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Kinetic discretization of one-dimensional nonlocal flow models ⋆

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Abstract: We show that one-dimensional nonlocal flow models in PDE form with Lighthill-Whitham-Richards flux supplemented with appropriate in- and out-flow terms can be spatially discretized with a finite volume scheme to obtain formally kinetic models with physically meaningful reaction graph structure. This allows the utilization of the theory of chemical reaction networks, as demonstrated here via the stability analysis of a flow model with circular topology. We further propose an explicit time discretization and a Courant-Friedrichs-Lewy condition ensuring many advantageous properties of the scheme. Additional characteristics, including monotonicity and the total variation diminishing property are also discussed.

Keywords: control of hyperbolic systems and conservation laws, kinetic modeling, modeling for control, stability of distributed parameter systems, stability of nonlinear systems

1. INTRODUCTION

Local conservation and balance laws have been widely used in aerodynamics and Eulerian gas dynamics (LeVeque, 1992), traffic flows (Kessels, 2019), ribosome flows (Reuveni et al., 2011) and many other fields (Smoller, 1994) in the past decades. In recent years nonlocality has been introduced in several applications, e.g., for modelling supply chains (Keimer et al., 2018) and traffic flows (Chiarello and Goatin, 2018). Spatial nonlocality is often defined as a continuum average or convolution with an appropriate weight function, which, in many applications, can be interpreted as the velocity distribution of the flow.

It is well-known that the conservation laws described by hyperbolic partial differential equations (PDEs) may develop irregularities even with smooth initial functions (LeVeque, 1992). This implies that solution concepts of these equations have to allow for discontinuous functions. Another consequence of the loss of regularity is that one is confined to a restricted class of applicable numerical schemes, such as, for example, finite volume methods (Eymard et al., 2000). Two of the most commonly used schemes in the field of traffic flows are the modified Lax-Friedrichs scheme and the Godunov scheme (Godunov, 1959). While these schemes possess numerous desired properties, the obtained form of ordinary differential equations (ODEs) computed via spatial discretization (also called semi-discretization) is often not optimal for dynamical analysis. However, a recently developed monotone flux scheme was shown to result in formally kinetic and compartmental ODEs called Traffic Reaction Models in case of local traffic flows, which allows us to use the well-developed theory of chemical reaction networks (Lipták et al., 2021). The aim of this paper is to generalize and further develop these results for nonlocal flow models.

In Section 2 we give a brief overview of nonlocal flow models and kinetic systems. Section 3 contains the spatial discretization of the introduced flow model, including the derivation of the kinetic property with the exact topology and interpretation of compartments and reactions. The discretized model is the subject of subsequent analysis in Section 4, where we demonstrate many advantageous properties of the spatial and the time-space discretization. In the latter case an appropriate CFL condition is formalized to ensure these features.

2. NOTATIONS AND BACKGROUND

2.1 Nonlocal flows

In this subsection we introduce the unidirectional nonlocal flow model based on the nonlocal pair-interaction model of (Du et al., 2017), supplemented with terms representing in- and out-flows.

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Spatial nonlocality allows us to model interaction pairs between points within a distance no larger than a given finite horizon while local models consist of interactions within infinitesimal range. Nonlocal interactions are weighted with an interaction kernel, which is a function of the distance between the two interacting points. Thus, considering nonlocal flows not only often results in more accurate models than their local counterpart (Kavallaris and Suzuki, 2018), but the horizon and the weighting kernel also enable the incorporation of different flow characteristics.

Let $\overline{\mathbb{R}}_+$ denote the set of nonnegative real numbers. Nonlocality is formally introduced as a continuum average of the finite difference approximation weighted with a bounded and nonnegative nonlocal interaction kernel $\omega \in \mathcal{L}^1(\mathbb{R})$ supported on $(0,\delta)$ with $\delta > 0$ and $\|\omega\|_{\mathcal{L}^1(\mathbb{R})} = 1$, as follows:

$$\begin{aligned} &\frac{\partial \rho}{\partial t} + \int_0^\delta \frac{F(\rho, \tau_h \rho) - F(\tau_{-h}\rho, \rho)}{h} \omega(h)\,\mathrm{d}h = r - s; \\ &\rho(x,0) = \rho_0(x), \end{aligned} \tag{1}$$

where $\rho : \mathbb{R} \times (0,T) \mapsto \overline{\mathbb{R}}_+$ is the conserved quantity at a given point and at a given time, $F : \mathbb{R} \times \mathbb{R} \mapsto \mathbb{R}$ is the flux function, $\tau_{\pm h}\rho(x,t) = \rho(x \pm h, t)$ denotes a spatial shift and $r, s : \mathbb{R} \times (0,t) \times \overline{\mathbb{R}}_+ \mapsto \overline{\mathbb{R}}_+$ are the source and sink terms, respectively. For the physical background and formal derivation of (1), we refer to (Du et al., 2013). Throughout the paper, we call (1) closed, if the functions r and s are identically zero; that is, the system does not have in- and out-flows. In any other case, the system is called open.

2.2 Chemical reaction networks

In this subsection we give a brief introduction of kinetic systems or chemical reaction networks (CRNs) based on (Horn and Jackson, 1972; Feinberg, 2019). In classical kinetic models we assume that the consumption of the reactants and the product formation are immediate. We can define chemical reaction networks with three sets as follows:

- A set of species: $\mathcal{S} = \{X_i | i = 1, 2, \ldots, n\}$.
- A set of complexes: $\mathcal{C} = \{C_j | j = 1, 2, \ldots, m\}$, where complexes are formally linear combinations of the species with nonnegative integer stoichiometric coefficients $\alpha_{i,j}$; that is,

$$\begin{aligned} C_j &= \sum_{i=1}^{n} \alpha_{i,j} X_i \qquad && j = 1, 2, \ldots, m \\ \alpha_{i,j} &\in \mathbb{N}_0 && i = 1, 2, \ldots, n,\ j = 1, 2, \ldots, m. \end{aligned}$$

  The stoichiometric coefficient vector of the complex C_j is $[\alpha_{1,j}\ \alpha_{2,j}\ \ldots\ \alpha_{n,j}]^{\mathrm{T}} \in \mathbb{R}^n$ such that $C_i \neq C_j$ for $i \neq j$. For the representation of the environment, we can use the so-called zero complex having zero stoichiometric coefficients.
- A set of reactions: $\mathcal{R} = \{\mathcal{R}_k | k = 1, 2, \ldots, r\}$ of the form

$$\mathcal{R}_k : C_l \xrightarrow{\kappa_k} C_{l'}, \quad l, l' \in \{1, 2, \ldots, m\},\ k = 1, 2, \ldots, r,$$

  where C_l and $C_{l'}$ are the reactant (or source) and product complexes, respectively. The positive real numbers κ_k are the reaction rate coefficients.

The stoichiometric coefficients are collected into the complex composition matrix $Y \in \mathbb{R}^{n \times m}$, where $Y_{i,j} = \alpha_{i,j}$ for $i = 1, 2, \ldots, n,\ j = 1, 2, \ldots, m$; that is, the jth column of Y, denoted with $Y_{\cdot,j}$, is the stoichiometric coefficient vector of complex C_j. We assume so-called mass action type reaction rates in the monomial form $\kappa_k x^{Y_{\cdot,l}}$ for $k = 1, 2, \ldots, r$. The general dynamic equations of kinetic systems are as follows:

$$\dot{x}(t) = \sum_{k=1}^{r} \big(Y_{\cdot,l'} - Y_{\cdot,l}\big) \kappa_k x^{Y_{\cdot,l}}. \tag{2}$$

A system of ODEs of the form $\dot{x} = f(x)$ with a polynomial function f is called kinetic if it can be written in the form (2) (Hárs and Tóth, 1981). Chemical reaction networks can be considered as universal descriptors of nonnegative dynamics (Érdi and Tóth, 1989). Another advantage of the model class is that the structure of the reaction graph can be related to qualitative properties of the system dynamics (Feinberg, 2019; Angeli, 2009).

3. NONLOCAL FLOW REACTION MODEL

In this section we consider nonlocal flows and carry out the spatial segmentation of the flow model, with clear compartmental interpretation. The resulting system is called Nonlocal Flow Reaction Model (NFRM) and will be the subject of subsequent analysis in Section 4.

Our main motivation comes from the theory of particle flows, thus ρ will denote particle density; that is, the number of particles per unit length. There are multiple flux functions appropriate for modeling such flows. One of the most widely used flux functions is the so-called Lighthill-Whitham-Richards (LWR) flux, which assumes that the speed of the flow is proportional to the particle density and available free spaces (Lighthill and Whitham, 1955; Richards, 1956). Note that this assumption is applicable in many areas, including ribosome flows (Reuveni et al., 2011). The local flux is given by

$$f(u) = \frac{v_{max}}{\rho_{max}} u(\rho_{max} - u) = wu(\rho_{max} - u),$$

where v_{max} and ρ_{max} are the maximal particle speed and density, respectively. The nonlocal flux is given by

$$F(u, v) = wu(\rho_{max} - v).$$

We assume that the in- and out-flows (source and sink terms) of an open system are of the form

$$\begin{aligned} r(x,t,\rho) &= 1_{in}(x) w(x) \rho_{in}(t) \big(\rho_{max} - \rho(x,t)\big) \\ s(x,t,\rho) &= 1_{out}(x) w(x) \rho_{out}(t) \rho(x,t), \end{aligned}$$

where $\rho_{in}, \rho_{out} : \mathbb{R}_+ \mapsto \overline{\mathbb{R}}_+$ are the rates of the in- and out-flows, respectively. The spatial positions are described by the indicator functions $1_{in}, 1_{out}$ defined by

$$1_{in}(x) = \sum_{i=1}^{\mathcal{I}} \chi_{\left[x_i^{in}, x_{i'}^{in}\right]}(x), \quad 1_{out}(x) = \sum_{j=1}^{\mathcal{J}} \chi_{\left[x_j^{out}, x_{j'}^{out}\right]}(x),$$

where the space coordinates defining the above intervals are strictly ordered as follows:

$$\begin{aligned} x_1^{in} < x_{1'}^{in} < \cdots < x_{\mathcal{I}}^{in} < x_{\mathcal{I}'}^{in}, \\ x_1^{out} < x_{1'}^{out} < \cdots < x_{\mathcal{J}}^{out} < x_{\mathcal{J}'}^{out}. \end{aligned}$$

We will use the finite volume approach to spatially discretize (also called semi-discretize) the flow model by introducing a grid defined by an increasing sequence of real

values $\left(x_{i+\frac{1}{2}}\right)_{i\in\mathbb{Z}}$ such that $\mathbb{R}=\bigcup_{i\in\mathbb{Z}}\left[x_{i-\frac{1}{2}},x_{i+\frac{1}{2}}\right]$. Then the grid is the set $\left\{K_i=\left(x_{i-\frac{1}{2}},x_{i+\frac{1}{2}}\right)\middle| i\in\mathbb{Z}\right\}$ where the length of the cell K_i is $h_i=x_{i+\frac{1}{2}}-x_{i-\frac{1}{2}}$. The derivation of the discretized model is analogous to the local case in (Lipták et al., 2021) with the additional approximation of the integral in (1).

We introduce the variables $\rho_i(t)$ approximating the average particle density in the ith cell at time t as

$$\rho_i(t)\approx\frac{1}{h_i}\int_{K_i}\rho(x,t)\,\mathrm{d}x$$

and the variables $1_{in,i}$ and $1_{out,i}$ as

$$1_{in,i}=\frac{1}{h_i}\int_{K_i}1_{in}(x)\,\mathrm{d}x\,,\quad 1_{out,i}=\frac{1}{h_i}\int_{K_i}1_{out}(x)\,\mathrm{d}x\,.$$

Let f_i be such that $\sum_{j=1}^{f_i}h_{i+j}\geq\delta$ and $\sum_{j=1}^{f_i-1}h_{i+j}<\delta$ and b_i be such that $\sum_{j=1}^{b_i}h_{i-j}\geq\delta$ and $\sum_{j=1}^{b_i-1}h_{i-j}<\delta$; that is, f_i and b_i denote the number of cells affected by the ith cell and the number of cells affecting the ith cell, respectively. Finally, define

$$W_{i,j}=\frac{1}{jh_{i+j}}\int_0^{h_{i+j}}\omega\left(\sum_{k=1}^{j-1}h_{i+k}+h\right)\mathrm{d}h\,,$$
$$W_{i,-j}=\frac{1}{jh_{i-j}}\int_0^{h_{i-j}}\omega\left(\sum_{k=1}^{j-1}h_{i-k}+h\right)\mathrm{d}h\,.$$

The approximation for the ith cell at time t is

$$\begin{aligned}&\int_0^{\delta}\frac{F(\rho,\tau_h\rho)-F(\tau_{-h}\rho,\rho)}{h}\omega(h)\,\mathrm{d}h\\&\approx\sum_{j=1}^{f_i}G(\rho_i,\rho_{i+j})W_{i,j}-\sum_{j=1}^{b_i}G(\rho_{i-j},\rho_i)W_{i,-j}\end{aligned}$$

where G is the so-called numerical flux. Since ω is of unit norm, we have

$$\sum_{j=1}^{f_i}jh_{i+j}W_{i,j}=1,\quad\sum_{j=1}^{b_i}jh_{i-j}W_{i,-j}=1.$$

The choice of the numerical flux G determines many important qualitative properties of the numerical scheme. The two most commonly used schemes especially in the field of traffic flows are the modified Lax-Friedrichs scheme and the Godunov scheme (LeVeque, 1992). The former uses

$$G(u,v)=\frac{f(u)+f(v)}{2}+D(u-v)$$

where $2D\geq v_{max}$ is the coefficient of the numerical diffusion term, and the latter utilizes

$$G(u,v)=\begin{cases}\min\limits_{s\in[u,v]}f(s) & \text{if } u\leq v,\\ \max\limits_{s\in[v,u]}f(s) & \text{otherwise.}\end{cases}$$

When used in time-space discretization of local conservation laws, both schemes are monotone flux schemes implying advantageous properties like the maximum principle, also called ℓ^∞-stability (Eymard et al., 2000), but the physical interpretation is not straightforward. Furthermore, these fluxes are complicated to handle from a control point of view. Note that while the theory of monotone flux schemes have been widely studied for local equations the theory is rather incomplete for nonlocal models. Recent advancements include the characterization of equidistant monotone flux schemes for closed nonlocal conservation laws and an appropriate Courant-Friedrichs-Lewy (CFL) condition under which the scheme is conservative, consistent, enjoys the maximum principle and is total variation diminishing (TVD) (Du et al., 2017).

Our main result is that using the naturally defined nonlocal flux as the numerical flux $G(u,v)=F(u,v)=wu(\rho_{max}-v)$ in the case of open conservation laws, the (not necessarily equidistant) discretization scheme will still have many desired qualitative properties mentioned above and the obtained system of ODEs is of a quite special form, namely, it is kinetic.

Definition 1. The NFRM is the spatial numerical segmentation of (1), given by

$$\begin{aligned}\dot\rho_i=&\sum_{j=1}^{b_i}w\rho_{i-j}(\rho_{max}-\rho_i)W_{i,-j}-\sum_{j=1}^{f_i}w\rho_i(\rho_{max}-\rho_{i+j})W_{i,j}+\\&+1_{in,i}w\rho_{in}(\rho_{max}-\rho_i)-1_{out,i}w\rho_{out}\rho_i,\quad(i,t)\in\mathbb{Z}\times\mathbb{R}_+;\\\rho_i(0)=&\frac{1}{h_i}\int_{K_i}\rho_0(x)\,\mathrm{d}x\,,\quad i\in\mathbb{Z}.\end{aligned}$$

For the sake of generality we may also consider variable maximal density and particle speed at different spatial points. These will be given by the functions $\rho_{max}:\mathbb{R}\mapsto\mathbb{R}_+$ and $v_{max}:\mathbb{R}\mapsto\mathbb{R}_+$, respectively. The local flux in this case is

$$\tilde f(u,x)=\frac{v_{max}(x)}{\rho_{max}(x)}u\big(\rho_{max}(x)-u\big)=w(x)u\big(\rho_{max}(x)-u\big)$$

and the nonlocal flux is

$$\tilde F(u,v,x,y)=w(x)u\big(\rho_{max}(y)-v\big).$$

We further introduce the variables $\rho_{max,i}$ and $v_{max,i}$ denoting the average maximal particle density and speed in cell K_i as

$$\rho_{max,i}=\frac{1}{h_i}\int_{K_i}\rho_{max}(x)\,\mathrm{d}x\,,\quad v_{max,i}=\frac{1}{h_i}\int_{K_i}v_{max}(x)\,\mathrm{d}x$$

and the variables $w_i=\frac{v_{max,i}}{\rho_{max,i}}$. Using the numerical flux

$$\tilde G(u,v,i,j)=w_iu(\rho_{max,j}-v)$$

we obtain a generalization of NFRMs.

Definition 2. The generalized NFRM is defined by

$$\begin{aligned}\dot\rho_i(t)=&\sum_{j=1}^{b_i}w_{i-j}\rho_{i-j}(t)\big(\rho_{max,i}-\rho_i(t)\big)W_{i,-j}\\&-\sum_{j=1}^{f_i}w_i\rho_i(t)\big(\rho_{max,i+j}-\rho_{i+j}(t)\big)W_{i,j}\\&+R_i(t,\rho_i)-S_i(t,\rho_i),\quad(i,t)\in\mathbb{Z}\times\mathbb{R}_+;\\\rho_i(0)=&\frac{1}{h_i}\int_{K_i}\rho_0(x)\,\mathrm{d}x\,,\quad i\in\mathbb{Z},\end{aligned}\tag{3}$$

where

$$\begin{aligned}R_i(t,\rho_i)&=1_{in,i}w_i\rho_{in}(t)\big(\rho_{max,i}-\rho_i(t)\big),\\S_i(t,\rho_i)&=1_{out,i}w_i\rho_{out}(t)\rho_i(t).\end{aligned}$$

Generalized NFRMs are formally kinetic, which ensures some advantageous properties of the model and most importantly, allows us to use the well-developed theory of

chemical reaction networks (Érdi and Tóth, 1989; Feinberg, 2019). Furthermore, the underlying CRN has physically meaningful compartments and topology. In fact, let N_i and S_i denote particles and available space slots for particles in the ith cell, respectively. Then the particle flow can be represented as transformations of complexes (that is, as reactions) as follows:

$$N_{i-j} + S_i \xrightarrow{k_{i-j,i}} N_i + S_{i-j} \qquad j = 1, 2, \dots, b_i \quad (4)$$

$$N_i + S_{i+j} \xrightarrow{k_{i,i+j}} N_{i+j} + S_i \qquad j = 1, 2, \dots, f_i \quad (5)$$

$$S_i \xrightarrow{k_{in,i}} N_i \quad (6)$$

$$N_i \xrightarrow{k_{out,i}} S_i. \quad (7)$$

Reaction (4) shows that during the particles' transition from the $(i-j)$th cell to the ith cell the available spaces increase in the $(i-j)$th cell and decrease in the ith cell, while the number of particles decrease in the $(i-j)$th cell and increase in the ith cell. Reaction (5) expresses the same transition from the ith cell to the $(i+j)$th cell. Finally, reactions (6) and (7) show the behaviour of in- and out-flows. Note that (4) and (5) are redundant when enumerating all reactions. Figure 1 shows the exact structure of the compartments and the topology of the intra- and intercell reactions.

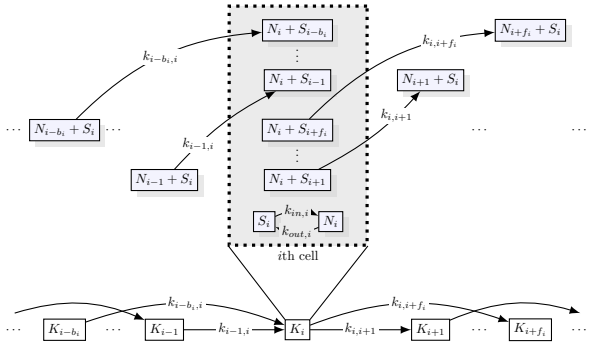

Fig. 1. Compartmental model of the generalized NFRM

Let n_i and s_i denote the continuous number of particles and available spaces in the ith cell per unit length, respectively. Using Eq. (2), the system of ODEs derived from the reactions are:

$$\dot{n}_i = \sum_{j=1}^{b_i} k_{i-j,i} n_{i-j} s_i - \sum_{j=1}^{f_i} k_{i,i+j} n_i s_{i+j} + k_{in,i} s_i - k_{out,i} n_i, \quad (8)$$

$$\dot{s}_i = -\sum_{j=1}^{b_i} k_{i-j,i} n_{i-j} s_i + \sum_{j=1}^{f_i} k_{i,i+j} n_i s_{i+j} - k_{in,i} s_i + k_{out,i} n_i.$$

We can see that $\dot{n}_i + \dot{s}_i = 0$; that is, the sum of particles and available spaces is conserved in each cell. Let $n_i + s_i = c_i$, and substitute $s_i = c_i - n_i$ into (8) to obtain

$$\dot{n}_i = \sum_{j=1}^{b_i} \big(k_{i-j,i} n_{i-j} c_i - k_{i-j,i} n_{i-j} n_i\big) + k_{in,i}(c_i - n_i) - \sum_{j=1}^{f_i} \big(k_{i,i+j} n_i c_{i+j} - k_{i,i+j} n_i n_{i+j}\big) - k_{out,i} n_i,$$

which is equivalent to (3) with $n_i = \rho_i$, $c_i = \rho_{max,i}$, $k_{i-j,i} = w_{i-j} W_{i,-j}$, $k_{i,i+j} = w_{i+j} W_{i,j}$, $k_{in,i} = 1_{in,i} w_{in} \rho_{in}$ and $k_{out,i} = 1_{out,i} w_i \rho_{out}$.

4. ANALYSIS OF THE NFRM

In this section we introduce some important properties of the spatial and the time-space discretization. General properties are established for open systems and then some stronger results are formalized for closed systems. We also briefly demonstrate the applicability of CRN theory for the analysis of NFRMs.

4.1 Spatial discretization

Theorem 3. The following statements hold for the proposed numerical scheme (3):

(i) It is nonnegative and capacitated; that is, we have $0 \le \rho_i(t) \le \rho_{max,i}$ for all $i \in \mathbb{Z}$ and $t \ge 0$.
(ii) It is conservative in the sense that

$$\sum_{i\in\mathbb{Z}} \rho_i(t) = \sum_{i\in\mathbb{Z}} \rho_i(0) + \int_0^t \big(R_i(\tau, \rho_i) - S_i(\tau, \rho_i)\big)\, \mathrm{d}\tau$$

holds for any $t \ge 0$.

Proof. (i) These are immediate consequences of the kinetic property (Feinberg, 2019).

(ii) Since

$$\sum_{i\in\mathbb{Z}} \dot{\rho}_i(t) = \sum_{i\in\mathbb{Z}} \big(R_i(t, \rho_i) - S_i(t, \rho_i)\big)$$

the scheme is conservative.

4.2 Discretization of the kinetic model in time

Consider the equidistant temporal grid $t_k = k\Delta t$, where $\Delta t > 0$ is the time step. Let ρ_i^k approximate the average particle density in the ith cell at time t_k; that is, we have

$$\rho_i^k \approx \frac{1}{h_i} \int_{K_i} \rho(x, t_k)\, \mathrm{d}x\,.$$

Consider the explicit Euler discretization of (3) as

$$\rho_i^{k+1} = \rho_i^k + \Delta t \sum_{j=1}^{b_i} w_{i-j} \rho_{i-j}^k \big(\rho_{max,i} - \rho_i^k\big) - \Delta t \sum_{j=1}^{f_i} w_i \rho_i^k \big(\rho_{max,i+j} - \rho_i^k\big) + R_i\big(t_k, \rho_i^k\big) - S_i\big(t_k, \rho_i^k\big) \quad (9)$$

for $(i,k) \in \mathbb{Z} \times \mathbb{N}$ and rewrite the scheme as

$$\rho_i^{k+1} = H\big(\rho_{i-b_i}^k, \dots, \rho_i^k, \dots, \rho_{i+f_i}^k\big). \quad (10)$$

Theorem 4. Under the CFL condition

$$2\Delta t \sup_{x,y\in\mathbb{R}} \big(w(x)\rho_{max}(y)\big) \le \inf_{i\in\mathbb{Z}} h_i \quad (11)$$

the following statements hold for the proposed spatio-temporal numerical scheme (9):

(i) It is nonnegative.
(ii) It is capacitated and $\rho_i^k \le \rho_{max,i}$ holds for all $i \in \mathbb{Z}$ and $k \in \mathbb{N}$.
(iii) It is conservative in the sense that

$$\sum_{i\in\mathbb{Z}} \rho_i^k = \sum_{i\in\mathbb{Z}} \rho_i^0 + \Delta t \sum_{i\in\mathbb{Z}} \sum_{l=0}^{k} \Big(R_i\big(t_l, \rho_i^l\big) - S_i\big(t_l, \rho_i^l\big)\Big)$$

holds for any $k \in \mathbb{N}$.

Proof. (i) Under the above CFL condition, we have

$$\rho_i^{k+1} \geq \rho_i^k - \rho_i^k \frac{\inf_{i\in\mathbb{Z}} h_i}{2\sup_{x,y\in\mathbb{R}}\big(w(x)\rho_{max}(y)\big)} \times \left(\sum_{j=1}^{f_i} w_i\rho_{max,i+j}W_{i,j} + 1_{out,i}w_i\rho_{max,i}\right) \geq$$
$$\geq \rho_i^k - \rho_i^k\frac{1}{2}\left(\sum_{j=1}^{f_i} h_{i+j}W_{i,j} + \inf_{i\in\mathbb{Z}} h_i\right) \geq 0$$

thus the scheme is nonnegative.

(ii) The proof is nearly identical to the proof of (i).

(iii) Summation over the cells and partial summation yield

$$\sum_{i\in\mathbb{Z}}\rho_i^{k+1} = \sum_{i\in\mathbb{Z}}\rho_i^k + \Delta t\sum_{i\in\mathbb{Z}}\sum_{j=1}^{b_i} w_{i-j}\rho_{i-j}\big(\rho_{max,i} - \rho_i^k\big)W_{i,-j}$$
$$- \Delta t\sum_{i\in\mathbb{Z}}\sum_{j=1}^{f_i} w_i\rho_i^k\big(\rho_{max,i+j} - \rho_{i+j}^k\big)W_{i,j}$$
$$+ \Delta t\sum_{i\in\mathbb{Z}}\big(R_i(t_k,\rho_i^k) - S_i(t_k,\rho_i^k)\big)$$
$$= \sum_{i\in\mathbb{Z}}\rho_i^k + \Delta t\sum_{i\in\mathbb{Z}}\big(R_i(t_k,\rho_i^k) - S_i(t_k,\rho_i^k)\big).$$

Induction shows that the scheme is conservative.

Theorem 5. Consider a closed NFRM. Under the CFL condition (11), the following statements hold for the proposed numerical scheme (9):

(i) It is monotone; that is, if $u_i^0 \leq v_i^0$ for all $i \in \mathbb{Z}$, then $u_i^k \leq v_i^k$ for all $i \in \mathbb{Z}$ and $k \in \mathbb{N}$.

(ii) It is ℓ^1-contractive; that is, if ρ^0 and η^0 are ℓ^1-summable sequences and ρ^k and η^k denote the result of scheme (9) after k steps using ρ^0 and η^0 as initial values, respectively, then for any $k > l$
$$\big\|\rho^k - \eta^k\big\|_{\ell^1} \leq \big\|\rho^l - \eta^l\big\|_{\ell^1}.$$

(iii) It satisfies the TVD property; that is, for any $k > l$
$$TV\big(\rho^k\big) \leq TV\big(\rho^l\big),$$
where $TV\big(\rho^k\big) = \sum_{i\in\mathbb{Z}}\big|\rho_i^k - \rho_{i-1}^k\big|$.

Proof. (i) It suffices to show that H given by (10) is monotone; that is,
$$\frac{\partial H(\rho_{i-b_i}^k,\dots,\rho_{i+f_i}^k)}{\partial\rho_{i+j}^k} \geq 0$$
holds for each $i, j \in \mathbb{Z}$. It is clear that
$$\frac{\partial H(\rho_{i-b_i}^k,\dots,\rho_{i+f_i}^k)}{\partial\rho_{i-j}^k} = 0 \qquad \text{for } j > b_i$$
$$\frac{\partial H(\rho_{i-b_i}^k,\dots,\rho_{i+f_i}^k)}{\partial\rho_{i+j}^k} = 0 \qquad \text{for } j > f_i$$
holds. Furthermore, we have that
$$\frac{\partial H(\rho_{i-b_i}^k,\dots,\rho_{i+f_i}^k)}{\partial\rho_{i-j}^k} = \Delta t w_{i-j}\big(\rho_{max,i} - \rho_i^k\big)W_{i,-j} \geq 0$$
for $j = 1, 2, \dots, b_i$. Similarly
$$\frac{\partial H(\rho_{i-b_i}^k,\dots,\rho_{i+f_i}^k)}{\partial\rho_{i+j}^k} = \Delta t w_i\rho_i^k W_{i,j} \geq 0$$
for $j = 1, 2, \dots, f_i$. Finally, using the same approximation as in the proof of Theorem 4(i), we obtain

$$\frac{\partial H}{\partial\rho_i^k} = 1 - \Delta t\left(\sum_{j=1}^{b_i} w_{i-j}\rho_{i-j}^k W_{i,-j} + \sum_{j=1}^{f_i} w_i\big(\rho_{max,i+j} - \rho_{i+j}^k\big)W_{i,j}\right)$$
$$\geq 1 - \frac{1}{2}\left(\sum_{j=1}^{b_i} h_{i-j}W_{i,-j} + \sum_{j=1}^{f_i} h_{i+j}W_{i,j}\right) \geq 0.$$

(ii) For the proof, we refer to (Harten et al., 1976, Appendix), where finite-difference schemes are considered, but the proof of ℓ^1-contractivity is detached from this fact.

(iii) The proof follows the proof of (LeVeque, 1992, Theorem 15.4). By denoting $\eta_i^k = \rho_{i-1}^k$ and using ℓ^1-contractivity, we have
$$TV\big(\rho^k\big) = \big\|\rho^k - \eta^k\big\|_{\ell^1} \leq \big\|\rho^{k-1} - \eta^{k-1}\big\|_{\ell^1} = TV\big(\rho^{k-1}\big).$$

Induction concludes the proof.

Theorem 6. Consider a closed NFRM with constant maximal particle density and speed. Under the CFL condition (11), the proposed numerical scheme (9) enjoys the maximum principle.

Proof. Since the scheme is monotone, we have
$$\rho_i^{k+1} = H\big(\rho_{i-b_i}^k,\dots,\rho_{i+f_i}^k\big) \leq H\big(\max_{j\in\mathbb{Z}}\rho_j^k,\dots,\max_{j\in\mathbb{Z}}\rho_j^k\big) = \max_{j\in\mathbb{Z}}\rho_j^k$$
and
$$\rho_i^{k+1} = H\big(\rho_{i-b_i}^k,\dots,\rho_{i+f_i}^k\big) \geq H\big(\min_{j\in\mathbb{Z}}\rho_j^k,\dots,\min_{j\in\mathbb{Z}}\rho_j^k\big) = \min_{j\in\mathbb{Z}}\rho_j^k.$$

Let $J_k = \big(k\Delta t, (k+1)\Delta t\big)$ and $\tilde\rho(x,t)$ denote the piecewise constant function defined by the grid values ρ_i^k; that is, let
$$\tilde\rho(x,t) = \sum_{k=0}^{\infty}\sum_{i\in\mathbb{Z}}\rho_i^k\chi_{K_i}(x)\chi_{J_k}(t).$$

Theorem 7. Consider a closed NFRM with constant maximal particle density and speed. Assume that $\rho_0 \in \mathcal{L}^1(\mathbb{R}) \cap \mathcal{L}^\infty(\mathbb{R}) \cap BV(\mathbb{R})$. Then, for any $t \geq 0$, we have
$$\|\tilde\rho(.,t)\|_Z \leq \|\rho_0\|_Z, \quad Z = \mathcal{L}^\infty(\mathbb{R}), BV(\mathbb{R}).$$

Proof. The case $Z = \mathcal{L}^\infty(\mathbb{R})$ follows from the maximum princple and $Z = BV(\mathbb{R})$ follows from (Crandall and Majda, 1980, (2.16)).

4.3 Stability analysis of a circular topology

In this subsection, as an extension of the results described in (Lipták et al., 2021), we consider closed NFRMs with constant maximal particle density and speed and with circular or ring-like topology obtained via equidistant spatial discretization. Let the number of compartments be N. In an equidistant setting $b_i = f_i =: r$ for $i = 1, 2, \dots, N$ and $W_{i,-j} = W_{i,j} =: W_j$ for $i = 1, 2, \dots, N$ and $j = 1, 2, \dots, r$. For simplicity of notations we assume that $N > 2r$; that is, the nonlocality does not loop. Under such assumptions ring topology means that $\rho_{N+j} = \rho_j$ and $\rho_{1-j} = \rho_{N-j}$ for $j = 1, 2, \dots, r$. An equilibrium point with densities ρ_i^* satisfies the following constraints

$$\sum_{j=1}^{r} w\rho_{i-j}^{*}(\rho_{max}-\rho_i^{*})W_j = \sum_{j=1}^{r} w\rho_i^{*}(\rho_{max}-\rho_{i+j}^{*})W_j$$

for $i = 1, 2, \ldots, N$. This shows that we obtain an equilibrium if each cell has equal density and since the number of particles is constant in the closed system we have

$$\rho_i^{*} = \overline{\rho} = \frac{1}{N}\sum_{i=1}^{N}\rho_i(0).$$

We will use the entropy-like Lyapunov function candidate well-known from the theory of chemical reaction networks (Feinberg, 2019, Section 7.7)

$$V(\rho) = \sum_{i=1}^{N}\rho_i\left[\log\left(\frac{\rho_i}{\overline{\rho}}\right)-1\right]+N\overline{\rho}.$$

Note that $\overline{\rho}=0$ is only possible when there are no particles in the system which is clearly not relevant.

It is easy to see that $V(\rho^*)=0$ and $\rho\neq\rho^*$ implies $V(\rho)>0$. Furthermore, partial summation yields

$$\begin{aligned}\dot{V}(\rho) &= \sum_{i=1}^{N}\log\left(\frac{\rho_i}{\overline{\rho}}\right)\dot{\rho}_i\\ &= \sum_{i=1}^{N}\log\left(\frac{\rho_i}{\overline{\rho}}\right)\sum_{j=1}^{r} w\big[\rho_{i-j}(\rho_{max}-\rho_i)-\rho_i(\rho_{max}-\rho_{i+j})\big]W_j\\ &= w\overline{\rho}\sum_{i=1}^{N}\sum_{j=1}^{r}\frac{\rho_i(\rho_{max}-\rho_{i+j})}{\overline{\rho}}\left[\log\left(\frac{\rho_{i+j}}{\overline{\rho}}\right)-\log\left(\frac{\rho_i}{\overline{\rho}}\right)\right]W_j.\end{aligned}$$

Using the inequality $e^a(b-a)\leq e^b-e^a$ with $a=\log\left(\frac{\rho_i}{\overline{\rho}}\right)$ and $b=\log\left(\frac{\rho_{i+j}}{\overline{\rho}}\right)$ and noting that equality holds if and only if $a=b$, we find that

$$\begin{aligned}\dot{V}(\rho) &\leq w\sum_{i=1}^{N}\sum_{j=1}^{r}(\rho_{max}-\rho_{i+j})(\rho_{i+j}-\rho_i)W_j\\ &= w\sum_{i=1}^{N}\sum_{j=1}^{r}\left(-\rho_{i+j}^2+\rho_i\rho_{i+j}\right)W_j\\ &= -\frac{w}{2}\sum_{i=1}^{N}\sum_{j=1}^{r}\left(\rho_i^2-2\rho_i\rho_{i+j}+\rho_{i+j}^2\right)W_j\\ &= -\frac{w}{2}\sum_{i=1}^{N}\sum_{j=1}^{r}(\rho_i-\rho_{i+j})^2W_j\leq 0.\end{aligned}$$

This shows that $\dot{V}(\rho^*)=0$ and $\rho\neq\rho^*$ implies $\dot{V}(\rho)<0$ and we conclude that this equilibrium point is asymptotically stable.

5. CONCLUSIONS

We showed that one-dimensional nonlocal particle flows with Lighthill-Whitham-Richards flux supplemented with appropriate in- and out-flow terms can be spatially discretized with a finite volume scheme to obtain formally kinetic models with physically meaningful reaction graph structure. To demonstrate the advantages of the kinetic property, the Lyapunov stability of a special, circular topology was shown with an entropy-like logarithmic Lyapunov function. An explicit temporal discretization of the kinetic model was also studied. An appropriate Courant-Friedrichs-Lewy condition was formulated to ensure many advantageous properties of the numerical scheme. For closed systems, additional characteristics including monotonicity and the total variation diminishing property was also discussed.

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