A Methodology to Generate Efficient Neural Networks for Classification of Scientific Datasets

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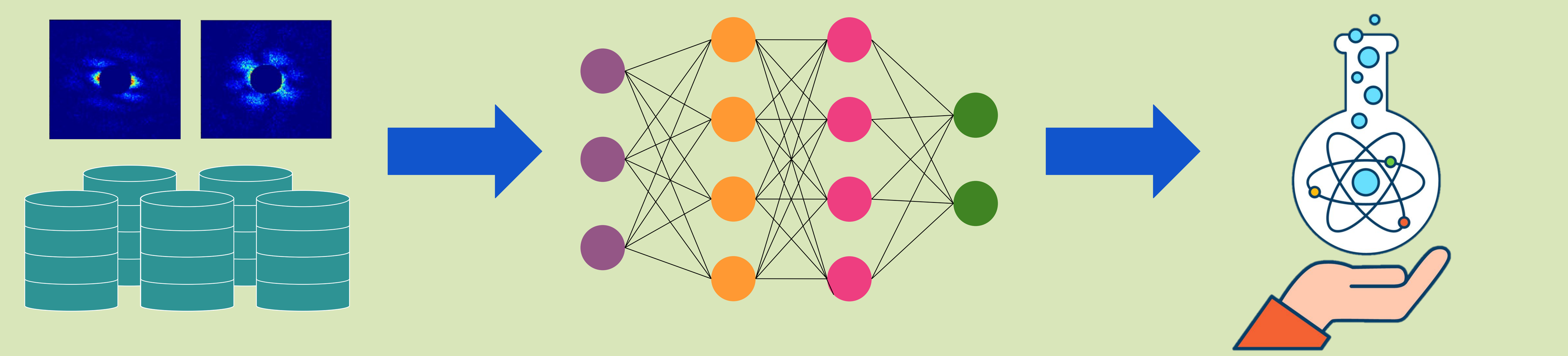
Using Neural Networks (NNs) for Scientific Discovery

Scientific Datasets | **Neural Networks** | **Scientific Discoveries**

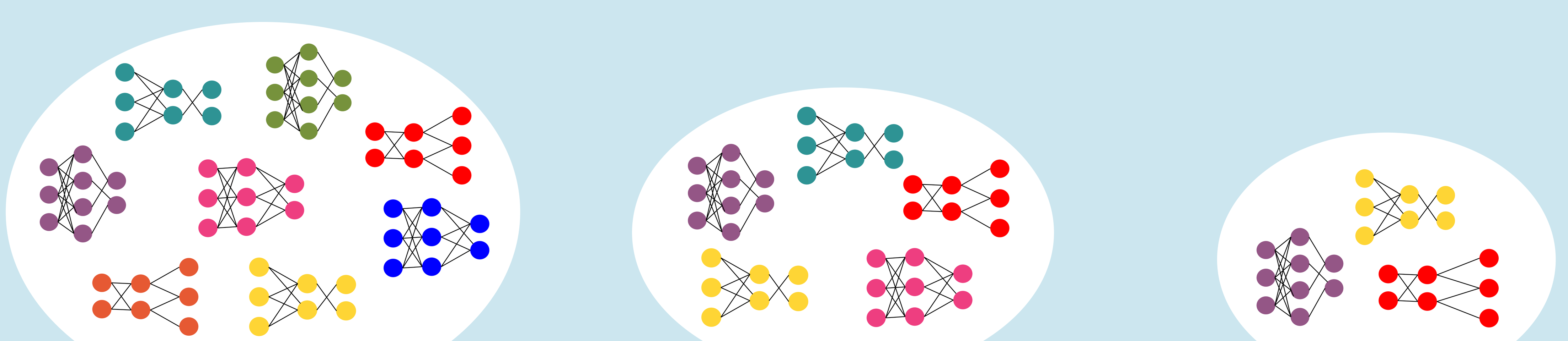


Achieving high accuracy and efficient performance is a challenge, so:

- We **define** a domain-agnostic methodology to find an efficient NN using a neural architecture search (NAS)
- We **optimize** for accuracy (minimize error) and for efficiency (minimize inference FLOPS).

Domain Agnostic Methodology for NNs Search

Our methodology efficiently utilizes a NAS to find a NN architecture optimized to classifying scientific datasets based on accuracy and performance.



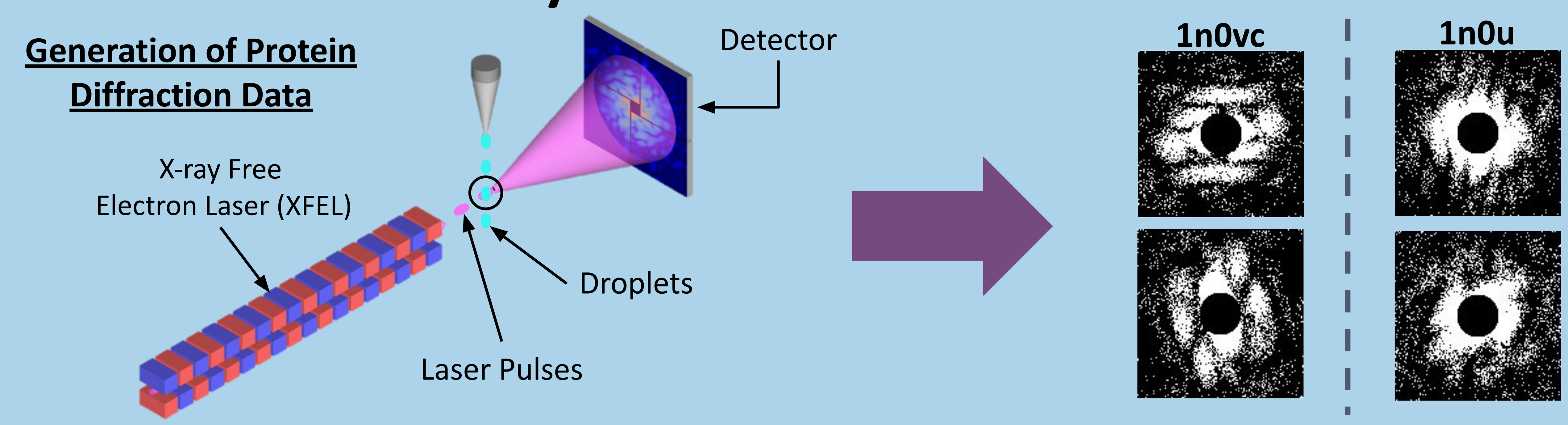
Generate NNs → **Select NNs** → **Refine NNs**

Generate NNs: Generate and train several generations of NNs on a dataset using a NAS of desired choice

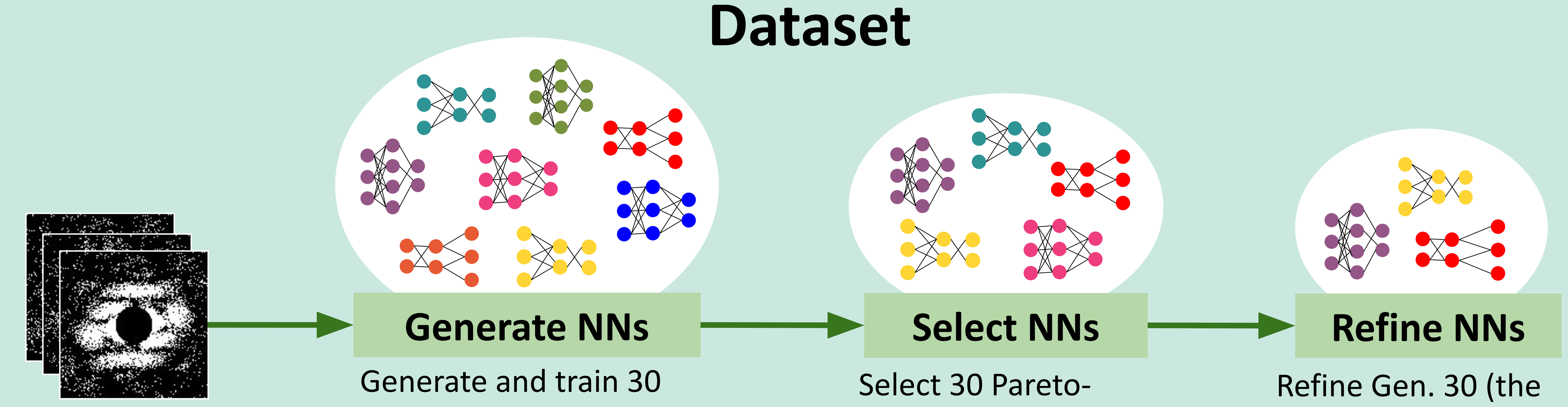
Select NNs: Select Pareto-optimal sets of NNs for *each generation* based on:
- high accuracy
- low FLOPS usage

Refine NNs: Refine by:
- choosing the optimal set of NNs
- establishing FLOPS cutoff
- long targeted training (more epochs)

Case Study: Protein Diffraction Dataset



Applying our Methodology to Classify Protein Diffraction Dataset



Generate NNs → **Select NNs** → **Refine NNs**

Generate NNs: Generate and train 30 generations of NNs with NSGA-Net's "macro-search" (750 NNs total)

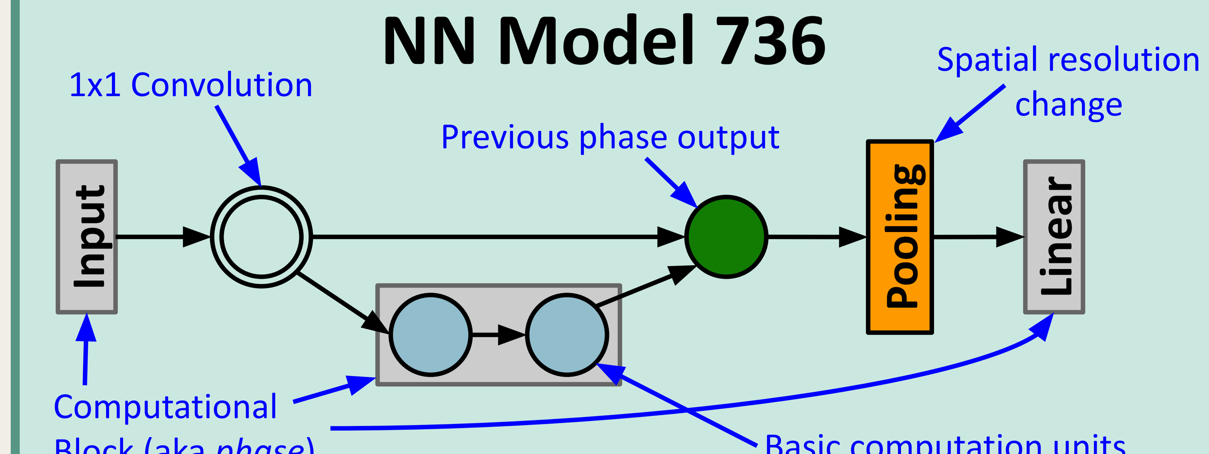
Select NNs: Select 30 Pareto-optimal sets of NNs based on objectives

Refine NNs: Refine Gen. 30 (the optimal set of NNs) with a 200 FLOPS cutoff to get the **3 most efficient NNs**

NN Model	FLOPS	Accuracy before refinement	Accuracy after refinement	Inference Time (s)
740	0.016	57.1	57.1	0.407
729	169.125	92.4	97.7	1.161
736	187.125	94.6	98.1	1.250

Best 2 NNs due to >97% accuracy and <200 FLOPS usage

NN Model 736



Our methodology leverages NAS to find accurate and efficient NN architectures tailored to any scientific dataset.

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