Why these tools?

Why these tools?

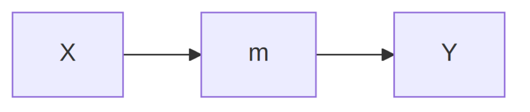
The story we are going to walk through is probably not new to most of you. Nonetheless, let's talk about it like a short story to refresh our minds.

ACKNOWLEDGEMENT: ChatGPT has been used for the preparation of these slides, everything has been reviewed and verified to the best of our capabilities. Errors and mistakes might still be present.

Complexities; Levels and Dimensions

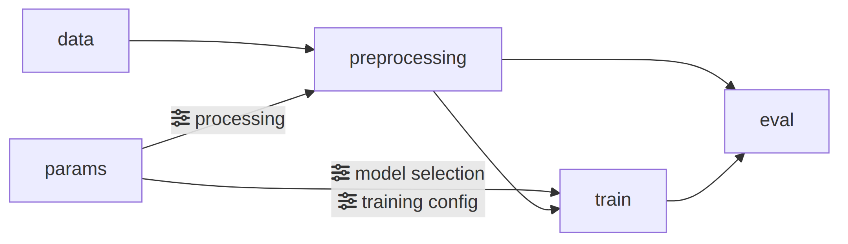
Pipeline i

We have data `X` and labels/targets `Y`. We want a model `m` that maps `X` to `Y`.



Pipeline ii

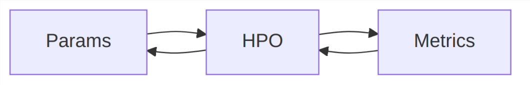
A typical pipeline looks like this:




```
X, Y = preprocessing(data, params)
model = select_model(params)
model.train(X, Y, params)
metrics = model.eval(X, Y)
```

Pipeline iii

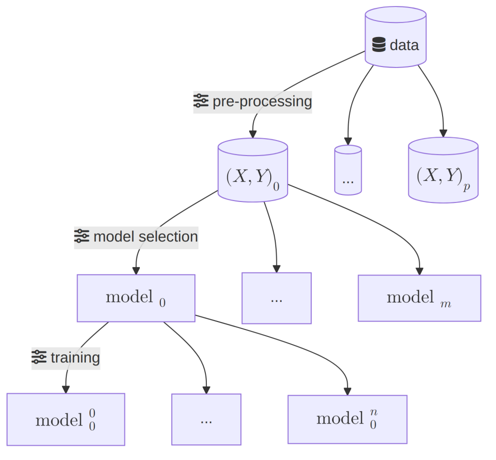
We start doing Hyper Parameter Optimization (HPO):



Neat and lovely, warm and cuddly, right?
But let's see what can get challenging.

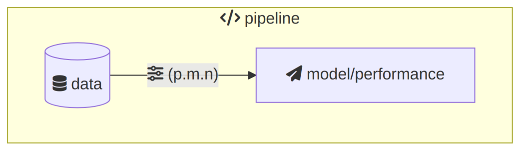
Complexity: Hyper Parameters i

Even for a simple supervised setting, we quickly branch into many variants (`p`, `m` and `n` are hyper-params for data pre-processing, models, and training respectively).



Complexity: Hyper Parameters ii

Let's simplify that to (with `p * m * n` total variations):

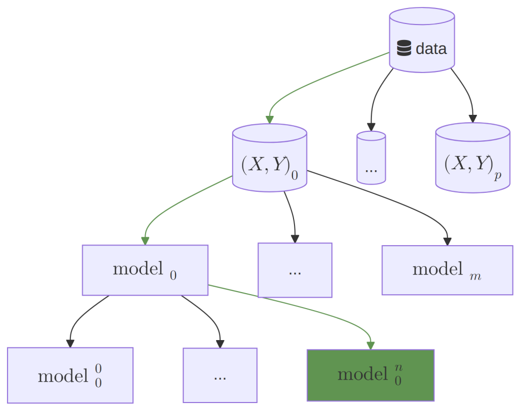


The "next Day/Week/Month" problem: auditability and reproducibility

We want to log/tag certain outputs (plots, tables, etc.) representing performance measures and params.

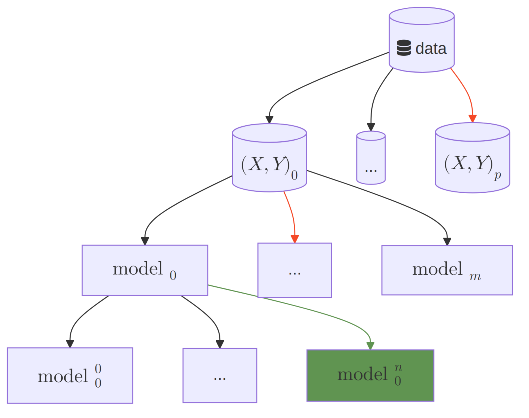
Complexity: Hyper Parameters iii

We would assume the green path produced our "tagged" results:



Complexity: Hyper Parameters iv

But how do we know we didn't make a mistake and its not actually the red ones?



Complexity: Hyper Parameters v

How do we know we got that right?

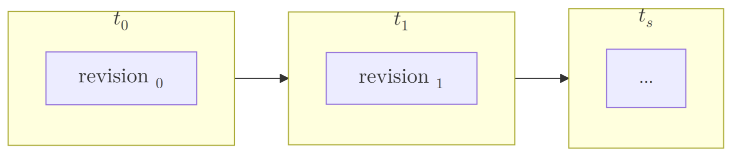
- Do we have a way to “audit” and show/prove what exact config did that result come from? Or is it implicit by the last values in the code?
- Can we **easily and reliably** trigger the whole pipeline to reproduce the same result, or did we hard code stuff?

Simple solution: all configs in a single place (**one source of truth**), and store the configs along the results.

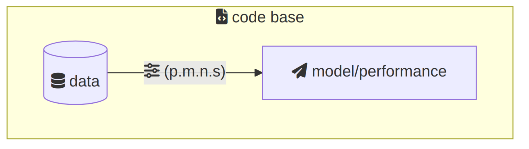
- Not easy in practice, if the run-time execution could be **non-linear** or without a proper **cache invalidation** (as is typical with jupyter notebooks).

Complexity: Implementation changes

Certain function's implementation changes that causes different results and is not explicitly noted in the configs.



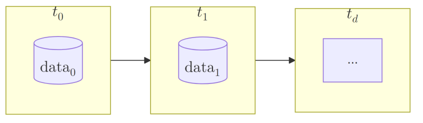
Let's update our model simplification with `s` for "source code":



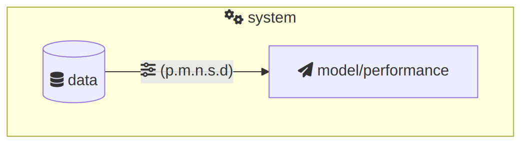
Simple solution: log the git commit hash along with the results (not bullet-proof, but can mitigate a lot of issues).

Complexity: Data can evolve over time i

Data changes over time, assumptions update, domain knowledge improve, etc. We started with `<X0, Y0>` at `[t0]`, followed by updates to `X` and `Y` over time.



Let's update our model simplification with `d` for data:



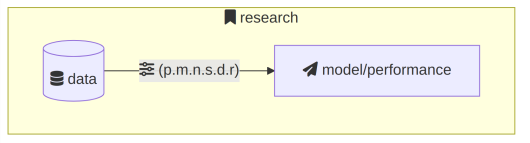
Simple solution: data versioning.

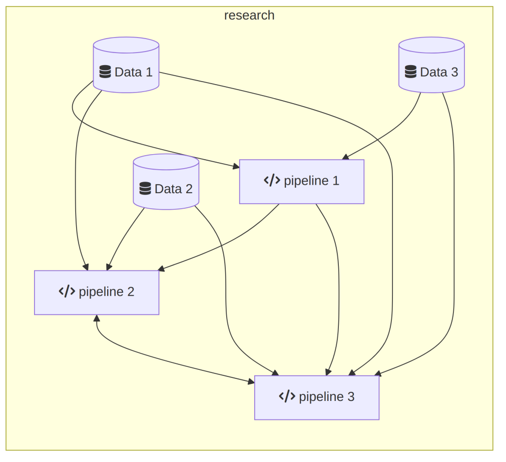
Complexity: Research and ideas i

Sometimes the bigger system is a composition of multiple different models. We'll have to maintain multiple pipelines if they are not a unified model.

- Now we have to deal with complexity at each level.

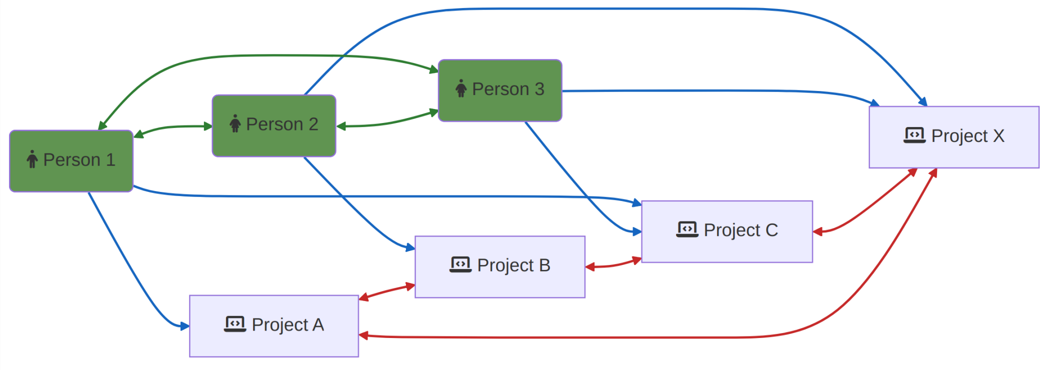
Let's update our model simplification with `r` for "research and ideas":





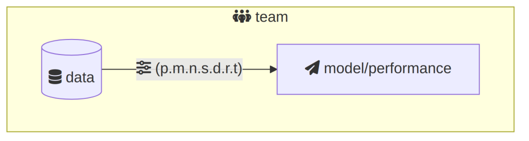
Complexity: Team work, communication, onboarding, documentation i

People moving between projects, projects influencing each other, and the cost of missing shared conventions.



Complexity: Team work, communication, onboarding, documentation ii

OK, this is getting out of hand (`t` for "team-work")!



"simple solution":

- documentation
- clean and maintainable code
- reproducible experiments
- ...

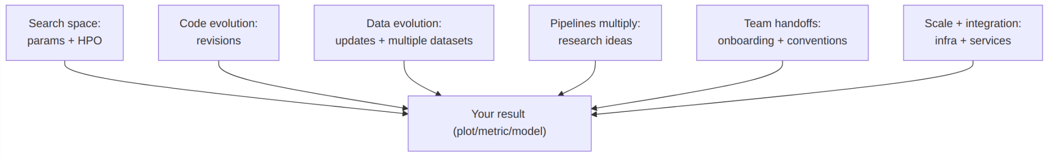
but, *we are way out of ML-specific realm, this is partly general team work and partly general software practices!*

More levels and dimensions i

The story so far was “inside the ML bubble” (params, code, data, research, team). In real projects, more dimensions show up:

- deployment
- big data
- distributed training
- heterogeneous systems
- optimization and constraints
- database and service integration
- ...

More levels and dimensions ii



These “dimensions” are present everywhere. We need a mental model that helps us recognize them early, and handle them intentionally.

No ring, but a coordinate system i

Bad news:

- There is no single way of handling every complexity. There are trade-offs.

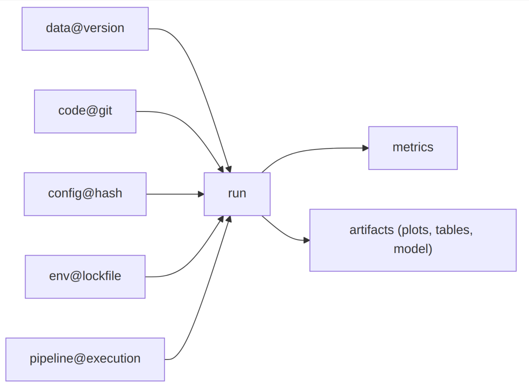
Good news:

- We almost never have to deal with all complexities at once.
- A small toolset can cover a large part of the pain, if we make "the hidden coordinates" explicit.

No ring, but a coordinate system ii

A result (a plot, a metric, a “best run”) should be locatable by a few coordinates:

- data snapshot
- code snapshot
- config/params
- environment
- pipeline execution



If we cannot point to these coordinates quickly, we do not really have a result we can defend.

Tooling and Ecosystem

Why tooling

Two questions:

- Which exact run produced this plot?
- Can you reproduce it today, on a clean machine, without manual steps?

If the honest answer is "not sure", then the problem is not the model. The problem is that the work is not *trackable*.

Tooling is how we turn:

- "I think I did this" -> "I can show exactly what I did"
- "best run somewhere on my laptop" -> "best run is findable and reproducible"
- "handoffs break" -> "handoffs are boring"

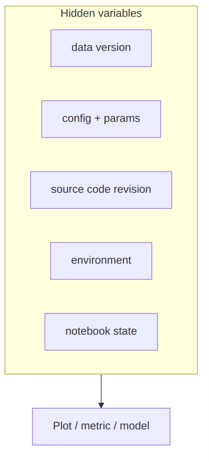
Why ML projects fail to be reproducible i

The usual culprits are not exotic. They are invisible.

- hidden data versions
- hidden configs
- invisible code changes
- notebook state and non-linear execution
- environment drift

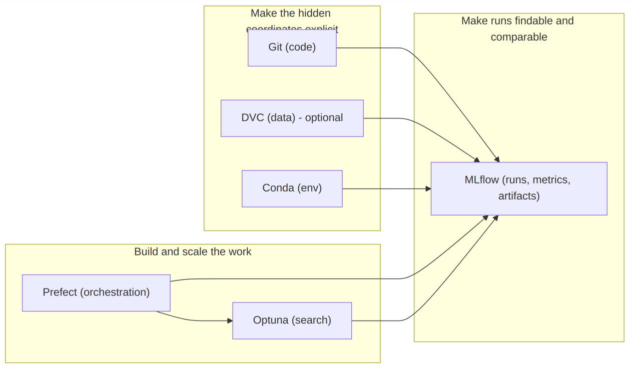
When this happens:

- "best run" cannot be found
- "best run" cannot be reproduced
- person-to-person and paper-to-paper handoffs break



Ecosystem map (pragmatic, not exhaustive) i

We do not need a giant framework. We need a small set of tools that make the hidden coordinates explicit, and keep them connected.



Ecosystem map (pragmatic, not exhaustive) ii

What each tool covers (and what it does not):

- Git: code history (not data snapshots, not runs)
- DVC (guided tour): data snapshots (not an experiment tracker)
- MLflow (guided build): runs, metrics, artifacts, provenance (not orchestration, not HPO)
- Optuna (guided build): HPO/search and study analysis (not reproducibility by itself)
- Prefect (guided tour): orchestration, retries, scheduling patterns (not tracking unless you log)

Alternatives exist in every box (see next slide).
We pick this set because it is simple, script-friendly, and covers a lot of the pain quickly.

Ecosystem: categories and what they answer (quick glance)

We can explain the tooling ecosystem via a small set of categories.
Each category answers a different question, and has a recognizable set of capabilities.

Putting it together (the short memory aid)

- Versioning answers: “Which data/code snapshot did we use?”
- Tracking answers: “Which run produced this result?”
- Optimization answers: “How did we search for better configs?”
- Orchestration answers: “How do we run this reliably and repeatedly?”

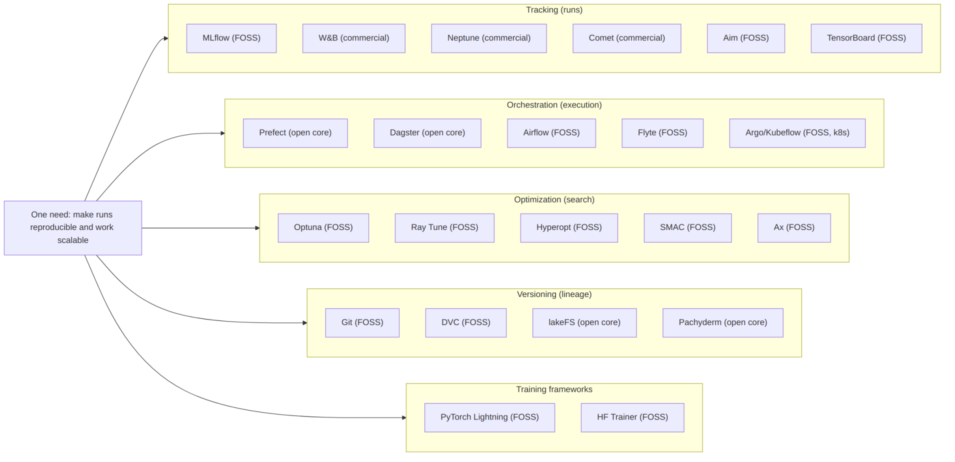
Or as a boundary

- Training frameworks help you write training loops faster.
- Trackers record what happened.
- Orchestrators make it repeatable and robust.
- Optimizers search the space.
- Versioning tools make data/code snapshots explicit.

Ecosystem: categories and what they answer - matrix (quick glance)

Category	Answers	Typical capabilities	Non-goals
Code versioning (Git)	* Which code snapshot did we use?	* history, diff, review, branching, tags * code provenance for papers and experiments	* does not version large data well * does not record “runs” or produced artifacts by itself
Data versioning and lineage (DVC, lakeFS, etc.)	* Which dataset snapshot did we use? * Which derived artifacts depend on which inputs?	* data snapshots / versions (often stored outside git) * lineage via declared deps/outs * reproducible data pipelines in terms of file dependencies * stage skip via cache and “nothing changed” detection (DVC-style)	* not a full experiment tracker UI * not a scheduler/queue/retry system (beyond simple stage execution)
Environment capture (conda/mamba, lockfiles)	* Which exact dependencies made this run work?	* pinned packages / versions * exportable environment spec (env.yml / lockfile) * reduces environment drift across machines	* does not track runs, metrics, or artifacts
Training frameworks (Lightning, HF Trainer, etc.)	* How do we write training loops faster and more consistently?	* training loop abstractions * standard callbacks, logging hooks * multi-GPU / mixed precision conveniences (depending on framework)	* not experiment tracking by itself * not orchestration by itself * not data versioning
Experiment tracking (MLflow, W&B, etc.)	* Which run produced this result? * What parameters, metrics, and artifacts did it generate?	* run records: params, metrics, tags * artifact logging: plots, tables, models, reports * comparison: search, filter, compare runs * provenance links (to code/config/data references) if you log them	* not HPO search engine (though it can integrate with one) * not orchestration/scheduling (though it can be triggered from one)
HPO optimization (Optuna, Ray Tune, etc.)	* How do we search the hyperparameter and design space systematically?	* define objective functions * search algorithms (samplers), pruning, early stopping * study analysis and visualizations * parallel trial execution (varies by tool and setup)	* does not guarantee provenance unless paired with tracking/versioning * does not replace broader evaluation surface (metrics beyond the objective)
Orchestration (Prefect, Dagster, Airflow, Argo/KFP)	* How do we run the workflow reliably and repeatedly, at scale?	* scheduling and triggers * retries, backoff, timeouts * concurrency / queues / distributed execution primitives * task caching / stage skip (orchestrator-style), idempotency patterns * observability of workflow runs (logs, states)	* not a tracker unless you log to a tracker * not a data versioning system (though it can call one)

Prominent alternatives by category (quick glance)



Prominent alternatives by category (quick glance)

Category	Tools
Tracking (runs, metrics, artifacts)	▪ MLflow (FOSS) ▪ Weights and Biases (commercial, free tier) ▪ Neptune (commercial, free tier) ▪ Comet (commercial, free tier) ▪ Aim (FOSS) ▪ TensorBoard (FOSS, strongest in TF ecosystems)
Orchestration (pipelines, retries, scheduling)	▪ Prefect (open source core) ▪ Dagster (open source core) ▪ Apache Airflow (FOSS) ▪ Flyte (FOSS) ▪ Argo Workflows / Kubeflow Pipelines (FOSS, Kubernetes-first)
Optimization (HPO, search, schedulers)	▪ Optuna (FOSS) ▪ Ray Tune (FOSS) ▪ Hyperopt (FOSS) ▪ SMAC (FOSS) ▪ Ax (FOSS) ▪ Nevergrad (FOSS)
Versioning and lineage (data, pipelines, artifacts)	▪ DVC (FOSS) ▪ lakeFS (open core) ▪ Pachyderm (open core) ▪ git-annex (FOSS)
Training loop frameworks (not tracking, not orchestration)	▪ PyTorch Lightning (FOSS) ▪ Hugging Face Trainer (FOSS) ▪ Keras/TensorFlow high-level APIs (FOSS) ▪ skorch (FOSS)

Tool comparison matrix (quick glance)

Tool	Tracking (runs)	Artifacts	Provenance (code/config/data link)	Orchestration (scheduling)	Retries	Parallelism / queues	Stage skip / caching	HPO optimization	Training framework	Versioning (code/data)	Typical deployment	License model
MLflow	X	X	X								self-host / local	FOSS
Weights and Biases	X	X	(x)					(x)			SaaS / enterprise	Commercial (free tier)
TensorBoard	(x)	(x)									local	FOSS
Prefect	(x)			X	X	X	X				self-host / cloud	Open core
Dagster	(x)		(x)	X	(x)	X	X				self-host / cloud	Open core
Airflow				X	(x)	X	(x)				self-host / managed	FOSS
Argo Workflows				X	(x)	X	(x)				Kubernetes	FOSS
Kubeflow Pipelines			(x)	X	(x)	X	(x)	(x)			Kubernetes	FOSS
Optuna						(x)		X			local / service-backed	FOSS
Ray Tune				(x)	(x)	X	(x)	X			Ray cluster	FOSS
DVC		(x)	X	(x)			X			X (data)	local / remote storage	FOSS
Git			X (code)							X (code)	everywhere	FOSS
lakeFS			X (data)				(x)			X (data)	service / storage layer	Open core
PyTorch Lightning		(x)							X		library	FOSS
Hugging Face Trainer		(x)							X		library	FOSS

Tool selection example: Experiment Tracking (quick glance)

Tool	Best at	Trade-offs	Cost / license
MLflow	run tracking, artifacts, provenance, self-host, script-friendly	UI less polished, collaboration features lighter	FOSS
W&B	UX, collaboration, dashboards, artifacts, team workflows	SaaS dependency for most users, costs for teams/scale	Commercial (free tier)
TensorBoard	training visualization (scalars/graphs), simple logging	not a full tracker, weak provenance/compare by itself	FOSS

Tool selection example: Orchestration (quick glance)

Tool	Best at	Trade-offs	Infra vibe
Prefect	pythonic workflows, quick adoption, retries, caching, scheduling	less "data-asset" centric than Dagster	light to medium
Dagster	assets/lineage, strong structure, great dev experience	steeper concepts, more opinionated	medium
Airflow	stable scheduling, huge ecosystem, classic DAG ETL	heavier, more boilerplate, not great for dynamic workflows	medium to heavy
Argo / KFP	Kubernetes-native pipelines, container-first scale	requires k8s maturity, more ops	heavy (k8s-first)

Tool selection example: HPO (quick glance)

Tool	Best at	Trade-offs	Scaling
Optuna	lightweight HPO, pruning, great ergonomics	less "cluster-native" out of the box	single-node to modest
Ray Tune	distributed tuning, large-scale parallel trials	more infra and concepts (Ray)	cluster-first

Recap

These are not “industry-only requirements”

We often assume certain tools, concerns, or discipline are irrelevant due to a false dichotomy:

“academic research” vs “industrial development”

Many of these are just ways-of-working under constraints, intended to optimize quality, throughput, and credibility. But guess where else these tricks can help?

Concern	Sounds like	In practice it also means
quality code	“product engineering”	research that survives handoffs and revision cycles
bigger data	“industry scale”	problems solvable beyond current scope
reproducibility and auditability	“regulation paperwork”	credible research claims and easier peer review
collaboration tooling	“company management”	major throughput boost (we cannot do it alone)
higher complexity and constraints	“real-world mess”	high-impact research questions become feasible
real-world metrics	“customer KPIs”	evaluation that matches the real objective
real-world integration	“business concerns”	research that can transition and live longer

Take away

None of this is new: you have seen it, suffered it, and learned to cope with it. But:

- Has it ever caused you to **limit the scope of your work**?
- Have you ever reached a point where you were **not sure about the result**?
- Have you ever had the "result" (plots) but **could not replicate** it despite your best housekeeping? (notebook / folders / Excel)

Has this complexity ever limited what you considered achievable?

One might say:

- "my data is super small, I do not care about challenges of bigger data"
- "I am a researcher, I do not care about deployment and delivering a service"
- "in academia knowledge (paper) is our output and not product (code), so code quality doesn't matter"

One should consider

- We live in the world we define and build
- those boundaries are blurrier than we think
- many practices are just to help us work better, not specific to academia or industry

So: **let's stop letting hidden complexity silently define our boundaries.**

And Remember:

- **If we cannot locate the run, we cannot build on it.**
- **Make work locatable, then make progress faster.**