

Autonomous X-ray Scattering



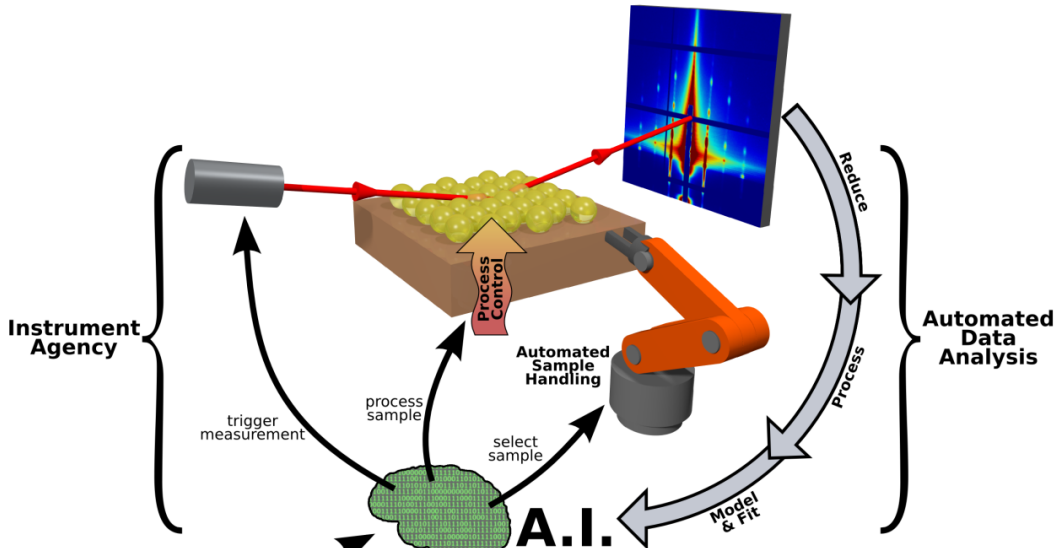
Kevin G. Yager (kyager@bnl.gov)

Acknowledgments

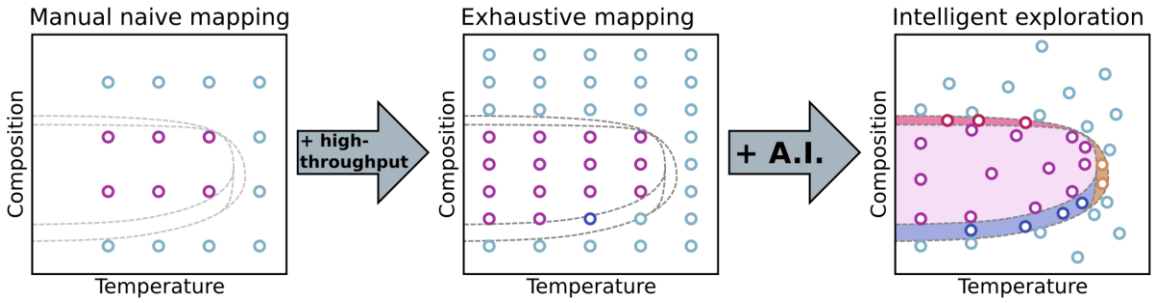
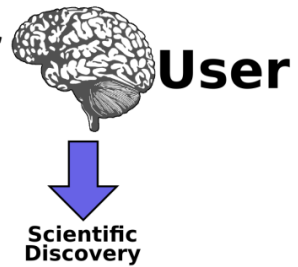
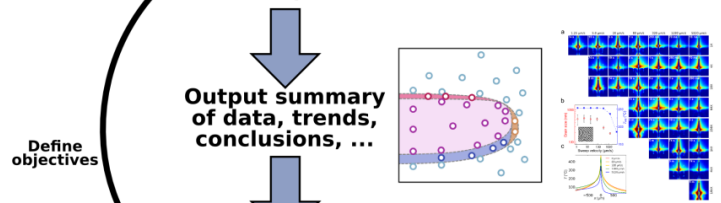
- Autonomous implementation
 - **Masa Fukuto** (BNL, NSLS-II)
 - **Marcus Noack** (CAMERA)
 - Jamie Sethian (CAMERA)
 - Ruipeng Li (BNL, NSLS-II)
 - **Esther Tsai** (BNL, CFN)
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Vision: Autonomous Experiments

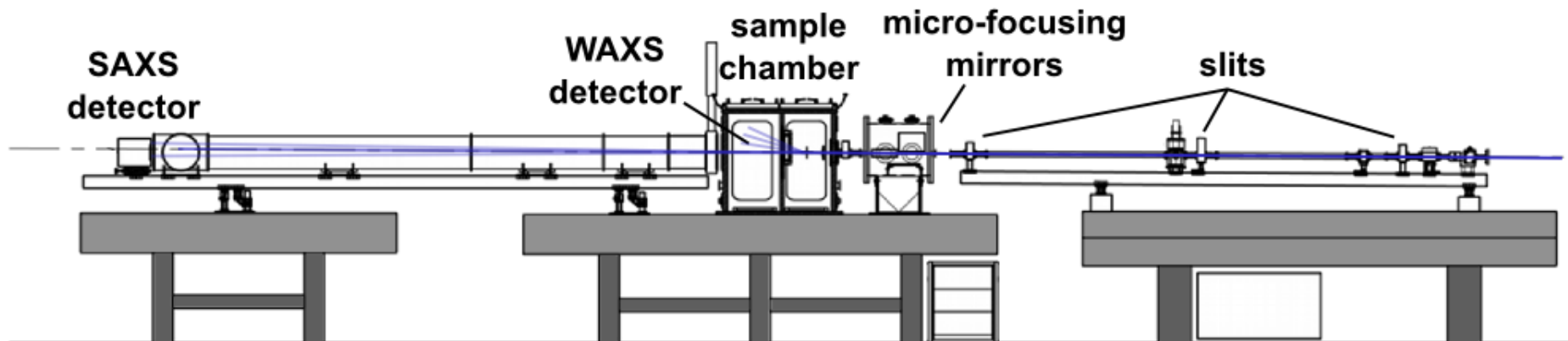
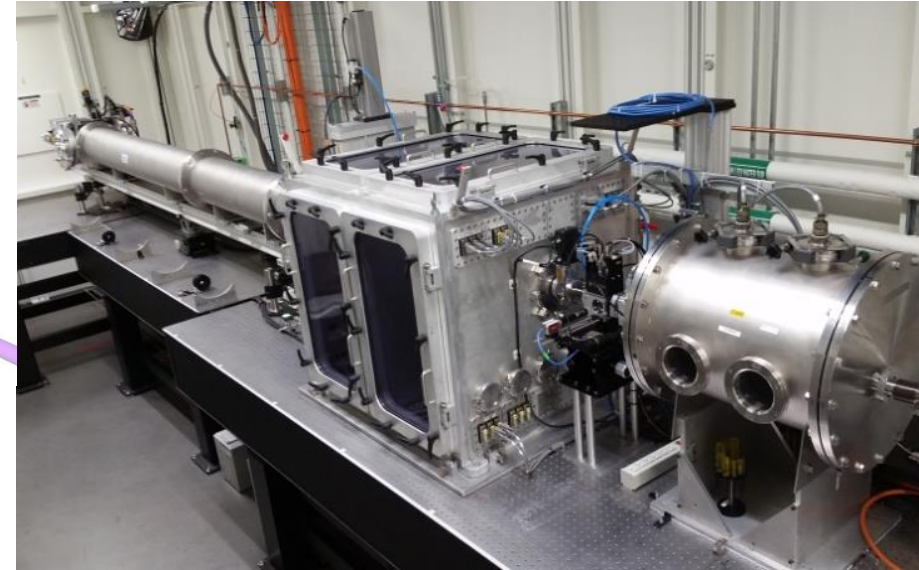
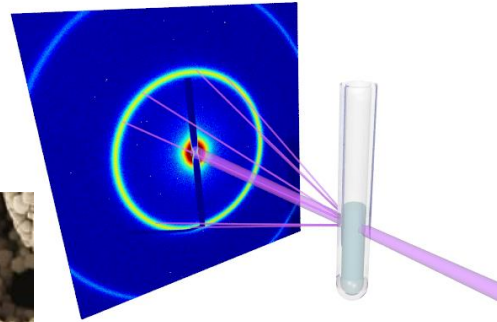
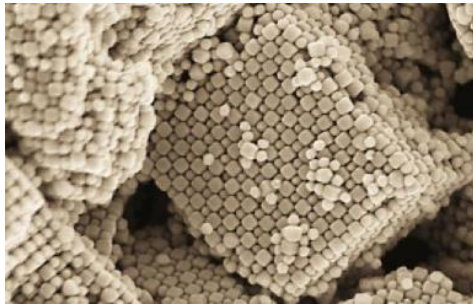


- Automate the entire experiment, including **decision-making**
- **Liberate** human scientist to focus on scientific insight
- Accelerate **materials discovery**



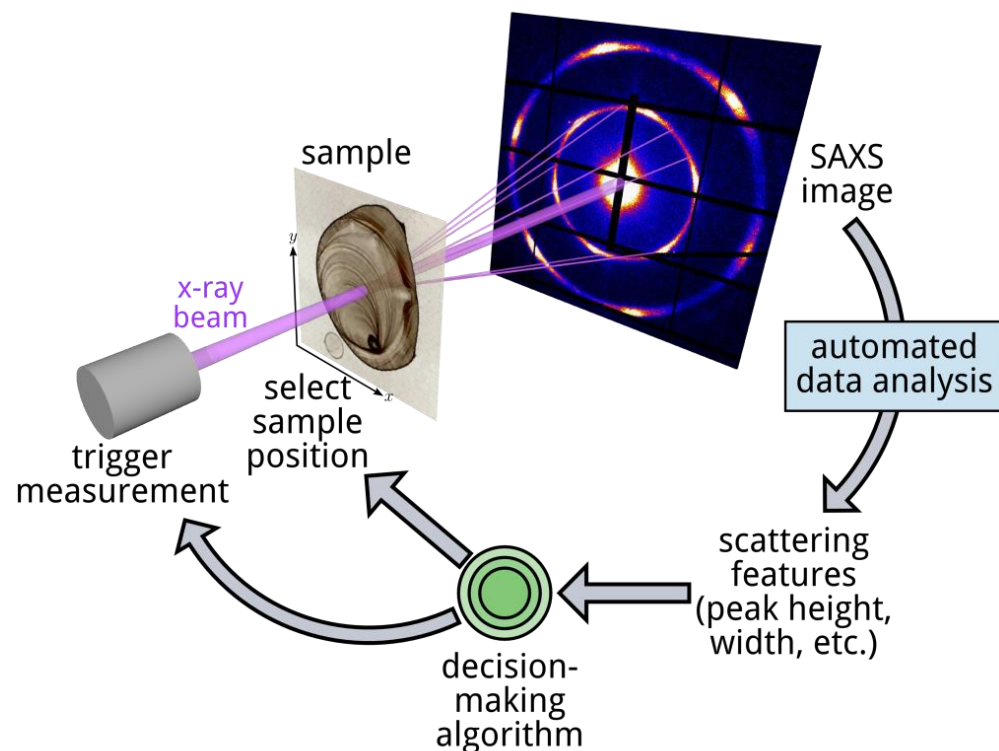
X-ray Scattering

- The goal in x-ray scattering is to determine the structure of a material



Autonomous X-ray Scattering

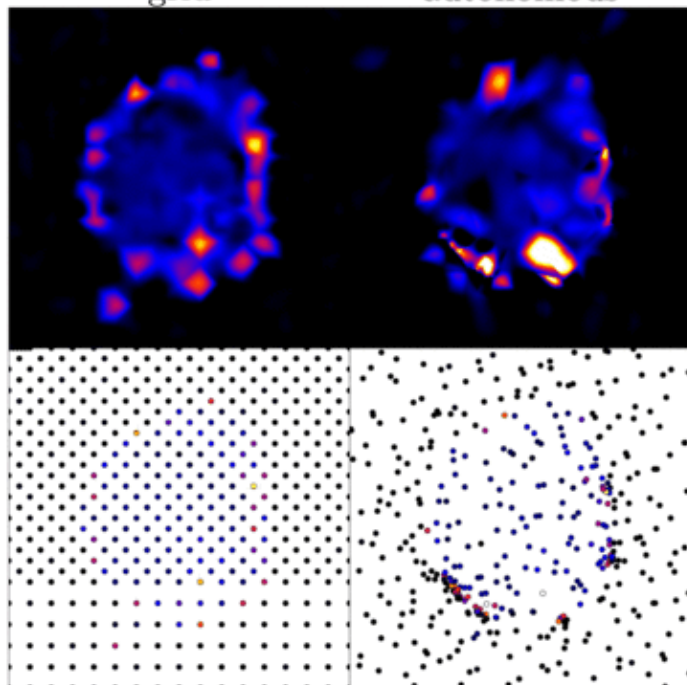
- Automate entire experiment
 - Instrument
 - Data analysis
 - **Decision-making**
- Improves efficiency, accelerates discovery
- **Liberates** humans to focus on science



$N=510$

grid

autonomous



Noack et al. *Scientific Reports* **2019**, 9, 11809;
2020, 10, 1325; **2020**, 10, 17663

Noack et al. *Nature Reviews Physics* **2021**, 3, 685

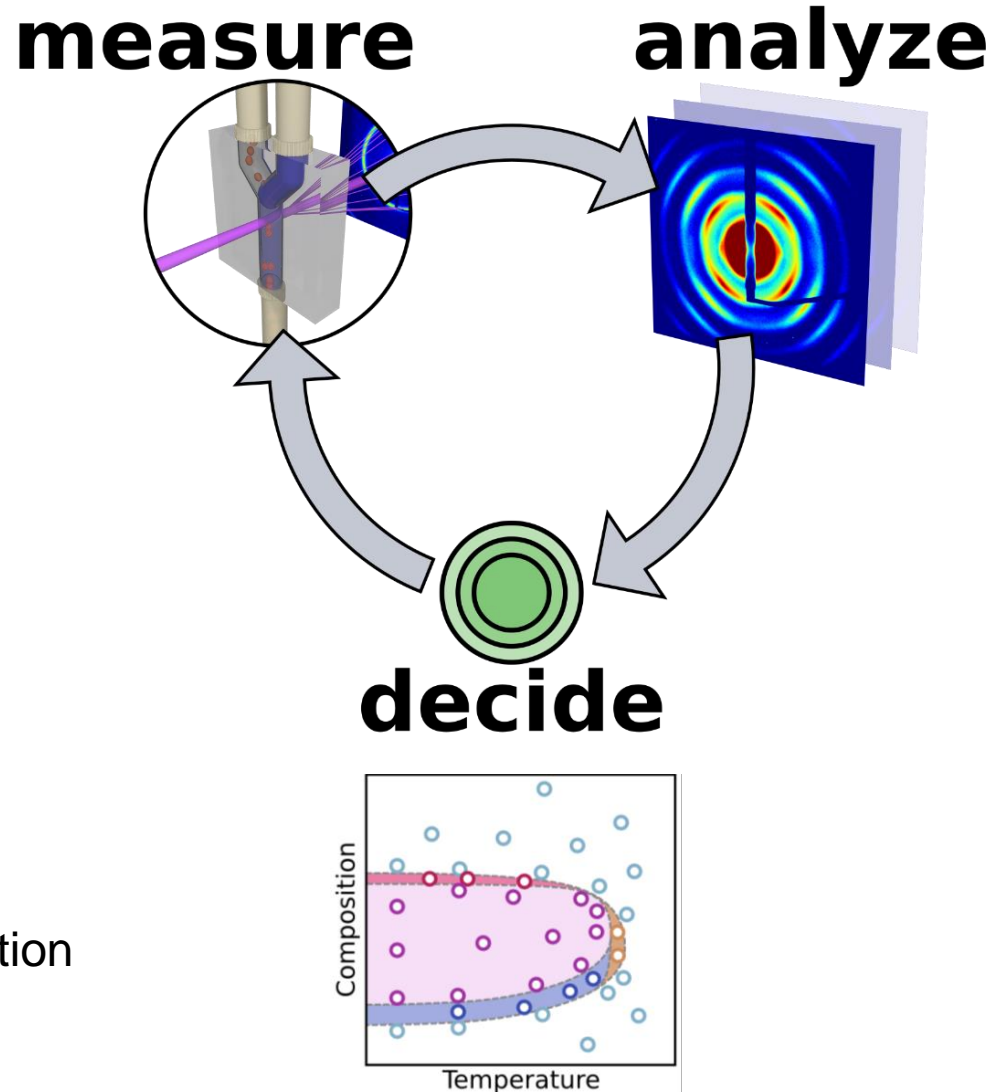
Yager et al. *Nanotechnology* **2023**, 34, 322001

Implementation

- Separate the data analysis from the decision-making
 - Dimensional reduction
 - Abstraction

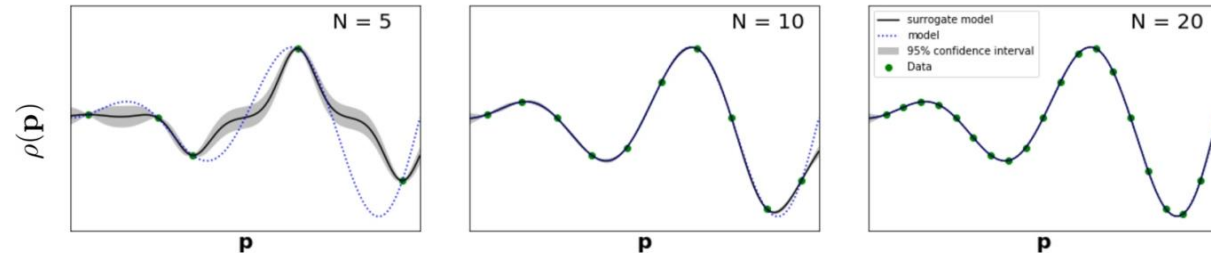
- Three processes (easy stop/restart)
 - **measure** (*Bluesky*)
 - **analyze** (*SciAnalysis*)
 - **decide** (*gpCAM*)

- Communication is “thin”
 - **m**→**a**: Pointer to data
 - **a**→**d**: Result vector
 - **d**→**m**: Parameter-space position



Algorithm: Gaussian Process

- Construct **surrogate model**
 - Fit/interpolate data
 - Select kernel to match physics
 - Estimate hyper-parameters that match data (lengthscales, periodicity, etc.)

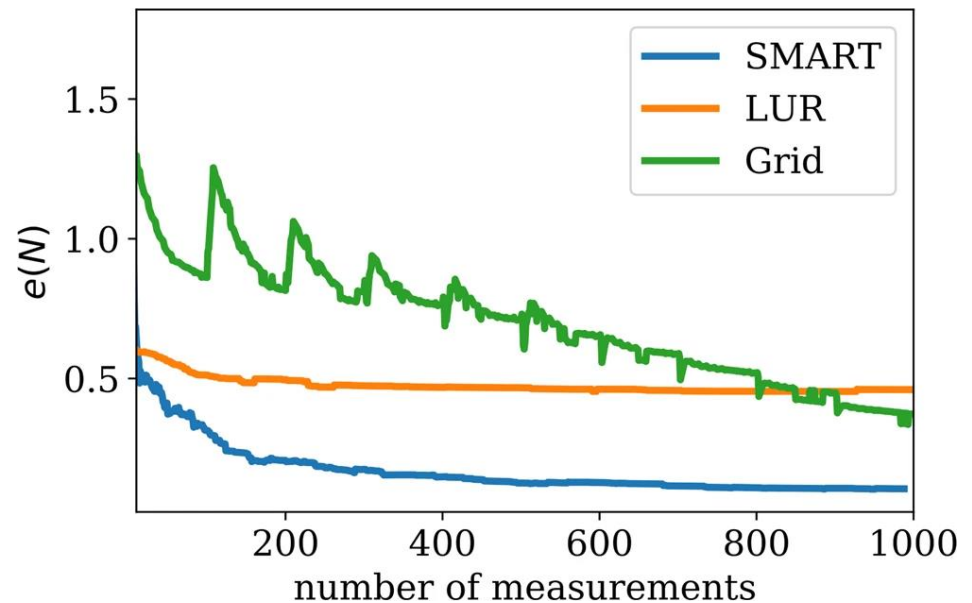


- Calculate **uncertainty surface**

- Construct **objective function**

- Search for maximum in objective
- Control behavior: gradients, cost, etc.

- As we **iterate**, errors decrease and surrogate model improves



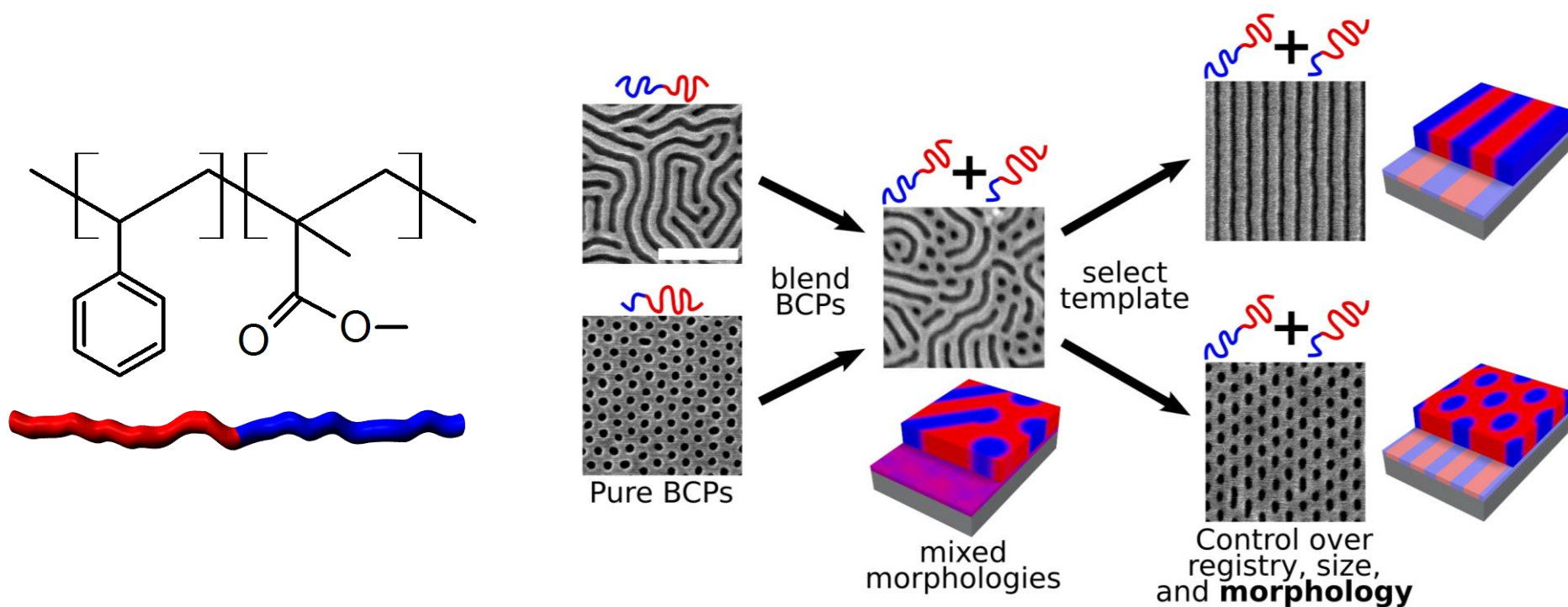
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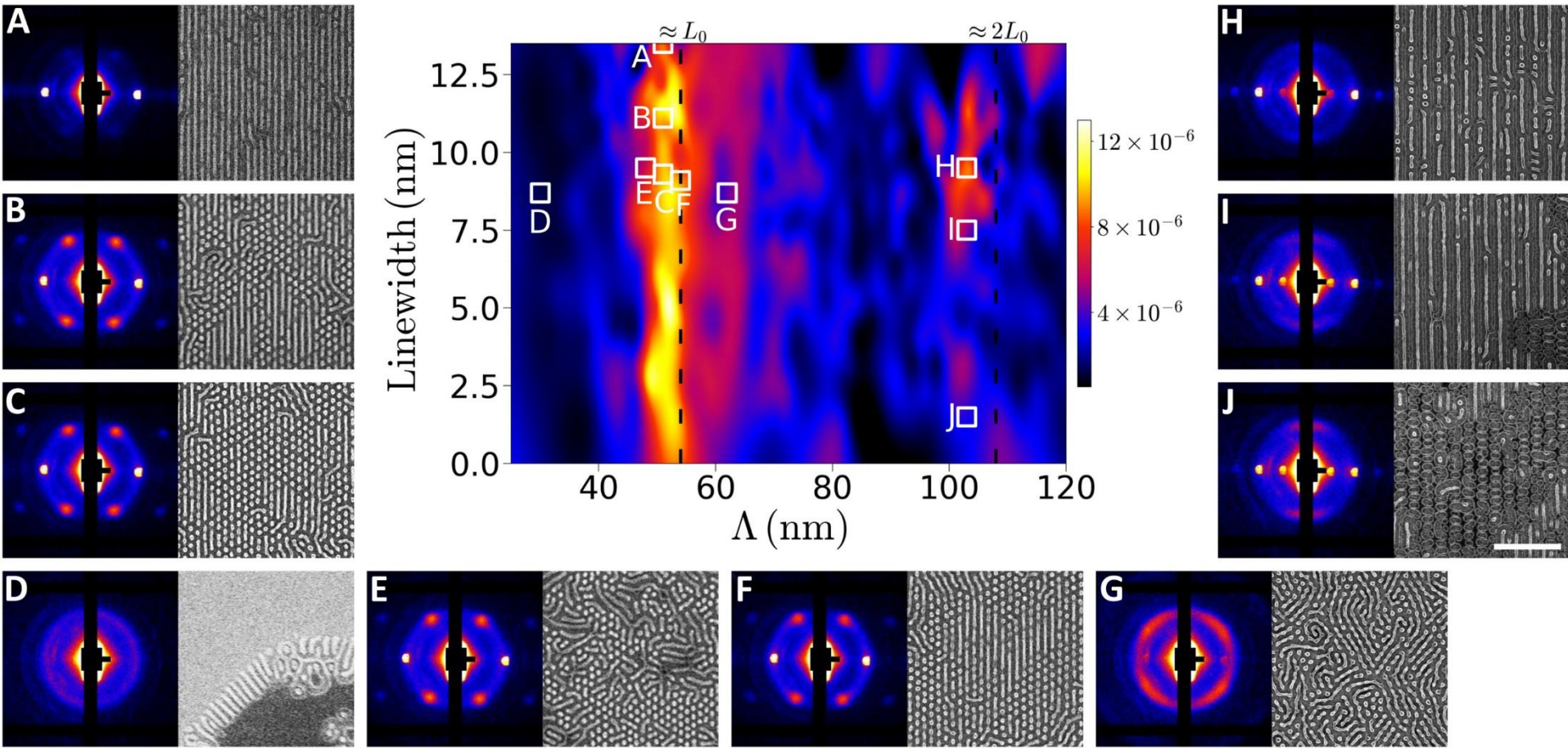
Self-Assembling Materials

- Blends of self-assembling materials become a 'responsive' resist
 - Template (pitch, duty cycle) selects morphology



Exploration of Self-Assembly

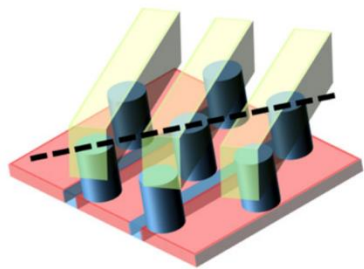
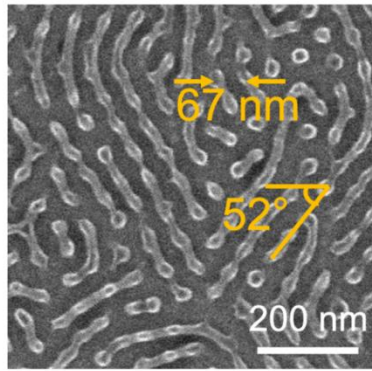
- Autonomy **discovered** numerous novel morphologies



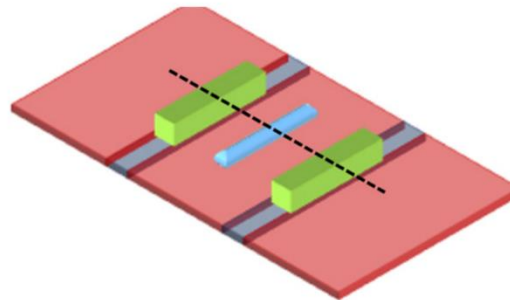
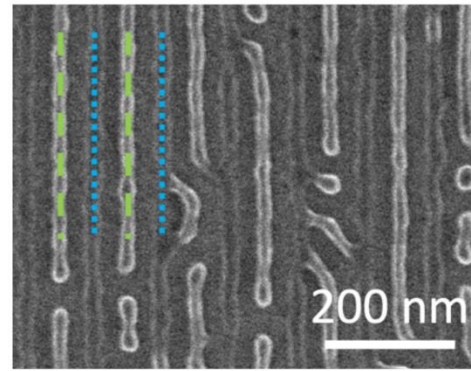
New Nano-structures

- Autonomy **discovered** numerous novel morphologies

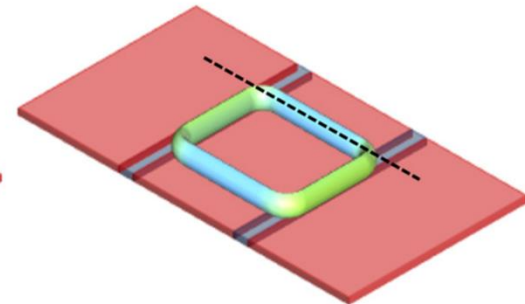
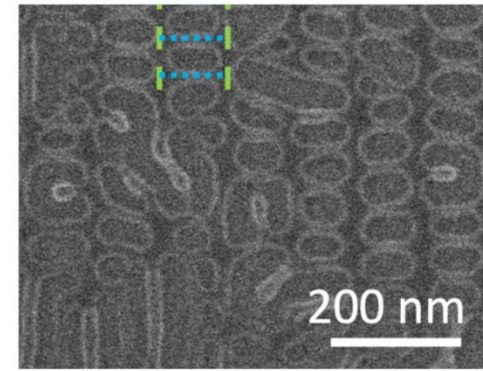
skew



alternating



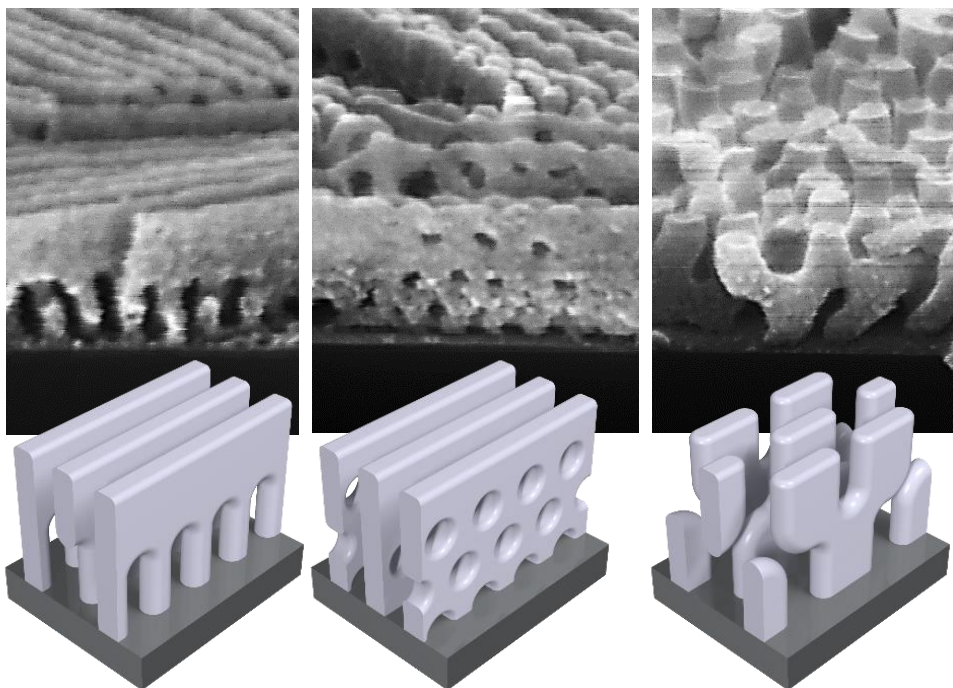
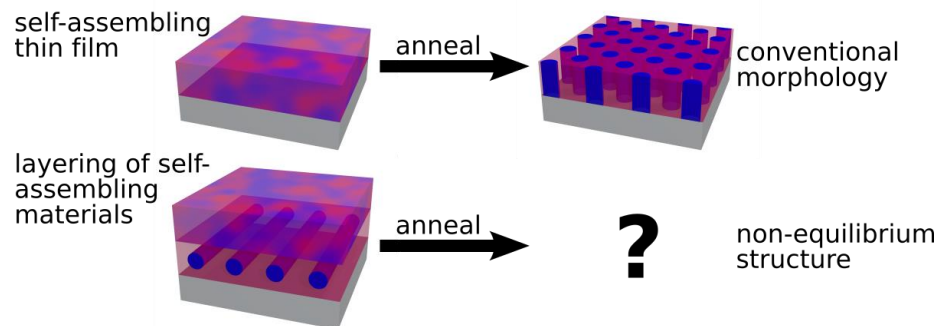
ladder



New Nano-structures

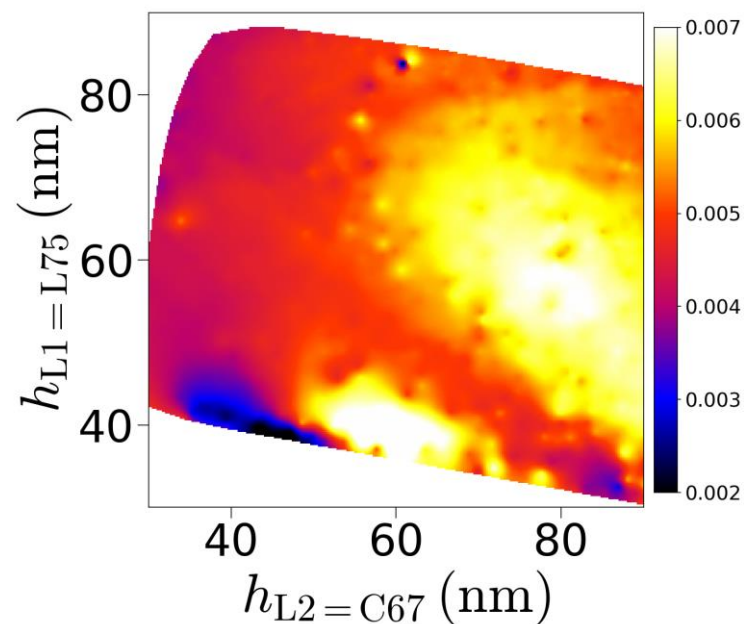
Materials science

- Layering self-assembling materials can generate new (non-equilibrium) structures



$N = 1, 249$

p (a. u.)

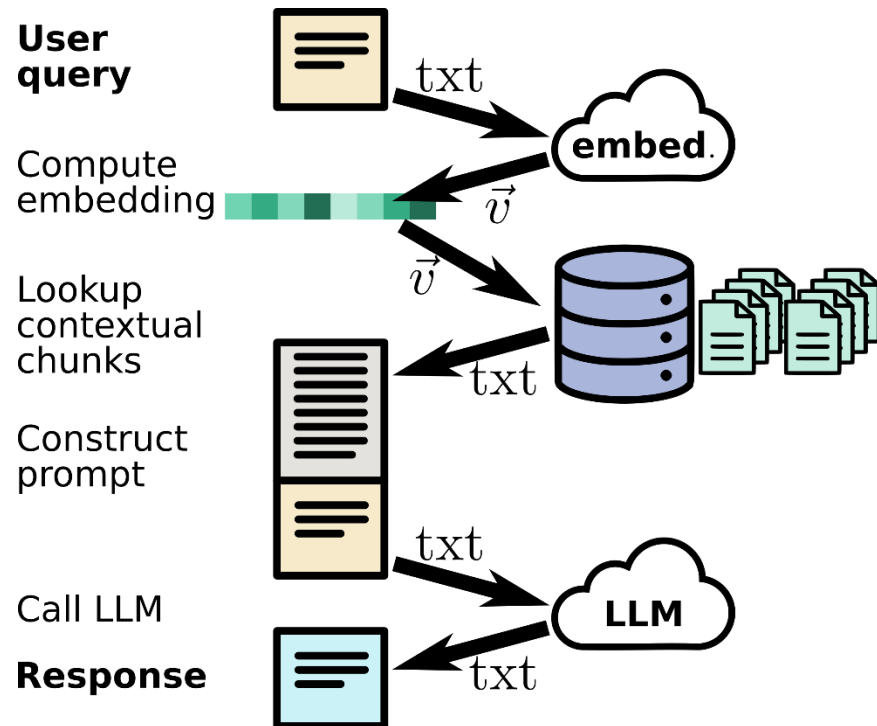
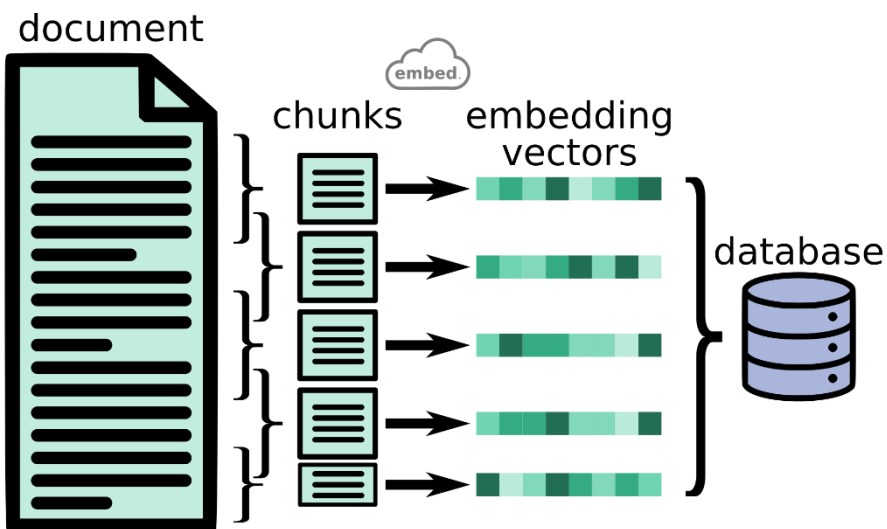


AI assistants

Domain-specific Chatbot

Large Language Models

- LLMs (c.f. ChatGPT) enable remarkably coherent dialog on any topic
- They sometimes “hallucinate”
- This can be solved by giving the bot domain-specific text



CFN Science ChatBot

Demo

This is a demo of a domain-specific ChatBot for science. The chatbot uses a large language model (LLM) for generative text, combined with a database of domain-specific text drawn from CFN publications.

User: I want to measure the orientation of a block copolymer morphology in a thin film (cylinders horizontal vs. vertical). Should I use **TSAXS, GISAXS, or GTSAXS**?

CFNBot: To measure the orientation of a block copolymer morphology in a thin film (cylinders horizontal vs. vertical), you can use either GISAXS (Grazing-Incidence Small-Angle X-ray Scattering) or GTSAXS (Grazing-Incidence Transmission Small-Angle X-ray Scattering). Both techniques provide valuable information about the structure of thin films.

GISAXS allows for the observation of monolayers of nanomaterials and **depth profiling of thin films**. It can provide information about the unit cell, morphology, repeat spacing, orientation distribution, and grain size in soft materials. However, analyzing the data obtained from GISAXS can be challenging due to refracted effects at the ambient-film interface causing distorted images of reciprocal-space.

On the other hand, **GTSAXS** is an alternative to GISAXS that **can obtain undistorted data** without requiring lengthy reconstruction. It involves aligning the incident x-ray beam on the downstream edge of a sample/substrate, rather than directing the beam towards the center of the sample as typically done in GISAXS. GTSAXS is simpler and can record an image without refraction-distortions or multiple-scattering complications. However, it requires arranging the sample of interest to be positioned near the edge of the substrate.

Type your message here...

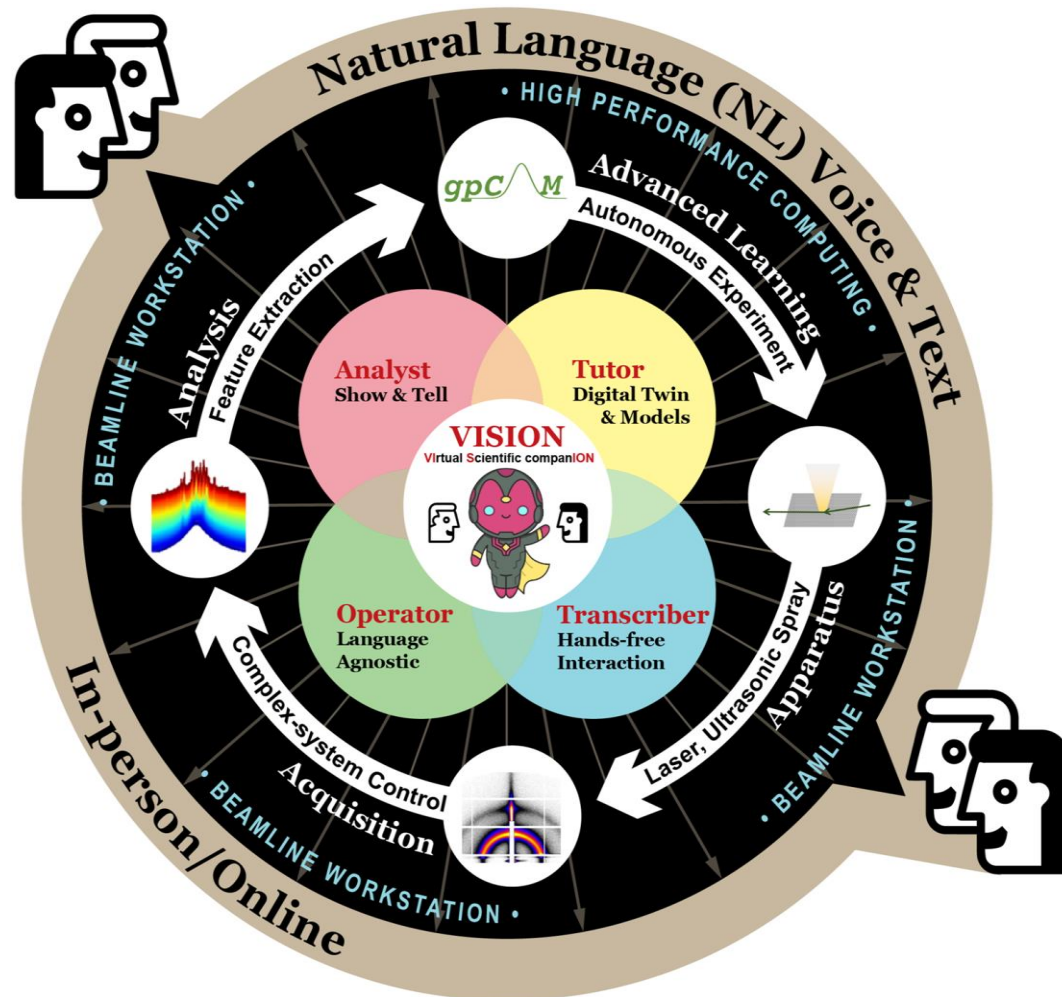
Send

Virtual Scientific Companion

- NLP allows scientist to plan experiments in natural language
- LLM helps refine experiment, generates Python code to execute at beamline
- Dialog with models and analysis pipelines



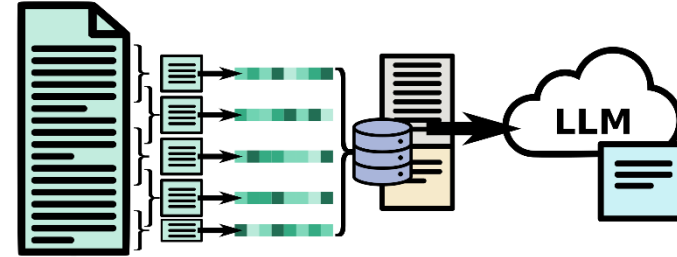
Esther Tsai
Early Career Award



Future: AI Assistants

Nanoscience Chatbot

- Find/discuss relevant information
- Brainstorming

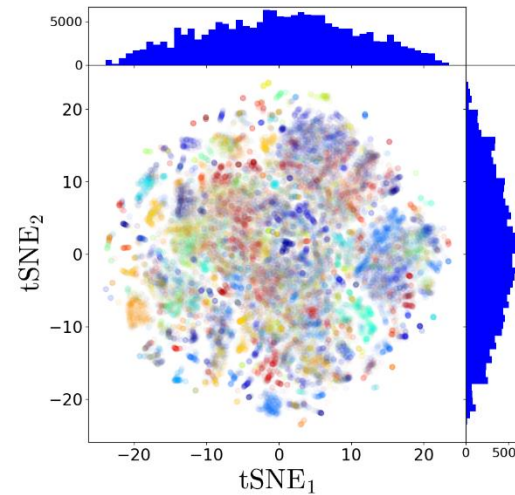


Data Navigator

- Organize data

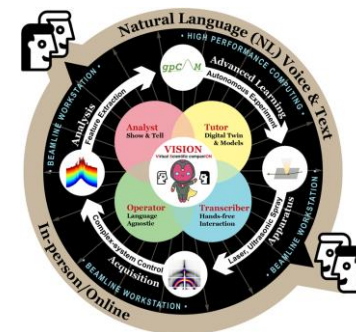
Experimental Assistant

- Plan/control experiments (including AE)



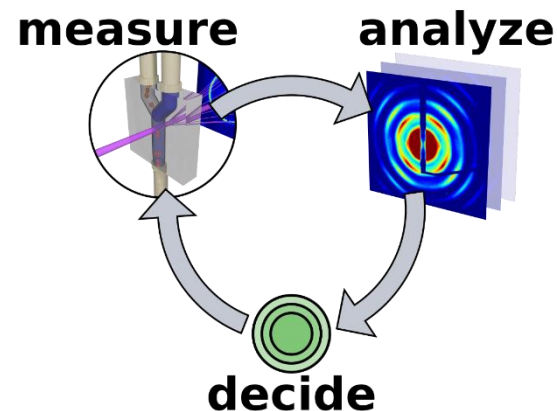
Future: Swarm of AI Agents

- Specialized agents for experiments, data, publications
- Agents talk to each other; surface only important topics to human
- Swarm effectively expands the human's memory, planning, and thinking

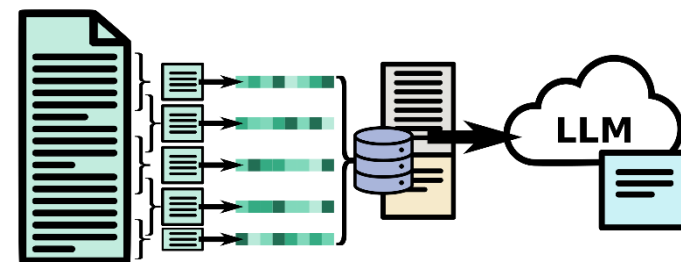


Summary

- **Autonomous experiments** can explore arbitrary science problems
 - Imaging/mapping
 - Combinatorial
 - Real-time synthesis/processing



- **Language models** can automate diverse science tasks



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