Karin Gatermann\textsuperscript{1}

Counting stable solutions of sparse polynomial systems in chemistry

\textsuperscript{1}FU Berlin

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Abstract. The polynomial differential system modeling the behavior of a chemical reaction is given by graph theoretic structures. The concepts from toric geometry are applied to study the steady states and stable steady states. Deformed toric varieties give some insight and enable graph theoretic interpretations. The importance of the circuits in the directed graph are emphasized. The counting of positive solutions of a sparse polynomial system by B. Sturmfels is generalized to the counting of stable positive solutions in case of a polynomial differential equation. The generalization is based on a method by sparse resultants to detect whether a system may have a Hopf bifurcation. Special examples from chemistry are used to illustrate the theoretical results.

1. Introduction

In chemistry a class of polynomial differential equations arise which has a lot of discrete structure in the coefficients and the monomials:

\[ \dot{x} = Y_a I_a I_K \Psi(x), \quad \Psi(x) = \begin{pmatrix} x^{n_1} \\ \vdots \\ x^{n_k} \end{pmatrix}, \]

is given by adjacency matrices and incidence matrices of two weighted graphs. A detailed description of the problem is given in Section 2. One is interested in the positive steady states, stable ones and Hopf points, especially depending on the structure of the graphs and for all positive values of the involved constants \(k_{ij}\). This fascinating problem shows a very rich mathematical structure and several mathematical disciplines may be applied.

Numerical methods are not suitable since several (too many) unknown constants are involved and one is interested in global statements while numerical investigations are local.

There are several known results. Especially, the early work in [Cl80] has influenced a lot the chemical literature like [EBSE96, E94, HS98]. The papers [F, F95a, F95b] (for explanation see also [GH99]) include special interesting results for a special subclass \(Y_a = Y_b\). In [MMN89] symbolic computation has been
applied to such chemical systems for the first time. They applied Gröbner bases as a black box neglecting the structure of the problem. Of course Gröbner bases are very important for the study of positive solutions ([GRRT99]), but in this problem class the computation of a Gröbner bases of the given polynomials ignore the graph theoretic structures. That’s why the use of Gröbner bases is restricted to study toric ideals which appear.

Toric varieties turn out to be very useful if they are adjusted to this particular application. The generalization is even suitable for the study of positive solutions. A realistic example illustrates this principle and nicely interpreted by substructures of the graphs.

But the main result is the counting of stable positive solutions by a generalization of ideas from [St94, St98]. For this reason the new polynomial $\text{Res}_{B,H}$ is introduced. The vanishing of $\text{Res}_{B,H}$ is a necessary condition that a dynamical system has a Hopf point.

The structure of the paper is as follows. Section 2 describes the given data and the structure of the differential equations precisely. Deformed toric varieties and graph theoretic investigation of a convex polyhedral cone are the topics of Section 3 while Section 4 investigates Hopf bifurcation with resultants and bilinear products. Finally, Section 5 gives the main result of this paper, the counting of positive stable steady states as a generalization of the counting of positive solutions in [St94, St98].

2. Mass action kinetics - a sparse polynomial system

An interesting system of ordinary differential equations consisting of sparse polynomials is defined by two graphs as presented in [GH99].

The first graph is a weighted bipartite graph. The two sets of vertices consist of $S_i$, $i = 1, \ldots, m$ and $C_j$, $j = 1, \ldots, n$. To each edge $\{S_i, C_j\}$ there are two weights $y_{ij} \in \mathbb{N}$ and $\eta_{ij} \in \mathbb{N}$ associated. This defines two weighted adjacency matrices whose relevant parts are $Y_s = (y_{ij})_{i=1, \ldots, m, j=1, \ldots, n}$ and $Y_k = (\eta_{ij})_{i=1, \ldots, m, j=1, \ldots, n}$. We denote the columns of $Y_s$ by $y_1, \ldots, y_n \in (\mathbb{Z}_{\geq 0})^m$ and the columns of $Y_k$ by $\eta_1, \ldots, \eta_n \in (\mathbb{Z}_{\geq 0})^m$. We assume that $Y_s$ and $Y_k$ have the same support (i.e. $y_{ij} = 0$ iff $\eta_{ij} = 0$ and $y_{ij} > 0$ iff $\eta_{ij} > 0$) and that $\eta_{ij} < y_{ij}$ for all $i = 1, \ldots, m, j = 1, \ldots, n$. Moreover, we assume that $y_i \neq y_j$ or $\eta_i \neq \eta_j$ for all $i \neq j$. Additionally, we assume that every vertex $S_i$ is adjacent at least to one vertex $C_j$. But there may be $C_j$ without incident edges.

Secondly, there is a weighted directed graph with vertices $C_i, i = 1, \ldots, n$ and oriented edges $C_j \rightarrow C_i$ for some $i, j \in \{1, \ldots, n\}$. Each oriented edge (arrow) $C_j \rightarrow C_i$ from reactant $C_j$ to product $C_i$ has a weight $k_{C_j \rightarrow C_i} = k_{ij} \in \mathbb{R}_+$. This information is encoded in the weighted adjacency matrix $K = (k_{ij}) \in (\mathbb{R}_{\geq 0})^{m,n}$ with $k_{ij} = 0$ if $C_j \rightarrow C_i$ is not an arrow. We assume that for each vertex $C_i$ there is at least one adjacent edge. An oriented edge $C_j \rightarrow C_i$ and its opposite $C_i \rightarrow C_j$ with two different associated constants are simultaneously possible. But there are parallel edges.

Beside the adjacency matrix the directed graph has two incidence matrices. The first incidence matrix is $I_s = (w_{ij})_{i=1, \ldots, m, j=1, \ldots, n}$ where $w_{ij} \in \{-1,0,1\}$ and $a$ denotes the number of arrows. Each column represents an oriented edge by containing one entry $-1$ for the reactant and 1 for the product. The second incidence matrix is $I_K = (u_{\mu\nu})_{\mu=1, \ldots, m, \nu=1, \ldots, n}$ with $u_{\mu\nu} \in \{k_{ij} \mid i, j = 1, \ldots, n\}$ or $u_{\mu\nu} = 0$. 

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Table 1. The algebra-chemistry dictionary.

<table>
<thead>
<tr>
<th>SNA stoichiometric network analysis</th>
<th>$Y_s$ stoichiometric matrix</th>
<th>$S = \text{im}(Y_sA)$ stoichiometric space</th>
<th>$v_i \perp \text{im}(Y_sA)$ conservation vector ($v_i \geq 0$)</th>
<th>$v'_i x - a_i$ conservation relations ($v_i \geq 0$)</th>
<th>$A \Psi(x)$ complex formation vector</th>
<th>$I_K \Psi(x)$ reaction velocity vector</th>
<th>$k_{ij}$ rate constant</th>
<th>$y_{ij}$ stoichiometric coeff. or molecularity</th>
<th>$C_i$ complexes</th>
<th>$\delta = \text{rank}(I_a) - \text{rank}(Y_s A)$ deficiency</th>
<th>$Y_s A \Psi(x)$ species formation vector</th>
<th>$S_i$ chemical species</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A = I_a I_K$ kinetic matrix</td>
<td>$\text{im}(Y_s A I_K) = \text{im}(Y_s A)$ kinetic space</td>
<td>$\exists v_i \perp \text{im}(Y_s A), v_i &gt; 0$ conservative</td>
<td>$\delta = \text{rank}(I_a) - \text{rank}(Y_s A)$ deficiency</td>
<td>$Y_s A \Psi(x)$ species formation vector</td>
<td>$S_i$ chemical species</td>
<td></td>
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</tr>
</tbody>
</table>

Each row corresponds to one oriented edge and has at most one non-zero entry. The $\mu$-th arrow $C_j \rightarrow C_i$ gives $u_{\mu ij} = k_{ij}$ encoding the weight and that $C_j$ is the reactant complex.

Altogether, this defines the following polynomial differential equation

$$
\dot{x} = Y_s A \Psi(x), \quad \text{with} \quad \Psi(x) = \begin{pmatrix} x^m \\ \vdots \\ x^m \end{pmatrix},
$$

where $A = I_a I_K = K - \text{diag}(K^t e)$ and $x = (x_1, \ldots, x_m) \in (\mathbb{R}_{\geq 0})^m$.

In [CL80] the matrix $\nu := Y_s I_a$ is used. With $v(x) = I_K \Psi(x)$ system (2.1) is written as

$$
\dot{x} = \nu v(x),
$$

Moreover, $v(x)$ may be written as $D \chi(x)$ with a diagonal matrix $D \in (\mathbb{R}_{\geq 0})^{d \times d}$ containing diagonal entries $d_{\mu \mu} = k_{ij}$ for the $\mu$-th arrow $C_j \rightarrow C_i$ and a vector of monomials $\chi(x) = (x^{e_1}, \ldots, x^{e_m})$, $\chi_{\mu}(x) = x^{e_{\mu}}$. The matrix $\kappa$ of exponents as used in [CL80] is formed from the columns of $Y_k$. More precisely they are formed from the columns of $Y_r$ which is given by those columns $\eta_k$ from $Y_k$ for which an arrow $C_i \rightarrow C_j$ exists.

A special case is that $Y_s$ can be chosen such that $Y_s = Y_k$. Then system (2.1) is a stoichiometric system or with mass action kinetics. This name stems from the fact that the graphs naturally arise in chemistry where (2.1) describes the evolution of the concentrations $x_i$ of the chemical species $S_i$. Also all other quantities have a special name as summarized in Table 1.

System (2.1) has flow-invariant subspaces of the form $(x_0 + \text{im}(Y_s A)) \cap (\mathbb{R}_{\geq 0})^m$, see Lemma 2.7 in [GH99]. Thus one restricts the investigation of steady states to those satisfying

$$
v'_i x - a_i = 0, \quad i = 1, \ldots, m - \text{rank}(Y_s A),
$$

\footnote{The precise definition of mass action kinetics is that it is not pathological ($\exists v_{ij} < 0, \kappa_{ij} = 0$) and for each pair of forward reaction $i$ and backward reaction $j$ we have $v_i = \kappa_j - \kappa_i$, where $v_i, \kappa_j, \kappa_i$ are columns of the matrices $\nu$ and $\kappa$.}
where \( v_i \) form an orthonormal basis of the orthogonal complement of \( \text{im}(Y_s A) \) and the \( a_i \in \mathbb{R} \) are given constants. In the literature often \( \text{im}(Y_s I_a) \) is used. But in case a connected component includes several terminal strong connected components then \( \text{rank}(I_a I_K) < \text{rank}(I_a) \). If \( \text{rank}(Y_s A) < \text{rank}(Y_s I_a) \) the \( v_i \) depend on the constants \( k_{ij} \) in general.

Even more one is interested in stable points (i.e. real parts of all eigenvalues of Jacobian negative) and Hopf points (eigenvalues \( \pm i\omega \)). Since \( \text{im}(Y_s A) \) is flow-invariant the notions of stability and Hopf points are modified in Section 4.

The graph theoretic definitions are explained by the following typical example which was taken from [EBSE96].

**Example 2.1.** Figure 1 and Figure 2 show the same information on a chemical reaction in an analogous way.

The differential equations are

\[
\begin{align*}
\dot{x}_1 &= -k_{2,1}x_1x_2^2 - 2k_{10,7}x_1^2 + 2k_{7,10}x_5^2 \\
\dot{x}_2 &= -2k_{2,1}x_1x_2^2 - 2k_{9,3}x_2^2 - 2k_{11,8}x_2x_4 + 2k_{3,9}x_5 \\
\dot{x}_3 &= k_{2,1}x_1x_2^2 + (-k_{5,4} - k_{9,4}) x_3 \\
\dot{x}_4 &= k_{5,4}x_3 - 2k_{10,6}x_4^2 - 2k_{11,8}x_2x_4 \\
\dot{x}_5 &= k_{2,1}x_1x_2^2 + k_{9,3}x_2^2 + k_{9,4}x_3 + 2k_{10,6}x_4^2 + 2k_{10,7}x_1 + 3k_{11,8}x_2x_4 - k_{3,9}x_5 - 2k_{7,10}x_5^2
\end{align*}
\]

where \( x_1, \ldots, x_5 \) are the concentrations of \( O, H, H_2O, H_2O_f \) and the amount of space on the metal, respectively.
FIGURE 2. Information from Figure 1 as a weighted directed graph and a weighted bipartite graph. An edge in the bipartite graph without number has weights \( y_{ij} = \eta_{ij} = 1 \). If one number is associated to the edge then \( y_{ij} = \eta_{ij} \) else \( y_{ij} > \eta_{ij} \).

We have \( \text{rank}(I_a I_K) = 6, \text{rank}(I_a) = 7, \text{rank}(Y_s I_a I_K) = \text{rank}(Y_s I_a) = 4 < 5 = m \). The additional linear restriction is given by

\[
v_1^T x - a_1 = (2, 1, 2, 2, 2) x - a_1 = 0.
\]

\( \Diamond \)

The nice thing about system (2.1) is that almost all mathematical terms have a graph theoretic meaning. For example we may consider the combined graph from the directed graph and the bipartite graph since the vertices \( C_i \) appear in both. If the combined graph has several connected components then system (2.1) decouples.

In [FH77] it is explained how the structure of the directed graph determines by connected components, strong connected components and terminal strong connected components the structure and the rank of the matrix \( A = I_a I_K \). This knowledge is exploited in the work [F], [F95a], [F95b]. An explanation of this is given in [GH99].

3. Deformed toric varieties and positive steady states

This section is started with the discussion of complex solutions \( x \in (\mathbb{C} \setminus \{0\})^n \) of \( Y_s A \Psi(x) = 0 \) with the help of toric varieties. If one neglects the property of normality they are defined as \( X_{\Gamma_K} = V(I_{\Gamma_K}) = \{ z \in \mathbb{C}^n | f(z) = 0 \forall f \in I_{\Gamma_K} \} \)

\( I_{\Gamma_K} = \{ f \in \mathbb{C}[z_1, \ldots, z_n]| f(x_0 z_1^m, \ldots, x_0 z_n^m) = 0 \} \). Binomial generators of \( I_{\Gamma_K} \) are computed by the usual implicitation of varieties with Gröbner bases or more
efficiently by Algorithms 12.3 and 12.6 in [St96]. See also [KM99] for efficient computation with ideals of this type.

The advantages of toric varieties are well-known. The degree of the toric variety (computed by the coefficient of the Hilbert polynomial [St96] p. 36 or by the mixed volume of the Newton polytopes by mixed subdivision [CLO98]) gives the number of toric solutions for generic coefficients since $I^*_X$ does not depend on the coefficients. The facets of the Newton polytopes are used to explain when for special values of the coefficients some solutions $x \in (\mathbb{C} \setminus \{0\})^n$ escape to points with components zero or to infinity ([CLO98] p. 309).

For positive real solutions one needs to discuss the intersection of the convex polyhedral cone $\text{ker}(Y_x A) \cap (\mathbb{R}_{\geq 0})^n$ (of dimension $n - \text{rank}(Y_x A)$) with $X_{Y_x}$ which is the basis of the deficiency-one-theorem [F95a] as explained in [GH99]. Once a generating vector $z$ of an intersection line is known $z = z_0 \Psi(x)$ is solved by Hermite normal form.

In this application one can take advantage of the special structure. The first obvious property is that not all monomials appear. Remember that the columns of $Y_x$ are formed by those $\eta_i$ for which an arrow $C_i \to C_j$ exists. Then one would consider the homogeneous toric ideal $I^*_X$. But one can even better take advantage of the structure. Because the coefficient matrix in our application is a product of $Y_x$, $I_a$ and $I_K$ and all constants are positive a variant of this principle has even more advantages. We use

$$I^*_z = \{ f \in C(\mathbb{A}) \mid z_1, \ldots, z_n \mid f(x) \equiv 0 \},$$

where $\mathbb{A}$ collects all appearing non-zero $k_{ij}$, and its variety $V(I^*_z)$ and the convex polyhedral cone $\text{ker}(Y_x I_a) \cap (\mathbb{R}_{\geq 0})^n$. The advantage in comparison to the standard approach is that the cone does not involve the constants $k_{ij}$. We denote the elements of a minimal set of generators by $E_i$.

**Lemma 3.1.** (i) If $\text{rank}(Y_x I_a) = \text{rank}(I_a)$ then the positive circuits of the directed graph generate the convex polyhedral cone $\text{ker}(Y_x I_a) \cap (\mathbb{R}_{\geq 0})^n$. Then the minimal generators $E_i$ are given by those positive circuits which are not a convex combination of other positive circuits.

(ii) Let the set of indices $\{1, \ldots, l\}$ decompose with respect to the connected components $L_\lambda$ and even further decompose with respect to terminal strong connected components $L_\lambda = T_\lambda^1 \cup \cdots \cup T_\lambda^{l_\lambda} \cup R_\lambda$. Define $I^*_\lambda = (w_{ij})_{i=1, \ldots, n; j=1, \ldots, l} \in T_\lambda$ where $I_a = (w_{ij})_{i=1, \ldots, n; j=1, \ldots, l}$. If $\text{rank}(Y_x I^*_\lambda) = \text{rank}(I^*_\lambda)$ then the positive circuits of the terminal strong connected components $(\lambda, \nu)$ which are not convex combinations of other positive circuits define minimal generators $E_i$.

While the positive circuits are oriented cycles in the directed graph the other minimal generators have an interpretation in the combined graph consisting of the directed graphs without weights $k_{ij}$ and the bipartite graph with weights $y_{ij}$, see the example below. Note that the cone is not necessarily simplicial, although in many practical situations this will be the case because $\text{rank}(I_a) - \text{rank}(Y_x I_a)$ is small and $\text{ker}(I_a) \cap (\mathbb{R}_{\geq 0})^n$ is a simplicial cone if the directed graph is not complicated.

The generators $E_i$ may be computed by the simplex algorithm from linear programming. But here no linear functional is optimized. A variant of the simplex algorithm is used to enumerate all vertex vectors. Of course one likes to take advantage of the graph theoretic information within this computation. Since $Y_x I_a$ is integer there is even a relation to Gröbner bases. Algorithm 4.3 in [St96] may be
used and an universal Gröbner basis may be computed which by Proposition 4.11 in [St96] includes all circuits. The circuits of type $z^E - 1$ will give our minimal generators. The computation of an universal Gröbner basis (equivalently the determination of the Gröbner fan and the state polytope) works for toric ideals efficiently even for larger problems as shown in [TH99].

Because of the importance of the cone $\ker(Y^t L_A) \cap (\mathbb{R}_{>0})^I$ the computation of a minimal set of generators $E_i$ is studied a lot in the chemical literature ([CI80], [HS98] and references therein). There the fact is used that each $z \in \ker(Y^t L_A) \cap (\mathbb{R}_{>0})^I$ gives a positive solution $x \in \mathbb{R}^m$ if the $k_{ij}$ are chosen appropriately. On the other hand if the constants $k_{ij}$ are given the vector $z \in \ker(Y^t L_A) \cap (\mathbb{R}_{>0})^I$ has to satisfy the condition $z \in V(I_{\mathbb{Z}})$.

**Lemma 3.2.** (i) The ideal $I_{\mathbb{Z}}$ in $\mathbb{C}(k)[z]$ is generated by binomials in $\mathbb{Q}(A)[z]$. (ii) Each vertex $C_i$ in the directed graph which is incident to two (or more) oriented edges pointing out from $C_i$ gives one (or several) linear polynomial(s) in $I_{\mathbb{Z}}$. (iii) $I_{\mathbb{Z}}$ and $I_{\mathbb{Q}}$ have the same Hilbert series and the same Hilbert polynomial.

**Proof.** (i) $I_{\mathbb{Z}}$ is clearly generated by binomials because a Gröbner basis of the elimination ideal $I_{\mathbb{Z}} = \langle \{z_i - x_0 v_i(x) \mid i = 1, \ldots, l \rangle \rangle \cap Q(k)[z]$ may be computed by the Buchberger algorithm where all involved polynomials are binomial if the input polynomials are binomial. (ii) Two arrows $C_i \xrightarrow{\alpha} C_j$ and $C_i \xrightarrow{\beta} C_r$ give $v_\alpha = k_{ij} x^\beta$, $v_\beta = k_{ij} x^\alpha$ and thus $k_{ij} z_\alpha - k_{ij} z_\beta$. (iii) The Hilbert series and the Hilbert polynomial are build from the vector space dimensions of $(\mathbb{C}[z_1, \ldots, z_n]/I_{\mathbb{Z}})_d$ and $(\mathbb{C}[z_1, \ldots, z_n]/I_{\mathbb{Q}})_d$ of degrees $d \in \mathbb{N}$. But for each additional variable in $z_1, \ldots, z_l$ there is a linear polynomial by (ii) such that the dimensions are equal.

Each binomial in $I_{\mathbb{Z}}$ has an interpretation in the combined graph formed from the directed graph with weights $k_{ij}$ and the bipartite graph with weights $\eta_{ij}$, see the example below.
Figure 4. Minimal generator $E_3$ of the cone. The numbers associated to the arrows are $E_3 = [2,0,3,0,2,0,0,1]$ while the weights on the vertices $C_i$ are given by the entries of $I_a E_3 = \{-2,2,3,-2,0,1,-1,-3,-1,1\}$. The computations associated to the vertices $S_i$ stand for $Y_s(I_aE_3)$.

Geometrically, the variation of values of all $k_{ij} > 0$ means that the variety $V(I_\lambda)$ just deforms without changing basic properties. The variety $V(I_{\lambda'})$ is clearly isomorphic to $V(I_{\lambda})$ in case all $k_{ij} = 1$ since for additional variables $z_i$ we have linear equations $z_i = z_{ji}0$. Thus for all positive choices of $k_{ij}$ the varieties $V(I_\lambda)$ and $V(I_{\lambda'})$ are isomorphic. While $X_{\lambda'}$ contains the orbit $O_1 = \{z \in (C \setminus \{0\})^n | \exists t_0, \ldots, t_m \text{ with } z = (t_0 \prod_{i=1}^m t_i^{\eta_{i1}}, \ldots, t_0 \prod_{i=1}^m t_i^{\eta_{in}})\}$ as an open and dense set the deformed toric variety $V(I_{\lambda'})$ contains the orbit $O_{K_0} = \{z \in (C \setminus \{0\})^i | \exists t_0, \ldots, t_m \text{ with } z = \text{diag}(t_0 \prod_{i=1}^m t_i^{\eta_{ij}}), \ldots, t_0 \prod_{i=1}^m t_i^{\eta_{in}})I_{K^0}\}$ as a dense and open set. Even more the structure of subvarieties corresponding to points at infinity or with zero-components is the same. That means that the property that toric solutions escape to infinity depends on the structure of the graphs, but not on their weights. It seems that the positive circuits in the directed graph often turn out to be important in this context.

Example 3.3. (Example 2.1 continued) A minimal set of generators of the convex polyhedral cone $\ker(Y_a I_a) \cap (R \geq 0)^I$ is found by elementary linear algebra

$$E_1 = [0,1,1,0,0,0,0,0,0] \quad E_2 = [0,0,0,0,0,1,1,0]$$

$$E_3 = [2,0,3,0,2,0,0,1,1]$$
$$E_4 = [2,0,2,0,2,1,0,1,0]$$
$$E_5 = [2,0,2,2,0,0,0,1,0].$$

While $I_a E_1 = I_a E_2 = 0$ because these two are positive circuits in the directed graph (see Figure 3) the other three are interpreted in the combined graph as
illustrated in Figure 4 for $E_8$. A Gröbner basis of the deformed toric ideal is computed by using

$$
\begin{align*}
  z_1 &= k_{2,1} \hat{x}_1 \hat{x}_2^2 \hat{x}_0 \quad z_2 = k_{9,3} \hat{x}_2^2 \hat{x}_0 \quad z_3 = k_{3,9} \hat{x}_5 \hat{x}_0 \\
  z_4 &= k_{9,4} \hat{x}_3 \hat{x}_0 \quad z_5 = k_{5,4} \hat{x}_3 \hat{x}_0 \quad z_6 = k_{10,6} \hat{x}_2^2 \hat{x}_0 \\
  z_7 &= k_{10,7} \hat{x}_2^2 \hat{x}_0 \quad z_8 = k_{7,10} \hat{x}_2^2 \hat{x}_0 \quad z_9 = k_{11,8} \hat{x}_2^2 \hat{x}_4 \hat{x}_0
\end{align*}
$$

giving

$$
- k_{9,4} z_4 + k_{9,4} z_5, \quad k_{11,8}^2 z_0 z_2 - k_{9,3} k_{10,6} z_2 z_3, \quad k_{10,7} k_{9,3}^2 k_{7,10} (2 \lambda_3 + 2 \lambda_4 + 2 \lambda_5) \lambda_1^2 \lambda_2 \lambda_3 \lambda_4 \lambda_5.
$$

Substituting $\sum_{i=1}^5 \lambda_i E_i$ gives three polynomials in $\lambda$

$$
-2 k_{9,4} \lambda_5 + k_{9,4} (2 \lambda_3 + 2 \lambda_4), \quad k_{11,8}^2 \lambda_4 \lambda_1 - k_{9,3} k_{10,6} \lambda_3^2, \quad k_{10,7} k_{9,3}^2 k_{7,10} (2 \lambda_3 + 2 \lambda_4 + 2 \lambda_5) \lambda_1^2 \lambda_2 \lambda_3 \lambda_4 \lambda_5.
$$

**CASE $\lambda_3 = 0$:** Then case $\lambda_1 = 0$ gives $\lambda_4 = \lambda_5 = 0$ and $\lambda_2$ arbitrary. The case $\lambda_4 = 0$ leads to $\lambda_5 = 0$ and $\lambda_1 = 0$ and $\lambda_2$ arbitrary or opposite $\lambda_2 = 0$ and $\lambda_1$ arbitrary.

**CASE $\lambda_3 \neq 0$:** Because we work in homogeneous coordinates we may choose $\lambda_3 = 1$ and receive from the first two equations

$$
\begin{align*}
  \lambda_5 &= \frac{k_{9,4} (k_{11,8} k_{1,4} + k_{9,3} k_{10,6})}{k_{11,8} k_{1,4} k_{9,4}}, \quad \lambda_4 = \frac{k_{9,3} k_{10,6}}{k_{11,8} k_{1,4}}.
\end{align*}
$$

Substitution into the third gives one polynomial in $\lambda_1, \lambda_2$

$$
 c_2 \lambda_1^4 \lambda_2^0 + (c_{14} \lambda_1^0 + c_{16} \lambda_1^0 + c_{18} \lambda_1^0) \lambda_2 - c_8 \lambda_1^0 - \cdots - c_0 \lambda_1^0
$$

which is quadratic in $\lambda_2$ having positive coefficients of $\lambda_2^0$ and $\lambda_2$ and negative constant $c_0 (\lambda_1, \lambda_2)$ if we consider $\lambda_1$ to be positive. There is one family of positive
solutions parameterized by \( \lambda_1 \geq 0 \). For given \( \lambda_2 \) there may be at most two values of \( \lambda_1 \) by Descartes' rule of signs.

The limits are of particular interest. Since points with zero-components or at infinity correspond to facets we investigated the 8 facets of the 5-dimensional polytope \( \text{conv} (\eta_1, \eta_3, \eta_4, \eta_7, \eta_8, \eta_9, \eta_{10}) \). Not all facets allow for non-negative real points. One facet corresponds to \( \lambda_5 = 0 \) while another corresponds to \( \lambda_3 = \lambda_4 = 0 \). Neighboring facets allow for real points only for \( \lambda_1 E_1 \) or \( \lambda_2 E_2 \). Since the real part of the variety is homeomorphic to the polytope ([F93] p. 81) the curve parameterized by \( \lambda_1 \) is homeomorphic to a curve within the 5-dimensional polytope. It connects two facets which are further investigated with the momentum map which projects a point on the toric variety to a convex combination of the vertices of the polytope. If \( \lambda_1 \to \infty \) then \( \lambda_2 \to c_2(k), \lambda_4 \to 0, \lambda_5 \to c_5(k) \). The limit of the image of the momentum map approaches \( k_{3,0}/(k_{3,9} + k_{3,0}) k_2 + k_{0,3}/(k_{3,9} + k_{0,3}) k_3 \) which corresponds to \( E_1 \). Then \( x \to (0,0,0,0,0) \). If \( \lambda_1 \to 0 \) then \( \lambda_2 \to \infty \) like \( 1/\lambda_1^3 \) and \( \lambda_4 \to \infty, \lambda_5 \to \infty \) the image of the momentum map goes to \( k_{7,10}/(k_{7,10} + k_{10,7}) k_7 + k_{10,7}/(k_{7,10} + k_{0,7}) k_8 \) which corresponds to \( E_2 \). Then \( x \) tends to infinity.

For arbitrary \( \lambda_1 \) we may solve for \( x_i (\hat{x}_i) \) in \( I_K \Psi (\hat{x}) \hat{x}_0 = z \) in terms of roots by Hermite normal form. This transforms the linear equation to

\[
2 \frac{w_1^3}{w_2^4 w_5^2} + 2 \frac{w_3^3}{w_4^4 w_5^2} + 2 \frac{w_4 w_3}{w_5^3 w_2^4} + 2 \frac{w_4 w_4}{w_5^4 w_2^4} - a_i = 0,
\]

where \( w_i = w_i(k, \lambda_1), i = 1, 2, 3, 4, 6 \) and \( w_5 = c_5(k) \cdot \frac{\sqrt{\lambda_1}}{\sqrt{\lambda_1}} \). Of course \( \lambda_1, \lambda_2 \) still need to satisfy the equation above from the toric ideal. Depending on the value of \( a_1 > 0 \) one expects several positive solutions.

\[\Box\]

An alternative way includes the linear conditions right from the beginning. Then

\[
\begin{pmatrix}
Y_s I_a & 0 \\
v_1^t & a_1 \\
0 & \vdots & \vdots \\
v_r^t & a_r
\end{pmatrix}
\begin{pmatrix}
v(x) \\
x_1 \\
\vdots \\
x_m \\
1
\end{pmatrix}
= B \chi (x) = 0.
\]

has the coefficient matrix \( B \) and monomial vector \( \chi \). The minimal set of generators of the convex polyhedral cone \( \ker(B) \cap (\mathbb{R}_\geq 0)^q \) are partially known as \( (E^t_1, 0) \) from the set of minimal generators of \( \ker(Y_s I_a) \cap (\mathbb{R}_\geq 0)^q \). Unfortunately, in general \( v_i \) will involve the constants \( k_{ij} \) as already \( a_i \) are entering the computation of the cone. Moreover, the discussion will be complicated and depend on the values of \( a_i \) for vectors \( v_i \) which are non-negative for conservative systems, but in general are not. The computation of the generators of the toric ideal is done analogously and substitution of a convex combination of the generators of the cone gives equations in \( \lambda \).

**Example 3.4.** (Example 2.1 and 3.3 continued)

Lifting \( \eta_1, \eta_3, \eta_4, \eta_7, \eta_8, \eta_9, \eta_{10}, e_1, e_2, e_3, e_4, e_5, 0 \) and computing a Gröbner basis of the toric ideal with Maple gives the Hilbert polynomial

\[
\frac{1}{5} \lambda^5 + \frac{13}{12} \lambda^4 + \frac{8}{3} \lambda^3 + \frac{47}{12} \lambda^2 + \frac{47}{15} \lambda + 1,
\]

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with degree 24 which means that the system has for generic values of coefficients at most 24 complex solutions and thus at most 24 real positive solutions.

For completeness we mention that one might as well work with Minkowski summands of the Newton polytopes, either by forming the sum of the two obvious summands or more tricky by distinguishing several Newton polytopes after linear manipulation of $Y_x A \Psi(x)$. This leads to higher dimensional convex polyhedral cones and toric ideals in rings with many variables. This may turn out to be inefficient.

4. Finding Hopf bifurcation with resultants

The aim of the next section is the generalization of the method of counting positive solutions valid for some parameter regions as explained in [St94] and [St98]. In this section we will give some necessary definitions from dynamical systems and prepare the generalization.

A dynamical system is given by $\dot{x} = f(x)$ where $f : \mathbb{R}^n \to \mathbb{R}^n$ is a $C^\infty$-function. A steady state $x_0 \in \mathbb{R}^n$ is called stable, if all eigenvalues of the Jacobian $D_x f(x_0) \in \mathbb{R}^{n \times n}$ have negative real part. We consider a system $\dot{x} = f(x, \lambda)$ where $f : \mathbb{R}^{n+1} \to \mathbb{R}^n$ depends on an additional parameter and like to know how the stable steady states depend on $\lambda$. Assume a $C^\infty$-branch $(x(s), \lambda(s))$ of steady state solutions then the eigenvalues of $D_x f(x(s), \lambda(s))$ depend $C^\infty$ on the parameter $s$. Starting with a stable point $x_0 = x(s_0)$ the real parts of the eigenvalues have two possibilities to turn positive. Either a real eigenvalue crosses 0 (in a bifurcation point) or a pair of complex eigenvalues crosses the imaginary axis. The last situation is called Hopf bifurcation because the pair of eigenvalues $\pm i \omega$ together with some genericity conditions guarantee the bifurcation of a branch of periodic solutions (oscillations). A good reference is [GH83] p. 151.

Criteria are known to decide numerically when a real matrix $C$ (which is a Jacobian $D_x f(x_0, \lambda_0) \in \mathbb{R}^{n \times n}$) has a pair of complex eigenvalues $\pm i \omega$. These methods use algebraic concepts.

The first method uses resultants and works efficiently for $n < 10$. From the characteristic polynomial $p(\mu) = \det(\mu \text{Id} - C)$ one constructs two polynomials $q_0(\mu^2) = p(\mu) + p(-\mu)$ and $q_0(\mu^2) = (p(\mu) - p(-\mu)) / \mu$ of degree $[n/2]$. Since $q_0(-\omega^2) = q_0(-\omega^2) = 0$ it follows for the Sylvester resultant $\text{Res}(D_x f) = \text{Res}(q_0, q_0, \mu) = 0$ if the matrix $C$ has a pair of eigenvalues $\pm i \omega$. This method has been successfully applied numerically in the program LocBif.

The second method uses the bialternate product of matrices (see e.g. [Go00] p. 94). This associates to $C$ a matrix $2C \odot \text{Id}$ of dimension $\frac{n(n-1)}{2}$.

$$(2C \odot \text{Id})_{(i,j),(k,l)} = \begin{cases} -a_{ij} & \text{if } k = j \\ a_{ik} & \text{if } k \neq i \text{ and } l = j \\ a_{ii} + a_{jj} & \text{if } k = i \text{ and } l = j \\ a_{jl} & \text{if } k = i \text{ and } l \neq j \\ -a_{jk} & \text{if } l = i \\ 0 & \text{else.} \end{cases}$$

The index pairs satisfy $i > j$ and $k > l$. If $C$ has eigenvalues $\pm i \omega$ then $2C \odot \text{Id}$ has eigenvalue zero. Thus $p_\odot = \det(2C \odot \text{Id}) = 0$ is a necessary condition for a dynamical system to have a Hopf point. This is used in the program Content.

These methods may be applied in order to check whether a system $\dot{x} = f(x, \lambda)$ where $f$ is polynomial in $x$ and $\lambda$ over a field $F$ may have a Hopf bifurcation at all.
Lemma 4.1. Let \( f(x, \lambda; \underline{k}) \in (F[\overline{k}][x, \lambda])^n \) be a polynomial vector where \( F \) is an appropriate field. Let \( \text{Res}(D_x f(x, \lambda; \underline{k})), p_\circ \in F[\overline{k}][x, \lambda] \) be the polynomials constructed above. If the system \( \dot{x} = f(x, \lambda; \underline{k}) \) has for some fixed values \( \underline{k}_0 \) a Hopf point at \( (x_0, \lambda_0) \) then \( \text{Res}(x_0, \lambda_0, \underline{k}_0) = 0 = p_\circ(x_0, \lambda_0, \underline{k}_0) \). If \( (x_0, \lambda_0) \) is a bifurcation point then det \( (D_x f(x_0, \lambda_0, \underline{k}_0)) = 0 \). If \( x_0 \) is positive then the toric Jacobian \( \det(\text{diag}(x_0), \ldots, (x_0)_n) D_x f(x_0, \lambda_0, \underline{k}_0)) \) has eigenvalue zero.

Since a bifurcation point satisfies \( n + 1 \) sparse polynomial equations in \( n \) variables \( x_1, \ldots, x_n \) the sparse resultant ([CLO98] Sec. 7.2) may be applied. Then \( \text{Res}_{B, T}(\lambda_0, \underline{k}_0) = 0 \) where \( B \) denotes the support of \( f \) as polynomials in \( x \) and \( T \) the support of the determinant of the toric Jacobian. This was used in [St98]. In analogy one may check for Hopf points by the sparse resultant \( \text{Res}_{B, H}(\lambda_0, \underline{k}_0) \) where \( H \) is the support of \( \text{Res}(D_x f) \) or of \( p_\circ \) as a polynomial in \( x \). For problems of moderate size it is possible to construct (multiples) of these sparse resultants ([EC95, EM99]).

For system (2.1) \( f(x; \underline{k}) = Y_a I_a I_K \Psi(x) \) is clearly polynomial, but the situation is slightly different. Since affine shifts of \( \text{im}(Y_a A) \) are flow-invariant a steady state \( x_0 \) is called to stable within \( x_0 + \text{im}(Y_a A) \) if the restricted Jacobian has the property that all eigenvalues have negative real part. Analogously, Hopf points within \( x_0 + \text{im}(Y_a A) \) are defined. Thus we use an orthonormal basis of \( \text{im}(Y_a A) \) and form a matrix \( U \in \mathbb{F}^{m, s} \) from these vectors where \( s \) is the dimension of \( \text{im}(Y_a A) \). Then \( C = U^T Y_a I_a I_K D_x \Psi(x) U \) is a polynomial matrix in \( F[\overline{k}]^{s, s} \). Then the resultant from the first method and the determinate of the bialternate product are polynomials in \( F[x, \underline{k}] \). We consider it as a polynomial in \( F[\overline{k}][x] \), as well as \( U^T Y_a I_a I_K \Psi(x) \) as \( s \) polynomials. The linear equations \( v_i^T x - a_i, i = 1, \ldots, m - s \) are polynomials in \( F[\overline{k}, \underline{a}][x] \). Then the sparse resultant is a polynomial in \( F[\overline{k}, \underline{a}] \). If system (2.1) undergoes some Hopf bifurcation for some value of some parameter \( \lambda = k_{ij} \) (and where the remaining \( k_{ij} \) are constant) then the sparse resultant vanishes for these values.

Example 4.2. (Example 2.1 simplified) We simplify the \( H_2 O \) example such that no \( H_2 O_f \) is involved \( (x_4 = 0) \). Then we compute \( \text{Res}(x; \underline{k}) \) and \( p_\circ(x, \underline{k}) \) explicitly in Maple. They turn out to be different. Unfortunately, the formulas are so complicated that no information can be extracted.

This example shows that in general this treatment of Hopf bifurcation is not efficient. Concepts in numerics and in symbolic computation are so different that methods from numerics can not be transferred without rethinking. Nevertheless the polynomials \( \text{Res}(x, \underline{k}) \) and \( p_\circ(x, \underline{k}) \) are important for theory and thus are used in the next section.

In [C180] it is suggested to use the minimal generators \( E_i \) of the convex polyhedral cone and the Routh-Hurwitz theorem to determine the stability of all steady states. This requires further research and a careful investigation with methods from algebraic geometry and analysis.

5. The number of stable solutions

In the beginning of this section we consider the general polynomial situation:

\[
\dot{x} = f(x; \underline{c}), \quad \text{where} \quad f_{ij} = \sum_{b < B_i} c_{ij}^b x^b, \quad i = 1, \ldots, r, j = 1, \ldots, k_i
\]

with \( k_1 + \cdots + k_r = n \) and supports \( B_i \subset (\mathbb{Z}_{\geq 0})^{n} \).
The theory in [HS95, St94, St98] is based on a special homotopy which enables to divide the polynomial system into binomial systems which are easily solved. This is

\[ H_{ij}(x,t) = \sum_{b \in B_i} c_{b,i}^t \omega_i(b), \]

where the integer values \( \omega_i(b) \) are chosen randomly. Geometrically, the Newton polytopes are lifted and the lower hull of the lifted polytopes gives a mixed subdivision of the Newton polytopes for generic lifting values. Moreover, generically one may assume that the mixed cells are even simple mixed.

**Definition 5.1.** ([HS95], [VG95])

(i) A subdivision of \( B = (B_1, \ldots, B_r) \) is a collection \( S = \{C_1, \ldots, C_s\} \) of \( s \) cells \( C_j = (C_j^{(1)}, \ldots, C_j^{(r)}) \) such that

(a) \( \dim(\text{conv}(C_j)) = n \) for \( j = 1, \ldots, s, \)

(b) \( \text{conv}(C_j) \cap \text{conv}(C_k) \) is a common face of \( \text{conv}(C_j) \) and of \( \text{conv}(C_k) \) for all pairs \( C_j, C_k \in S, \)

(c) \( \bigcup_{j=1}^r \text{conv}(C_j) = \text{conv}(B). \)

(ii) The subdivision is called **mixed** if the additional property

(d) \( \sum_{\lambda=1}^r \dim(\text{conv}(C_j^{(\lambda)})) = n \) for all cells \( C_j \in S \) holds.

(iii) A cell \( C_j \) is called **mixed**, if

(e) \( \dim(\text{conv}(C_j^{(\lambda)})) = k_\lambda, \quad \lambda = 1, \ldots, r. \)

(iv) A mixed cell \( C_j \) is called **simple**, if

(f) \( \sum_{\lambda=1}^r (\#(C_j^{(\lambda)}) - 1) = n \)

holds.

(v) A mixed subdivision is called a **simple mixed** subdivision if all mixed cells are simple mixed cells.

The idea is that each mixed cell gives a small subsystem of the original system \( f(x; \xi) = 0 \) corresponding to a facet of the lower hull. Along the homotopy this generically continues to solutions of \( f(x; \xi) = 0 \). Additionally, one may check the stability for \( t = 0 \). If no bifurcation or Hopf bifurcation occurs along the homotopy then the number of stable, positive solutions at \( t = 0 \) equals the number of stable, positive solutions at \( t = 1 \), i.e. for the original system \( f(x, \xi) = 0 \).

Motivated by the signed Newton polytopes a mixed cell of the subdivision is called **alternating** in [IR96], if the associated binomial system has precisely one positive solution.

**Theorem 5.2.** Consider \( f, H \) as above with generic lifting values \( \omega_i(b) \in \mathbb{Z} \). Assume that the induced mixed subdivision is simple mixed and that the coefficients \( \xi \) are such that the following conditions are satisfied.

(i) The sparse resultant \( \text{Res}_{B,T}(\xi, \xi, t) \) has no zero for \( t \in (0,1] \).

(ii) None of the small systems associated to a facet has infinitely many solutions.

(iii) The sparse resultant \( \text{Res}_{B,H}(\xi, \xi, t) \) has no zero for \( t \in (0,1] \).

Then the number of stable positive solutions is the same for \( t = 0 \) and \( t = 1 \).
PROOF. The proof of Bernstein’s theorem in [HS95] is based on Puiseux expansions

\[
x(t) = \left( \begin{array}{c}
  u_1 t^{\gamma_1} \\
  \vdots \\
  u_n t^{\gamma_n}
\end{array} \right) + \text{higher order terms in } t,
\]

where \((\gamma, 1)\) is an inner normal to one of the facets of the lower hull of the lifted Newton polytopes. The complex solutions of the associated binomial system are candidates for \(u\). By Hensel’s lemma they give rise to a Puiseux expansion. In [St94, St98] it was observed that \(x(t)\) is real and positive for all \(t \in (0, \varepsilon)\) with \(\varepsilon\) sufficiently small iff \(u\) is real and positive. This argumentation uses the coordinate transformation \(x_i = u_i t^{\gamma_i}, 1 = 1, \ldots, n\) and

\[
g_{ij}(u, t) = \frac{1}{t^{m_i}} H_{ij}(ut^j, t) = \sum_{b \in C(l)} c_b^i x^b + \text{hot in } t, \quad j = 1, \ldots, k_i, \quad i = 1, \ldots, r,
\]

where \(C = (C^{(1)}, \ldots, C^{(r)})\) is a simple mixed cell defined by the facet of the lower hull and \(m_i\) is the minimal value of the linear functional defined by \((\gamma, 1)\) on the lifted Newton polytope. A positive solution \((u, 0)\) gives by the theorem of implicit functions a branch of positive solutions \((u(t), t)\) for \(t\) small which yields a branch of positive solutions \((x(t), t)\).

By the first two conditions it is guaranteed that the homotopy paths stay positive, finite and do not undergo a bifurcation. Then the number of positive solutions of \(f(x; \varepsilon) = 0\) equals the number of alternating cells.

According stability we observe that generically \(D_u g(u, 0)\) is regular and thus one may decide on stability. Suppose all eigenvalues have negative real part. Since the eigenvalues depend \(C^\infty\) on the parameter \(t\) the points \((u(t), t)\) are stable for \(\dot{u} = g(u, t)\) for sufficiently small \(t\). The Jacobian matrices are related as

\[
\text{diag}(\frac{1}{t^{m_i}}) D_x H(x(t), t) \text{diag}(t^{m_i}) = D_u g(u(t), t).
\]

Multiplication with positive diagonal matrices from both sides does not change the signs of the real parts of the eigenvalues. This implies stability of \((x(t), t)\) for small \(t\). One may use the equivalent characterization of stability

\[
\xi^T BJ \xi < -\delta \xi^T J \xi \quad \forall \xi \in \mathbb{R}^n,
\]

where \(J\) is the Jacobian, \(\delta > 0\) a constant, and \(B\) a symmetric positive definite matrix. With this criterion the desired conclusion is easily observed.

By the third condition there is no Hopf bifurcation along the homotopy. Thus the number of alternating cells whose positive solution is stable equals the number of stable steady states of \(\dot{x} = f(x; \varepsilon)\).

\[\square\]

In the chemical reaction system (2.1) the situation is slightly different since there are flow-invariant subspaces. But a modified version is still valid.

**Theorem 5.3.** Assume a chemical reaction system

\[
\dot{x} = Y_s I_a I_K \Psi(x), \quad \Psi(x) = \left( \begin{array}{c}
  x^{\eta_1} \\
  \vdots \\
  x^{\eta_n}
\end{array} \right),
\]

defined by a weighted bipartite graph and a weighted directed graph together with the conservation relations \(\psi_i^T x - a_i, i = 1, \ldots, m - \text{rank}(Y_s I_a I_K)\). Assume that the
lifting values of the two supports \( B_1 = \{ \eta_i \mid \eta_i \text{ column in } Y_r \} \) and the \( m \)-simplex \( B_2 = \{0, e_1, \ldots, e_m\} \) are chosen such that the mixed subdivision is simple. The lifting values define a homotopy

\[
H_1(x, t; \mathbf{a}) = Y_s I_a I_K \left( \begin{array}{c} x^m t^{\omega x(e_1)} \\ \vdots \\ x^m t^{\omega x(e_m)} \end{array} \right)
\]

\[
H_2_j(x; t; \mathbf{a}) = (x_1 t^{\omega x(e_1)}, \ldots, x_m t^{\omega x(e_m)}) v_j - a_j t^{\omega x(0)},
\]

where \( j = 1, \ldots, m - \text{rank}(Y_s A) \). Assume the constants \( k_{ij} \in \mathbb{R}_+ \) and parameter \( a_i \) are chosen such that the following conditions are satisfied along the homotopy.

(i) The sparse resultant \( \text{Res}_{BH,T}(\mathbf{k}, \mathbf{a}, t) \) has no zero for \( t \in (0, 1] \).

(ii) None of the small systems associated to a facet has infinitely many solutions.

(iii) The sparse resultant \( \text{Res}_{BH,T}(\mathbf{k}, \mathbf{a}, t) \) has no zero for \( t \in (0, 1] \). This sparse resultant is constructed from the equations \( Y_s I_a I_K \Psi(x) t^{\omega x} = 0 \), the conservation relations \( v_j^T x t^{\omega x} - a_j t^{\omega x(0)} = 0 \) and the determinant of the bi-alternate product of the Jacobian matrix \( U^T Y_s I_a I_K D_x \Psi(x) t^{\omega x} U \), where the columns of \( U \) form an orthonormal basis of \( \text{im}(Y_s I_a I_K) \).

Then the number of stable positive points of \( Y_s I_a I_K \Psi(x) = 0 \) within a subspace \( x_0 + \text{im}(Y_s A) \) \( \cap (\mathbb{R}_+)^m \) equals the number of stable positive points of the binomial systems.

Of course it will be difficult to compute the sparse resultants as polynomials in \( k, a \), but for given values \( k_0, a_0 \) one might evaluate its value numerically.
A mixed cell \((C^{(1)}, C^{(2)})\) of the supports have graph theoretic meaning. It corresponds to a subgraph of the combined graph.

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COUNTING STABLE SOLUTIONS OF SPARSE POLYNOMIAL SYSTEMS IN CHEMISTRY


KONRAD-ZUSE-ZENTRUM BERLIN, TAKUSTR. 7, D-14195 BERLIN, GERMANY OR INSTITUT FÜR MATHEMATIK I, FACHBEREICH MATHEMATIK UND INFORMATIK, FREIE UNIVERSITÄT BERLIN, ARNIMALLEE 2-6, D-14195 BERLIN, GERMANY.

E-mail address: gatermann@zib.de, URL: http://www.zib.de/gatermann