Modeling traffic flows with reaction networks

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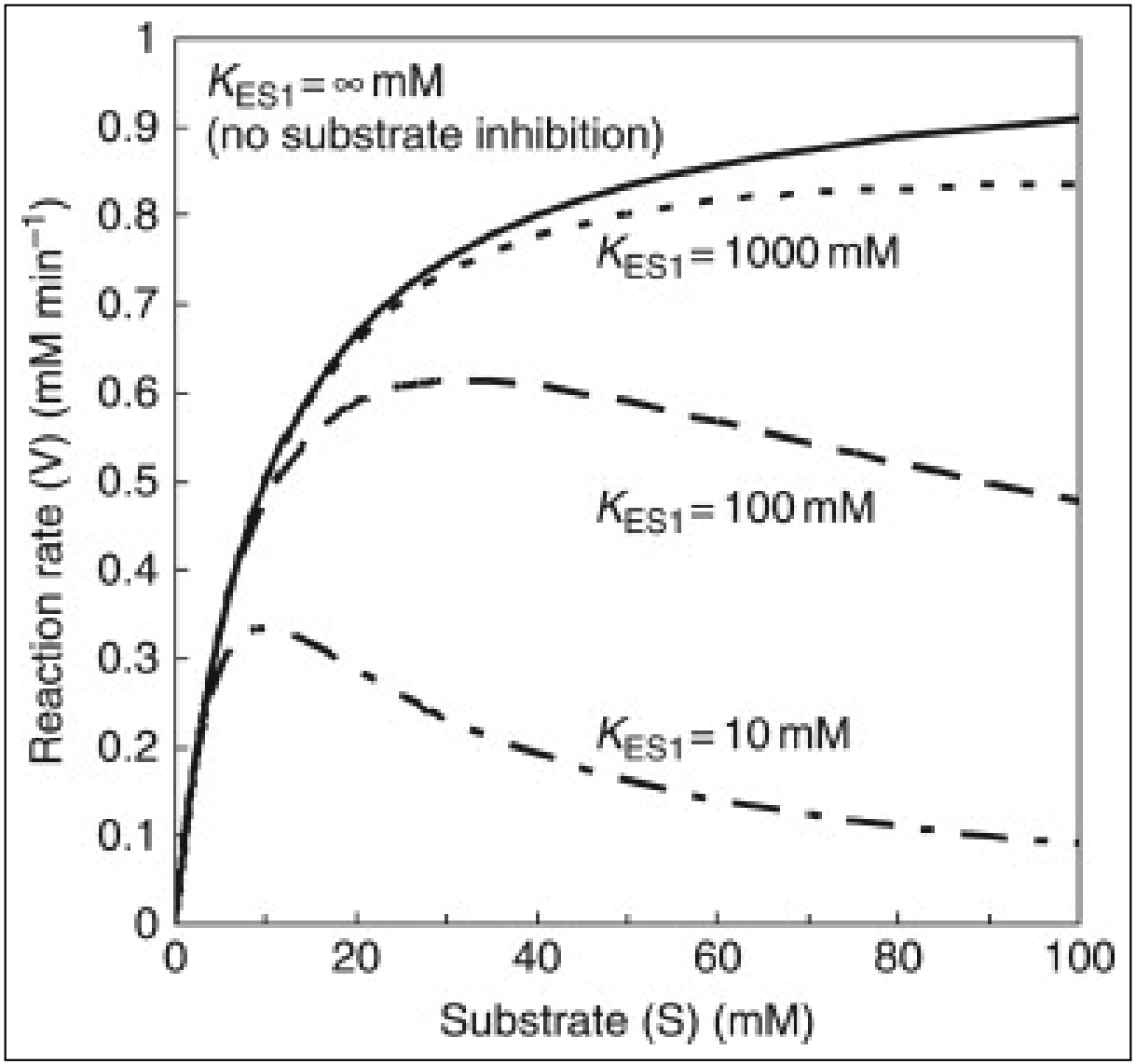
Outline

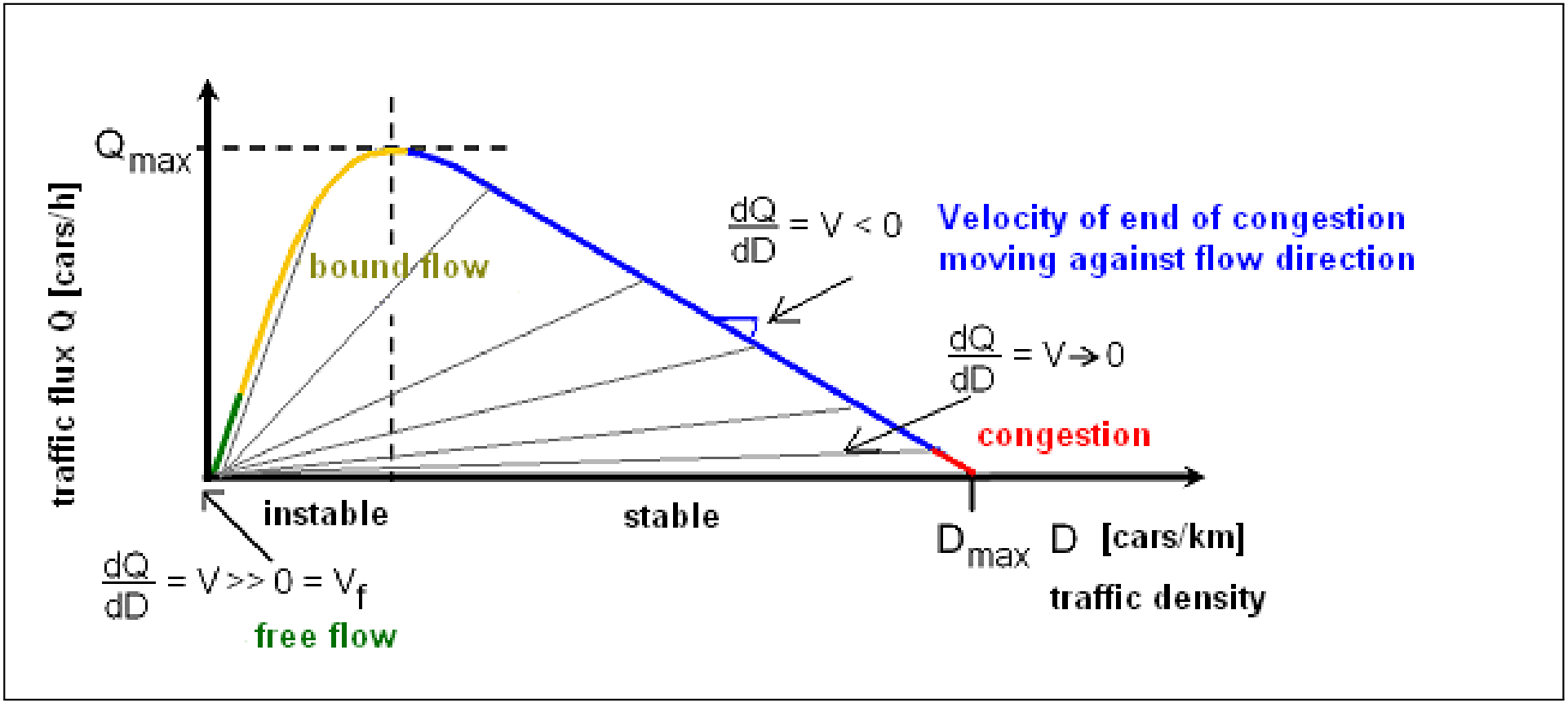
Problem statement

Substrate inhibition



Problem statement

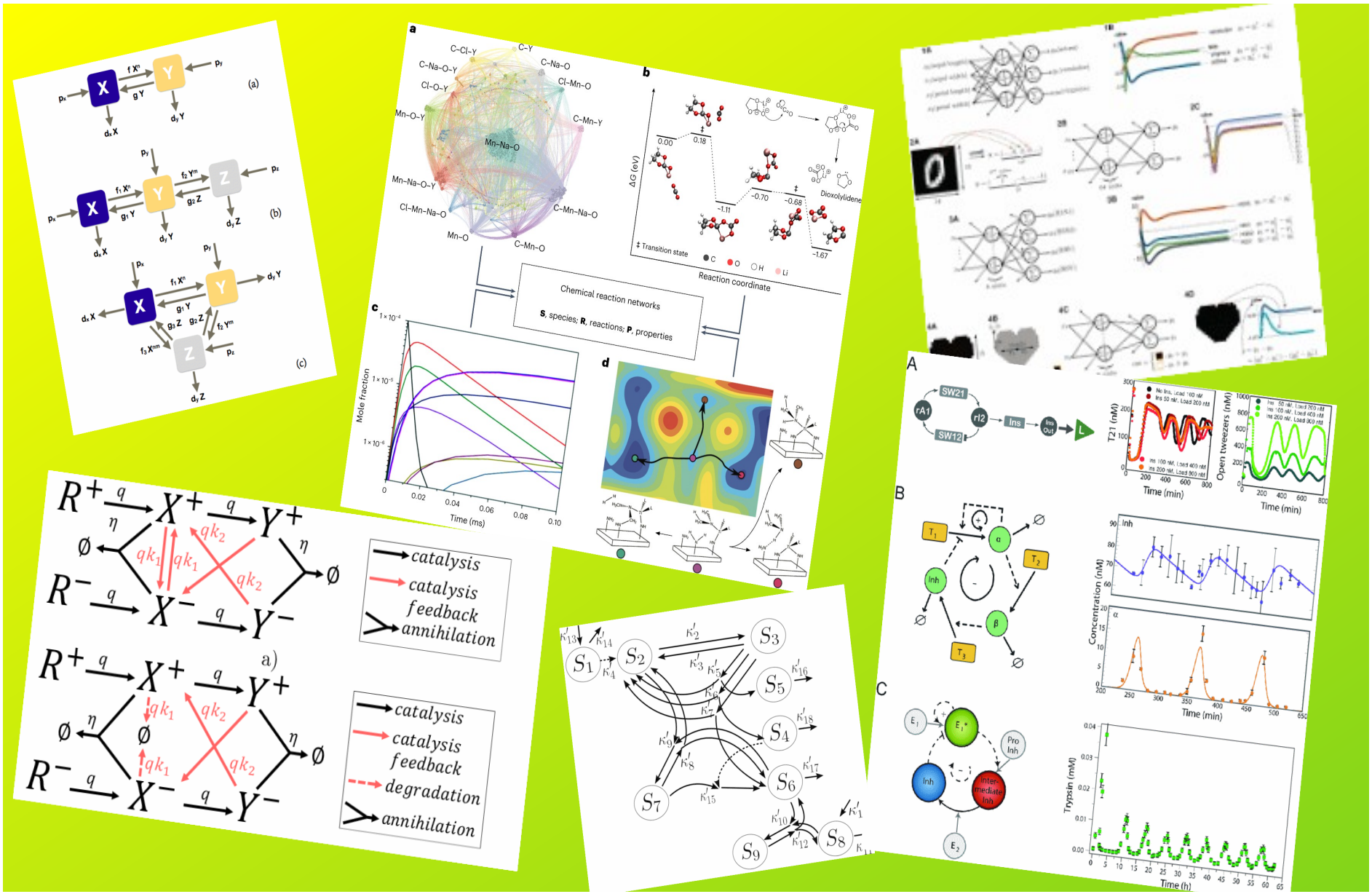
Fundamental diagram of traffic flows (flux-density)



Introduction, motivation

- Recently, several different research problems have led to compartmental models (epidemic processes, ribosome flows, traffic flows)
- These models are nonnegative and (can be) kinetic
- Such models are widely used to describe the transition (flow) of 'items' (molecules, ribosomes, vehicles, pedestrians etc.) between compartments or (abstract states)
- Interests, problem statements:
  - fundamental dynamical properties
  - possible generalizations
  - relations between different application fields
  - control-related tasks

Kinetic systems (CRNs)



Kinetic systems (CRNs)

- dynamical models which can be *formally* represented as a set of "chemical reactions" (transformations)

Molecules taken individually:

- stochastic discrete event systems
- Petri net representation: places $\rightsquigarrow$ species, transitions $\rightsquigarrow$ reactions, tokens $\rightsquigarrow$ available molecules
- Turing complete computer' with an arbitrarily small probability of error

Continuous concentrations considered:

- nonnegative nonlinear dynamical systems (ODEs)
- relatively simple mathematical model with a network (directed graph) structure
- all kinds of complex dynamical phenomena (multiplicities, oscillations, chaos, etc.) can be described in a kinetic framework

Kinetic systems (CRNs)

- recall from chemistry: $2H_2 + O_2 \longrightarrow 2H_2O$
- M species denoted by $\mathcal{X} = \{X_1, \ldots, X_M\}$, species vector: $X = [X_1 \ \ldots \ X_M]^T$
- reactions: $C_j \to C'_j, \quad j = 1, \ldots, R$
- source (reactant) and product complexes: $C_j = y_j^T X$ and $C'_j = {y'_j}^T X$, where $y_j, y'_j \in \overline{\mathbb{Z}}_+^M$ for $j = 1, \ldots, R$
- reaction graph: directed graph containing the complexes as vertices and reactions as directed edges
- graph related notions: *strongly connected graph*: there exists a directed path between any pair of its vertices in both directions; *strong component*: a maximal strongly connected subgraph; *weakly connected component*: subgraph where all vertices are connected to each other by some (not necessarily directed) path; *weakly reversible graph*: each weakly connected component is a strong component

Kinetic systems (CRNs)

- The evolution of species concentrations' ($x(t) \in \overline{\mathbb{R}}_+^M$):

$$\dot{x} = \sum_{i=1}^{R} \mathcal{K}_i(x)[y_i' - y_i], \quad x(0) \in \overline{\mathbb{R}}_+^M$$

  where $\mathcal{K}_i : \overline{\mathbb{R}}_+^M \longrightarrow \overline{\mathbb{R}}_+$ is the rate function corresponding to reaction step i

- Assumptions on $\mathcal{K}$:

  (A1) $\mathcal{K}_i$ is differentiable,

  (A2) $\dfrac{\partial \mathcal{K}_i(x)}{\partial x_j} \geq 0$ if $[y_i]_j > 0$, and $\dfrac{\partial \mathcal{K}_i(x)}{\partial x_j} = 0$ if $[y_i]_j = 0$,

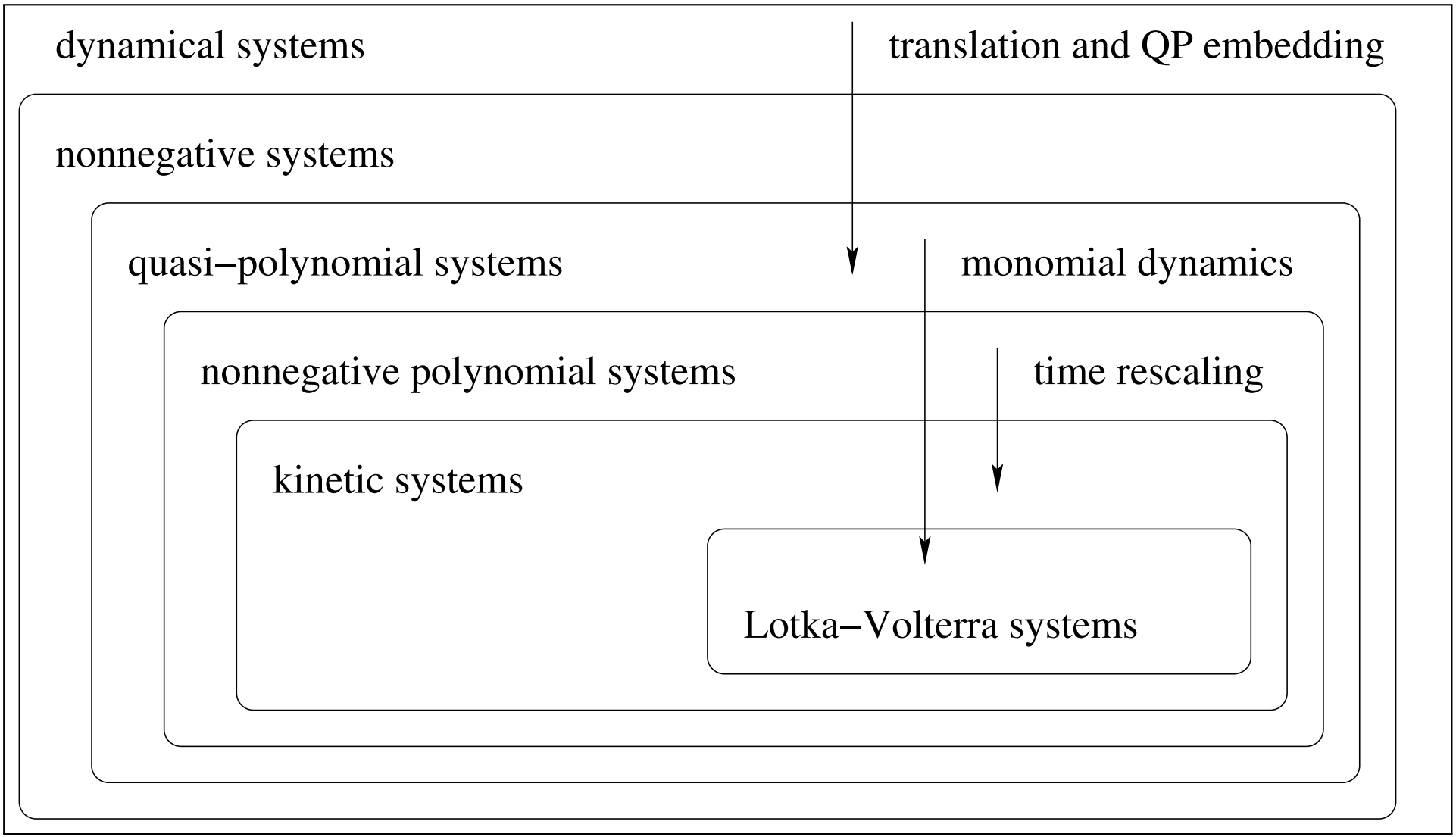
  (A3) $\mathcal{K}_i(x) = 0$ whenever $x_j = 0$ such that $j \in \mathrm{supp}(y_i)$.

  These guarantee local existence and uniqueness of the solutions as well as the invariance of the nonnegative orthant for the dynamics

- special case – mass action kinetics: $\mathcal{K}_j(x) = k_j \prod_{i=1}^{M} x_i^{[y_j]_i}$ (polynomial nonlinearities)

Kinetic systems can be considered as general descriptors of nonlinear dynamics

Generality of kinetic systems



Compartmental models

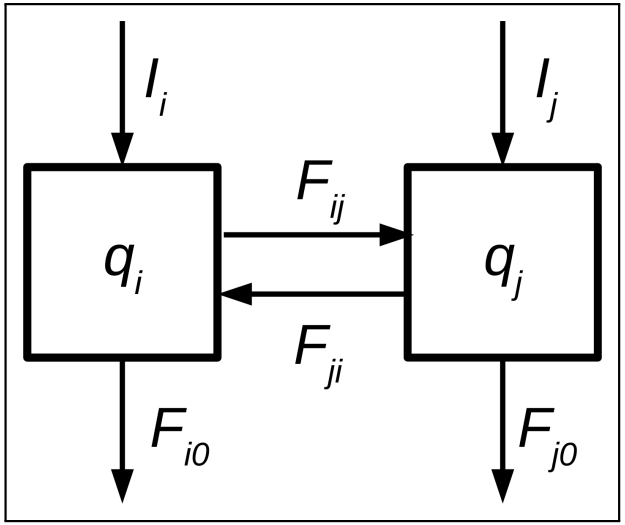
- $Q = \{q_1, q_2, \ldots, q_m\}$ set of compartments and state variables
- $F_{ij}(q) \geq 0$: flow from q_i to q_j
- $F_{i0}(q) \geq 0$: outflow from q_i to the environment
- $I_i \geq 0$: inflow to q_i
- $q_i = 0 \implies F_{ij} = F_{i0} = 0$
- can be written as $F_{ij}(q) = f_{ij}(q)q_i$

$$\dot{q}_i = -\left(f_{i0} + \sum_{i \neq j} f_{ij}\right) q_i + \sum_{i \neq j} f_{ji} q_j + I_i$$

$$\dot{q} = f(q)$$

- $\rightsquigarrow$ Jacobian of f is Metzler matrix with nonpositive column sums

Some properties of compartmental dynamics



- Compartmental systems are nonnegative
- Chemical reactions without diffusion can be written in compartmental form
- Dynamically, *"anything can happen"* in a nonlinear compartmental system
- Linear compartmental systems behave nicely (graph/eigenvalues, Lyapunov functions, diagonal stability, controllability, observability, identifiability etc.)
- In many cases, graph structure alone is informative about the qualitative dynamics even in the nonlinear case

Generality of compartmental dynamics

- Any stable nonnegative linear dynamics can be linearly transformed into compartmental form
- Any bounded dynamics in $\mathbb{R}^n$ can be embedded into a compartmental system having $n+1$ compartments:

Theorem (Jacquez, Simon 1993); constructive proof

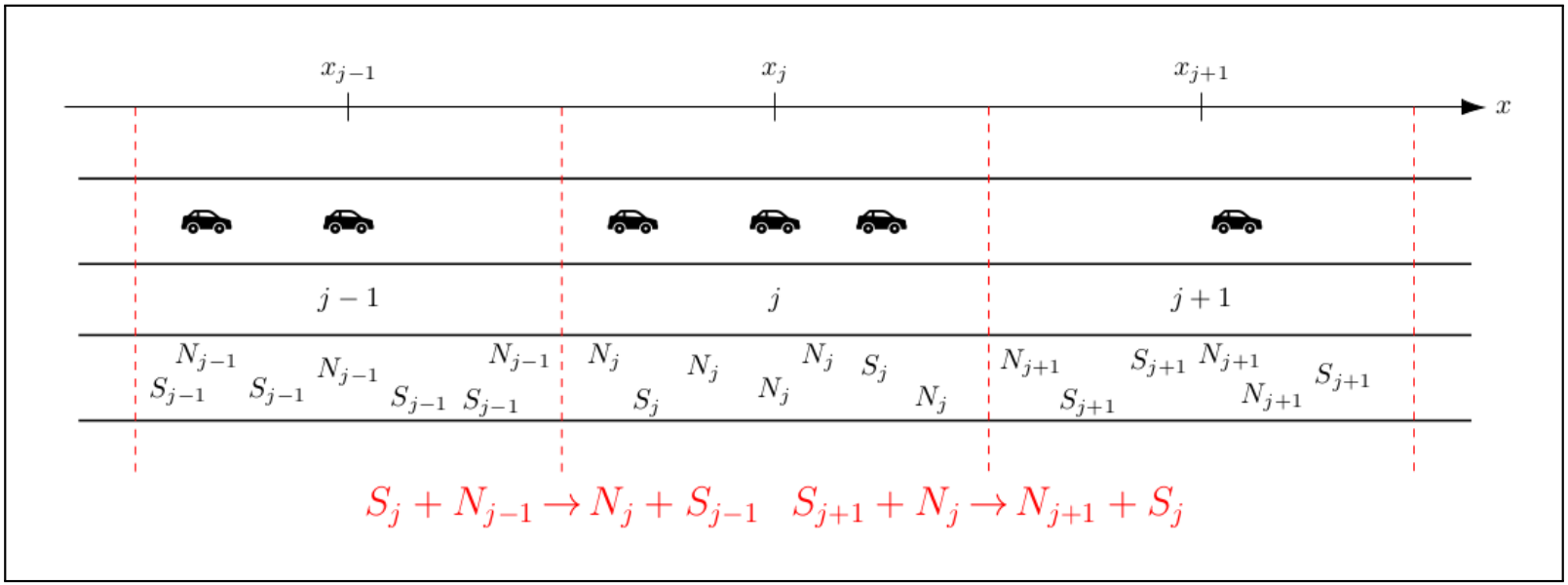
Let $\dot{x} = f(x)$ be a C^k system of n differential equations on an n-dimensional simplex

$$\Sigma_1^n = \left\{ (x_1, \ldots, x_n) \ : \ x_i \geq 0, \ \sum_{i=1}^{n} x_i \leq 1 \right\}$$

which points into Σ_1^n on its boundary. Then, there exists an autonomous C^k closed compartmental system $\dot{x} = \tilde{f}(x)$ defined on an $(n+1)$-dimensional simplex $\Sigma_{1+\epsilon}^{n+1}$ and an invariant n-dimensional subsimplex Σ of $\Sigma_{1+\epsilon}^{n+1}$ isomorphic to Σ_1^n such that $\tilde{f}$ restricted to Σ is the original f.

(Traffic) flow models

Compartments: road sections



- the basic flow equation: $\rho_t + f(\rho)_x = r - s$
- approximating ODEs (e.g., compartmental ones) can be obtained by various spatial discretization methods
- properties of the obtained ODEs are important for analysis and control (smoothness, conservation, nonnegativity, kinetic property, etc.)

Flow models in PDE form

- $\rho(x,t) \in \Omega = [0, \rho_{max}]$: traffic density (e.g., in [cars/km])
- Consider the conservation law

$$\frac{d}{dt}\int_{x_l}^{x_r} \rho(x,t)\,dx = f(\rho(x_l,t)) - f(\rho(x_r,t)) + \int_{x_l}^{x_r} r(x,t,\rho(x,t)) - s(x,t,\rho(x,t))\,dx,$$

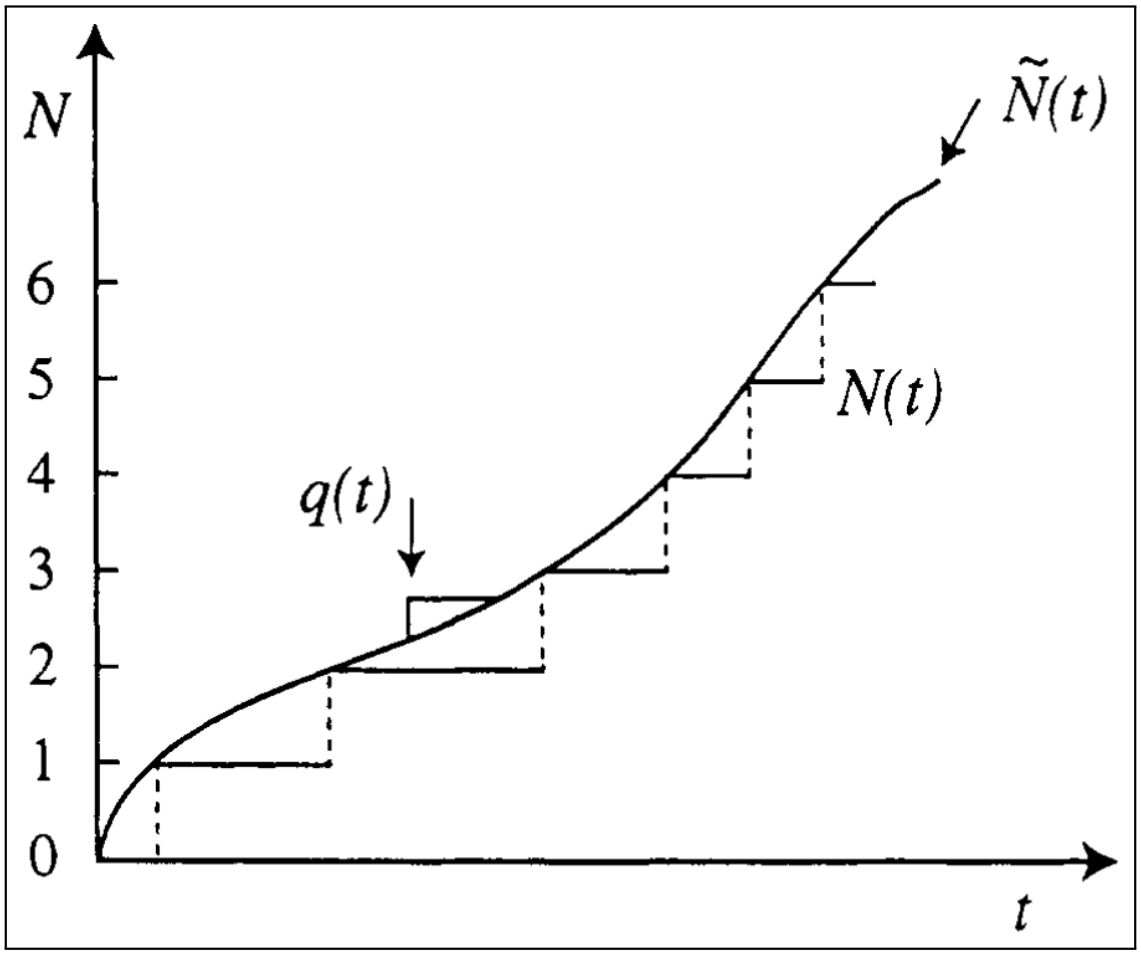
  for any $x_l < x_r$, and where the function $\rho : \mathbb{R} \times \overline{\mathbb{R}}_+ \to \mathbb{R}$ denotes the modeled quantity, the function $f \in \mathcal{C}^1 : \mathbb{R} \to \mathbb{R}$ is called flux function (often denoted by Q), source r and sink terms s are functions $\mathbb{R} \times \overline{\mathbb{R}}_+ \times \mathbb{R} \to \mathbb{R}$, respectively
- this can be reformulated in PDE form as

$$\rho_t + f(\rho)_x = r - s$$

  Lighthill–Whitham–Richards (LWR) model, 1955
- critical density: ρ_{crit}, where $f(\rho_{crit}) = f_{max}$

Flow models in PDE form

$N(t)$: cumulative number of vehicles to have passed an observer by time t
$\tilde{N}(t)$: smooth approximation of N



(Daganzo, C. F. (1997). *Fundamentals of transportation and traffic operations.* Emerald Group Publishing Limited.)

Flow models in PDE form

- introducing spatial dependence as well: $N(t,x)$, $\tilde{N}(t,x)$
- density:

$$\rho(t,x) = -\frac{\partial \tilde{N}(t,x)}{\partial x} \quad \left[\frac{\text{cars}}{\text{km}}\right]$$

- flux:

$$f(t,x) = \frac{\partial \tilde{N}(t,x)}{\partial t} \quad \left[\frac{\text{cars}}{\text{h}}\right]$$

- $\tilde{N}$ fulfills:

$$\frac{\partial^2 \tilde{N}(t,x)}{\partial x \partial t} = \frac{\partial^2 \tilde{N}(t,x)}{\partial t \partial x}$$

- therefore,

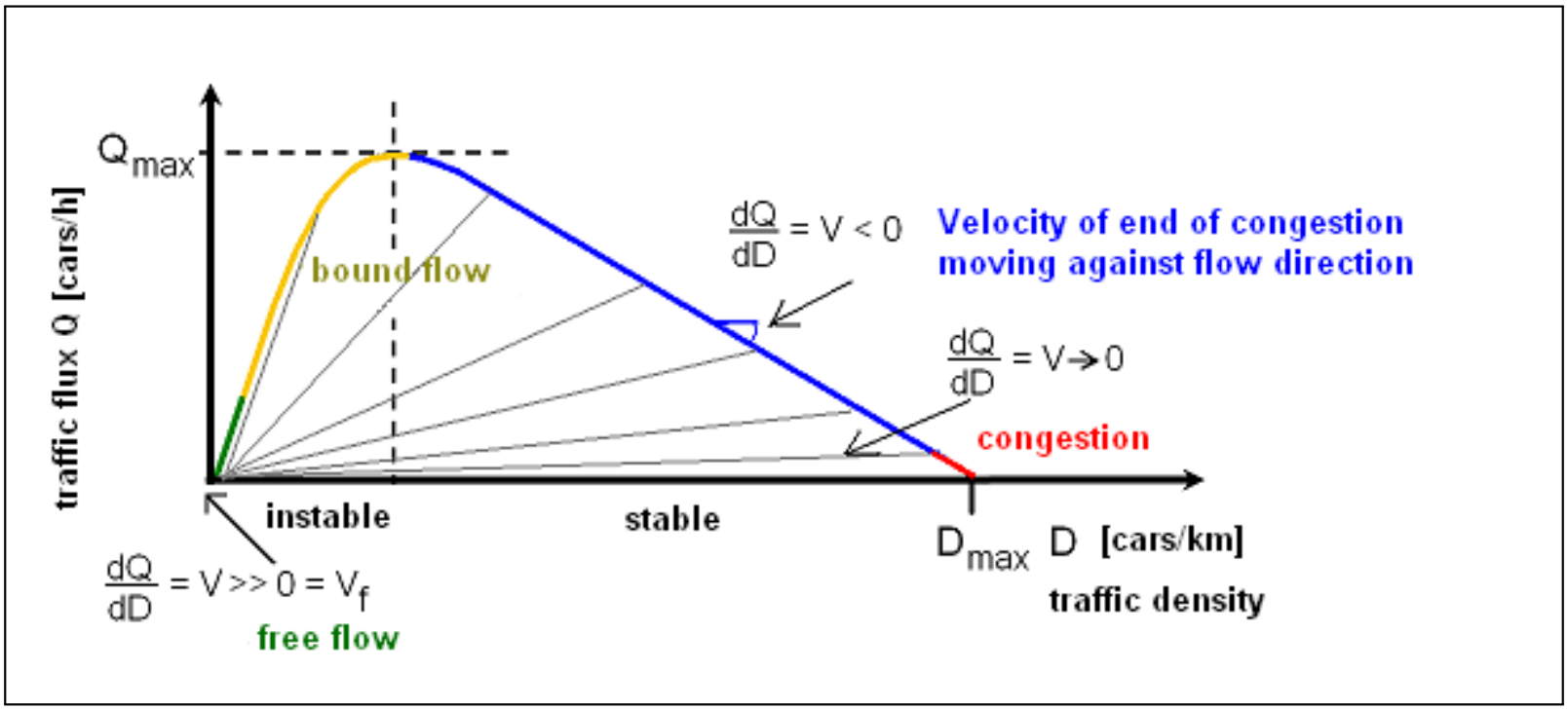
$$-\frac{\partial \rho(t,x)}{\partial t} = \frac{\partial f(t,x)}{\partial x}$$

assuming no on and off-ramps (conservation relation)

Fundamental diagrams of traffic flow

Basic relationship: $Q = D \cdot V$
(Q [cars/h]: flux, D [cars/km]: density, V [km/h]: speed)

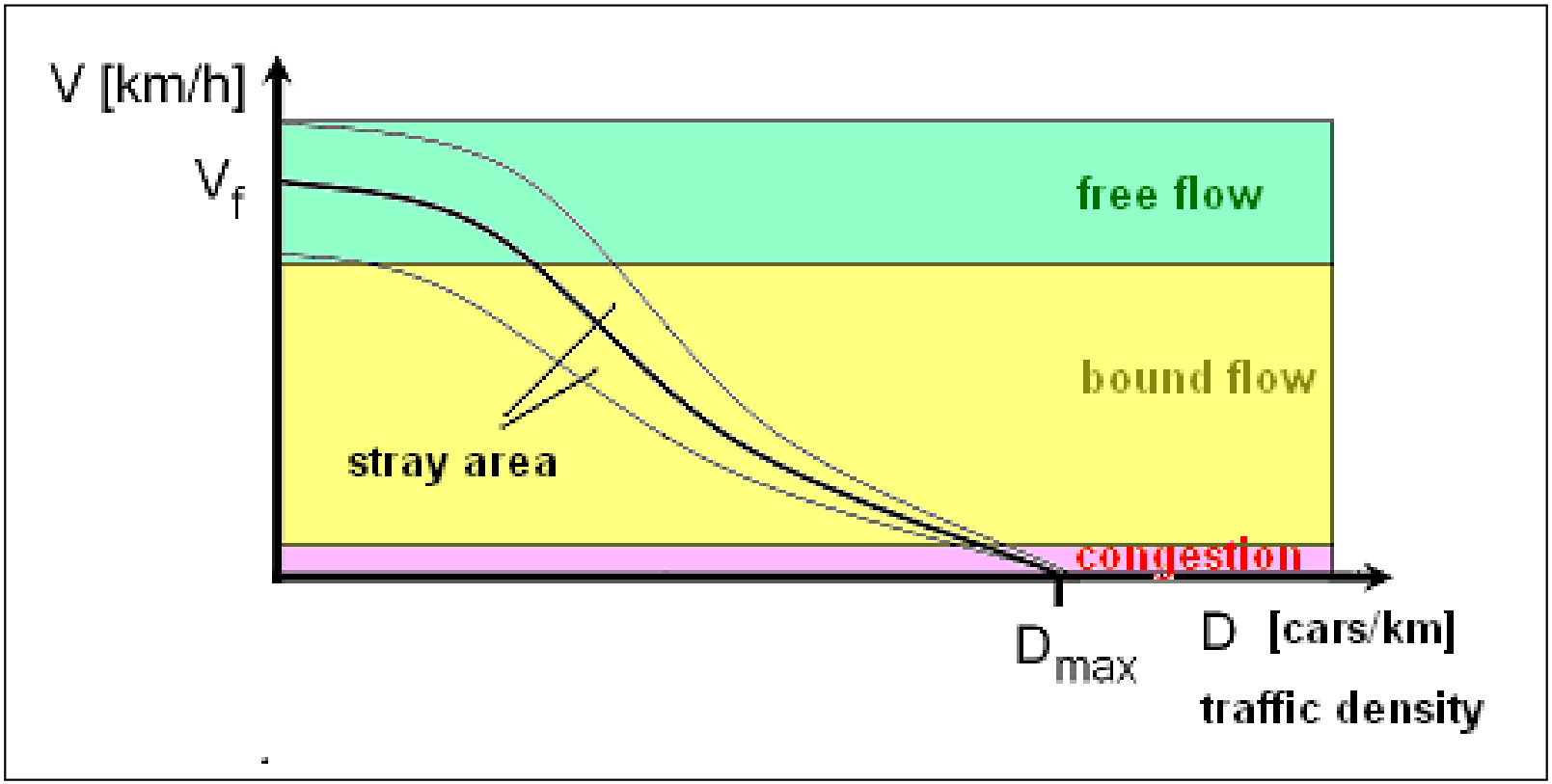
flux-density diagram:



source: https://en.m.wikipedia.org/wiki/File:Fundamental_Diagram.PNG

Fundamental diagrams of traffic flow

speed-density diagram:



source: https://en.m.wikipedia.org/wiki/File:Fundamental_Diagram.PNG

The flux function

- dual variable: density of free space $\nu = \rho_{\max} - \rho$
- assumption: the flux function has the form

$$f(\rho) = g(\rho, \rho_{\max} - \rho) = g(\rho, \nu)$$

where $g : \Omega \times \Omega \mapsto \overline{\mathbb{R}}_+$ satisfies the following assumptions:

A1 g is Lipschitz continuous w.r.t. both arguments, with associated Lipschitz constants $K_1 > 0$ and $K_2 > 0$,

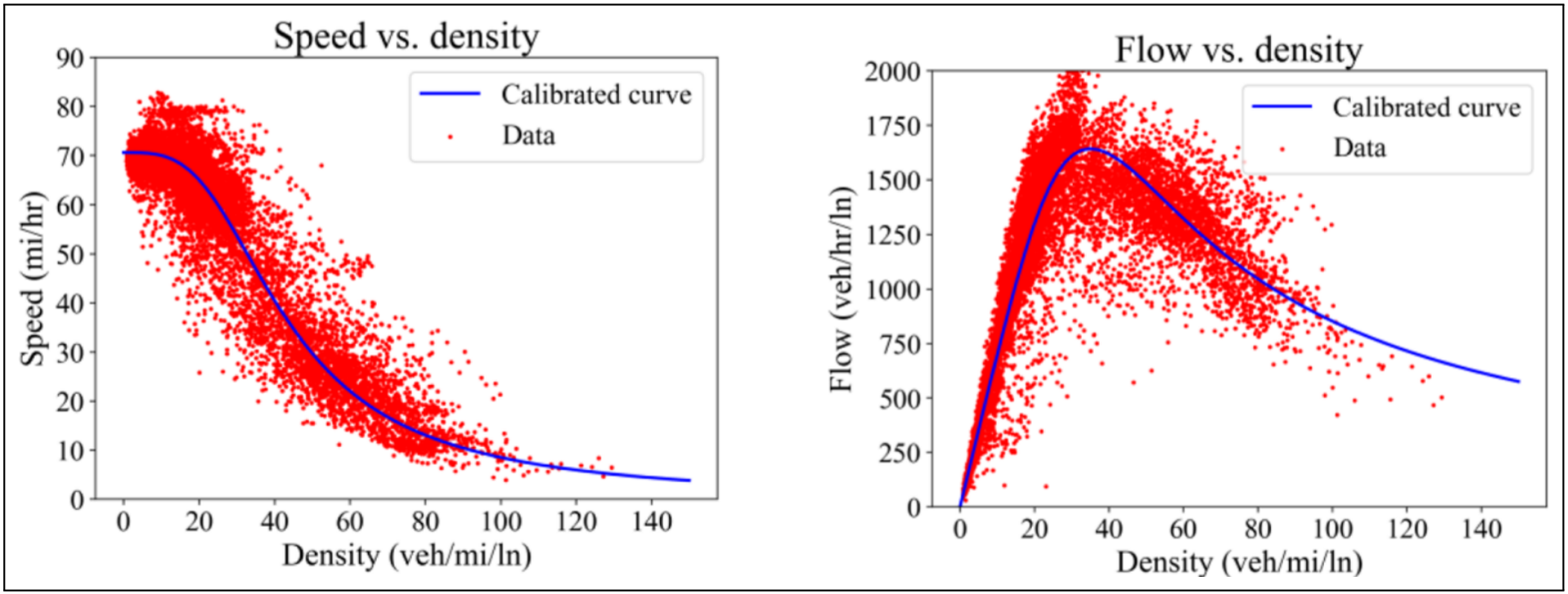
A2 g is non-decreasing in each argument,

A3 $g(\rho, 0) = g(0, \nu) = 0$ for all $\rho, \nu \in \Omega$ (which ensures that no vehicles is removed (resp. added) if the road is empty (resp. at capacity).

(above properties motivated by CRN theory)

Uncertainty of measurements and modeling

fundamental diagrams in practice



(Cheng, Q. et al. (2021). An S-shaped three-parameter (S3) traffic stream model with consistent car following relationship. *Transportation Research Part B: Methodological*, 153, 246-271.)

Generality of the flux function

- any flux function f that can be written as

$$f(\rho) = g_1(\rho) g_2(\rho_{\max} - \rho), \quad \rho \in \Omega,$$

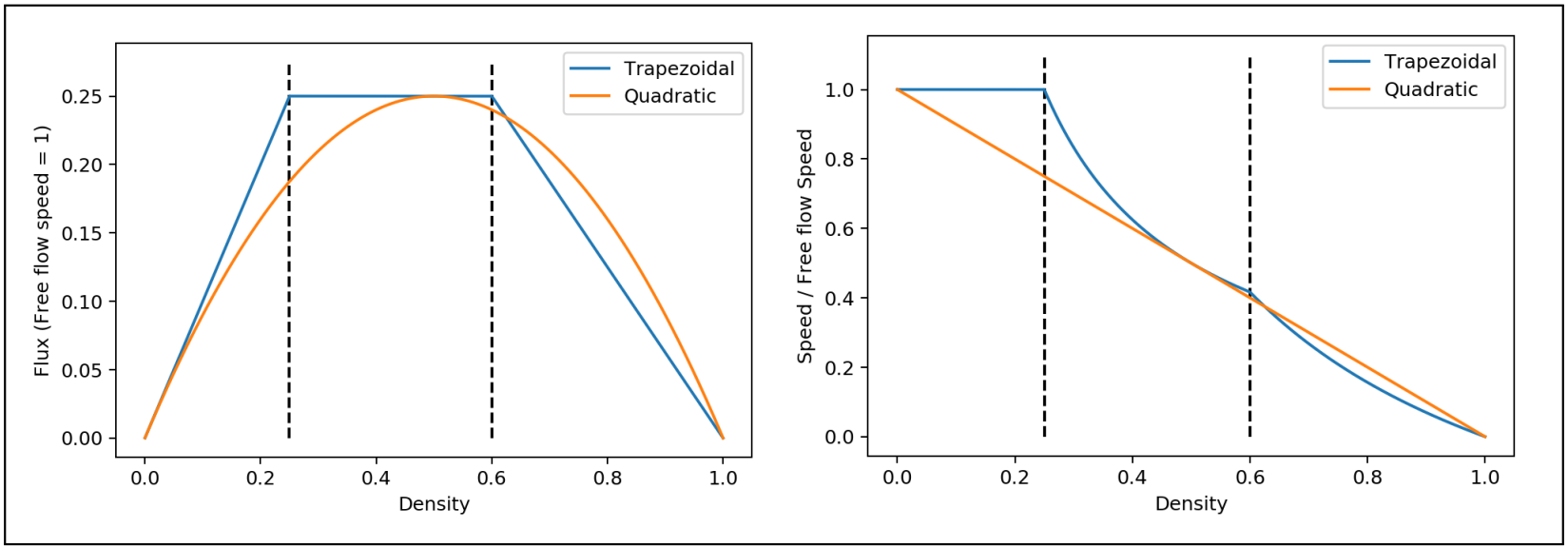
  where g_1 and g_2 are non-decreasing Lipschitz-continuous functions with $g_1(0) = g_2(0) = 0$, satisfy Assumptions A1–A3
- if we take $g_1(\rho) = \rho$, then $\rho \mapsto g_2(\rho_{\max} - \rho)$ can be interpreted as the speed-density relationship of the fundamental diagram
- taking $g_2(\nu) \propto \nu$ yields the so-called Greenshields (quadratic) flux function (mass action case)
- can also retrieve trapezoidal fundamental diagrams by considering g_2 as

$$g_2(\nu) = \begin{cases} v_{\max} \frac{\rho_{\max} - \nu_1}{\rho_{\max} - \nu} \frac{\nu}{\nu_2} & \text{if } 0 \le \nu \le \nu_2, \\ v_{\max} \frac{\rho_{\max} - \nu_1}{\rho_{\max} - \nu} & \text{if } \nu_2 \le \nu \le \nu_1, \\ v_{\max} & \text{if } \nu_1 \le \nu \le \nu_{\max}, \end{cases}$$

  where $v_{\max}$: free flow speed, and $\rho_1 = \rho_{\max} - \nu_1$, $\rho_2 = \rho_{\max} - \nu_2$: critical densities of the fundamental diagram which satisfy $0 < \rho_1 \le \rho_2 < \rho_{\max}$

Generality of the flux function

quadratic and trapezoidal fundamental diagrams



On and off ramps

assumed form of source and sink terms:

$$r(x,t,\rho) = 1_{\text{on}}(x) g_{\text{on}}(\rho_{\text{on}}(x,t),\nu), \quad s(x,t,\rho) = 1_{\text{off}}(x) g_{\text{off}}(\rho,\nu_{\text{off}}(x,t)),$$

where

- ρ_{on} and ν_{off}: traffic density of the on-ramp and the free space density of the off-ramp, respectively, and are assumed to be taking values in Ω;
- $g_{\text{on}} : \Omega \times \Omega \mapsto \overline{\mathbb{R}}_+$ and $g_{\text{off}} : \Omega \times \Omega \mapsto \overline{\mathbb{R}}_+$: the traffic flows of the on- and off-ramp, respectively, and assumed to satisfy Assumptions A1–A3;
- spatial position of the on- and off- ramps: indicator functions 1_{on} and 1_{off} defined as

$$1_{\text{on}}(x) = \begin{cases} 1, & \text{if } \underline{x}_{\text{on}} \le x \le \overline{x}_{\text{on}} \\ 0, & \text{otherwise} \end{cases}, 1_{\text{off}}(x) = \begin{cases} 1, & \text{if } \underline{x}_{\text{off}} \le x \le \overline{x}_{\text{off}} \\ 0, & \text{otherwise} \end{cases},$$

for some $\underline{x}_{\text{on}} \le \overline{x}_{\text{on}}$ and $\underline{x}_{\text{off}} \le \overline{x}_{\text{off}}$.

Spatial discretization of flow models in PDE form

- average (traffic) density in the i-th cell:

$$\rho_i(t) \approx \frac{1}{\Delta x} \int_{x_{i-1/2}}^{x_{i+1/2}} \rho(x,t)\, dx,$$

  where $\Delta x = x_{i+1/2} - x_{i-1/2}$ is the length of a cell.
- this gives a finite volume (semi)discretization scheme (called TRM):

$$\dot{\rho}_i = \frac{1}{\Delta x}\big[F(\rho_{i-1},\rho_i) - F(\rho_i,\rho_{i+1}) + R_i(\rho_i,t) - S_i(\rho_i,t)\big], \quad (1)$$

  with the so-called numerical flux

$$F(u,v) = g(u, \rho_{\mathsf{max}} - v),$$

  and initial condition $\rho_i(0) = \frac{1}{\Delta x}\int_{x_{i-1/2}}^{x_{i+1/2}} \rho(x,0)\, dx \in \Omega$

Flux properties

Theorem

The numerical flux F is consistent with the flux function f (i.e. it satisfies for any $u \in \Omega$, $F(u,u) = f(u)$) and is monotone. As for the TRM defined in (1), it preserves nonnegativity and capacity, and it is a conservative finite volume scheme.

different decompositions of $f = g(\rho, \rho_{\max} - \rho)$ can be proposed, e.g.:

$$
\begin{aligned}
&g_{\mathrm{MAK}}(\rho,\nu) = \omega\rho\nu = \omega\rho(\rho_{\max}-\rho), \quad (\omega = v_{\max}/\rho_{\max}) \\
&g_{\mathrm{Gdnv}}(\rho,\nu) = \min(D(\rho), Q(\rho_{\max}-\nu)), \\
&g_{\mathrm{Cap}}(\rho,\nu) = D(\rho)Q(\rho_{\max}-\nu)/f_{\max},
\end{aligned}
\tag{2}
$$

where $D(\rho) = f(\min\{\rho, \rho_{\mathsf{crit}}\})$, $Q(\rho) = f(\max(\rho, \rho_{\mathsf{crit}}))$: supply and demand functions, respectively, $f_{\max}$: maximal flux value
note that $g_{\mathrm{Gdnv}}(\rho,\nu)$ in (2) is the Godunov flux $\Longrightarrow$ the Godunov scheme can be seen as a particular instance of the proposed model class

The polynomial (mass action) case

the numerical flux is given as

$$F(\rho_{i-1},\rho_i) = g_{\mathrm{MAK}}(\underbrace{\rho_{i-1}}_{\rho}, \underbrace{\rho_{\max}-\rho_i}_{\nu}) = \omega\rho_{i-1}(\rho_{\max}-\rho_i)$$

the semi-discretized model is

$$\dot{\rho}_i = \frac{1}{\Delta x}\Big[\underbrace{\omega\rho_{i-1}(\rho_{\max}-\rho_i)}_{\text{inflow from previous cell}} - \underbrace{\omega\rho_i(\rho_{\max}-\rho_{i+1})}_{\text{outflow to next cell}} + \underbrace{R_i(\rho_{\max}-\rho_i,t)}_{\text{on ramp}} - \underbrace{S_i(\rho_i,t)}_{\text{off ramp}}\Big]$$

transition rate between cells i and $i+1$ depends on

- number (density) of vehicles in cell i
- amount of free space in cell $i+1$

this is clearly kinetic, but what can be a meaningful reaction network behind?

Kinetic interpretation of transition between compartments

- Q: set of compartments (cells)
- $A \subset Q \times Q$ set of transitions (no loops)
- if $(q_i, q_j) \in A$, then q_i is the **donor** of q_j and q_j is the **recipient** of q_i
  - set of donors $\mathcal{D}_i$ and recipients $\mathcal{R}_i$
- kinetic representation of $(q_i, q_j) \in A$

$$N_i + S_j \xrightarrow{\mathcal{K}_{ij}} N_j + S_i$$

where N_i and S_i denote the amount of modeled items (objects) and available space units in q_i, respectively

- dynamics in a redundant state space (may have any network structure)

$$\dot{n}_i = \sum_{j \in \mathcal{D}_i} \mathcal{K}_{ji}(n_j, s_i) - \sum_{j \in \mathcal{R}_i} \mathcal{K}_{ij}(n_i, s_j)$$

$$\dot{s}_i = -\sum_{j \in \mathcal{D}_i} \mathcal{K}_{ji}(n_j, s_i) + \sum_{j \in \mathcal{R}_i} \mathcal{K}_{ij}(n_i, s_j)$$

- compartmental in the sense of Jacquez et al. (1993)
- capacities of compartments are bounded $(n_i(t) + s_i(t) = n_i(0) + s_i(0) =: c_i)$

Reduced state space

- $c_i := n_i(t) + s_i(t)$ is the constant capacity of q_i
  - let $c^{(m)} \in \mathbb{R}^m$ be such that $c_i^{(m)} = c_i$
- reduced state space $C := [0, c_1] \times [0, c_2] \times \cdots \times [0, c_m]$

$$\dot{n}_i = \sum_{j \in \mathcal{D}_i} \mathcal{K}_{ji}(n_j, c_i - n_i) - \sum_{j \in \mathcal{R}_i} \mathcal{K}_{ij}(n_i, c_j - n_j)$$

This has the same structure as the semi-discretized flow model with $n_i \rightsquigarrow \rho_i$, and $c_i \rightsquigarrow \rho_{\max}$

- including on and off ramps:

$$S_i \xrightarrow{\mathcal{K}_{\text{on},i}(t)} N_i, \quad N_i \xrightarrow{\mathcal{K}_{\text{off},i}(t)} S_i$$

Relation between the models

- discretized flow model recalled:

$$\dot{\rho}_i = \frac{1}{\Delta x}[g(\rho_{i-1}, \rho_{\max} - \rho_i) - g(\rho_i, \rho_{\max} - \rho_{i+1}) + R_i(\rho_{\max} - \rho_i, t) - S_i(\rho_i, t)],$$

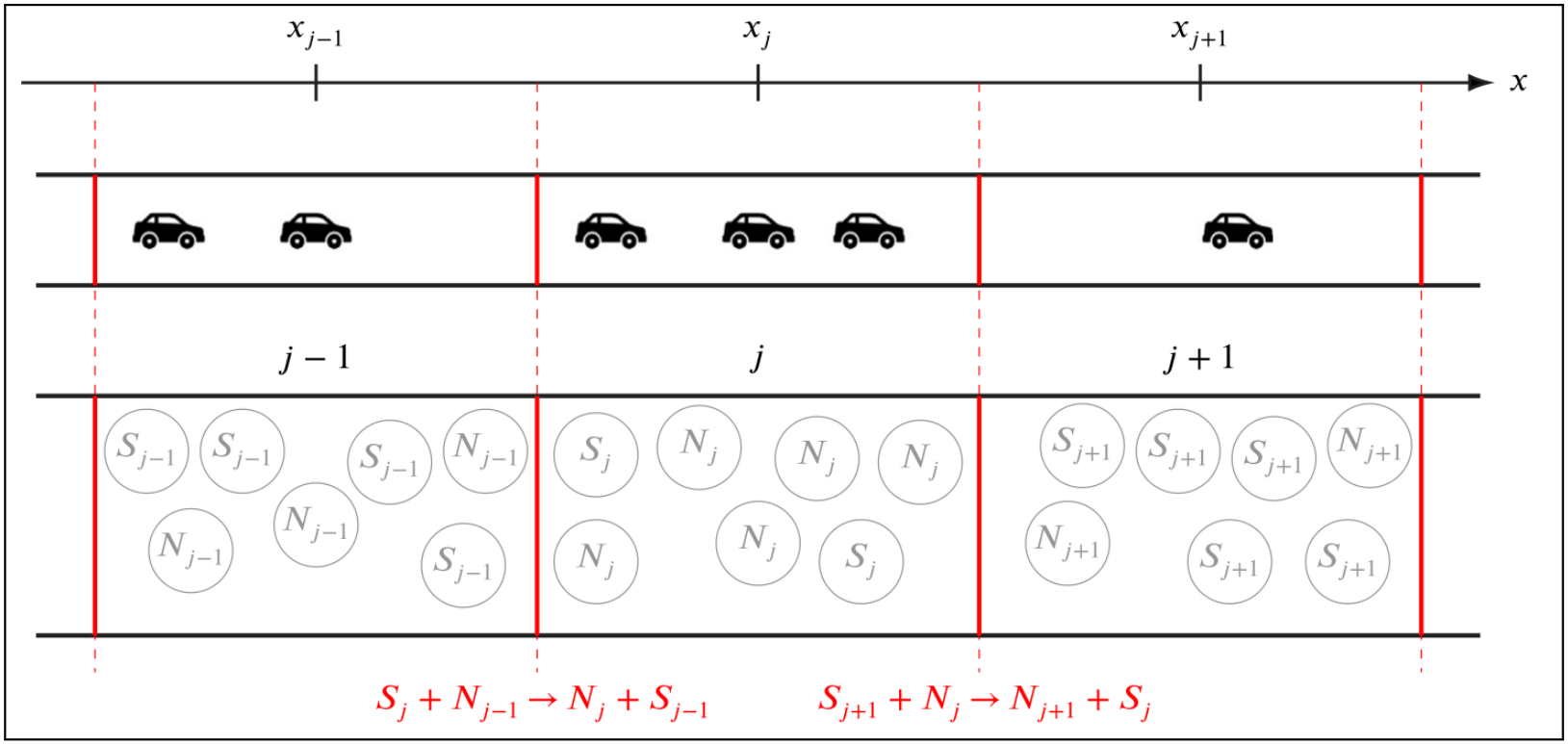
- kinetic equations of the simple tubular (road) structure

$$\dot{n}_i = \mathcal{K}_{i-1,i}(n_{i-1}, c_i - n_i) - \mathcal{K}_{i,i+1}(n_i, c_{i+1} - n_{i+1}) + \mathcal{K}_{\mathsf{on},i}(c_i - n_i, t) - \mathcal{K}_{\mathsf{off},i}(n_i, t)$$

- relation: $\mathcal{K}_{i,i+1}(\rho, \nu) = \frac{1}{\Delta x} g(\rho, \nu)$
- mass action case:

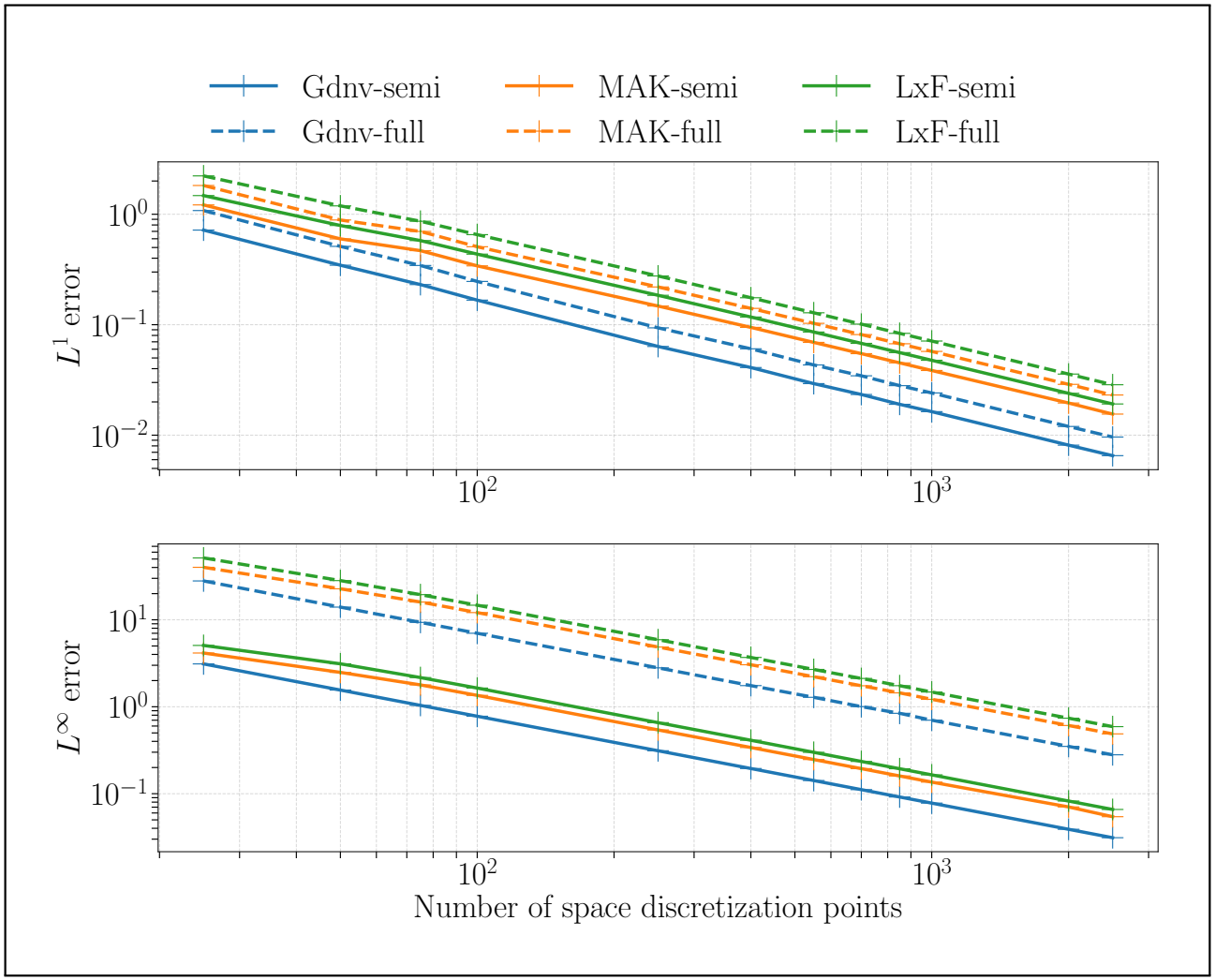
$$g_{\mathrm{MAK}}(\rho_{i-1}, \rho_{\max} - \rho_i) = \omega \rho_{i-1}(\rho_{\max} - \rho_i)$$
$$\mathcal{K}_{i-1,i}(n_{i-1}, c_i - n_i) = k n_{i-1}(c_i - n_i)$$

Kinetic view of traffic flows



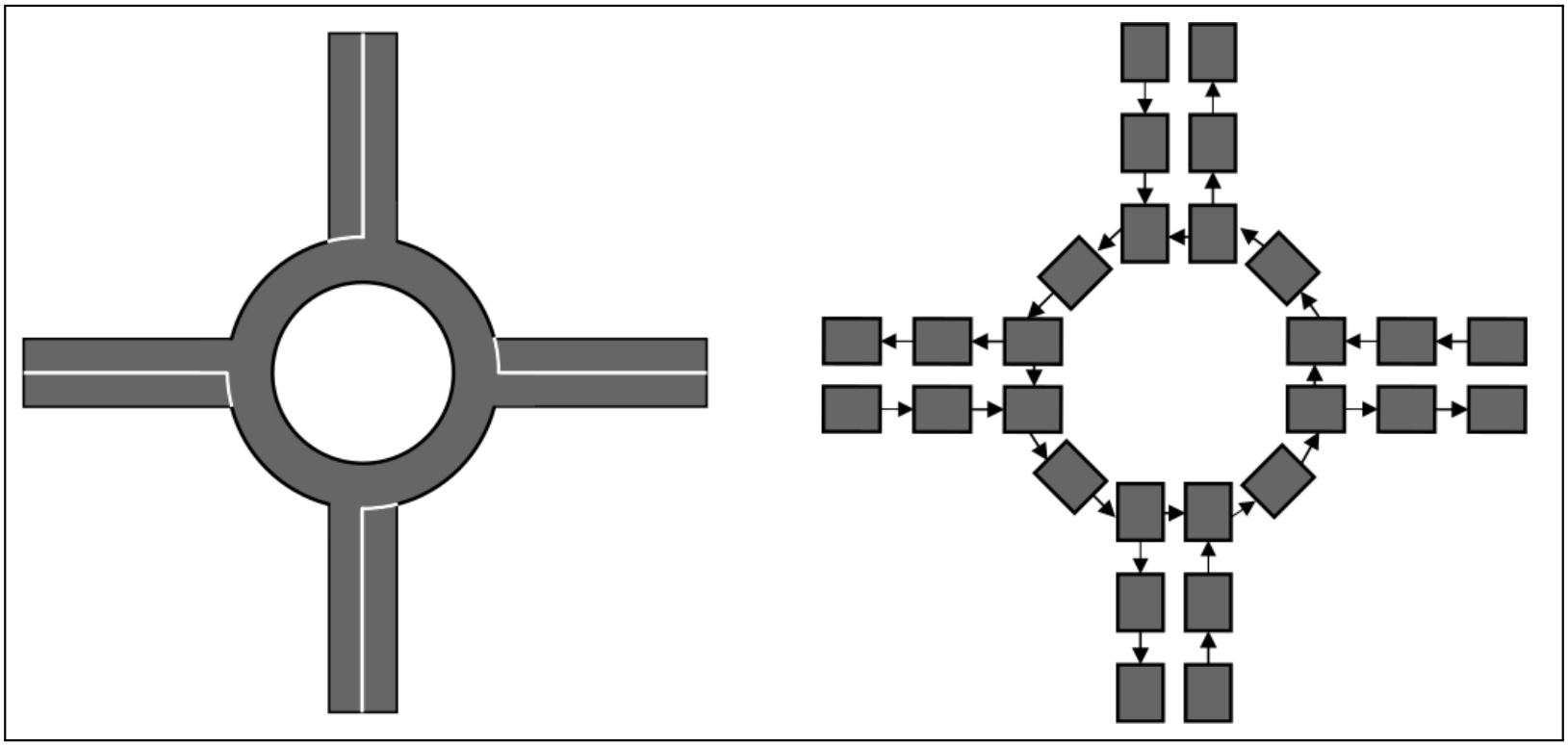
Numerical comparison: solution with a shock wave

$$\rho(x,0) = \begin{cases} 0.1\rho_{\max} & \text{if } x < L/2 \\ 0.8\rho_{\max} & \text{otherwise,} \end{cases}$$



Networked model

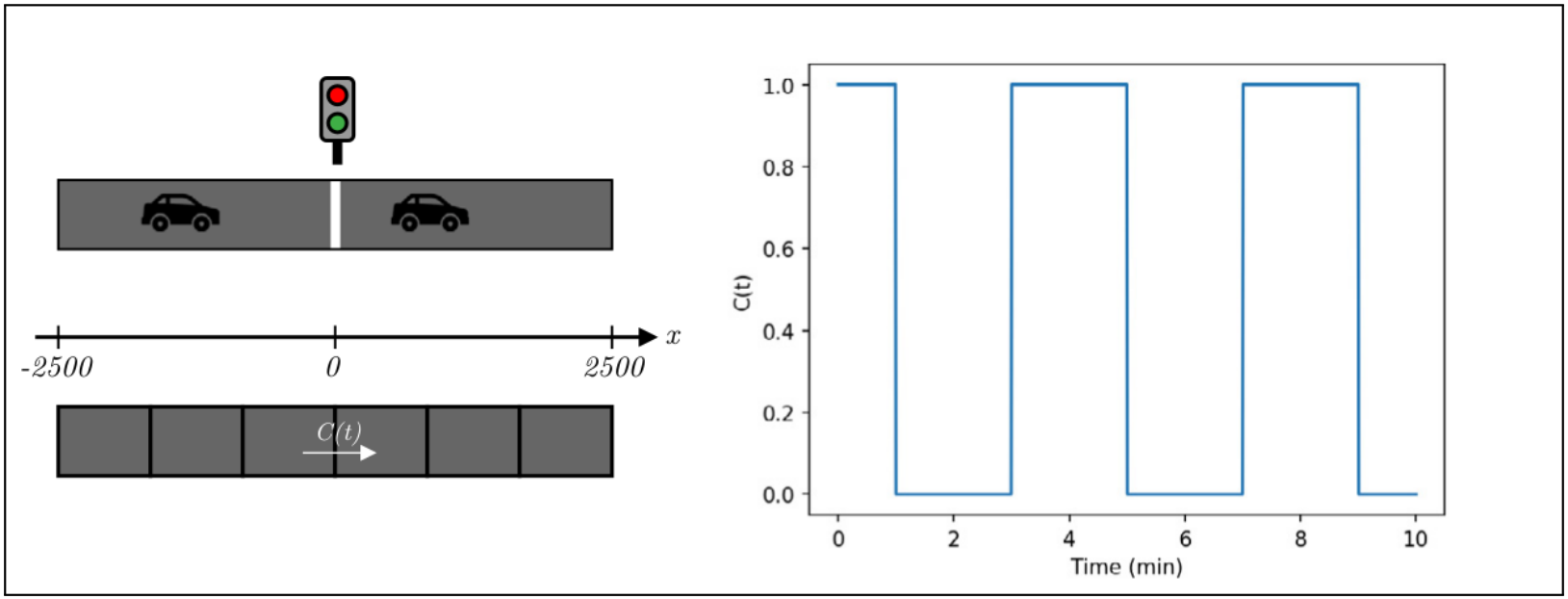
possible application: discretization of a roundabout



Traffic control: time-varying reaction rates

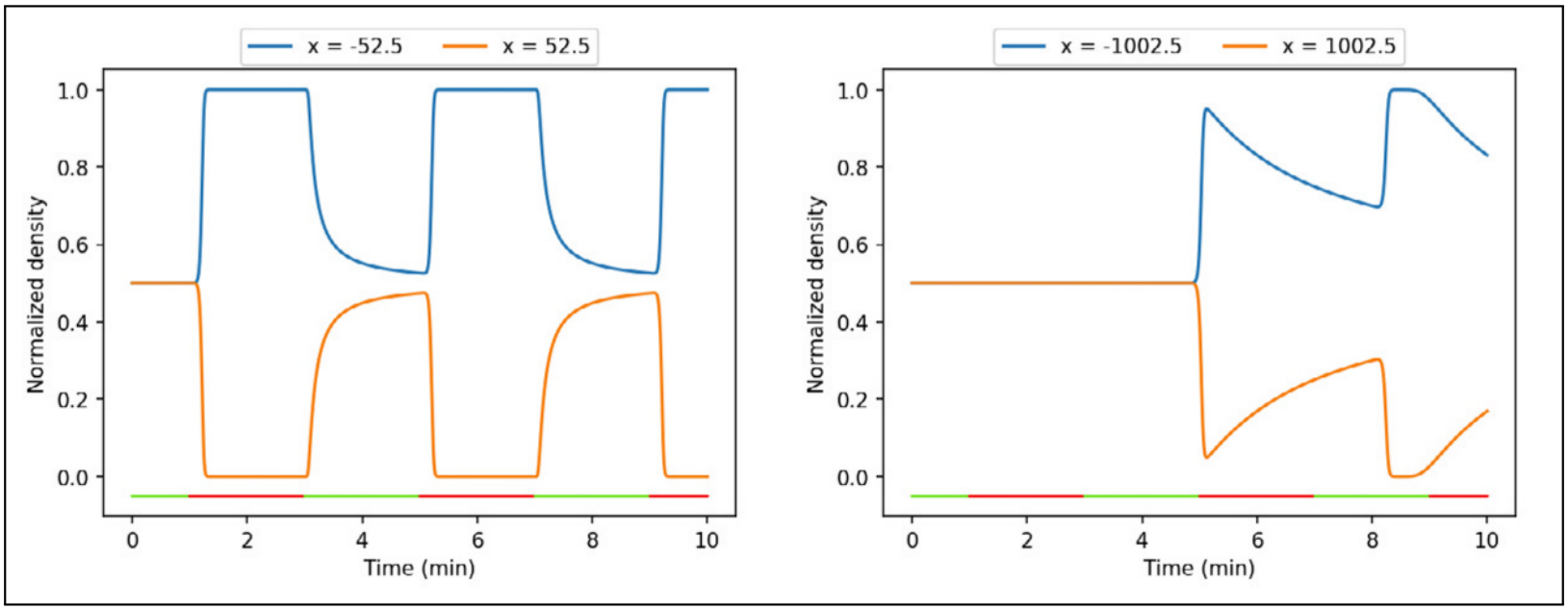
extended model:

$$\dot{\rho}_i(t) = \frac{1}{\Delta x}\left(C_i(t)F_i(\rho_{i-1},\rho_i) - C_{i+1}(t)F_{i+1}(\rho_i,\rho_{i+1}) + R_i(\rho_i,t) - S_i(\rho_i,t)\right)$$



Traffic control: time-varying reaction rates

densities near and far



Further remarks

- the studied models belong to the class of generalized ribosome flow models (GRFMs)
- the reaction rates do not need to be mass action: practically any fundamental diagram can be described
- we know a lot about persistence and the existence and uniqueness of equilibria
- we have a whole family of logarithmic Lyapunov functions
- we have a port-Hamiltonian description
- model calibration (fitting) is quite straightforward
- many advantageous properties are preserved in the time-varying case

Summary

- the kinetic representation of (traffic) flow models was studied
- the same model structure can be obtained from
  1. a special FVM-type semi-discretization of the flow PDE
  2. the kinetic description of compartmental transitions between cells
  3. (statistical physics, asymmetric simple exclusion processes)
- main relationship:

  species $\rightsquigarrow$ vehicles and space units
  reactions $\rightsquigarrow$ cell transitions

- (numerical) flux is transparently related to the reaction rate
- several popular discretization schemes are kinetic with various reaction rates (not all)
- the MAK scheme is numerically not the 'best', but still converges well, and gives a second order polynomial model which is advantageous for analysis, control etc.
- road networks can also be described in an ODE setting
- CRNT can be used in another interesting application domain

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Co-authors, students

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Related publications

- Pereira, M., Kulcsár, B., Lipták, G., Kovács, M., & Szederkényi, G. (2024). The Traffic Reaction Model: A kinetic compartmental approach to road traffic modeling. *Transportation Research Part C: Emerging Technologies*, 158, 104435.
- Vághy, M. A., & Szederkényi, G. (2023). Persistence and stability of generalized ribosome flow models with time-varying transition rates. *PLoS One*, 18(7), e0288148.
- Szederkényi, G., Ács, B., Lipták, G., & Vághy, M. A. (2022). Persistence and stability of a class of kinetic compartmental models. *Journal of Mathematical Chemistry*, 60(6), 1001-1020.