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FROM BENCHMARKING TO AGENTIC WORKFLOWS

Foundation Models For X-ray Data Analysis

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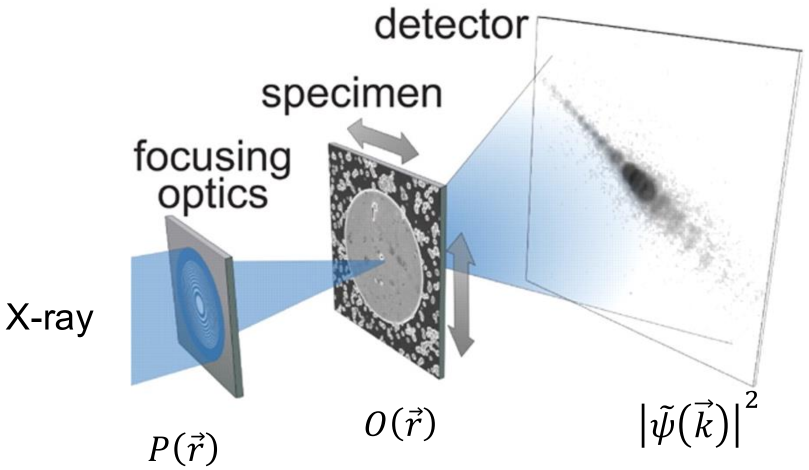
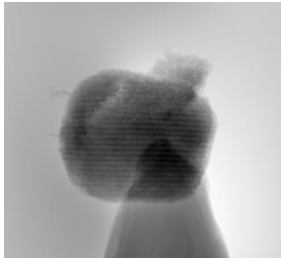
Ptychography



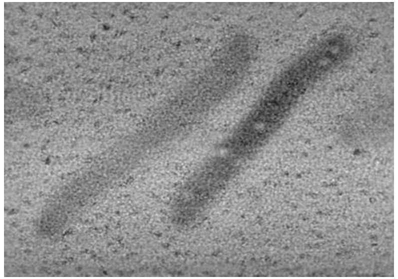
Retrieve object $O(\vec{r})$ (and phase $P(\vec{r})$) from a series of scanning diffraction patterns ($|\tilde{\psi}(\vec{r}_p,\vec{k})|^2$)

Sensitive to reconstruction parameters and prone to artifacts



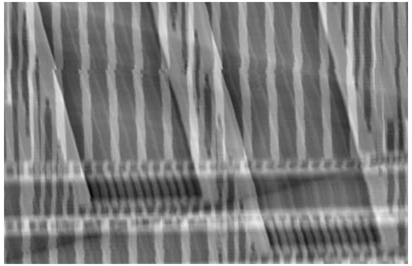
Sample: integrated circuit
Instrument: 2xfm
Diagnosis:
- Local scan drift

Actions:
- Turn on position correction
- Crop data to 64x64
- Increase the number of iterations



Sample: Ecoli
Instrument: Bionanoprobe
Diagnosis :
- Slowly-varying background
- Noisy artifacts

Actions:
- Use variable probe correction
- Use Poisson noise model



Sample: super crystal
Instrument: Ptycho-SAXS
Diagnosis :
- Non-unform background
- Singularity artifacts in the object

Actions:
- Use compact batch scheme with momentum acceleration
- Multislice ptychography

Benchmark LLMs/VLMs on Ptychography Tasks

Task 1: Visual artifact detection

Find artifacts (e.g., grid/aliasing/ring) in reconstructed ptychography images.

Input: reconstructed image
Output: diagnosis

Task 2: Parameter recommendation

Given a dataset's metadata, recommend new/better reconstruction parameters.

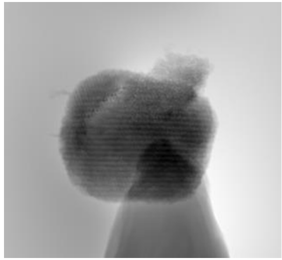
Input: sample metadata
Output: actions

Strategies compared

In-context learning (ICL): prompting w. examples

Sample-specific few-shot (SSFS): fetch relevant examples

Supervised fine-tuning (SFT): train adaptors w. few examples



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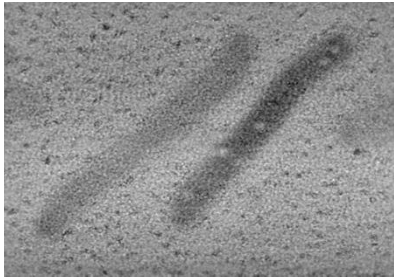

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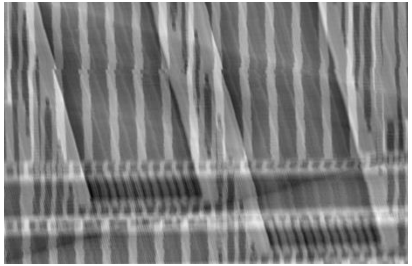

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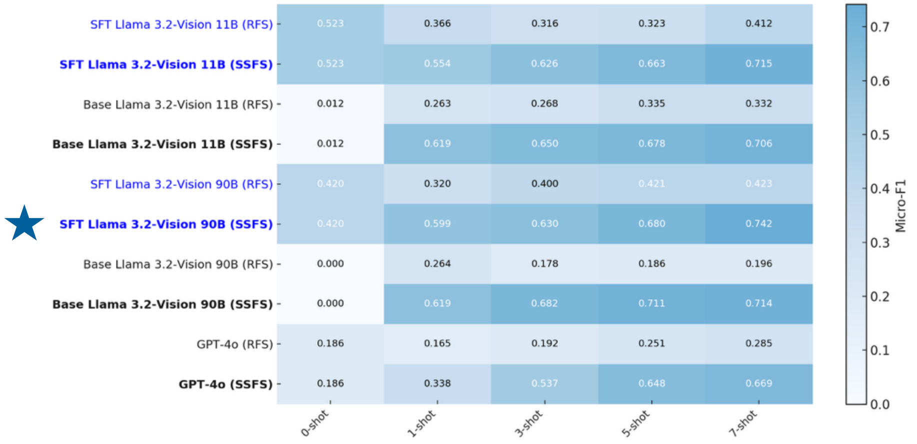

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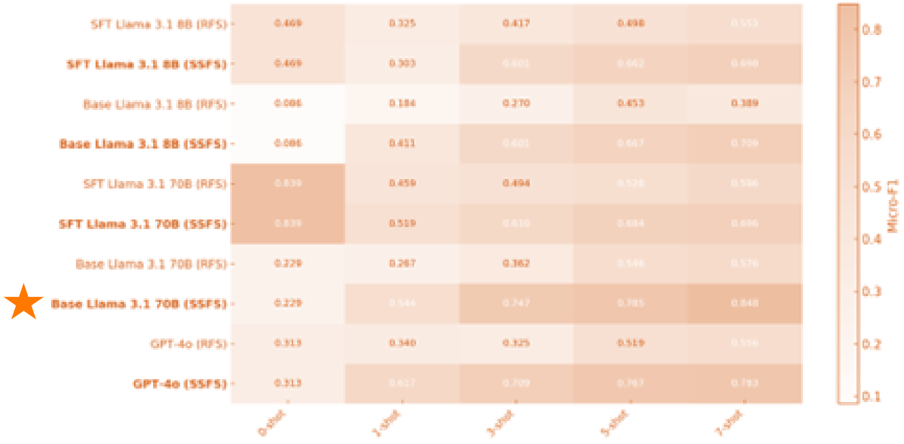


Task 2: Parameter recommendation

Best recipe:
SFT + sample-specific few-shot examples

Example relevancy matters most, irrelevant context can hurt performance

Best recipe:
large base + sample-specific few-shots

SFT can produce “rigid expert”: great 0-shot but few shots degrades performance

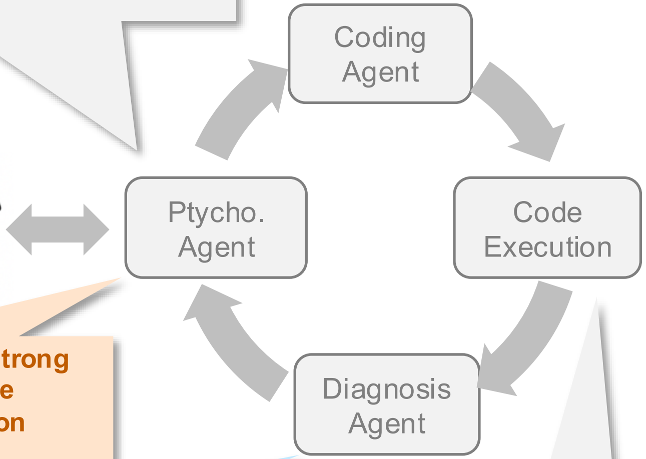
Build Workflows around Tested Models and Recipes

Can you help me process my ptychography dataset?

Certainly! Please answer some questions so that I can figure out your problem settings.

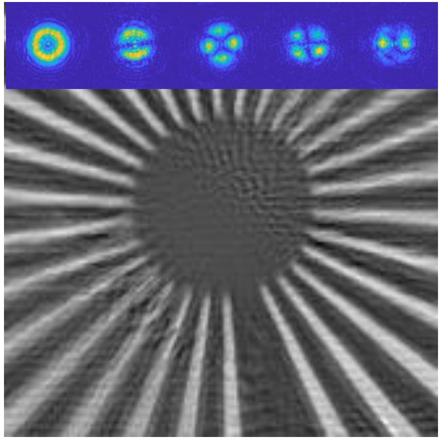
1. Which instrument did you use to acquire this data?
2. Was the data acquired in step-scan or fly-scan mode?
3. …

I suggest using 5 probe modes and single slice model.




```
% initialize parameters
par = {};
par.z = 1.92;
par.energy = 8.8;
par.Ndp = 256;
...
par.multislice_ptycho = false;
par.Nprobe = 5;
par.Niter = 1000;
...
% start reconstruction
ptycho_recon_exp_data(par);
```

Here are the reconstructed object and probe:



The reconstructed object seems to exhibit some grid or line artifacts. The final probe mode shows clear structures and a high-power percentage.

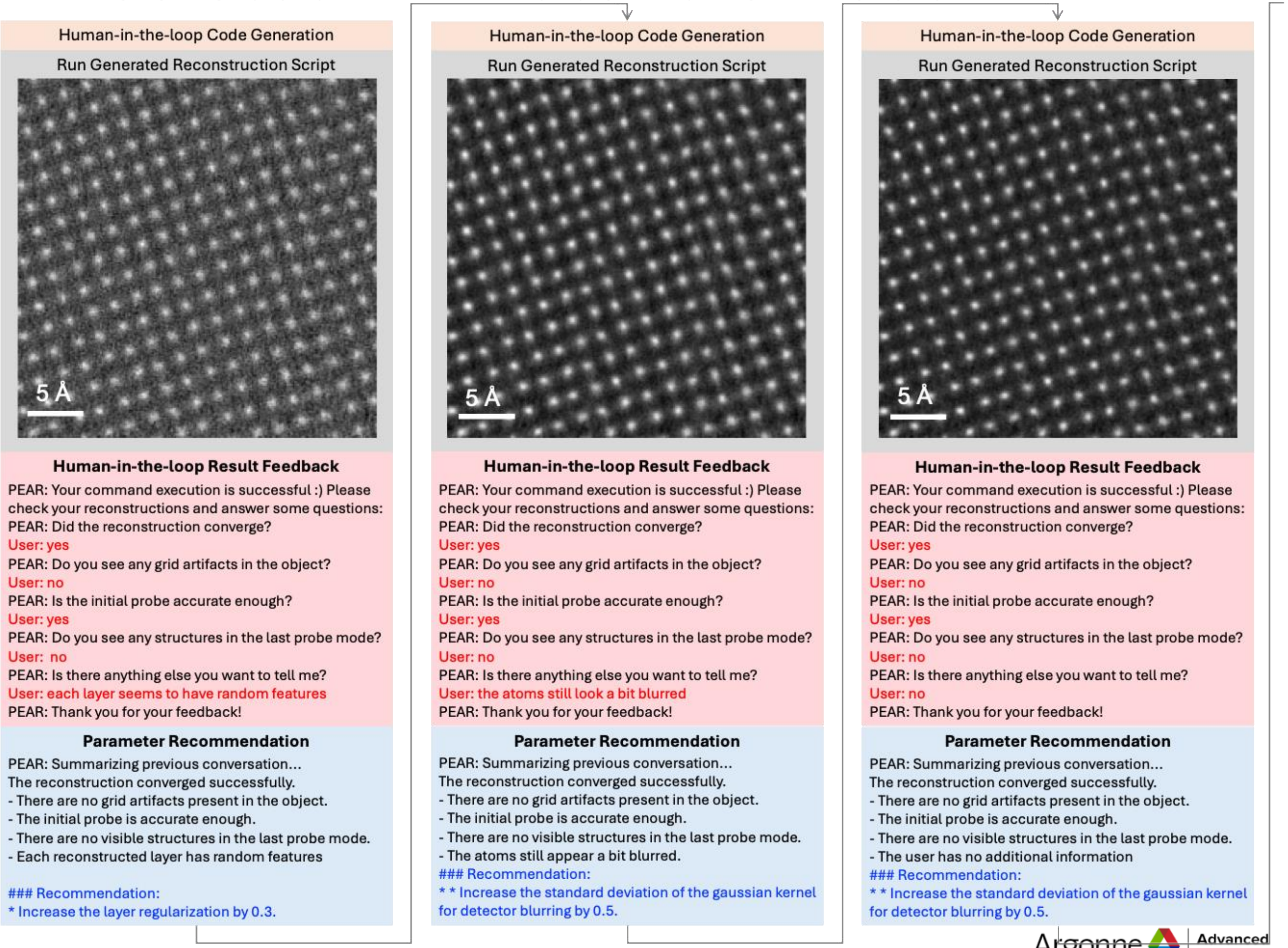
The artifacts could be caused by strong beam vibrations. Try increasing the number of probe modes and turn on variable probe correction.

Case Study: AI-Assisted 2D Materials Recon.

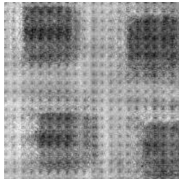
arXiv:2410.09034

AI workflow can improve reconstruction quality in a few iterations

Bayesian optimization can take tens/hundreds of iterations



From Parameter Tuning to Algorithm Discovery



Can you help me find a regularizer to suppress grid artifacts in IC dataset

Action: GENERATE

```
def regularize_llm(self):
"""Physics-aware
regulariser for hard-X-ray
IC ptycho."""
<function content>
self.set_data(updated_obj)
```

Here are the reconstructed object and probe:

Research Agent

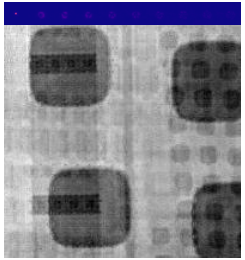
Coding Agent

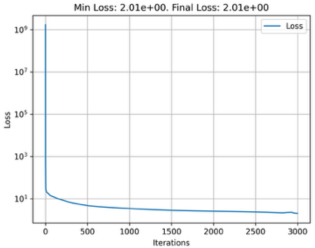
Code Execution

Evaluation Agent

Analysis Agent

ptychi





- **(Ground truth) metrics mode**
- **Human-in-the-loop mode**
- **Auto mode (tools & VLMs)**

Below is a compact "look-up sheet" you can keep next to your reconstruction script. It lists the regularizers, constraints and mitigation steps that have proved useful for hard-X-ray ptychography of planar integrated-circuit (IC) samples acquired in step-scan mode with (i) an inaccurate initial probe, (ii) very sparse/large scan steps and (iii) visible raster-grid artifacts.

Regularization techniques that work for this experiment

A. Spatial-domain sparsity & piece-wise constancy

- Isotropic Total-Variation (TV) or Total-Generalised-Variation (TGV) penalties suppress noise and fill in missing pixels when the overlap is small; TV was shown to recover 100 nm IC lines at only 15 % overlap (arxiv.org).
- Structure-Tensor or directional TV priors preserve the long, straight metal lines typical of IC routings (arxiv.org).

B. Frequency-domain / smoothness penalties

- L2/Tikhonov or gradient-penalising terms on the object and/or probe, implemented in modern autodiff engines (e.g. phaser/ptyRAD), keep high-frequency probe noise from leaking into the object (arxiv.org, ar5iv.labs.arxiv.org).

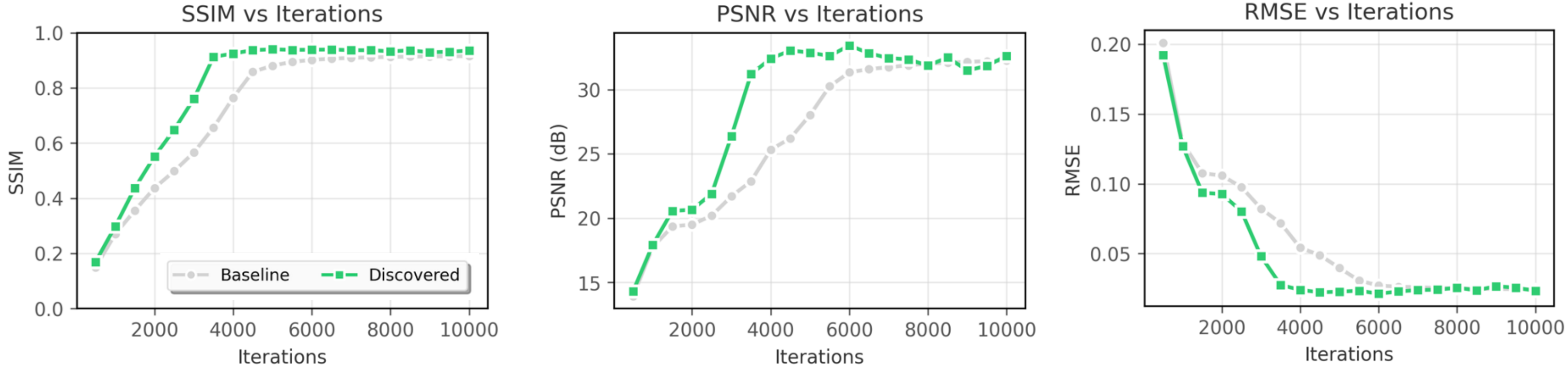
Action: EVOLVE

```
def regularize_llm(self):
"""Multi-scale anisotropic
DTGV-Huber regulariser with
adaptive notch filtering."""
<function content>
self.set_data(updated_obj)
```

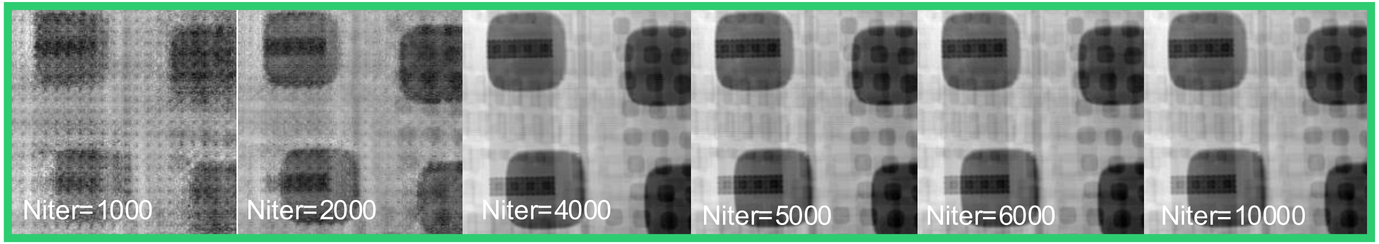
- Expose the main hyper-parameters (gamma, lam_init/min/max, huber_eps_factor, phase_tv_strength, softplus_beta_scale) through the external API so they can be tuned per dataset; grid/Bayesian search typically yields ≥2 dB PSNR
- Keep the Barzilai-Borwein step length as a tensor (do not call .item()) and compute it in full complex arithmetic; this preserves autograd graphs for unrolled or meta-learning pipelines.

…

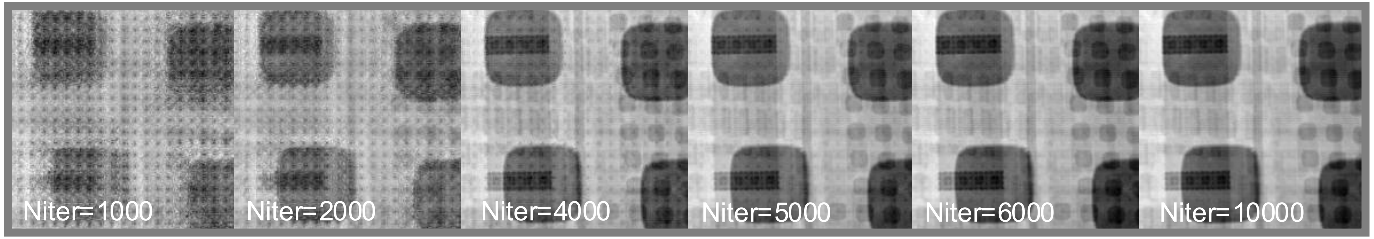
Discovered Regularizer v.s. the Hand-Crafted Baseline



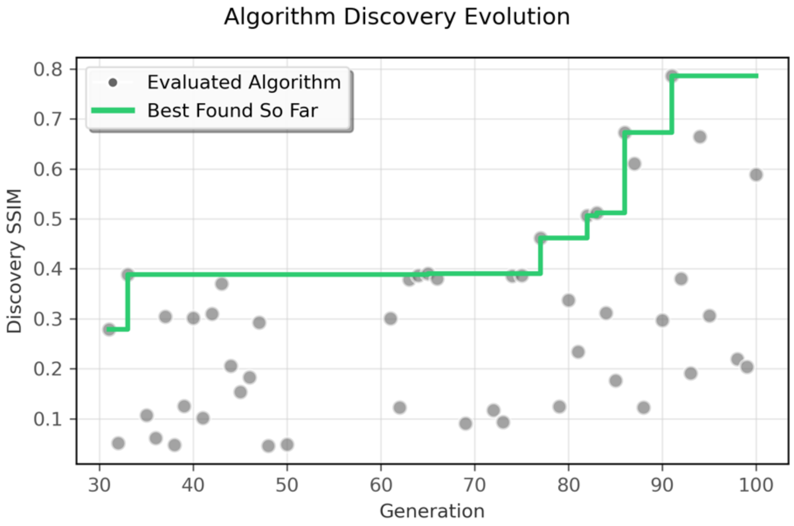
Discovered

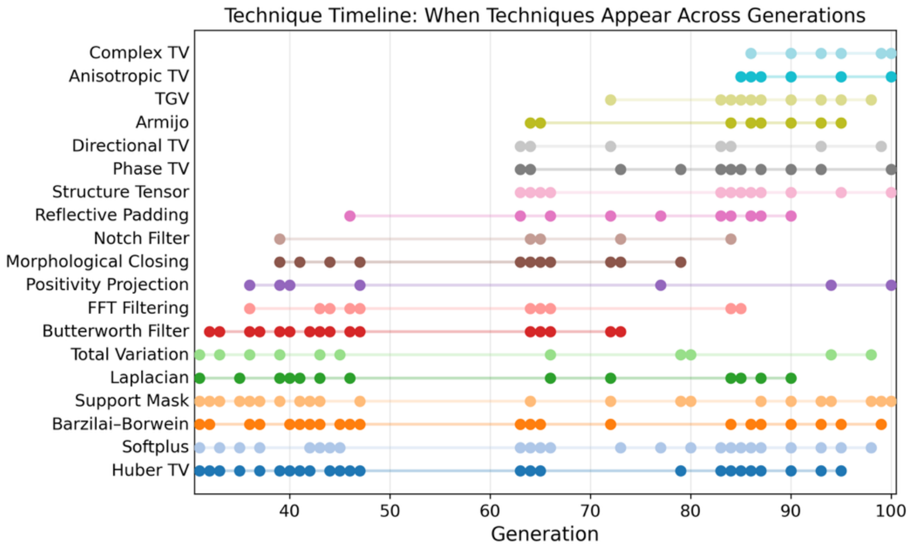


Baseline



Algo. Evolution History Recorded for Insights





Key Technical Insights:

Adaptive notch filtering:	FFT-based grid artifact suppression
Structure-tensor TV:	Edge-aware anisotropic smoothing
Barzilai-Borwein:	Adaptive step size acceleration

Most Data Analysis Problems are Unstructured

Ming Du

Structured problem

Optimizer

Loss

Model | Data & labels

Unstructured problem

Numerical optimization

A pool of TIFF images

Filtering

All sort of transforms

Morphological operations

Challenges for unstructured analysis

Development environment setup

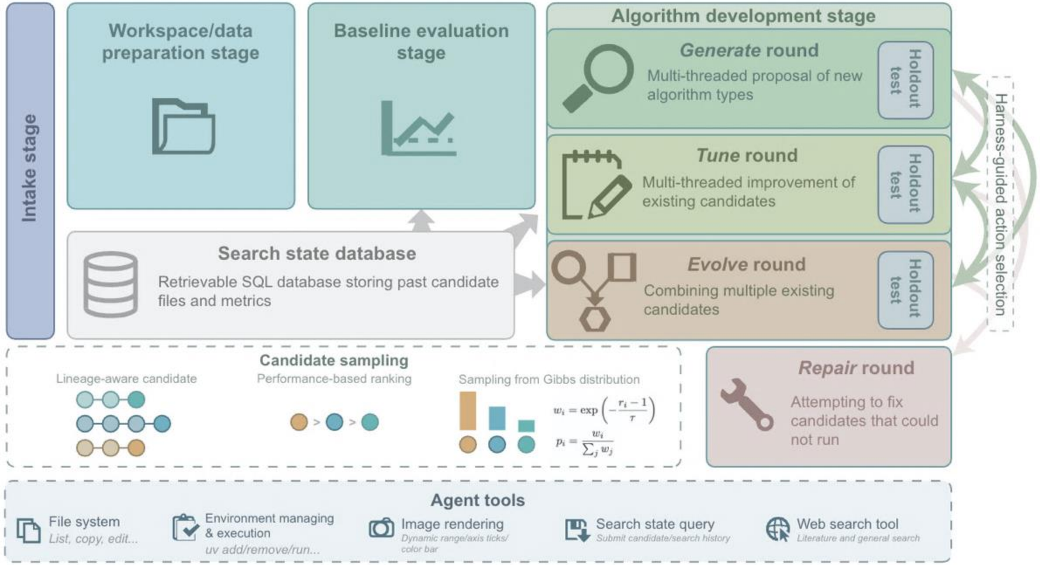
Evaluation script

Troubleshooting

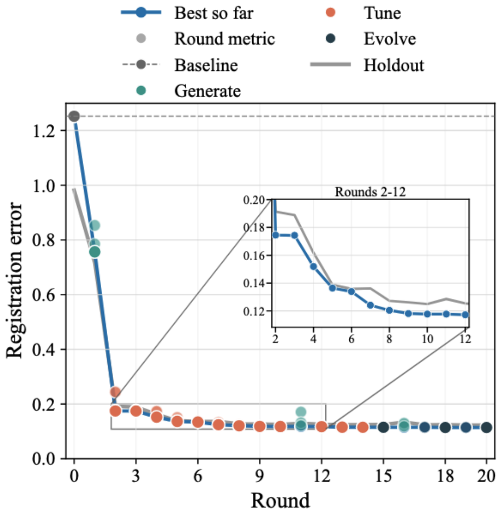
Exploration-exploitation tradeoff

Automated Agentic System for Unstructured Analysis

Ming Du



Example: finding a translational registration algorithm for small, noisy fluorescence images



Algorithm	Development set	Holdout set
Brute-force error minimization	1.25	0.98
Phase correlation	5.28	5.59
OpenEvolve	0.20	0.23
ERA	0.46	0.50
CVEvolve	**0.11**	**0.12**

Du, M., Yin, X., Luo, Y., Beniwal, D., Tang, S., Sharma, H., & Cherukara, M. J. (2026). CVEvolve: Autonomous Algorithm Discovery for Unstructured Scientific Data Processing. *arXiv preprint arXiv:2605.11359*.

https://github.com/AdvancedPhotonSource/CVEvolve

Skills + General Agent for Interactive Flexible Analysis

Yi Jiang

Ptycho Skills

If you need...	See...
Data formats & required HDF5 keys	references/data_formats.md
Parameter reference & suggestions (pear wrapper params)	references/ptychox_parameters.md
Troubleshooting artifacts & failures	references/troubleshooting.md
Quality assessment & "what to change next"	references/quality_assessment.md
Physics background & key equations	references/theoretical_foundations.md
Deep API customization (Options, Schedule, constraints, losses)	references/ptychox_api_guide.md
Warm-start optimization (multi-stage refinement)	references/warm_start_guide.md
Batch reconstruction (many scans)	references/batch_reconstruction.md
X-ray template (step-scan)	templates/ptychox_xray_standard.py
X-ray template (fly-scan)	templates/ptychox_flyscan.py
Near-field template	templates/ptychox_nearfield.py
Multislice template	templates/ptychox_multislice.py
Electron (4D-STEM) template	templates/ptychox_electron_stem.py
Custom regularizer template	templates/ptychox_custom_regularizer.py
JSON schema & sample configs	examples/
Running on ALCF (Polaris/Aurora)	See "Running on ALCF" section below
What makes PtychoX different (vs pty-chi/ptyrad/phaser/foldslice)	docs/unique_features.md
PtychoX vs pty-chi (algorithm-level differences, ported bug fixes)	docs/vs_ptychi.md

Self-updating of Ptycho Skills

"Can you process a new data?"

↓

"Explore more parameters/strategies to improve image quality"

↓

"Summarize the lessons we learned and update the Ptycho Skill"

The AI era in X-ray data science is not about replacing physics and scientists with black boxes.

It is about rebuilding data analysis systems so physics, AI, and human expertise work together.

Thanks! I look forward to the discussion.

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