

Generating Process Explanations in Nuclear Astrophysics

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Abstract. In this paper we describe ASTRA, a computational aid for generating process explanations in nuclear astrophysics. The system operates in two stages, the first using knowledge of quantum theory to produce a set of legal reactions among elements and the second searching for pathways of such reactions that explain the construction of some element from lighter ones. ASTRA has found apparently novel reactions that involve proton and neutron capture, as well as novel fusion reactions that produce neutrons and deuterium. The system has also generated reaction pathways for helium, carbon, and oxygen that do not appear in the scientific literature. However, ASTRA also finds many other reaction pathways that are less interesting and that suggest priorities for future research.

1 Introduction

The computational study of scientific discovery has made important strides in its short history. Early research focused on replicating discoveries from the history of science, covering results from disciplines as diverse as physics, chemistry, and biology. The types of discoveries also ranged widely, including numeric laws (e.g., Langley, 1981), qualitative relations (e.g., Jones, 1986), structural models (e.g., Zytков & Simon, 1986), and process models (e.g., Kulkarni & Simon, 1990). Nevertheless, some critics questioned these results because they involved scientific relations already known to the developers.

In recent years, some researchers have turned their efforts toward the computational discovery of new scientific knowledge, with some success. For instance, Mitchell, Sleeman, Duffy, Ingram, and Young (1997) report their DAVICCAND system finding a new numeric relation in metallurgy, whereas Buchanan and Lee (1995) describe novel results on whether chemicals cause cancer. Another important example is Valdes-Perez' (1995) MECHEM system, which has found new reaction pathways in physical chemistry. His progress has encouraged us to examine other branches of science in which reaction pathways occupy a central position.

In this paper, we focus on scientific discovery in the field of astrophysics. In the section that follows, we briefly

review this discipline's basic problems and methods. After this, we describe ASTRA, an *astrophysical research aid* designed to support scientists in explaining the synthesis of elements and their relative abundance in stars. After explaining the inputs, outputs, and operation of the system, we report the reactions and reaction pathways that ASTRA produces for some astrophysical problems. One challenge in research on scientific reasoning is to determine the quality of new discoveries in terms relevant to the field at hand; we devote some attention to this issue, using a careful literature search to evaluate ASTRA's outputs. This analysis reveals some limitations of the system and suggests directions for future research.

Our aim in developing ASTRA is not to automate the scientific process, but rather, as with Valdes-Perez' MECHEM, to provide scientists with computational support. Astrophysics has a strong theoretical framework, which it largely shares with particle physics. However, constructing process models for particular phenomena is a tedious task that involves considering many alternative fusion reactions and exploring many potential reaction pathways. We hypothesize that published accounts of such stellar phenomena are not the only such process models that astrophysicists would find acceptable, and our results with ASTRA suggest that it can find explanations that are consistent with existing theory but that human researchers have overlooked. We anticipate that scientists will welcome a tool of this sort to help them identify candidate process explanations.

2 Process Explanations in Astrophysics

The field of astrophysics addresses a number of issues, including the the formation of the stars and their thermal equilibria. The subfield of nuclear astrophysics focuses on a more specific topic: the nucleosynthesis of chemical elements in stars. The basic problem is to explain the transformation of hydrogen (H) and helium (4He), thought to have emerged early in the history of the universe, into heavier elements. Another important problem concerns the distribution of the elements, in particular the abundance of carbon (${}^{12}C$), nitrogen (${}^{14}N$), and oxygen (${}^{16}O$) relative to lighter elements like lithium (7Li), beryllium (9Be), and boron (${}^{11}B$).

Theoretical accounts in astrophysics are closely related to those found in particle physics and nuclear physics. In their attempts to explain nucleosynthesis, theorists first

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identify particle reactions that are consistent with quantum physics and that are likely to occur in the stellar medium. They then combine these primitive processes into reaction pathways that transform hydrogen, helium, and other components into new elements, ideally with the distribution observed in nature.³

According to the current astrophysical theories, stars develop through several stages in their lifetimes. The first stage, which follows the star’s initial formation by the condensation of cosmic clouds and hydrogen gas, involves ‘hydrogen burning’. During this period, stars radiate energy emitted by a series of hydrogen fusion reactions. Astrophysicists have proposed three different pathways (see Adouze & Vauclair, 1990, p. 52; Williams, 1991, p. 351) to account for hydrogen burning in stars the size of the sun and smaller. Later stages consist of more complex reactions, typically involving heavier elements.

Assuming a stellar model in thermal equilibrium, and drawing on known fusion and decay reactions, astrophysicists propose reaction pathways to explain the synthesis of particular elements. The reactions come either from the results of fusion experiments or from current theories using quantum constraints. Taking these reactions as building blocks, astrophysicists construct reaction pathways to explain transitions from lighter to heavier elements, presumably by reasoning forward from the chain’s first elements or reasoning backward from the final one.

Naturally, there exist many possible pathways that might account for the nucleosynthesis of a given element. Astrophysicists focus their attention on only a few of these candidates, relying on heuristics to constrain the generation of explanatory hypotheses. The main heuristic, at least as reported in the literature, concerns a bias toward using component processes with high reaction rates, a property that should determine their frequency of occurrence in the stellar medium. The reaction rate depends in turn on factors like the nuclear cross section, the energy released, the temperature and density of stellar plasma, and the concentrations of reacting nuclei.

This behavior, heuristic search guided by domain-specific constraints, is consistent with other findings about human cognition on nonroutine problems. Yet the fact that astrophysicists find effective ways to limit their search does not mean they find the best solutions to their problems. We hypothesize that one might uncover alternative process models, overlooked by scientific theorists, with a more systematic search of the same space, to which we now turn.

3 The ASTRA System

Before we describe our application of ASTRA to astrophysical phenomena, we should first describe its inputs, outputs, and procedures, which include two main stages. The first generates reactions that are legal according to quantum theory, whereas the second produces reaction pathways to explain the nucleosynthesis of new elements.

³ We have based our analysis on standard texts in astrophysics, including Adouze and Vauclair (1990), Clayton (1983), Fowler (1986), Fowler, Caughlan, and Zimmermann (1967, 1975), Kippenhahn and Weigert (1994), Lang (1974), and Williams (1991).

3.1 Generating Reactions

The first stage of ASTRA takes as input descriptions for a set of elements and isotopes. Each entity is characterized in terms of five quantum properties: rest mass (in MeV/c²), electric charge, spin, lepton number, and baryon number. We also give ASTRA theoretical knowledge about conservation relations over these quantum properties that hold in reactions among the elements and isotopes. Finally, we constrain the system to consider only exothermic reactions, which produce energy, since endothermic reactions play a minor role in astrophysics.

Based on this information, ASTRA systematically generates all reactions among these elements that obey the conservation laws and that take one of six forms: $A \rightarrow C$, $A \rightarrow C + D$, $A \rightarrow C + D + E$, $A + B \rightarrow C$, $A + B \rightarrow C + D$, and $A + B \rightarrow C + D + E$. The algorithm simply instantiates each form in all possible ways and retains each proposed reaction only if it conserves all the relevant properties. The basic operation at this stage is equivalent to one module of the BR-4 system, which we have described elsewhere (Kocabas & Langley, 1995). Note that this process generates not only fusion reactions, considered the mainstay of nuclear astrophysics, but also decay reactions, in which one element breaks into others.

For the runs described in this paper, we provided ASTRA with the elements from hydrogen to oxygen, their isotopes, and a few elementary particles like the electron, proton, neutron, and neutrino, giving a total of 36 distinct entities. From these, the system generated some 350 different reactions, but some were minor variations on one another, such as ${}^3\text{He} + {}^9\text{Be} \rightarrow {}^{12}\text{C} + e + \bar{e}$ and ${}^3\text{He} + {}^9\text{Be} \rightarrow {}^{12}\text{C} + \nu + \bar{\nu}$. We eliminated such near repetitions manually, leaving 276 reactions that included 262 fusion relations and 14 decays.

3.2 Generating Reaction Pathways

ASTRA’s second stage takes as input these primitive reactions, along with an element E whose evolution we want explained and the basic elements/isotopes $\{B\}$ that we are willing to assume as given (typically hydrogen and deuterium). In response, the system generates all pathways that lead from the starting elements to the final element through the various reactions identified in the first stage.

The system uses a depth-first, backward-chaining search to construct these process explanations. On the first step, ASTRA finds those reactions that give as an output the final element E . Upon selecting one of these reactions, R , it recursively finds those reactions that give as output one or more of R ’s input elements. The algorithm continues this process, halting its recursion when it finds a reaction pathway for which all the starting elements are in $\{B\}$ or when it cannot find a reaction off which to chain. ASTRA generates all possible reaction pathways in this systematic manner.

This basic process is very similar in spirit to that used in Valdes-Perez’ MECHEM. Both systems find reaction pathways that explain how one set of entities transforms

into another set, and both use extensive search through the space of pathways, constrained by knowledge of legal reactions. MECHEM focuses on pathways in physical chemistry, whereas ASTRA deals with certain astrophysical phenomena, but that difference is less important than the fact that our system also generates its reactions from a deeper background theory. This provides another layer of reasoning at which scientists may have overlooked processes, and thus gives ASTRA additional opportunities for novel discoveries. In more recent work, Valdes-Perez (1997) has extended MECHEM to accept component reactions from an external source, thus reducing the difference between our two approaches.

4 Experimental Results in Astrophysics

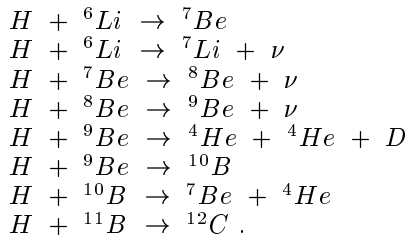
As we have noted, one primary concern of astrophysics is the nucleosynthesis of chemical elements in stars, so our studies of ASTRA's behavior have focused on this topic. In this section we report the results of these tests, which we have organized around conceptual distinctions in the scientific literature. We first address two broad classes of reactions that astrophysicists believe play an important role in stellar nucleosyntheses, then turn to reaction pathways that explain the generation of heavier elements from lighter ones.

4.1 Proton and Neutron Captures

The building blocks of astrophysical explanations are the reactions among elements and isotopes. Because the main phenomena involve the creation of heavier elements from lighter ones, scientists focus on fusion reactions. Although many such reactions are possible, astrophysicists emphasize the role of two main reaction types – proton capture and neutron capture – so we will concentrate on those here.

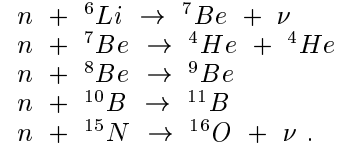
Proton capture involves an exothermic reaction between some element and hydrogen that produces a heavier element, an isotope, and/or helium atoms. Such reactions take part in processes called ‘hydrogen burning’, in which hydrogen atoms are continuously transformed into helium atoms. We have found 33 examples of proton captures given in astrophysics texts (e.g., Fowler et al., 1967, 1975) for elements from hydrogen (H) to oxygen (^{16}O); most concern strong interactions, although some, identified by neutrino emissions, involve weak interactions.

ASTRA's first stage predicts that all elements from hydrogen to nitrogen (^{15}N), with the exception of 4He , participate in proton capture. The program produces 46 such reactions, including all 33 examples we have found in texts, but also 13 others, some of which are:



We have not seen these reactions in any of the astrophysics texts that we have examined. Thus, they may be proton captures that scientists would accept as theoretically possible but that they have overlooked due to the nonsystematic nature of their generation strategies.

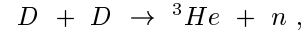
In fusion reactions that involve neutron capture, an element combines with a neutron to form a heavier isotope of the same element. We found 17 neutron captures for light elements in the literature, while ASTRA predicts 59 such reactions that are theoretically possible for the same elements. These include five reactions that we did not see in the texts:



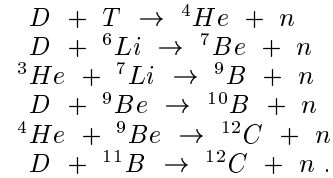
The third reaction may play an important role in stellar reaction pathways, which we will consider shortly.

4.2 Neutron and Deuteron Production

Neutron capture requires a continuous supply of neutrons in the stellar plasma, so that it relies on some neutron-producing reaction. Astrophysicists (e.g., Adouze & Vauclair, p. 89) suggest that

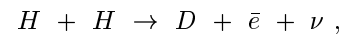


which combines deuterons (an isotope of hydrogen), is the only reaction that releases neutrons in the hydrogen-burning stage of main-sequence stars. Yet ASTRA also predicts six additional reactions that produce neutrons:

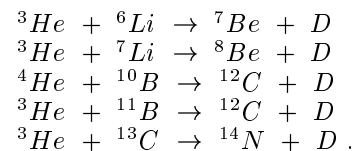


The first two of these reactions appear likely in main-sequence stars, as 6Li , D , and T (tritium, another isotope of hydrogen) all exist in them. The second reaction seems especially important, as both D and 6Li are stable, and thus could play a role in stellar reaction pathways.

Many of the neutron-producing reactions rely on a deuteron (D) as one of their inputs. The best known deuteron-generating reaction is



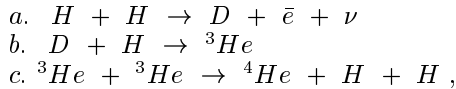
in which two hydrogens react, and we have found in astrophysics texts two other reactions that produce deuterium ($T + {}^3He \rightarrow {}^4He + D$ and $H + {}^9Be \rightarrow {}^8Be + D$). However, the first stage of ASTRA predicts 15 other reactions of this sort. These include:



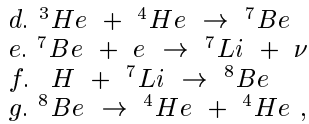
The first two of these reactions should be possible in main-sequence stars, as ${}^6\text{Li}$ and ${}^7\text{Li}$ are known to exist there, yet we have not found either reaction in the scientific literature.

4.3 Generation of Helium

Having established the reactions possible in the stellar medium, the most basic explanatory task in nuclear astrophysics concerns the transformation of hydrogen into helium. Scientists assume that this hydrogen-burning process is the principal energy source in main-sequence stars. The standard reaction pathway given by astrophysicists (e.g., Adouze & Vauclair, p. 52; Williams, 1991, p. 351) to explain this effect is:

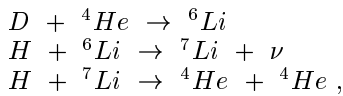


which they refer to as the ‘proton-proton chain’. The net effect of this reaction pathway, when reaction (a) occurs twice, is $4 H \rightarrow {}^4\text{He} + \nu + 26.72 \text{ Mev}$. Another pathway hypothesized by scientists, which they call an ‘alpha-catalysed chain’, is:

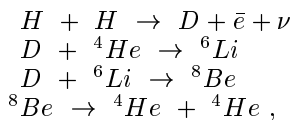


in which reactions *b* and *c* provide both the ${}^3\text{He}$ and the ${}^4\text{He}$ needed by reaction *d*. An alternative pathway, which also appears in texts, replaces reaction *e* with $H + {}^7\text{Be} \rightarrow {}^8\text{B}$ and *f* with ${}^8\text{B} \rightarrow {}^8\text{Be} + \bar{e} + \nu$, which produce the ${}^8\text{Be}$ needed by the final reaction through a different mechanism. Astrophysicists refer to these three pathways as the *pp1*, *pp2*, and *pp3* chains, respectively.

When asked to generate reaction pathways from hydrogen to helium, the ASTRA system finds all of these reaction pathways, along with one other main helium-producing pathway, called the ‘CNO cycle’ in texts, that involves carbon, nitrogen, and oxygen atoms, and that takes place in stars more massive than the sun. The program also finds some 44 other process accounts of helium generation that differ in their last link of the chains. These include the two reaction pathways:



which has the net effect of $2 H + D \rightarrow {}^4\text{He} + \nu$, and

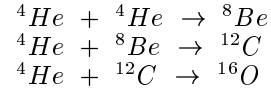


which has the net effect of $4 H \rightarrow {}^4\text{He} + \bar{e} + \bar{e} + \nu + \nu$. Both Cujec and Fowler (1980) and Harris, Fowler, Caughlan, and Zimmerman (1983) argue that reactions involving *D* are unlikely due to its relatively low abundance.

However, Clayton (1983, pp. 371–2) notes that the density of deuterium in the interstellar medium and the sun remains unknown, and suggests that the substance might be more common than usually believed. From this perspective, the above reaction pathways provide plausible novel accounts of helium production.

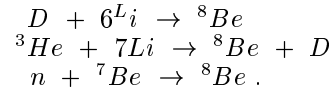
4.4 Generation of Carbon and Oxygen

As we have noted, astrophysicists are especially concerned with explaining the origin of carbon and oxygen. The standard account supposes a process called ‘helium burning’, in which helium atoms react with a light element to produce a heavier one. For example, Fowler (pp. 5–6) proposes the pathway

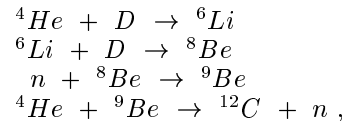


to explain the synthesis of carbon and oxygen from helium. However, there are theoretical problems with this account; although these reactions are allowed by quantum theory, the first one is endothermic and the lifetime of ${}^8\text{Be}$ is very short ($2 \times 10^{-16} \text{ sec}$). The only other published pathway that we have found, the fusion of three helium atoms into carbon, has a low reaction rate. Despite these acknowledged problems, current theories rely on the above reaction chains to explain helium burning.

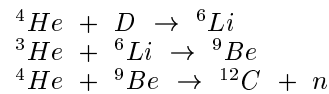
ASTRA does not find the reaction ${}^4\text{He} + {}^4\text{He} \rightarrow {}^8\text{Be}$ because it is slightly endothermic, but the system finds 20 other reactions that produce ${}^8\text{Be}$, such as:



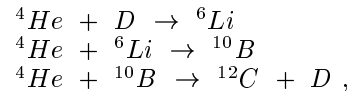
Once ${}^8\text{Be}$ is available, ${}^4\text{He} + {}^8\text{Be} \rightarrow {}^{12}\text{C}$ can take place exothermically, so ASTRA formulates this reaction. The system produces 24 additional pathways that differ in their final steps to ${}^{12}\text{C}$, which contribute to a total of 8.2×10^{14} more pathways for ${}^{12}\text{C}$ synthesis than astrophysicists appear to have entertained. These include:



which relies on one of the neutron-capture reactions we discussed earlier. Briefly, if ${}^8\text{Be}$ captures a neutron before it decays, then it transforms into its stable isotope. This in turn produces carbon by reacting with ${}^4\text{He}$, where the emitted neutron from the latter reaction can combine with another ${}^8\text{Be}$. Two other novel pathways are:

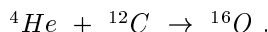


and

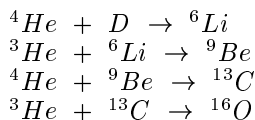


in which the net effect is $3\ ^4\text{He} \rightarrow\ ^{12}\text{C}$, providing yet another account of carbon production that complements the standard explanations.

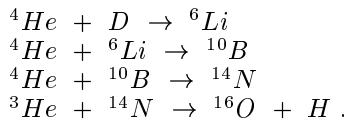
Once ^{12}C has formed, in whatever manner, it can react with ^4He exothermically to produce oxygen, as stated in the existing literature:



Astrophysicists favor this reaction because of the relative abundance of ^4He , but ASTRA also finds other pathways to oxygen. These include variations on the last two carbon chains shown above:



and



In summary, ASTRA finds a number of reaction pathways to carbon and oxygen that physicists appear to have missed, just as they have done in the case of the lighter element helium. All of these pathways are theoretically possible, but final judgement about their scientific value requires further evaluation, as we discuss next.

5 Discussion of Results

We have been careful to compare ASTRA's outputs, at both the reaction and pathway level, to those available in astrophysics texts (Adouze & Vauclair, 1990; Clayton, 1983; Kippenhahn & Weigert, 1994; Lang, 1974; Fowler et al., 1967, 1975) and particle physics (Williams, 1991). Of course, an exhaustive comparison to these fields' literatures would be intractable, but we have combined our search with analyses by an established plasma physicist, whose expertise should complement that available in our sample of the written record.

We can evaluate our results with ASTRA on two main fronts. The first concerns false negatives or errors of omission. Here the system fares very well, in that we have found only one reaction and one reaction pathway that appear in the literature but that our program fails to generate. Both involve endothermic (energy using) reactions, and we intentionally forbid ASTRA from considering such reactions, as they play a minor role in astrophysics and as this constrained the search space of reaction pathways considerably. Otherwise, the system has found all basic reactions we have seen in texts, along with all pathways for proton and neutron capture, for neutron and deuterium creation, and for helium, carbon, and oxygen production.

The second main issue concerns false positives or errors of commission, and here issues of evaluation become more complex. ASTRA generates only those reactions consistent with quantum theory, so in some sense it can have no false positives at this level. But not all possible reactions are interesting to astrophysicists; for many the reaction

rates, which determine the yield of a reaction, are so low they cannot play much role in stellar processes.

In fact, the current system generates about 8×10^9 reaction pathways for helium creation and even more, over 7×10^{20} pathways, to oxygen. As we have noted, astrophysicists appear to use low rates of component reactions to rule out the vast majority of these pathways. Existing theory states how to predict these factors, but the calculation is a complicated one that involves the nuclear radii, the temperature, pressure, and density of the plasma, and the relative concentrations of the elements. But, clearly, incorporating rate constraints into ASTRA should be our highest priority for future work.

Nevertheless, preliminary analysis suggests that some of the novel reaction pathways, in particular those in Sections 4.3 and 4.4, have viable reaction rates. Moreover, our expert in plasma physics maintains that these pathways constitute plausible explanations that hold scientific interest. We must still confirm their relevance through more extensive calculations, but the preliminary analysis is encouraging. Of course, publication of these results in the scientific literature would be even stronger evidence, but that too must await additional work.

6 Related Research on Scientific Discovery

Our approach to computational discovery draws many ideas from earlier work on the topic. As we noted in Section 3, our system shares many goals and techniques with Valdes-Perez' MECHEM, which discovers reaction pathways in physical chemistry. Another close relative is SYNGEN (Hendrickson, 1995), which addresses the task of chemical synthesis in which one must determine not only the reaction paths but also the starting molecules. A more detailed similarity is that both ASTRA and SYNGEN generate pathways by chaining backward from the final products using known reactions.

Our system differs mainly from these earlier algorithms in its focus on astrophysics and in its ability to generate the basic reactions from the elements involved and the principles of quantum physics. ASTRA inherits this latter ability from our previous BR-4 system (Kocabas & Langley, 1995), which carries out theory revision in particle physics, much like its predecessor BR-3 (Kocabas, 1991). The BR-3 system in turn descends directly from STAHL (Zytkow & Simon, 1986) and STAHLp (Rose & Langley, 1986), which modeled qualitative discovery in chemistry. Unlike its ancestors, BR-4 includes a module that predicts reactions from its current theory, which forms the basis for ASTRA's capacity along these lines.

Other discovery systems that formulate process theories seem less closely related. Kulkarni and Simon's (1990) KEKADA generates reaction pathways but relies on experimental data to determine intermediate steps. Karp (1990), Rajamoney (1990), and O'Rourke, Morris, and Schulenberg (1990) describe systems that produce process explanations in biology, physics, and chemistry, respectively, but all start with given accounts and revise them in response to unexpected observations. Our work has focused on generating process models from a deeper theory, rather than on their revision.

7 Concluding Remarks

In this paper we described ASTRA, which we designed to serve as an aid for astrophysical research. Given a set of elements, isotopes, and particles, the system determines all valid reactions among these entities that are consistent with quantum theory. We found that ASTRA generates all reactions we have seen in the astrophysics literature involving proton and neutron captures, as well as neutron and deuteron production. Moreover, given an element observed within stars and the likely starting elements, the algorithm generates all reaction pathways that can explain the latter's transformation into the former. Again, studies have revealed that ASTRA reproduces all reaction pathways that, to our knowledge, scientists have proposed for the creation of helium, carbon, and oxygen.

However, the system also generates many reactions and pathways that we have not found in the scientific literature. Discussions with an expert in plasma physics indicate that some of these results hold theoretical interest, in that they may provide viable alternatives to generally accepted accounts. But the vast majority of generated reactions and pathways appear to be implausible due to low reaction rates. This suggests that ASTRA needs to use constraints about these factors, and we intend to incorporate them in future versions. Nevertheless, the system shows considerable promise as an aid to astrophysical theory development, and some of its current outputs already appear to constitute valuable scientific results.

Acknowledgements

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