From Physics-Informed AI to National Impact: Hybrid Approaches for Science, Security, and Energy

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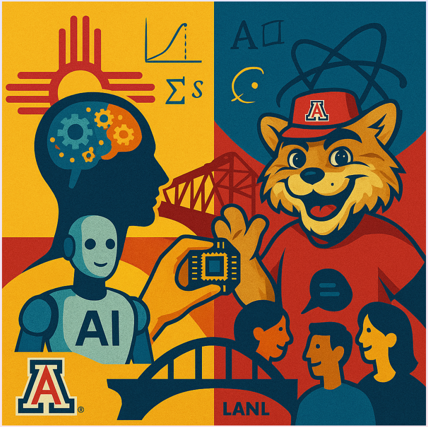
Applied Math @ UArizona



Invitation to Collaborate

During my possible mini-sabbatical at LANL, I invite collaboration on a set of projects under the theme:

Physics-informed, Hybrid AI, and Mathematics for Engineering and Sciences (PHAMES)

PHAMES aims to unite applied math, physics-based modeling, engineering, and social sciences to build a robust AI infrastructure – positioning the team as a leader in responsible, high-impact research for national security, energy, and societal resilience.

AI – Elephant in the Room

- **Dream** New AI Models
- Explain the Models

- **Grow** the Models from – Stochastic Calculus, Optimal Control, Non-Equil Stat Mech

Worth Climbing the Beanstalk

From Ugly (?) Duck to Swan

AI – Elephant in the Room

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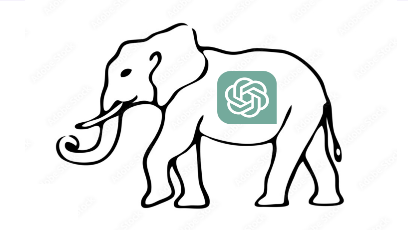
From Ugly (?) Duck to Swan

Artificial Intelligence ⊂ Applied Math

Applied Math '21

- **Traditional Applied Math:** Driven by sciences & engineering
- **Contemporary Applied Math:** Foundations and frontiers in AI
- **Synthesis:** Integration of Traditional and Contemporary Approaches



Upcoming Example of Advancing AI ⊂ Applied Math

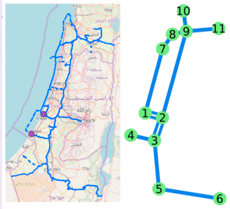
- Sampling Decisions = Synthesis of **Generative AI** tools
  - **Diffusion Models** (Stochastic ODEs, Optimal Contol)
  - **Transformers** (Tokens + Auto-Regression)
  - **Reinforcement Learning** (Markov Decision Processes)

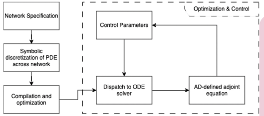
Instead of Introduction: Subjective = Personal Reflection on

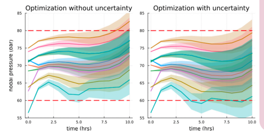
- How Does Applied Math Enable AI? – AM → AI
- How Do We Use AI in Sciences & Engineering (Applications)? – AI → AM
- MC, *Mixing artificial and natural intelligence: from statistical mechanics to AI and back to turbulence*, Topical Review in J. Phys. A: Math. Theor. 57, 33 (333001), 2024

- Automatic Differentiation (AD):
  - Computes derivatives efficiently using elementary operations and the chain rule.
  - Major engine behind efficient optimization (billions of parameters) critical for “everything" AI
- Deep Learning:
- Reinforcement Learning (RL):
- Generative Models:

- Automatic Differentiation (AD):







- Focus on rare interruptions - multi-scenario optimization under uncertainty + sensitivity analysis
- Progress: **Augmenting AD with Symbolic Differentiation**
- Neural Network Free/minimal

- Academy & Industry (NOGA - energy system operator of Israel) Collaboration: Model Reduction & open-source via Julia
- Pipe Line Simulation Interest Group - best student award C. Hyett, et al, arXiv:2304.01955, 2310.18507, 2311.08686

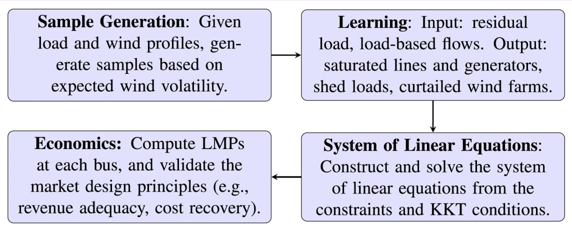
- Deep Learning:
- Reinforcement Learning (RL):
- Generative Models:

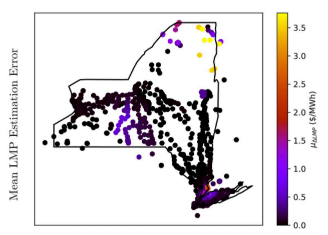
- Automatic Differentiation (AD):
- Deep Learning:
  - Represents functions through many-layered (deep), parameterized nonlinear transformations, expressed via Neural Networks (NN).
  - Employs Automatic Differentiation for optimizing NNs.
- Reinforcement Learning (RL):
- Generative Models:

- Automatic Differentiation (AD):
- Deep Learning:

Physics-Informed Machine Learning for Electricity Market

- R. Ferrando, et al, IEEE Transactions on Energy Markets, 2/1 (2024), DOI: 10.1109/TEMPR.2023.3318197



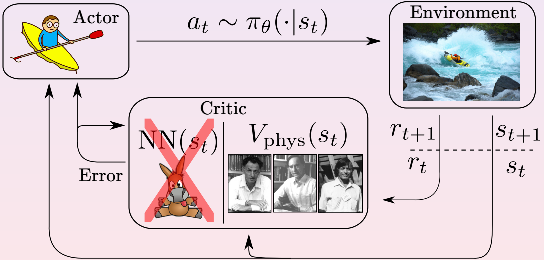


- Identify least understood bottleneck (stressed power lines)
  - Reinforcement Learning (RL):
  - Generative Models:
- Utilize Deep Learning to resolve the bottleneck

- Automatic Differentiation (AD):
- Deep Learning:
- Reinforcement Learning (RL):
    - A data-driven approach to optimal control under uncertainty using Deep Learning to predict and control actions.
    - Adaptive/dynamic approach – reinforces decisions based on the information, e.g. reward, received in the process of learning/exploration, to get better inference/exploitation.
- Generative Models:

- Automatic Differentiation (AD):
- Deep Learning:
- Reinforcement Learning (RL):

Physics-Guided Actor-Critic Reinforcement Learning for Swimming in Turbulence



- identify least understood bottleneck (weak NN critic)
- utilize Theory (Stochastic Hydrodynamics) to fix it
- C. Koh, L. Pagnier, MC, Phys. Rev. Research 7, 013121 (2025), 10.1103/PhysRevResearch.7.013121

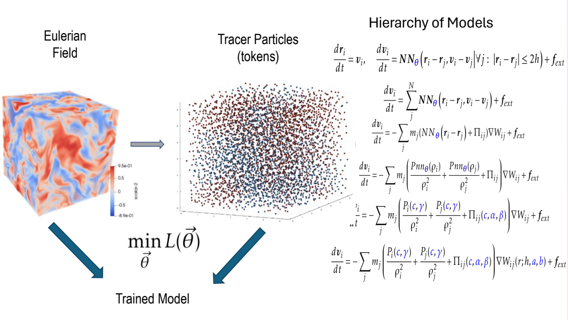
- Generative Models:

- Automatic Differentiation (AD):
- Deep Learning:
- Reinforcement Learning (RL):
- Generative Models:
  - Outputs new data from existing (ground truth) data. The new data may be statistically similar to the ground truth (e.g., diffusion) or comes in response to prompts (e.g., transformers).
  - Leverages Deep Learning to generate synthetic data and elements of optimal control/Reinforcement Learning, in achieving optimality

GPT-4 prompt: Show UArizona bobcat swimming butterfly style in a turbulent river.

- Automatic Differentiation (AD):
- Deep Learning:
- Reinforcement Learning (RL):
- Generative Models:

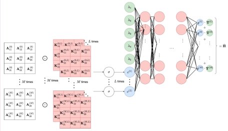
Neural Smooth Particle Hydrodynamics = Tokens in Turbulence



- quasi-particles = tokens
- "physical" attentions via particles & fields
- Lagrangian Large Eddy Simulations = New Reduced Order Model of Turbulence – M. Woodward, et al, 10.1103/PhysRevFluids.8.054602 & Y. Tian, et al, 10.1073/pnas.2213638120

- Automatic Differentiation (AD):
- Deep Learning:
- Reinforcement Learning (RL):
- Generative Models:

Lagrangian Attention Tensor NN – Auto-Regression in Turbulence



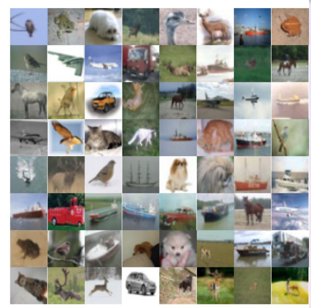
$\hat{\boldsymbol{H}} = \sum_{n=1}^{10} g_\theta^{(n)}(\lambda_1, \ldots, \lambda_5, c^{(1)}, \ldots, c^{(L)}) \boldsymbol{T}^{(n)}$

$c^{(\ell)}\left(\boldsymbol{A}^{(0)}, \cdots, \boldsymbol{A}^{(M)}\right) = \sigma\left(K_{ij}^{(m,\ell)} A_{ij}^{(m)}\right)$

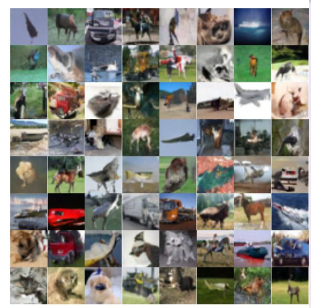
Neural Representation of the Pressure Hessian, $\hat{\boldsymbol{H}}$, via the Velocity Gradient, $\boldsymbol{A}$, along Lagrangian Trajectories. The tensor basis $\{\boldsymbol{T}^{(n)}\}_{n=1}^{10}$ is according to Pope (1975).

- Physics-informed, Neural Stochastic ODE model for the Velocity Gradient Tensor in Turbulence
- LATN generalizes the Tensor Basis Neural Network (TBNN) by incorporating temporal memory through **auto-regressive**, convolutional – **attention-like** – structures that encode Lagrangian history
- LATN: *Improving Velocity Gradient Statistical Topology using Parameterized Lagrangian Attention Tensor Networks* – C. Hyett, et al, arxiv:2502.07078
- TBNN: *Physics-informed machine learning of the Lagrangian dynamics of velocity gradient tensor* – Y. Tian, D. Livescu, MC, Phys Rev Fluids (2021)

Stat Phys ⇒ AI: Score-Based Diffusion



Train on Ensemble of Samples



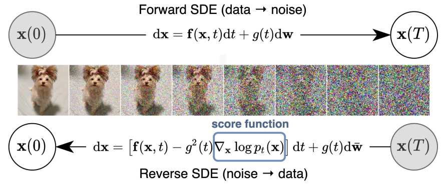
Generate Synthetic Samples

Generate Synthetic Samples which are i.i.d. from a target probability distribution, $p_{\text{target}}(\cdot)$, represented

- implicitly via Ground Truth samples
- or explicitly via energy function, $p_{\text{target}}(\cdot) \propto \exp(-E(\boldsymbol{x}))$

Diffusion Models = Non-Autonomous Stochastic ODE

Score Based Diffusion (SBD)



- Reverse-Time Diffusion [1,2]
- Reference (vague) to Stat. Thermodynamics [2]

- Continuous time SBD – state-of-the-art in GenAI [4]

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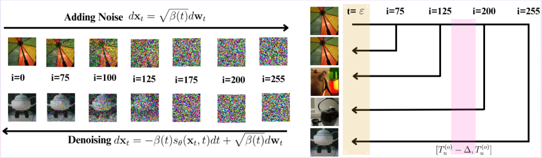
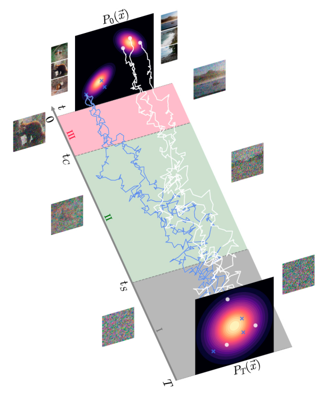
[1] B. Anderson, Reverse-time diffusion equation models, 1982
[2] H. Fölmer, Time Reversal on Wiener Spaces, 1986
[3] J. Sohl-Dickstein, et al, Deep Unsupervised Learning using Nonequilibrium Thermodynamics, 2015
[4] Y. Song, et.al., Score-Based Generative Modeling through Stochastic Differential Equations, 2021

Dynamic Phase Transitions in Score Based Diffusion





- When to U-turn? – Memorization/Collapse Transition [1,2]
- Spontaneous Choice of the Specie/Class – Speciation Transition [2]

[1] H. Behjoo, MC, U-turn Diffusion, 2023 (published in Entropy, 2025)

[2] G. Biroli, et al, Dynamical Regimes of Diffusion Models, 2024

Score Based Diffusion & Stochastic Optimal Control

Score Based Diffusion as "Integrable" Stochastic Optimal Control

$$\min_{\boldsymbol{u}(0\to 1;\boldsymbol{x}(0\to 1))} \mathbb{E}\left[\int_0^1 dt \frac{|\boldsymbol{u}(t;\boldsymbol{x}(t))|^2}{2} \middle| \text{Eqs. } (*,**)\right]$$

$$\text{s.t. } t\in[0,1]:\ d\boldsymbol{x}(t)=\boldsymbol{u}(t;\boldsymbol{x}(t))dt+d\boldsymbol{W}(t),\ \boldsymbol{x}(0)=0\ (*)$$

$$p(\boldsymbol{x}(1)) = p_{\text{target}}(\boldsymbol{x}(1)) \qquad (**)$$

- Grow target distribution from point source
- Theory for sampling from $p_{\text{target}}(\cdot)$ [1], based on
  - "Integrability": Nonlinear HJB ⇒ Hopf '50 -Cole '51 ⇒ Diffusion (Mitter '81, Pavon '89)

[1] M.Tzen, M.Ragynsky, Theoretical guarantees .. with latent diffusions, 2019

Integrable SOC with Potential, Forced & Gauged

(Top Level) Integrable SOC in a Potential. Forced (& Gauged)

$$\min_{\boldsymbol{u}(\cdot;\boldsymbol{x}(\cdot))} \mathbb{E}\left[\int_0^1 dt \left(\frac{|\boldsymbol{u}(t;\boldsymbol{x}(t))|^2}{2} + V(t;\boldsymbol{x}(t)) + \dot{\boldsymbol{x}}^T(t)\boldsymbol{A}(t;\boldsymbol{x}(t))\right) \Big| \text{Eqs. } (*,**)\right]$$

$$\text{s.t. } t \in [0,1]: \ d\boldsymbol{x}(t) = \boldsymbol{f}(t;\boldsymbol{x}(t)) + \boldsymbol{u}(t;\boldsymbol{x}(t))dt + d\boldsymbol{W}(t), \ \boldsymbol{x}(0) = 0 \ (*)$$

$$p(\boldsymbol{x}(1)) = p_{\text{target}}(\boldsymbol{x}(1)) \qquad (**)$$

Path Integral Diffusion – H. Behjoo, MC (2024, IEEE Access 2025)

- "Integrable" SOC in a Potential, Forced and Gauged
  - Grow target distribution from a point source
  - Based on Path Integral Control (PIC) [1]
    - control & diffusion are co-dimensional

[1] H. J. Kappen, *Path integrals ... for optimal control theory*, 2005.

[2] V. Chernyak, MC, J. Bierkens, H.J. Kappen, *SOC as Non-Eq Stat Mech: Calculus of Variations over Density and Current*, 2013

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  - Grow target distribution from a point source
  - Based on Path Integral Control (PIC) [1]
  - Field & Gauge Extension of PIC [2]

[1] H. J. Kappen, *Path integrals ... for optimal control theory*, 2005.

[2] V. Chernyak, MC, J. Bierkens, H.J. Kappen, *SOC as Non-Eq Stat Mech: Calculus of Variations over Density and Current*, 2013

Path Integral Diffusion – (Top Level) Integrability

Hamilton-Jacobi Bellman for Cost-to-go (from t to 1)

$$-\partial_t J = V + \frac{1}{2}\left(\boldsymbol{\nabla}^T(\boldsymbol{\nabla} J + \boldsymbol{A}) - |\boldsymbol{\nabla} J + \boldsymbol{A}|^2\right) + \boldsymbol{f}^T(\boldsymbol{\nabla} J + \boldsymbol{A})$$

Optimal Control: $\boldsymbol{u}^* = -\boldsymbol{\nabla} J - \boldsymbol{A}$

Hopf-Cole: $J(t;\boldsymbol{x}) = -\log\psi(t;\boldsymbol{x})$

$-\partial_t\psi + \tilde{V}\psi + \tilde{\boldsymbol{A}}^T\boldsymbol{\nabla}\psi = \frac{1}{2}\Delta\psi, \quad \psi(1;\boldsymbol{x}) = \exp\left(-\phi(\boldsymbol{x})\right)$, $\phi(\cdot)$ is the terminal cost correspondent to $p_{\text{target}}(\cdot)$

$$\tilde{V} \doteq V + \frac{1}{2}\boldsymbol{\nabla}^T\boldsymbol{A} + \boldsymbol{f}^T\boldsymbol{A} - \frac{1}{2}|\boldsymbol{A}|^2, \quad \tilde{\boldsymbol{A}} \doteq \boldsymbol{A} - \boldsymbol{f}$$

$$\partial_t p^* + \boldsymbol{\nabla}^T\left(p^*(\boldsymbol{\nabla}\log\psi - \tilde{\boldsymbol{A}})\right) = \frac{1}{2}\Delta p^*, \quad p^*(0;\boldsymbol{x}) = \delta(\boldsymbol{x}), \quad p^*(1;\boldsymbol{x}) = p_{\text{target}}(\boldsymbol{x})$$

Optimal Control via Green Functions:

$$u^*(t;\boldsymbol{x}(t)) = \nabla_{\boldsymbol{x}}\log\left(\int d\boldsymbol{y}\; p_{\text{target}}(\boldsymbol{y})\frac{G_-(t;\boldsymbol{x}(t);\boldsymbol{y})}{G_+(1;\boldsymbol{y};0)}\right)$$

$$t\in[1\to 0]: \quad -\partial_t G_- + \tilde{V}(\boldsymbol{x};t)G_- + \tilde{\boldsymbol{A}}^T\boldsymbol{\nabla} G_- = \frac{1}{2}\Delta G_-, \quad G_-(1;\boldsymbol{x}) = \delta(\boldsymbol{x}-\boldsymbol{y})$$

$$t\in[0\to 1]: \quad \partial_t G_+ + \tilde{V}(\boldsymbol{x};t)G_+ - \boldsymbol{\nabla}^T(\tilde{\boldsymbol{A}}G_+) = \frac{1}{2}\Delta G_+, \quad G_+(0;\boldsymbol{x}) = \delta(\boldsymbol{x}-\boldsymbol{y})$$

Harmonic Path Integral Diffusion (H-PID) – Integrability

H-PID – Mid Level Integrability

- **Green Functions are Gaussian** when
  - Potential is Quadratic:
    $V(t;\boldsymbol{x}(t)) = \boldsymbol{x}^T\hat{\beta}(t)\boldsymbol{x}/2 +$ linear and const terms
  - Force and Gauge are Affine in $\boldsymbol{x}$
- Akin to Quant Mech (in imag. time) in Harmonic Potential
- $u^*(t;\boldsymbol{x}(t)) = \nabla_{\boldsymbol{x}} \log\left(\int d\boldsymbol{y}\ p_{\text{target}}(\boldsymbol{y})\frac{G_-(t;\boldsymbol{x}(t);\boldsymbol{y})}{G_+(1;\boldsymbol{y};0)}\right) =$
  $a(t)\boldsymbol{x}(t) - b(t)\hat{\boldsymbol{x}}(t;\boldsymbol{x}(t))$

Special case, also discussed in [1] – Low Level Integrability

- $\boldsymbol{A}, \boldsymbol{f} = 0$ – zero gauge, zero force

[1] A. Teter, W, Wang & A. Halder, *Schrödinger bridge with quadratic state cost is exactly solvable*, 2024

Use Case – Harmonic, Uniform – Low Level Integrability

$V(t;\boldsymbol{x}) = \beta|\boldsymbol{x}|^2 \Rightarrow$ Explicit Expression for the Green Functions

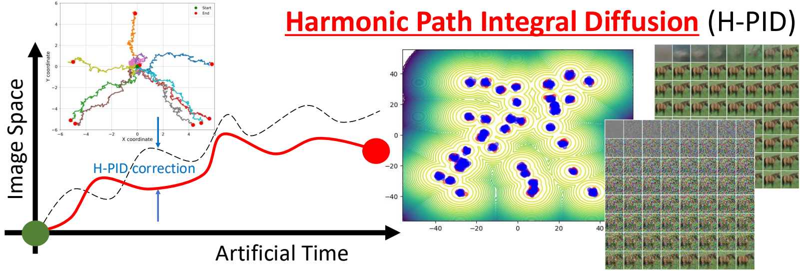
- $u^*(t;\boldsymbol{x}(t)) = \nabla_{\boldsymbol{x}} \log\left(\int d\boldsymbol{y}\; p_{\text{target}}(\boldsymbol{y})\frac{G_-(t;\boldsymbol{x}(t);\boldsymbol{y})}{G_+(1;\boldsymbol{y};0)}\right) = a(t)\boldsymbol{x}(t) - b(t)\hat{\boldsymbol{x}}(t;\boldsymbol{x}(t))$
- $u^*(t;\boldsymbol{x}) = \frac{\sqrt{\beta}}{\sinh((1-t)\sqrt{\beta})}\left(\hat{\boldsymbol{x}}(t;\boldsymbol{x}) - \boldsymbol{x}\cosh((1-t)\sqrt{\beta})\right)$
- **Weighted State:** $\hat{\boldsymbol{x}}(t;\boldsymbol{x}) \doteq \int d\boldsymbol{y}\boldsymbol{y}\, w(\boldsymbol{y}|t;\boldsymbol{x}) = \mathbb{E}_{\boldsymbol{y}\sim w(\cdot|t;\boldsymbol{x})}[\boldsymbol{y}]$
- **Weight (probability):** $w(\boldsymbol{y}|t;\boldsymbol{x}) \propto p_{\text{target}}(\boldsymbol{y})\frac{G_-(t;\boldsymbol{x};\boldsymbol{y})}{G_+(1;\boldsymbol{y};0)}$

$$\frac{G_-(t;\boldsymbol{x};\boldsymbol{y})}{G_+(\mathbf{1};\boldsymbol{y};\mathbf{0})} = \sqrt{\frac{\sinh(\sqrt{\beta})}{\sinh((\mathbf{1}-t)\sqrt{\beta})}}\exp\left(-\frac{\sqrt{\beta}}{\mathbf{2}}\left((\boldsymbol{x}^{\mathbf{2}}+\boldsymbol{y}^{\mathbf{2}})\coth\left((\mathbf{1}-t)\sqrt{\beta}\right) - \boldsymbol{y}^{\mathbf{2}}\coth\left(\sqrt{\beta}\right) - \frac{\mathbf{2}(\boldsymbol{x}^T\boldsymbol{y})}{\sinh((\mathbf{1}-t)\sqrt{\beta})}\right)\right)$$

Experiments & Analysis (ask me about)

- Dependence on β – **strength of the potential**
- What is the meaning/significance of the **Weighted State**

(Harmonic) Path Integral Diffusion – Summary



- From zero to high-quality sample via *Stochastic Optimal Control*

Three Levels of ***Integrability****:*

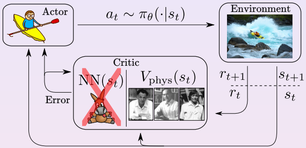
- ❑ **Top:** Any Potential, Force & Gauge [two linear ODEs for Green Functions]
- ❑ **Mid:** Equivalent to Quantum Harmonic Oscillator
- ❑ **Low:** Uniform Quadratic Potential [implemented in algorithm]

H. Behjoo, MC, IEEE Access **13**, 42196 - 42213 (2025), 10.1109/ACCESS.2025.3548396

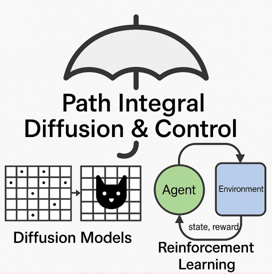
Insight #1: Diffusions & Reinforcement Learning

Diffusions = GREAT tools of GenAI

- ... BUT ... time is artificial
- **Dream:** Can we link diffusion to a physical process of sample growth?
- and BTW ... Path Integral Diffusion links Diffusion to Stochastic Optimal Control (SOC)



- ... and in AI data-driven version of SOC = Reinforcement Learning

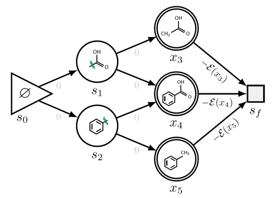


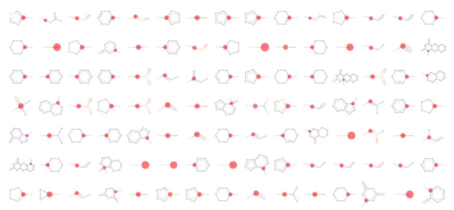
Key Insight #1:
Path Integral Diffusion & Control bridge RL and Diffusion

Insight #2: Reinforcement Learning & Auto-Regression

Generative Flow Networks (GFN)

- GFN [1]: view sampling as sequential decisions on a Directed Acyclic Graph
- Built on discrete space-time RL = Markov Decision Processes
- Samples are built step-by-step: $s_0 = \emptyset \to s1 \to \ldots \to s_T$.
- History-dependent, auto-regressive construction like **transformers**.





[a] E. Bengio, et. al, Flow Network based Generative Models for Non-Iterative Diverse Candidate Generation, 2021

Key Insight #2: GFN bridges RL and Transformer paradigms

Insight #2: Reinforcement Learning & Auto-Regression

Generative Flow Networks (GFN)

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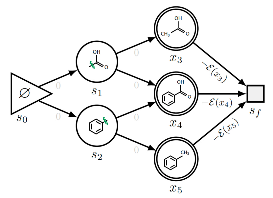
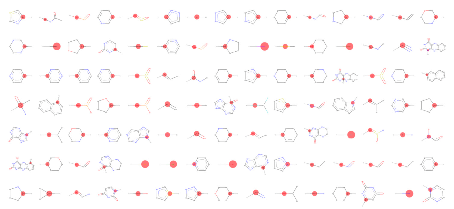
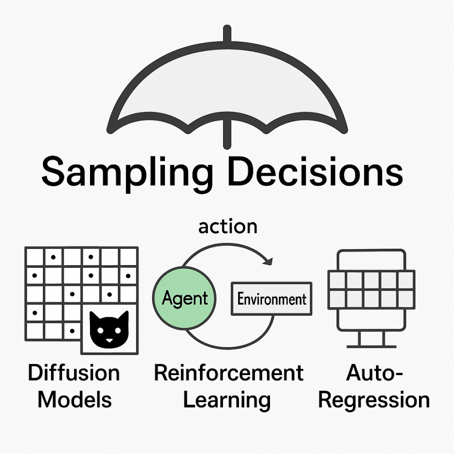
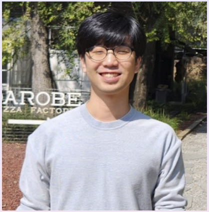




Key Insight #2: GFN bridges RL and Transformer paradigms

- Can we brought it all together — Diffusions, RL, Auto-Regression?





MC, S. Ahn, H. Behjoo, **Sampling Decisions**, arxiv:2503.14549

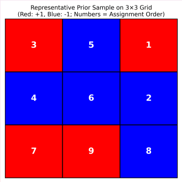
Decision Flow Framework

Goal: Generate Samples: $\boldsymbol{\sigma} \sim \exp(-E(\boldsymbol{\sigma}))$ – from the Energy/Graph Model

- **Sequentially:** $\emptyset = s_0 \to \{s_1 \to \cdots \to s_T = \boldsymbol{\sigma}$, **Given:** Prior Markov Process $p^{\text{prior}}(\cdot|\cdot)$

Solution: $$p_t^*(s_{t+1}|s_t) \propto p_t^{(\text{prior})}(s_{t+1}|s_t) \sum_{s'_T} \frac{e^{-E(s'_T)} G_{t+1}(s_{t+1}|s'_T)}{\pi_T^{(\text{prior})}(s'_T)},$$

$$G_t(s_t|s_T) = \sum_{s_{t+1}} p_t^{(\text{prior})}(s_{t+1}|s_t) G_{t+1}(s_{t+1}|s_T), \quad G_T(s_T|s'_T) = \delta(s_T, s'_T)$$



Illustrative Example:

Ising model : $E(\sigma) =$
$-\sum_{(a,b)\in\mathcal{E}} J_{ab}\sigma_a\sigma_b - \sum_{a\in\mathcal{V}} h_a\sigma_a$

Integrable = Solution of a Markov Decision Process (MDP)

- $G_\bullet(\bullet|\bullet)$ – (time-reverse) Green function of the prior MP
- Akin to a Linearly Solvable MDP [1] with an extra terminal condition, where [1] a Discrete Time & Space generalization of the Path Integral Control [2]

[1] E. Todorov, *Linearly-solvable Markov decision problems, NeurIPS 2007*
[2] H. J. Kappen, *Path integrals ... for optimal control theory*, 2005.

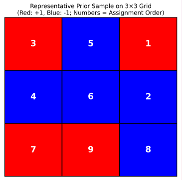
Decision Flow Framework

Goal: Generate Samples: $\boldsymbol{\sigma} \sim \exp(-E(\boldsymbol{\sigma}))$ – from the Energy/Graph Model

- **Sequentially:** $\emptyset = s_0 \to \{s_1 \to \cdots \to s_T = \boldsymbol{\sigma}$, **Given:** Prior Markov Process $p^{\text{prior}}(\cdot|\cdot)$

Solution: $$p_t^*(s_{t+1}|s_t) \propto p_t^{(\text{prior})}(s_{t+1}|s_t) \sum_{s'_T} \frac{e^{-E(s'_T)} G_{t+1}(s_{t+1}|s'_T)}{\pi_T^{(\text{prior})}(s'_T)},$$

$$G_t(s_t|s_T) = \sum_{s_{t+1}} p_t^{(\text{prior})}(s_{t+1}|s_t) G_{t+1}(s_{t+1}|s_T), \quad G_T(s_T|s'_T) = \delta(s_T, s'_T)$$



$$\min_{p_{0\to T-1}, \pi_{0\to T-1}} \sum_{t=0}^{T-1} \sum_{s_t, s_{t+1}} \pi_t(s_t) p_t(s_{t+1}|s_t) \log\left(\frac{p_t(s_{t+1}|s_t)}{p_t^{(\text{prior})}(s_{t+1}|s_t)}\right)$$

$$\text{s.t.} \quad \pi_{t+1}(s_{t+1}) = \sum_{s_t} p_t(s_{t+1}|s_t)\pi_t(s_t),$$

$$\sum_{s_{t+1}} p_t(s_{t+1}|s_t) = 1$$

Illustrative Example:

Ising model : $E(\sigma) = -\sum_{(a,b)\in\mathcal{E}} J_{ab}\sigma_a\sigma_b - \sum_{a\in\mathcal{V}} h_a\sigma_a$

NN-Free Decision Flow Algorithm

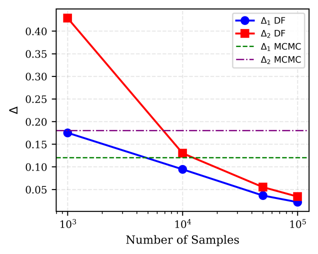
Solution: $$p_t^*(s_{t+1}|s_t) \propto p_t^{(\text{prior})}(s_{t+1}|s_t) \sum_{s'_T} \frac{e^{-E(s'_T)} G_{t+1}(s_{t+1}|s'_T)}{\pi_T^{(\text{prior})}(s'_T)} \quad (1),$$

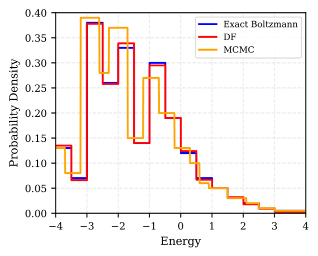
$$G_t(s_t|s_T) = \sum_{s_{t+1}} p_t^{(\text{prior})}(s_{t+1}|s_t) G_{t+1}(s_{t+1}|s_T), \quad G_T(s_T|s'_T) = \delta(s_T, s'_T), \quad (2)$$

- **Given:** $p_t^{(\text{prior})}(\bullet|\bullet),\ t = 1, \cdots, T$ – pre-trained algorithm
- **Generate** K Paths from the algorithm, $\Xi^{(k)} = (s_0 = \emptyset, s_1^{(k)}, \cdots, s_T^{(k)}), \cdots k = 1, \cdots, K$
- Build $p_\bullet^{(\text{prior-emp})}(\bullet|\bullet)$
- Build empirical version of the Green function according to (1)
- Build $p_\bullet^{(\text{post-emp})}(\bullet|\bullet)$ according (2)
- Generate S posterior samples to test performance

Decision Flow Example: Sampling from Ising

- Apply DFA to sample from Glassy Ising (3×3), $h_a, J_{ab} \sim \text{Uniform}[-1, 1]$
- $m_a^* = \frac{1}{S} \sum_{s=1}^{S} \sigma_{T;a}^{(s)}$
  $c_{ab}^* = \frac{1}{S} \sum_{s=1}^{S} \sigma_{T;a}^{(s)} \sigma_{T;b}^{(s)}$
- $\Delta_1 = \sum_a \frac{\| m_a - m_a^{(\text{ref})} \|}{T \, \| m_a^{(\text{ref})} \|}$,
  $\Delta_2 = \sum_{(a,b)} \frac{2 \| c_{ab} - c_{ab}^{(\text{ref})} \|}{T(T-1) \, \| c_{ab}^{(\text{ref})} \|}$
- Posterior vs MCMC (benchmark) – better convergence in small-sample regime





Conclusion and Path Forward

Key Takeaways

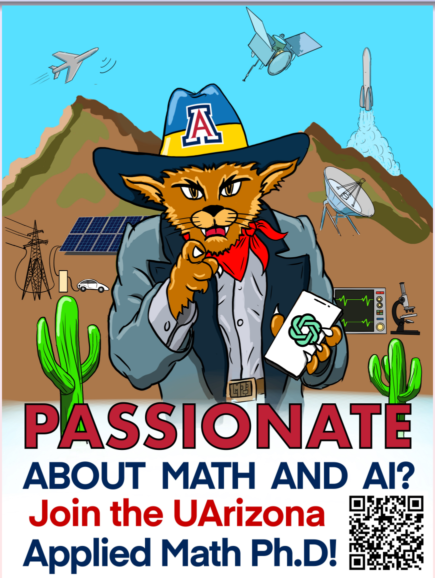
- **Decision Flow (DF)** provides a unifying framework for GenAI.
- Integrates core ideas from **Diffusion Models**, **Reinforcement Learning**, and **Transformers**.
- Rooted in stochastic control and Green function techniques.
- Especially suited for problems with:
  - an inherent time-line or sample growth process
  - emphasis on **sampling** rather than classical optimization

Conclusion and Path Forward

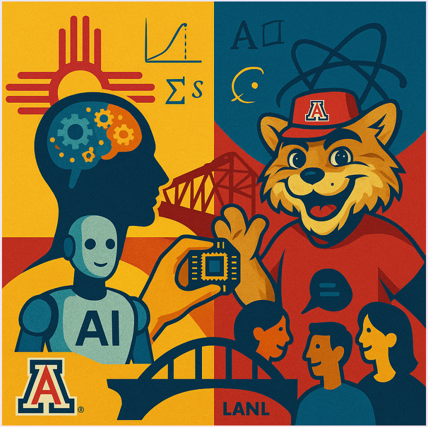
Next Steps: Methodology & Applications

- **Scalability**: Neural implementations for large systems; batched empirical averaging
- **Hybrid Input**: Combine ground-truth samples with energy-based models
- **Expert-Informed Models**: Incorporate constraints, domain knowledge, and rare events
- **Target Applications**:
  - Material discovery and design
  - Control of physical (e.g., complex fluids) and engineered (e.g., power grids, drone swarms) systems
  - Modeling epidemics—both social and viral
  - Open to discuss other Applications

Applied Math @ UArizona



- **Research** focused, since 1976, one of the US first in Applied Mathematics
- **Interdisciplinary**: 130+ professors/ 27 departments / 8 colleges across UA campus (Science & Engineering & Optics – top 3)
- **Mixing** traditional contemporary AM
- **65** PhD students (12/12/12/13/16/10 enrolled in 2024/23/22/21/20/19)
- 3 Core Courses to Qualify (Methods, Analysis, Algorithms) - **re-designed** to incorporate **AI** in 2019-20; + three **research rotations** in the first 3 semesters with at least two professors
- Strong collaborations with National – **DOE** – & Industrial – **DOD+** – Labs, e.g. via **NSF** (Graduate Innovation in Education) support – **pipeline**: recruitment, internerships, co-advising (triads), partial employment



Invitation to Collaborate

During my possible mini-sabbatical at LANL, I invite collaboration on a set of projects under the theme:

Physics-informed, Hybrid AI, and Mathematics for Engineering and Sciences (PHAMES)

PHAMES aims to unite applied math, physics-based modeling, engineering, and social sciences to build a robust AI infrastructure – positioning the team as a leader in responsible, high-impact research for national security, energy, and societal resilience.

Physics-informed, Hybrid AI, and Math for Eng and Sciences (PHAMES): Addressing National Defense, Security, and Energy

Focus Areas:

- Integrated Energy Systems: power, gas, nuclear, and fusion
- Flying Devices: airplanes, drones, satellites
- Communications & Computing: optical, radio, sound, quantum
- New Materials: tailored for the above
- Networks of Influence: disease, beliefs, behaviors

- 23 professors from 5 colleges of UArizona
- Under umbrella of RII Institutes & Applied Math GIDP
- UA "Big Idea" proposal

UA Participants:

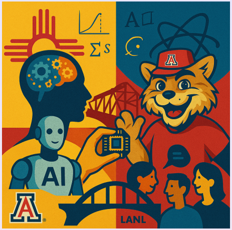
- M. Chertkov (Math) – PI 📐 🔬 ⚒ 🌍
- F. Mashayek (AME) – Co-PI 📐 🔬 ⚒
- D. Apai (Astro) 📐 🔬
- J. Aubrey (Math) 📐 🌍
- L. Brandimarte (MIS) 🌍
- CK Chan (Astro) 📐 🔬
- G. Cipolloni (Math) 📐
- P. Deymier (MSE) ⚒ 🔬
- H. Fasel (AME) ⚒
- I. Gabitov (Math & Optics) 📐 🔬 ⚒
- Y. Ge (MIS) 📐 🌍
- H. Hahn (MSE+RII) ⚒ 🔬
- K. Hanquist (AME) ⚒
- M. Latypov (MSE) 📐 ⚒
- X. Lu (IS) 🌍
- B. Maccabe (CoI+RII) 📐 ⚒
- K. Muralidharan (MSE) ⚒ 🔬
- L. Pagnier (Math) 📐 🔬 ⚒
- M. Rychlik (Math) 📐 🔬
- P. Shipman (Math) 📐 🌍
- M. Stepanov (Math) 📐 🔬
- J. Zavisca (Sociology) 🌍
- C. Zhang (CS) 📐

Legend:

- 📐 Math & AI
- 🔬 Physical Sciences
- ⚒ Engineering Sciences
- 🌍 Social & EDU Sciences

- **Hybrid AI** + **Physics/Math** to tackle **defense**, and **security** challenges.
- Focus: Energy systems, aerospace, comms, materials, and social dynamics.
- Building shared AI infrastructure with National & Industrial Labs

- Looking for Los Alamos Partners !!



Background & Existing Collaboration

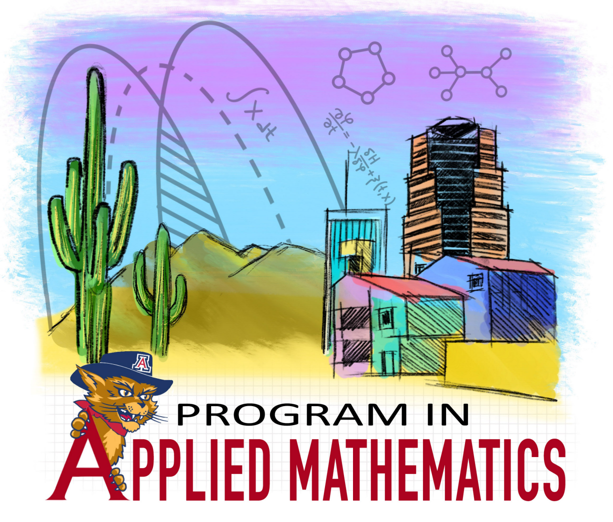
- **LANL – UA MOU since March 2024**
- History of Collaboration – CNLS@LANL and AM GIDP@UA
  - Multiple interns, GRAs -> Postdocs
  - Annual Arizona - Alamos Days
  - 40+ alumni of UA at LANL

Vision for Strategic Expansion

- **Joint Strategic Appointments**
- **Triangle Model: LANL-UA-Grad Students**
- **LANL Teaching @ UA**
  - Courses of joint interest (optimization, PIML)

Joint Project Potential

- **Next Steps**
  - UA & LANL leadership Meeting (07/25)
  - Align funding
- **Targeted Outcomes**
  - Co-sponsored **DOE/NSF proposals**
  - Collaborative infrastructure



Thank You!

Score Based Diffusion & Stochastic Optimal Control

Score Based Diffusion as "Integrable" Stochastic Optimal Control

$$\min_{\boldsymbol{u}(0\to 1;\boldsymbol{x}(0\to 1))} \mathbb{E}\left[\int_0^1 dt \frac{|\boldsymbol{u}(t;\boldsymbol{x}(t))|^2}{2} \middle| \text{Eqs. } (*, **)\right]$$

$$\text{s.t. } t\in[0,1]: \ d\boldsymbol{x}(t) = \boldsymbol{u}(t;\boldsymbol{x}(t))dt + d\boldsymbol{W}(t), \ \boldsymbol{x}(0)=0 \ (*)$$

$$p(\boldsymbol{x}(1)) = p_{\text{target}}(\boldsymbol{x}(1)) \qquad (**)$$

- Grow target distribution from point source
- Theory for sampling from $p_{\text{target}}(\cdot)$ [1], based on
  - "Integrability": Nonlinear HJB ⇒ Hopf '50 -Cole '51 ⇒ Diffusion (Mitter '81, Pavon '89)

[1] M.Tzen, M.Ragynsky, Theoretical guarantees .. with latent diffusions, 2019

Score Based Diffusion & Stochastic Optimal Control

Score Based Diffusion as "Integrable" Stochastic Optimal Control

$$\min_{\boldsymbol{u}(0\to 1;\boldsymbol{x}(0\to 1))} \mathbb{E}\left[\int_0^1 dt \frac{|\boldsymbol{u}(t;\boldsymbol{x}(t))|^2}{2}\Big|\text{Eqs. }(*,**)\right]$$

$$\text{s.t. } t\in[0,1]:\ \ d\boldsymbol{x}(t)=\boldsymbol{u}(t;\boldsymbol{x}(t))dt+d\boldsymbol{W}(t),\ \ \boldsymbol{x}(0)=0\ (*)$$

$$p(\boldsymbol{x}(1)) = p_{\text{target}}(\boldsymbol{x}(1)) \qquad (**)$$

- Grow target distribution from point source
- Efficient Algorithms
  - Path Integral Sampling – Fitting Control with NN, Expansive (repetitive forward propagation of SDE) [3]
  - Iterative Denoising Energy Matching – sampling to estimate score-function – [4]

[3] Q.Zhang, Y.Chen, Path Integral Sampler, 2022

[4] T. Akhound-Sadegh, et al, Iterative Denoising Energy Matching, 2024

Integrable SOC with Potential, Forced & Gauged

Integrable SOC with a "Potential"

$$\min_{\boldsymbol{u}(0\to 1;\boldsymbol{x}(0\to 1))} \mathbb{E}\left[\int_0^1 dt \left(\frac{|\boldsymbol{u}(t;\boldsymbol{x}(t))|^2}{2} + V(t;\boldsymbol{x}(t))\right) \Big| \text{Eqs. } (*), (**)\right]$$

$$\text{s.t. } t \in [0,1]: \quad d\boldsymbol{x}(t) = \boldsymbol{u}(t;\boldsymbol{x}(t))dt + d\boldsymbol{W}(t), \quad \boldsymbol{x}(0) = 0 \; (*)$$

$$p(\boldsymbol{x}(1)) = p_{\text{target}}(\boldsymbol{x}(1)) \qquad (**)$$

Path Integral Diffusion – HB, MC (2024)

- "Integrable" SOC in a Potential, Forced and Gauged
  - Grow target distribution from a point source
  - Based on Path Integral Control (PIC) [1]
    - control & diffusion are co-dimensional

[1] H. J. Kappen, *Path integrals ... for optimal control theory*, 2005.

Integrable SOC with Potential, Forced & Gauged

(Top Level) Integrable SOC in a Potential. Forced (& Gauged)

$$\min_{\boldsymbol{u}(\cdot;\boldsymbol{x}(\cdot))} \mathbb{E}\left[\int_0^1 dt\left(\frac{|\boldsymbol{u}(t;\boldsymbol{x}(t))|^2}{2} + V(t;\boldsymbol{x}(t)) + \dot{\boldsymbol{x}}^T(t)\boldsymbol{A}(t;\boldsymbol{x}(t))\right)\middle|\text{Eqs. } (*,**)\right]$$

$$\text{s.t. } t\in[0,1]:\ d\boldsymbol{x}(t) = \boldsymbol{f}(t;\boldsymbol{x}(t)) + \boldsymbol{u}(t;\boldsymbol{x}(t))dt + d\boldsymbol{W}(t),\ \ \boldsymbol{x}(0)=0\ (*)$$

$$p(\boldsymbol{x}(1)) = p_{\text{target}}(\boldsymbol{x}(1)) \qquad (**)$$

Path Integral Diffusion – HB, MC (2024)

- "Integrable" SOC in a Potential, Forced and Gauged
  - Grow target distribution from a point source
  - Based on Path Integral Control (PIC) [1]
  - Field & Gauge Extension of PIC [2]

[1] H. J. Kappen, *Path integrals ... for optimal control theory*, 2005.

[2] V. Chernyak, MC, J. Bierkens, H.J. Kappen, *SOC as Non-Eq Stat Mech: Calculus of Variations over Density and Current*, 2013

Path Integral Diffusion – (Top Level) Integrability

Hamilton-Jacobi Bellman for Cost-to-go (from t to 1)

$-\partial_t J = V + \frac{1}{2}\left(\boldsymbol{\nabla}^T(\boldsymbol{\nabla} J + \boldsymbol{A}) - |\boldsymbol{\nabla} J + \boldsymbol{A}|^2\right) + \boldsymbol{f}^T(\boldsymbol{\nabla} J + \boldsymbol{A})$

Optimal Control: $\boldsymbol{u}^* = -\boldsymbol{\nabla} J - \boldsymbol{A}$

Hopf-Cole: $J(t;\boldsymbol{x}) = -\log\psi(t;\boldsymbol{x})$

$-\partial_t\psi + \tilde{V}\psi + \tilde{\boldsymbol{A}}^T\boldsymbol{\nabla}\psi = \frac{1}{2}\Delta\psi, \quad \psi(1;\boldsymbol{x}) = \exp\left(-\phi(\boldsymbol{x})\right)$, $\phi(\cdot)$ is the terminal cost correspondent to $p_{\text{target}}(\cdot)$

$\tilde{V} \doteq V + \frac{1}{2}\boldsymbol{\nabla}^T\boldsymbol{A} + \boldsymbol{f}^T\boldsymbol{A} - \frac{1}{2}|\boldsymbol{A}|^2, \quad \tilde{\boldsymbol{A}} \doteq \boldsymbol{A} - \boldsymbol{f}$

$\partial_t p^* + \boldsymbol{\nabla}^T\left(p^*(\boldsymbol{\nabla}\log\psi - \tilde{\boldsymbol{A}})\right) = \frac{1}{2}\Delta p^*, \quad p^*(0;\boldsymbol{x}) = \delta(\boldsymbol{x}), \quad p^*(1;\boldsymbol{x}) = p_{\text{target}}(\boldsymbol{x})$

Optimal Control via Green Functions:

$u^*(t;\boldsymbol{x}(t)) = \nabla_x \log\left(\int d\boldsymbol{y}\ p_{\text{target}}(\boldsymbol{y})\frac{G_-(t;\boldsymbol{x}(t);\boldsymbol{y})}{G_+(1;\boldsymbol{y};0)}\right)$

$t\in[1\to 0]: \quad -\partial_t G_- + \tilde{V}(\boldsymbol{x};t)G_- + \tilde{\boldsymbol{A}}^T\boldsymbol{\nabla} G_- = \frac{1}{2}\Delta G_-, \quad G_-(1;\boldsymbol{x}) = \delta(\boldsymbol{x}-\boldsymbol{y})$

$t\in[0\to 1]: \quad \partial_t G_+ + \tilde{V}(\boldsymbol{x};t)G_+ - \boldsymbol{\nabla}^T(\tilde{\boldsymbol{A}}G_+) = \frac{1}{2}\Delta G_+, \quad G_+(0;\boldsymbol{x}) = \delta(\boldsymbol{x}-\boldsymbol{y})$

Harmonic Path Integral Diffusion (H-PID) – Integrability

H-PID – Mid Level Integrability

- **Green Functions are Gaussian** when
  - Potential is Quadratic: $V(t;\boldsymbol{x}(t)) = \boldsymbol{x}^T\hat{\beta}(t)\boldsymbol{x}/2 +$ linear and const terms
  - Force and Gauge are Affine in $\boldsymbol{x}$
- Akin to Quant Mech (in imag. time) in Harmonic Potential
- $u^*(t;\boldsymbol{x}(t)) = \nabla_{\boldsymbol{x}} \log\left(\int d\boldsymbol{y}\ p_{\text{target}}(\boldsymbol{y})\frac{G_-(t;\boldsymbol{x}(t);\boldsymbol{y})}{G_+(1;\boldsymbol{y};0)}\right) = a(t)\boldsymbol{x}(t) - b(t)\hat{\boldsymbol{x}}(t;\boldsymbol{x}(t))$

Special case, also discussed in [1] – Low Level Integrability

- $\boldsymbol{A}, \boldsymbol{f} = 0$ – zero gauge, zero force

[1] A. Teter, W, Wang & A. Halder, *Schrödinger bridge with quadratic state cost is exactly solvable*, 2024

Use Case – Harmonic, Uniform – Low Level Integrability

$V(t;\boldsymbol{x}) = \beta|\boldsymbol{x}|^2 \Rightarrow$ Explicit Expression for the Green Functions

- $u^*(t;\boldsymbol{x}(t)) = \nabla_{\boldsymbol{x}} \log\left(\int d\boldsymbol{y}\; p_{\text{target}}(\boldsymbol{y}) \frac{G_-(t;\boldsymbol{x}(t);\boldsymbol{y})}{G_+(1;\boldsymbol{y};0)}\right) = a(t)\boldsymbol{x}(t) - b(t)\hat{\boldsymbol{x}}(t;\boldsymbol{x}(t))$
- $u^*(t;\boldsymbol{x}) = \frac{\sqrt{\beta}}{\sinh((1-t)\sqrt{\beta})}\left(\hat{\boldsymbol{x}}(t;\boldsymbol{x}) - \boldsymbol{x}\cosh((1-t)\sqrt{\beta})\right)$
- **Weighted State:** $\hat{\boldsymbol{x}}(t;\boldsymbol{x}) \doteq \int d\boldsymbol{y}\boldsymbol{y}\, w(\boldsymbol{y}|t;\boldsymbol{x}) = \mathbb{E}_{\boldsymbol{y}\sim w(\cdot|t;\boldsymbol{x})}[\boldsymbol{y}]$
- **Weight (probability):** $w(\boldsymbol{y}|t;\boldsymbol{x}) \propto p_{\text{target}}(\boldsymbol{y}) \frac{G_-(t;\boldsymbol{x};\boldsymbol{y})}{G_+(1;\boldsymbol{y};0)}$

$$\frac{G_-(t;\boldsymbol{x};\boldsymbol{y})}{G_+(\boldsymbol{1};\boldsymbol{y};\boldsymbol{0})} = \sqrt{\frac{\sinh(\sqrt{\beta})}{\sinh((\boldsymbol{1}-t)\sqrt{\beta})}}\exp\left(-\frac{\sqrt{\beta}}{\boldsymbol{2}}\left((\boldsymbol{x}^{\boldsymbol{2}}+\boldsymbol{y}^{\boldsymbol{2}})\coth\left((\boldsymbol{1}-t)\sqrt{\beta}\right) - \boldsymbol{y}^{\boldsymbol{2}}\coth\left(\sqrt{\beta}\right) - \frac{\boldsymbol{2}(\boldsymbol{x}^T\boldsymbol{y})}{\sinh((\boldsymbol{1}-t)\sqrt{\beta})}\right)\right)$$

Next – Experiments & Analysis

- Dependence on β – **strength of the potential**
- What is the meaning/significance of the **Weighted State**

How to estimate the optimal control?

$p_{\text{target}}(\boldsymbol{x}) \propto \exp(-E(\boldsymbol{x}))$ – the Energy function is known explicitly

- $u^*(t;\boldsymbol{x}) = \nabla_{\boldsymbol{x}} \log \left(\int d\boldsymbol{y} \;\; \exp(-E(\boldsymbol{y})) \frac{G_-(t;\boldsymbol{x};\boldsymbol{y})}{G_+(1;\boldsymbol{y};0)} \right)$
- How to Estimate the Integral?

Importance Sampling !!

$$\int d\boldsymbol{y} \;\; \exp(-E(\boldsymbol{y})) \frac{G_-(t;\boldsymbol{x};\boldsymbol{y})}{G_+(\boldsymbol{1};\boldsymbol{y};\boldsymbol{0})} = \mathbb{E}_{\boldsymbol{y}\sim\mathcal{N}\left(\cdot;\boldsymbol{y}^*;\hat{\boldsymbol{H}}^{-\boldsymbol{1}}\right)} \left[\frac{\exp(-E(\boldsymbol{y}))}{\mathcal{N}\left(\boldsymbol{y};\boldsymbol{y}^*;\hat{\boldsymbol{H}}^{-\boldsymbol{1}}\right)} \frac{G_-(t;\boldsymbol{x};\boldsymbol{y})}{G_+(\boldsymbol{1};\boldsymbol{y};\boldsymbol{0})} \right]$$

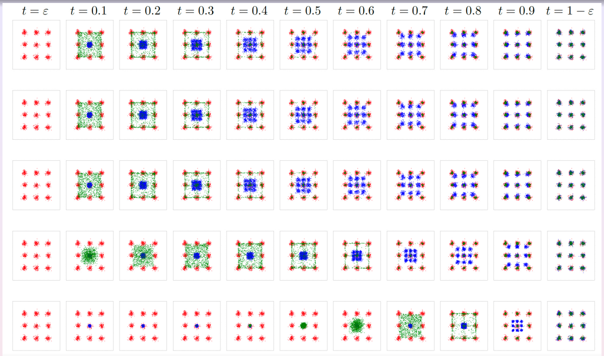
$$\nabla_{\boldsymbol{y}} \log \left(\frac{G_-(t;\boldsymbol{x};\boldsymbol{y})}{G_+(\boldsymbol{1};\boldsymbol{y};\boldsymbol{0})} \right) = \sqrt{\beta} \left(\boldsymbol{y} \left(\coth(\sqrt{\beta}) - \coth\left((\boldsymbol{1}-t)\sqrt{\beta}\right) \right) + \boldsymbol{x} \frac{\boldsymbol{1}}{\sinh((\boldsymbol{1}-t)\sqrt{\beta})} \right)$$

$$H_{ij} = -\partial_{y_i}\partial_{y_j} \log \left(\frac{G_-(t;\boldsymbol{x};\boldsymbol{y})}{G_+(\boldsymbol{1};\boldsymbol{y};\boldsymbol{0})} \right) \Bigg|_{\boldsymbol{y}\to\boldsymbol{y}_*} = \delta_{ij}\sqrt{\beta} \left(\coth\left((1-t)\sqrt{\beta}\right) - \coth(\sqrt{\beta}) \right)$$

$$\boldsymbol{y}_* = \frac{\boldsymbol{x}}{\cosh((\boldsymbol{1}-t)\sqrt{\beta}) - \sinh((\boldsymbol{1}-t)\sqrt{\beta}) \coth(\sqrt{\beta})}$$

- Rely on stationary-point approximation
- Exact asymptotically at $t \to 1$
- Importance Samples are Universal – do not depend on $E(\boldsymbol{x})$

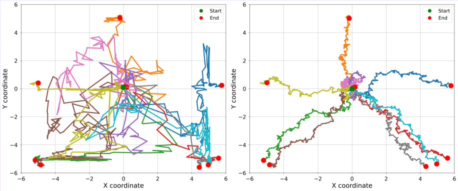
Universal Harmonic Importance Sampling (UHIC)

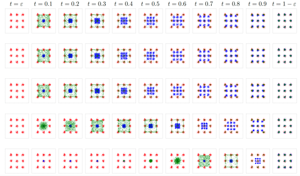


- Gaussian Mixture over (3×3) grid
- Difficult for PIS Alg.
- $s = 1, \cdots, 1000$ - samples of UHIC:
  Red - exact
  Blue - $\boldsymbol{x}^{(s)}(t)$
  Green $\hat{\boldsymbol{x}}^{(s)}(t; \boldsymbol{x}(t))$
- Rows:
  $\beta = 0, 0.1, 1, 10, 100$

Energy Function Sampling

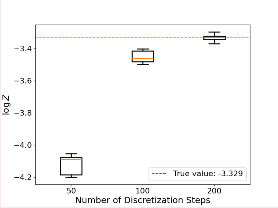
- **Speciation Transition**: 9 Gaussians = 9 species
- Seen earlier in $\hat{\boldsymbol{x}}^{(s)}(t; \boldsymbol{x}(t))$ – **the order parameter**
- Transition time depends on β. Fastest at $\beta \approx 0.1$

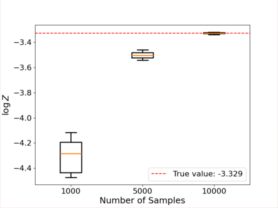




Space-Time Evolution of Samples [1]

- Dynamics is "direct" in $\boldsymbol{x}(t)$
- Much more of "exploration" meandering in $\hat{\boldsymbol{x}}(t; \boldsymbol{x}(t))$





- Good **Convergence** – in # t-steps & # of samples

[1] HB, MC, Space-Time Bridge Diffusion, 2024

Sampling from Ground Truth Samples

$$u^*(t;\boldsymbol{x}) = \nabla_{\boldsymbol{x}} \log\left(\int d\boldsymbol{y}\, p_{\text{target}}(\boldsymbol{y})\, \frac{G_-(t;\boldsymbol{x};\boldsymbol{y})}{G_+(1;\boldsymbol{y};0)}\right)$$

$$\approx \nabla_{\boldsymbol{x}} \log\left(\frac{1}{S}\sum_{s=1}^{S} \frac{G_-(t;\boldsymbol{x};\boldsymbol{y}^{(s)})}{G_+(1;\boldsymbol{y}^{(s)};0)}\right)$$

$$\approx \frac{\sqrt{\beta}\left(\hat{\boldsymbol{x}}(t;\boldsymbol{x}) - \boldsymbol{x}\cosh((1-t)\sqrt{\beta})\right)}{\sinh((1-t)\sqrt{\beta})}$$

- Memorization Regime $\Rightarrow$ Ground Truth samples
- Focus on **Analysis** of **Memorization transition** [1,2]

$$\hat{\boldsymbol{x}}(t;\boldsymbol{x}(t)) \doteq \textstyle\sum_s \boldsymbol{y}^{(s)} w(\boldsymbol{y}^{(s)}|t;\boldsymbol{x}(t))$$

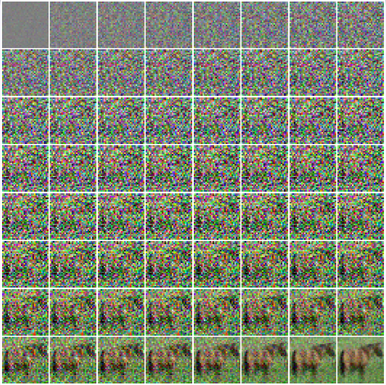
$$w(\boldsymbol{y}|t;\boldsymbol{x}) \propto \exp\left(-\frac{\sqrt{\beta}}{2}\left((\boldsymbol{x}^2+\boldsymbol{y}^2)\coth\left((1-t)\sqrt{\beta}\right) - \boldsymbol{y}^2\coth\left(\sqrt{\beta}\right) - \frac{2(\boldsymbol{x}^T\boldsymbol{y})}{\sinh\left((1-t)\sqrt{\beta}\right)}\right)\right)$$

[1] HB, MC, U-turn Diffusion, 2023
[2] G. Biroli, et al, Dynamical Regimes of Diffusion Models, 2024

Sampling from CIFAR-10

$\beta = 0.1$

$\hat{\boldsymbol{x}}(t;\boldsymbol{x}(t)) \doteq \sum_s \boldsymbol{y}^{(s)} w(\boldsymbol{y}^{(s)}|t;\boldsymbol{x}(t))$



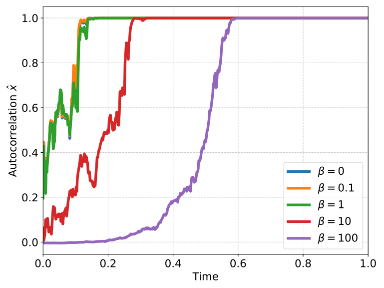
$\boldsymbol{x}(t)$

Analysis of the Memorization Transition

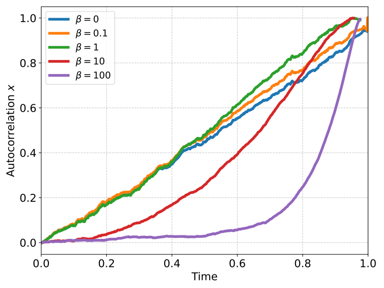
- Emergence of Two Phases
- See it earlier in the **Weighted State = Order Parameter**

Sampling from CIFAR-10

Auto-Correlations in Dynamics of a Single Sample



$(\hat{\boldsymbol{x}}^T(t; \boldsymbol{x}(t))\boldsymbol{x}(1))$



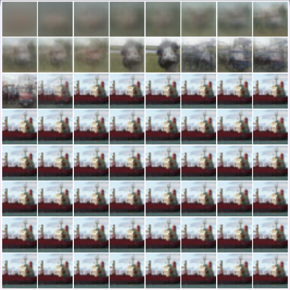
$(\boldsymbol{x}^T(t)\boldsymbol{x}(1))$

Analysis of the Memorization Transition

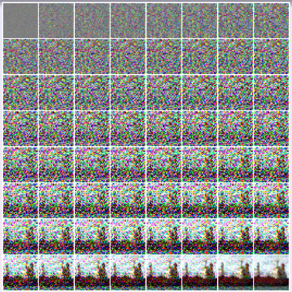
- Emergence of Two Phases
- See it earlier in the **Weighted State = Order Parameter**
- Transition time increases with β

Sampling from CIFAR-10

$\beta = 10$



$\hat{\boldsymbol{x}}(t;\boldsymbol{x}(t)) \doteq \sum_s \boldsymbol{y}^{(s)} w(\boldsymbol{y}^{(s)}|t;\boldsymbol{x}(t))$



$\boldsymbol{x}(t)$

Analysis of the Memorization Transition

- Emergence of Two Phases
- See it earlier in the Weighted State = Order Parameter
- Transition time increases with β
- Much more of "exploration" meandering in $\hat{\boldsymbol{x}}(t;\boldsymbol{x}(t))$

Summary – Harmonic Path Integral Diffusion (H-PID) framework

- Expressive **Stochastic Optimal Control** for Bridge Diffusion
- **"Integrable"** – Three Levels

  Top **Potential** + **Force** + **Gauge** ⇒ Linearly Solvable = log-ratio-of backward & forward Green Functions

  Mid Potential - quadratic, Force + Gauge are affine ⇒ **Green Functions are Gaussian** = akin **Quantum Harmonic Oscillators**

  Low Uniform Quadratic Potential ⇒ control is a **convolution** of the **Target Distribution** with a kernel expressed via **elementary functions**
- H-PID Algorithms is **Neural Networks – FREE**, works better on **CPUs**
- Experiments on Gaussian mixtures and CIFAR-10: **Weighted State** is **Order Parameter** of a **Dynamic Phase Transition** - early pre-cursor of the resulting sample