconservative well-balanced scheme (right). The upper two pictures show a static equilibrium configuration. With the standard discretization

a velocity field (represented by the arrows) of order of the mesh size arises immediately and remains as time tends to infinity. The nonconservative well-balanced scheme approaches a perfect static equilibrium state on the discrete level. Similar velocity fields (parasitic currents) have been observed in [5]. The lower two pictures show the total physical energy which is not monotonically decreasing for the numerical solution given by the standard scheme.

The basic first order well-balanced scheme can be generalized to higher order schemes by application of the Discontinuous Galerkin approach as proposed by Cockburn and Shu, see for example the review paper [1] and the references therein. The difficulty that arises is the handling of the nonconservative terms in equation (5). The discretization of nonconservative terms within the framework of the Discontinuous Galerkin method can be done using the definition of nonconservative products [2], for details see [3]. By construction, all higher order methods have the well-balanced property and, as long as local mesh adaption is omitted, the numerical solutions given by the higher order methods have a monotonically decreasing total energy on the discrete level.

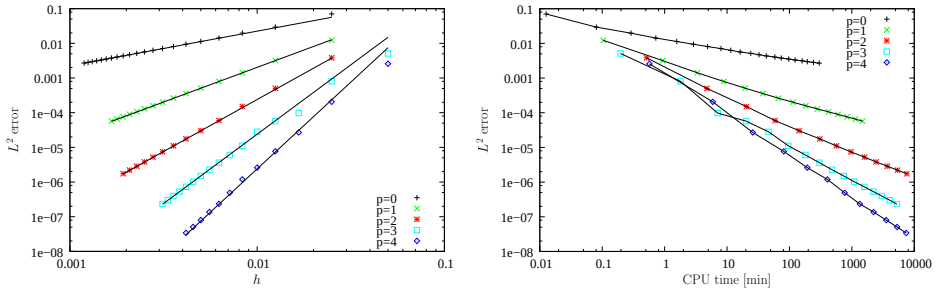

FIGURE 2. Left: mesh size versus L^2-error (black lines indicate the expected order of the method $p+1$). Right: CPU time versus L^2-error.

Figure 2 shows the result of a convergence test. The left part of the figure shows that the expected order of the method, which is $p+1$ where p denotes the polynomial degree in the Discontinuous Galerkin method, is achieved. The right part of this figure shows that a higher polynomial degree leads to more efficient schemes. For this convergence test we have used special solutions of the Navier-Stokes-Korteweg system that have been constructed numerically (but very accurately) by ODE techniques, for details see [3].

For application to real world problems a Discontinuous Galerkin code for general evolution equations in multiple space dimensions (1,2,3) has been designed using local mesh refinement and coarsening, MPI-based parallelization [6] and

ParMETIS-based load-balancing [7]. The discretization of the isothermal Navier-Stokes-Korteweg system as well as the discretization of the full temperature dependent model is done using this general purpose code.

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From the Global Entropy Inequality to Kinetic Relations

Wolfgang Dreyer

Background and Objectives. The local form of the *2nd law of thermodynamics* is used to control the evolution of initial and boundary value problems for systems for PDEs. In particular it restricts the admissible class of *constitutive functions*, and it yields inequalities on which for example *kinetic relations* are based. However, the local form of the *2nd law* is not a unique consequence of some universally stated axioms. This study discusses the subtleties of its derivation and application.

A piece of history. A heat engine converts heat power $\dot{Q}$ into mechanical power W and runs between a lower temperature T_{L} and an upper temperature T_{U}. In order to improve its efficiency, in 1824 Sadi Carnot found an upper bound for the produced maximal mechanical work, viz. $W_{\max} \leq f(T_{\mathrm{L}}, T_{\mathrm{U}})\dot{Q}$, where f indicates a universal function, that is independent of the agency and to the path of the process .

However, Carnots paper contains many serious errors. For example, even the conservation law of energy, the *1st Law of Thermodynamics*, is found to be violated, i.e. Carnot assumed that the heat that is needed to produce mechanical work is conserved during the process. Surprisingly, Carnots final result is correct and Rudolf Clausius rederived it from the simple axiom: *Heat cannot flow by it itself from a colder body to a hotter body.* This is the first version of the *2nd Law of Thermodynamics*. Based on his axiom Clausius derived in 1865 a further law that goes far beyond the characterization of efficiencies of heat engines. Nowadays this law is called the *2nd Law of Thermodynamics*, and it reads:

$$\frac{\mathrm{d}S}{\mathrm{d}t} \geq \frac{\dot{Q}}{T} \quad \text{or} \quad \frac{\mathrm{d}}{\mathrm{d}t}\int_V \rho\eta \,\mathrm{d}V \geq -\frac{1}{T}\oint_{\partial V} q^i n^i \,\mathrm{d}A\,. \tag{1}$$

The inequality concerns an arbitrary body with volume V, whose surface ∂V may exchange heat with the enviroment with rate $\dot{Q}$ at homogeneous temperature T. By means of this version of the 2nd Law, Clausius introduced a new additive quantity, that he called the *entropy* of the body. The equality sign holds in equilibrium and in non-equilibrium the variation of the entropy is larger than $\dot{Q}/T$.

Various attempts were undertaken in the past to find the local form of this inequality, in particular to determine the general form for the entropy flux. The most obvious way is to simply "write" the temperature T under the integral. The resulting equation is called the CLAUSIUS-DUHEM inequality:

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_V \rho\eta \,\mathrm{d}V \geq -\oint_{\partial V} \frac{q^i n^i}{T}\,\mathrm{d}A \quad \Rightarrow \quad \frac{\partial \rho\eta}{\partial t} + \nabla_i\left(\rho\eta v^i + \frac{q^i}{T}\right) \geq 0\,. \tag{2}$$

Consequently the entropy flux is $\phi^i = q^i/T$. However, this form of ϕ^i already fails in case of fluid mixtures, radiation problems and even in ideal gases we have $\phi^i = q^j/T(\delta^{ji} + 2\sigma^{<ji>}/5p)$, where $\sigma^{<ji>}$ denotes the stress deviator and p is the pressure.

In 1968 this shortcoming was remedied by the seminal works of Ingo Müller. Here, in contradiction to the preliminary definition of the local form of ϕ^i, the entropy flux is considered to be a material dependent quantity and thus relies on a constitutive law whose explicit form results from the exploitation of the 2nd law according to the strategies of Müller. We present a revision of the entropy principle based on five, well accepted statements. In particular, it relies on a prescribed form of the entropy production ζ based on established thermodynamical concepts.

Example: 1D elasticity with strain gradients The following example gives a simple illustration. A state of a 1D body at time t is assumed to be given by the variables internal energy density $e(t,x)$ and the displacement $u(t,x)$. The field equations for the variables rely on the equations of balance for momentum and internal energy

$$\ddot{u} - \frac{\partial \sigma}{\partial x} = 0, \quad \dot{e} + \frac{\partial q}{\partial x} = \sigma \dot{u}_x\,. \tag{3}$$

In order to end up with a closed set of field equation we have to relate the two quantities stress, σ, and heat flux, q, which are not among the basic variables, via constitutive laws to the variables and their derivatives. Within the setting of a phase field model, we assume that the entropy density s is given by the function $s = h(e, u_x, u_{xx}, u_{xxx})$. We form the time derivative of s and proceed with elimination of $\dot{e}$ by means of the balance equation $(3)_2$. Hereafter the product rule is used to rearrange terms. The resulting identity forms the basis of a local entropy inequality, that we obtain by 2 definitions, Clausius axiom and a conclusion.

1. We define the (absolute) temperature, T, and subsequently define the entropy flux, ϕ, according to

$$\frac{1}{T} = \frac{\partial h}{\partial e}, \quad \text{and} \quad \phi = \frac{q}{T} - \left(\frac{\partial h}{\partial u_{xx}} - \frac{\partial}{\partial x}\frac{\partial h}{\partial u_{xxx}}\right)\dot{u}_x + \frac{\partial h}{\partial u_{xxx}}\dot{u}_{xx}\,. \tag{4}$$

2. We satisfy Clausius axiom, whereupon heat cannot flow by itself from a cold to a hot place, by

$$q\frac{\partial\frac{1}{T}}{\partial x} \geq 0, \tag{5}$$

i.e. the heat flux must be antiparallel to the temperature gradient.
3. In order that (5) is the only contribution to the entropy production ζ, we must have

$$\frac{\sigma}{T} = -\frac{\partial h}{\partial u_x} + \frac{\partial}{\partial x}\frac{\partial h}{\partial u_{xx}} - \frac{\partial^2}{\partial x^2}\frac{\partial h}{\partial u_{xxx}} \ . \tag{6}$$

Thus the local entropy inequality, viz.

$$\dot{s} + \frac{\partial \phi}{\partial x} = q\frac{\partial\frac{1}{T}}{\partial x} \geq 0; , \tag{7}$$

results here as a consequence of the field equations and some assumptions. Note (i) that the entropy production is of the form *irreversible flux* $\times$ *driving force*, which is in a thermoelastic body the heat flux times the derivative of $1 \ / \ T$, and (ii) that the described strategy requires in particular a prerequisite identification of the irreversible fluxes and the corresponding driving forces in the system of field equations. These are those that are known to be zero in equilibrium.

On the 2^{nd} law across singular surfaces. Within sharp interface models, two adjacent phases of a body are separated by a singular surface with normal speed w^ν, where the thermodynamic quantities may suffer a discontinuity. For example, if the adjacent phases are Euler fluids, the jump conditions for mass density ρ and velocity v^i including anisotropic surface tension read

$$[[\rho(v^\nu - w^\nu)]] = 0, \quad \rho(v^\nu - w^\nu)[[v^i]] + [[p]]\nu^i = (S^{\alpha\beta}\tau^i_\beta + S^\alpha \nu^i)_{;\alpha} \ . \tag{8}$$

Here the double brackets denote the jumps, the semicolon indicates covariant derivatives along the surface and τ^i_β respectively ν^i are its tangential and normal vector. The surface force is decomposed into tangential, $S^{\alpha\beta}$, and normal, S^α, components.

Likewise to the bulk, there is a 2^{nd} law of thermodynamics across the interface, which can be formulated in a similar manner to the above. For example, the temperature axiom, which corresponds to $(4)_1$ states the continuity of temperature across the interface, i.e. $[[T]] = 0$, and the analogon to (6) allows the calculation of the surface stresses if the interfacial free energy γ were known as a function of the metric tensor $g_{\alpha\beta}$ and the normal vector ν^i:

$$S^{\alpha\beta} = \gamma g^{\alpha\beta} + \frac{1}{2}\frac{\partial \gamma}{\partial g_{\alpha\beta}} \ , \quad S^\alpha = -g^{\alpha\beta}\tau^i_\beta \frac{\partial \gamma}{\partial \nu^i} \ . \tag{9}$$

The inequality that corresponds to (5) involves the specific free energy ψ and the stress σ^{ij} of the bulk phases, and it has likewise the form of a product *flux* $\times$ *driving force*:

$$\rho(v^\nu - w^\nu)[[\psi - \frac{1}{\rho}\sigma^{ij}\nu^i\nu^j + \frac{1}{2}(v-w)^2]] \geq 0 \ . \tag{10}$$

Recall that the inequality (5) may be used to motivate Fourier's law, viz. $q \sim \nabla(1/T)$, as the simplest possibility to satisfy (5). In a similar manner we read off from (10) $\rho(v^\nu - w^\nu) \sim [[\psi + \frac{1}{\rho}\sigma^{ij}\nu^i\nu^j + \frac{1}{2}(v-w)^2]]$ as the simplest possibility to satisfy (10). Usually this law is called *kinetic relation*.

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Supersonic Rarefaction Phase Boundaries

Haitao Fan

(joint work with X. Lin)

The isothermal fluid flow involving liquid/vapor phase transitions can be modelled by

$$\begin{aligned} &v_t - u_x = 0, \\ &u_t + p(\lambda, v)_x = \varepsilon u_{xx}, \\ &\lambda_t = \frac{a}{\varepsilon} w(\lambda, v) + b\varepsilon\lambda_{xx}, \end{aligned} \tag{1}$$

where v is the specific volume, u the velocity of the fluid, λ the weight portion of vapor in the liquid/vapor mixture. The constants ε is the viscosity, ε/a the typical reaction time, and $b\varepsilon$ the diffusion coefficient. The pressure function in (1), $p(\lambda, v)$, satisfies

$$p_v < 0, \quad p_\lambda > 0. \tag{2}$$

In this paper, we further assume

$$p_{vv} > 0. \tag{3}$$

The function $w(\lambda, v)$ represents the rate of vapor initiation and growth. For studying the travelling waves of (1) and the related issues, we take

$$w(v, \lambda) = (p(\lambda, v) - p_e)\lambda(\lambda - 1), \tag{4}$$

where p_e is the equilibrium pressure. The system (1-3) not only exhibits all major one-dimensional wave patterns observed in actual experiments on retrograde fluids, [3], but also explains the puzzling ring formations observed experiments, [4]. Retrograde fluids are fluids with high molar heat capacity and hence can be approximated by isothermal flows. Existence and nonexistence conditions for liquefaction and evaporation waves are given in [5]. Existence and uniqueness of solutions of Riemann problems under a kinetic relation motivated be the behavior of liquefaction and evaporation waves is proved in [2]. There are variational

solutions of the non-isothermal multi-dimensional case of (1) under various assumptions, [6]. The inviscid case of (1) with $a = b = 0$ has global solutions for a class of initial data of large total variations, [1].

The travelling waves equations for (1) are

$$\begin{aligned} &-cv' - u' = 0,\\ &-cu' + p' = u'',\\ &-c\lambda' = aw(\lambda, v) + b\lambda'',\\ &(u, v, \lambda)(\pm\infty) = (u_\pm, v_\pm, \lambda_\pm). \end{aligned} \tag{5}$$

Collapsing waves are travelling waves of (1) with end values $(v_\pm, \lambda_\pm) := (v, \lambda)(\pm\infty)$ satisfying

$$\begin{aligned} &0 < \lambda_- < 1, \quad p(\lambda_-, v_-) = p_e,\\ &\lambda_+ = 1, \quad p(\lambda_+, v_+) > p_e, \end{aligned} \tag{6}$$

The end value of an explosion waves satisfy

$$\begin{aligned} &0 < \lambda_- < 1, \quad p(\lambda_-, v_-) = p_e,\\ &\lambda_+ = 0, \quad p(\lambda_+, v_+) < p_e, \end{aligned} \tag{7}$$

A necessary and sufficient condition for the existence of collapsing wave is

$$c^2 \geq 4ab|p(\lambda_+, v_+) - p_e|, \quad c^2 \geq -p_v(\lambda_\pm, v_\pm). \tag{8}$$

For explosion waves, (8) is a sufficient condition for their existence. When $c^2 < 4ab|p(\lambda_+, v_+) - p_e|$, there is no explosion wave. These collapsing and explosion waves shown to exist are monotone. Note that since physically meaningful solutions lies in the range $0 \leq \lambda \leq 1$, the non-existence of travelling waves in this paper means that there is no travelling wave satisfying $0 \leq \lambda \leq 1$ everywhere.

¿From (8), we see that collapsing waves are supersonic on both side of the wave, and it is a rarefaction shock. In the explanation of the ring formation phenomenon, [4], the front of the outer ring is found to be a collapsing wave. Actual experiments show that the outer front of the ring is indeed supersonic.

Given (v_+, λ_+) satisfying (6) and (8), there are travelling waves connecting infinitely many different (v_-, λ_-) to the given (v_+, λ_+). Which one of them will actually appear in the solution of (1) for large t? The last equation in (1) is similar to the KPP equation

$$\lambda_t = \lambda(\lambda - 1) + \lambda_{xx}, \tag{9}$$

The travelling wave showing up in the solution of initial value problem of (9) for large t is the one with the same decay rate as that of the initial value as $x \to \infty$. With Riemann initial data, we expect that collapsing and explosion waves of (1) with slowest possible speed for the given the downstream state to appear in the solution. Our numerical computation supports this expectation.

To study the behavior of (1-3) when $\varepsilon > 0$ is small, we assume the strong limit $\lim_{\varepsilon \to 0+}$ of the solution exist, and study the behavior of the limit. Such limit will

satisfy

$$\begin{aligned} &v_t - u_x = 0, \\ &u_t + p_x = 0, \\ &(p - p_e)\lambda(\lambda - 1) = 0. \end{aligned} \tag{10}$$

In [2], existence and uniqueness of the solution of the Riemann problem is established under kinetic relations mimicking the behavior of the slowest liquefaction and evaporation waves. Now, we have proved the existence of collapsing and explosion waves, and hence we should include these waves into the kinetic relation. However, admitting collapsing and explosion waves resulting in two solutions for the same Riemann initial data. For example, one of the solution has a collapsing wave, while the other does not. To resolve this nonuniqueness, we have to set up the criterion on when to use which solution. Our numerical tests show that when a pure phase is in contact with mixture or the other pure phase, then collapsing and explosion waves of the slowest speed are preferred if they exist. Whether this criterion will settle the nonuniqueness of the Riemann problem is left for future research.

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Analysis and Numerical Approximation of a Traffic Flow Model with Phase Transitions

Paola Goatin

(joint work with C. Chalons, R.M. Colombo, F.S. Priuli)

I consider a traffic flow model with phase transitions, that has been introduced by R.M. Colombo in [7]. For low densities, the flow is *free* and is described by a scalar conservation law usually referred to as the Lighthill-Whitham [11] and Richards [12] model. At high densities, the flow is *congested* and is described by

a 2×2 system. More precisely, we have

$$
(1) \qquad \begin{array}{ll} \text{Free flow:} & \text{Congested flow:} \\ (\rho, q) \in \Omega_f, & (\rho, q) \in \Omega_c, \\ \partial_t \rho + \partial_x(\rho v) = 0, & \left\{ \begin{array}{l} \partial_t \rho + \partial_x(\rho v) = 0, \\ \partial_t q + \partial_x \left((q - Q) v \right) = 0, \end{array} \right. \\ q = \rho V, & \\ v = v_f(\rho) = V \left(1 - \frac{\rho}{R} \right), & v = v_c(\rho, q) = \left(1 - \frac{\rho}{R} \right) \frac{q}{\rho}. \end{array}
$$

The conserved quantity $\rho \in [0, R]$ is the mean traffic density, and v is the mean traffic velocity. The parameter R is the positive maximal density, V the maximal speed and Q is a parameter depending on the road under consideration. The weighted linear momentum q is originally motivated by gas dynamics. It approximates the real flux ρv for ρ small compared to R.
The coupling is achieved by introducing a transition dynamics from free to congested flow. A detailed description of the Riemann solver, and analogies between solutions to (1) and real traffic features are given in [7]. Here I just want to recall that the 2×2 system describing the congested flow turns out to be hyperbolic, the second characteristic field being linearly degenerate, while the first has an inflection point along the curve $q = Q$. Moreover, shock and rarefaction curves coincide, hence system (1), right, belongs to Temple class [13].
The domains Ω_f and Ω_c are taken to be invariant sets for the corresponding conservation laws in (1). The resulting domain is given by $\Omega = \Omega_f \cup \Omega_c$, with

$$
\begin{array}{rcl} \Omega_f & = & \{(\rho, q) \in [0, R] \times [0, +\infty[\, : \, v_f(\rho) \geq V_f, \, q = \rho \cdot V\} \, , \\ \Omega_c & = & \left\{ (\rho, q) \in [0, R] \times [0, +\infty[\, : \, v_c(\rho, q) \leq V_c, \, \frac{q - Q}{\rho} \in \left[\frac{Q_- - Q}{R}, \frac{Q_+ - Q}{R} \right] \right\} \, , \end{array}
$$

where $V_f > V_c$ are the threshold speeds, i.e. above V_f the flow is free and below V_c the flow is congested. The parameters $Q_- \in]0, Q[$ and $Q_+ \in]Q, +\infty[$ depend on the environmental conditions and determine the width of the congested region. The domain Ω turns out to be a disconnected set in $\mathbb{R}^2$, its two connected components representing the free and the congested phases.
Other traffic flow models with phase transitions have been considered in the literature since the 60-ties, in order to explain empirical flow-density relations. In particular, we refer the reader to the scalar model of Drake, Schofer and May [9]. Another model has been introduced recently by myself [10]. It consists in coupling the LWR equation with the 2×2 Aw-Rascle model [1].

In collaboration with R.M. Colombo and F.S. Priuli [8], I proved the well posedness (in the L^1-norm) of the solutions to the Cauchy and initial-boundary value problems for (1), for data with bounded total variation. More precisely, we construct a *Riemann Semigroup* of solutions defined on a set of functions with bounded total variation, which is Lipschitz continuous with respect to initial (and eventually boundary) data and time. The semigroup trajectories are obtained as limit of approximate solutions constructed by wave-front tracking (see [2] for a well posedness result for classical Temple systems).
¿From the traffic point of view, the result is useful in view of applications to control and optimization problems.

As far as numerical approximations are regarded, we observe that, due to the lack of convexity of the domain $\Omega_f \cup \Omega_c$, the classical Godunov method does not apply. In fact, in the presence of phase transitions, the projection step of the algorithm can give values which are not in the domain. C. Chalons and I present a new version of the Godunov scheme, based on a modified averaging strategy and a sampling procedure [6]. More precisely, we modify the mesh cells following the phase boundaries, so that the projection involves only values belonging to the same phase. In order to come back to the original cells, we complete the projection step with a Glimm-type sampling technique.
This scheme is essentially first order accurate, and hence introduces a considerable dissipation away from phase transitions. In order to improve accuracy, we also present an extension of the method to second-order accuracy in space and time, which is L^1-stable in space.
The averaging procedure on modified cells has first been used (up to our knowledge) in [14] but in a different context and a slightly different form. However, the idea of going back to the initial cells by means of a sampling procedure is new and allows us to avoid dealing with moving meshes (as in [14]). Similar numerical techniques have recently been proposed by C. Chalons for approximating nonclassical solutions arising in certain nonlinear hyperbolic equations (see [3], [4] and the references therein), and very recently by Chalons and Coquel in [5] for computing sharp discrete shock profiles.
I conclude by emphasizing that due to the sampling procedure, the proposed algorithm is not conservative in the classical sense of finite volumes methods. However, we numerically demonstrate that it is actually "weakly" conservative in the following sense: phase transitions propagate with the right speeds (given by Rankine-Hugoniot conditions) and conservation errors seem to tend to zero with the mesh size. Of course, the random choice method (Glimm's scheme) could be applied successfully in this case. Nevertheless, our method doesn't need to compute all the values in the Riemann solution, but only the values on both sides of the phase transition, and is then cheaper. Moreover, our algorithm coincides with the classical Godunov scheme, and hence it is conservative, away from phase transitions.

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Phase Transitions and Interface Conditions for Two Phase Flows

Dietmar Kröner
(joint work with K. Hermsdörfer, C. Kraus)

In this talk we consider a mathematical model of liquid-vapour flows including phase transition which was proposed by Korteweg already in 1901 [2] and which is known as the Navier-Stokes-Korteweg model. It is an extension of the compressible Navier-Stokes equation and given by the following system.

$$\begin{aligned} \partial_t \rho + \nabla \cdot (\rho v) &= 0 \\ \partial_t(\rho v) + \nabla \cdot (\rho v v^t + p(\rho) I) &= \mu \Delta v + \lambda \rho \nabla \Delta \rho. \end{aligned} \tag{1}$$

This is a one fluid model where $\rho, v, p(\rho)$ and μ denote the density, velocity, pressure and the viscosity of the fluid/vapour respectively. Compared to the original Navier–Stokes equation the system (1) contains the term $\gamma\varepsilon^2\rho\nabla\Delta\rho$ (in which λ is replaced by $\gamma\varepsilon^2$) which is supposed to model capillarity effects close to phase transitions. The pressure $p(\rho)$ as a function of the density ρ is defined as

$$p(\rho) = \rho^2 \psi'(\rho) \tag{2}$$

where ψ is a smooth function of ρ such that $\rho\psi(\rho)$ is the total free energy density and of the form of a double well potential (up to a linear function).

The values α_1 and α_2 are defined by the extrema of p. The conservation of energy is neglected in (1). Different phases of the fluid are defined by the size of ρ. If $\rho \leq \alpha_1$ we are in the vapour phase and if $\rho \geq \alpha_2$ we are in the liquid phase. The equation (2) is known as the van der Waals equation of state.

In this contribution we study the behaviour of the pressure across the interface. Since a rigorous theory about this question is not available and difficult, we will concentrate on the static version of (1), i.e.

$$\nabla p(\rho) \quad = \quad \gamma\varepsilon^2\rho\nabla\Delta\rho. \tag{3}$$

In particular we will study the behaviour of the pressure in the limit if $\varepsilon \to 0$. First we will repeat some recent results [1], [4], which show that the difference of the pressures $[p]$ on both sides of the interface is of order ε:

$$[p] = ck_m\varepsilon + o(\varepsilon), \tag{4}$$

where k_m is the mean curvature of the interface. This seems to contradict the classical result of Landau and Lifschitz [3], which says that the difference of the pressures on both sides of the interface is proportional to the mean curvature of the interface:

$$[p] = c_1 k_m. \tag{5}$$

Now let us consider the low Mach number limit of (1) and assume, that we have an asymptotic expansion of all quantities with respect to the Mach number M, in particular

$$p(x,t) \quad = \quad p(\rho(x,t)) = p_0(x,t) + Mp_1(x,t) + M^2p_2(x,t) + O(M^3).$$

The non-dimensionalization form of (1) for small Mach number M is given by:

$$\partial_t(\rho v) + \nabla\cdot(\rho vv^t + \frac{1}{M^2}p(\rho)I) \quad = \quad \frac{1}{Re}\Delta v + \frac{\lambda b^2}{M^2}\rho\nabla\Delta\rho.$$

Then we show that the scaling/capillarity quantity λ can be related to the Mach number under certain conditions such that we get the expected jump relation for the difference of the pressures p_2 on both sides of the interface. Similarly in a second approach we can obtain the expected pressure relation across the interface by a modified definition of the pressure on the basis of a special scaling of the free energy density compared to the gradient term. Instead of the energy

$$J_\varepsilon(\rho) := \int_\Omega W(\rho) + \frac{\varepsilon^2}{2}|\nabla\rho|^2dx + \tilde{M} \to \text{Minimum} \tag{6}$$

we use the modification

$$I_\varepsilon(\rho) := \frac{1}{\varepsilon}\int_\Omega W(\rho) + \frac{\varepsilon^2}{2}|\nabla\rho|^2dx + \tilde{M} \to \text{Minimum} \tag{7}$$

where W denotes the free energy density up to a linear function, $\frac{\varepsilon^2}{2}|\nabla\rho|^2$ penalizes the occurrence of a large interface and $\tilde{M}$ is a constant.

It turns out that the functional in (7) satisfies the following identity.

$$I_\varepsilon(\rho) \quad = \quad \int_\Omega \frac{1}{\varepsilon} W(\rho) + \frac{\varepsilon}{2}|\nabla\rho|^2 dx + \tilde{M} = \int_\Omega \rho\psi_\varepsilon(\rho) + \frac{\varepsilon}{2}|\nabla\rho|^2 dx$$

where $\psi_\varepsilon(\rho)$ is defined as $\rho\psi_\varepsilon(\rho) := \frac{1}{\varepsilon}(\rho\psi(\rho) - l(\rho)) + l(\rho)$ and $l(\cdot)$ is the Maxwell-line.

Therefore instead of (6) we consider the functional

$$I_\varepsilon(\rho) \quad = \quad \int_\Omega \rho\psi_\varepsilon(\rho) + \frac{\varepsilon}{2}|\nabla\rho|^2 dx. \tag{8}$$

Similar as in (2) we define for this new scaling the pressure $p_\varepsilon(\rho) := \rho^2\psi'_\varepsilon(\rho)$ and the relation to $p(\rho)$ is given by

$$p_\varepsilon(\rho) = \frac{1}{\varepsilon}p(\rho) + \frac{1-\varepsilon}{\varepsilon}d_1 \tag{9}$$

where $p(\rho) = \rho^2\psi'(\rho)$ is defined as in (2) (see also [1]). Now putting (4) and (9) together we obtain the expected jump condition (5) for p_ε .

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Kinetic Relations for Undercompressive Shocks

Philippe G. LeFloch

I presented a review of the theory of kinetic relations for systems of nonlinear conservation laws of hyperbolic or of hyperbolic-elliptic type. One important issue is understanding the effect of *singular perturbations* including diffusion, dispersion, and/or relaxation terms, for instance

$$u^\varepsilon_t + f(u^\varepsilon)_x = \big(R(\varepsilon u^\varepsilon_x, \varepsilon^2 u^\varepsilon_{xx}, \ldots)\big)_x,$$

where $u^\varepsilon : \mathbb{R}_+ \times \mathbb{R} \to \mathbb{R}^N$ is the unknown of the problem. Such systems of equations arise in the dynamics of complex materials undergoing phase transitions and in the dynamics of van der Waals fluids with viscosity and capillarity effects included.

The importance of small scales is central and a key objective is to determine the "sharp interface" *hyperbolic theory* for the system

$$u_t + f(u)_x = 0$$

associated with the given singular perturbation problem.

One need to establish the existence of the limit $u := \lim_{\varepsilon \to 0} u^\varepsilon$ and then investigate its qualitative properties. Which propagating discontinuities are admissible ? What is the structure of the corresponding Riemann solution ? One is led to distinguish between (classical) *compressive* shock waves and (nonclassical) *undercompressive* ones. For the latter, for the sake of uniqueness (at least for the Riemann problem) one need to impose a *kinetic relation,* which comes in addition to the usual entropy inequality.

The *analytical properties* (monotonicity, dependence upon parameters) of the kinetic relation associated with a given *continuous or discrete* approximation model have been investigated. This goal has been achieved by a detailed study of the existence and qualitative properties of associated traveling wave solutions.

Numerical approximation of both nonclassical shocks and the kinetic relation associated with Glimm-type, front-tracking, or finite difference schemes has been extensively studied.

In particular, in the recent work [15] we have investigated the role of the *equivalent equation* associated with a finite difference scheme. We stated a conjecture and provided numerical evidences demonstrating its validity. We have shown that the kinetic function associated with a finite difference scheme approaches the (exact) kinetic function derived from a given (viscosity, capillarity) regularization. Interestingly, the accuracy improves as its equivalent equation coincides with the diffusive-dispersive model at a higher and higher order of approximation.

These small scale features can not be quite the same at the continuous and at the discrete levels, since a *continuous* dynamical system of ordinary differential equations can not be exactly represented by a *discrete dynamical system* of finite difference equations. The effects of the regularization coefficients on the kinetic functions were also investigated.

In [15] we have also considered fourth-order models and demonstrated that a kinetic function can be associated with the *thin liquid film model.* We also investigated a *generalized Camassa-Holm model,* and discovered nonclassical shocks for which we could determine a kinetic relation. In both models, the kinetic function was found to be monotone decreasing, as required in the general theory [13].

We also investigated to what extent a kinetic function can be associated with *van der Waals fluids,* whose flux-function admits two inflection points. We established that the Riemann problem admits several solutions whose discontinuities have viscous-capillary profiles, and we exhibited *non-monotone kinetic functions.*

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Numerical Simulation of Cavitation Bubbles by Compressible Two-Phase Fluids

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(joint work with P. Helluy, M. Bachmann, J. Ballmann)

Motivation. Cavitation is induced by a pressure drop in the liquid below vapor pressure. Such a pressure decrease may occur due to local acceleration of the liquid flow caused by geometrical constraints, e.g., if the liquid flows through a narrow orifice or around an obstacle. In this case, the pressure drops below vapor pressure, the liquid bursts and creates a free surface filled with gas and vapor – the bubble. Due to changes in the flow field, the pressure in the liquid may increase again causing the bubble to collapse. The collapse is accompanied by strong shock and rarefaction waves running into the bubble and the surrounding liquid. The inwards running shock wave focuses in the center of the bubble. This leads to extreme physical states in the interior. In addition, the shrinking of the bubble leads to a strong compression of the vapor. Both effects evoke an increase of pressure which bulges the bubble. Hereby, a dynamic oscillation process is initiated which finally leads to the collapse of the bubble. If the collapse takes place next to a boundary, flow and pressure fields become asymmetric and a liquid jet develops which is either directed towards or away from the boundary, depending on its compliance.

The processes taking place in the interior and exterior of the collapsing and oscillating bubble and the prediction of onset and extent of cavitation damage are still subject of theoretical and experimental research. However, small time and space scales as well as the complicated dynamics make any theoretical and experimental approach a challenge. Therefore, advanced numerical investigations are needed to reveal further information about the highly unsteady flow dynamics in the fluid. Here the main challenge is the high difference of the acoustic impedance caused by the density jump across the phase boundary.

Mathematical Model. Compressible fluid flow is characterized in continuum mechanics by the fields of density ρ, velocity $\mathbf{v}$, internal energy e and pressure p distributions. The balances of mass, momentum and energy for inviscid flow lead to the Euler equations in conservation form

$$\begin{aligned} &\rho_t + \operatorname{div}(\rho\mathbf{v}) = 0, \\ &(\rho\mathbf{v})_t + \operatorname{div}(\rho\mathbf{v}\otimes\mathbf{v} + p\mathbf{I}) = \mathbf{0}, \\ &(\rho E)_t + \operatorname{div}(\rho\mathbf{v}(E + p/\rho)) = 0, \end{aligned} \tag{1}$$

where $E = e + 0.5\,\mathbf{v}^2$ is the total energy. In order to take into account the two different fluids (a gas and a liquid) we introduce a new unknown φ that we call the fraction of gas. We make the convention that $\varphi = 0$ and $\varphi = 1$ correspond to pure liquid and gas, respectively. Because we are interested in very high speed flows and very short observation times we suppose that the phase transition can be neglected so that there is no mass transfer between the two fluids, i.e.,

$$\varphi_t + \mathbf{v}\cdot\nabla\varphi = 0. \tag{2}$$

In order to close the system, we have to provide a pressure law. Here we consider the stiffened gas pressure law:

$$p(\rho, e, \varphi) = (\gamma(\varphi) - 1)\rho e - \gamma(\varphi)\pi(\varphi). \tag{3}$$

For the continuous model it would be sufficient to provide the pressure law coefficients γ and π for $\varphi = 0$ or $\varphi = 1$. But because of the numerical mixture, it is necessary to interpolate γ and π for $0 < \varphi < 1$. An arbitrary choice of interpolation would lead to numerical difficulties. In [7] it is suggested to use a linear interpolation of the two special quantities $\beta_1 = 1/(\gamma - 1)$ and $\beta_2 = \gamma\pi/(\gamma - 1)$.

Numerical Discretization. For the discretization of the stiffened gas model the approach of Saurel and Abgrall [7] is employed where the flow equations (1) for the conserved quantities are approximated by a finite volume scheme and an upwind discretization is used for the non-conservative transport equations of the gas fraction (2) by which the different phases are indicated. The original 1st order discretization is extended to higher order applying 2nd order ENO reconstruction to the primitive variables. In order to derive an appropriate non-conservative upwind discretization for the gas fraction on arbitrary unstructured grids we apply the key idea by Saurel and Abgrall: the resulting discretization has to preserve homogeneous pressure and velocity fields to avoid pressure oscillations. Hence we are not free in the discretization of the evolution equation for the gas fraction but it is closely related to the finite volume approximation of the flow equations.

Multiscale-based grid adaptation techniques [3] have been employed to improve the efficiency of the scheme. This allows for a locally high resolution that is needed to resolve accurately the local physical effects in the bubble collapse process. Since this process is highly dynamical the time discretization is explicit. Therefore the CFL condition is very restrictive because of the small cells sitting on the high refinement levels. For the cells on the coarser discretization levels we use a multilevel time stepping strategy that allows for larger time steps on coarser scales. This strategy has been recently developed in combination with the multiscale-grid adaptation, cf. [6]. It had to be modified taking into account the non-conservative upwind discretization of the evolution equations (2), cf. [5].

Numerical Results. The scheme is applied to the planar collapse of a gas bubble of radius $r = 1$ [mm] near to a rigid wall located at a distance of $r/2$. The bubble is filled with air at $\rho = 0.026077$ [kg/m^3] and $p = 2118$ [Pa] surrounded by water at $\rho = 1000$ [kg/m^3] and $p = 5 \times 10^7$ [Pa]. The dynamics of the resulting flow field can be separated into three stages. In a first stage, a low pressure regime is developing between the wall and the vapor bubble. This is caused by expansion and compression waves running between the wall and the bubble where they are reflected. At the same time, a shock wave is running inside the bubble towards the bubble center. Due to transmitted expansion and compression waves at the interface, the pressure distribution becomes asymmetric also inside the bubble. When the shock wave focuses in the bubble center a second stage starts where a liquid jet is forming that penetrates the bubble at the symmetry line and is directed towards the wall. This process is caused by the formation of two vortices inside the vapor bubble by which the vapor is concentrating in two almost rotational

symmetric vapor bubbles above and below the symmetry axis. The small distance between the two vortices causes a bottleneck for the liquid which acts as a nozzle where the liquid is significantly accelerated. In front of this bottleneck a high pressure zone is forming in the liquid where the pressure is about 5 times higher than in the undisturbed liquid. This high pressure liquid is then squeezing through the bottleneck and directed towards the wall where it hits with high pressure. The impact of the high pressure might be the cause of material damage. But this analysis requires considering of the coupled fluid-structure problem with the appropriate modeling of elastic-plastic stress waves in the solid wall. When the jet hits the wall, the third stage of the flow process starts. The liquid supplied by the jet is deflected at the wall to both sides of the symmetry axis and pushes away the water supplied from the free stream from above and below. In the wake of the jet the system of the splitted bubbles and the vortices start moving towards the wall where they are deflected upward and downward the symmetry axis. Details on the computation can be found in [5].

Validation. In order to investigate the influence of numerical phase transition on the numerical results the scheme has been validated by means of laser-induced cavitation bubbles, cf. [4]. For this purpose the Saurel-Abgrall approach has been applied to investigate the spherical bubble collapse of laser-induced cavitation bubbles. Initial data have been derived by first fitting the equilibrium radius in the Keller-Miksis model [2] to optimize the least square error to the experimental movement of the bubble wall. Then the gas state for an arbitrary bubble radius is deduced applying an ideal and adiabatic gas law.

The computations verify that the SA approach results in a severe numerical phase transition regime that is unphysical because mass transfer is excluded in the underlying physical model. This can be reduced by grid refinement but grid convergence is too slow and the needed resolution to reduce this effect significantly can not be afforded. Hence, discretizations using sharp interface models such as the real ghost fluid method might be more convenient.

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On a Non-Local Phase Field Model for Phase Transitions

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(joint work with A. Dressel, J. Haink)

1. The Mathematical Model

We consider the spatially one-dimensional dynamics of a fluid or a solid that can occur in two phases. ¿From the point of view of modelling phase boundaries can be either viewed as sharp or as diffuse interfaces. The first ansatz typically leads to mixed hyperbolic-elliptic systems of conservation laws where phase boundaries can be characterized as undercompressive shock waves (see [6] for an overview). Here we focus on a diffuse-interface or phase field model. Phase field models contain additional terms that contribute to the surface energy and regularize the equations. One obtains as phase transitions smooth functions with steep gradients. In contrast to the classical local Van-der-Waals (or Cahn-Hilliard) energy term we focus here on a non-local version. Some new well-posedness results will be presented. By numerical experiments we show that the non-local approach offers interesting modelling possibilities.
Using the notions of solid mechanics we search for strain $w = w(x,t) : (0,1) \times [0,\infty) \to \mathbb{R}$ and velocity $v = v(x,t) : (0,1) \times [0,\infty) \to \mathbb{R}$ satisfying the system

$$\begin{aligned} w_t - v_x &= 0, \\ v_t - [\sigma(w)]_x &= \mu v_{xx} - [\phi * w - w]_x, \end{aligned} \tag{1.1}$$

subject to the initial and (self-consistent) Dirichlet boundary conditions

$$\begin{gathered} v(x,0) = v_0(x), \quad w(x,0) = w_0(x), \\ \int_0^1 w(x,t)\,dx = \int_0^1 w_0(x)\,dx, \quad v(0,t) = v(1,t) = 0 \ \ \forall t \in [0,\infty). \end{gathered} \tag{1.2}$$

In (1.1) the stress-strain relation σ is chosen as the non-monotone function $\sigma(w) = w^3 - w$ such that the w-intervals which correspond to increasing branches of σ define the two different phases. For the potential $\phi \in L^1(\mathbb{R}) \cap L^\infty(\mathbb{R})$ we assume $\int_{\mathbb{R}} \phi = 1$. The functions $w_0, v_0 \in L^2(0,1)$ are given and $\mu > 0$ is the viscosity parameter. The operator $*$ denotes convolution.
A straightforward computation shows that solutions of (1.1), (1.2) dissipate the energy

$$E[v,w] = \int_0^1 \left(\Sigma(w(x)) + \frac{v(x)^2}{2} + \frac{1}{4} \int_0^1 \phi(x-y)(w(x) - w(y))^2\,dy \right) dx, \tag{1.3}$$

where we suppressed the t-dependency. In (1.3) Σ is a primitive of σ.

2. Wellposedness and Stability

We are interested in weak solutions of (1.1), (1.2). By a weak solution we mean functions $(w,v) \in C^0([0,\infty), (L^2(0,1))^2)$ such that (1.1) is satisfied in the distributional sense, the initial conditons are assumed weakly and $v \in L^2(0,\infty; H_0^{1,2}(0,1))$

holds. For the initial functions we only impose the energy bound

$$E[v_0, w_0] < \infty. \tag{2.4}$$

Theorem 2.1: *Let* (2.4) *be satisfied. Then there exists a unique weak solution* (w, v) *of* (1.1), (1.2) *such that we have*

$$E[w(.,t), v(.,t)] \leq E[w_0, v_0] \text{ for } t \geq 0$$

and

$$(w, v) \in L^\infty((0,1) \times (\delta, \infty)) \text{ for } \delta > 0. \tag{2.5}$$

The proof of Theorem 2.1 can be found in [3]. The existence part is verified via finite-difference approximations. It can also be obtained by other methods and also for the multidimensional case (see e.g. [5] for another result). More delicate and –up to our knowledge– restricted to the spatially one-dimensional case is the regularity bound (2.5). It is derived following the work of Andrews [1] and using the fact that the convolution operator in (1.1) is continuous. The a-priori L^∞-bound on w in (2.5) is the key step to obtain

Theorem 2.2: *Let the weak solution* $(w, v) \in C^0([0,\infty), (L^2(0,1))^2)$ *of* (1.1), (1.2) *from Theorem 2.1 be given. Then there is a* $P \in \mathbb{R}$ *such that we have*

$$\begin{aligned} \lim_{t\to\infty} v(.,t) &= 0 \text{ in } H^{1,2}(0,1), \\ \lim_{t\to\infty} w(.,t) &= \bar{w} \text{ in } L^2(0,1), \end{aligned}$$

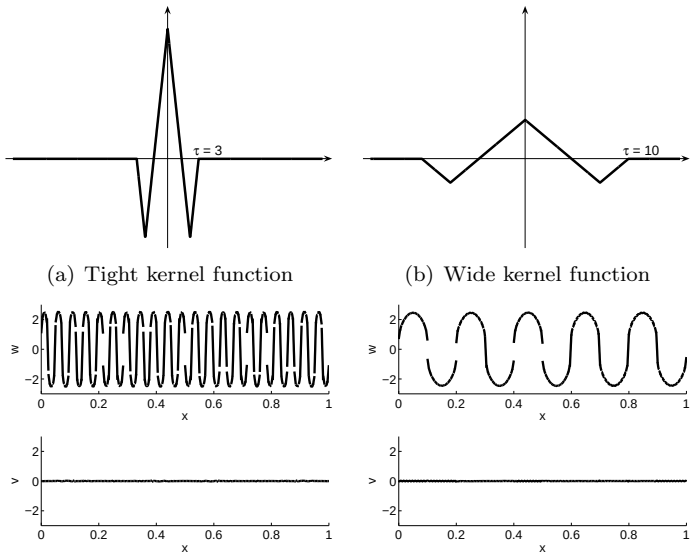
where $\bar{w}$ *is a solution of the elasto-static equation*

$$(K * \bar{w} - \bar{w}) - \sigma(\bar{w}) = P.$$

The proof from [4] is motivated by the work in [8] where an asymptotic stability result is derived for a local model. Furthermore we exploit that the convolution operator in (1.1) is even compact (for appropriate spaces).

3. Numerical Modelling by Discontinuous-Galerkin Schemes

The problem (1.1) can be seen as a hyperbolic-parabolic system. A quite flexible numerical approach that is able to take into account convective effects is given by the class of Local-Discontinuous-Galerkin Schemes [2]. We have adopted this approach in [7]. In particular we performed experiments for (non-positive!) kernels as in the first row of Fig. 1 below. As the initial datum we have chosen $v_0(x) = 0$ $w_0(x) = \pm 1.2$ for $x \in [0, 0.5]/x \in (0.5, 1]$. The computations show that in the time-asymptotic limit the solution converges to an oscillating equilibrium where the frequency of the oscillations depend on the structure of the kernel. Theorem 2.2 applies in this case.



(a) Tight kernel function (b) Wide kernel function

(c) $t = 5$. (d) $t = 5$.

FIGURE 1. Numerical solution for (1.1), (1.2) at $t = 5.0$ (lower row) with two different kernels (upper row).

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Stability of Traveling Waves in which an Insoluble Surfactant Influences the Flow of a Thin Liquid Film Down an Inclined Plane.

Michael Shearer

The flow of thin liquid films is important in a variety of contexts, including the chemical engineering of processes to manufacture industrial coatings, and the medical use of surfactant replacement therapy [6]. In this paper, we consider a system of PDE derived from the Stokes equations using the lubrication approximation, and including an equation for the propagation of surfactant on the free surface. Surfactant is treated as a layer of zero thickness, transported by the local speed of the free surface, but also subject to diffusion of surfactant molecules on the surface.

Specifically, the system of equations is

$$
\begin{aligned}
h_t - \nabla\cdot\left[\tfrac{1}{2}h^2\nabla\Gamma\right] + \alpha\left[\tfrac{1}{3}h^3\right]_x &= -\kappa\nabla\cdot\left[\tfrac{1}{3}h^3\nabla\nabla^2 h\right] + \beta\nabla\cdot\left[\tfrac{1}{3}h^3\nabla h\right] \\
\Gamma_t - \nabla\cdot\left[h\Gamma\nabla\Gamma\right] + \alpha\left[\tfrac{1}{2}h^2\Gamma\right]_x &= -\kappa\nabla\cdot\left[\tfrac{1}{2}h^2\Gamma\nabla\nabla^2 h\right] \\
&\quad +\beta\nabla\cdot\left[\tfrac{1}{2}h^2\Gamma\nabla h\right] + \delta\nabla^2\Gamma,
\end{aligned}
\tag{1}
$$

in which the dependent variables $h = h(x, y, t), \Gamma = \Gamma(x, y, t)$ represent the height of the free surface, and the surfactant concentration, respectively. The dimensionless non-negative parameters $\alpha > 0, \beta, \kappa, \delta$ are related to parallel and normal components of gravity, capillarity (i.e., surface tension), and diffusion on the free surface, respectively.

Somewhat surprisingly, for $\beta = \delta = \kappa = 0$, system (1) possesses one-parameter families of traveling waves of the form $(h(x - st; m), \Gamma(x - st; m)$ in which $h(\pm\infty, m) = h_\pm, \Gamma(\pm\infty, m) = 0$, and the parameter $m = max_x\Gamma(x; m)$. Details of the construction of these waves are given in [9, 13]. The traveling waves have speed $s = \frac{1}{3}(h_+^2 + h_+h_- + h_-^2)$, they are piecewise constant in h, with three jumps. Correspondingly, Γ is continuous, piecewise linear, zero both ahead of the leading jump in h, and behind the trailing jump. Traveling waves with this structure with $m > 0$ exist if and only if the upstream and downstream heights are well separated: $h_- > \frac{1}{2}(\sqrt{3} + 1)h_+$. Interestingly, the waves are *overcompressive* [12] in the sense that small disturbances ahead of and behind the wave propagate towards the wave.

For $\kappa = 0$, $\beta \geq 0$, and $\delta \geq 0$, the traveling waves are easily seen to have smooth counterparts, using phase plane analysis. However, for $\kappa > 0$, phase portraits are in $\mathbb{R}^4$ and are consequently difficult to analyze. Nonetheless, for small values of m, it seems likely that the trajectories can be proved to exist by perturbing away from the $\Gamma = 0$ traveling wave [10].

Stability of these traveling waves in one dimension, with at least one of β and κ positive, and $\delta > 0$ can be studied using an Evans function, as was done for a single fourth-order equation in [1]. Important steps in making the connection from linear to nonlinear stability have been achieved by Zumbrun and Howard [7, 11], including for fourth-order scalar equations. Preliminary results suggest

that traveling waves near $\Gamma = 0$ are stable. A complete proof in the case $\kappa = 0$ may rely on energy methods, similar to the analysis of Freistuhler and Liu [5] on overcompressive waves in a rotationally symmetric system.

In two dimensions, the traveling waves are thought to be unstable, consistent with numerical evidence for solutions related to the traveling waves [3, 4]. Theoretical verification comes from an asymptotic analysis, similar to the one done in [1, 2]. (See also [8].) However, zero is a double eigenvalue for the linearized problem, so that two eigenvalues have to be tracked as the wave number q varies away from zero. Preliminary results indicate that one eigenvalue is $-\delta q^2$, and the other eigenvalue is aq^2 to leading order, with the parameter a given by the same integral as in [2]. The interpretation is that perturbations due to diffusion of the surfactant on the free surface are mildly stabilizing, but do not help to stabilize the free surface itself. Since these results are for small values of $m \geq 0$, it would be interesting to see if the waves can be stabilized if there is more surfactant present, i.e., with larger values of m.

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Multi-Phase Mixture Balances with Phase Transitions

Gerald Warnecke
(joint work with W. Dreyer, F. Duderstadt, M. Hantke)

The aim of our work is to obtain and study multi-phase mixture conservation laws with phase change. We want to predict the flow of bubbly liquids or liquid droplets in a gas/vapor mixture. Without phase change this is a well studied subject in analysis and numerics. Still there are many open problems, which is no surprise in the field of systems of conservation laws. In order to obtain macroscopic equations for mixtures we study a specific averaging technique. The most important issue is to obtain the transfer terms for mass, momentum and energy transfer due to the phase change. For this we consider a bubble of vapor surrounded by the corresponding liquid phase. We study the behavior of the bubble due to phase change, i.e. condensation and evaporation, at the interface in some detail under spherical symmetry. The work reported here is joint work with Maren Hantke in Magdeburg as well as Wofgang Dreyer and Frank Duderstadt of the Weierstraß-Institut für angewandte Analysis and Stochastik (WIAS) in Berlin, Germany.

Our approach is based on volume averaging techniques due to Voinov and Petrov [4]. These were studied in detail in a diploma thesis of Rydzewski [2]. In our approach we aim at taking the compressible Euler equations to describe the microscopic flow in the carrier phase whereas Voinov and Petrov [4, 5, 3] assumed a potential flow field and made explicit use of the known solution of potential flow around a sphere. Our results are aimed to be more general than those. But we do take up the idea to use a potential flow in the farfield in order to determine the interfacial terms on the spherical surfaces between the phases.

We average by using a type of sliding average over a ball of radius $a > 0$ in space. The diameter of the ball $d = 2a$ is the scale at which we want to derive macroscopic equations for the mixture of a carrier phase C occupying most of the space and a dispersed phase D consisting of small balls with radii considerably smaller than a. For the dispersed phase we make strongly simplified homogeneity assumptions in the balls. This averaging is a specific case of volume averaging as described in Drew and Passman [1]. The treatment of the dispersed phase is considerably simplified. Transport theorems for averaged quantities of each phase are derived via the Reynolds transport theorem for the continuous phase and a distributional calculus for the disperse phase. Also quantities conserved at the microscopic level remain conserved at the macroscopic level. The closure of the macroscopic system while considering phase transition is still under discussion.

For the latter purpose we are studying the case of one spherical bubble centered at the origin. For this we have derived a system of three ordinary differential equations to describe the mass and volume change of the bubble due to the phase transition. Without the mass transfer term this system can be reduced to a version of the well known Rayleigh-Plesset equation. The connection to extended Rayleigh-Plesset theories with phase change is still under investigation. Further,

the system is being tested numerically and compared to experimental data. A next step will be to incorporate these microscopic results into the averaged macroscopic equations.

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