Discrete Kinetic Models for Dynamical Phase Transitions

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Abstract

In this paper, we shall describe discrete kinetic models, which serve as a novel and systematic way to regularized a mixed-type system describing the dynamical phase transitions. In the limit of zero mean free path, it is expected to provide abundant reasonable kinetic relations and nucleation criteria for constructing Riemann solvers. Some particular models have been investigated theoretically and numerically.

1 Introduction

Phase transitions occur in many physical systems, such as water-vapor mixture, liquid crystal, shape-memory alloy, etc. [5, 17, 20, 29]. Despite of the efforts by many ingenious scientists, it remains an interdisciplinary challenge to mathematicians, physicists, as well as engineers. There are two main aspects for the study: the constitutive theory, and the dynamics. In this paper we shall concern only with the dynamics, namely the evolution of a system for phase transitions.

Some of the crucial features, also difficulties for phase transitions are the sharp free interface, non-local interaction, and instability. Mathematical models reflecting these features are typically partial differential equations of mixed-type. For instance, the well-known van der Waals gas is described in the Lagrangian coordinates by

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

where v is the density, u the velocity, and $p(v)$ the pressure. The function $p(v)$ here is non-monotone, hence the characteristics $\lambda = \pm\sqrt{-p'(v)}$ might be either pure imaginary or real. Accordingly, the system (1) becomes elliptic or hyperbolic.

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As is well-known, the Cauchy problem for such a system is ill-posed. Numerical simulation is thus impossible due to the immediate blow-up. To resolve this difficulty, appropriate regularization is needed. One way is to add high order dissipation terms. As viscosity alone in the momentum equation is not enough to control the instability [15], further dissipation mechanisms are included, such as capillarity [25, 6], artificial viscosity in the mass equation [16], and heat diffusion [13, 27]. However, this approach is quite restrictive, as we do not know how to include high-order terms to make the system stable and physically reasonable. Moreover, the resolution of high-order derivatives usually cause tough numerical difficulties.

Meanwhile, there is another way to resolve the instability, namely to specify a Riemann solver. The crucial issue is to identify the class of discontinuities that is allowed (admissible). In the current system for phase transitions, we should distinguish two kinds of sharp discontinuities, namely the supersonic phase boundary and the subsonic one. The supersonic phase boundary is indeed a normal shock as in hyperbolic systems. Usually an entropy condition (e.g. the Lax geometrical entropy condition) singles out the physically correct shock. The discontinuity that demands special care is the subsonic phase boundary, for which the propagating speed determined by the Rankine-Hugoniot relation is smaller than the sound speeds at both end-states. It can be shown that normal entropy conditions are not valid any more. To specify a Riemann solver, one either generalizes entropy conditions arising in the study of hyperbolic systems [11, 14, 24], or investigates the limiting behavior of the systems with high-order dissipations [25]. Since the supersonic phase boundaries are subject to normal entropy condition, essentially what is done here can be regarded as specifying a kinetic relation for subsonic phase boundaries [1, 4, 7, 9, 10, 8, 21]. More precisely, a kinetic relation confines the two end-states across a subsonic phase boundary with certain relation, which is usually algebraic. In certain case when multiple solutions appear according to the prescribed kinetic relation, a nucleation criterion is also specified for the uniqueness. The idea of kinetic relation broadens the viewpoint of Riemann solver approach. Nevertheless, it can hardly reach far, unless we discovered a big variety of reasonable kinetic relations and nucleation criteria.

In this paper, we shall describe a new and systematic way of regularization, namely the discrete kinetic models (DKM's). A DKM is a semilinear hyperbolic system with source terms. The DKM's are easy to construct and to simulate. In the limit of zero mean free path, it is consistent with the original system of mixed-type partial differential equations, and provides a variety of reasonable kinetic relations and nucleation criteria.

We shall construct general discrete kinetic models in Sections 2. In Section 3, the scheme is presented. Then we shall describe three particular examples, namely Suliciu's model, Jin-Xin's relaxation model, and a six-speed model in Section 4. We conclude by some general remarks in Section 5.

2 General formulation

Consider phase transitions for:

$$\begin{cases} u_t + v_x & = 0, \\ v_t + \sigma(u)_x & = 0, \end{cases} \tag{2}$$

where u is the strain, v the speed, and $\sigma(u)$ the stress. The non-monotone constitutive relation $\sigma(u)$ makes the system of mixed-type.

We shall approximate the solution by $\begin{pmatrix} u^\epsilon \\ v^\epsilon \end{pmatrix} = \tilde{P}\tilde{f}$ where $\tilde{f}$ solves a discrete kinetic model (DKM) system

$$\tilde{f}_t + \tilde{\Lambda}\tilde{f}_x = \frac{1}{\epsilon}(\tilde{M}(\tilde{P}\tilde{f}) - \tilde{f}), \qquad \tilde{f}, \tilde{M} \in R^k. \tag{3}$$

Here $\tilde{\Lambda} = diag(\tilde{\lambda}_1, \cdots, \tilde{\lambda}_k)$, $\tilde{P} = (\tilde{p}_{ij})$ is a $2 \times k$ matrix, and $\tilde{M}(\tilde{P}\tilde{f})$ is the local Maxwellian. As the so-called mean free path $\epsilon \to 0$, formally $\tilde{f}$ tends to the local Maxwellian, and we expect the resulting approximating solution would solve (2) at the leading order. Therefore, naturally come the compatibility conditions

$$\tilde{P}\tilde{M}\begin{pmatrix} w_1 \\ w_2 \end{pmatrix} = \begin{pmatrix} w_1 \\ w_2 \end{pmatrix}, \tag{4}$$

$$\tilde{P}\tilde{\Lambda}\tilde{M}\begin{pmatrix} w_1 \\ w_2 \end{pmatrix} = \begin{pmatrix} w_2 \\ \sigma(w_1) \end{pmatrix}, \tag{5}$$

for any $(w_1, w_2) \in R^2$.

The general form of DKM (3) can be put into a canonical form.

Proposition 1 *The system (3) is equivalent to*

$$\begin{pmatrix} f_{1+} \\ f_{2+} \\ f_{1-} \\ f_{2-} \end{pmatrix}_t - \begin{pmatrix} \Lambda & & & \\ & \Lambda & & \\ & & -\Lambda & \\ & & & -\Lambda \end{pmatrix} \begin{pmatrix} f_{1+} \\ f_{2+} \\ f_{1-} \\ f_{2-} \end{pmatrix}_x = \frac{1}{\epsilon}\left[\begin{pmatrix} M_{1+}(u^\epsilon, v^\epsilon) \\ M_{2+}(u^\epsilon, v^\epsilon) \\ M_{1-}(u^\epsilon, v^\epsilon) \\ M_{2-}(u^\epsilon, v^\epsilon) \end{pmatrix} - \begin{pmatrix} f_{1+} \\ f_{2+} \\ f_{1-} \\ f_{2-} \end{pmatrix}\right]. \tag{6}$$

Here $f_{1\pm}, f_{2\pm}, M_{1\pm}, M_{2\pm}$ are columns of length N, $\Lambda = diag(\lambda_1, \cdots, \lambda_N)$ with $\lambda_1 > \lambda_2 > \cdots > \lambda_N \geq 0$. Denote 1_N the row vector with N entries identically 1,

$$P = \begin{pmatrix} 1_N & 0 & 1_N & 0 \\ 0 & 1_N & 0 & 1_N \end{pmatrix}, \qquad f = \begin{pmatrix} f_{1+} \\ f_{2+} \\ f_{1-} \\ f_{2-} \end{pmatrix}.$$

The primitive variables are recovered from $\begin{pmatrix} u^\epsilon \\ v^\epsilon \end{pmatrix} = Pf$, *i.e.*

$$\begin{aligned} u^\epsilon = &\quad 1_N(f_{1+} + f_{1-}), \\ v^\epsilon = &\quad 1_N(f_{2+} + f_{2-}). \end{aligned} \tag{7}$$

Proof Without loss of generality, assume that there are N distinct absolute values of propagating speeds in (3) as $\lambda_1 > \lambda_2 > \cdots, \lambda_N \geq 0$. Assume further that there are $\tilde{f}_1, \cdots, \tilde{f}_k$ corresponding to speed λ_1, and $\tilde{f}_{k+1}, \cdots, \tilde{f}_s$ corresponding to speed $-\lambda_1$. Let

$$\begin{pmatrix} f_{1,1+} \\ f_{1,1-} \\ f_{1,2+} \\ f_{1,2-} \end{pmatrix} = \begin{pmatrix} \sum_{i=1}^k \tilde{p}_{1i}\tilde{f}_i \\ \sum_{i=1+k}^s \tilde{p}_{1i}\tilde{f}_i \\ \sum_{i=1}^k \tilde{p}_{2i}\tilde{f}_i \\ \sum_{i=1+k}^s \tilde{p}_{2i}\tilde{f}_i \end{pmatrix}, \quad \begin{pmatrix} M_{1,1+} \\ M_{1,1-} \\ M_{1,2+} \\ M_{1,2-} \end{pmatrix} = \begin{pmatrix} \sum_{i=1}^k \tilde{p}_{1i}\tilde{M}_i \\ \sum_{i=1+k}^s \tilde{p}_{1i}\tilde{M}_i \\ \sum_{i=1}^k \tilde{p}_{2i}\tilde{M}_i \\ \sum_{i=1+k}^s \tilde{p}_{2i}\tilde{M}_i \end{pmatrix}.$$

Then $f_{1,1\pm}, f_{1,2\pm}$ satisfy

$$\begin{aligned} f_{1,1+;t} + \lambda_1 f_{1,1+;x} &= \frac{1}{\epsilon}(M_{1,1+} - f_{1,1+}), \\ f_{1,1-;t} - \lambda_1 f_{1,1-;x} &= \frac{1}{\epsilon}(M_{1,1-} - f_{1,1-}), \\ f_{1,2+;t} + \lambda_1 f_{1,2+;x} &= \frac{1}{\epsilon}(M_{1,2+} - f_{1,2+}), \\ f_{1,2-;t} - \lambda_1 f_{1,2-;x} &= \frac{1}{\epsilon}(M_{1,2-} - f_{1,2-}). \end{aligned} \tag{8}$$

Note that if there is no $\tilde{f}_i$ corresponding to λ_1, we take $f_{1,1\pm}$ as dumb variables, and corresponding local Maxwellian functions are set to be zero. Performing the same treatment with other λ_i's, the canonical form is obtained. If we take the initial data (and boundary data) accordingly, the two systems (3) and (6) are equivalent in the sense of giving the same approximating solution.

As the discontinuities of (2) are the limit of traveling waves of (6), one requires the end-states of the heteroclinic orbit of (6) satisfying the Rankine-Hugoniot relation. This is actually true for our DKM under the compatibility conditions.

Proposition 2 *Under the the compatibility conditions (4)-(5), the end-states of a traveling wave with speed c to (6) verify the Rankine-Hugoniot relation*

$$\begin{cases} -c[u^\epsilon] + [v^\epsilon] &= 0, \\ -c[v^\epsilon] + [\sigma(u^\epsilon)] &= 0, \end{cases} \tag{9}$$

where $[\cdot] = (\lim_{x-ct\to+\infty} - \lim_{x-ct\to-\infty})(\cdot)$ *is the jump between the two end-states.*

Proof Take $W_i = Pdiag(\lambda_1^i, \cdots, \lambda_N^i)f$, and $M_i = Pdiag(\lambda_1^i, \cdots, \lambda_N^i)M$, then the equations for W_0 and W_1 are, with the help of the compatibility conditions,

$$\left\{\begin{array}{lll} W_{0t}+W_{1x}= & W_0-M_0 & =0, \\ W_{1t}+W_{2x}= & W_1-M_1 & =W_1-\begin{pmatrix} v^\epsilon \\ \sigma(u^\epsilon) \end{pmatrix}. \end{array}\right.$$

For a traveling wave $f(x-ct)$, we have

$$-cW_0'+W_1'=0,$$

or

$$-cW_0+W_1=C_1,$$

with C_1 a constant vector. In particular, at the end-states, we have

$$\lim_{x-ct\to-\infty}[-cW_0+W_1]=\lim_{x-ct\to+\infty}[-cW_0+W_1]=C_1.$$

Meanwhile, as the end-states are stationary points, the second equation requires

$$\lim_{x-ct\to\pm\infty}\left[W_1-\begin{pmatrix} v^\epsilon \\ \sigma(u^\epsilon) \end{pmatrix}\right]=0.$$

Noticing that $W_0=\begin{pmatrix} u^\epsilon \\ v^\epsilon \end{pmatrix}$, we get the Rankine-Hugoniot relation (9) from

$$\lim_{x-ct\to+\infty}\left[-c\begin{pmatrix} u^\epsilon \\ v^\epsilon \end{pmatrix}+\begin{pmatrix} v^\epsilon \\ \sigma(u^\epsilon) \end{pmatrix}\right]=\lim_{x-ct\to-\infty}\left[-c\begin{pmatrix} u^\epsilon \\ v^\epsilon \end{pmatrix}+\begin{pmatrix} v^\epsilon \\ \sigma(u^\epsilon) \end{pmatrix}\right].$$

To make the models more specific, we confine DKM's with the following reasonable assumptions. In the text followed, we shall drop the super-scription ϵ for clarity.

1. "Linear" local Maxwellian: the local Maxwellians are linear combinations of $u, v, \sigma(u)$.
2. Symmetry: if there is a right-going traveling wave $f(x-ct)$ connecting (u^-, v^-) to (u^+, v^+), then there exists a left-going traveling wave $\hat{f}(x+ct)$ connecting $(u^-, -v^-)$ to $(u^+, -v^+)$, and *vice versa.*

Proposition 3 *If we take the local Maxwellian as*

$$M=\begin{pmatrix} m_1 & m_2 & m_3 \\ m_4 & m_5 & m_6 \\ m_1 & -m_2 & m_3 \\ -m_4 & m_5 & -m_6 \end{pmatrix}\begin{pmatrix} u \\ v \\ \sigma(u) \end{pmatrix}, \tag{10}$$

then the system (6) possesses the symmetry described above. The compatibility conditions then become

$$1_N m_1 = 1_N m_5 = 1_N \Lambda_1 m_2 = 1_N \Lambda_1 m_6 = 0.5, \qquad 1_N m_3 = 1_N \Lambda_1 m_4 = 0. \tag{11}$$

Proof The traveling wave $f(x-ct)$ is the solution to $(' = \epsilon \frac{d}{d(x-ct)})$

$$
\begin{aligned}
-cf_{1+}' + \Lambda f_{1+}' &= (m_1 u + m_2 v + m_3 \sigma(u)) - f_{1+}, \\
-cf_{1-}' - \Lambda f_{1-}' &= (m_1 u - m_2 v + m_3 \sigma(u)) - f_{1-}, \\
-cf_{2+}' + \Lambda f_{2+}' &= (m_4 u + m_5 v + m_6 \sigma(u)) - f_{2+}, \\
-cf_{2-}' - \Lambda f_{2-}' &= (-m_4 u + m_5 v - m_6 \sigma(u)) - f_{2-},
\end{aligned} \tag{12}
$$

and

$$
\begin{aligned}
\lim_{x-ct\to-\infty} 1_N(f_{1+}+f_{1-}) &= u^-, \\
\lim_{x-ct\to-\infty} 1_N(f_{2+}+f_{2-}) &= v^-, \\
\lim_{x-ct\to+\infty} 1_N(f_{1+}+f_{1-}) &= u^+, \\
\lim_{x-ct\to+\infty} 1_N(f_{2+}+f_{2-}) &= v^+.
\end{aligned}
$$

Then $(\hat{f}_{1+}(\xi), \hat{f}_{1-}(\xi), \hat{f}_{2+}(\xi), \hat{f}_{2-}(\xi)) = (f_{1-}(-\xi), f_{1+}(-\xi), -f_{2-}(-\xi), -f_{2+}(-\xi))$ solves $(` = \epsilon \frac{d}{d(x+ct)})$

$$
\begin{aligned}
c\hat{f}_{1+}` + \Lambda \hat{f}_{1+}` &= (m_1 \hat{u} + m_2 \hat{v} + m_3 \sigma(\hat{u})) - \hat{f}_{1+}, \\
c\hat{f}_{1-}` - \Lambda \hat{f}_{1-}` &= (m_1 \hat{u} - m_2 \hat{v} + m_3 \sigma(\hat{u})) - \hat{f}_{1-}, \\
c\hat{f}_{2+}` + \Lambda \hat{f}_{2+}` &= (m_4 \hat{u} + m_5 \hat{v} + m_6 \sigma(\hat{u})) - \hat{f}_{2+}, \\
c\hat{f}_{2-}` - \Lambda \hat{f}_{2-}` &= (-m_4 \hat{u} + m_5 \hat{v} - m_6 \sigma(\hat{u})) - \hat{f}_{2-},
\end{aligned} \tag{13}
$$

and

$$
\begin{aligned}
\lim_{x+ct\to-\infty} 1_N(\hat{f}_{1+}+\hat{f}_{1-}) &= u^+, \\
\lim_{x+ct\to-\infty} 1_N(\hat{f}_{2+}+\hat{f}_{2-}) &= -v^+, \\
\lim_{x+ct\to+\infty} 1_N(\hat{f}_{1+}+\hat{f}_{1-}) &= u^-, \\
\lim_{x+ct\to+\infty} 1_N(\hat{f}_{2+}+\hat{f}_{2-}) &= -v^-.
\end{aligned}
$$

Substituting the particular form of local Maxwellians (10) into (4) and (5), we obtain the compatibility conditions as (11).

As a summary, a DKM under our consideration takes the form

$$
\begin{aligned}
&\begin{pmatrix} f_{1+} \\ f_{2+} \\ f_{1-} \\ f_{2-} \end{pmatrix}_t - \begin{pmatrix} \Lambda & & & \\ & \Lambda & & \\ & & -\Lambda & \\ & & & -\Lambda \end{pmatrix} \begin{pmatrix} f_{1+} \\ f_{2+} \\ f_{1-} \\ f_{2-} \end{pmatrix}_x \\
= \; & \frac{1}{\epsilon} \left[\begin{pmatrix} m_1 u + m_2 v + m_3 \sigma(u) \\ m_4 u + m_5 v + m_6 \sigma(u) \\ m_1 u - m_2 v + m_3 \sigma(u) \\ -m_4 u + m_5 v - m_6 \sigma(u) \end{pmatrix} - \begin{pmatrix} f_{1+} \\ f_{2+} \\ f_{1-} \\ f_{2-} \end{pmatrix} \right],
\end{aligned} \tag{14}
$$

with $u = 1_N(f_{1+} + f_{1-}), v = 1_N(f_{2+} + f_{2-})$.

Remark 4 *As a DKM is devised to model the mixed-type system (2), namely not only to resolve the phase boundaries in a correct way, but also the hyperbolic waves. It is well-known that hyperbolic systems, in general, possesses such symmetries. For phase boundaries, on the other hand, these symmetries also come naturally from the basic physical considerations of the invariance under the change of reference frame.*

Remark 5 *For the sake of such symmetries, a "linear" local Maxwellian turns out to be the simplest model one may think of. Some particular nonlinear Maxwellians may also serve the purpose, yet neither easy to construct, nor easy to prove the symmetry. At this moment, as the general nonlinear Maxwellian does not provide us any advantages, we shall confine ourselves with the current model.*

Remark 6 *There are many different ways to generalize our model, for certain specific purposes. For instance, taking a non-constant relaxation parameter as in*

$$\begin{cases} u_t + w_x &= 0, \\ v_t + z_x &= 0, \\ w_t + \lambda^2 u_x &= \dfrac{u^{5/2}}{\epsilon}(v - w), \\ z_t + \lambda^2 v_x &= \dfrac{u^{5/2}}{\epsilon}(\sigma(u) - z), \end{cases} \tag{15}$$

one essentially obtains the same kinetic relation, at least at the traveling wave analysis level, as the viscosity-capillarity model

$$\begin{cases} u_t + v_x &= 0, \\ v_t + \sigma(u)_x &= (2u^{-5/2}u_x)_x - u^{-1}[u^{-1}(u^{-3}u_x)_x]_x. \end{cases} \tag{16}$$

According to the ideas proposed by T.P. Liu [22], to understand the dissipative role of the kinetic approximations we have to perform a Chapman-Enskog type expansion as in [2], which fixes some stability dissipation conditions. In the present case these conditions are contained in the following statement.

Proposition 7 *A DKM (14) is dissipative if*

$$\min(1_N \Lambda^2(m_1 - \dot{\sigma} m_3) - 0.5\dot{\sigma}, 1_N \Lambda^2 m_5 - 0.5\dot{\sigma}) \geq 0. \tag{17}$$

Proof As in [2], multiplying P to (14), we have

$$Pf_t + P\Lambda f_x = 0,$$

or,

$$\begin{pmatrix} u \\ v \end{pmatrix}_t + P\Lambda f_x = 0.$$

Substituting $f = M - \epsilon(f_t + \Lambda f_x)$ into it, retaining only terms up to the order of ϵ, we have, with the help of the compatibility conditions,

$$
\begin{array}{ll}
& P\begin{pmatrix} u \\ v \end{pmatrix}_t + \begin{pmatrix} v \\ \sigma(u) \end{pmatrix} \\
= & \epsilon P\Lambda(f_t + \Lambda f_x)_x \\
= & \epsilon(P\Lambda M_t + P\Lambda^2 M_x)_x + O(\epsilon^2) \\
= & \epsilon\left[\begin{pmatrix} v \\ \sigma(u) \end{pmatrix}_t + P\Lambda^2 M_x\right]_x + O(\epsilon^2) \\
= & \epsilon\left[-\begin{pmatrix} \dot\sigma(u)u_x \\ \dot\sigma(u)v_x \end{pmatrix} + 2\begin{pmatrix} 1_N\Lambda^2(m_1 - \dot\sigma m_3)u_x \\ 1_N\Lambda^2 m_5 v_x \end{pmatrix}\right]_x + O(\epsilon^2). \\
= & 2\epsilon\left[-\begin{pmatrix} 1_N\Lambda^2(m_1 - \dot\sigma m_3) - 0.5\dot\sigma(u) & 0 \\ 0 & 1_N\Lambda^2 m_5 - 0.5\dot\sigma(u) \end{pmatrix}\begin{pmatrix} u_x \\ v_x \end{pmatrix}\right]_x + O(\epsilon^2).
\end{array}
$$

The dissipativity condition then follows.

Remark 8 *This Chapmann-Enskog expansion yields normal subcharacteristic condition [22], and it is worth mentioning that no further restriction is caused due to the non-monotonicity.*

For some systems of dynamical phase transitions, e.g. in van der Waals fluids, it is known from physics that stationary phase boundary solution must follow the Maxwell construction of equal-area law. More precisely, besides the Rankine-Hugoniot relation for the two states across the discontinuity, namely

$$[v] = [\sigma(u)] = 0,$$

it also requires that the two regions separated by the curve $\sigma(u)$ and the level line of $\sigma(u^-)$ take equal area, i.e.

$$\int_{u^-}^{u^+} \sigma(u) - \sigma(u^-)du = 0. \tag{18}$$

This is not true in general for the DKM's. However, a sub-category of our DKM's admit solutions with this property. In particular, if we take $m_1 = m_5 \equiv \alpha, m_2 = m_6 \equiv \beta = \frac{1}{2\sum_{i=1}^{N} \lambda_i^2 \alpha_i}\Lambda_1\alpha, m_3 = m_4 = 0_N$, then a stationary wave of (14) solves ($' = \epsilon\frac{d}{dx}$)

$$
\left\{\begin{array}{lll}
\Lambda f'_{1+} & = & \alpha u + \beta v - f_{1+}, \\
\Lambda f'_{2+} & = & \alpha v + \beta\sigma(u) - f_{2+}, \\
-\Lambda f'_{1-} & = & \alpha u - \beta v - f_{1-}, \\
-\Lambda f'_{2-} & = & \alpha v - \beta\sigma(u) - f_{2-}.
\end{array}\right. \tag{19}
$$

It admits a special solution

$$\begin{pmatrix} f_{1+} \\ f_{2+} \\ f_{1-} \\ f_{2-} \end{pmatrix} = \begin{pmatrix} u\alpha + v^-\beta \\ v\alpha + \sigma(u^-)\beta \\ u\alpha - v^-\beta \\ v\alpha - \sigma(u^-)\beta \end{pmatrix},$$

where (u, v) satisfies

$$(2\sum_{i=1}^{N} \lambda_i^2 \alpha_i^2) \begin{pmatrix} u \\ v \end{pmatrix}' = \begin{pmatrix} v - v^- \\ \sigma(u) - \sigma(u^-) \end{pmatrix}. \tag{20}$$

It is then easily verified that along each trajectory, we have the following constant energy

$$H = \frac{(v - v^-)^2}{2} - \int_{u^-}^{u} (\sigma - \sigma(u^-))du. \tag{21}$$

As (u^+, v^+) is a stationary point of (20), we know that $v^+ = v^-$. Therefore, the equal area law is implied as

$$\int_{u^-}^{u^+} (\sigma - \sigma(u^-))du = 0.$$

Moreover, the characteristic width of the phase boundary is $\epsilon(2\sum_{i=1}^{N} \lambda_i^2 \alpha_i^2)$.

3 Numerical schemes

As the DKM here is of the same form as that for approximating hyperbolic systems, it takes all the same nice properties, such as easy to implement, relatively low computing load, easy to generalize to multi-dimensional problems in coding, etc. Please refer to [2] for details. Here we only describe the framework of the scheme.

We employ the first-order splitting method in solving the DKM (14). Given data $f(x, 0)$ at time $t = 0$, we first solve the homogeneous system

$$\hat{f}_t + \Lambda \hat{f}_x = 0, \quad \hat{f}(x, 0) = f(x, 0), \tag{22}$$

for a time step $\triangle t$. As this is a linear system, we may take either an upwind scheme, or a second order scheme. In fact, since it is diagonal, we may even get the solution explicitly. The numerical simulations shown in this paper are performed by a second order scheme with minmod limiter.

Then, we solve the ordinary differential equations with source terms

$$\tilde{f}_t = \frac{1}{\epsilon}(M(P\tilde{f}) - \tilde{f}), \quad \tilde{f}(x, 0) = \hat{f}(x, \triangle t), \tag{23}$$

for one time step, and take $f(x, \triangle t) = \tilde{f}(x, \triangle t)$. This step can also be made explicit. Due to the fact that the primary variables (u, v) remain unchanged in this step, and M depends only on (u, v), we get the exact solution as

$$\begin{aligned}\tilde{f}(x, \triangle t) = \quad & \exp(-\frac{\triangle t}{\epsilon})\tilde{f}(x, 0) \\ & +(1 - \exp(-\frac{\triangle t}{\epsilon}))M(P\tilde{f}(x, 0)).\end{aligned}$$

We may even directly take the limit $\epsilon = 0$ in this step, namely $\tilde{f}(t, x) = M(P\tilde{f}(0, x))$. The resulting relaxed scheme consists of a wave propagation updated with local Maxwellian. Numerical simulations reported here are performed with this relaxed scheme. In our numerical experiments, it is observed that non-zero ϵ gives the same result but with slightly stronger smoothing effect, the same as what happens with DKM's for hyperbolic systems [2].

In our simulations, we use the local Maxwellians as the initial or boundary data for $f_i's$. A non-Maxwellian data will cause a thin initial layer or boundary layer, which will be a topic for future study.

We have also applied a second-order splitting scheme proposed by Jin. A semi-discrete version for the relaxed scheme has also been implemented, which allows a natural high-order time splitting, e.g. with fourth-order Runge-Kutta method. The accuracy is of great importance for general initial boundary value problems, particularly, when there are interactions among waves. Nevertheless, as we shall describe in the following sections, the main issue in the current paper is the kinetic relation that changes along with different models. Unless mentioned, the numerical results exposed here are performed with a first-order time splitting.

4 Specific models

In this section, we shall describe some specific DKM's. To illustrate better the idea instead of stepping into the complexities caused by the interaction of hyperbolic waves, we shall take the tri-linear constitutive relation, i.e.

$$\sigma(u) = \begin{cases} 2u, & \text{for} \quad u < 1, \\ 3 - u, & \text{for} \quad 1 < u < 1.5, \\ u, & \text{for} \quad u > 1.5. \end{cases} \tag{24}$$

As mentioned before, a DKM has two-fold usages. First, it may serve as a systematic way to regularized the ill-posed dynamical phase transition system (2). Indeed, it may be used to solve general initial value problems or initial-boundary value problems. Secondly, a DKM dictates a particular kinetic relation and nucleation criterion.

As a first step of the study, we only present here the solution of Riemann problems, namely, the Cauchy problem with Riemann initial data

$$(u(x, 0), v(x, 0)) = \begin{cases} (u^-, v^-), & \text{for} \quad x < 0, \\ (u^+, v^+), & \text{for} \quad x > 0. \end{cases} \tag{25}$$

In particular, we shall investigate traveling waves of (14) to obtain elementary waves and kinetic relations, analyze Riemann problem with these elementary waves, and perform numerical simulations to verify our Riemann solver, as well as to get the nucleation criterion when necessary.

4.1 Suliciu's model

This model was proposed by Suliciu in studying viscoelasticity [26]. It takes the form of

$$\begin{cases} u_t + v_x &= 0, \\ v_t + w_x &= 0, \\ w_t + \lambda^2 v_x &= \dfrac{1}{\epsilon}(\sigma(u) - w). \end{cases} \tag{26}$$

Using the technique in proving Proposition 1, we may recast it into an equivalent system (14) with

$$\Lambda = \begin{bmatrix} \lambda & \\ & 0 \end{bmatrix}, \quad M = \begin{bmatrix} 0 & \frac{1}{2\lambda} & \frac{1}{2\lambda^2} \\ \frac{1}{2} & 0 & -\frac{1}{2\lambda^2} \\ 0 & \frac{1}{2} & \frac{1}{2\lambda} \\ 0 & 0 & 0 \\ 0 & -\frac{1}{2\lambda} & \frac{1}{2\lambda^2} \\ \frac{1}{2} & 0 & -\frac{1}{2\lambda^2} \\ 0 & \frac{1}{2} & -\frac{1}{2\lambda} \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} u \\ v \\ \sigma(u) \end{bmatrix}.$$

The stability condition can be found as

$$P\Lambda^2 M' - \begin{pmatrix} \dot{\sigma} & 0 \\ 0 & \dot{\sigma} \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & \lambda^2 - \dot{\sigma} \end{pmatrix} \geq 0.$$

Or, $\lambda^2 - \dot{\sigma} \geq 0$.

A smooth traveling wave of (26) at speed c satisfies

$$\begin{cases} -cu' + v' &= 0, \\ -cv' + w' &= 0, \\ -cw' + \lambda^2 v' &= \dfrac{1}{\epsilon}(\sigma(u) - w). \end{cases} \tag{27}$$

By integration, this amounts to

$$c(\lambda^2 - c^2)u' = \frac{1}{\epsilon}(\sigma(u) - c^2 u + C), \tag{28}$$

where C is a constant. By standard phase plane analysis, it is easy to know that a traveling wave solution exists if and only if the chord connecting the Riemann data keeps on one side of the constitutive curve $\sigma(u)$.

Meanwhile, we observe that (26) admits stationary phase boundary solutions as well, with $v_l = v_r, \sigma(u_l) = \sigma(u_r)$. We shall call it $0^{\#}$-wave and 0^{b}-wave, depending on the relative position of u_l and u_r.

As a summary, there are five classes of elementary waves.

- Backward and forward slip line ($\pm\sqrt{2}$- and ± 1- wave): The end-states are in the same stable phase, v may either increase or decrease. By Rankine-Hugoniot condition, the speed is $\pm\sqrt{2}$ or ± 1 depending on the phase it falls in.

- Subsonic phase boundary with one end-state as $u = 1$ ($T\pm$-wave): The other end-state is in the phase $u > 2$, v decreases when crossing the discontinuity from left to the right. The speed is given by the Rankine-Hugoniot condition with absolute value less than 1, positive if $u = 1$ is the right end-state, and negative if left.

- Subsonic phase boundary with one end-state as $u = 1.5$ ($B\pm$-wave): The other end-state is in the phase $u < 0.75$, v increases when crossing the discontinuity from left to the right. The speed is given by the Rankine-Hugoniot condition with absolute value less than 1, positive if $u = 1.5$ is the left end-state, and negative if right.

- Supersonic phase boundary or shock ($S\pm$-wave): The two end-states are in the different phases $u \leq 0$ and $u \geq 1.5$, respectively, and v may either decrease or increase across the discontinuity. The speed is given by the Rankine-Hugoniot condition with absolute value no less than 1.

- Stationary phase boundaries ($0^{\#}$-, 0^{b}-wave: The two end-states are in different stable phases. The propagating speed is 0, and v keeps unchanged across the boundary.

For better comprehension, please refer to Table 1 and Figure 1, where the arrow is from the left end-state to the right end-state.

Remark 9 *The traveling wave equation (28) is the same as that yielded from the viscosity formulation of (2). The kinetic relation is the same as chord criterion studied by Shearer [24].*

Table 1. Elementary waves in Suliciu's model

Wave	Speed c	u	[v]
$+\sqrt{2}$-	$\sqrt{2}$	$u_{l,r} \leq 1$	$\sqrt{2}[u]$
$-\sqrt{2}$-	$-\sqrt{2}$	$u_{l,r} \leq 1$	$-\sqrt{2}[u]$
$+1$-	1	$u_{l,r} \geq 1.5$	$[u]$
-1-	-1	$u_{l,r} \geq 1.5$	$-[u]$
$0^{\#}$-	0	$u_r = 2u_l \in [1.5, 2]$	0
$0^{\flat}$-	0	$u_l = 2u_r \in [1.5, 2]$	0
T_+-	$\sqrt{\frac{u_l - 2}{u_l - 1}}$	$u_r = 1, u_l > 2$	$-\sqrt{(u_l - 2)(u_l - 1)}$
T_--	$-\sqrt{\frac{u_r - 2}{u_r - 1}}$	$u_r > 2, u_l = 1$	$-\sqrt{(u_r - 2)(u_r - 1)}$
B_+-	$\sqrt{\frac{1.5 - 2u_l}{1.5 - u_l}}$	$u_r = 1.5, u_l \in (0, 0.75)$	$\sqrt{(1.5 - 2u_l)(1.5 - u_l)}$
B_--	$-\sqrt{\frac{1.5 - 2u_l}{1.5 - u_l}}$	$u_r \in (0, 0.75), u_l = 1.5$	$\sqrt{(1.5 - 2u_r)(1.5 - u_r)}$
S_+-	$\sqrt{\frac{u_r - 2u_l}{u_r - u_l}}$	$u_r > 1.5, u_l \leq 0$	$\sqrt{(u_r - 2u_l)(u_r - u_l)}$
S_--	$-\sqrt{\frac{u_l - 2u_r}{u_l - u_r}}$	$u_r \leq 0, u_l > 1.5$	$\sqrt{(u_l - 2u_r)(u_l - u_r)}$

Now we shall construct a Riemann solver with these elementary waves. Let $(u^*, v^*) = (u(0-, t), v(0-, t))$, by studying the elementary waves, we may find that starting from (u^-, v^-), the jump in v led by left-going waves is

$v^* - v^- =$

if $u^- \leq 1$,

$$\begin{cases} -\sqrt{2}(u^* - u^-), & \text{for} \quad u^* \leq 1, \quad \text{by } -\sqrt{2}\text{-wave}, \\ -\sqrt{2}(1 - u^-) - \sqrt{(u^* - 1)(u^* - 2)}, & \text{for} \quad u^* > 2, \quad \text{by } -\sqrt{2}, T_-\text{-wave}; \end{cases} \tag{29}$$

and if $u^- \geq 1.5$,

$$\begin{cases} -(u^* - u^-), & \text{for} \quad u^* \geq 1.5, & \text{by } -1\text{-wave}, \\ -(1.5 - u^-) + \sqrt{(1.5 - u^*)(1.5 - 2u^*)}, & \text{for} \quad u^* \in (0, 0.75), & \text{by } -1, B_-\text{-wave}, \\ \sqrt{(u^- - 2u^*)(u^- - u^*)}, & \text{for} \quad u^* \leq 0, & \text{by } S_-\text{-wave}. \end{cases} \tag{30}$$

It is observed that for any given u^-, $v^* - v^-$ is a monotonically decreasing function of u^*, with a gap in $(1, 2)$ or $(0.75, 1)$. See Figure 2 (a)(b).

Meanwhile, starting from (u^+, v^+), the jump in v led by right-going and stationary waves is

$v^* - v^+ =$

if $u^+ \leq 1$,

$$\begin{cases} \sqrt{2}(u^* - u^+), & \text{for} \quad u^* \le 1, & \text{by } +\sqrt{2}\text{-wave}, \\ \sqrt{2}(0.5u^* - u^+), & \text{for} \quad u^* \in [1.5, 2], & \text{by } 0^b, +\sqrt{2}\text{-wave}, \\ \sqrt{2}(1 - u^+) + \sqrt{(u^* - 1)(u^* - 2)}, & \text{for} \quad u^* > 2, & \text{by } T_+, +\sqrt{2}\text{-wave}; \end{cases} \tag{31}$$

and if $u^+ \ge 1.5$,

$$\begin{cases} u^* - u^+, & \text{for} \quad u^* \ge 1.5, & \text{by } +1\text{-wave}, \\ 2u^* - u^+, & \text{for} \quad u^* \in [0.75, 1], & \text{by } 0^\#, +1\text{-wave}, \\ 1.5 - u^+ - \sqrt{(1.5 - u^*)(1.5 - 2u^*)}, & \text{for} \quad u^* \in (0, 0.75), & \text{by } B_+, +1\text{-wave}, \\ -\sqrt{(u^+ - 2u^*)(u^+ - u^*)}, & \text{for} \quad u^* \le 0, & \text{by } S_+\text{-wave}. \end{cases} \tag{32}$$

It is observed that for any given u^+, $v^* - v^+$ is a piecewise monotonically increasing function of u^*, with a gap in $(1, 2)$ or $(0.75, 1)$. See Figure 2(c)(d).

We note here that the wave profiles listed here exhaust all the possible combinations of the elementary waves, except the combination of $0^\#$-wave with 0^b-wave. The latter indeed means a single line $x = 0$ in (x, t)-plane, across which the solution is continuous. It is equivalent to no discontinuity in weak sense, and the numerical simulations show that it is unstable, thus excluded here.

Now to solve a Riemann problem (2)-(25), one solves the algebraic equations (29) (or (30)) and (31) (or (32)) to find u^*. Or equivalently, one finds the intersection point of the two curves in Figure 2 (a) (or (b)) and (c) (or (d)). It can be easily shown that there exists one and only one such intersection point. It is interesting that the gap in the first two curves just fits in the non-monotone part of the latter two curves, and in turn unique intersection point follows if u^* lies in the interval.

The Riemann solver is described in Table 2 and Figure 3. Numerical experiments with (14)-(25) reveal that the Riemann solver listed here describes correctly the limiting behavior of the Suliciu's model. For example, we compute the solution with $(u^-, v^-) = (-0.2, 0), (u^+, v^+) = (3, 0)$. By the Riemann solver, the solution for (2) comprises a $-\sqrt{2}$-wave, a $0^\#$-wave, and a $+1$ wave, i.e. falls into the category C in Table 2. The numerical results with $\lambda = 2, \triangle x = 0.01, \triangle t = 0.005$ is plotted in Figure 4. The data shows that the intermediate state (u^*, v^*) agrees very well with that obtained with the Riemann solver.

Let us now take an example to illustrate the elementary waves, and the generic profiles. We consider the profile A, which constitutes consequently, from left to right in the (t, x) plane, $-\sqrt{2}$-wave, T_+-wave, T_--wave, and $+\sqrt{2}$-wave, as shown in Figure 5. Because both $+\sqrt{2}$-wave and $-\sqrt{2}$-wave take end-states in $u < 1$, this profile only solves Riemann problem with $u_-, u_+ \le 1$. Moreover, by Rankine-Hugoniot relation, we know that

$$v_1 - v^- = -\sqrt{2}(u_1 - u^-).$$

For T_--wave, the left end-states, i.e. $u_1 = 0$, and

$$v^* - v_1 = -\sqrt{(u^* - 1)(u^* - 2)}.$$

Therefore, for these two left-going waves, we have,

$$v^* - v^- = -\sqrt{2}(1 - u^-) - \sqrt{(u^* - 1)(u^* - 2)},$$

which is exactly the second line of (29).

Similarly, for T_+-wave, the right endstates, i.e. $u_2 = 0$, and

$$v_2 - v^* = -\sqrt{(u^* - 1)(u^* - 2)}.$$

Meanwhile, by $+\sqrt{2}$-wave, one has

$$v^+ - v_2 = \sqrt{2}(u^+ - 1).$$

Therefore, for these two right-going waves, we have,

$$v^+ - v^* = \sqrt{2}(u^+ - 1) - \sqrt{(u^* - 1)(u^* - 2)},$$

which is the third line of (31).

As a result, we have an equation for u^*,

$$v^+ - v^- = -\sqrt{2}(2 - u^+ - u^-) - 2\sqrt{(u^* - 1)(u^* - 2)}. \tag{33}$$

By some basic calculations, one knows that this quadratic equation admits two real solutions if and only if

$$v^+ - v^- \leq -\sqrt{2}(2 - u^+ - u^-).$$

Moreover, as the sum of these two roots equals to 3, we select the bigger one as u^* to satisfy the condition of $u^* \geq 1.5$ for T_+, T_--waves. So, in Figure 3, profile A solves uniquely, and in fact continuously, Riemann problems with $u^+, u^- < 1, v^+ - v^- \leq -\sqrt{2}(2 - u^+ - u^-)$.

Other generic wave profiles can be derived in the same fashion.

We may conclude this section by summarize the results.

Proposition 10 *Kinetic relation yielded by Suliciu's model (26) is the chord criterion. With this kinetic relation, the Riemann problem is uniquely solvable.*

Table 2. Generic wave profiles for Riemann problem ($u_* = u(0-,t)$)

	Profile	$[v]$	Parameter
A	$-\sqrt{2} \to T_- \to T_+ \to +\sqrt{2}$	$\sqrt{2}(u^+ + u^- - 2u_*) - 2\sqrt{(u_*-2)(u_*-1)}$	$u_* > 2$
B	$-\sqrt{2} \to T_- \to +1$	$-\sqrt{2}(1-u^-) - \sqrt{(u_*-2)(u_*-1)} + u^+ - u_*$	$u_* > 2$
C	$-\sqrt{2} \to 0^\# \to +1$	$-\sqrt{2}(u_* - u^-) + (u^+ - 2u_*)$	$u_* \in [0.75, 1]$
D	$-\sqrt{2} \to B_+ \to +1$	$-\sqrt{2}(u_* - u^-) + \sqrt{(1.5-2u_*)(1.5-u_*)} + u^+ - 1.5$	$u_* \in (0, 0.75)$
E	$-\sqrt{2} \to S_+$	$-\sqrt{2}(u_* - u^-) + \sqrt{(u^+ - 2u_*)(u^+ - u_*)}$	$u_* \leq 0$
F	$-\sqrt{2} \to +\sqrt{2}$	$\sqrt{2}(u^- + u^+ - 2u_*)$	$u_* \leq 1$
G	$S_- \to S_+$	$\sqrt{(u^- - 2u_*)(u^- - u_*)} + \sqrt{(u^+ - 2u_*)(u^+ - u_*)}$	$u_* \leq 0$
H	$S_- \to +\sqrt{2}$	$\sqrt{(u^- - 2u_*)(u^- - u_*)} + \sqrt{2}(u^+ - u_*)$	$u_* \leq 0$
I	$-1 \to B_- \to B+ \to +1$	$(u^- + u^+ - 2u_*) + 2\sqrt{(1.5-2u_*)(1.5-u_*)}$	$u_* \in (0, 0.75)$
J	$-1 \to B_- \to +\sqrt{2}$	$u^- - u_* + \sqrt{(1.5-2u_*)(1.5-u_*)} + \sqrt{2}(u^+ - u_*)$	$u_* \in (0, 0.75)$
K	$-1 \to 0^b \to +\sqrt{2}$	$u^- - u_* + \sqrt{2}(u^+ - u_*/2)$	$u_* \in [1.5, 2]$
L	$-1 \to T_+ \to +\sqrt{2}$	$u^- - u_* - \sqrt{(u_*-2)(u_*-1)} + \sqrt{2}(u^+ - u_*)$	$u_* > 2$
M	$-1 \to +1$	$u^- + u^+ - 2u_*$	$u_* \geq 1.5$

4.2 Jin-Xin's relaxation model

Jin and Xin proposed a relaxation model to approximate a hyperbolic system [18]. By an example, Jin shows that it also applies to mixed-type partial differential equations [19]. The model is

$$\left\{ \begin{aligned} u_t + w_x &= 0 \\ v_t + z_x &= 0 \\ w_t + \lambda^2 u_x &= \frac{1}{\epsilon}(v - w) \\ z_t + \lambda^2 v_x &= \frac{1}{\epsilon}(\sigma(u) - z) \end{aligned} \right. \tag{34}$$

In this case, we have

$$\Lambda = (\lambda), \qquad M = \frac{1}{2\lambda} \begin{bmatrix} \lambda & 1 & 0 \\ 0 & -\lambda & 1 \\ \lambda & -1 & 0 \\ 0 & \lambda & -1 \end{bmatrix} \begin{bmatrix} u \\ v \\ \sigma(u) \end{bmatrix}.$$

The stability condition is $\lambda^2 - \dot{\sigma} \geq 0$.

We start with the study of traveling waves to find the kinetic relation. A traveling wave with speed c satisfies a set of ordinary differential equations $(` = \epsilon\dfrac{d}{d(x-ct)})$

$$\left\{\begin{array}{ll} -cu` + w` & = 0, \\ -cv` + z` & = 0, \\ -cw` + \lambda^2 u` & = v - w, \\ -cz` + \lambda^2 v` & = \sigma(u) - z. \end{array}\right. \tag{35}$$

The first two equations can be integrated, and the integration constant in the first one can be set to 0, by virtue of the translation invariance of v. After a rescaling, i.e. taking $' = \dfrac{d}{d\xi}$ with $\xi = \dfrac{x-ct}{\epsilon(\lambda^2 - c^2)}$, we have

$$\left\{\begin{array}{ll} u' & = v - cu, \\ v' & = \sigma - cv - C_1. \end{array}\right. \tag{36}$$

We observe that (36) is the same as the traveling wave equations in Slemrod's viscosity-capillarity model [25]. Consequently the kinetic relation is the same. In particular, a stationary traveling wave must verify the Maxwell construction of equal area law.

There are two kinds of subsonic phase boundaries according to the traveling wave equations. One is exactly the $T\pm$- or $B\pm$-waves as in the Suliciu's model. In fact, by phase plane analysis it can be shown that corresponding traveling wave always exists if the chord connects $(u^-, \sigma(u^-))$ and $(u^+, \sigma(u^+))$ lies on one side of the constitutive curve on the $(u, \sigma(u))$-plane, that is, there are only two critical points in (u, v)-plane for the dynamical system (36), i.e. (u^+, v^+) and (u^-, v^-). However, through numerical experiments, it is found that these waves are not stable. For instance, taking Riemann data exactly corresponding to a T_+-wave, $(u^-, v^-) = (1, 0), (u^+, v^+) = (3, -1)$, the numerical solution turns out to comprise a $-\sqrt{2}$-wave, a left-going subsonic phase boundary (known as D_--wave in the coming discussion), and a $+1$-wave. See $(u(x,1), v(x,1))$ in Figure 6. These $T_\pm$-, $B_\pm$-waves are thus excluded from the elementary waves for constructing the Riemann solver.

For the other kind of subsonic phase boundaries, there are three critical points in (36), namely (u^+, v^+), (u^-, v^-), and (u_0, v_0) which lies in the unstable phase. For the tri-linear constitutive relation (24), we shall work out explicitly the relation between (u^-, v^-) and (u^+, v^+) for supporting an heteroclinic orbit, i.e. the kinetic relation. Without loss of generality, we consider here only the case $c < 0$.

Lemma 11 *For any heteroclinic orbit for system (36), $u(\xi)$ must be monotone.*

This is proved in [28], and is only sketched here. First, we rewrite (36) as

$$\left\{\begin{array}{ll} u' & = w, \\ w' & = \sigma - c^2 u - C_1 - 2cw. \end{array}\right. \tag{37}$$

Then we compare the vector field generated by (37) along any curve Γ^+ on the upper half phase plane and the vector field on the reflected curve (with respect to the u-axis) $-\Gamma^+$,

$$\frac{dw}{du}\Big|_{-\Gamma^+} = -4c - \frac{dw}{du}\Big|_{\Gamma^+} < -\frac{dw}{du}\Big|_{\Gamma^+}.$$

The eigenvalues at a fix point is $-c \pm \sqrt{\sigma}$, so (u_0, v_0) is a stable focus, and $(u_\pm, v_\pm)$ are saddles. The monotonicity of the profile in u then follows from the geometrical analysis with the well-known fact that an intersection of trajectories occurs only at critical points.

Using this monotonicity, we can express explicitly the solution of the piecewise linear system (37) as, if $u^- < 1$, and $u^+ > 1.5$ (noted as U_--wave),

$$u(\xi) = \begin{cases} u^- + Ae^{(\sqrt{2}-c)\xi}, & \text{for} \quad \xi \le \xi_1, \\ u_0 + Be^{-c\xi}\sin(\xi), & \text{for} \quad \xi \in [\xi_1, \xi_2], \\ u^+ + Ce^{-(1+c)\xi}, & \text{for} \quad \xi \ge \xi_2, \end{cases} \tag{38}$$

with C^1 continuity conditions

$$\begin{cases} u^- + Ae^{(\sqrt{2}-c)\xi_1} & = 1, \\ u_0 + Be^{-c\xi_1}\sin\xi_1 & = 1, \\ u_0 + Be^{-c\xi_2}\sin\xi_2 & = 1.5, \\ u^+ + Ce^{-(1+c)\xi_2} & = 1.5, \\ (-c+\sqrt{2})Ae^{(\sqrt{2}-c)\xi_1} & = Be^{-c\xi_1}(-c\sin\xi_1 + \cos\xi_1), \\ -(1+c)Ce^{-(1+c)\xi_2} & = Be^{-c\xi_2}(-c\sin\xi_1 + \cos\xi_2). \end{cases} \tag{39}$$

Together with the stationary point equations

$$\sigma(u^+) - c^2u^+ = \sigma(u_0) - u_0 = \sigma(u^-) - c^2u^-,$$

we can find

$$\begin{aligned} \xi_1 &= ctg^{-1}\left(\frac{\sqrt{2}c-1}{\sqrt{2}+c}\right) - \pi, \\ \xi_2 &= ctg^{-1}\left(\frac{1+c}{1-c}\right) + k\pi, \\ A &= (1-u^-)e^{-(\sqrt{2}-c)\xi_1} > 0, \\ B &= (1-u_0)e^{c\xi_1}/\sin\xi_1. \\ C &= (1.5-u^+)e^{(1+c)\xi_2} \end{aligned} \tag{40}$$

The monotonicity of u is verified in $\xi \in (-\infty, \xi_1) \cup (\xi_2, +\infty)$ as $A > 0, C < 0$. In the interval $[\xi_1, \xi_2]$, the monotonicity requires $B(-c\sin\xi + \cos\xi) \ge 0$. This is equivalent to $(\xi_1, \xi_2) \subseteq (ctg^{-1}c - \pi, ctg^{-1}c)$. Thus, we should choose $k = 0$, and

$$\xi_2 = ctg^{-1}\left(\frac{1+c}{1-c}\right).$$

By a straightforward calculation, we find that

$$
\begin{aligned}
u_0 = \phi_0(-c) \equiv & \quad \frac{\sqrt{1.5}(1-c) + 1.5(\sqrt{2}+c)e^{-c(\xi_1-\xi_2)}}{\sqrt{1.5}(1-c) + (\sqrt{2}+c)e^{-c(\xi_1-\xi_2)}}, \\
u^+ = \phi_2(-c) \equiv & \quad \frac{3-(1+c^2)\phi_0(-c)}{1-c^2}, \\
u^- = \phi_1(-c) \equiv & \quad \frac{3-(1+c^2)\phi_0(-c)}{2-c^2}.
\end{aligned}
\tag{41}
$$

So for each $c \in (-1,0)$, there is a unique u_0, u^+ and u^-. It is quite unexpected that the range of u_0 does not cover the whole interval $[1, 1.5]$. As $c \to -1$, we find $u_0 \to 1.0144$, $u^- \to 0.9712$, whereas $u^+ \to +\infty$.

Similarly, for the case $u^- \geq 1.5, u^+ \leq 1$ (noted as D_--wave), we can find the heteroclinic orbit as

$$
u(\xi) = \begin{cases} u^- + (u_2 - u^-)e^{(1-c)(\xi-\xi_1)}, & \text{for} \quad \xi \leq \xi_1, \\ u_0 + (u_2 - u_0)e^{-c(\xi-\xi_1)} \sin\xi / \sin\xi_1, & \text{for} \quad \xi \in [\xi_1, \xi_2], \\ u^+ + (u_1 - u^+)e^{-(\sqrt{2}+c)(\xi-\xi_2)}, & \text{for} \quad \xi \geq \xi_2, \end{cases}
\tag{42}
$$

with

$$
\begin{aligned}
\xi_1 \quad &= ctg^{-1}\left(\frac{c-1}{c+1}\right) - \pi \\
\xi_2 \quad &= ctg^{-1}\left(\frac{1+\sqrt{2}c}{\sqrt{2}-c}\right)
\end{aligned}
\tag{43}
$$

and

$$
\begin{aligned}
u_0 = \psi_0(-c) \equiv & \quad \frac{1.5(\sqrt{2}-c) + \sqrt{1.5}(1+c)e^{-c(\xi_1-\xi_2)}}{(\sqrt{2}-c) + \sqrt{1.5}(1+c)e^{-c(\xi_1-\xi_2)}}, \\
u^- = \psi_1(-c) \equiv & \quad \frac{3-(1+c^2)\psi_0(|c|)}{2-c^2}, \\
u^+ = \psi_2(-c) \equiv & \quad \frac{3-(1+c^2)\psi_0(|c|)}{1-c^2}.
\end{aligned}
\tag{44}
$$

For this one, though the range of u_0 covers $[1, 1.5]$, and that of u^+ covers $[0, 1]$, u^- tends to about 1.5445 as $c \to -1$.

For the case $c > 0$, i.e. the U_+- and D_+-waves, the kinetic relation is obtained by a change of variables as $(u, v, \xi; c) \longrightarrow (u, -v, -\xi; -c)$.

We demonstrate the kinetic relation in Figure 7. Instead of $u^\pm$, we denote the end-states of the subsonic wave as $u_{r,l}$, to avoid confusion with the Riemann data in the Riemann solver described soon. It is noticed that $u_l(c)$ for D_--wave and T_+-wave is smooth at $c = 0$, and this can be rigorously proved.

We may then summarize the elementary waves in the following table. Please see Figure 8 as well.

Table 3. Elementary waves in Jin-Xin's model

Wave	Speed c	u	[v]
$+\sqrt{2}$-	$\sqrt{2}$	$u_{l,r} \leq 1$	$\sqrt{2}[u]$
$-\sqrt{2}$-	$-\sqrt{2}$	$u_{l,r} \leq 1$	$-\sqrt{2}[u]$
$+1$-	1	$u_{l,r} \geq 1.5$	$[u]$
-1-	-1	$u_{l,r} \geq 1.5$	$-[u]$
U_+-	$c \geq 0$	$u_r = \phi_1(c), u_l = \phi_2(c)$	$c[u] \leq 0$
U_--	$c \leq 0$	$u_r = \phi_2(-c), u_l = \phi_1(-c)$	$c[u] \leq 0$
D_+-	$c \geq 0$	$u_r = \psi_2(c), u_l = \psi_1(c)$	$c[u] \geq 0$
D_--	$c \leq 0$	$u_r = \psi_1(-c), u_l = \psi_2(-c)$	$c[u] \geq 0$
S_+-	$\sqrt{\dfrac{u_r - 2u_l}{u_r - u_l}}$	$u_r > 1.5, u_l \leq 0$	$\sqrt{(u_r - 2u_l)(u_r - u_l)}$
S_--	$-\sqrt{\dfrac{u_l - 2u_r}{u_l - u_r}}$	$u_r \leq 0, u_l > 1.5$	$\sqrt{(u_l - 2u_r)(u_l - u_r)}$

Table 4. Generic wave profiles for Riemann problem

	Profile	$[v]$	Parameter
A	$-\sqrt{2} \to U_- \to U_+ \to +\sqrt{2}$	$\sqrt{2}(u_+ + u_- - 2\phi_1(c)) + 2c(\phi_1(c) - \phi_2(c))$	$c \in [0,1]$
B	$-\sqrt{2} \to U_- \to +1$	$-\sqrt{2}(\phi_1(c) - u_-) + c(\phi_1(c) - \phi_2(c)) + u_+ - \phi_2(c)$	$c \in [0,1]$
C	$-\sqrt{2} \to D_+ \to +1$	$-\sqrt{2}(\psi_1(c) - u_-) + c(\psi_2(c) - \psi_1(c)) + u_+ - \psi_2(c)$	$c \in [0,1]$
D	$-\sqrt{2} \to S+$	$-\sqrt{2}(u_* - u_-) + \sqrt{(u_+ - 2u_*)(u_+ - u_*)}$	$u_* \leq 0$
E	$-\sqrt{2} \to +\sqrt{2}$	$\sqrt{2}(u_- + u_+ - 2u_*)$	$u_* \leq 1$
F	$-1 \to U_+ \to +\sqrt{2}$	$u_- - \phi_2(c) + c(\phi_1(c) - \phi_2(c)) + \sqrt{2}(u_+ - \phi_1(c))$	$c \in [0,1]$
G	$-1 \to D_- \to D_+ \to +1$	$(u_- + u_+ - 2\psi_2(c)) + 2c(\psi_2(c) - \psi_1(c))$	$c \in [0,1]$
H	$-1 \to D_- \to +\sqrt{2}$	$u_- - \psi_2(c) + c(\psi_2(c) - \psi_1(c)) + \sqrt{2}(u_+ - \psi_1(c))$	$c \in [0,1]$
I	$-1 \to +1$	$u_- + u_+ - 2u_*$	$u_* \geq 1.5$
J	$S- \to S+$	$\sqrt{(u_- - 2u_*)(u_- - u_*)} + \sqrt{(u_+ - 2u_*)(u_+ - u_*)}$	$u_* \leq 0$
K	$S- \to +\sqrt{2}$	$\sqrt{(u_- - 2u_*)(u_- - u_*)} + \sqrt{2}(u_+ - u_*)$	$u_* \leq 0$

The same as what has been done for Suliciu's models, we may solve a Riemann problem by finding the appropriate $u^* = u(0-, t)$. Note that when a U_-- or D_--wave appears in the wave profile, there is a one-to-one correspondence between u^* and the speed c. Therefore, it causes no confusion to use c as the parameter instead of u^* in this case. We exhaust all possibilities of wave profiles, and list them in Table 4.

Like in Suliciu's model, again we have the monotonicity with respect to the parameters. However, there are overlapped regions for the profiles A with E, and G with I. See Figure 9, where the overlapped regions are shaded. This means that multiple solutions appear if (u^+, v^+) falls into the shaded region. For instance, for the overlapped region of A and E, a wave profile comprising a $-\sqrt{2}$-wave and a $+\sqrt{2}$-wave solves the Riemann problem, and so does the one comprising consequently a $-\sqrt{2}$-wave, a U_--wave, a U_+-wave and a $+\sqrt{2}$-wave. For the first one, the solution keeps in the same phase $u \leq 1$, whereas the second one jumps into the other phase $u \geq 1.5$. A nucleation criterion is thus needed here. Though an rigorous stability analysis would be quite complicated, numerical experiments suggests that the system select the wave profile E rather than A. For instance, with Riemann data $(u^-, v^-) = (0.3, 0), (u^+, v^+) = (0.8, -1)$ which falls into the overlapped region of A and E, The solution by Jin-Xin's model is depicted in Figure 10, containing only the $\pm\sqrt{2}$-waves.

To summarize this subsection, we have the following Proposition.

Proposition 12 *Kinetic relation yielded by Jin-Xin's relaxation model (34) is the Slemrod's viscosity-capillarity criterion. In case of tri-linear constitutive relation (24), it can be expressed parametrically by $\phi_1(c)$ and $\phi_2(c)$, or $\psi_1(c)$ and $\psi_2(c)$. the nucleation criterion is: new phase is generated only when there exists no solution that keeps in the same phase. With this kinetic relation and nucleation criterion, the Riemann problem is uniquely solvable.*

4.3 A six-speed model

With our general formulation of DKM's, we may construct system of larger size. For instance, a six-speed system takes the form of

$$\left\{\begin{array}{ll} u_t + \lambda p_x & = 0, \\ v_t + \lambda q_x & = 0, \\ p_t + \lambda r_x & = \frac{1}{\epsilon}(\frac{v}{\lambda} - p), \\ q_t + \lambda s_x & = \frac{1}{\epsilon}(\frac{\sigma(u)}{\lambda} - q), \\ r_t + \lambda p_x & = \frac{1}{\epsilon}(2m_1 u + 2m_3\sigma(u) - r), \\ s_t + \lambda q_x & = \frac{1}{\epsilon}(2m_2 v - s). \end{array}\right. \tag{45}$$

Here $m_1 \in [0, 0.5], m_2 \in [0, 0.5], m3 \geq 0$ are constants. In this case,

$$\Lambda = \begin{bmatrix} \lambda & 0 \\ 0 & 0 \end{bmatrix}, \qquad M = \begin{bmatrix} m_1 & \frac{1}{2\lambda} & m_3 \\ 0 & m_2 & \frac{1}{2\lambda} \\ 1-2m_1 & 0 & -2m_3 \\ 0 & 1-2m_2 & 0 \\ m_1 & -\frac{1}{2\lambda} & 0 \\ 0 & m_2 & -\frac{1}{2\lambda} \end{bmatrix} \begin{bmatrix} u \\ v \\ \sigma(u) \end{bmatrix}.$$

The stability condition is $\min((\ 2\lambda^2(m_1 + m_3\dot{\sigma}) - \dot{\sigma}, 2\lambda^2 m_2 - \dot{\sigma} \ ) \geq 0$.

Again, we take traveling wave analysis for seeking the kinetic relations. The equations read $(' = \epsilon \dfrac{d}{d(x-ct)})$

$$\begin{cases} -cu' + \lambda p' & = 0, \\ -cv' + \lambda q' & = 0, \\ -cp' + \lambda r' & = (\dfrac{v}{\lambda} - p), \\ -cq' + \lambda s' & = (\dfrac{\sigma(u)}{\lambda} - q), \\ -cr' + \lambda p' & = (2m_1 u + 2m_3\sigma(u) - r), \\ -cs' + \lambda q' & = (2m_2 v - s). \end{cases} \tag{46}$$

We may integrate the first two equations, and obtain

$$\begin{cases} \lambda^2 r' - c^2 u' & = v - cu - C_1, \\ \lambda^2 s' - c^2 v' & = \sigma(u) - cv - C_2, \\ cu' - cr' & = 2m_1 u + 2m_3\sigma(u) - r, \\ cv' - cs' & = 2m_2 v - s. \end{cases} \tag{47}$$

It seems impossible to describe the heteroclinic orbit for this fourth-order dynamical system in general. Nevertheless, there are a few facts clear.

First, for $m_3 = 0$, a stationary phase boundary solution must verify the equal-area law.

Secondly, the existence of a heteroclinic orbit depends also on λ. For trilinear structure relation, we may try the approach as for Jin-Xin's model for a kinetic relation. However, the heavy calculation makes it virtually impossible by hand. We only make a numerical comparison here. Taking the same initial data $(u^-, v^-) = (0.8, 0), (u^+, v^+)(1.7, 0.8)$, the different solutions at time $t = 1$ for $\lambda = 1.6$ and $\lambda = 10$ are displayed in Figure 11.

Thirdly, in general, the existence of a heteroclinic orbit depends also on m_1, m_2, m_3. For example, consider $m_2 = 1/3, m_3 = 0$, and vary m_1. Taking initial data $(u^-, v^-) = (0.8, 0), (u^+, v^+) = (1.6, 0.4)$, the solutions at time $t = 1$ for $m_1 = 0.1, 0.3, 0.5$ are displayed in Figure 12.

Fourthly, for $m_1 = m_2 \neq 0$, when λ becomes large, we may find the kinetic relation approaches to that of Jin-Xin's model. In fact, from (47), the spatial scale is of order λ^2. Let

$$
\begin{cases}
u &= u_0 + \dfrac{1}{\lambda^2} u_1 + \cdots, \\
v &= v_0 + \dfrac{1}{\lambda^2} v_1 + \cdots, \\
r &= r_0 + \dfrac{1}{\lambda^2} r_1 + \cdots, \\
s &= s_0 + \dfrac{1}{\lambda^2} s_1 + \cdots.
\end{cases}
\tag{48}
$$

Then, up to the leading order, we have

$$
\begin{cases}
r_0' &= v_0 - cu_0 - C_1, \\
s_0' &= \sigma(u_0) - cv_0 - C_2, \\
0 &= 2m_1 u_0 - r_0. \\
0 &= 2M - 2v_0 - s_0.
\end{cases}
\tag{49}
$$

As $m_1 = m_2$, this is equivalent to Jin-Xin's model. The characteristic phase boundary width is $\epsilon\lambda^2$.

Finally, if we take $m_1 = 0, m_2 > 0, m_3 > 0$, then there are stationary phase boundary solutions as in Suliciu's model. Positive m_2, m_3 may ensure the stability conditions. However, both stationary phase boundary and moving phase boundary have been observed. For instance, the solutions $u(x, 1)$ with initial data $(u^-, v^-) = (0.8, 0), (u^+, v^+) = (1.7, 0)$, and $(u^-, v^-) = (0.8, 0), (u^+, v^+) = (1.7, 0.4)$, are depicted in Figure 13(a) and Figure 13(b), respectively.

5 Discussions

In this paper, we have constructed a general DKM model for modeling dynamical phase transitions. As stable regularization-s, DKM's are expected to provide a variety of reasonable kinetic relations and nucleation criteria, which may then be applied to approximate those appearing in real systems or experiments. DKM therefore may serve as a uniform and flexible approach of providing Riemann solvers to dynamical phase transition problems. Moreover, the Particular models have also been studied both theoretically and numerically. It is found that the kinetic relation yielded by Suliciu's model is indeed the chord criterion, and that by Jin-Xin's relaxation model is the viscosity-capillarity criterion. For a tri-linear constitutive relation, it is shown that the Riemann problem is uniquely solvable, with certain nucleation criterion prescribed for Jin-Xin's model.

The objective of studying DKM's is two-fold. First, this is a new and systematic-Al way to regularized the ill-posed system (2). As demonstrated by our preliminary theoretical and numerical investigations, this approach provides stable pictures of the phase transition phenomena, and different DKM's give different profiles in general. The numerics are simple and easy to implement, and without Riemann solver. Meanwhile, the study of DKM's, particularly the traveling wave profiles, naturally yields admissibility conditions of discontinuities, in particular, kinetic relations for subsonic phase boundaries, when we take $\epsilon \longrightarrow 0+$. Nucleation criteria also follows from a theoretic study, and/

or numerical study of the stability of wave profiles. A Riemann solver thus is obtained for such a DKM.

It would be very interesting to see how the wave patterns differs along with the DKM's, for general initial boundary data. Moreover, in high dimensions [3], the behavior of the model is still to be explored, mainly numerically.

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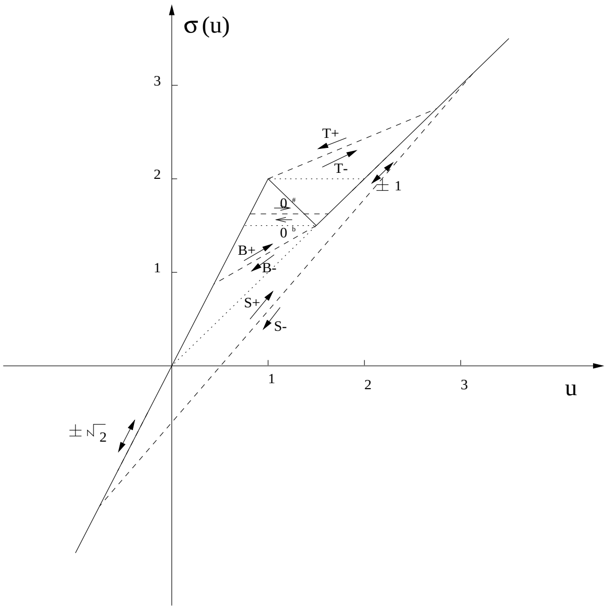

Figure 1: Elementary waves in Suliciu's model.

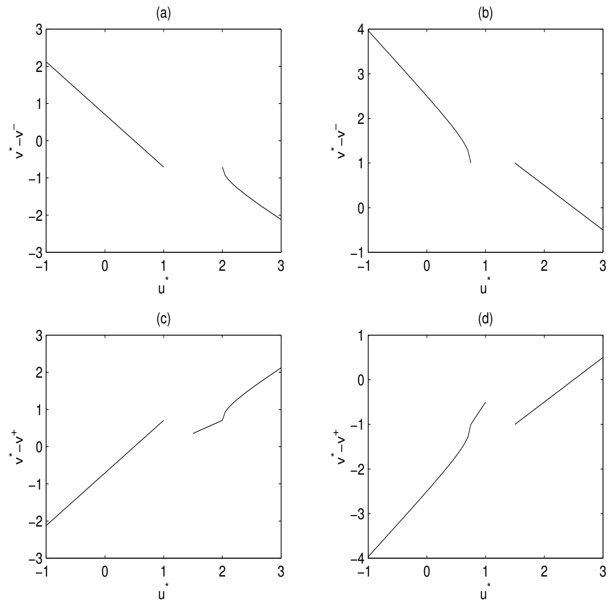

Figure 2: The jump in v through (a) left-going wave(s) with $u^- \leq 1$; (b) left-going wave(s) with $u^- \geq 1.5$; (c) right-going and stationary wave(s) with $u^+ \leq 1$; (d) right-going and stationary wave(s) with $u^+ \geq 1.5$.

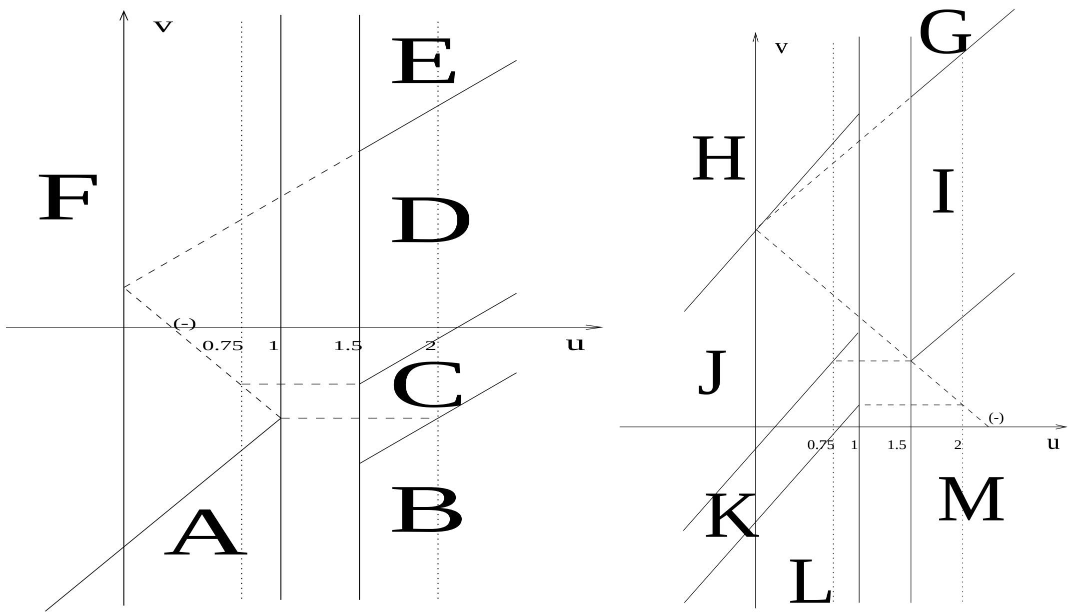

Figure 3: Riemann problem for Suliciu's model: $u^- \leq 1$, and $u^- \geq 1.5$.

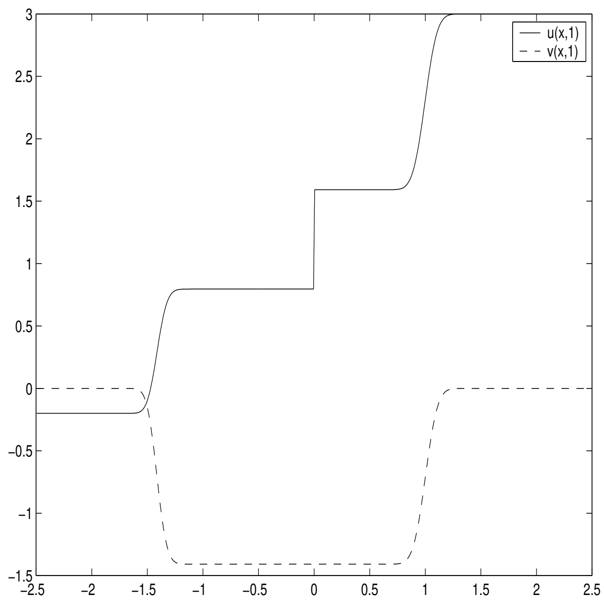

Figure 4: Solution to Riemann initial data in Suliciu's model.

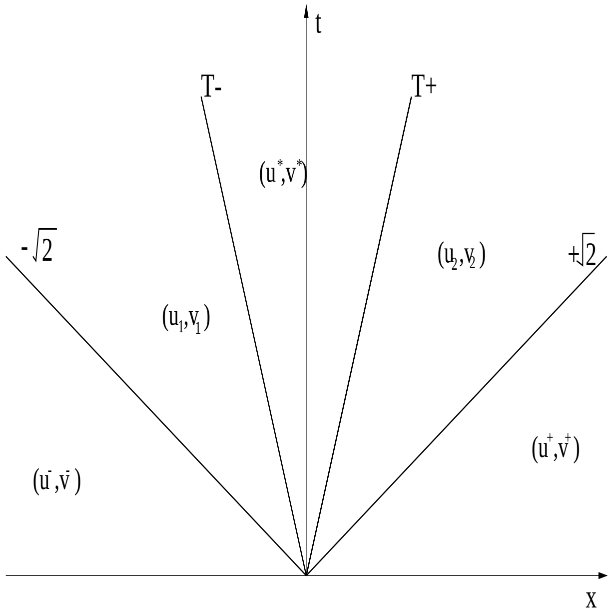

Figure 5: Wave profile A in Suliciu's model.

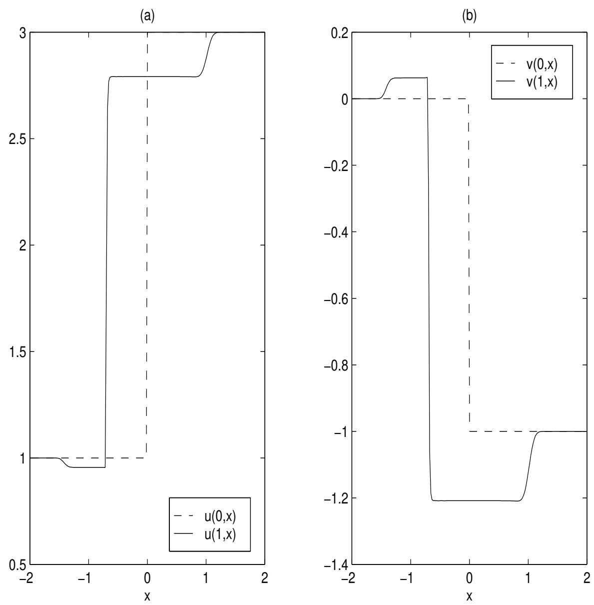

Figure 6: Instability of T_+-wave.

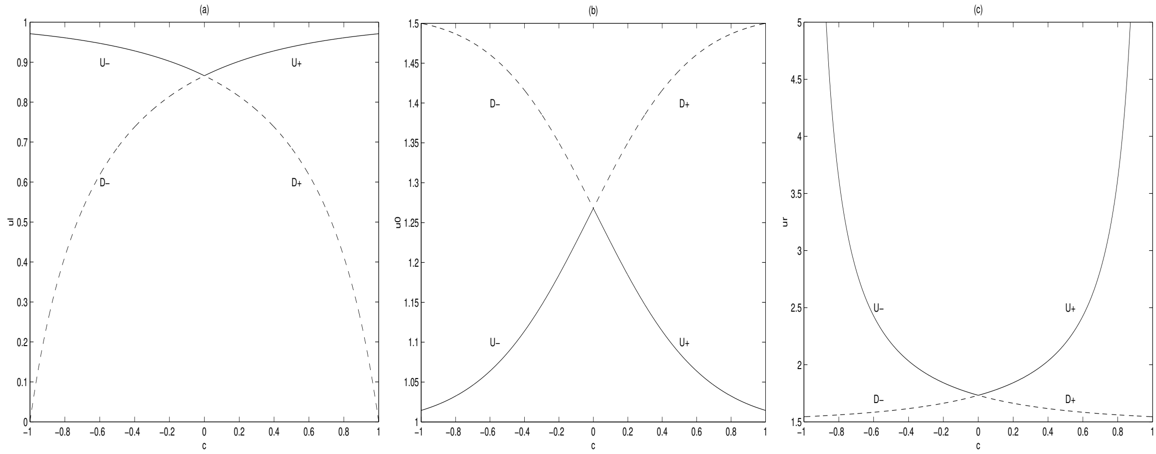

Figure 7: Kinetic relation for Jin-Xin's model.

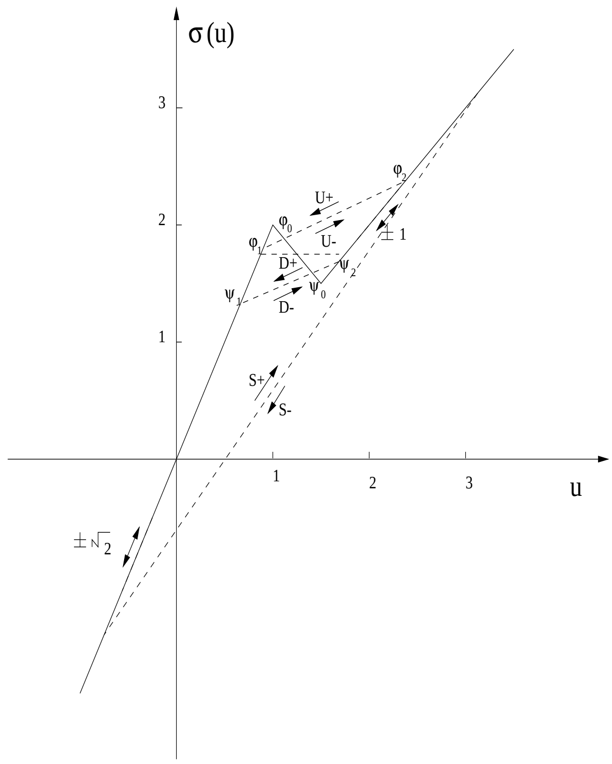

Figure 8: Elementary waves in Jin-Xin's model.

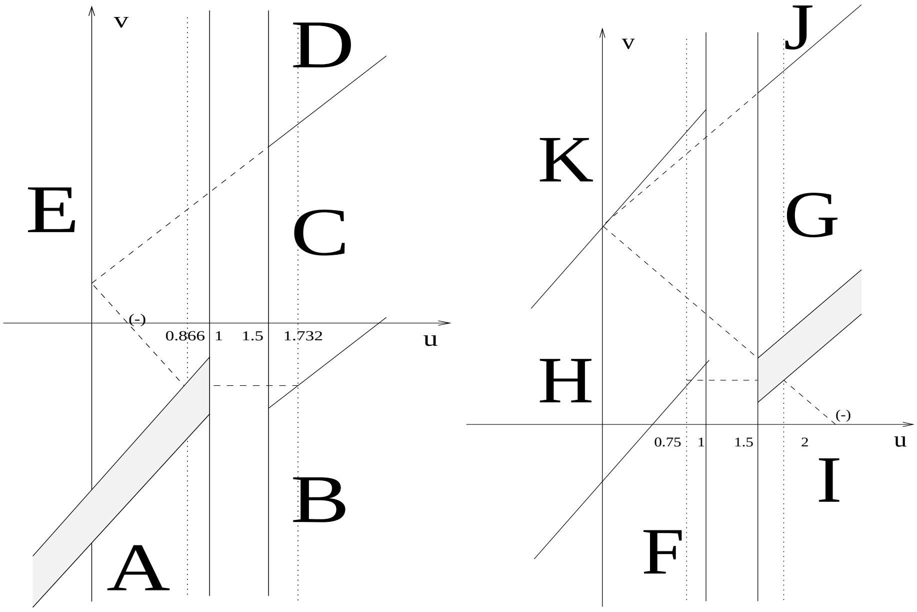

Figure 9: Riemann problem for Jin-Xin's model: $u_- < 1$, and $u_- > 1.5$.

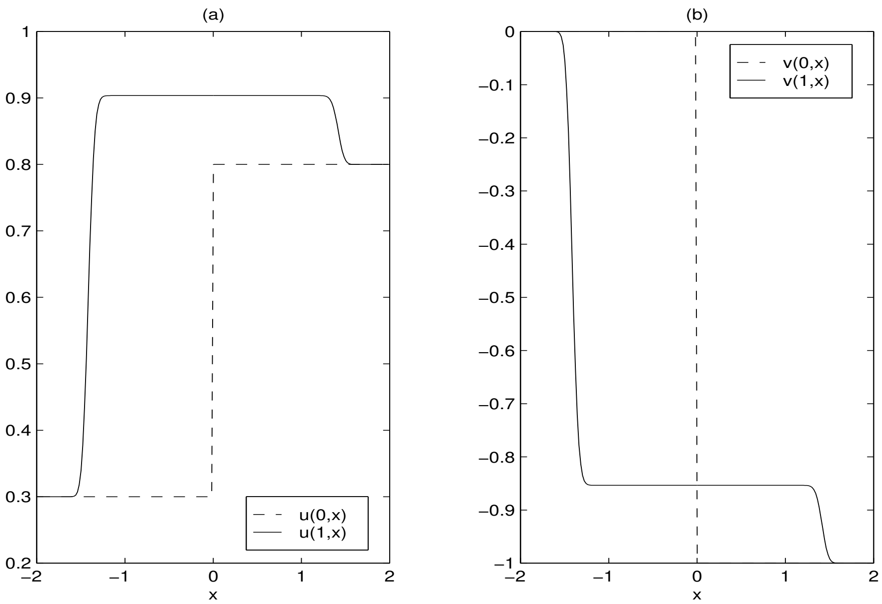

Figure 10: Nucleation criterion for Jin-Xin's model.

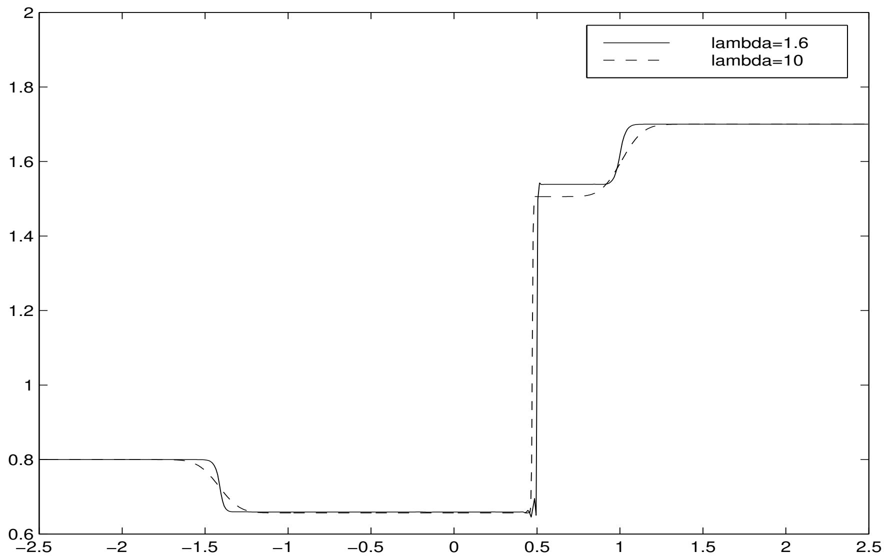

Figure 11: Comparison between the six-speed models with different λ.

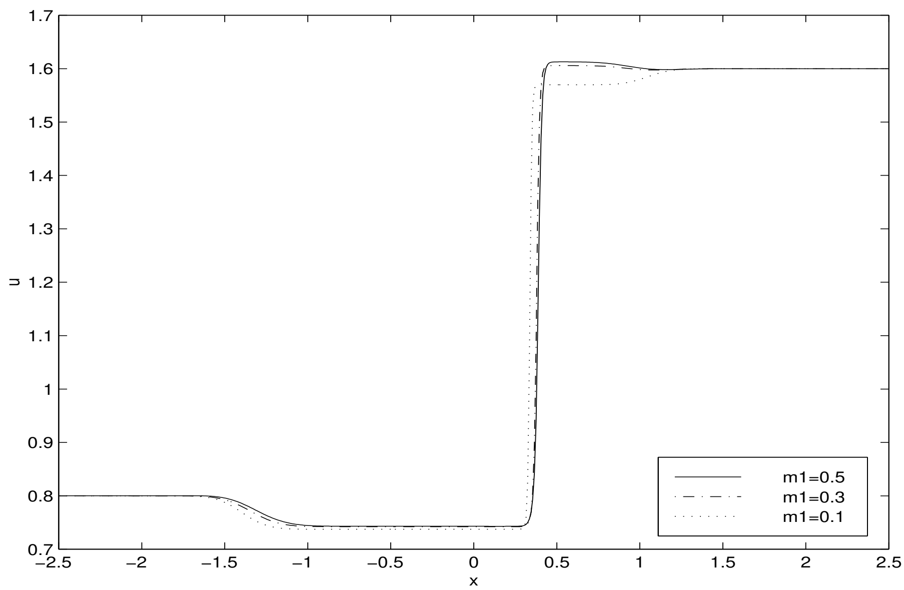

Figure 12: Comparison between the six-speed models with different m_1.

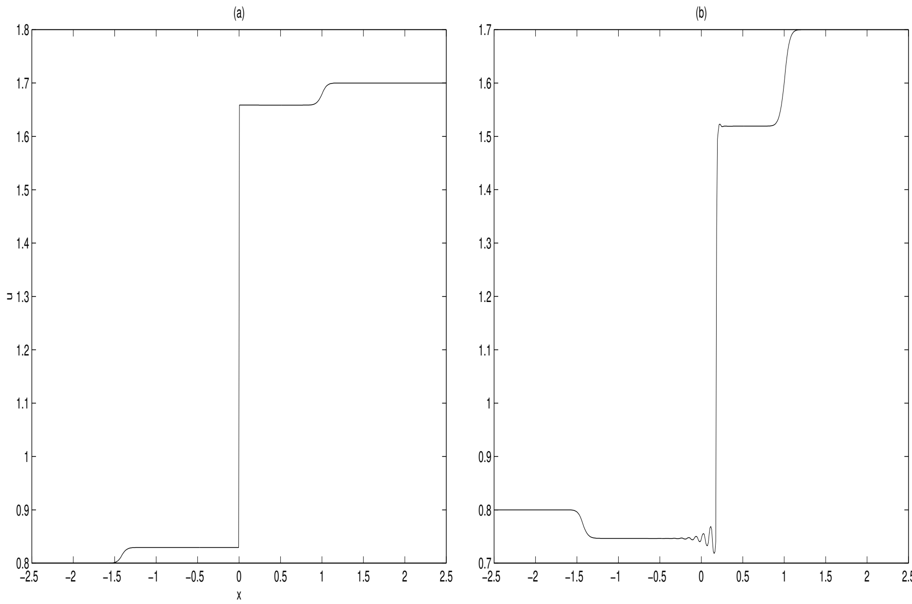

Figure 13: Stationary and moving phase boundaries.