

Libraries used are:

1. **Catlab**: Provides tools for category theory, allowing manipulation of mathematical structures and creation of wiring diagrams.
2. **AlgebraicPetri**: Facilitates modeling and simulating Petri nets, useful for representing distributed or concurrent systems.
3. **AlgebraicDynamics.UWDDynam**: Supports modeling open dynamical systems with external interactions and evolving states.
4. **DifferentialEquations**: Solves differential equations, enabling simulation of time-dependent dynamical systems.
5. **LabelledArrays**: Creates arrays with labeled elements, simplifying tracking of variables in systems with named components.
6. **Plots**: Offers comprehensive plotting tools for visualizing mathematical models and simulation results.

```
1 using Catlab, Catlab.CategoricalAlgebra, Catlab.Programs, Catlab.WiringDiagrams,  
Catlab.Graphics
```

```
1 using AlgebraicPetri
```

```
1 using AlgebraicDynamics.UWDDynam
```

```
1 using DifferentialEquations
```

```
1 using LabelledArrays
```

```
1 using Plots
```

Functions which takes in *"place names"* and *"transition names"* and creates an **open petri-net** using Catlab's *"OpenLabelledPetriNet"* method.

- HE\_addition creates petri-nets which represent **He-4 addition reactions**.
- decay\_reaction creates petri-nets which represent **decay chains**.

HE\_addition (generic function with 1 method)

```
1 # Function to generate binary fusion reactions (He_ + Element => Product)
2 function HE_addition(elements::Tuple, transition_name::Symbol)
3     return Open(LabelledPetriNet(
4         elements, # Places: Input and Output elements
5         transition_name => ((elements[1], elements[2]) => (elements[3])) #
6         Transition rule
7     ))
8 end
9 # Function to generate decay reactions (Element => Intermediate => Product)
```

decay\_reaction (generic function with 1 method)

```
1 function decay_reaction(elements::Tuple, transition_names::Tuple)
2     return Open(LabelledPetriNet(
3         elements, # Places: Input and Output elements
4         transition_names[1] => ((elements[1]) => (elements[2])), # First Decay
5         transition_names[2] => ((elements[2]) => (elements[3])) # Second Decay
6     ))
7 end
```

Creating open petri-nets for each reaction in the "**alpha process**".

```
StructuredMulticospan(Multicospan(
    AlgebraicPetri.LabelledPetriNet {T:2, S:3, I:2, O:2, Name:0}
```

T	tname
1	Ni_Co
2	Co_Fe

S	sname
1	Ni
2	Co
3	Fe_stable

I	it	is
1	1	1
2	2	2

O	ot	os
1	1	2
2	2	3

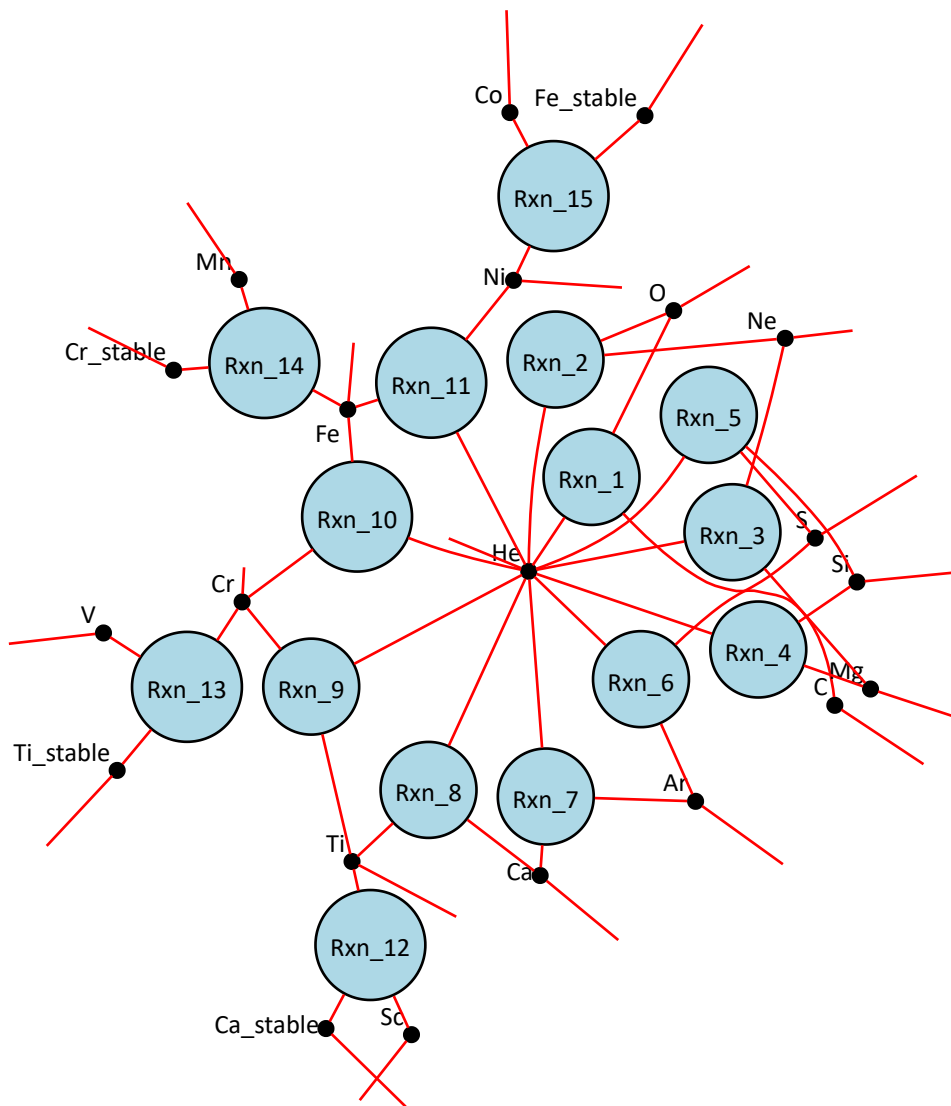
```
1 begin
2   # Generate all the fusion reactions
3   Rxn_1 = HE_addition(:He, :C, :O), :He_C)
4   Rxn_2 = HE_addition(:He, :O, :Ne), :He_O)
5   Rxn_3 = HE_addition(:He, :Ne, :Mg), :He_Ne)
6   Rxn_4 = HE_addition(:He, :Mg, :Si), :He_Mg)
7   Rxn_5 = HE_addition(:He, :Si, :S), :He_Si)
8   Rxn_6 = HE_addition(:He, :S, :Ar), :He_S)
9   Rxn_7 = HE_addition(:He, :Ar, :Ca), :He_Ar)
10  Rxn_8 = HE_addition(:He, :Ca, :Ti), :He_Ca)
11  Rxn_9 = HE_addition(:He, :Ti, :Cr), :He_Ti)
12  Rxn_10 = HE_addition(:He, :Cr, :Fe), :He_Cr)
13  Rxn_11 = HE_addition(:He, :Fe, :Ni), :He_Fe)
14
15  # Generate all the decay reactions
16  Rxn_12 = decay_reaction(:Ti, :Sc, :Ca_stable), (:Ti_Sc, :Sc_Ca))
17  Rxn_13 = decay_reaction(:Cr, :V, :Ti_stable), (:Cr_V, :V_Ti))
18  Rxn_14 = decay_reaction(:Fe, :Mn, :Cr_stable), (:Fe_Mn, :Mn_Cr))
19  Rxn_15 = decay_reaction(:Ni, :Co, :Fe_stable), (:Ni_Co, :Co_Fe))
20
21 end
```

Thanks to Hirithik, the below code snippet helps to visualise the composition more clearly.

display\_uwd (generic function with 1 method)

```
1 display_uwd(ex) = to_graphviz(ex, box_labels=:name, junction_labels=:variable,  
graph_attrs=Dict(  
2     "layout" => "neato",  
3     "bgcolor" => "white",  
4     "overlap" => "false",  
5     "splines" => "true"  
6 ),  
7 node_attrs=Dict(  
8     "shape" => "circle",  
9     "style" => "filled",  
10    "fillcolor" => "lightblue",  
11    "fontname" => "Calibri",  
12    "fontsize" => "10"  
13 ),  
14 edge_attrs=Dict(  
15     "color" => "red",  
16     "penwidth" => "1"  
17 ))
```

Using @relation to create a composition pattern, in which the relation between each individual reaction (open petri-net) is described.



```

1 begin
2   alpha_chain_composition_pattern = @relation (He, C, O, Ne, Mg, Si, S, Ar, Ca,
3     Ti, Cr, Fe, Ni, Sc, Ca_stable, V, Ti_stable, Mn, Cr_stable, Co, Fe_stable) where
4     (He, C, O, Ne, Mg, Si, S, Ar, Ca, Ti, Cr, Fe, Ni, Sc, Ca_stable, V, Ti_stable,
5     Mn, Cr_stable, Co, Fe_stable) begin
6     # Rxn_1 through Rxn_15 mapped to the respective elements in the alpha chain
7     Rxn_1(He, C, O)
8     Rxn_2(He, O, Ne)
9     Rxn_3(He, Ne, Mg)
10    Rxn_4(He, Mg, Si)
11    Rxn_5(He, Si, S)
12    Rxn_6(He, S, Ar)
13    Rxn_7(He, Ar, Ca)
14    Rxn_8(He, Ca, Ti)
15    Rxn_9(He, Ti, Cr)
16    Rxn_10(He, Cr, Fe)
17    Rxn_11(He, Fe, Ni)
18    Rxn_12(Ti, Sc, Ca_stable)
19    Rxn_13(Cr, V, Ti_stable)
20    Rxn_14(Fe, Mn, Cr_stable)
21    Rxn_15(Ni, Co, Fe_stable)
22  end

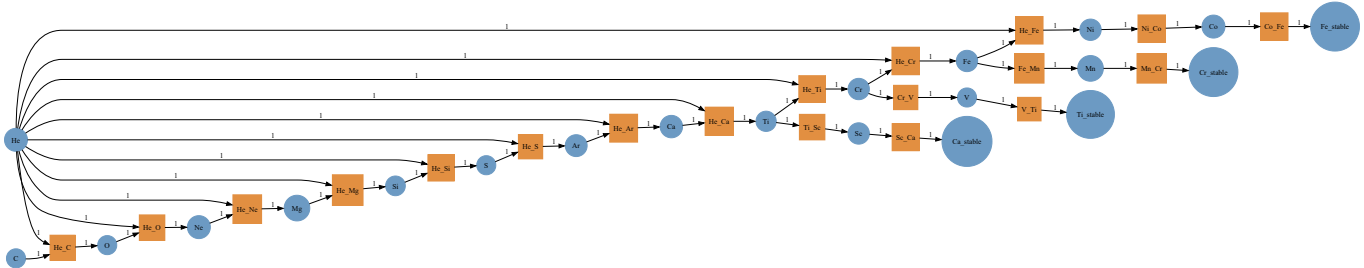
```

```

20
21 # Visualizing the forest composition pattern with to_graphviz
22 #to_graphviz(alpha_chain_composition_pattern, box_labels = :name,
23             junction_labels = :variable)
24 display_uwd(alpha_chain_composition_pattern)

```

oapply is used to apply the composition pattern on the open petri-nets.



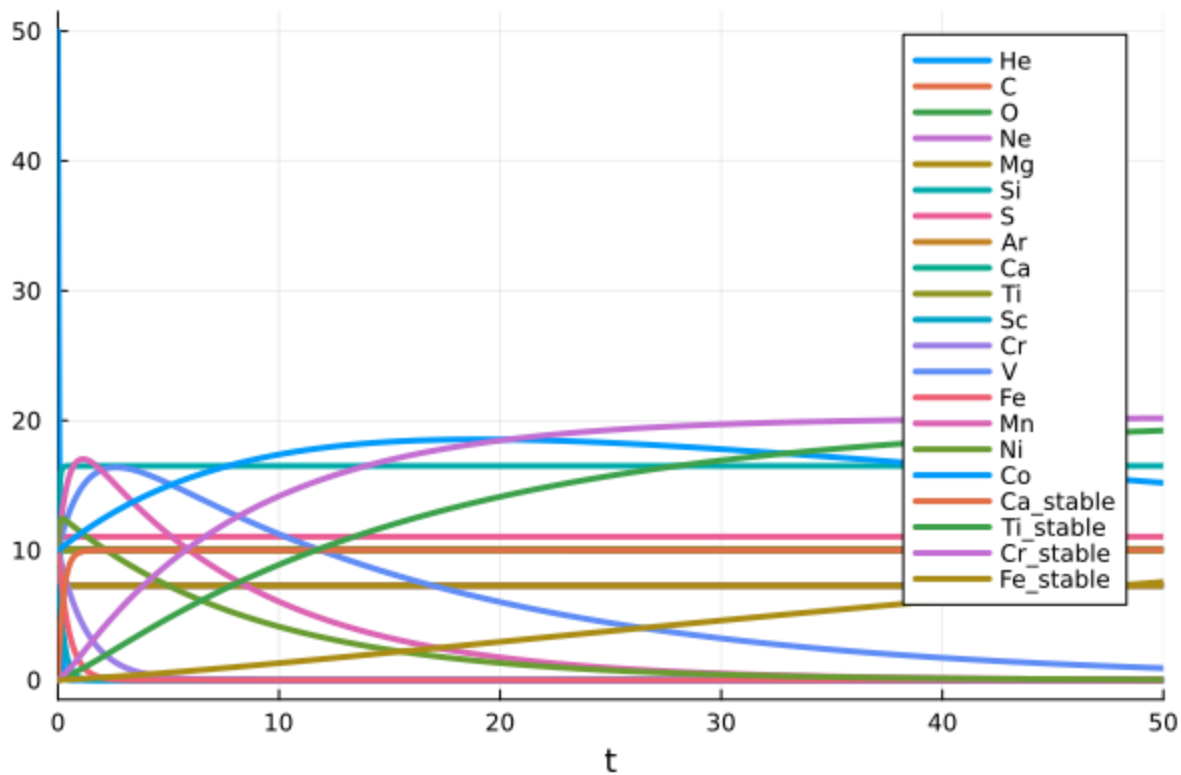
```

1 begin
2   rxn_composite = oapply(alpha_chain_composition_pattern,
3     Dict(
4       :Rxn_1 => Rxn_1,
5       :Rxn_2 => Rxn_2,
6       :Rxn_3 => Rxn_3,
7       :Rxn_4 => Rxn_4,
8       :Rxn_5 => Rxn_5,
9       :Rxn_6 => Rxn_6,
10      :Rxn_7 => Rxn_7,
11      :Rxn_8 => Rxn_8,
12      :Rxn_9 => Rxn_9,
13      :Rxn_10 => Rxn_10,
14      :Rxn_11 => Rxn_11,
15      :Rxn_12 => Rxn_12,
16      :Rxn_13 => Rxn_13,
17      :Rxn_14 => Rxn_14,
18      :Rxn_15 => Rxn_15
19    )
20  )
21
22  to_graphviz(rxn_composite, program="osage")
23 end

```

Now using appropriate rate constants and initial conditions, we can solve this dynamical system by taking the ODEs using `ODEProblem()` and using `solve()` to find the solution to the differential equations. The solution is then plotted using `plot()`.

Transition	Half-Life	Rate Constant (/day)
Cr-48 → V-48	21.6 hours	0.77
Ti-44 → Sc-44	60 years	3.208e-5
Sc-44 → Ca-44	3.97 hours	4.189
V-48 → Ti-48	15.9735 days	0.0626
Fe-52 → Mn-52	8.275 hours	2.01
Mn-52 → Cr-52	5.59 days	0.124
Ni-56 → Co-56	6.1 days	0.1136
Co-56 → Fe-56	77.1 days	0.009



```

1 begin
2   # Assigning parameter values and initial conditions and finding the solution for
   this Dynamical System
3   p = LVector(
4     He_C = 0.1,
5     He_O = 0.2,
6     He_Ne = 0.3,
7     He_Mg = 0.4,
8     He_Si = 0.1,
9     He_S = 0.1,
10    He_Ar = 0.1,
11    He_Ca = 0.1,
12    He_Ti = 0.1,
13    He_Cr = 0.1,
14    He_Fe = 0.1,
15    Ti_Sc = 3.208e-5,
16    Sc_Ca = 4.189,
17    Cr_V = 0.77,
18    V_Ti = 0.0626,
19    Fe_Mn = 2.01,
20    Mn_Cr = 0.124,
21    Ni_Co = 0.1136,
22    Co_Fe = 0.009
23  )
24  u0 = LVector(
25    He = 50,
26    C = 10,
27    O = 10,
28    Ne = 10,
29    Mg = 10,
30    Si = 10,
31    S = 10,

```



```
32      Ar = 10,  
33      Ca = 10,  
34      Ti = 10,  
35      Sc = 10,  
36      Cr = 10,  
37      V = 10,  
38      Fe = 10,  
39      Mn = 10,  
40      Ni = 10,  
41      Co = 10,  
42      Ca_stable = 0,  
43      Ti_stable = 0,  
44      Cr_stable = 0,  
45      Fe_stable = 0  
46  )  
47  soln = solve(ODEProblem(vectorfield(apex(rxn_composite)), u0, (0.0, 50.0), p))  
48  plot(soln, linewidth=3)  
49  end
```

You can also view the solution curve for each element using the command:

`plot(soln.t, soln[20, :], label="Cr_stable", linewidth=3)` (Cr\_stable is the 20th component of soln vector)

