Decompositional Modeling through Caricatural Reasoning

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Abstract

Many physical phenomena are sufficiently complex that the corresponding equations afford little insight, or no analytical method provides an exact solution. *Decompositional modeling (DM)* captures a modeler's tacit skill at solving nonlinear algebraic systems. DM divides statespace into a patchwork of simpler subregimes, called *caricatures,* each of which preserves only the dominant characteristics of that regime. It then solves the simpler nonlinear system and identifies its *domain of validity.* The varying patchwork reflects how variations in the parameters change the dominant characteristics. The patchwork is built by extracting equational features consisting of the relative strength of terms, and then exagerating and merging these features in different combinations, resulting in the different caricatural regimes. DM operates by providing strategic guidance to a pair of symbolic manipulation systems for qualitative sign and order of magnitude algebra. The approach is sufficient to replicate a broad set of examples from acid-base chemistry.

Introduction

Much work within the qualitative reasoning community (Addanki, S. and R. Cremonini and J. S. Penberthy 1989; Falkenhainer & Forbus 1991; Nayak, Joskowicz, & Addanki 1991; Weld 1991) has concentrated on methods for selecting and composing sets of models with a diversity of underlying modeling assumptions, and a strong emphasis has been placed on managing the diversity of these models. This is a fruitful avenue. Yet it is also important to realize that this diversity arises in each physical domain from a small, core set of principles, such as Newton's laws or Maxwell's equations. The application of these principles are taught from the start of a modeler's education. Thus of equal importance is the skill of a modeler to adapt these principles to the phenomena being accounted for.

In this paper we introduce a complementary, domain independent approach called *decompositional modeling (DM).* The task we address is finding analytic solutions to systems of nonlinear equations, couched in the domain of analytical chemistry. Instead of solving a system directly, DM partitions the behavior of each equation into a patchwork of regimes where different behaviors dominate, and the equations in each regime are simplified to reflect only what is significant. Regimes for the overall system are then constructed by composing the regions of the individual equations, and then solving the system of simplified equations, to describe the behavior within each of the system's regimes. In addition to the overall decompositional process, this work is novel for its use of the concept of a *caricature* to extract the appropriate regimes, and the demonstration of the power of *qualitative algebraic resolution* at all stages of the modeling process.

An Example From Chemistry

To ground our approach, consider the application of decompositional modeling to the analysis of the equilibrium behavior of a simple reaction — the dilution of acid molecules, AH, into water. The dilution is characterized by the reactions $\mathrm{H_2O} \rightleftharpoons \mathrm{H^+} + \mathrm{OH^-}$ and $\mathrm{AH} \rightleftharpoons \mathrm{H^+} + \mathrm{A^-}$; its equilibrium is governed by:

$$
\begin{array}{llcl}
\text{(I1) Charge balance:} & \mathrm{h^+} & = & \mathrm{oh^-} + \mathrm{a^-}, \\
\text{(I2) Mass balance:} & \mathrm{C}_a & = & \mathrm{ah} + \mathrm{a^-}, \\
\text{(I3) Water equilibrium:} & \mathrm{K}_w & = & \mathrm{h^+ oh^-}, \\
\text{(I4) Acid equilibrium:} & \mathrm{K}_a \mathrm{ah} & = & \mathrm{h^+ a^-},
\end{array}
$$

where ah, $\mathrm{a^-}$, $\mathrm{h^+}$, $\mathrm{h_2o}$, and $\mathrm{oh^-}$ denote concentration at equilibrium of the species AH, $\mathrm{A^-}$, $\mathrm{H^+}$, $\mathrm{H_2O}$, and $\mathrm{OH^-}$, respectively. Note that although the concentration of species S is traditionally denoted $[S]$, this conflicts with the use of [ ], within qualitative reasoning, to denote a quantity's sign. K_w and K_a are equilibrium constants for the water and acid ionization, and C_a denotes the initial concentration of AH.

Determining the equilibrium concentrations in terms of constants K_w, K_a and AH directly requires the solution of four nonlinear equations in four unknowns. For example, solving for $\mathrm{H^+}$ ions yields the *equilibrium concentration equation*:

$$\mathrm{h^+}^3 + \mathrm{K}_a \mathrm{h^+}^2 - (\mathrm{K}_a \mathrm{C}_a + \mathrm{K}_w)\mathrm{h^+} = \mathrm{K}_a \mathrm{K}_w .$$

The derivation of this equation was highlighted in text (Beckwith 1985) (chapter 5) to demonstrate the dangers of using brute force. Even for this simple case the concentration equation is a third degree polynomial in h^+, whose roots are difficult to solve for by hand. Recent developments in the automatic solution of nonlinear equations provides some additional latitude. However, problems arise for slightly more complicated cases. For example, for polyprotic acids — acids with more than one replaceable hydrogen ion H^+, such as H_3PO_4 — the degree of the equations increases with the number of replaceable ions. Thus for example H_3PO_4 has three replaceable ions and results in a concentration equation of degree five. There are no general closed form solutions to algebraic equations of degree five or higher (by Galois), and it is difficult to derive insight from such equations directly. For more interesting chemical systems, such as those studied in atmospheric modeling, the number of reactions range in the hundreds. In this situation the application of a direct method clearly breaks down and even when numeric methods are applied, approximations are performed liberally.

Instead, a chemist is taught to proceed as follows (taken from (Beckwith 1985), chapter 5). First, having introduced equations I1–I4 governing the reaction's equilibrium, the chemist guesses several interesting simplifying assumptions (A1-4) about what the dominant species may be:

A1: The acid is weak ($a^- \ll C_a$).

A2: The acid is strong ($ah \ll C_a$).

A3: The solution is essentially neutral ($a^- \ll h^+$).

A4: The solution is strongly acidic ($oh^- \ll h^+$).

Combining, for example, assumptions A2 and A4 and applying them to the charge and mass balance equations (I1,I2) produces $h^+ \approx a^-$ (I1') and $C_a \approx a^-$ (I2'). Solving for h^+ results in $h^+ \approx C_a$, a far simpler result than produced through a direct solution without simplification. Applying other combinations of assumptions produces:

Asump.	Reg.	Simplified Concentration Eqns.			
A2,A4	R1	h^+	$\approx$	C_a	E1
A3	R2	h^{+2}	$\approx$	K_w	E2
A2	R3	$h^{+2} - C_a h^+$	$\approx$	K_w	E3
A4	R4	$h^{+2} + K_a h^+$	$\approx$	$C_a K_a$	E4
A1,A4	R5	h^{+2}	$\approx$	$C_a K_a$	E5
A1	R6	h^{+2}	$\approx$	$C_a K_a + K_w$	E6
none	R7	$h^{+3} + K_a h^{+2} - (K_a C_a + K_w) h^+$	$=$	$K_a K_w$	E7

The remaining step is to determine the *domain of validity* for each set of assumptions — the constraints that the assumptions impose on the givens, K_a, K_w and C_a. Returning to the pair of assumptions A2 and A4, from A2 ($ah \ll C_a$) the chemist derives $C_a^2/K_a \ll C_a$ by substituting for ah and a^- using the simplified acid equilibrium (I4), acid concentration (E1) and mass balance (I2') equations. And from A4 ($oh^- \ll h^+$) the chemist derives $K_w/C_a \ll C_a$ by substituting for oh^- and h^+ using the simplified acid concentration (E1) and water equilibrium (I3) equations. These two constraints define a region, R1, whose fringe corresponds to the two bold lines in the upper right corner of the region diagram in figure 1 (taken from (Beckwith 1985), p. 75). The domains of validity R2–R7 for the remaining sets of assumptions partitions the reaction's behavior into simpler regimes according to the values of C_a and K_a. Given these results, the problem of identifying a solution's acidity for given values of C_a and K_a involves identifying the appropriate region and applying the corresponding simplified concentration equation.

Figure 1: The different combinations of simplifying assumptions divide the space of values for C_a and K_a into simpler regimes of dominant behavior. Its given that $K_w = 10^{-14}$ and $a \ll b$ when $a/b < 0.1$.

Decompositional Modeling and Caricatures

In this example we saw that the analytical chemistry task is in essence one of solving a system of simultaneous, nonlinear equations, and that the modeling process is fundamentally decompositional. This approach results in behavioral descriptions that are more tractable to manipulate and provide greater insight. The example also demonstrates the five major steps of DM: 1) identify simplifying assumptions about the dominance of parameters, 2) combine these assumptions to define different subregimes of dominant behavior, 3) simplify the system of equations based on the assumptions of a particular subregime, 4) solve the simplified equations to obtain the system's dominant behavior over that subregime, and 5) identify the domain of validity over which the simplified behavior is valid.

This provides a layer of structure for the modeling process, but it doesn't explain where the simplifying assumptions come from, or provide a conceptual viewpoint of the overall process. For this we use the metaphor of a *caricature*. In decompositional modeling the patchwork of regimes, corresponding to dominant behaviors are derived by reinforcing the "prominent features" of the system's behavior.

¿From a commonsense standpoint a caricature of an object is a description which exagerates prominent features and eliminates insignificant features. For example caricatures of Richard Nixon reduce his face to little more than a nose with an exaggerated slope. Applying this concept to modeling, given a system of initial equations DM constructs a *caricature of the system* by exagerating one or more of the equation's prominent features. In this paper, we take "prominent" to mean that one term a of an equation E dominates another term b: $|a| > |b|$; that is, a is further from zero than b. DM exagerates this feature by making $|a|$ much greater than $|b|$, thus making a dominant and b insignificant: $|a| > |b| \rightsquigarrow a \gg b$. We call this relation a *caricatural assumption*. By using this assumption to simplify E, DM produces a *caricatural equation*, that eliminates the insignificant features.

For example, given that all concentrations are positive, two prominent features of equation I2 ($\mathrm{C}_a = \mathrm{ah} + \mathrm{a}^-$) are $|\mathrm{C}_a| > |\mathrm{ah}|$ and $|\mathrm{C}_a| > |\mathrm{a}^-|$ (note that all concentrations are positive). Exagerating $|\mathrm{C}_a| > |\mathrm{ah}|$ introduces the caricatural assumption $\mathrm{C}_a \gg \mathrm{ah}$, and allows I2 to be replaced by the caricatural equation $\mathrm{C}_a \approx \mathrm{a}^-$. This corresponds to the chemist's notion of a strong acid (i.e., essentially all AH dissociates). Conversely, exagerating $|\mathrm{C}_a| > |\mathrm{a}^-|$ introduces the assumption $\mathrm{C}_a \gg \mathrm{a}^-$, and produces the caricature $\mathrm{C}_a \approx \mathrm{ah}$, the chemist's notion of a weak acid (i.e., a negligible fraction of the acid AH dissociates).

Of course an alternative approach might take a quantity or subterm from *any* two equations and presume one dominates another. However, the number of potential assumptions would be prohibitively large. Instead the concept of caricature allows us to use existing features of the initial equations as clues to what relations are worth exaggerating. What is striking is that the restricted set generated through caricatures matches the simplifying assumptions introduced in a variety of acid-base chemistry examples.

Summarizing the observations of this section, the DM algorithm is:

Decompositional Modeling: Given a system of non-linear equations $\mathbf{E}$ with state variables $\mathbf{x}$ and parameters $\mathbf{p}$:

1. Generate the caricatural assumptions C_i for each $E_i \in \mathbf{E}$.
2. Merge the sets of assumptions of the E_i, producing a set C whose elements are sets of combined assumptions corresponding to dominance regimes.

   Then, **for each set** $c \in C$,
3. use c to extract the caricature of each $E_i \in \mathbf{E}$, producing $\mathbf{E}'$;
4. solve for $\mathbf{x}$ in the system of caricatures $\mathbf{E}'$, and
5. derive from c and $\mathbf{E}$ the domain of validity.

DM relies heavily on the computational machinery of qualitative algebraic reasoning(Williams 1991; Raiman 1991) to perform tactical inferences. This corresponds to the rote algebraic manipulations taught informally to a modeler early on, and is discussed in the next section. The art of the modeler is the strategic guidance given to these manipulations. This is the contribution of this paper, and is the focus of the remaining sections.

Qualitative Algebraic Inference

DM operates by strategically guiding the inferences of two symbolic manipulation systems, one for a sign algebra, and a second for order of magnitude equations. We provide here an overview of the algebraic foundation underlying DM. Representationally it is unified as a set algebra that captures knowledge of order and dominance. Computationally it is unified through *qualitative resolution.* Decompositional modeling involves reasoning about three types of information: non-linear equations, such as $\mathrm{K}_a\mathrm{ah} = \mathrm{h}^+\mathrm{a}^-$, inequalities between magnitudes, such as $|\mathrm{a}^-| < |\mathrm{h}^+|$, and order of magnitude information, such as $|\mathrm{a}^-| \ll |\mathrm{h}^+|$ and $|\mathrm{a}^-| \approx |\mathrm{h}^+|$. Both equations and inequalities are expressed as equations in the hybrid qualitative/quantitative algebra SR1 (Williams 1991) (an algebra combining signs and reals). The domain of SR1 extends the reals to include signs (i.e., $\hat{+} \equiv (0, \inf)$, $\hat{-} \equiv (-\inf, 0)$ and $\hat{?} \equiv (-\inf, \inf)$). The operators of SR1 extend the standard operators of the reals ($+, -, \times$ and $/$) to this larger domain, resulting for example in the combination of a real and sign algebra. As usual $[r]$ maps a real r to its sign. In SR1 an inequality, such as $\mathrm{C}_a > \mathrm{ah}$ is expressed by the hybrid equation $[\mathrm{C}_a - \mathrm{ah}] = \hat{+}$, and $|\mathrm{C}_a| > |\mathrm{ah}|$ is expressed by $[\mathrm{C}_a^2 - \mathrm{ah}^2] = \hat{+}$. Since the elements of the algebra are sets, expressions are related using $\subset$ as well as $=$. In addition, the set relation $\approx$ represents non-empty intersection.

Dominance relations and other types of order of magnitude information are captured as equations in the algebra of *Estimates* (Raiman 1991). The domain of Estimates extends the reals to include ϵ, a set of infinitesimal values around 0 that are negligible with respect to 1. Like SR1, Estimates' algebra extends the standard operators and includes the same set relations as SR1. The dominance relations are represented by: $a \gg b \equiv b \subset \epsilon a$, and $a \approx b \equiv a \subset (1+\epsilon)b$. Intuitively ϵa denotes the set of all values much smaller than a, and $(1+\epsilon)a$ denotes all values close to a.

Note that, although seemingly disparate, SR1 and Estimates are both instances of set algebras over the reals, and as such share many properties — in particular a common algebraic inference structure. For both algebras the basic inference involves combining two equations, and is performed through three steps: solve for a shared variable in one equation, substitute

Initial Eqns		Sign Eqns	prominent feature	caricatural assumptions
$h^+ = oh^- + a^-$	(I1)	$[a^-] = \hat{+}, [oh^-] = \hat{+}$	$\|h^+\| > \|oh^-\|$	$h^+ \gg oh^-$ (A4)
$h^+ = oh^- + a^-$	(I1)	$[oh^-] = \hat{+}, [a^-] = \hat{+}$	$\|h^+\| > \|a^-\|$	$h^+ \gg a^-$ (A3)
$C_a = ah + a^-$	(I2)	$[ah] = \hat{+}, [a^-] = \hat{+}$	$\|C_a\| > \|a^-\|$	$C_a \gg a^-$ (A1)
$C_a = ah + a^-$	(I2)	$[a^-] = \hat{+}, [ah] = \hat{+}$	$\|C_a\| > \|ah\|$	$C_a \gg ah$ (A2)
$K_w = h^+ oh^-$	(I3)		none	none
$K_a ah = h^+ a^-$	(I4)		none	none

Figure 2: The complete set of caricatural assumptions and equations.

the solution into the second equation, and simplify the composite result. For example, consider the composition of SR1 equations $s + [a] \approx u$ and $t - [a] \approx v$. First, the shared variable $[a]$ is solved for in the first equation, resulting in $[a] \subset u - s$. Next, the result is substituted for $[a]$ in the second equation using substitution of supersets, and results in $t - (u - s) \approx v$. Finally the result is simplified, producing $t - u + s \approx v$ or equivalently $t + s \approx v + u$. The following are the results of additional examples for the two algebras:

$$\begin{array}{lll} s + [a] \approx u, \quad t - [a] \approx v & \Rightarrow & s + t \approx u + v \\ [a - b] = s, \quad [b - c] = t & \Rightarrow & [a - c] \subset s + t \\ s + a \approx u, \quad t - a \approx v & \Rightarrow & s + t \approx u + v \end{array}$$

An important property of each example is that it has the flavor of propositional resolution. A term and its negation are identified in the two equations (e.g., $[a]$ and $-[a]$), they are eliminated from both equations, and the respective sides of the two equations are combined. We refer to this process as *qualitative resolution.* The details of qualitative resolution for SR1 (performed by *Minima* and Estimates) are described extensively in (Williams 1991) and (Raiman 1991), respectively. For our purposes we can think of Minima and Estimates together as a qualitative resolution black box. What is striking is that each step of decompositional modeling (DM) maps to a particular set of qualitative resolutions. DM is then performed by framing a qualitative resolution problem at each step. This process is the focus of the remaining sections.

Step 1 & 2. Caricatural Assumptions

DM first extracts and then exagerates the prominent features of each $E_i \in \mathbf{E}$, where a prominent feature is a partial order between the absolute values of any two terms. For each $E_i \in \mathbf{E}$ this involves:

1. Nondeterministically select a pair of terms $a, b \in E_i$.
2. Infer the ordering $(<, =, >)$ between $|a|$ and $|b|$.
   (a) Create ordering expression $O = [a^2 + b^2]$.
   (b) Repeatedly resolve O with all E_i, and constraints on variable signs ($[v] = s$).
   (c) If a sign constant $\hat{+}$ or $\hat{-}$ results, map to an ordering (e.g., $[a^2 - b^2] = \hat{+} \rightarrow |a| > |b|$).
3. Exagerate any ordering using $|a| > |b| \leadsto a \gg b$.

For example, given the mass balance equation $C_a = ah + a^-$ (I2) and the fact that a^- is positive ($[a^-] = \hat{+}$ (P1)), then DM selects C_a and ah, constructs $[C_a^2 + ah^2]$, and performs the following sequence of resolutions:

$[C_a^2 - ah^2]$	Given.
$= [(ah + a^-)^2 - ah^2]$	Resolve with $C_a = ah + a^-$.
$= [2aha^- + (a^-)^2]$	Simplification.
$\subset [2(\hat{+})a^- + (a^-)^2]$	Resolve with $ah \subset \hat{+}$.
$\subset [2(\hat{+})(\hat{+}) + (\hat{+})^2]$	Resolve with $a^- \subset \hat{+}$.
$\subset \hat{+}$	Simplification.

Thus $[C_a^2 - ah^2] = \hat{+}$ or equivalently $|C_a| > |ah|$. Finally, exagerating this feature according to $|a| > |b| \leadsto a \gg b$ produces $C_a \gg ah$, which is equivalent to assumption A2 of the example section. The derivation of each feature and its corresponding caricature for all equations is summarized in figure 2.

The assumptions just generated for each equation induce a patchwork of dominant subregimes local to that equation. DM then combines these local regimes into a set of global regimes. To do this step 2 combines the sets of assumptions. For the moment presume all possible combinations of assumptions are explored separately. We return later with a more sophisticated approach. Having combined the assumptions, the next two steps construct a caricature of the system's composite behavior for some subregime. Step 5 makes explicit the boundaries of that subregime.

Step 3. Extracting Dominant Behaviors

Given a set of caricatural assumptions c defining a subregime, each of the E_i is simplified using c by Estimates, producing a set of *caricatural equations.* Estimates provides a sophisticated strategy for guiding resolution during simplification (see (Raiman 1991)). For completeness we sketch here an extremely simple strategy. Recall that an assumption $a \ll b$ is encoded as the equation $a \subset \epsilon b$. Then given E_i and assumptions c, simplification involves repeatly:

1. Identifying variables $a, b \in E_1$ such that $(a \ll b) \in c$.
2. Resolving E_i and $a \subset \epsilon b$ using variable a.

For example, consider the pair of caricatural assumptions: $C_a \gg ah$ (A2) and $h^+ \gg oh^- (A4)$, corresponding to the example at the beginning of the paper. To simplify the mass balance equation $C_a = ah + a^-$ (I2), DM identifies that the pair of variables C_a and ah also appear in A2, and then through resolution DM derives the caricatural equation $C_a \approx a^-$ (I2'):

$ah + a^- = C_a$	Equation I2 to simplify.
$ah \subset \epsilon C_a$	Estimates equation for A2.
$a^- = C_a - ah$	Cancellation on I2.
$a^- \subset C_a - \epsilon C_a$	Resolving for ah in I2, A2.
$a^- \subset (1+\epsilon)C_a$	Simplification.

This caricatural equation is equivalently $a^- \approx C_a$. Likewise, to simplify charge balance $h^+ = a^- + oh^-$ (I1), DM resolves it with A4, resulting in $h^+ \approx a^-$ (I1'). Finally, resolving I3 and I4 with A2 and A4 provides no simplification.

Step 4. Solving Caricatural Equations

Next the caricatural equations are solved for the unknown concentrations. Specifically, given a set of knowns K, caricatural equations $\mathbf{E}'$ and unknowns U, DM repeatedly resolves all pairs of equations that share an unknown. A solution is a resulting equation that contains exactly one unknown. For example, DM solves for h^+ in terms of the givens K_w, K_a and C_a, using the caricatural equations just derived:

$(1+\epsilon)h^+ - a^- \supset 0$	Estimates eqn. for I1'.
$(1+\epsilon)C_a - a^- \supset 0$	Estimates eqn. for I2'.
$(1+\epsilon)h^+ - (1+\epsilon)C_a \supset 0$	Resolving a^-.

Equivalently $h^+ \approx C_a$ (E1). Equilibrium concentrations for ah, a^- and oh^- are derived analogously. Solving systems of equations by resolution will be costly for large systems. A more desirable alternative is to use a package for solving nonlinear systems of equations. Such a package, however, must be able to manipulate error terms to ensure that the cancellation of two dominant terms does not cause the error, introduced during exageration, to become significant.

Step 5. Identifying Domains of Validity

Having just constructed a caricature of the composite system's behavior, the final step identifies the domain over which the caricatural assumptions are valid. Each bound of the domain of validity corresponds to one of the caricatural assumptions (figure 1), where an assumption $a \gg b$ produces bound $a +/- \epsilon b = 0$. A boundary is derived from an assumption A by repeatedly resolving one of the unknown variables of U that appears in A, with one of the equations in $\mathbf{E}'$. A solution is reached when no variables of U remain. For example, from $C_a \gg ah$ (A2) DM derives $K_a \gg C_a$ using I4 ($K_a ah = h^+ a^-$), I2' ($h^+ \approx C_a$), and E1 ($C_a \approx a^-$). Using a less mechanical notation:

$C_a \gg ah$	Assumption A2
$C_a \gg h^+ a^- / K_a$	Resolving ah with I4.
$C_a \gg h^+ C_a / K_a$	Resolving a^- with E1.
$C_a \gg C_a^2 / K_a$	Resolving h^+ with I2'.
$K_a \gg C_a$	Simplification.

This completes DM's process of constructing the caricature of a single subregime. The bounds and concentration equations derived through these five steps correspond exactly to those in the example section.

Step 2 (cont.) Creating a Patchwork

In the section on steps 1 & 2 we glossed over the step of merging assumptions, saying only that all combinations of assumptions were explored. DM provides a more intelligent coordination based on the interrelationship between sets of assumptions. These are depicted using the subset/superset lattice of figure 3.

Figure 3: Subset/superset lattice of caricatural assumptions considered by DM.

First, note that the bottom of the lattice is rooted in the original model — since no assumptions are made and no approximations are performed. Moving upwards through the lattice results in simpler models, since each new assumption makes an additional term insignificant, which then drops out of the equations.

Second, although models higher in the lattice are simpler, their domain of validity is more restrictive. That is, each caricatural assumption introduces a new subregime boundary; thus, the region corresponding to the domain of validity of one caricature is a subset of any caricature appearing below it in the lattice.

Third, when moving up the lattice the added assumptions do not always result in simplification. For example, $\{A2, A3\}$ produces the same equation for h^+ as does $\{A3\}$.[1] This explains why Schaum's outline (Beckwith 1985) includes a region $R3$ for $\{A2\}$, but no region for $\{A2, A3\}$ (see figure 1). The same argument applies to the absence of $\{A1, A3\}$. These eliminated sets are depicted by squares in the lattice. Likewise, additional assumptions do not always restrict the domain of validity, particularly when the boundary they introduce is outside the existing region.

Fourth, in some cases a set of caricatural assumptions is mutually inconsistent, for example, as we pointed out earlier for $\{A1, A2\}$. This is recognized when the result of a resolution is detected to be incon-

[1] But this depends on how many of the equilibrium concentrations we are interested in. $\{A2, A3\}$ may allow additional simplification over $\{A3\}$ for other species.

sistent by Estimates or Minima. For example, from $\{A1, A2\}$ Estimates derives $C_a \gg C_a$.

While all caricatures could be generated by simply repeating steps 3-5 on all combinations of caricatural assumptions, the different combinations share two properties that DM exploits to make this process more efficient. First, by monotonicity each superset of an inconsistent set of assumptions is also inconsistent. Thus to avoid exploring potentially large sections of the lattice, DM creates caricatures of each regime by starting at the bottom of the lattice and moving monotonically upwards, ignoring anything above an inconsistent set. In our example, of 16 potential sets of assumptions, 9 prove consistent, 2 are explicitly demonstrated inconsistent, and 5 are supersets of them and thus need not be explored. The 7 inconsistent sets are marked by X's in the lattice. Finally, caricatures of regimes are generated incrementally by exploiting monotonicity. Given the caricatural equations $\mathbf{E}'$ for a set of assumptions S, the caricatural equations of its immediate supersets $S \cup \{A_i\}$ are computed by further exagerating $\mathbf{E}'$ using assumptions A_i.

Discussion

Decompositional modeling has been demonstrated on several analytical chemistry examples taken from (Beckwith 1985). The first step of DM is implemented in Lisp on top of Minima (Williams 1991). The remaining four steps are implemented in Prolog on top of Estimates (Raiman 1991). The solutions DM produces are guaranteed to be correct within the conditions of negligibility for order of magnitude. This paper makes precise the caricature's metaphor first introduced in (Raiman 1988), and the decompositional modelling process introduced in (Raiman & Williams 1992).

One clear need of DM is the ability to bound error, such as is available in a variety of approximate or order of magnitude systems, such as (McAllester 1981; Mavrovouniotis & Stephanopoulos 1988; Weld 1991; Shirley & Falkenhainer 1990; Nayak 1991; Yip 1993). A second need, highlighted at the end of the section on step 4, is to exploit recent advances in solving nonlinear systems, by embodying them with sufficient error bounding capabilities. (Nayak 1991) provides an alternative to Estimates for performing order of magnitude inference, based on a very interesting mapping to linear programming.

An earlier example of a decompositional approach is (Sacks 1987) on piecewise linear approximations. An important difference is that the approximated behaviors of decompositional modeling remain non-linear. The claim is that the approximation should preserve the essential characteristics of the behavior, and this is often nonlinear. Until recently linear approximations were necessary for a system to be solvable. This is dramatically changing, however, given recent advances in nonlinear symbolic algebra.

Finally, note that our approach only addresses decompositional modeling applied to algebraic systems, not for example dynamical systems. In this context a caricature would, for example, characterize an ever so slightly decaying satellite's orbit as a limit cycle (Raiman 1988). A variety of authors have explored this context, including (Weld 1988; Davis 1987).

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