Predicting Band-gap of Inorganic Materials using Neuromorphic Graph Learning

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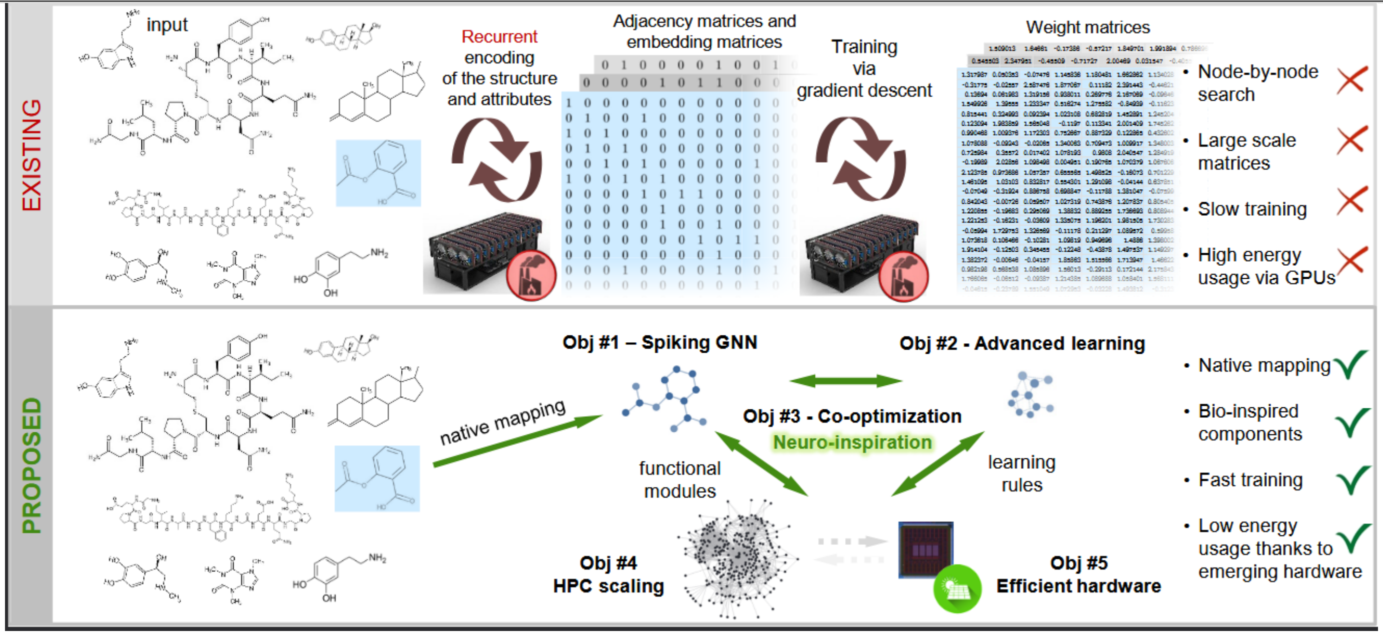
ENGAGE: (E)nergy-efficient (N)ovel Al(g)orithms and (A)rchitectures for (G)raph L(e)arning

Hypotheses: (1) Science-aware graph learning mapped onto spiking neural networks (SNNs) can overcome the limitations of current graph neural networks (GNNs) on graphic processing units (GPUs), **(2)** such networks are naturally smaller in size with energy-consumption advantages, **(3)** this new paradigm for graph learning opens up new front for AI advancements and for hardware architecture design, **(4)** when trained naively using approaches beyond gradient descent on emerging CMOS-compatible nonvolatile memory device technologies, hereafter referred to as (CMOS + X), they can perform faster, more accurately, and with greater energy efficiency for a wide range of the U.S. Department of Energy (DOE) mission-critical applications.



Components:

- SNN for Graph Learning
- Advanced learning – local learning rules and genetic algorithms beyond gradient descent
- Simulation and co-design guiding algorithm and device design
- Scalability – scaling to large number of neurons
- Energy efficient hardware – cross bars

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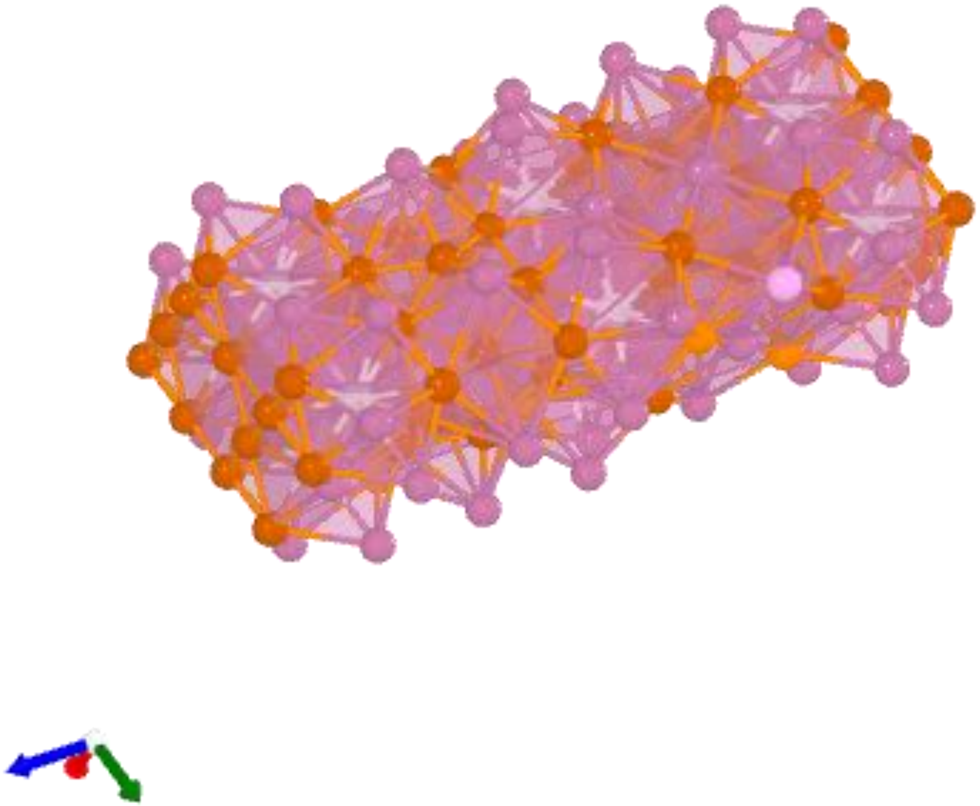
Why Inorganic Materials

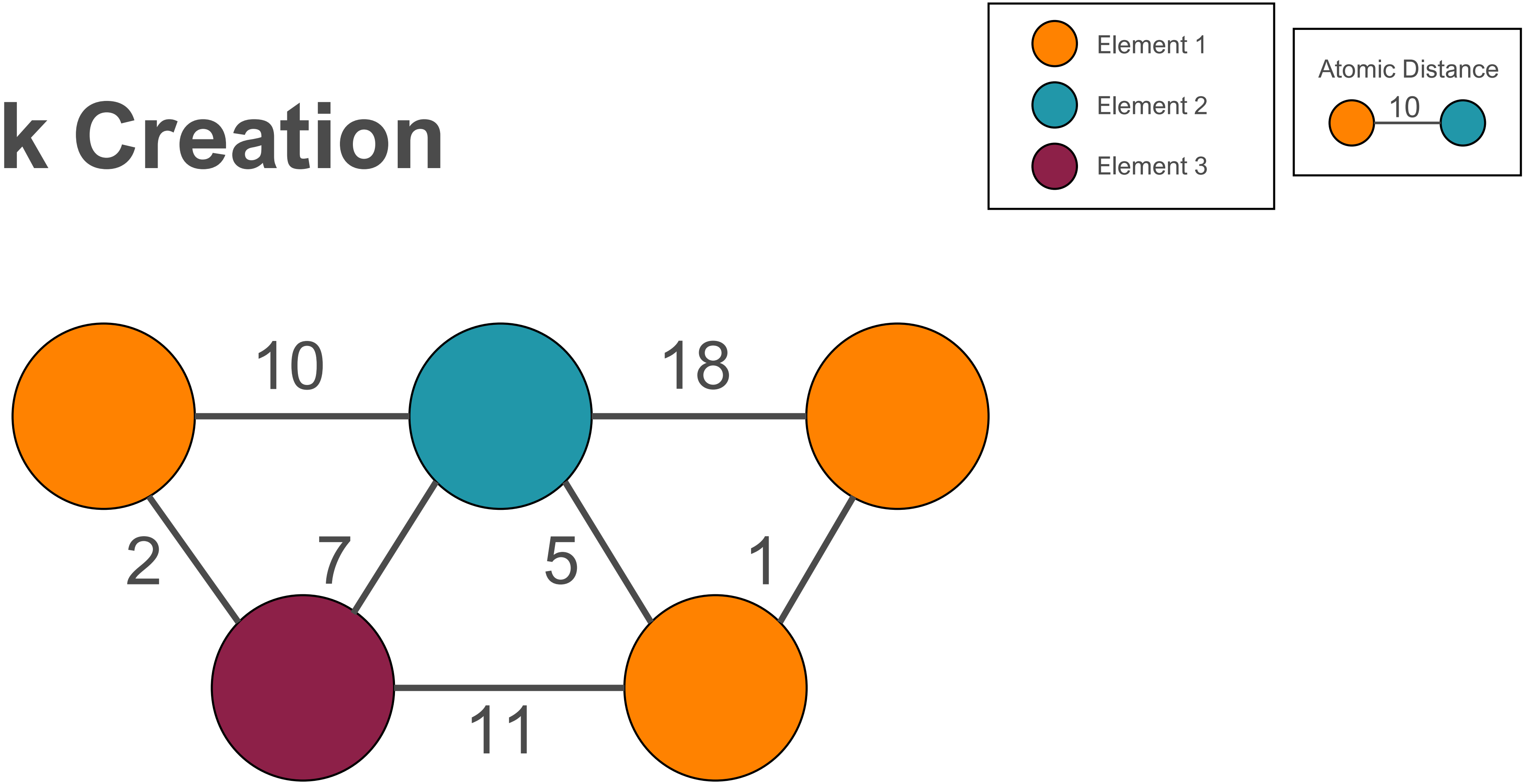
- Inorganic materials can be treated as a 3D graph.
- Materials have several properties that are desirable for prediction such as:
  - Refractive Index
  - **Band Gap**
  - Formation Energy
  - Shear and Bulk Modulus
- One goal of regression is to aid material discovery



Our Approach

- We leverage the structure of the material for the creation of our spiking neural networks using a method of Neuromorphic Graph Learning (NGL).
- We have two approaches to predict the band-gap of inorganic materials:
  - *Evolutionary Algorithm*
  - *Spike Pipeline for Raster Analysis (SPIRE)*

Network Creation



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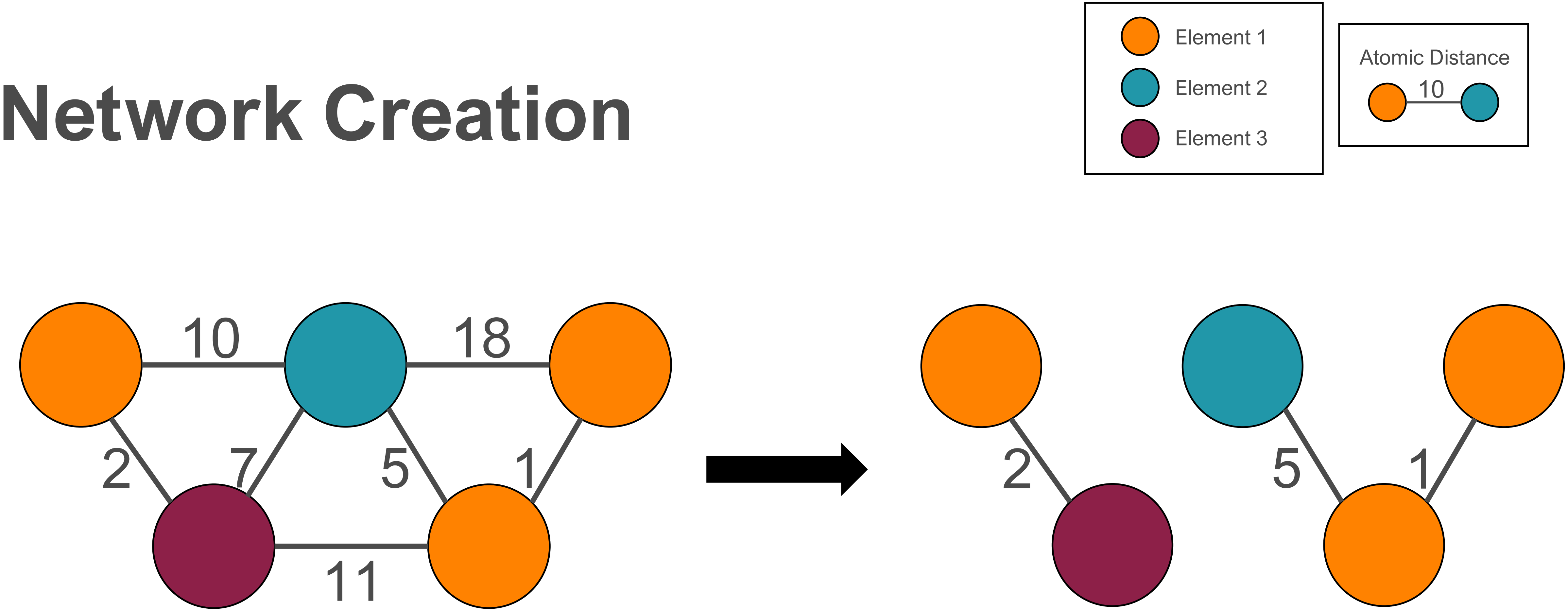

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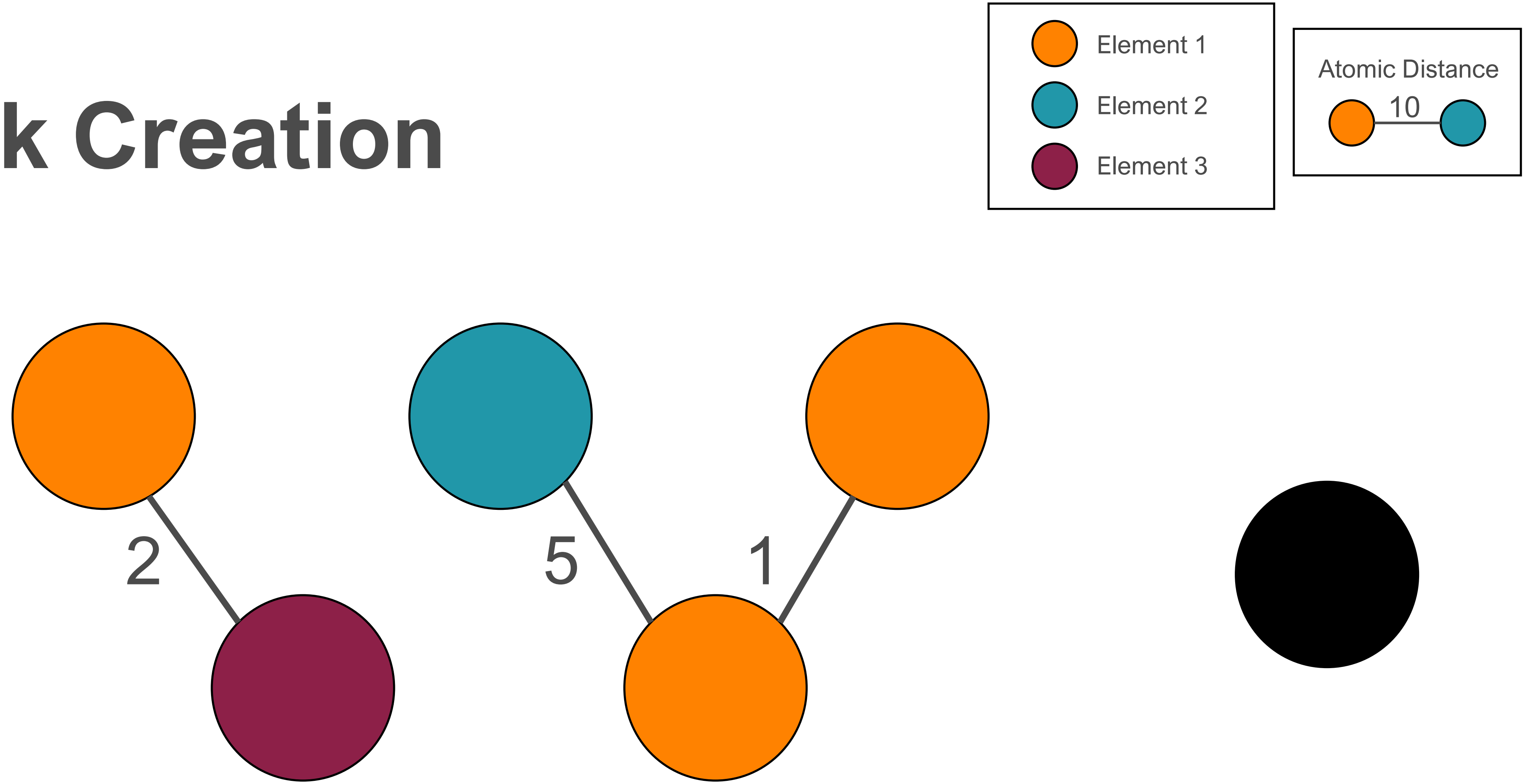

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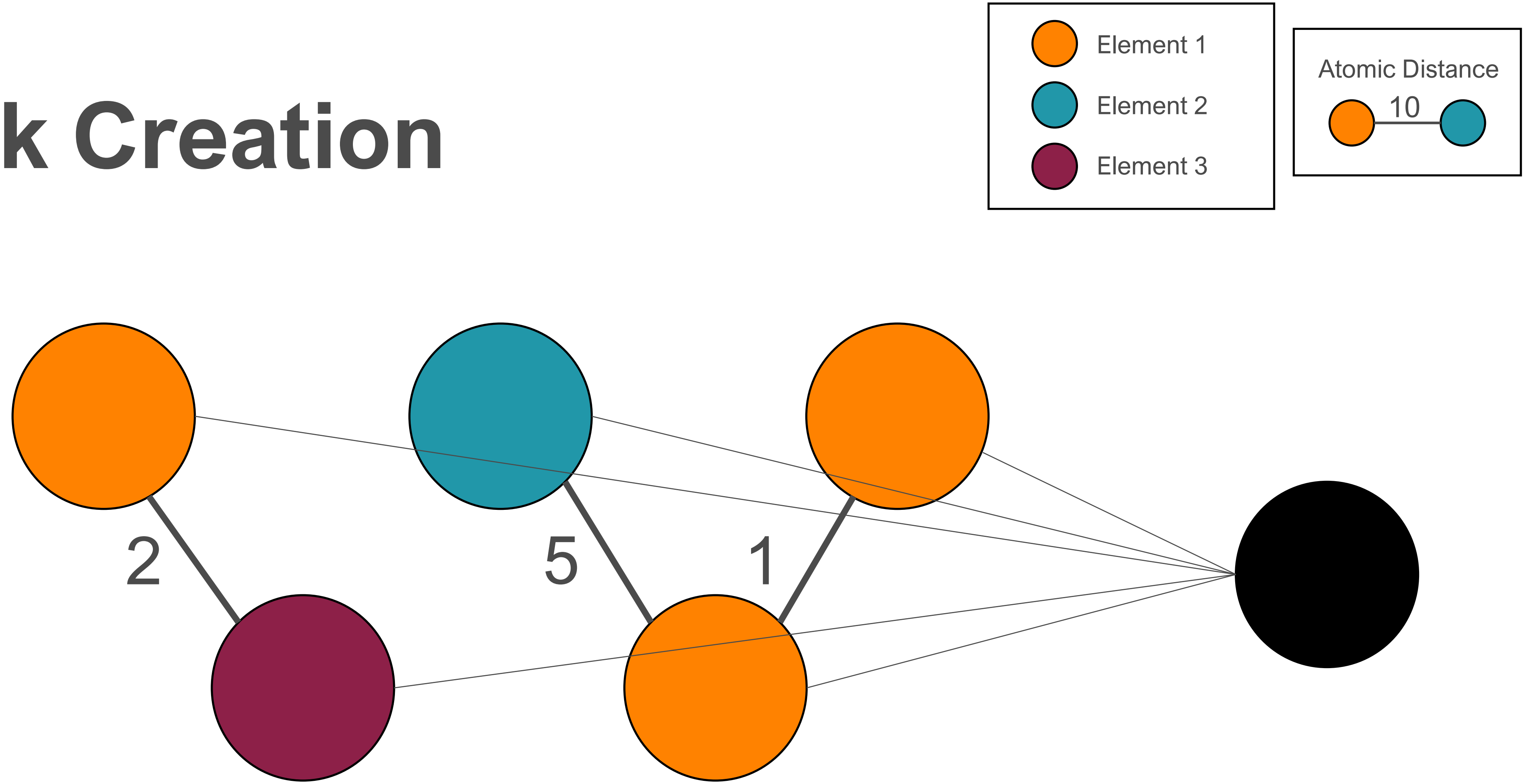


Encoder/Decoder

Encoding:

- We have every element spike with a threshold of 16 at timestep *n.*

Element	Timestep
Hydrogen	1
Oxygen	2
Lead	3
Zinc	4
…	…

Default Decoding:

- Rate decoding (i.e. number of spikes on the output neuron)

$$output = \frac{\sum_{t=0} output\_neuron\_spikes_t}{total\_timesteps}$$

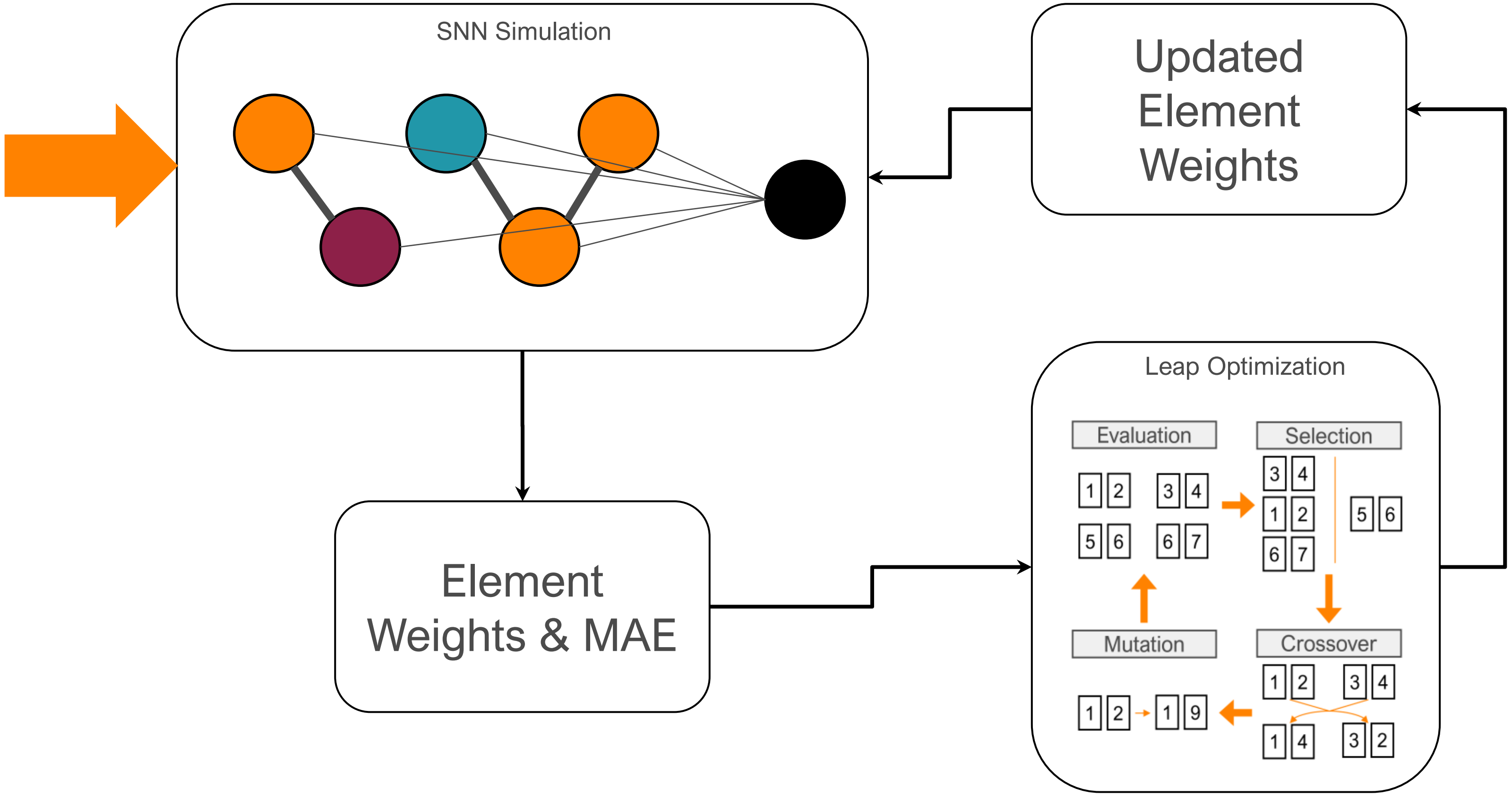
$$error = |\, output - label \,|$$

$$Mean\ Absoulute\ Error = \frac{\sum_{e=0} error_e}{total\_dataset\_size}$$

Experimental Setup

- The dataset was obtained from the Matbench *mp_gap* repository. This contains over 100,000 materials in which we sampled 1000 materials.
- We utilized the SuperNeuroMAT simulator for simulation of the SNN’s.
- Each test was run on an AMD Ryzen 7800X3D with 32GB of RAM

Evolutionary Algorithm



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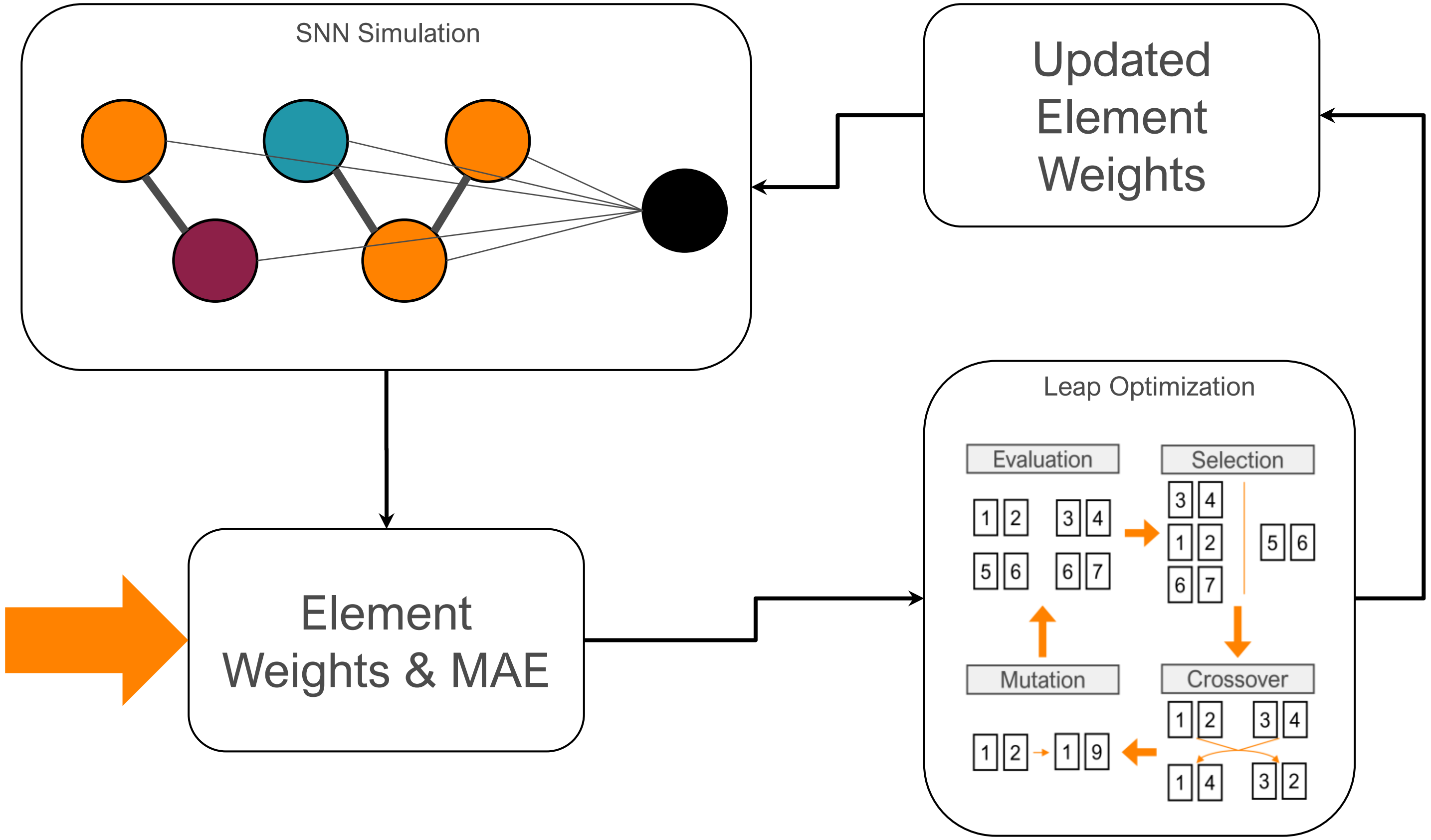

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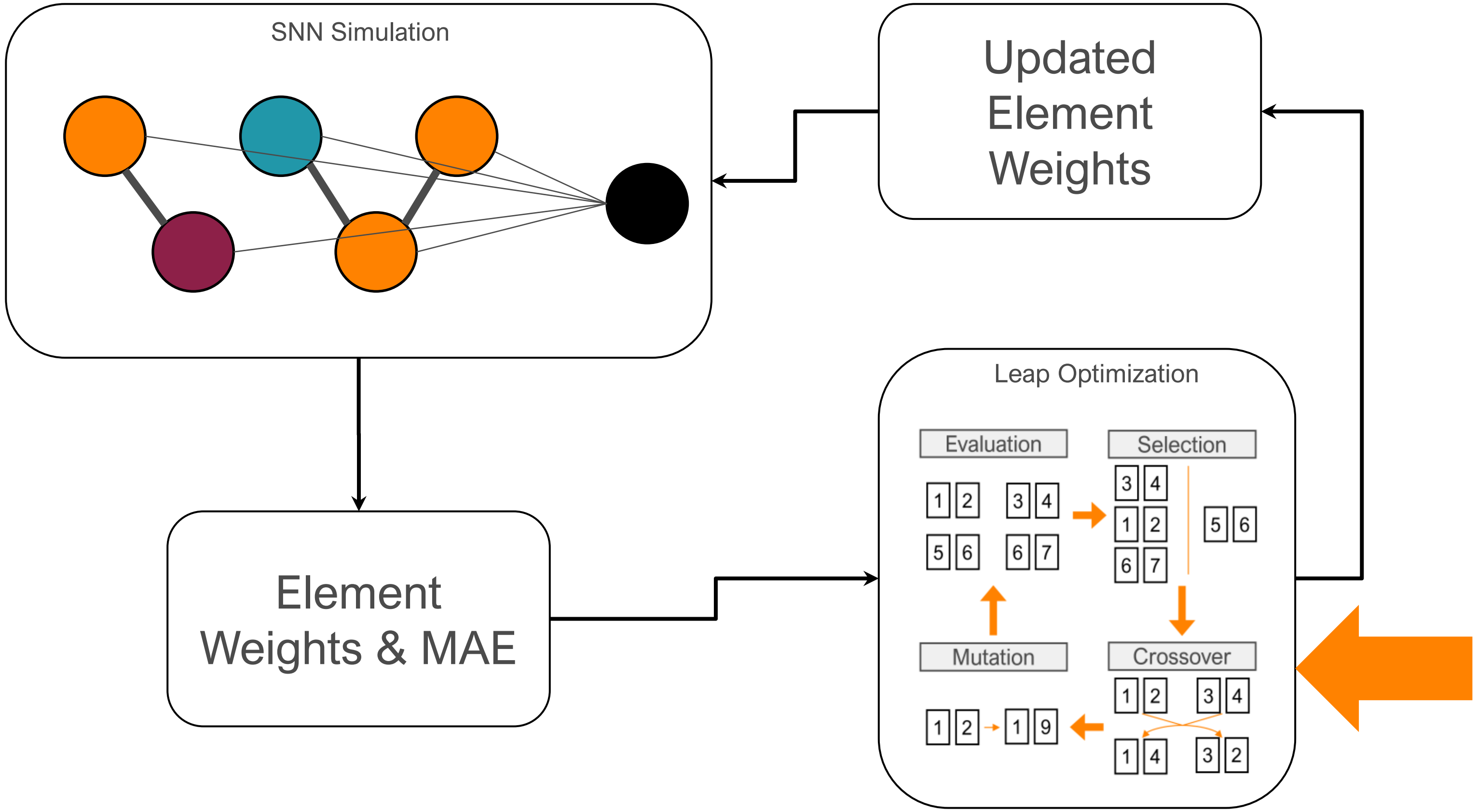

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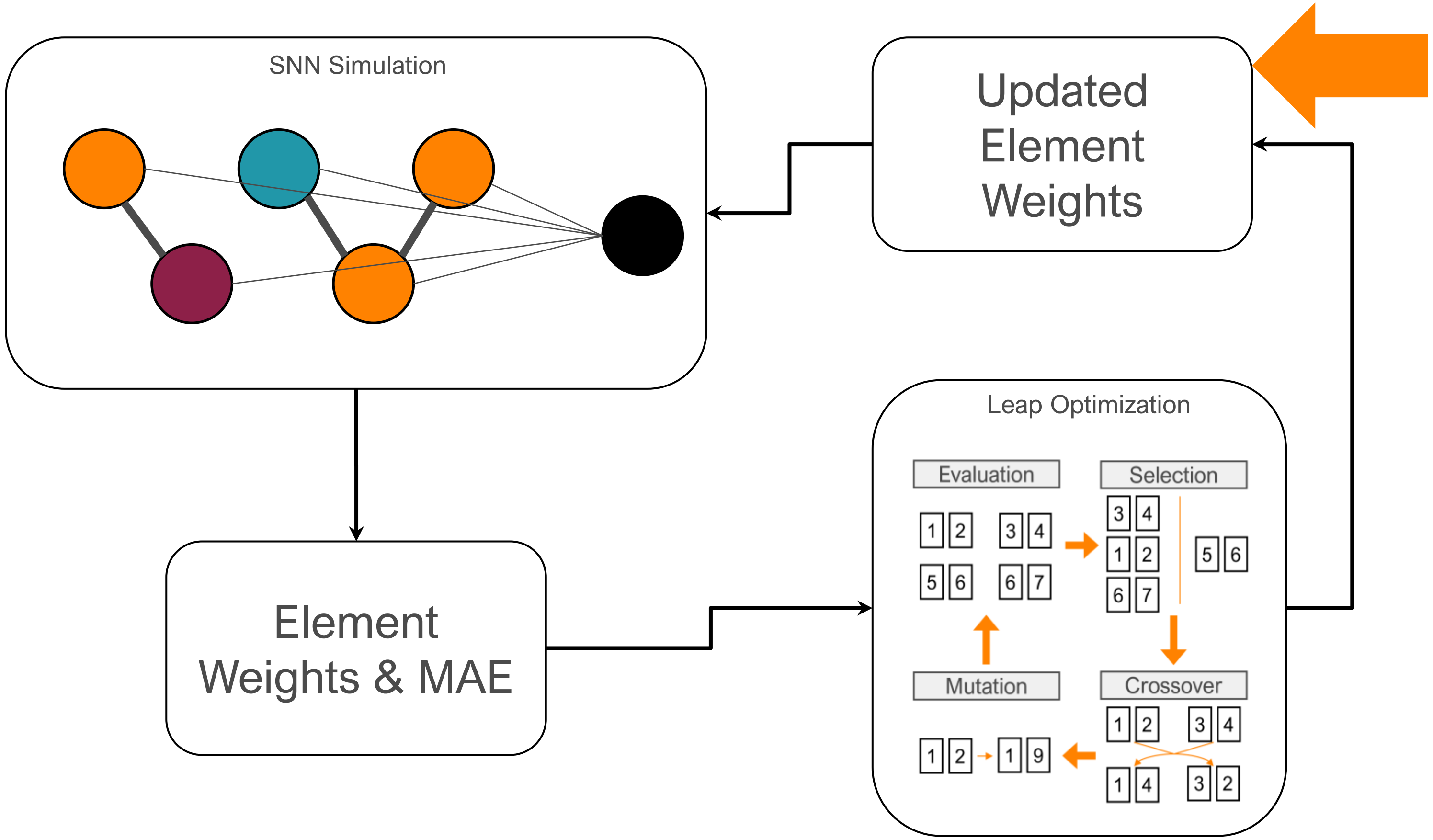

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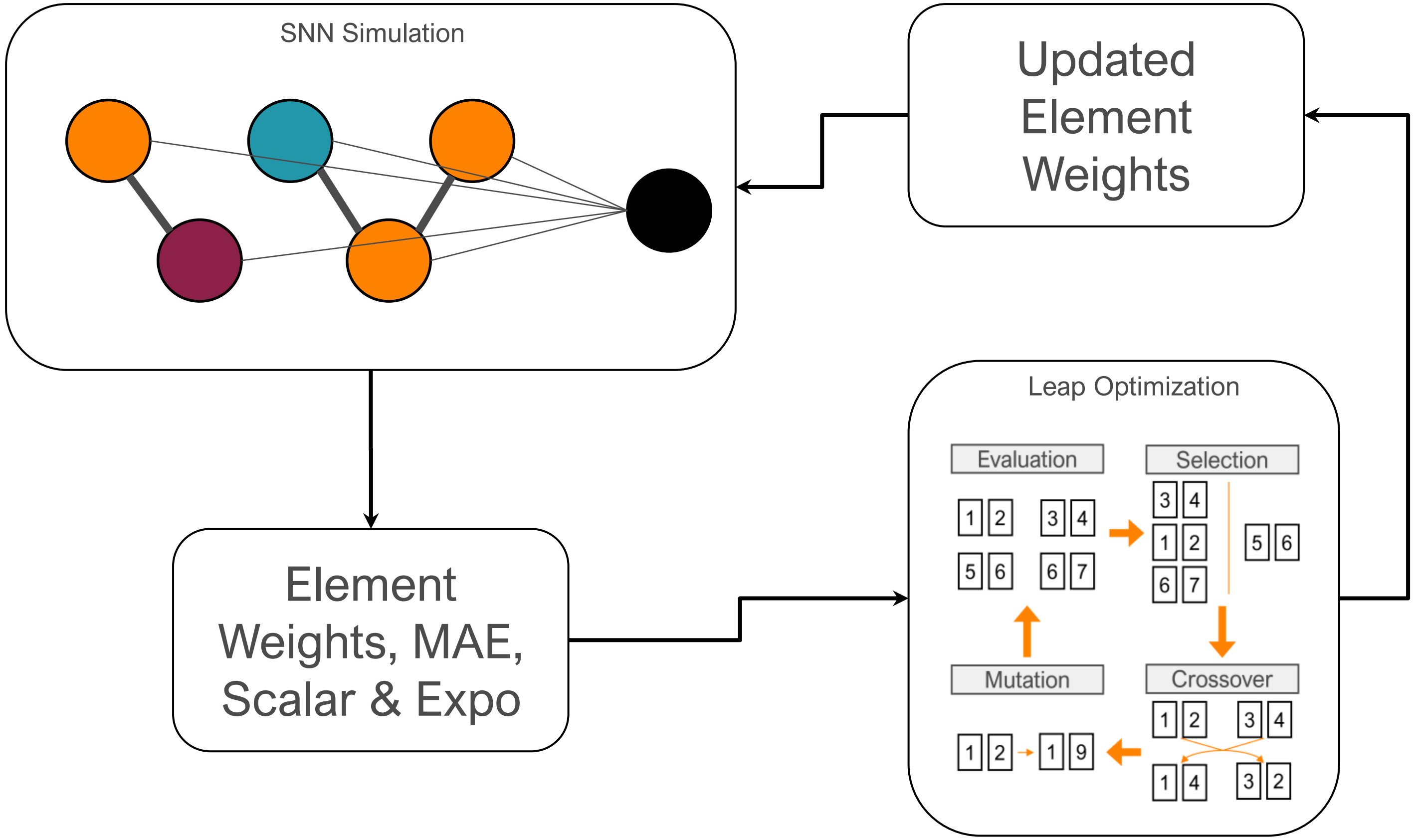
Evolutionary Algorithm

Linear Decoding:

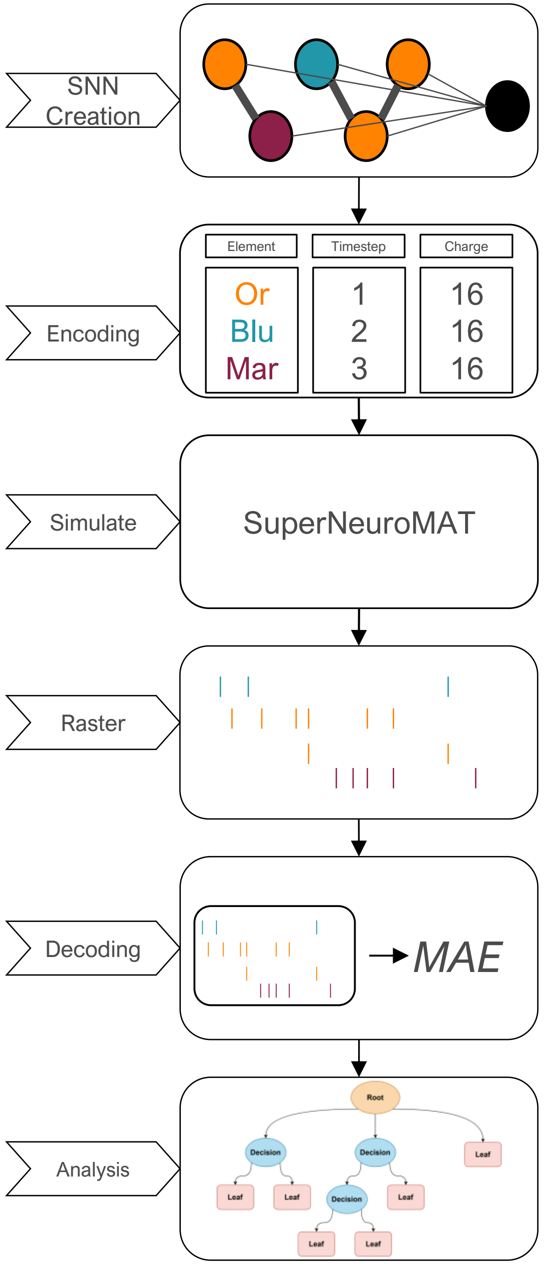
$$output = \frac{\sum_{t=0} output\_neuron\_spikes_t}{total\_timesteps}$$

Exponential Decoding:

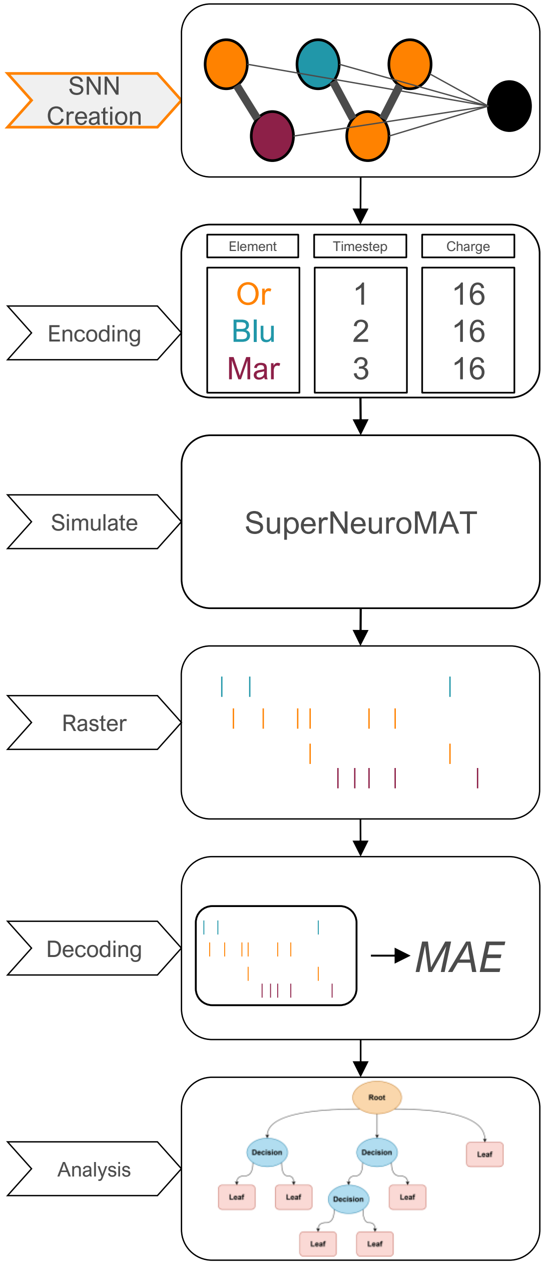
$$ex\_output = s * output^{\alpha}$$



SPIRE


SNN Creation
Encoding
Element
Timestep
Charge
Or
Blu
Mar
1
2
3
16
16
16
Simulate
SuperNeuroMAT
Raster
Decoding
MAE
Analysis
Root
Decision
Leaf

SPIRE



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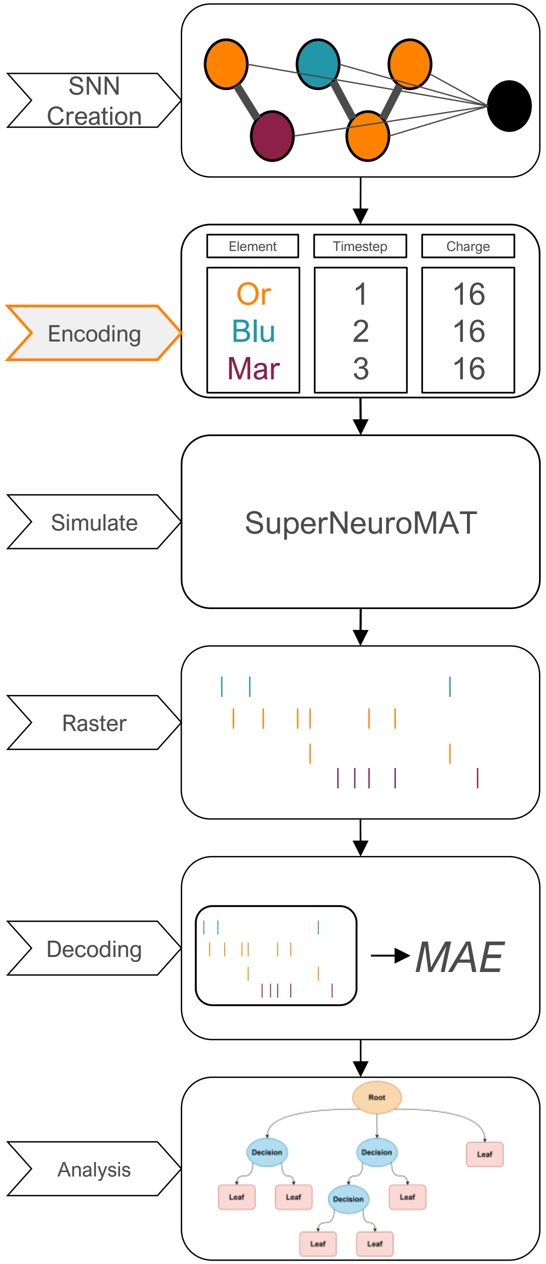
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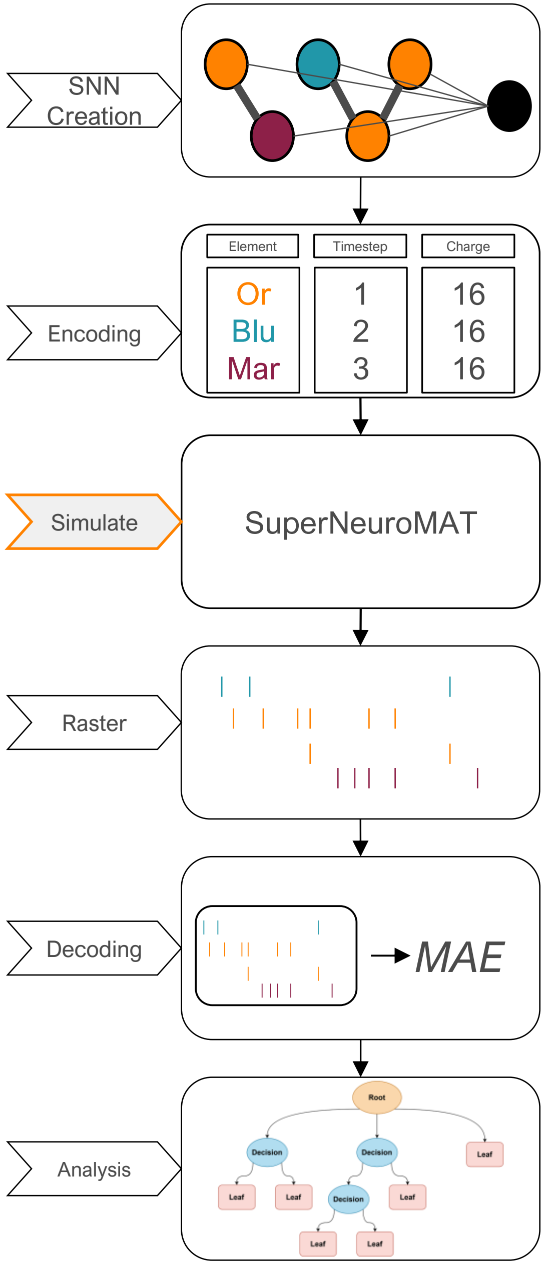
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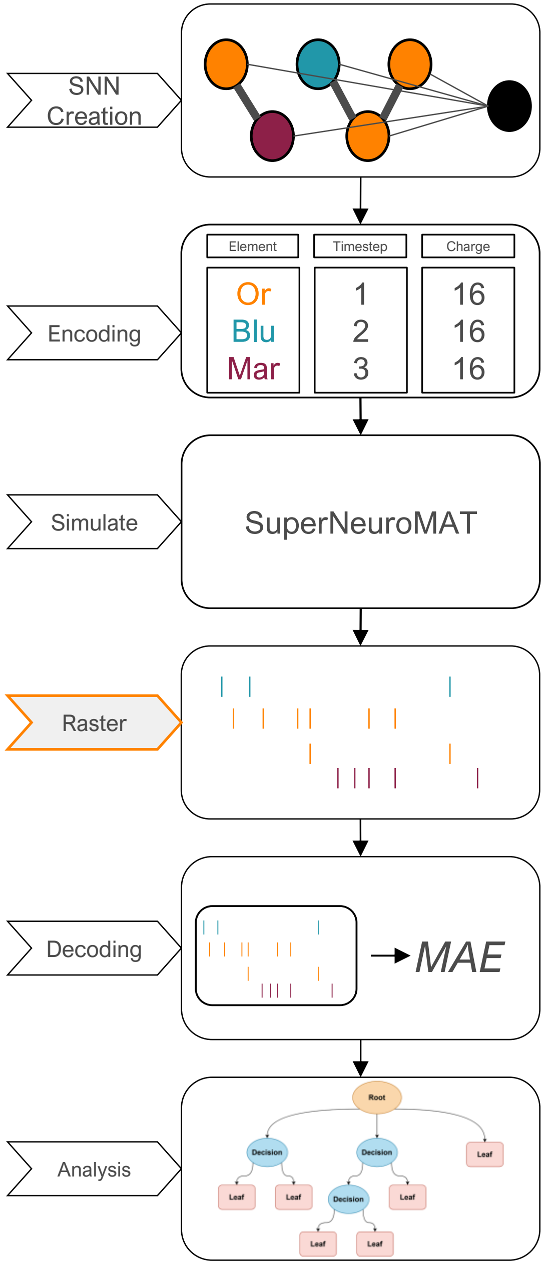

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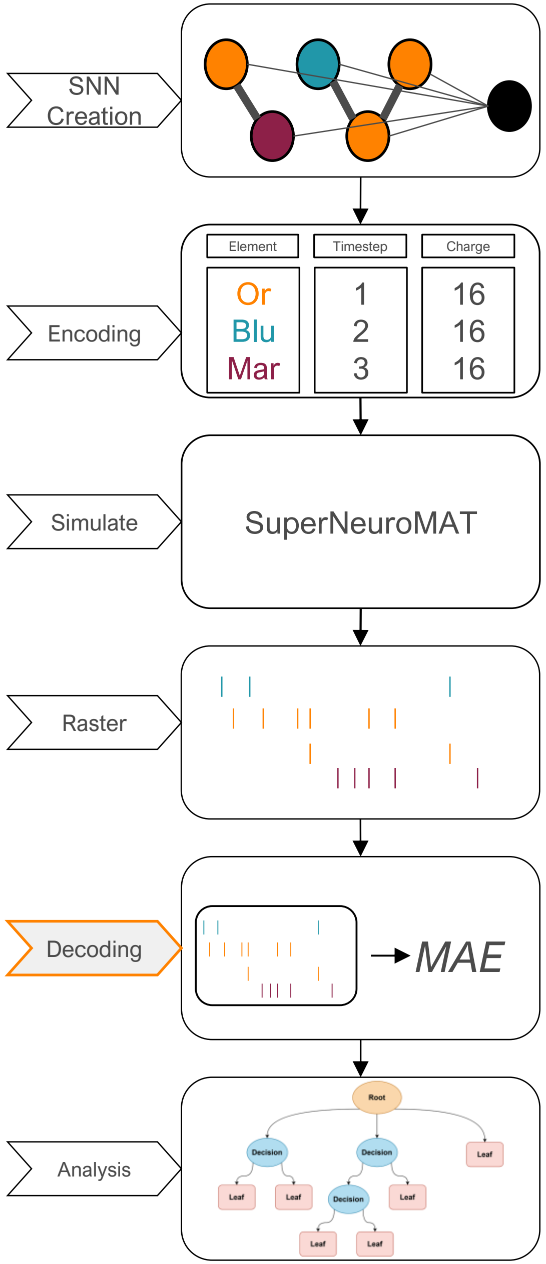

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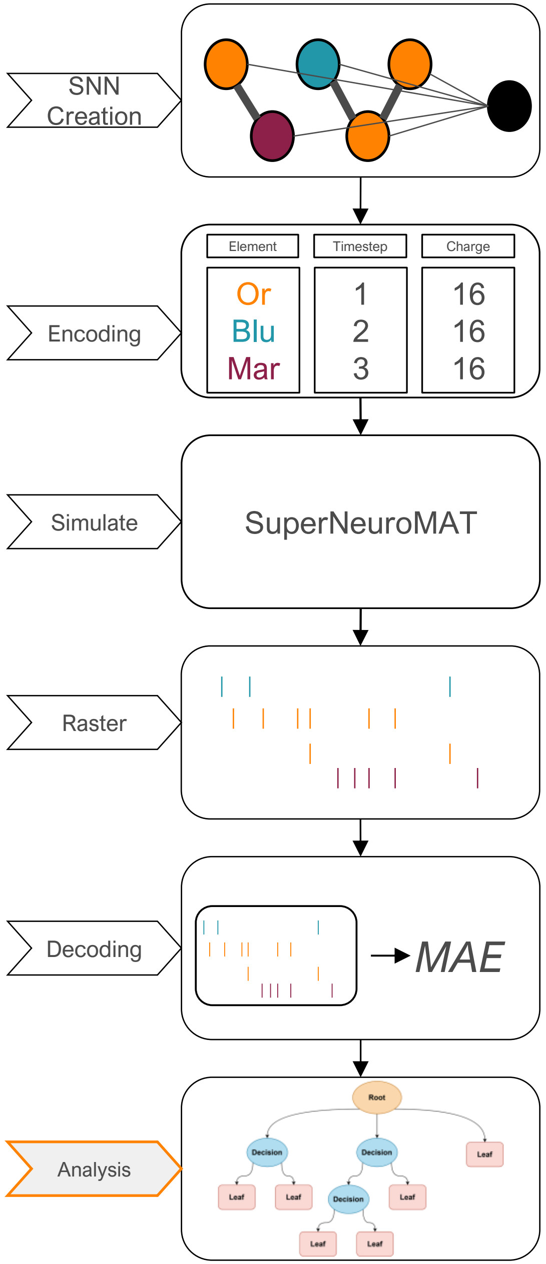

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	NGL EA Linear	NGL EA Exponential	SPIRE	ALIGNN	GraphHD
Average MAE	1.073	0.981	1.368	0.7656	1.312

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Results

	Linear		Exponential		SPIRE
Run	Train	Test	Train	Test	Test
1	1.027	1.053	0.868	0.982	1.377
2	1.039	0.993	0.866	0.939	1.355
3	1.035	1.033	0.829	0.948	1.373
4	1.039	1.045	0.906	0.874	1.396
5	1.054	0.975	0.872	0.921	1.259
6	1.004	1.147	0.895	0.991	1.380
7	1.003	1.119	0.825	1.029	1.442
8	0.992	1.215	0.794	1.202	1.431
9	0.997	1.162	0.863	0.982	1.436
10	1.056	0.986	0.861	0.941	1.230
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Conclusion

- Key Points
  - New novel algorithms utilizing SNN's in the prediction of band-gap
  - Evolutionary algorithms show promise for prediction of band-gap
  - A new avenue for encoding spike rasters into datasets for analysis

- Future works
  - Sweep hyper-parameters (complete)
  - New encoding methods (in-progress)
  - New decoding methods
  - Move to hardware to measure energy efficiency
  - Utilize new algorithms for analyzing spike rasters (in-progress)

Questions?

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