Mechanism Reduction via Adjacency Matrix Power

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***Abstract*— Mechanism reduction is badly needed in large scale chemical simulations. Most graph based approaches, such as Directed Relation Graphs, derive the dependency of a species on all the others using single paths between them, which is not optimal. But since calculating the optimal solution has prohibitive costs, in this paper we propose the use of all the paths of a given large size to approximate the dependency.**

I. Introduction

Mechanism reduction is an essential step prior to simulation due to the computation of simulating a full mechanism. Several approaches to reduction exist, being graph based approaches prominent. Graph based approaches normally calculate, for each pair of species that appear in a chemical equation, how much they directly affect each other's production and consumption; these *Direct Interaction Coefficients (DIC)* are the weights of the edges connecting the vertexes corresponding to the given species in a directed graph that represent the whole mechanism, the *dependency* graph[]. Given a set of target species, for example pollutants or desired products, the dependency graph is used to calculate the *Overall Interaction Coefficient (OIC)* of each target, i.e., how much it is affected by each of the other species[]. Because calculating the OIC precise values is too costly in computational terms, current methods provide only approximations, such as that given by considering only the paths from the target to the species that have the biggest DIC product and ignoring other paths.

In this paper we provide a an approximation to the OIC that consider all the paths from target to species of a given size. By considering a large size and considering that complex mechanisms have very small cycles in their graphs, and hence that a large path will likely include many small paths, our approach can better approximate the OIC. Our technique uses large powers of the adjacency matrix, equivalent to the dependency graph. Our algorithm performs O($\log p$) multiplications, where p is the power of the matrix.

We built our approach using Cantera. It automatically builds the *dependency* graph and calculates the OIC of all species of a loaded mechanism, and also reduces the mechanism using user provided parameters, e.g., the target number of reactions.

II. Directed Relation Graph

A. Directed Interaction Coefficient

A directed graph $G = (V, E)$ is composed by a set of vertexes V and edges E, such that $\forall (v, w) \in E, v, w \in V$, and the edge is directed from v to w. Graph based reduction methods build graphs in which vertexes represent chemical species (We use species' names and corresponding vertexes interchangeably.) and a directed edge (A, B) denotes the presence of a reaction that consumes b and produces or consumes A in the mechanism, Directed Relation Graph (DRG). The weight of each (A, B) edge in the DRG is the coefficient of how much species B directly affects the production and consumption of species A, i.e., their **Direct Interaction Coefficient** (DIC), noted r_{AB}. The method to calculate r_{AB} was proposed by [Pepiot-Desjardins and Pitsch, 2008] and extended by [Niemeyer, 2013].

B. Path-Independent and Overall Interaction Coefficients

A directed path or, in the context of this work, a path from v to w in a directed graph (V, E) is a sequence of vertexes $s = \langle v_1 = v, v_2, \ldots, v_n = w \rangle$, such that $v_i \in V, 1 \leq i \leq n$ and the edge $(v_i, v_{i+1}) \in E$, where n is the length of sequence s and v_i is the i-th element of s. Hence, there exists a path $\langle v, \ldots, w \rangle$, from v to w, in a graph corresponding to a chemical mechanism if and only if there is at least one chain of reactions in the mechanism where the first reaction consumes species w and the last one produces v.

The the DIC of a path connecting a target species to a source species may be combined to produce a *Path-Dependent Interaction Coefficient* (PIC); the formula to calculate $r_{AB,p}$ is given by Equation 1, where p is the corresponding path from A to B and n is the number of reactions in the sequence.

$$r_{AB,p} = \Pi_{j=1}^{n} r_{p[j],p[j+1]} \tag{1}$$

Finally, the PIC may be combined to produce an *Overall Interaction Coefficient* (OIC). However, the precise value of the OIC would be a combination of all the paths connecting the two species, but finding all paths in a graph is computationally too expensive for any reasonably sized mechanism, with complexity O($n!$). This is why reduction methods use approximated OIC, based a single path in the graph.

C. Path Based OIC Approximations

Since finding all the paths is too expensive, an alternative is to find one path that is representative of all the others, and use its PIC as an approximation to the OIC. Nyemeyer compared the performance of three path searching algorithms, Breath-First Search, Depth-First Search, and Dijkstra shortest path [Niemeyer, 2013]. Ultimately, all of these algorithms use a "special" path to approximate the OIC, such as the one with biggest PIC or whose smallest DIC is the biggest.

The problem with using a single path to approximate the OIC is that even though the resulting coefficient might show a low dependency between species, the actual value could show otherwise. This is true even in the case the path with biggest PIC is used, as given by the Dijkstra algorithm, since there could be a multitude of alternative paths.

Alternative approaches to OIC approximation exist, such as the Path-flux propagation [Sun et al., 2010], but they seem to have similar problems, and we do not review it here.

III. Proposal

A directed and weighted graph may be represented as adjacency matrix, and our proposal consists in using simple matrix multiplication and, ultimately, matrix large powers, to approximate the value of the OIC, for any given pair of species, as we now explain.

In the adjacency matrix lines and columns correspond to the graph's vertexes and the cells value is the weight of the edge from the line vertex to the column vertex; if no such edge exists, the value is 0. In other words, if M is the adjacency matrix corresponding to a DRG (V, E), then

$$M_{A,B} = \begin{cases} r_{AB} = r_{AB,\langle A,B\rangle} & \text{if} A, B \in V \text{ and } (A,B) \in E \\ 0 & \text{otherwise} \end{cases} \tag{2}$$

Also, if $M_{A,B}$ is the direct dependency of A in B, then $M_{A,C} * M_{C,B}$ is the dependency of A in B via chain reactions of size two, in which the second reaction involves B, that is,

$$M_{A,C} * M_{C,B} = \begin{cases} r_{AB,\langle A,C,B\rangle} & \text{if } A, B, C \in V \\ & \text{and } (A,C), (C,B) \in E \\ 0 & \text{otherwise} \end{cases} \tag{3}$$

Moreover, $\sum_{C \in V} M_{A,C} * M_{C,B}$ measures the dependency of A in B through all chain reactions of size two, that is,

$$\sum_{C \in N} r_{AB,\langle A,C,B\rangle} \tag{4}$$

But since $\sum_{C \in V} M_{A,C} * M_{C,B}$ is exactly the value of cell $M^2_{A,B}$, it may be calculated, along with the other dependencies through chain reactions of size two, by raising M to the second power.

Finally, the same is true for any power; for example, $M^{100}_{A,B}$ has the dependency of A in B considering *all chains of one hundred reactions*, i.e., $\sum_p r_{AB,p}$ where $p = \langle s_1 = A, s_2, \ldots, s_{101} = B\rangle$.

We propose to use $M^x_{A,B}$, for a large x, as an approximation for the OIC of A and B. Since the paths considered include cycles, if we assume that there are cycles of most sizes in the DRG and that huge paths are concatenations of smaller ones, then a large power will include cycles of various sizes and be a good approximation to using all possible paths. We believe this assumption is true by analyzing different mechanisms, such as GRIMech3.0, whose DRG is depicted in Figure 1.

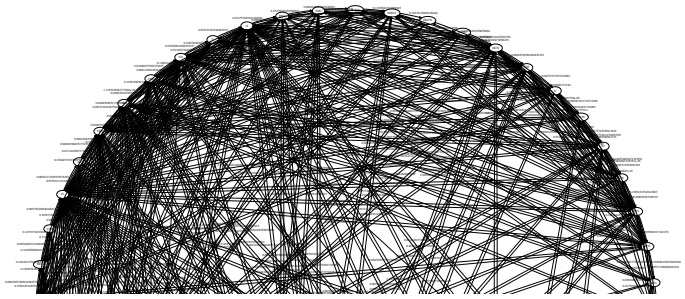

Fig. 1. GRIMech3.0 DRG excerpt.

A. Calculating the Matrix Power Efficiently

Multiplying two matrices takes O($n^{2.373}$ time. Hence, calculating the power matrix by successive multiplications is impractical. Instead, we use the equality $M^x * M^x = M^{2x}$ in our approach, presented in Algorithm1; it has complexity $log(x) * n^{2.373}$, where x is the power desired and n the number of species.

Algorithm 1 Matrix power algorithm.

```
function RAISE(M, P)
    A ← I
    while P > 0 do
        if P mod 2 = 1 then A ← A * M
        P ← P/2
        if P > 0 then M ← M * M
    return A
```

IV. Conclusion and Future Work

We have implemented our proposal in Cantera[1] to reduce any mechanism to one with a given fraction of the original size, using different methods to rank the equations using the approximated OIC. In a qualitative approach we verified that our reduced mechanisms maintain a behavior close to the original one while cutting up to 70% of the reactions.

Our next steps include performing an extensive evaluation and combining our method with others.

Last, we note that this work is the product of scientific collaboration between the Fluid Mechanics Laboratory (MFLab) of the Federal University of Uberlândia and Petrobras.

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[1] `http://www.cantera.org`