J. Differential Equations 254 (2013) 1359–1374

Contents lists available at SciVerse ScienceDirect

Journal of Differential Equations

www.elsevier.com/locate/jde

Global convergence in systems of differential equations arising from chemical reaction networks

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ARTICLE INFO

Article history:
Received 8 May 2012
Available online 1 November 2012

Keywords:
Global attractivity
Monotone dynamical systems
Chemical reactions
Network structure
DSR graph

ABSTRACT

It is shown that certain classes of differential equations arising from the modelling of chemical reaction networks have the following property: the state space is foliated by invariant subspaces each of which contains a unique equilibrium which, in turn, attracts all initial conditions on the associated subspace.

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1. Introduction

There are difficult and interesting open questions about allowed asymptotic behaviour in systems of differential equations arising in the modelling of chemical reaction networks (CRNs for short). The main goal in this area is to make claims about the behaviour of these systems which are as far as possible independent of the particular choices of functions or parameters which describe the rates of reaction or "kinetics". Classical results in this direction [1,2] rely strongly on the choice of "mass action kinetics" leading to particular polynomial differential equations. Mathematically, such results involve proving that solutions of certain parameterised families of polynomial differential equations have certain asymptotic behaviours regardless of the values of the parameters, but provided these have fixed sign. However when the kinetics is constrained only by loose qualitative laws, the family of possible differential equations describing a reaction network becomes much larger, and results become fewer. Here, we provide a general result based on the theory of monotone dynamical systems [3,4], and use it to prove global convergence in certain classes of CRNs where only very mild assumptions are made on the kinetics.

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0022-0396/$ – see front matter © 2012 Elsevier Inc. All rights reserved.
http://dx.doi.org/10.1016/j.jde.2012.10.018

The key geometrical insight on which the results are built was provided in [5] and generalised in [6]. Stated very briefly, these results show that sometimes the existence of an integral of motion in a strongly order-preserving dynamical system allows the construction of a Liapunov function on each level set, which increases along nontrivial orbits. This in turn has strong implications for the convergence of orbits. While in general it may be an unusual conjunction of affairs to have a first integral, strong monotonicity, and moreover integral and order cone related in a particular way, it actually appears that this situation is not uncommon in CRNs. However identifying when this situation occurs is nontrivial, and explicit construction of families of CRNs satisfying all these conditions becomes important.

The results at several points will be presented in considerably less generality than possible in order to simplify the presentation and highlight the key geometrical points, although where a theoretical result allows greater generality, this may be mentioned.

2. A convergence result

The result presented in this section, and applied in subsequent sections, is essentially derived from Theorem 2.4 in [6], with slight modification and specialisation for our purposes. Note that Theorem 2.4 in [6] stated that all orbits on a level set of the system in question converge to a unique equilibrium, provided the equilibrium exists, while what was actually proved was that all *bounded* orbits converge to the unique equilibrium. As remarked in [7], it remains an open question whether the word "bounded" can be dropped from the statement of the main result as erroneously done in [6]. However for the purposes of this paper all orbits will be bounded and only convergence of bounded orbits is required. Note also that much of the difficulty in the proof of Theorem 2.4 in [6] stemmed from the fact that the integrals of motion considered were in general nonlinear whereas here only the linear case is required.

Standard notions from convex geometry (as in [8–10] for example) will be assumed. Closed, convex and pointed cones in $\mathbb{R}^n$ define partial orders on $\mathbb{R}^n$. Following [8], cones in $\mathbb{R}^n$ which are closed, convex, pointed and solid will be referred to as *proper*. Standard results in the theory of monotone dynamical systems [3,4] will also be assumed.

Notation. The symbols $<, >, \leqslant, \geqslant, \ll, \gg$ will refer to the usual partial ordering of vectors in $\mathbb{R}^n$ derived from the nonnegative orthant $\mathbb{R}^n_{\geqslant 0}$. So, given $a, b \in \mathbb{R}^n$, $a \leqslant b$ means $b - a \in \mathbb{R}^n_{\geqslant 0}$, $a < b$ means $b - a \in \mathbb{R}^n_{\geqslant 0}\backslash\{0\}$ and $a \ll b$ means $b - a \in \mathrm{int}(\mathbb{R}^n_{\geqslant 0})$. When the ordering is defined by some other closed, convex and pointed cone K, the alternative symbols $\prec, \succ, \preccurlyeq, \succcurlyeq, \lll, \ggg$ will be used. So, for example, $a \lll b$ means $b - a \in \mathrm{int}\, K$, and so forth.

Let Y, K be proper cones in $\mathbb{R}^n$ with $K \supseteq Y$. Define K^* to be the dual cone to K, i.e., $K^* = \{y \in \mathbb{R}^n \mid \langle y, k\rangle \geqslant 0 \text{ for all } k \in K\}$. Consider a system

$$\dot{x} = F(x) \tag{1}$$

on Y, and assume that (1) defines a local semiflow ϕ on Y.

2.1. Three conditions

We define three conditions on (1) and the associated semiflow which will be referred to as Conditions 1, 2 and 3:

1. ϕ is *monotone* with respect to K, i.e., given $x, y \in Y$ with $x \prec y$ and any $t > 0$ such that $\phi_t(x)$ and $\phi_t(y)$ are defined, $\phi_t(x) \prec \phi_t(y)$. Moreover, ϕ is *strongly monotone* in $\mathrm{int}\, Y$ in the following sense: given $x \prec y$ with at least one of x or y in $\mathrm{int}\, Y$, then $\phi_t(x) \lll \phi_t(y)$ for all $t > 0$ such that $\phi_t(x)$ and $\phi_t(y)$ are defined.

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