

# Powering Generative AI for HPC

Geetika Gupta

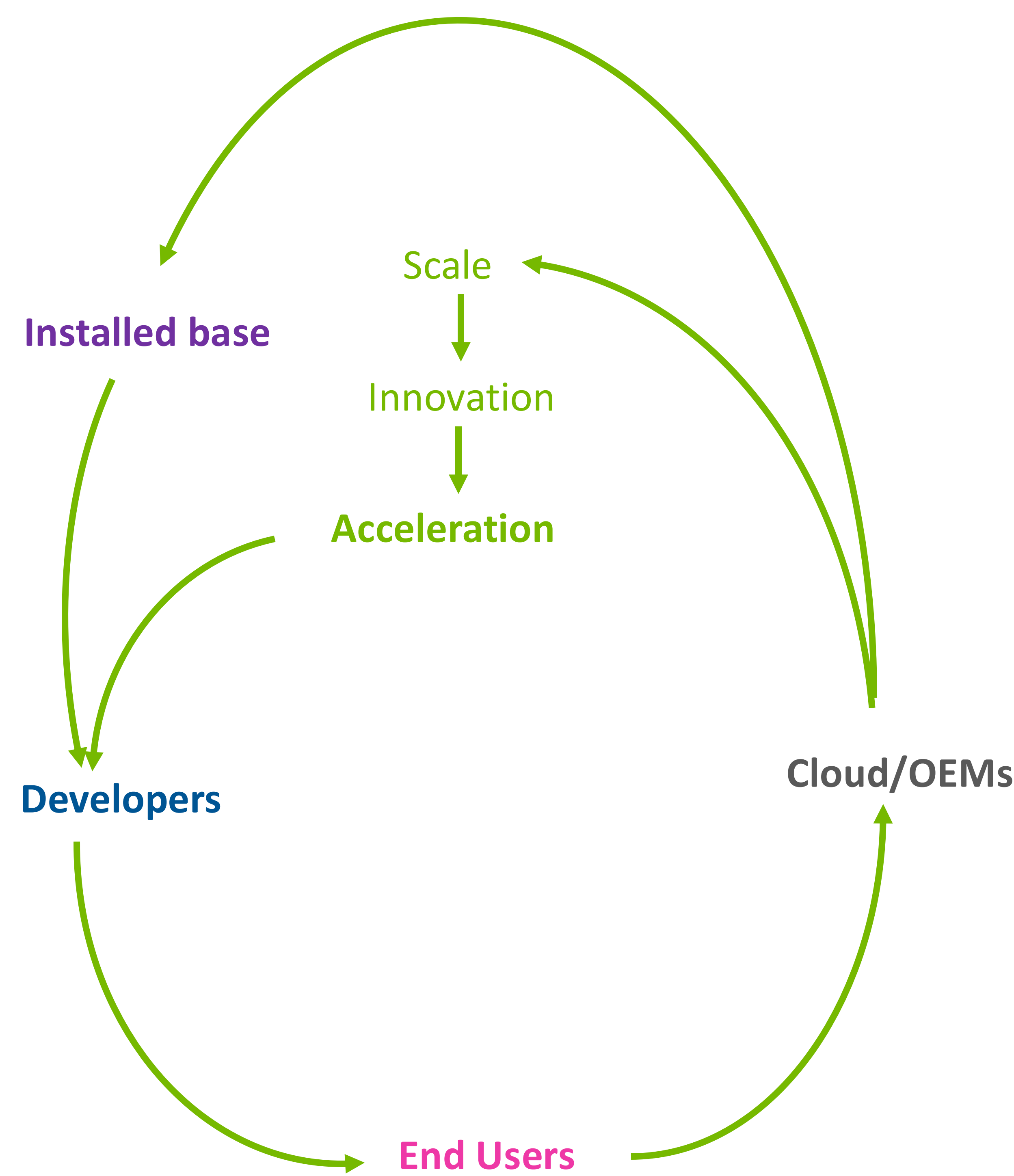
Sr Dir Product Management AI for Science

Wenjie Ong Sr Product Mgr NVIDIA ALCHEMI

Sept 2025



# The Accelerated Computing Cycle

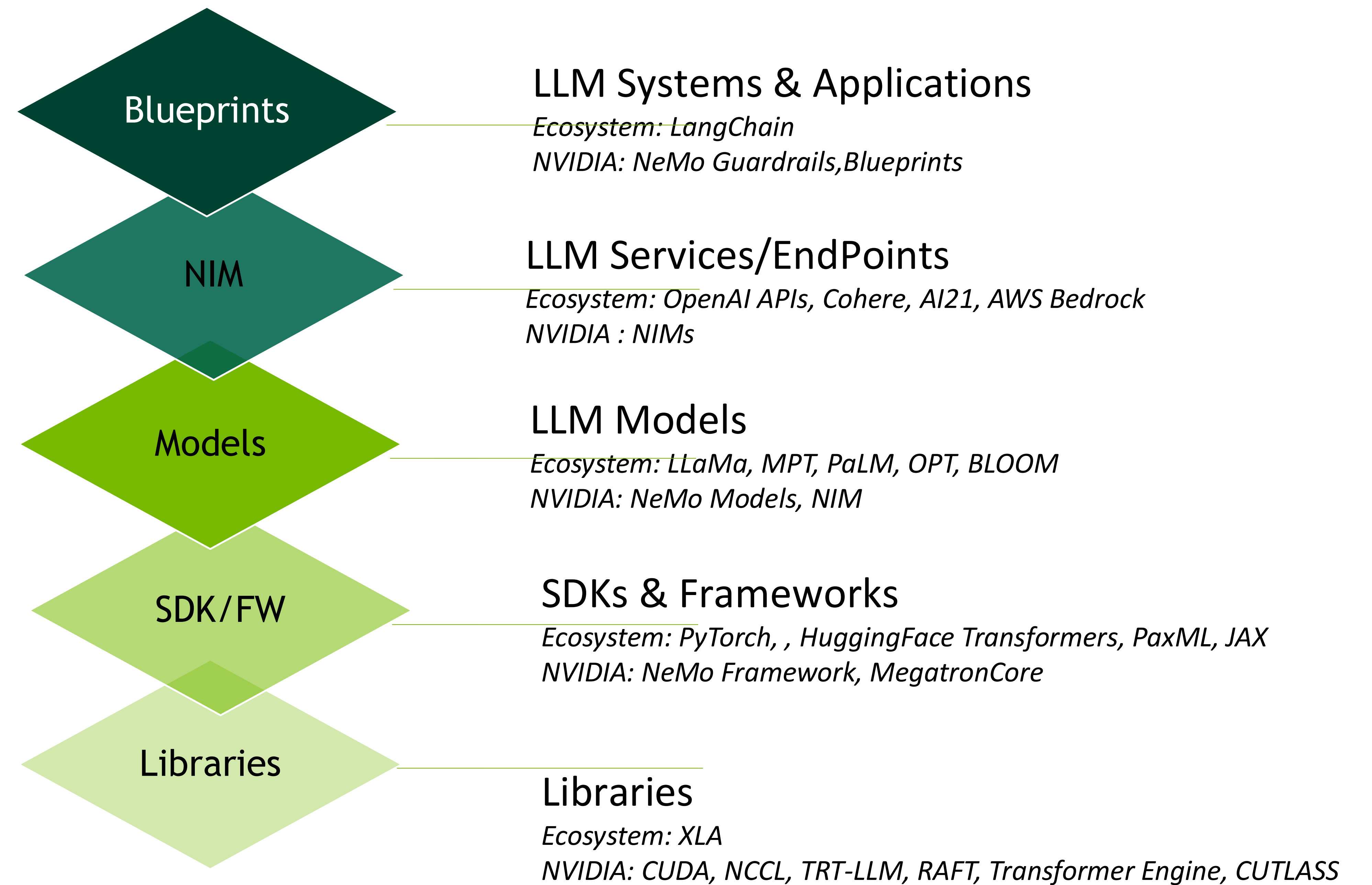
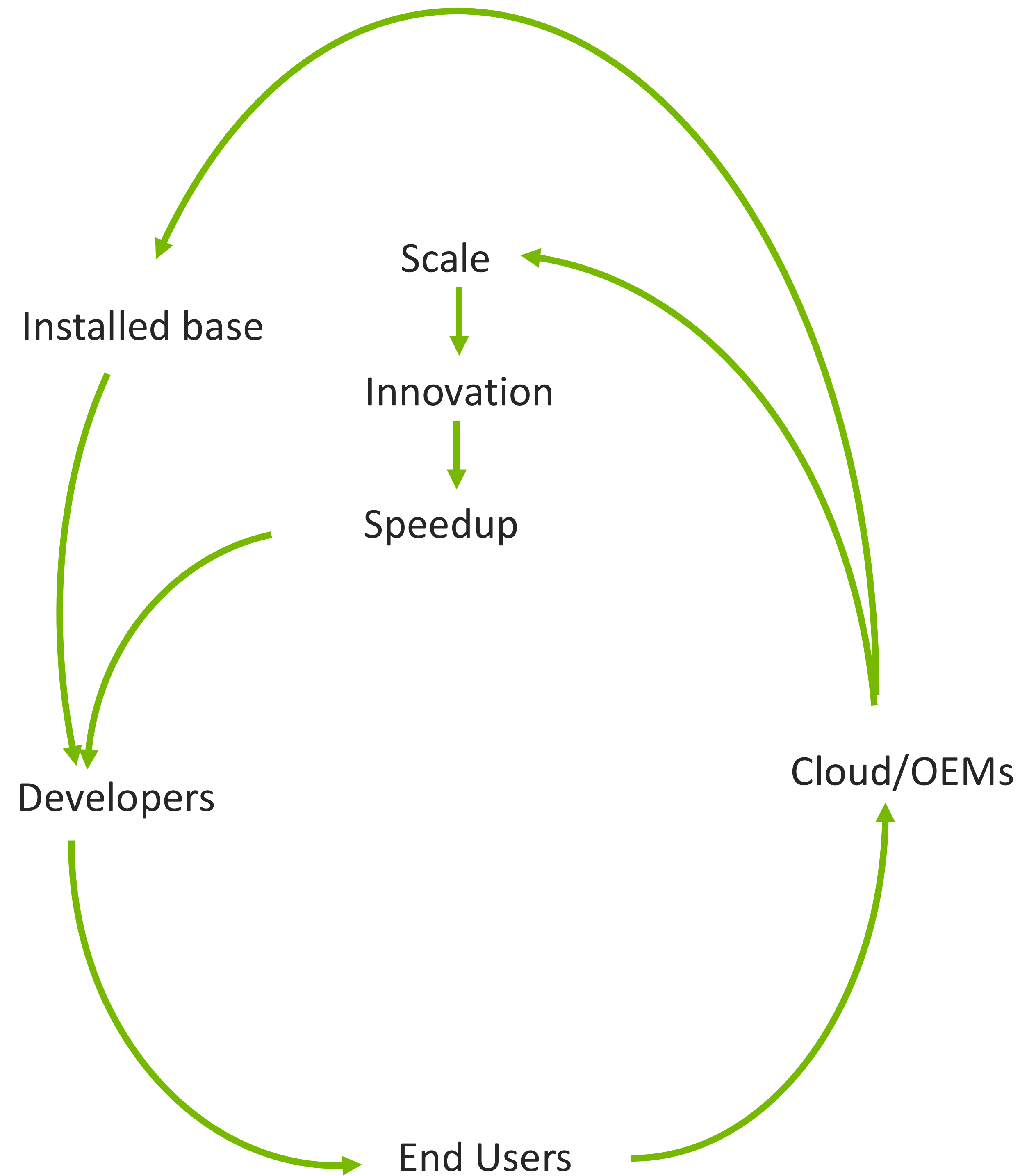


# Generative AI Ecosystem

1600+ Gen AI Companies Building on NVIDIA Platform



# Multiple Entry Points For Developers and Users

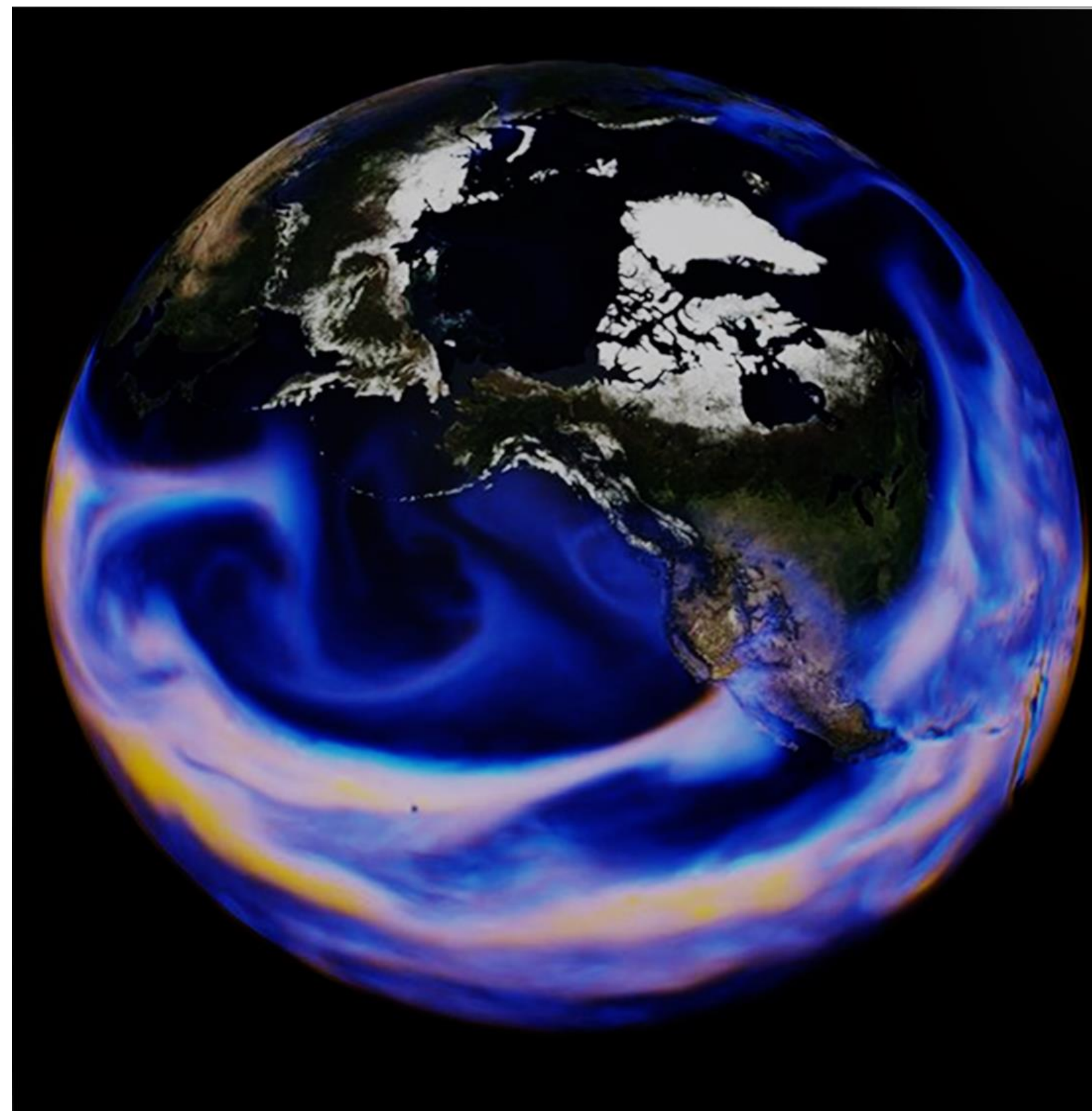




# Democratizing AI for Science and Discovery

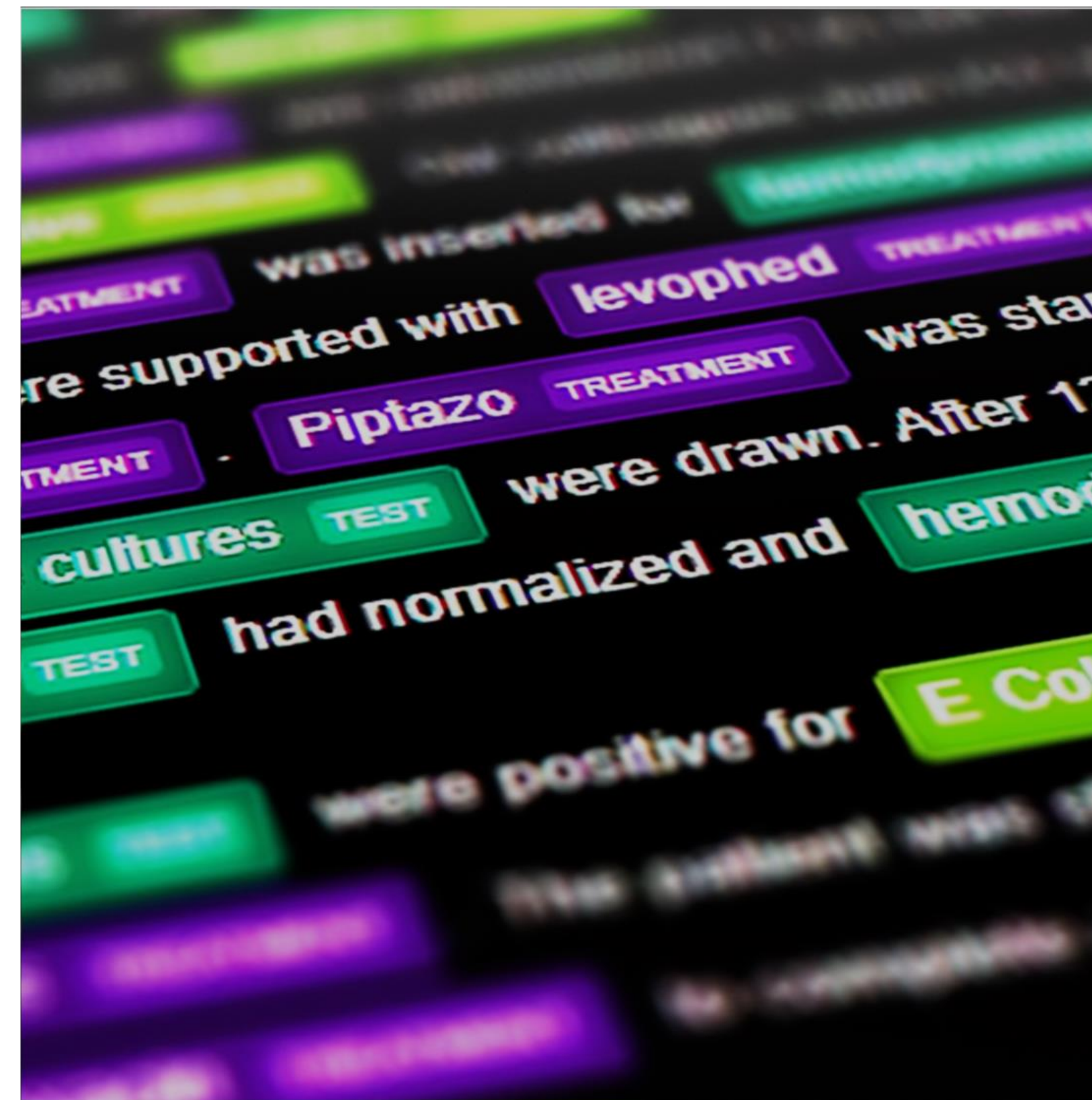
## PhysicsNemo

Physics-ML Model Training and Inference



## NEMO FRAMEWORK

Developing Scientific Foundational Models at Scale



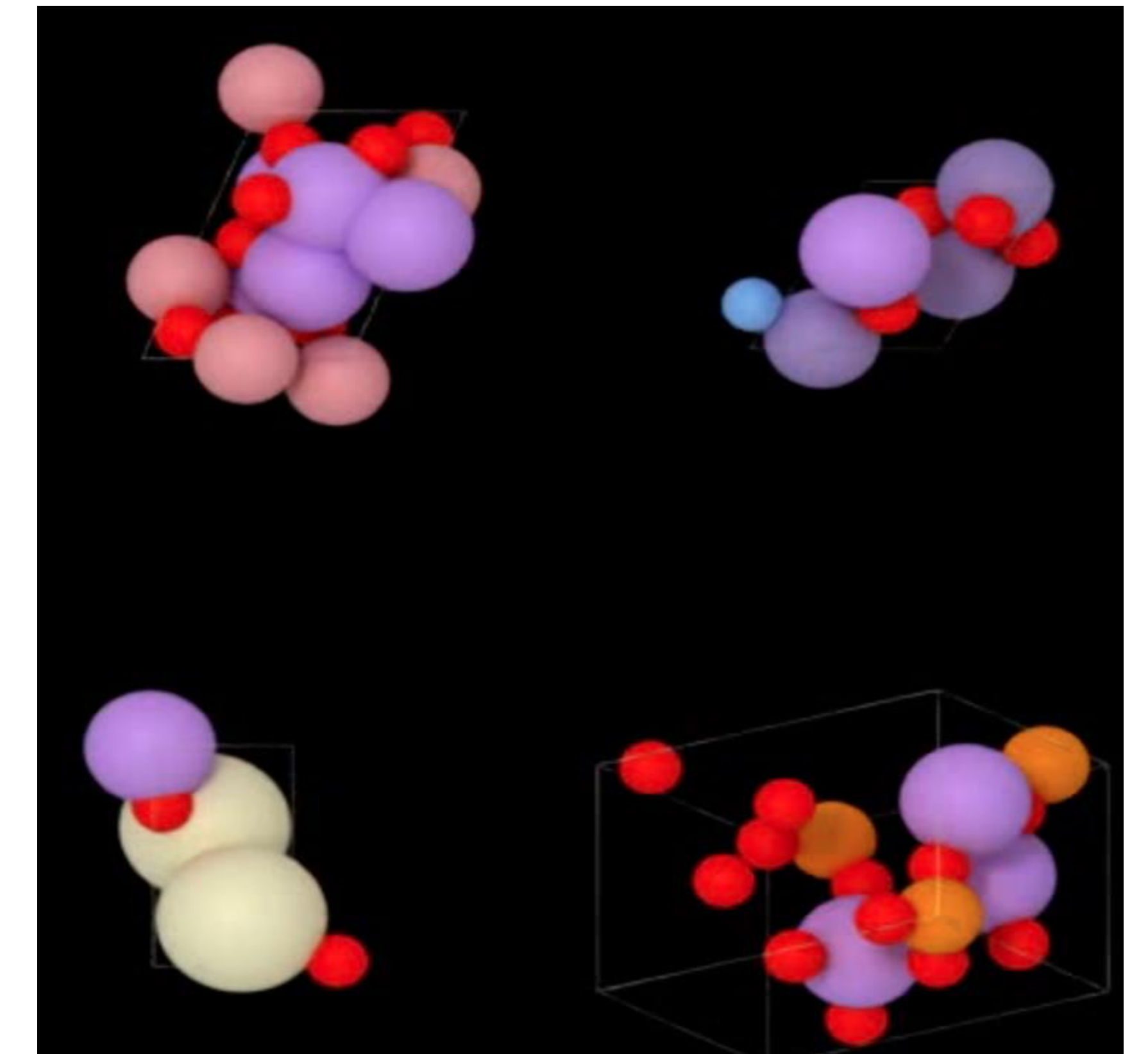
## BIONEMO

AI-Driven Drug Discovery

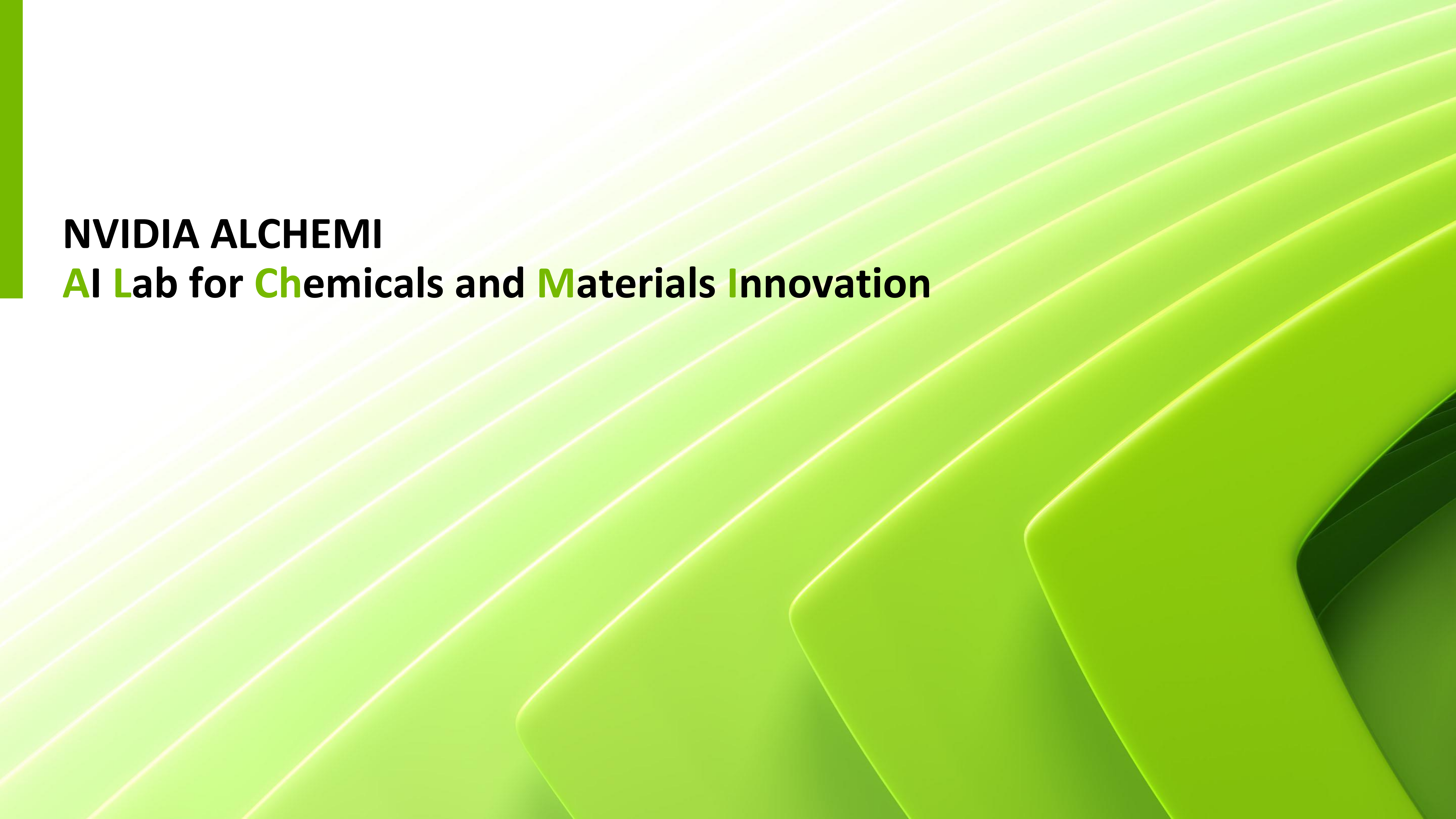


## ALCHEMI

AI-Driven Materials and Chemical Discovery





The background features a series of overlapping, diagonal, wavy bands in various shades of green, ranging from light lime to dark forest green. These bands create a sense of depth and movement, resembling a stylized landscape or a modern architectural design. The text is positioned on the left side, with the first line in black and the second line in a mix of green and black.

**NVIDIA ALCHEMI**

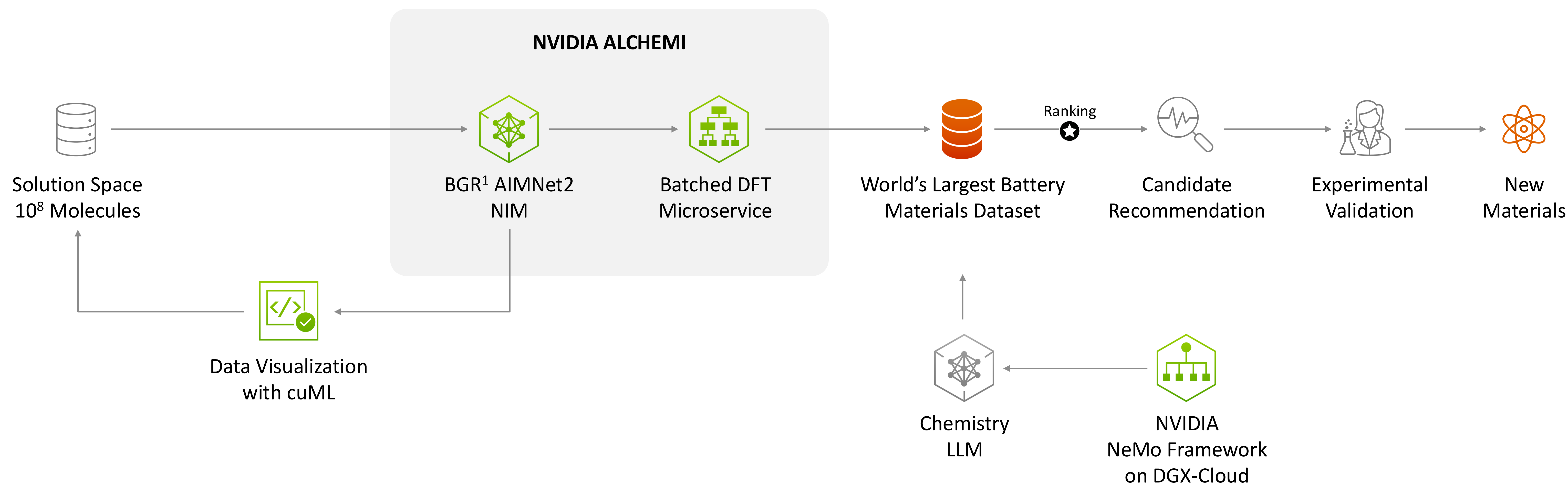
**AI Lab for Chemicals and Materials Innovation**



# 1: AI-accelerated molecular and materials discovery

Case study: SES AI created world's largest battery materials dataset with NVIDIA ALCHEMI

Green icon = NVIDIA product



**1,600x Acceleration<sup>2</sup>** (20 years to 4 days)

1. Batched Geometry Relaxation
2. 80x acceleration with NVIDIA ALCHEMI software and 20x acceleration from moving workloads to 500 H100s from CPU equivalence



# NVIDIA ALCHEMI DEMO

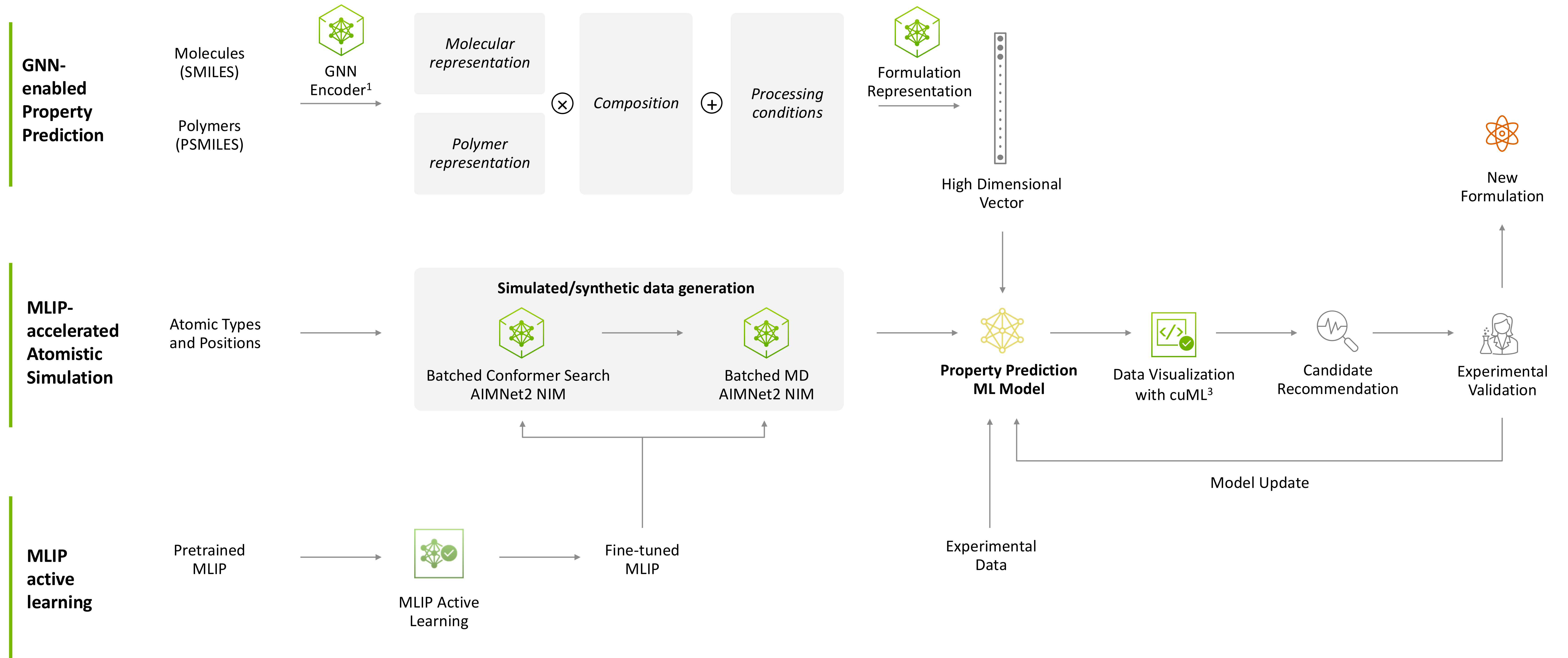
<https://www.youtube.com/watch?v=O-2TLhaTcuw>



# AI-accelerated formulation optimization

Effective property prediction enables finding global optimal candidate in fewer experimental iterations

Green icon = NVIDIA product



1. Graph Neural Network encoder (e.g., KPGT, GROVER)

2. Machine Learning Interatomic Potential

3. E.g., UMAP (Uniform Manifold Approximation and Projection) and clustering





**Thank You**



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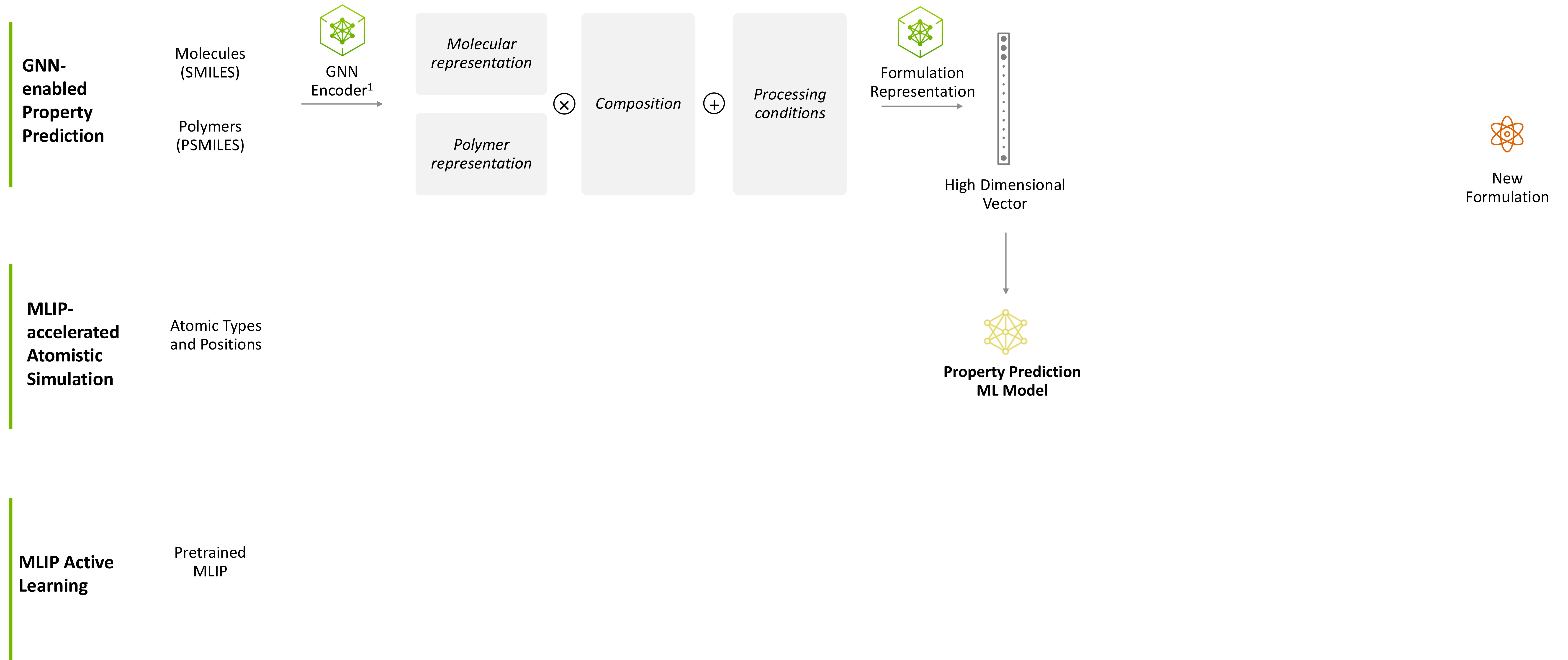
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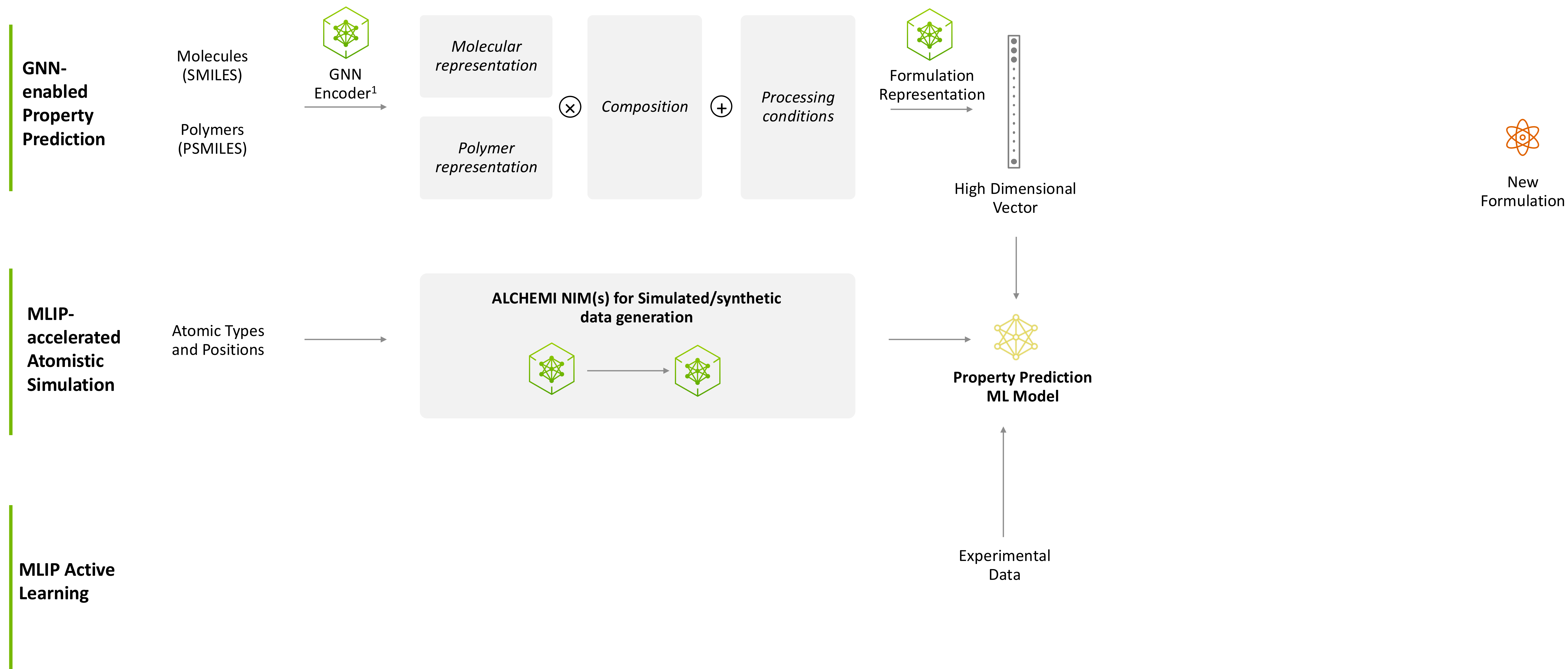
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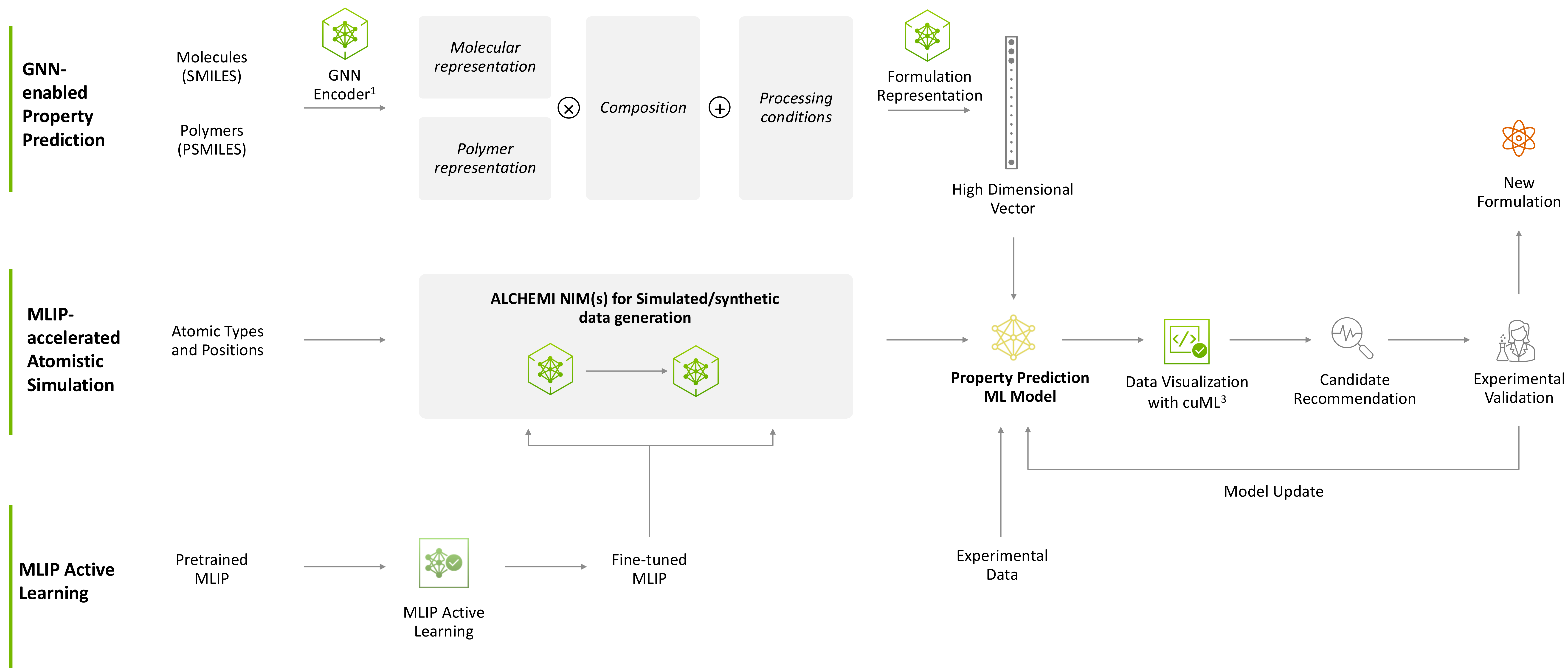
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