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# Pathways to medical isotope production for a given flux

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# Medical isotope production

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Medical isotope production is a key part of future/modern cancer treatment.

Production methods:

1. Nuclear reactors, currently most medical isotopes are produced in nuclear reactors (e.g. Tc99 ..)
2. Proton beam, usually cheaper than neutron beams (e.g. Ac225, Ga67, Cu64 ...)
3. Neutron beam, greater spread of nuclei to produce (e.g. Mo99, Tc99 ...)

A lot of nuclear reactors are going to be decommissioned, also there is a supply chain pinch point, which could greatly affect medical isotope supply.

Potentially the majority of medical isotopes will be produced in beam facilities in the future.

# How to identify isotope production process

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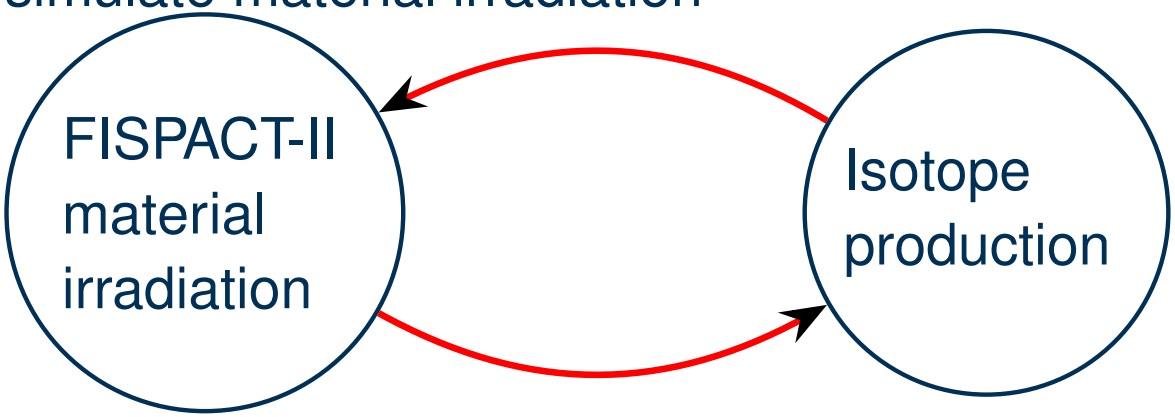
Many existing beam facilities are not exclusively designed for medical isotope production (beam spectrum)

-> Many are for material engineering design

-> Fusion development

One process is to use 'our' (UKAEA) software FISPACT-II to simulate material irradiation




Work flow would be slow.

# Build a framework to interrogate nuclear data

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The intention is to use aspects of Mathematics to build a framework to interrogate nuclear data as a whole.

- Computer friendly
  - optimal data structure
  - easily implementable
  - simple to interogate
- Computationally efficient
  - make use of existing computing libraries
  - optimal for modern (and advanced) computer architectures

## Adjacency matrix and algebra

Our aim is to use the fact that every directed graph can be expresses as an adjacency matrix. This matrix has an algebra (a ring) associated with graphical operations.

# Nuclear data as a graph

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Instead of iteratively sampling from the space of possible materials, consider nuclear data as a graph

- Nuclear data is a concatenation of $\{\text{decay}\} \cup \{\text{activation}\}$.
  - $\sigma_{ij}$ is a matrix of transmutation cross sections and decay coefficients
  - Graph is link between nuclei $i$ to $j$ if $\int_0^\infty \sigma_{ij} dE > 0$

Figure: Graph of $\{\text{Tendl17}\} \cup \{\text{decay2012}\}$ - not very useful

- Investigating the entire nuclear data graph will not elucidate much about how to produce key nuclei.

# Cross section spectrum collapse

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transmutation coefficients matrix:

$$A_{ij} = \frac{\int \sigma_{ij}(E)\phi(E)dE}{\int \phi(E)dE}, \tag{1}$$

where $\sigma_{ij}$ are the cross-section distribution as a function of energy, $E$, and projectile flux $\phi$.
This coefficients matrix is conventionally used to predict the nuclear inventory (or nuclei production) via the inventory equation,

$$\dot{\boldsymbol{n}}(t) = A\boldsymbol{n}(t). \tag{2}$$

# Cross section spectrum collapse

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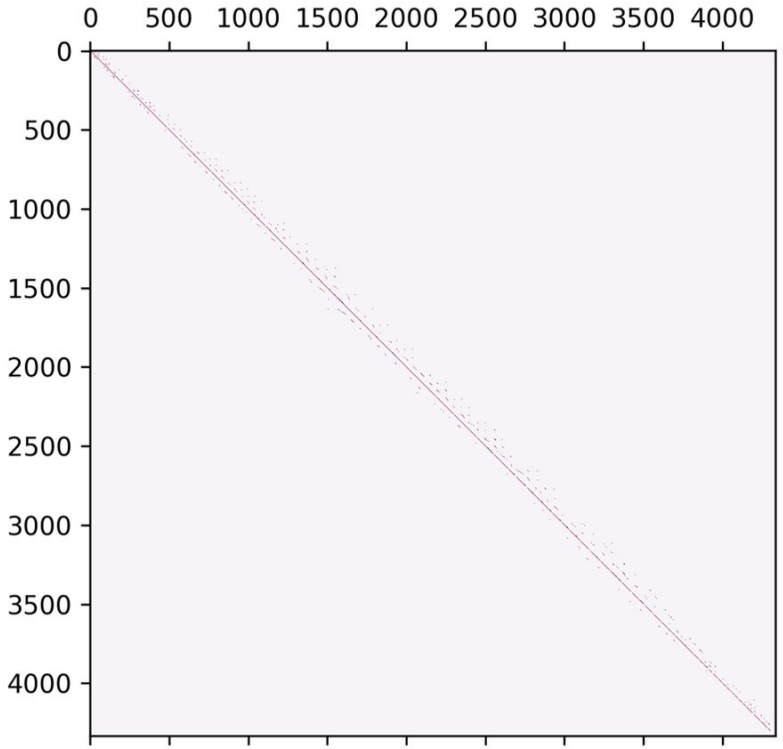
$A_{ij}$ is a sparse matrix

- mostly zeros (97% ish)
- if $\phi = 0$ $A$ can be arranged to be a lower triangle matrix
- only the non-zero components are stored




representation of a nuclear data sparse matrix - yellow corresponds to a non-zero term in the matrix (P. Kanth)

# Collapse graph

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In terms of graphs this collapse is a pruning of the transmutation/decay nuclear data graph - i.e. reduces the number of links/nodes (threshold reactions)

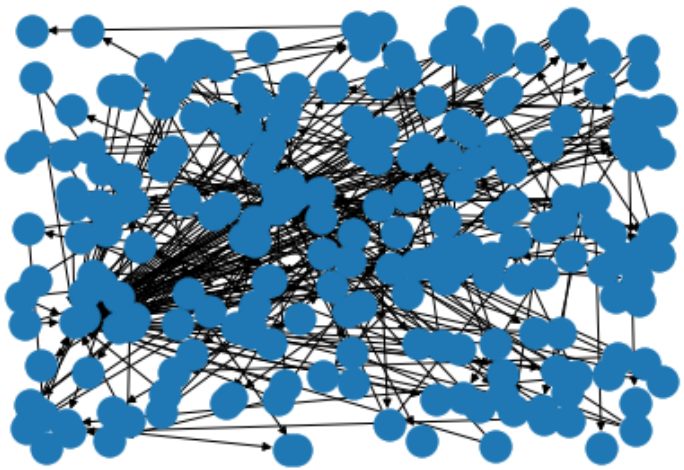

Figure: Collapsed pruned graph of 10MeV projectile - with cut off

So it is a more efficient and holistic approach to consider the collapsed graph/matrix, and identify the initial material. Opposed to randomly sampling from the space of possible material.

- supply a flux, identify key nuclei and how to produce them.

# Graph exploration

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Conventionally this would be investigated using a graph search algorithm.

- One to one relation between a graph and its adjacency matrix,

$$A_{ij} = \begin{cases} 1 & \text{if } A_{ij}^{\text{coeff}} > 0 \\ 0 & \text{else,} \end{cases} \tag{3}$$

this is an algebraic representation of the graph, where $A_{ij} = 1$ represents a directed edge from $i$ to $j$.

- note: this adjacency matrix can contain elements along the diagonal, $A_{ii} \neq 0$.

# Adjacency matrix

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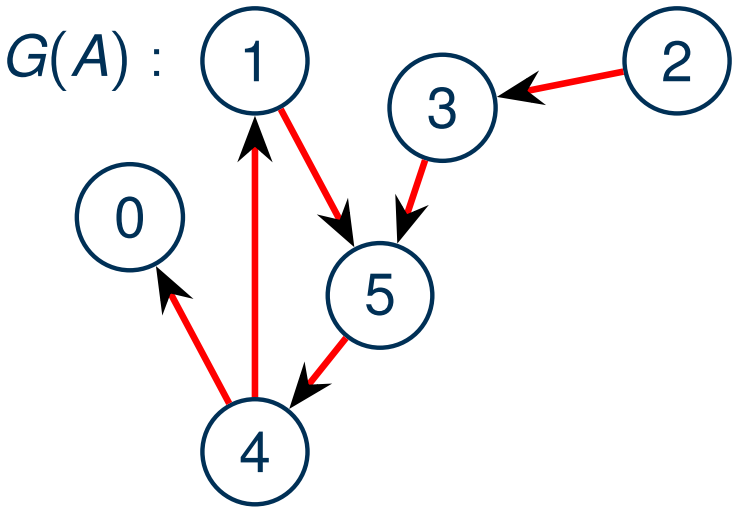
Example graph $G$:

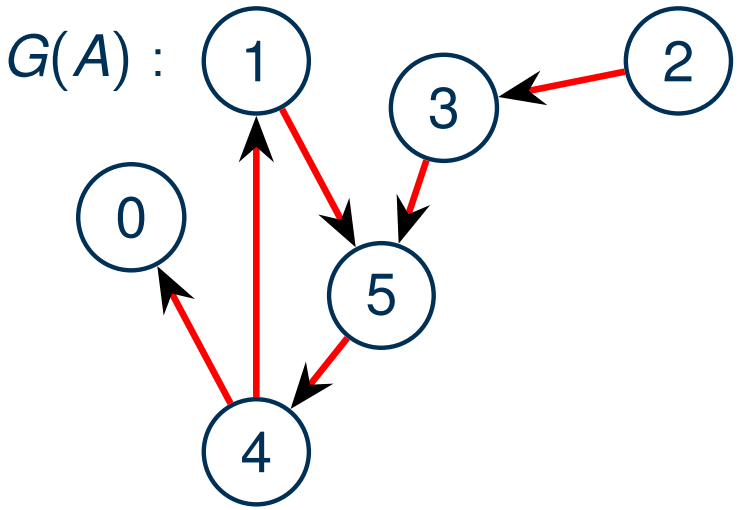



$$A = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix} \tag{4}$$

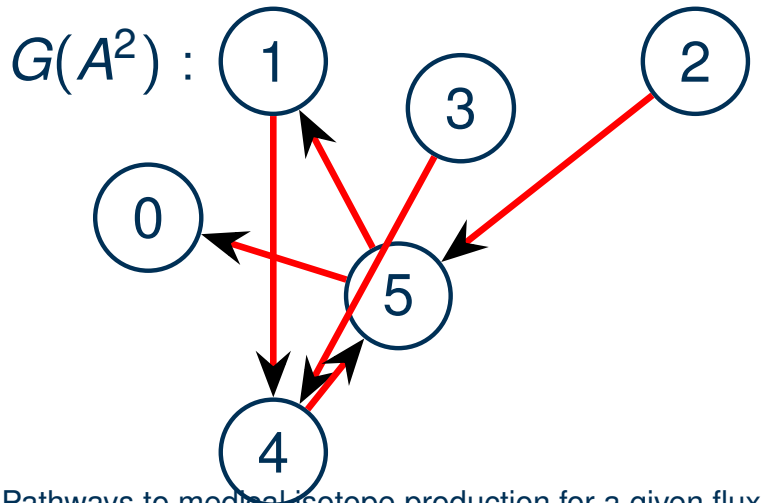
Node $i$ links to node $j$
i.e. node 4 links to nodes 0 and 1.

# Paths

*n*th power of the adjacency matrix show distance *n* paths.




$$A = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}$$




$$A^2 = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 1 & 0 & 0 & 0 & 0 \end{pmatrix}$$

# Paths

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- $A$ represents a transmutation/decay path of nuclei $i$ to $j$
- $A^2$ represents a two step transmutation/decay path of nuclei $i$ to $j$
- $A^n$ represents an $n$ step transmutation/decay path of nuclei $i$ to $j$

Transitive closure, $A^+$, of $A$,

$$A_n^+ = A \cup A^2 \cup A^3 ... \cup A^n, \tag{5}$$

contains all possible paths from $i \rightarrow j$, up to length $n$.
Can be used to identify disconnected subgraphs - sub-matrix identifying nuclei that cannot transmute/decay into each other (for a given irradiation).

# Identifying paths

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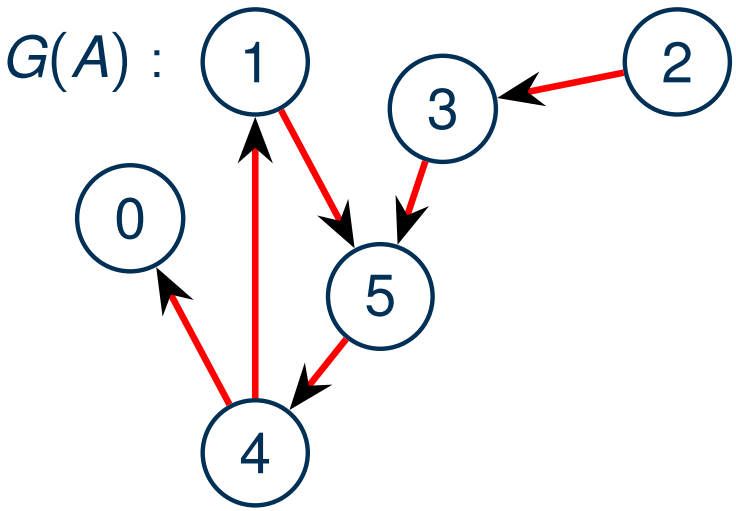


$$A = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}$$

$$A_7^+ = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 2 & 2 & 0 & 0 & 2 & 3 \\ 2 & 2 & 0 & 1 & 2 & 2 \\ 2 & 2 & 0 & 0 & 2 & 3 \\ 3 & 3 & 0 & 0 & 2 & 2 \\ 2 & 2 & 0 & 0 & 3 & 2 \end{pmatrix}$$

All paths up to length 7

# Identifying disconnected graphs

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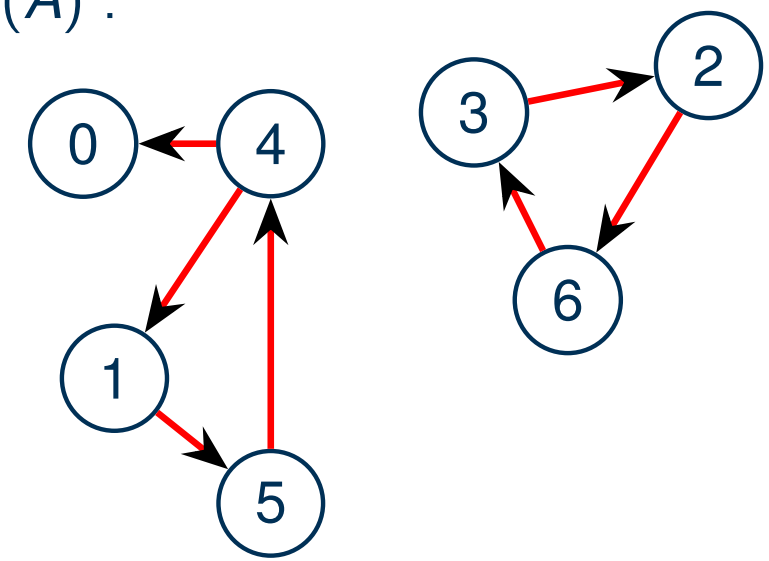
$G(A)$ :




$$A = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \end{pmatrix}$$

$$A_7^\top = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 2 & 2 & 0 & 0 & 2 & 3 & 0 \\ 0 & 0 & 2 & 2 & 0 & 0 & 3 \\ 0 & 0 & 3 & 2 & 0 & 0 & 2 \\ 3 & 3 & 0 & 0 & 2 & 2 & 0 \\ 2 & 2 & 0 & 0 & 3 & 2 & 0 \\ 0 & 0 & 2 & 3 & 0 & 0 & 2 \end{pmatrix}$$

# Identifying cycles

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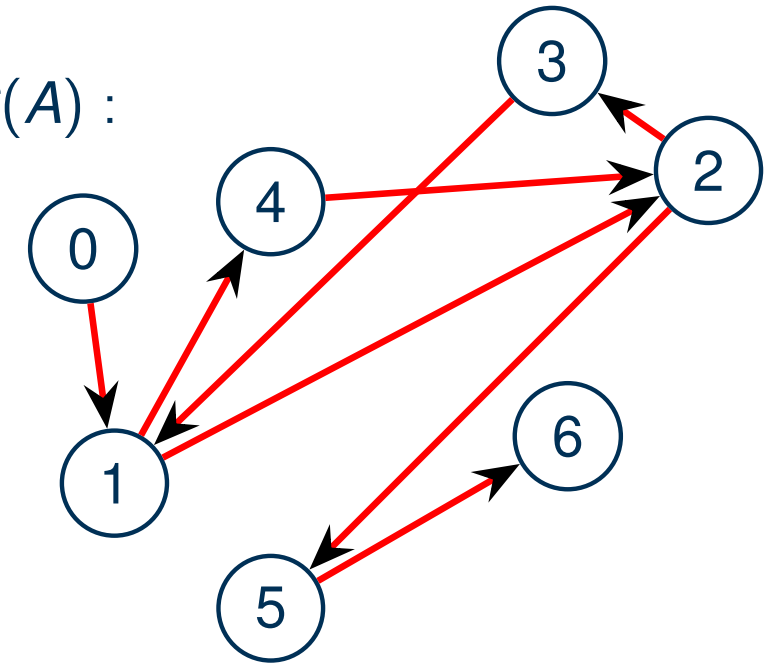
Cycles correspond to non-Bateman terms in the solution. They correspond to exponentially suppressed oscillating terms.

$G(A)$ :




$$A = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

$$A_7^{\top} = \begin{pmatrix} 0 & 0 & 1 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 1 & 1 \\ 0 & 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

# Cycles (triangles)

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Triangles deviate away from the Bateman type solution. The general solution of the inventory equation, $\dot{\boldsymbol{n}} = A_{coeff}\boldsymbol{n}$ is:

$$n_i(t) = e^{A_{ij}t}N_j(0), \tag{6}$$

which is expanded in terms of an eigen-basis. by introducing a time varying term $(\sin(\omega t))$ - complex eigenvalue:

- identify the nature of a transmutation from topology
- important for numerical integration of inventory equation - first time step estimation

$$\dot{\boldsymbol{n}}(t) = A_{coeff}\boldsymbol{n}(t), \tag{7}$$

$$A_{coeff}\boldsymbol{n} = \sigma\boldsymbol{n}, \tag{8}$$

$$\therefore \dot{\boldsymbol{n}} = \sigma\boldsymbol{n}. \tag{9}$$

# Finding nuclei

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The set of nuclei, $\tilde{n}$, with paths to the nuclei $i$, $n^i$ can identified by

$$\tilde{n} = An^i, \tag{10}$$

where $n^i = (0, 0, 0, ..., 1, ...)^T$ $\tilde{n}$ contains 1's on the position of the neighbours with paths to $i$.
Itterativly applying

$$n_{i+1} = An^i, \tag{11}$$

produces a list of connected nuclei up to $m$ links $\{n_1, n_2, n_3, ...., n_m\}$.

# Path connected nuclei

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We can identify a path, of length $m$, between nuclei:

1. Is there a component $i \to j$ in the order $m$ transitive closure $A_m^+$
2. $n_1 = A_{m-1}^+ e_j$ identifies all of the neighbour to $j$ of length $m-1$
3. $n_{1a} = A_1^+ e_i - n_1$ removes the neighbours not linked to node $j$ ($-$ is over a semi ring). Producing the set of nodes (nuclei) distance $m-1$ from $j$ and 1 from $i$
4. $n_2 = A_{m-2}^+ e_j$ identifies all of the neighbour to $j$ of length $m-2$
5. $n_{2a} = A_1^+ n_{1a} - n_2$ removes the neighbours not linked to node $j$ ($-$ is over a semi ring). Producing the set of nodes (nuclei) distance $m-2$ from $j$ and 2 from $i$ (and 1 from the list $n_2$)

-> Repeat $2 \to 5$, storing $n_i$ until the set is complete

# Conclusion

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- Nuclear data shows how nuclei transform, and currently can be used on a sample by sample basis to inform material choice in isotope production facilities
- We are proposing a new approach which takes the entirety of nuclear data into account in one go
- The algebraic framework lends itself to modern computing architectures and libraries
- This technique has the potential to show what isotopes can be produced within an existing facility
- The matrix structure and algebraic operations mean that the algorithms can make use of modern HPC architectures and libraries.

-> Next phase is to apply to real data and optimise symbolic LU factorisation

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