Université Grenoble Alpes

Inria

PhD Thesis Defence Presentation

High Performance Online Deep Neural Network Training from Synthetic Data with Active Learning

by **Sofya DYMCHENKO**

April 21, 2026 — Université Grenoble Alpes & INRIA

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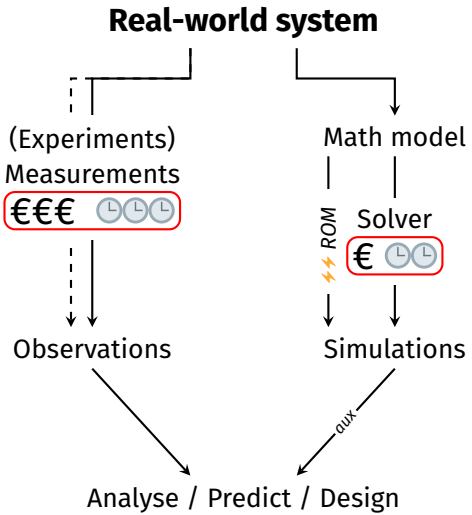
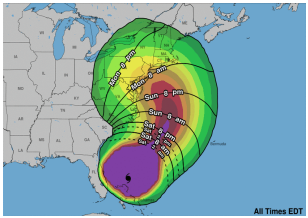
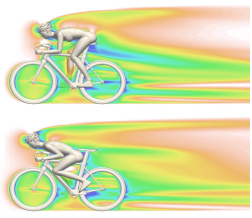
Thesis Director:	**Bruno RAFFIN**, Univ. Grenoble Alpes & INRIA

Scientific computing: simulate real-world







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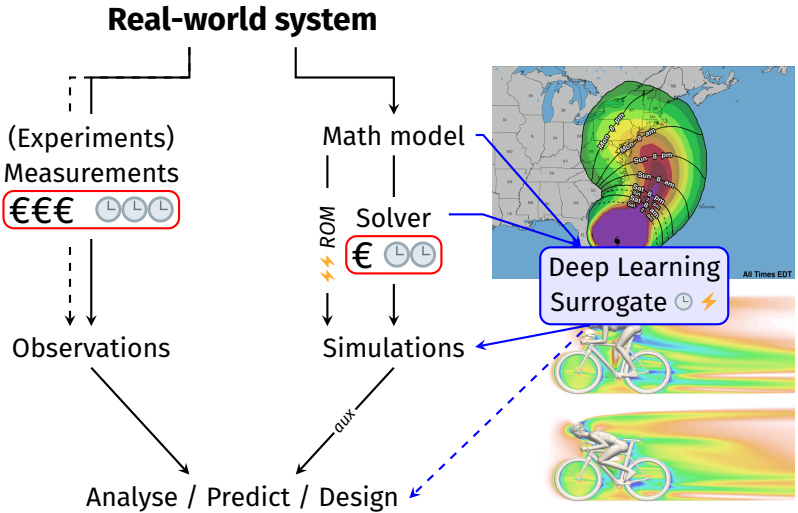
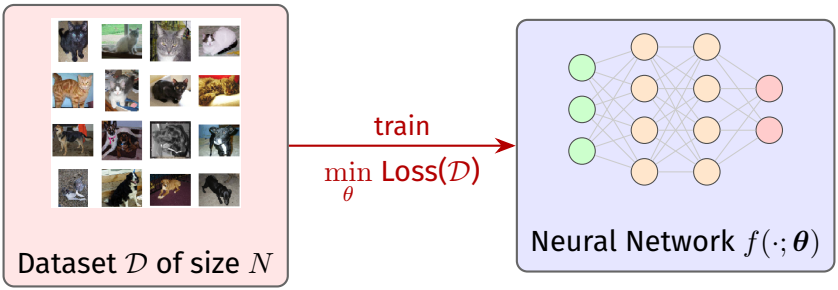
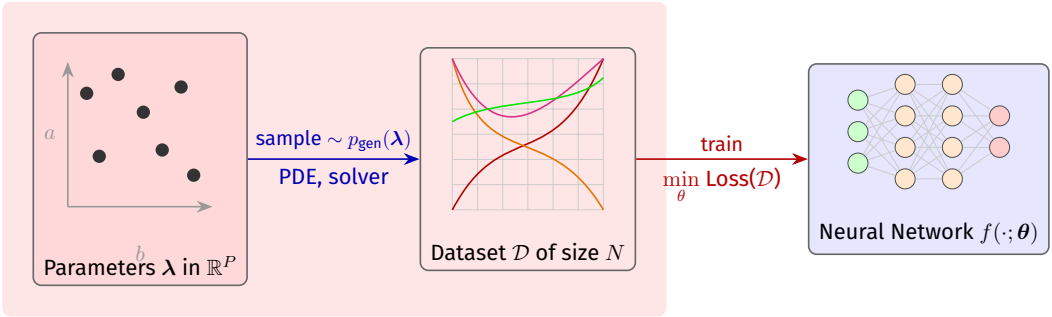


Deep learning training: observational data



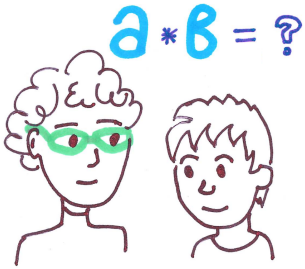
Deep learning training: synthetic data



💡 Which data to create to train well?

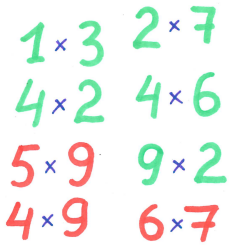
Analogy: active learning

Exam: multiplication for $a, b \in \{1, 2, ..., 20\}$



📝 Choose a and b?

Passive: no prior information, sample many uniform a and b



😐 Redundant exercises

Active: acquire information, prepare relevant a and b

💯 Only useful practice

Active learning (AL) for deep learning

(Settles, 2009)

Given set of data without labels

select

Pool-based AL

Train NN

Label data

CAT

Continuous parameter space Λ

sample

Discrete set

select

Pool-based AL

Train NN

Create data

sample

Query-synthesis AL

🤔 How to apply query-synthesis AL for surrogate training?

C1: *Breed* method

Query-synthesis active learning for NN training

Dynamical system example: a rolling ball on the surface

Parameter: initial position $x \in X \subset \mathbb{R}^D$

Black-box oracle $\mathcal{O}$ output:

$$x \xrightarrow{x^{(i+1)}=x^{(i)}-\eta\nabla f(x^{(i)})} x^{\min} \in \{x^A, x^B\}$$

NN predicts $f_\theta(x) \approx \mathcal{O}(x)$ for any $x \in X$

Loss: $\mathbb{E}_{\mathcal{D}}\left[\ell(f_\theta(x_i) - x_i^{\min})\right] \xrightarrow{\theta} 0$

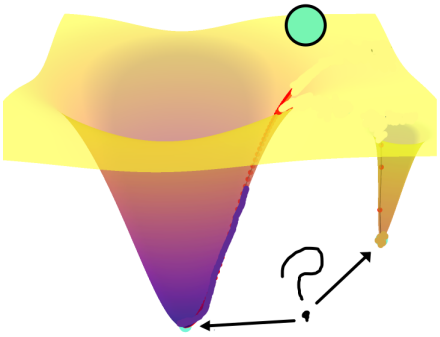
Training data:

(0) Choose prior $p_{\text{gen}}(X)$

(1) Sample $\mathcal{P} = \{x_i \sim p_{\text{gen}}(X)\}_{i=1}^N$

(2) Create $\mathcal{D} = \{(x_i, \mathcal{O}(x_i) = x_i^{\min}) \mid x_i \in \mathcal{P}\}_{i=1}^N$

What samples are useful and not?



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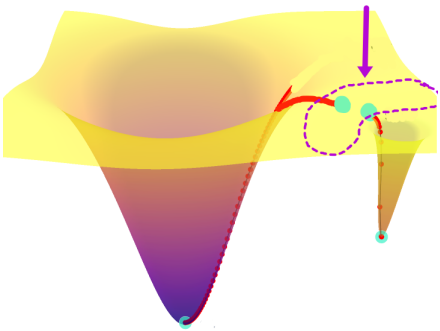


What samples are useful and not?

💡 Uncertain = useful!

🤔 How to get $p_{\text{gen}} \sim p(\text{uncertainty})$

Challenges and inspired solutions

Estimation:

No closed form for uncertainty, can't sample from it
↪ approximate with a weighted density estimator

Uncertainty estimates are costly (Nabian et al., 2021)
↪ cheaper proxy NN loss

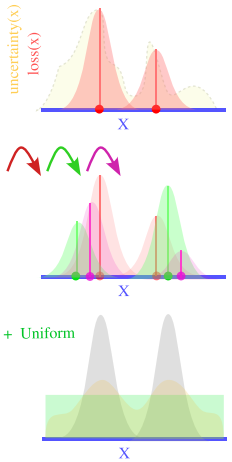
Adaptation:

NN evolves, can't fix $p_{\text{gen}}(x)$
↪ update training data in rounds

Sudden data distribution shift, NN destabilisation (Cappé et al., 2004)
↪ generate new samples close to previous

Regularisation:

Overfitting, closed loop, mode collapse (Sutton and Barto, 2018)
↪ mix with uniform distribution to explore



(these ideas intersect with: population Monte-Carlo, reinforcement learning exploration-exploitation trade-off, inference, and more)

(Dymchenko and Raffin, 2023)

Breed: progressively populate high-error regions

Initialise dataset $\mathcal{S} = \{N \text{ samples } \sim \mathrm{Unif}(X)\}$

1. Train NN for p iterations on $\mathcal{S}$
2. Compute loss l_i for each sample $x_i \in \mathcal{S}$
3. Build proposal $\mathrm{GM}(x) \propto \sum_1^N l_i \cdot \mathcal{N}(x_i; \sigma\mathbb{I})$
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5. Sample $N_c = \alpha \cdot N$ concentrated samples:

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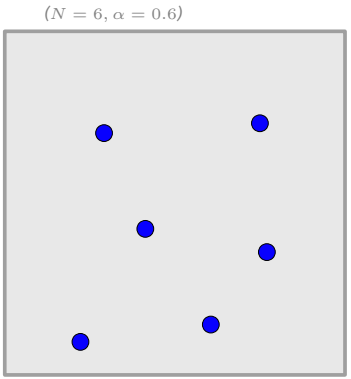

p: adaptivity control (fixed)
σ: diversity control (fixed)
α: mixing control, linearly increasing:
$\alpha = \max(\alpha_1 \cdot i + \alpha_0, \alpha_{\max}) \in [0, 1]$

(curriculum learning: from exploration to exploitation)

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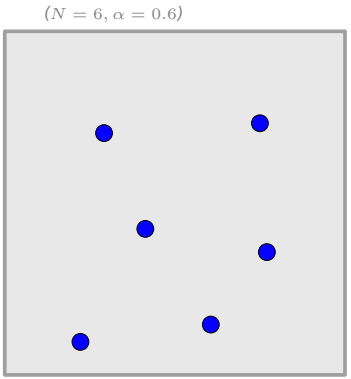

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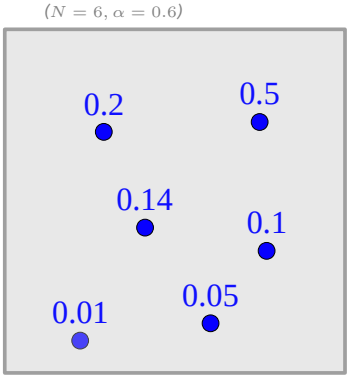

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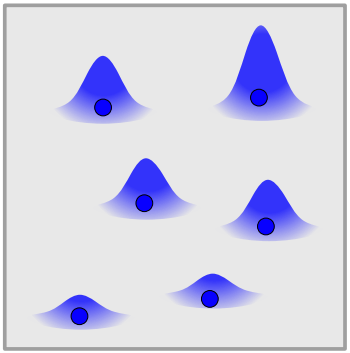

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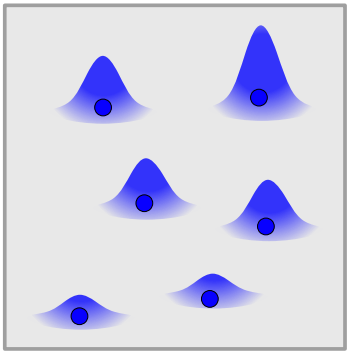

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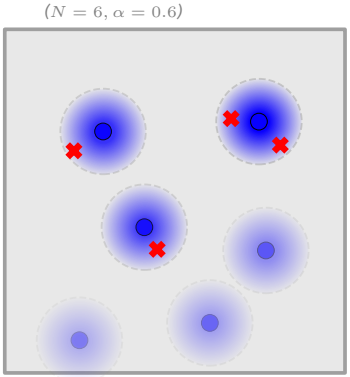

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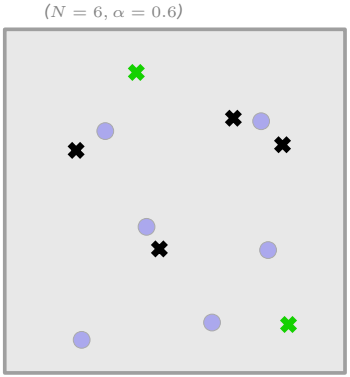

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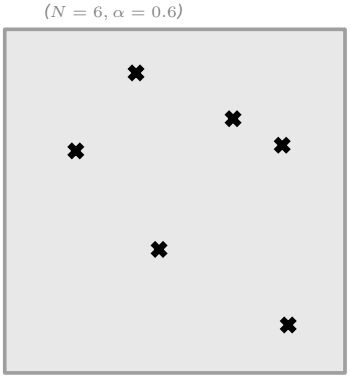

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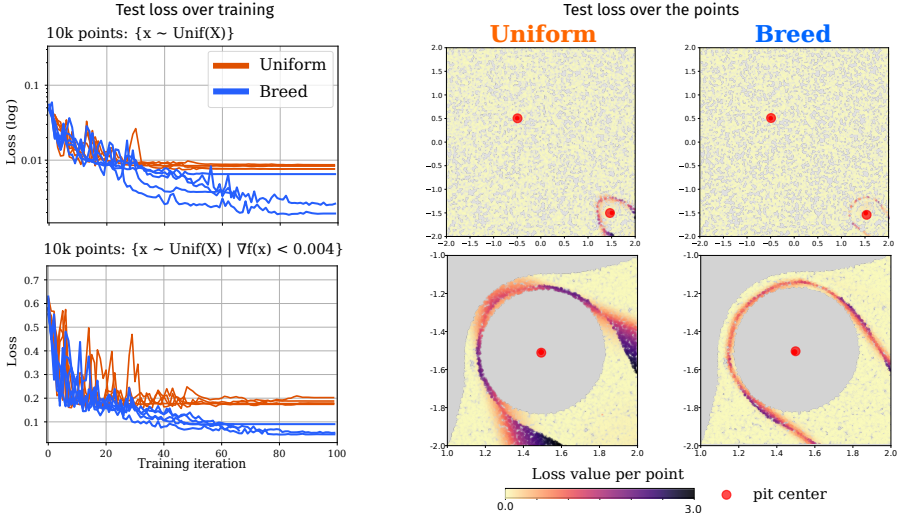
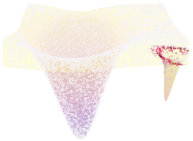
Toy benchmark results: two validation sets





(Raissi et al., 2017)

Physics-Informed NNs: learn from governing equations

Idea: use a mathematical model for training

System example: *1D Allen-Cahn equation*

$$F[u](x,t) = u_t - 0.0001u_{xx} + 5u^3 - 5u = 0$$

(reaction-diffusion, sharp gradients) for $(\boldsymbol{x}, t) \in \Omega \subset \mathbb{R}^2$

NN approximates unknown solution:

$$u_\theta(\boldsymbol{x}, t) \approx u(\boldsymbol{x}, t) \text{ over } \Omega$$

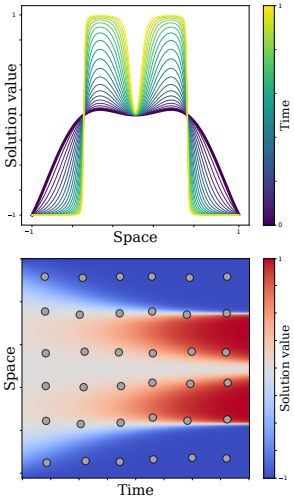
Constraint: *(generally, can include initial/boundary conditions)*

u_θ satisfies system F across the domain

Imposing constraint:

Collocation points: $\mathcal{S} = \{(\boldsymbol{x}_i, t_i) \sim p_{\text{gen}}(\Omega)\}_{i=1}^N$

Residual loss: $\frac{1}{N}\sum_{i=1}^N F[u_\theta](\boldsymbol{x}_i, t_i) \overset{\boldsymbol{\theta}}{\to} 0$



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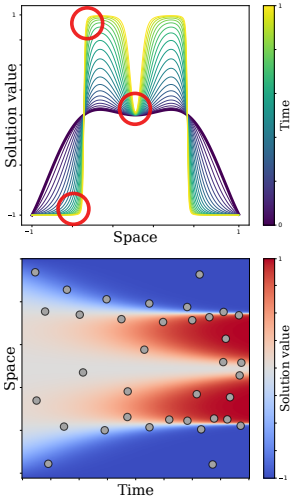


Data-driven surrogates: generation bottleneck (Kovachki et al., 2021)

Idea: use simulation data, reuse DL methodology

↪ create ground-truth data with solver

Solver S_λ for system $F[u](\boldsymbol{x}, t; \boldsymbol{\lambda})$

Solution state is discretised spatially:

$$u(\boldsymbol{x}, t; \boldsymbol{\lambda}) \overset{h}{=} \boldsymbol{X}_\lambda^{(t)} \in \mathbb{R}^{N_x^D}$$

Trajectory of solution states $t \to t + \Delta t$:

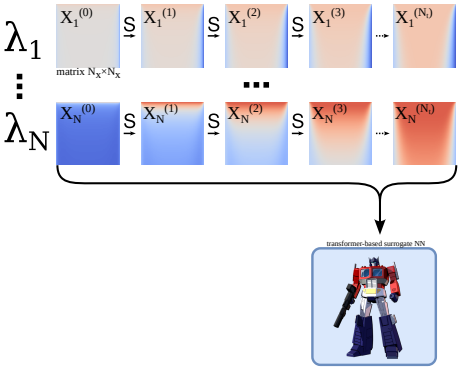
$$S_\lambda(\boldsymbol{X}_\lambda^{(i)}) = \boldsymbol{X}_\lambda^{(i+1)} \text{ for } i = 0, \ldots, N_t$$

Simulation data:

↪ many $\boldsymbol{\lambda}_i \in \Lambda \subseteq \mathbb{R}^P$

↪ large series of meshes

↪ computationally expensive



Every data sample comes at a **large cost**!

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$$S_\lambda(\boldsymbol{X}_\lambda^{(i)}) = \boldsymbol{X}_\lambda^{(i+1)} \text{ for } i = 0, \ldots, N_t$$

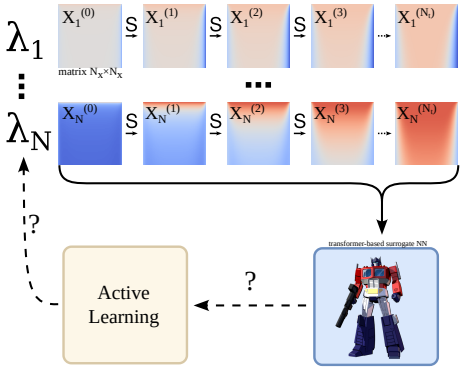
Simulation data:

↪ many $\boldsymbol{\lambda}_i \in \Lambda \subseteq \mathbb{R}^P$

↪ large series of meshes

↪ computationally expensive

Every data sample comes at a **large cost**!



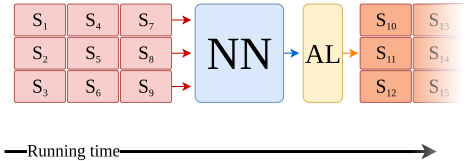
🤔⚡ How to make every solver call $S_{\boldsymbol{\lambda}_i}$ count?

C2: Online active learning

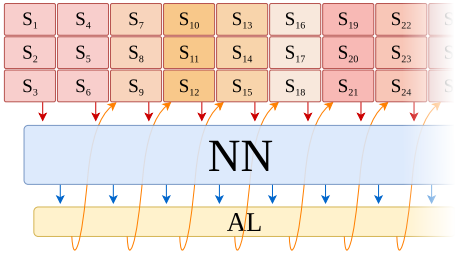
Active sampling mechanism in Melissa and online Breed

Offline rounds vs. online continuous integration

Instead of proceeding in rounds...



...everything runs simultaneously?



🔀🔄 Continuous feedback loop ⇒ increase impact of each solver run

🤔 How to achieve this?

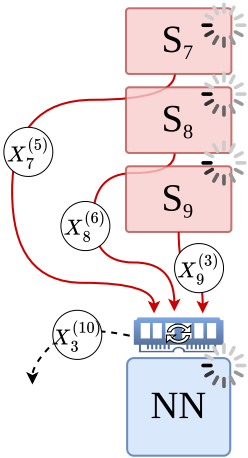
Online training: setting

(Schouler et al., 2023)

MELISSA framework: online surrogate training

- Asynchronous parallel:
  K concurrent solvers clients and training server
- Avoids storage:
  produced states $\boldsymbol{X}_{\lambda_j}^{(t)}$ are sent directly to a fixed capacity memory buffer $\mathcal{B}$
- Avoids idle resources:
  training is on while $\mathcal{B} \neq \emptyset$, solvers are on while $\mathcal{B}$ contains "seen" samples

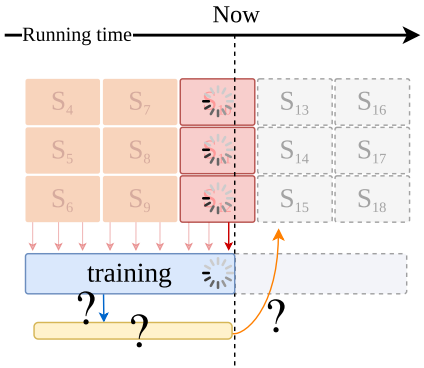
🤔🔄 How to implement an infrastructure for active learning?



Online training: challenges

Goal for AL process:

- no experiment walltime overheads
- low latency between feedback and data exposure



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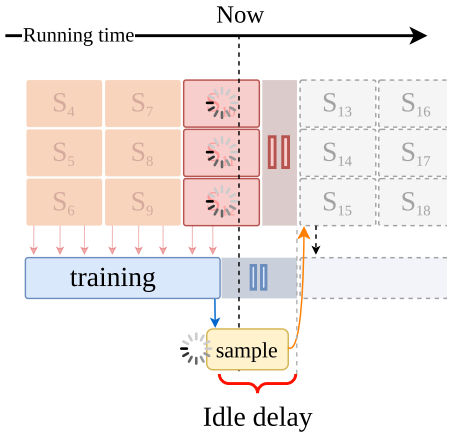

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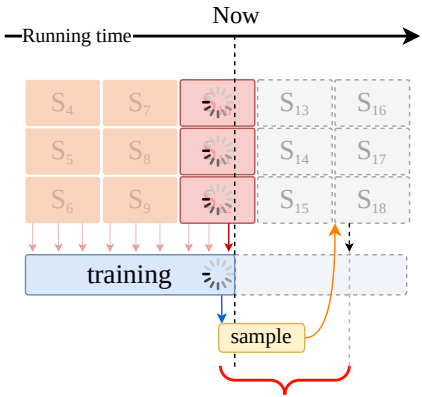


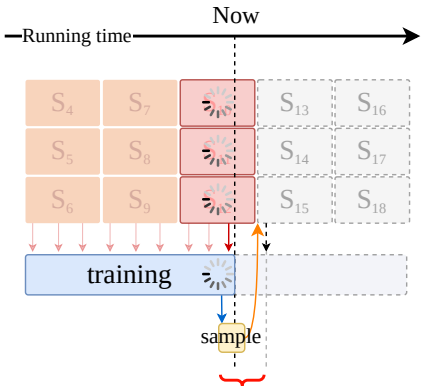
Online training: challenges

Goal for AL process:

- no experiment walltime overheads
- low latency between feedback and data exposure

NEW Implemented active sampling mechanism in Melissa!

Separate server rank, optimised to continuously:
- receive AL information from training process
- update solver parameters for immediate next clients



(Dymchenko et al., 2024)

Breed online: moving population aggregated historical losses

Obstacle: No set of all past samples, no additional loss scoring allowed

Adaptations:

↪ $\mathcal{Q}$ population of M parameters linked to the most-recently-seen training samples
↪ l_{jti}: use already computed loss from training iterations
↪ ∂l_{jti}: normalise by batch statistics and threshold harder samples
↪ ∂l_j: aggregate over trajectory and training steps

$$l_{jti} = \ell(\boldsymbol{X}_{\lambda_j}^{(t)}; \boldsymbol{\theta}_i), \quad m_i = \underset{\boldsymbol{X} \in \text{batch}}{\text{mean}}\ \ell(\boldsymbol{X}; \boldsymbol{\theta}_i), \quad s_i = \underset{\boldsymbol{X} \in \text{batch}}{\text{deviation}}\ \ell(\boldsymbol{X}; \boldsymbol{\theta}_i)$$

$$\partial l_{jti} = \max\left(\frac{l_{jti} - m_i}{s_i}, 0\right), \quad \partial l_j = \underset{t,i}{\text{mean}}\ \partial l_{jti}, \quad \text{GM}(\boldsymbol{\lambda}) \propto \sum_{\lambda_j \in \mathcal{Q}} \partial l_j \cdot \mathcal{N}(\boldsymbol{\lambda}_j; \sigma \mathbb{I}_P)$$

✅ Up-to-date proposal focused on samples with above-average loss over trajectory exhibited during training

Experiments: 1D PDEs of different difficulty and dynamics (using APEBench)

(Koehler et al., 2024)

(we combine in total 10 cases with fixed a_i, b, including conservative KS with $(u^2)_x$)

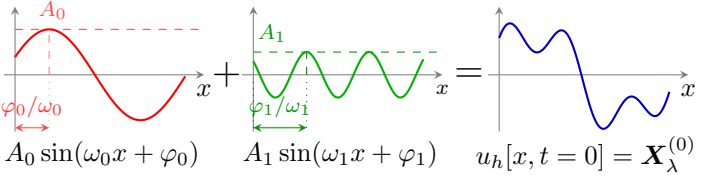
Nonlinear *Kortweg-de Vries* (KdV)

$$u_t = a_3 u_{xxx} - a_4 u_{xxxx} - 0.5b(u^2)_x$$

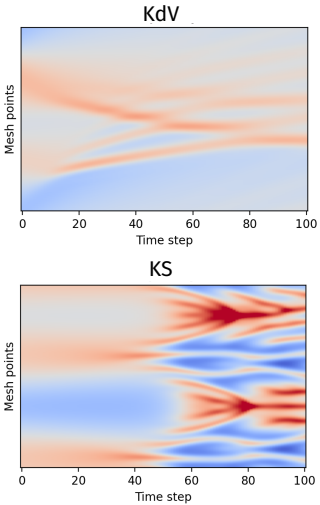
Chaotic *Kuramoto-Sivashinsky* (KS)

$$u_t = -a_2 u_{xx} - a_4 u_{xxxx} - 0.5b(u_x)^2$$

Initial condition: waves superposition

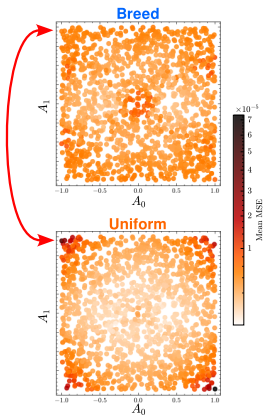


AL: curate initial state – parameters $\boldsymbol{\lambda} = (A_0, A_1, \varphi_0, \varphi_1)$

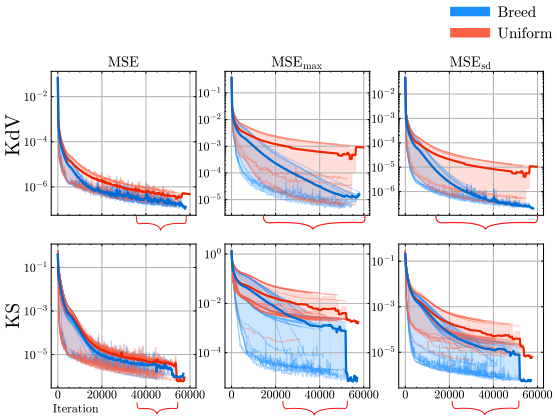


Experiments: results *(not published work)*

Test loss over A_0, A_1



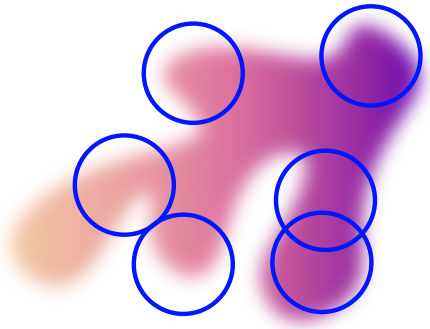
Test loss over training (9 seeds)



⚡🏆 More reliable performance with fewer data ⇒ lower cost!

Limitation of Breed

- **Local**:
  proposal is anchored to visited samples
  $\hookrightarrow$ no global view
- **Rigid**:
  fixed isotropic Gaussian kernels
  $\hookrightarrow$ blind to local geometry
- **Statistically poor**:
  degrades as $D = \dim(\Lambda)$ grows;
  full-covariance requires $O(D^3)$
  $\hookrightarrow$ not scalable



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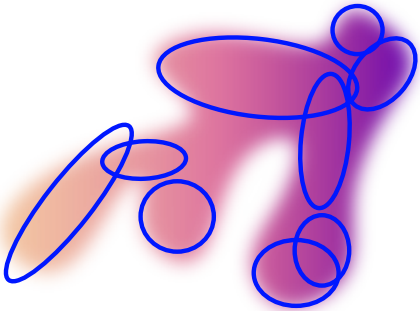

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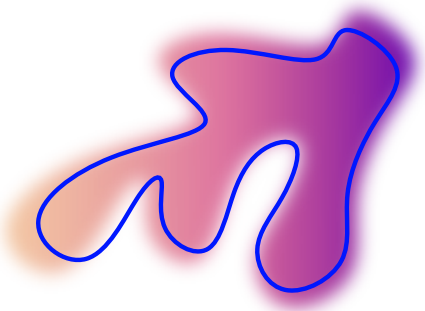


🧠🤔 How can we approximate it better?

C3: *OGAS* method

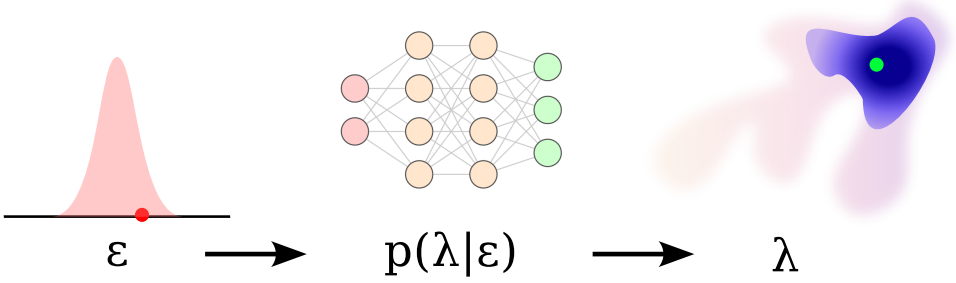
Generative AL for high-dimensional parameter spaces

Neural proposal: learn where to sample

Define: $\varepsilon \propto$ expected error level

Train: a conditional generative NN $\hat{p}(\boldsymbol{\lambda}|\varepsilon)$ on pairs $(\boldsymbol{\lambda}, \ell_{jti})$

Proposal: sample desired ε, obtain $\boldsymbol{\lambda}$ from generator



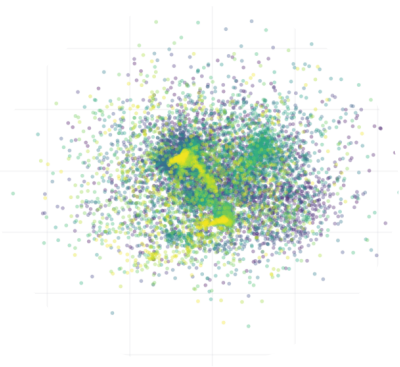
OGAS: Online Generative Active Sampling *(under review for ICML'26)*

Generator:
fast MLP-based conditional diffusion model (Ho et al., 2020)

Training:
ε is a z-standardised $\ell(\boldsymbol{X}_j^{(t)}; \boldsymbol{\theta}_i)$ with moving statistics
pairs $(\boldsymbol{\lambda}, \varepsilon)$ sent to a FIFO buffer for generator training
objective is corrected with importance weights

New parameters:
proportional prior over ε to focus on harder data
mix with $\mathrm{Unif}(\Lambda)$ to ensure exploration

Evaluation:
three 2D PDEs, three surrogate architectures
AL: curate IC and PDE parameters with $\dim(\Lambda) \leq 308$



Experiments: example results

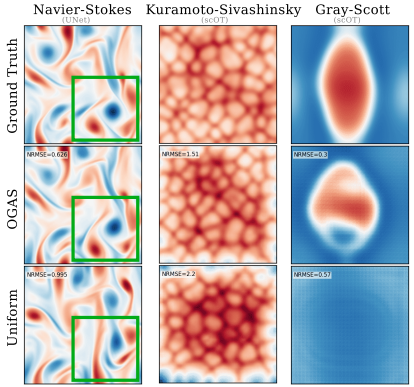
FNO (28M parameters) on Kuramoto-Sivashinsky PDE

Strategy	Mean ($\times 10^{-3}$)	Std ($\times 10^{-3}$)	Max ($\times 10^{-2}$)
OGAS-L	9.49 ± 0.28	1.76 ± 0.06	3.26 ± 0.18
Breed	11.32 ± 0.35	2.53 ± 0.41	5.02 ± 0.58
SBAL	9.26 ± 0.36	3.23 ± 0.42	3.34 ± 0.11
Uniform	8.30 ± 0.32	4.02 ± 0.16	5.95 ± 0.12

scOT (180M parameters) on Navier-Stokes PDE

Strategy	Mean ($\times 10^{-2}$)	Std ($\times 10^{-3}$)	Max ($\times 10^{-2}$)
OGAS-L	1.72 ± 0.19	4.42 ± 0.23	5.45 ± 0.34
Breed	2.15 ± 0.21	7.96 ± 1.07	10.10 ± 1.44
SBAL	1.82 ± 0.18	6.30 ± 0.29	8.32 ± 0.34
Uniform	1.91 ± 0.22	6.54 ± 0.47	8.83 ± 0.99

Overhead delay:
0.2% for OGAS, 0.7% for Breed, 10% for SBAL

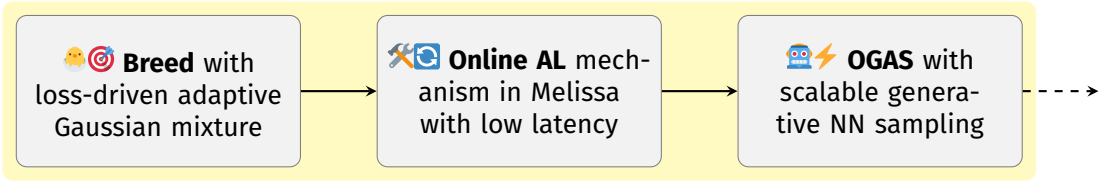


⚡🏆 Minimal delays, robustness for tail-metrics, mean improvement for capable models

Conclusion

Main takeaways

RQ: How to improve training of deep learning surrogates with QSAL?



- ⚙️ Improved training data – not surrogate's NN architectures
- 🚀 Effective navigation of parameters space – reduced data cost
- 📈 AL gains scale with model capacity – the better the model, the more AL helps
- ♾️ Continuous online feedback – each solver call is maximally exploited

What is next?

Short-term for online QSAL in deeper surrogate training:

- **Foundation models:** (McCabe et al., 2025)
  - require huge amount of data for pretraining (Ashton et al., 2025)
  - choosing PDEs and ICs, heterogeneous parameters, ...
- **Geometry-aware AL**: beyond regular grids, choosing geometries or points... (Alkin et al., 2025)
- **Connecting to related frameworks:**
  Simulation-Based Inference (Cranmer et al., 2022), Reinforcement Learning (Rolnick et al., 2019)

Open question:

⚖️ At what point does **learning how to learn become harder than learning itself**?

🌱🌍 Finding the efficient path itself comes at a cost...
...≈**4 tons** CO_2eq emitted along the way of this thesis.

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