Generative Models for Physicists

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https://wangleiphy.github.io

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Lecture Note http://wangleiphy.github.io/lectures/PILtutorial.pdf

Generative Models for Physicists

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Beijing 100190, China

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Abstract

Generative models generate unseen samples according to a learned joint probability distribution in the high-dimensional space. They find wide applications in density estimation, variational inference, representation learning and more. Deep generative models and associated techniques (such as differentiable programing and representation learning) are cutting-edge technologies physicists can learn from deep learning.

This note introduces the concept and principles of generative modeling, together with applications of modern generative models (autoregressive models, normalizing flows, variational autoencoders etc) as well as the old ones (Boltzmann machines) to physics problems. As a bonus, this note puts some emphasize on physics-inspired generative models which take insights from statistical, quantum, and fluid mechanics.

The latest version of the note is at http://wangleiphy.github.io/. Please send comments, suggestions and corrections to the email address in below.

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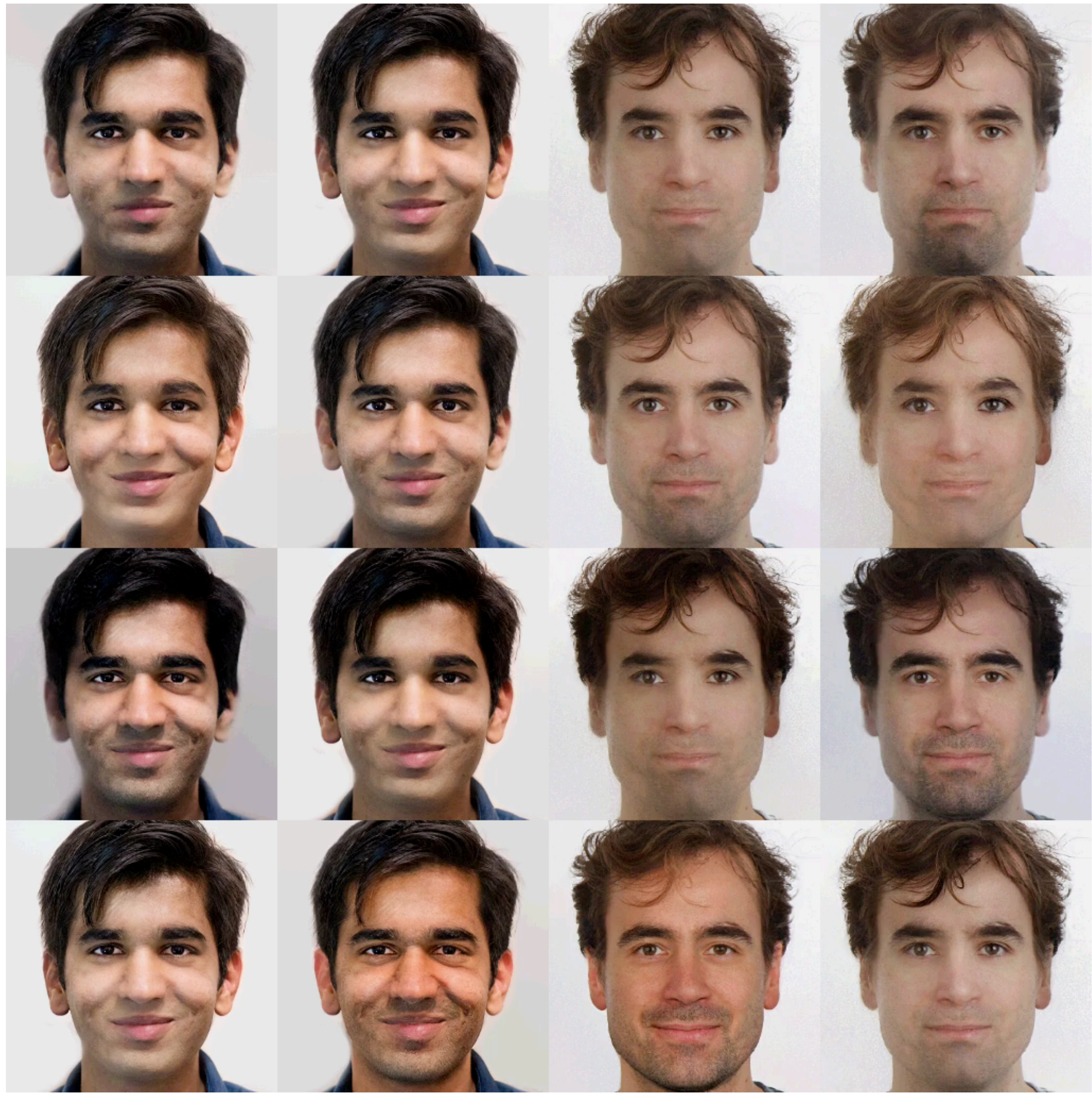
Generative Models



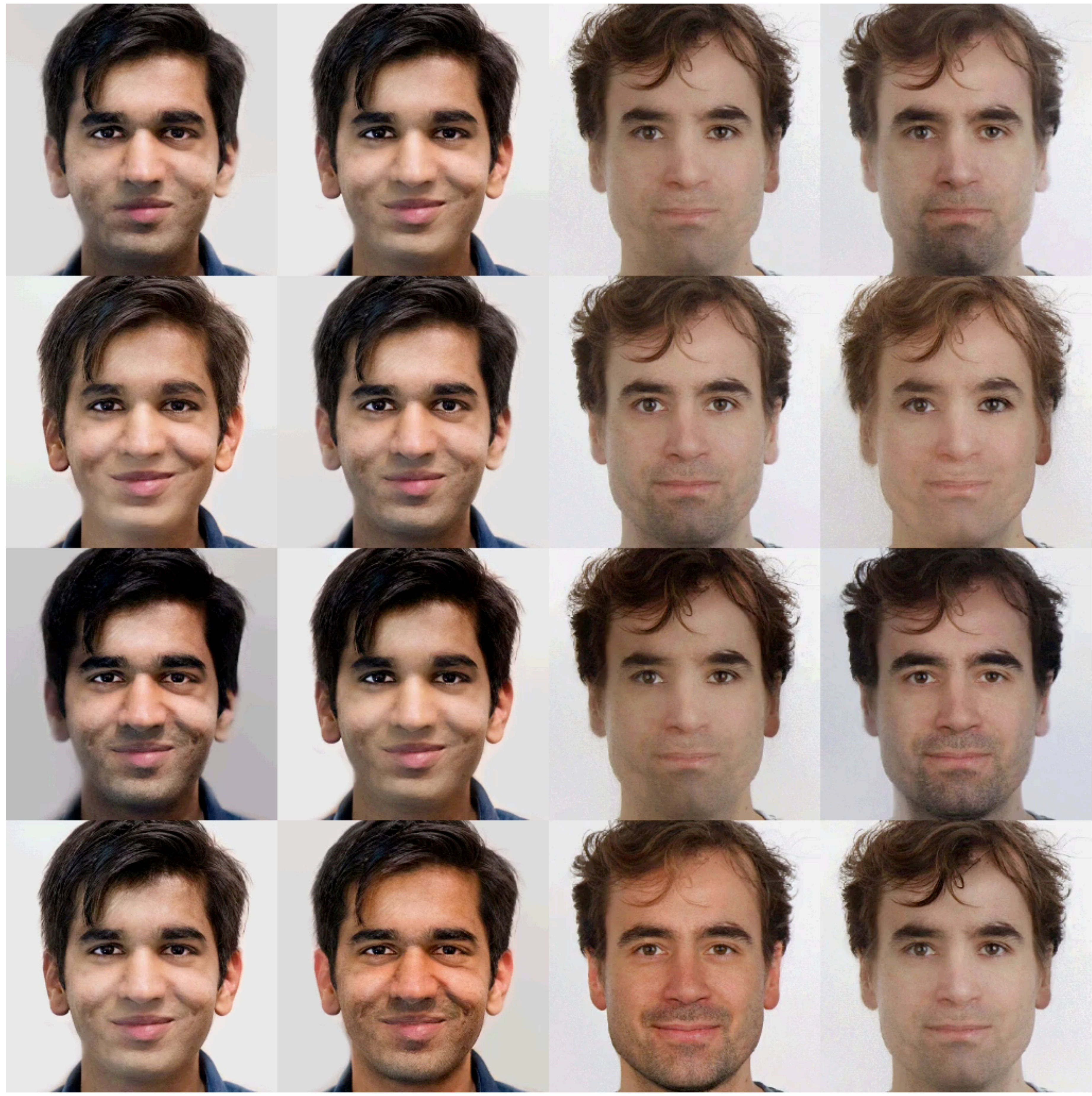
Wavenet 1609.03499 1711.10433

https://deepmind.com/blog/wavenet-generative-model-raw-audio/
https://deepmind.com/blog/high-fidelity-speech-synthesis-wavenet/

Glow 1807.03039

https://blog.openai.com/glow/

Generative Models



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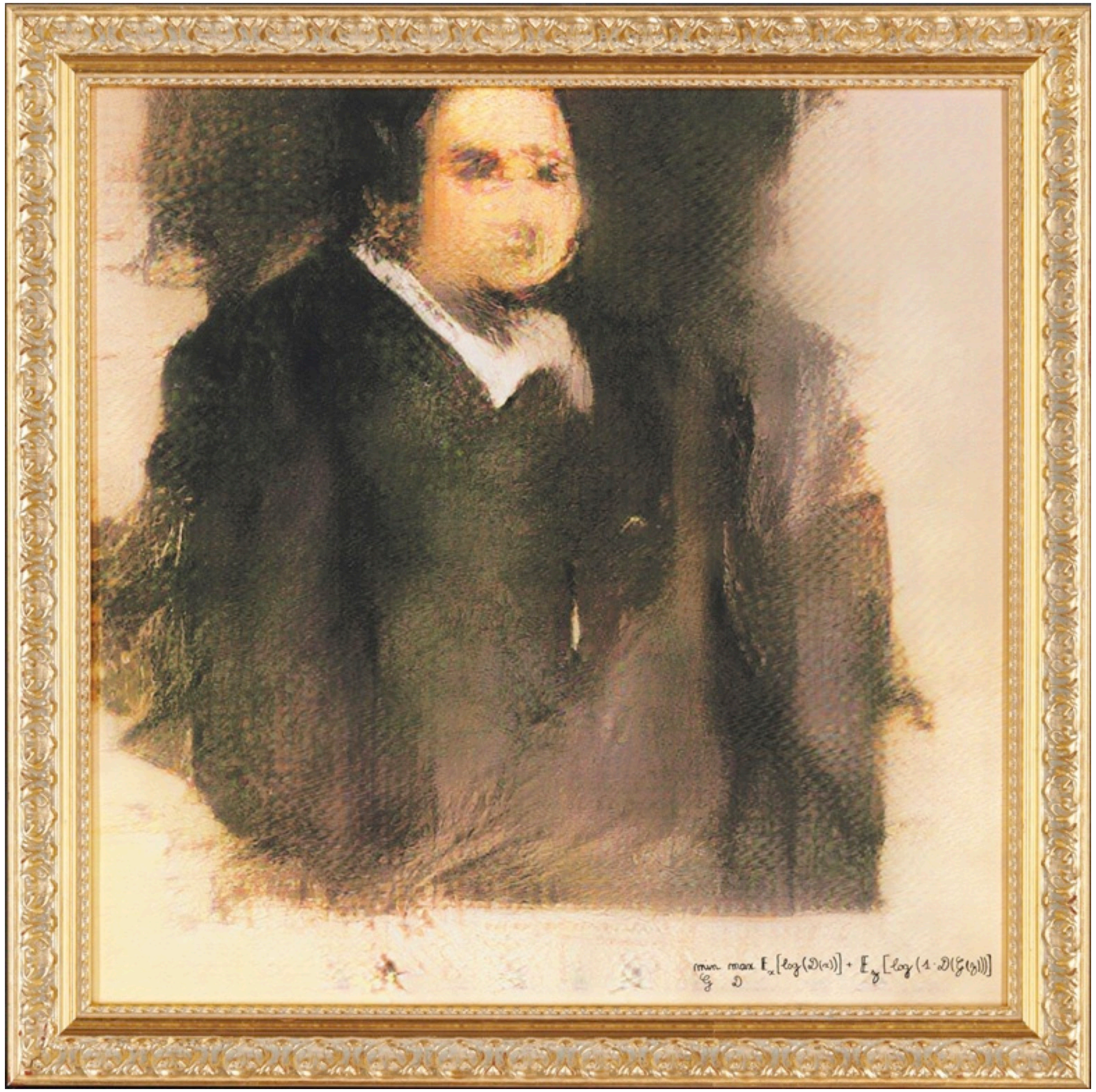
Glow 1807.03039

https://blog.openai.com/glow/

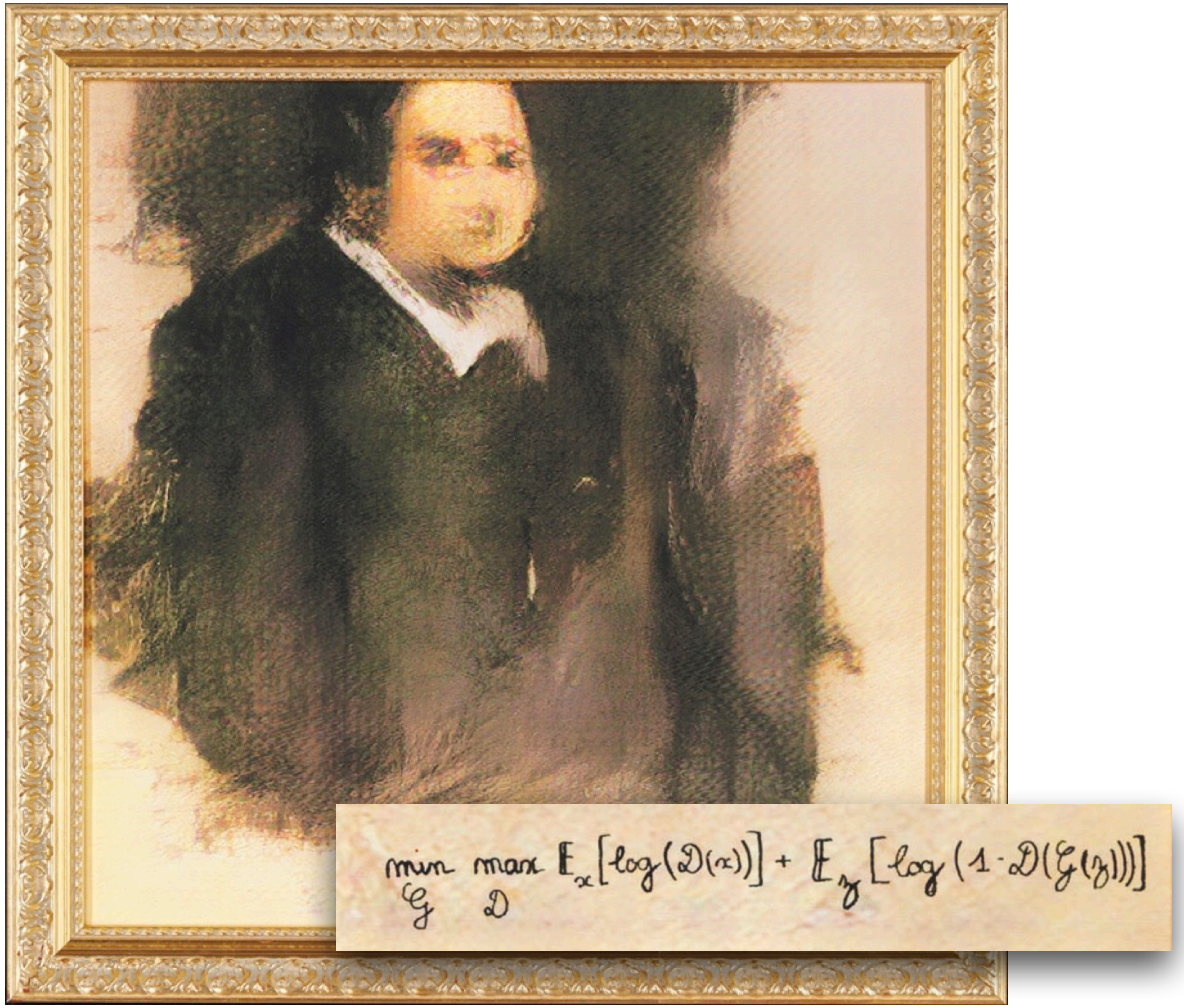
Generative Artwork



Sold for $432,500 on 25 October 2018 at Christie’s in New York

https://www.christies.com/Features/A-collaboration-between-two-artists-one-human-one-a-machine-9332-1.aspx

Generative Artwork



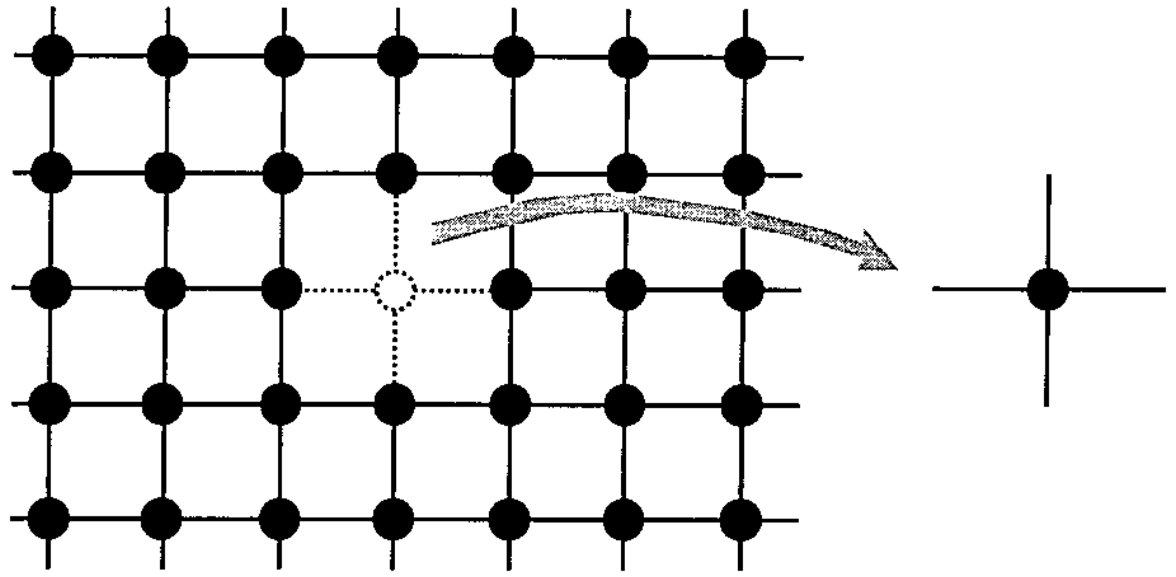
Sold for $432,500 on 25 October 2018 at Christie's in New York

https://www.christies.com/Features/A-collaboration-between-two-artists-one-human-one-a-machine-9332-1.aspx

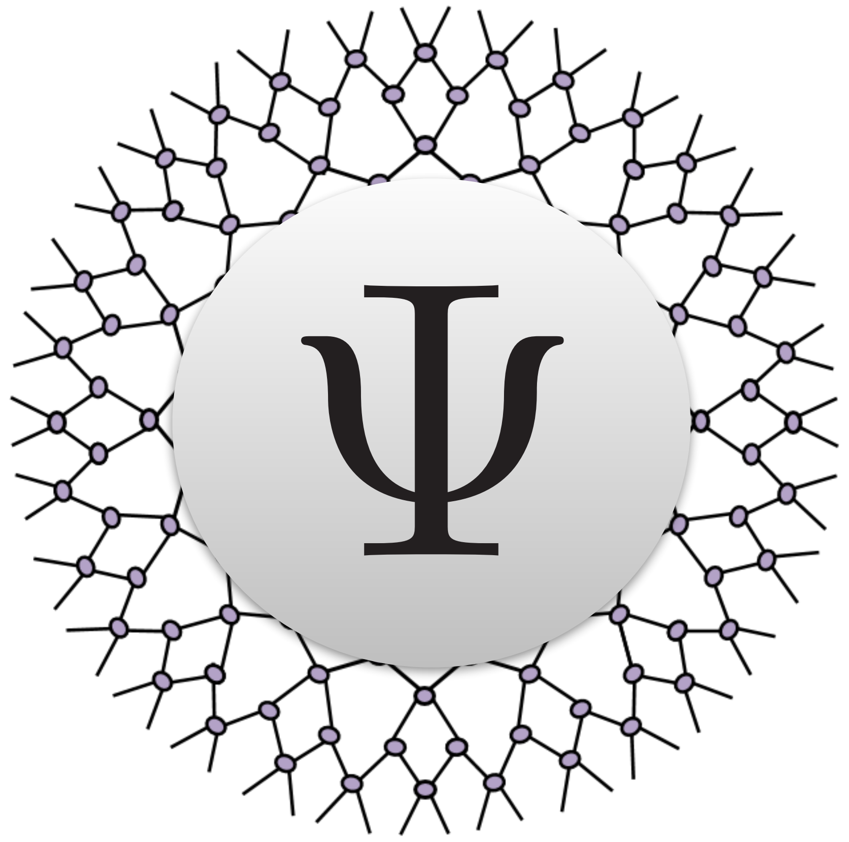
What can we do for physics ?

Physicists' gifts to Machine Learning

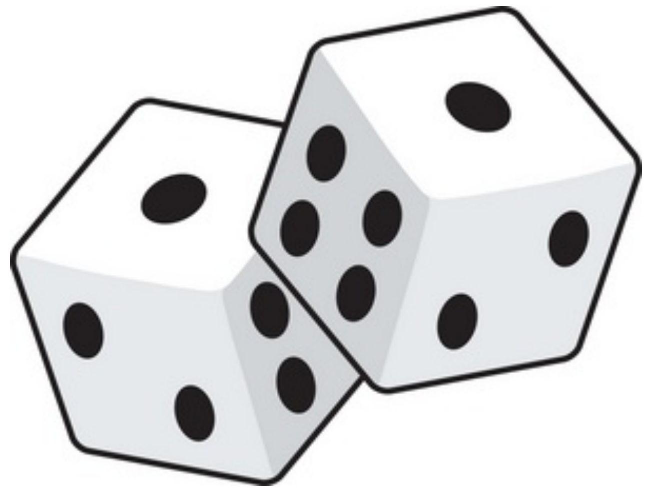
Mean Field Theory



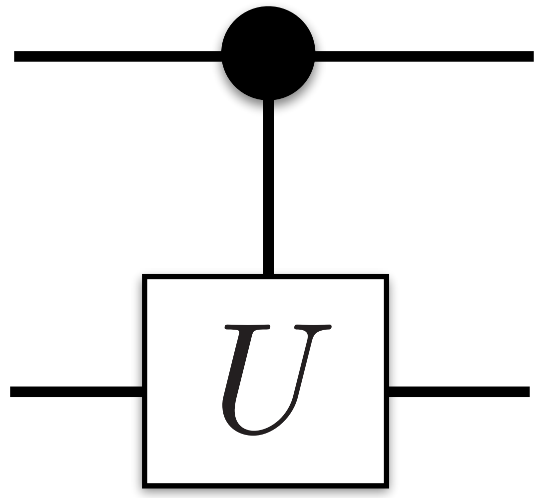
Tensor Networks



Monte Carlo Methods

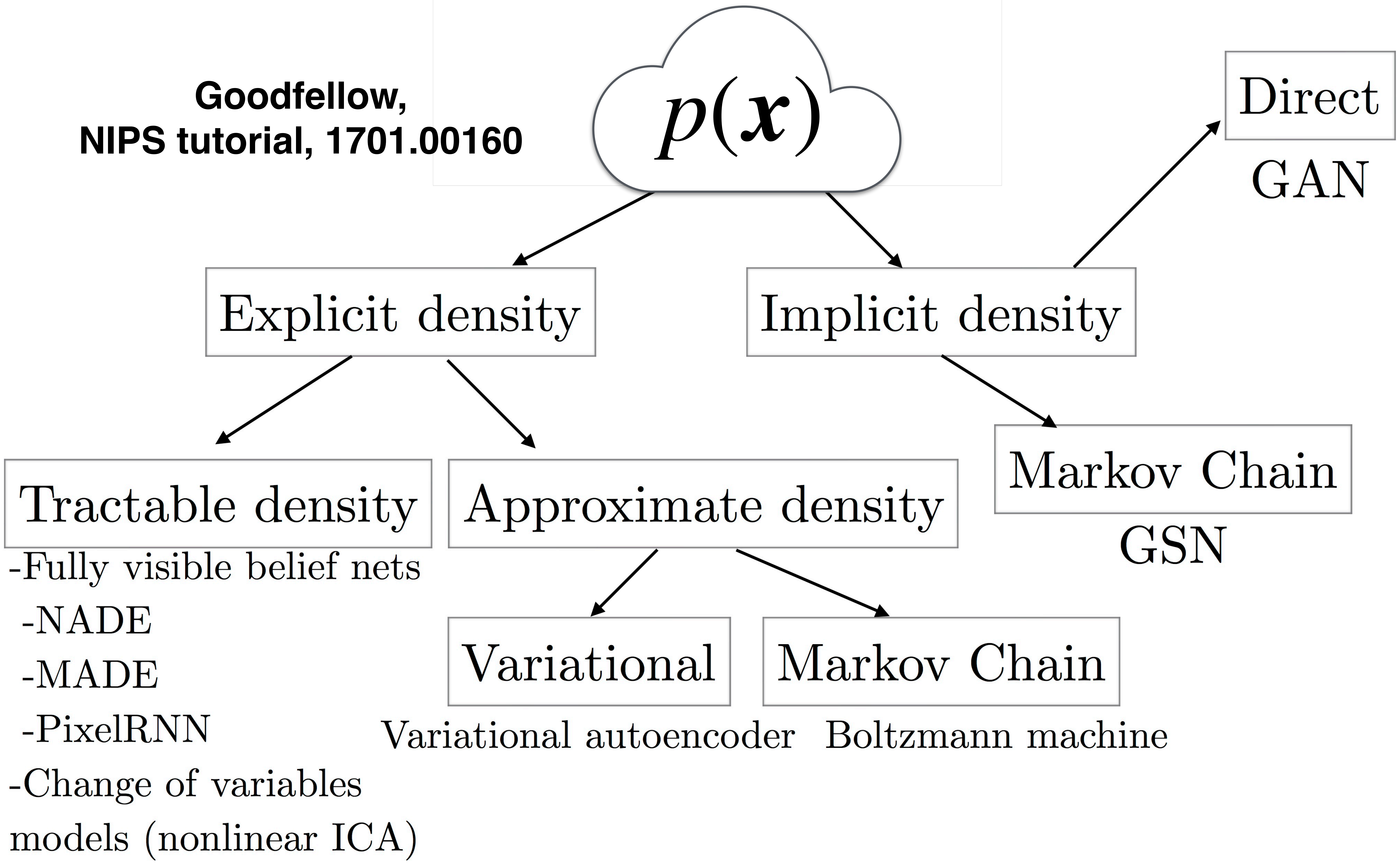


Quantum Computing



Physics genes of generative models

Goodfellow,
NIPS tutorial, 1701.00160



Physics genes of generative models

Goodfellow,
NIPS tutorial, 1701.00160

$p(\boldsymbol{x})$

Explicit density

Implicit density

Direct

GAN

Tractable density

-Fully visible belief nets

-NADE

-MADE

-PixelRNN

-Change of variables models (nonlinear ICA)

Approximate density

Markov Chain

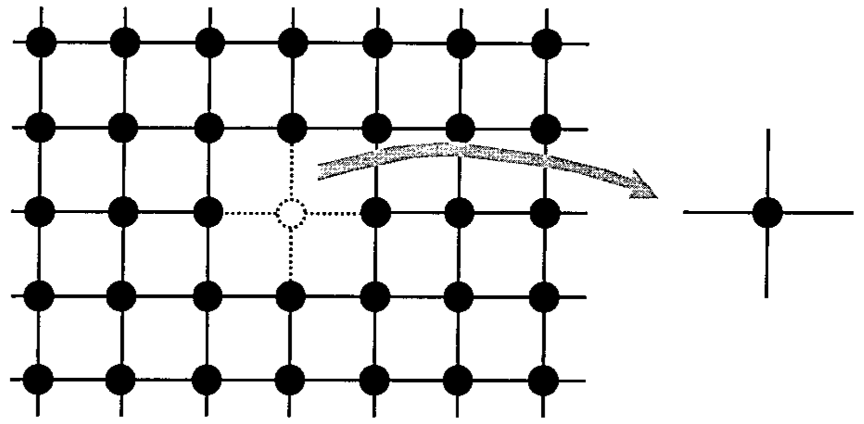
GSN

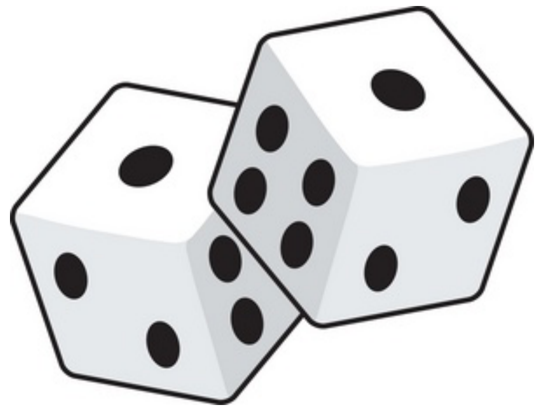
Variational

Variational autoencoder

Markov Chain

Boltzmann machine





Physics genes of generative models

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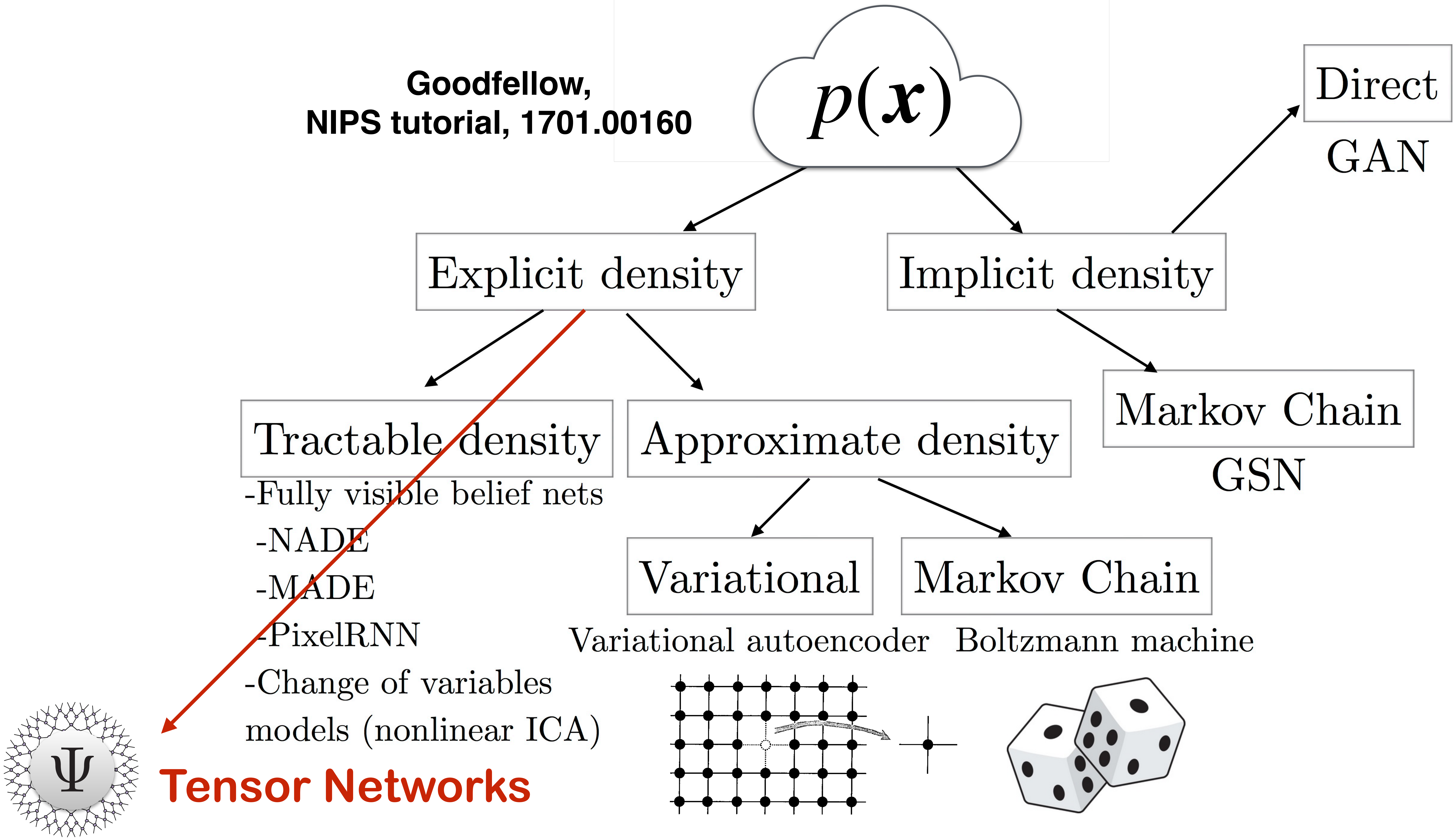
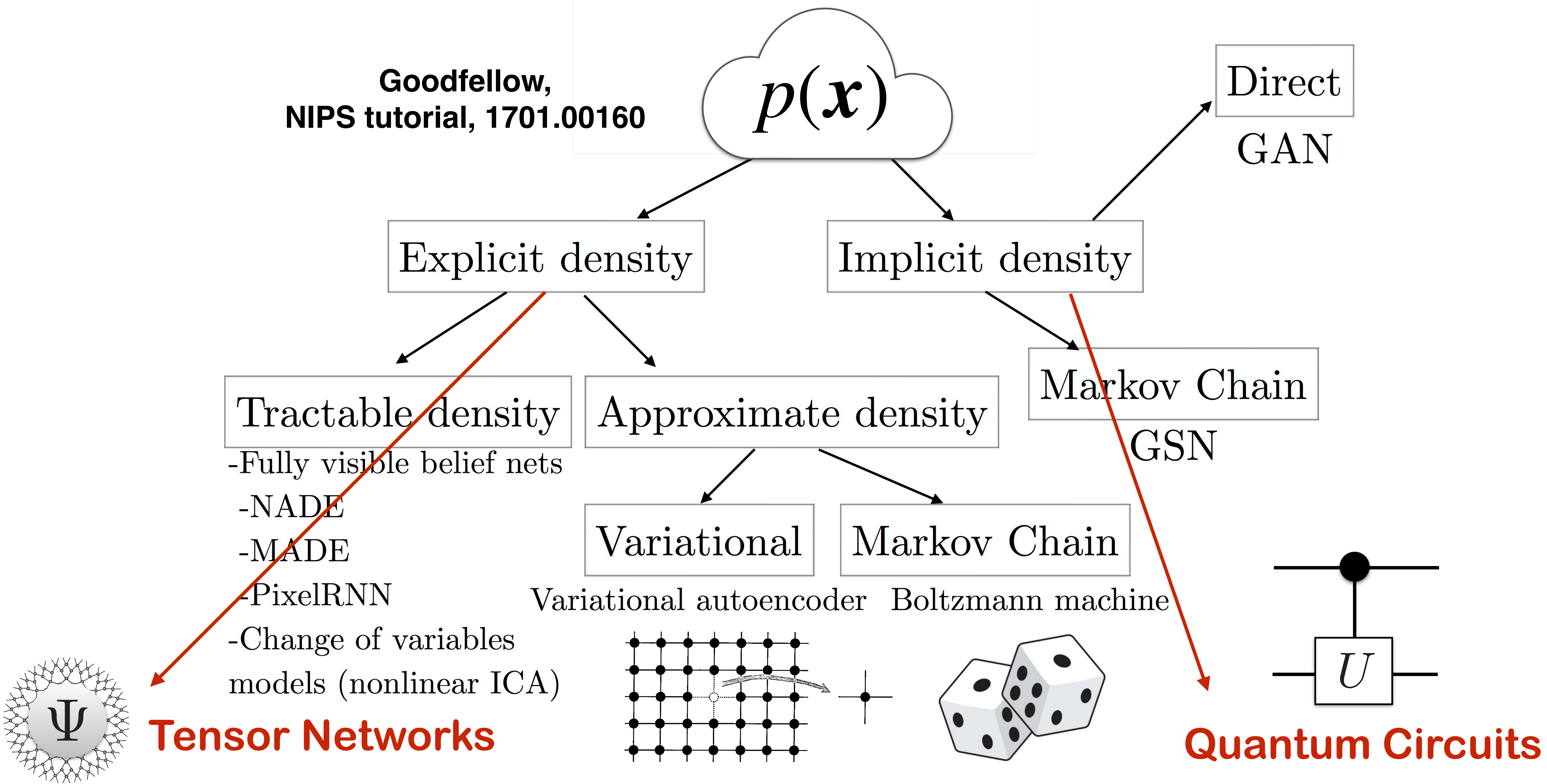


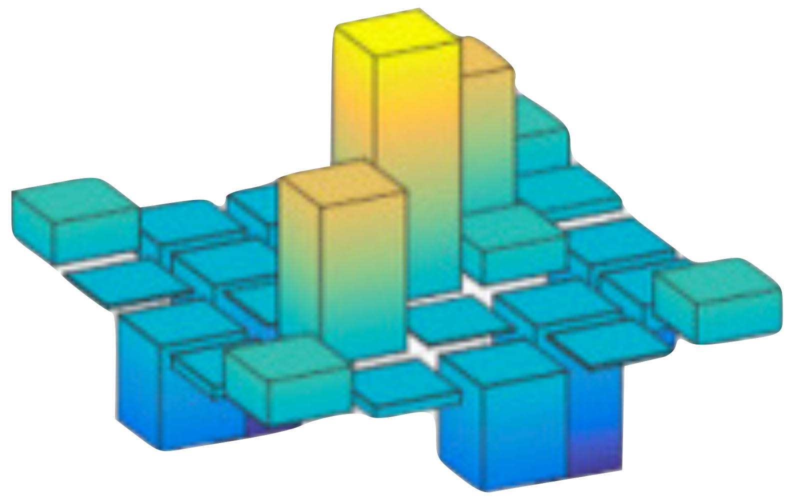
Physics genes of generative models



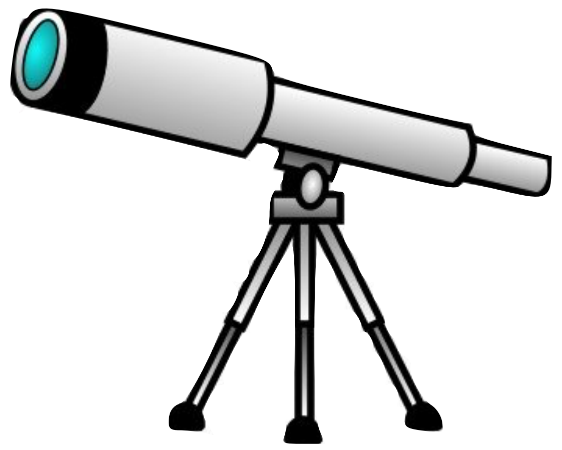
Applications in Physics

Ψ

Wavefunctions ansatz



Quantum tomography

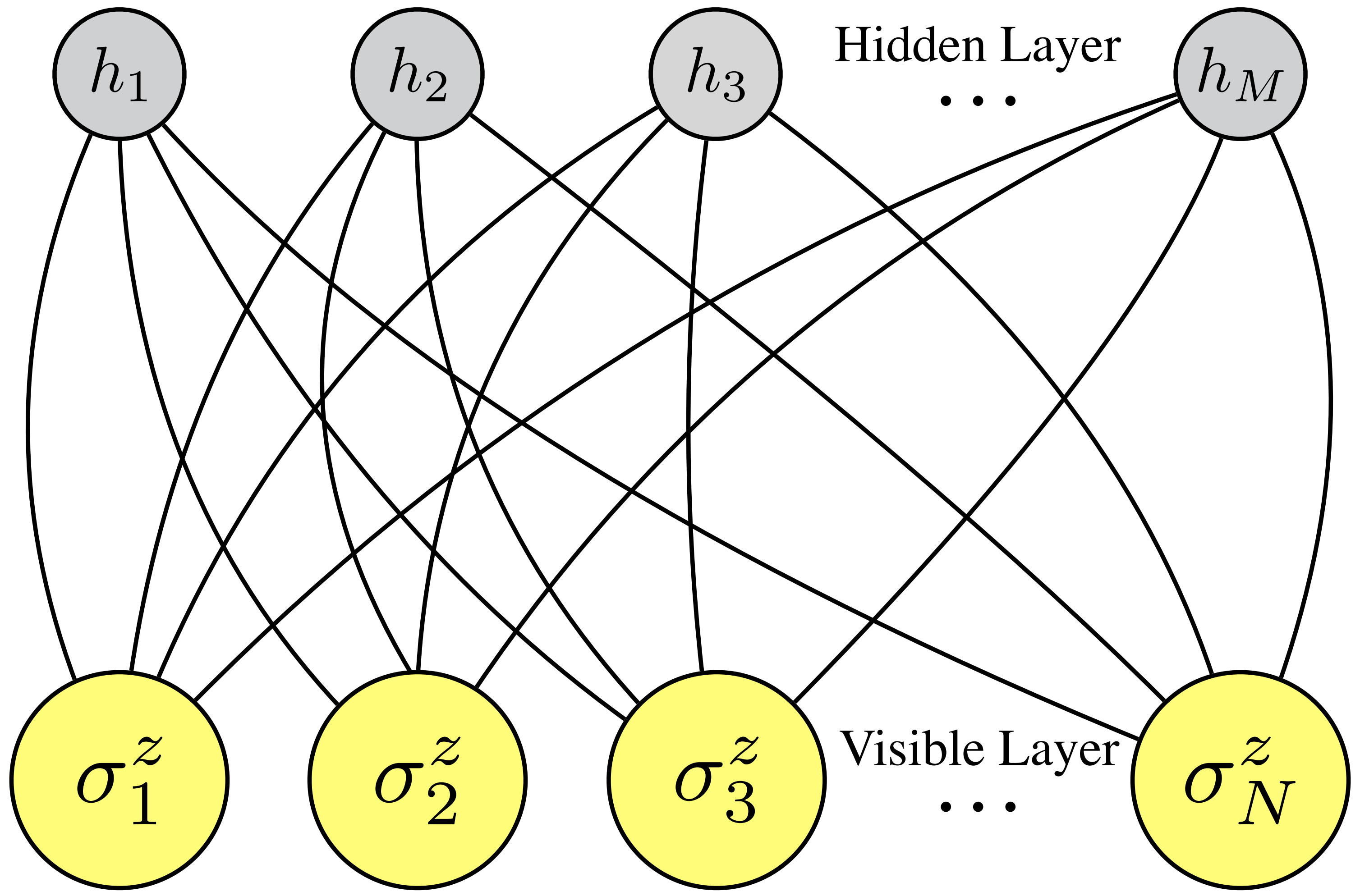


Renormalization group

Monte Carlo update

RBM as a variational ansatz

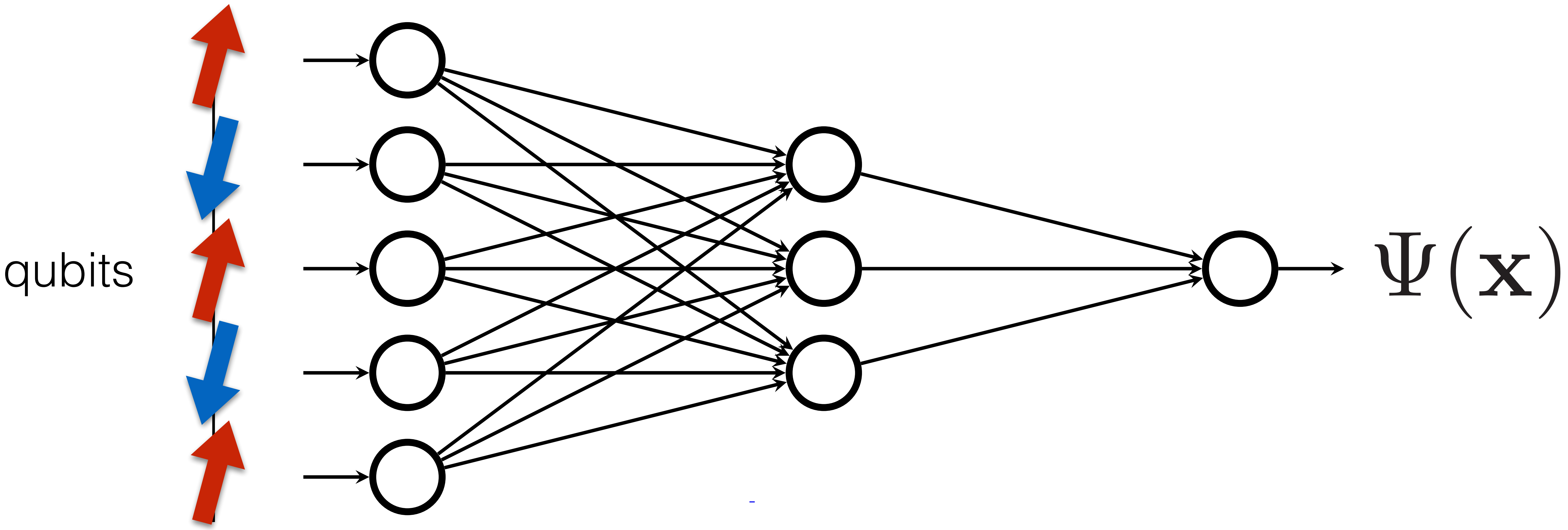
Carleo and Troyer, Science 2017



- Exact construction for 1d SPT, 2d toric code state etc
- Related to tensor network, string-bond, correlator product states
- **Killer app ?** Long-range, volume law entanglement, chiral state, improved Jastrow/Backflow

Deng, Li, Gao, Chen, Cheng, Xiang, Clark, Glasser, Cirac, Carl Budich, Imada…

Ψ Boltzmann machine as a quantum state



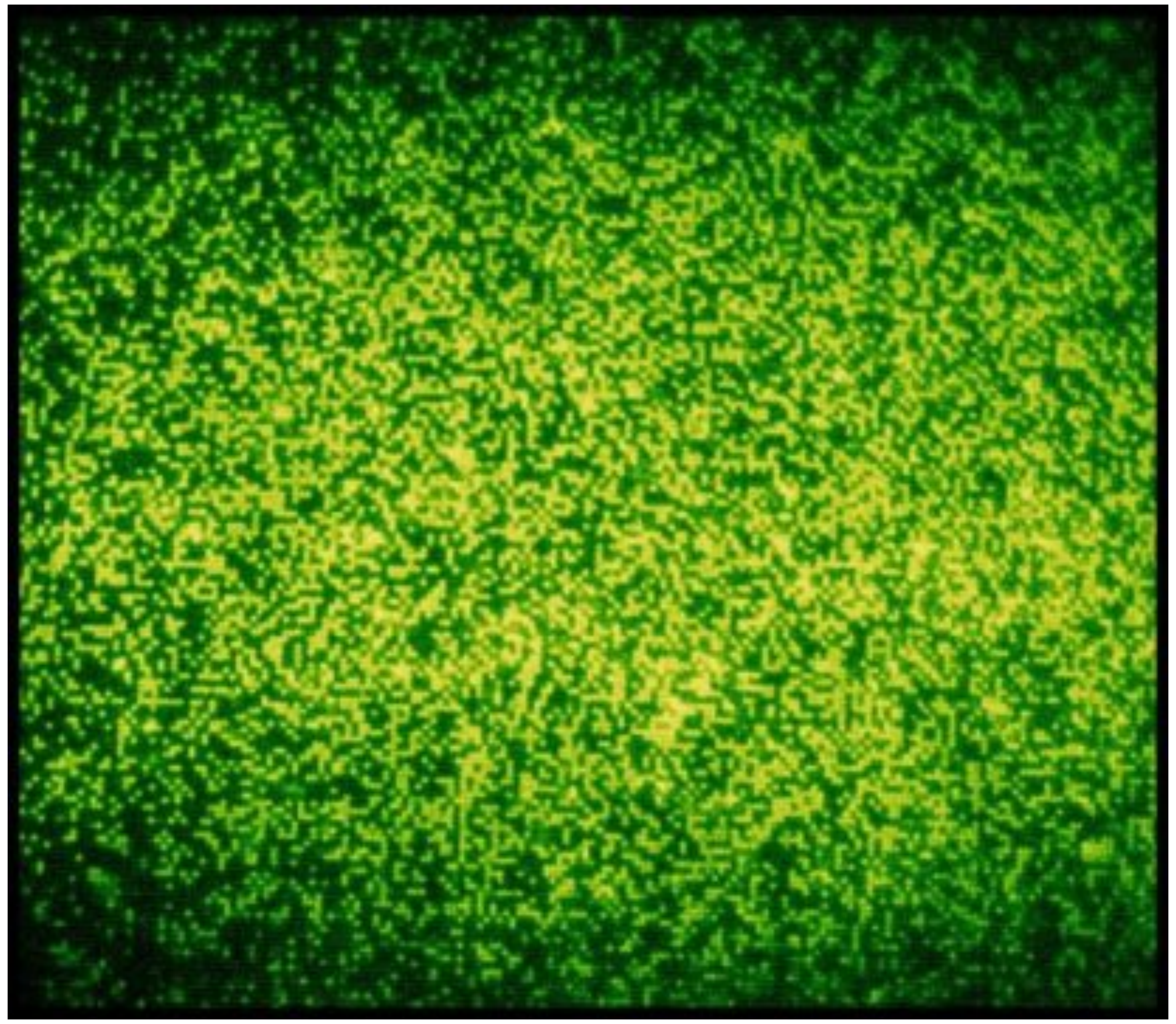
- Stronger feature detection of deep hierarchical structure
- BackProp for efficient gradient computation
- **Beyond VMC**: variational autoregressive networks (VAN)

"Teach a neural network quantum & statistical physics"

Cai, Liu, Han, He, Clark, Wu, Zhang…

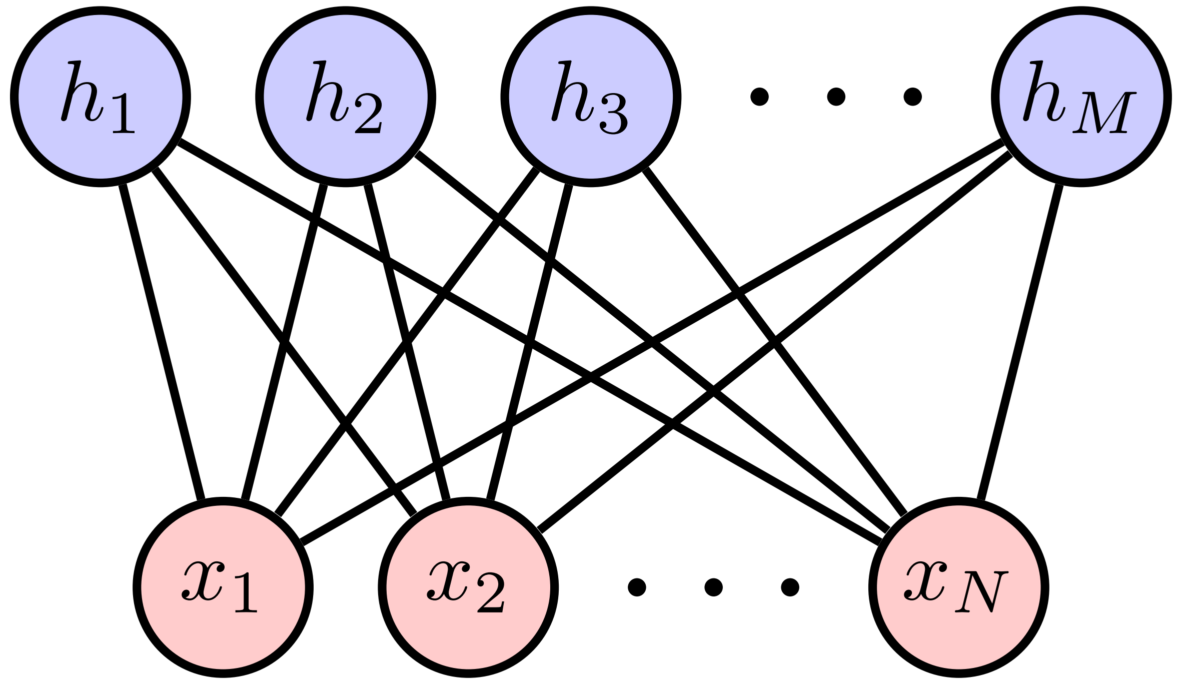
Quantum State Tomography

Ψ $\xrightarrow{\text{Measure}}$



$\xrightarrow{\text{Reconstruction}}$

$$\psi_{\lambda,\mu}(\mathbf{x}) = \sqrt{\frac{p_\lambda(\mathbf{x})}{Z_\lambda}}\, e^{i\phi_\mu(\mathbf{x})/2}$$



RBMs
(but other generative models also work)

"Reconstruct quantum state as a neural network"

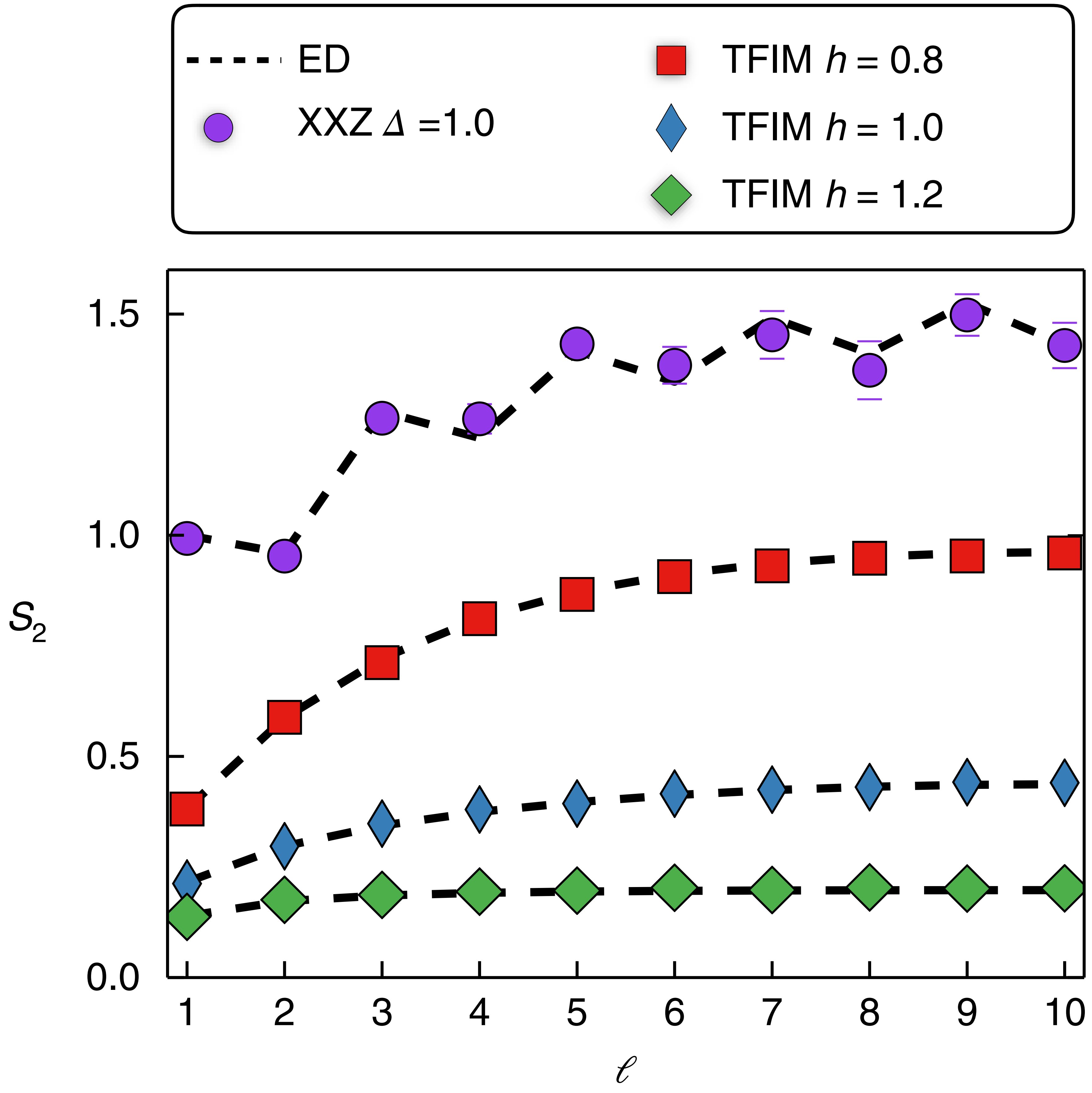
Torlai et al, Nature Physics 2017, Carrasquilla et al 1810.10584

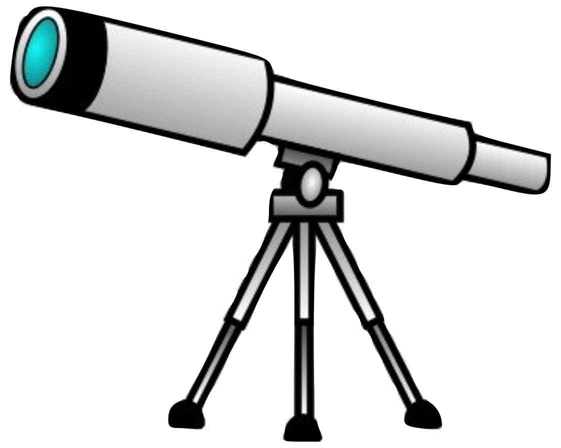
Applications of QST

Observables inaccessible
to the experiment

XX spin correlations
(unpublished)

Entanglement entropy





RG and Deep Learning

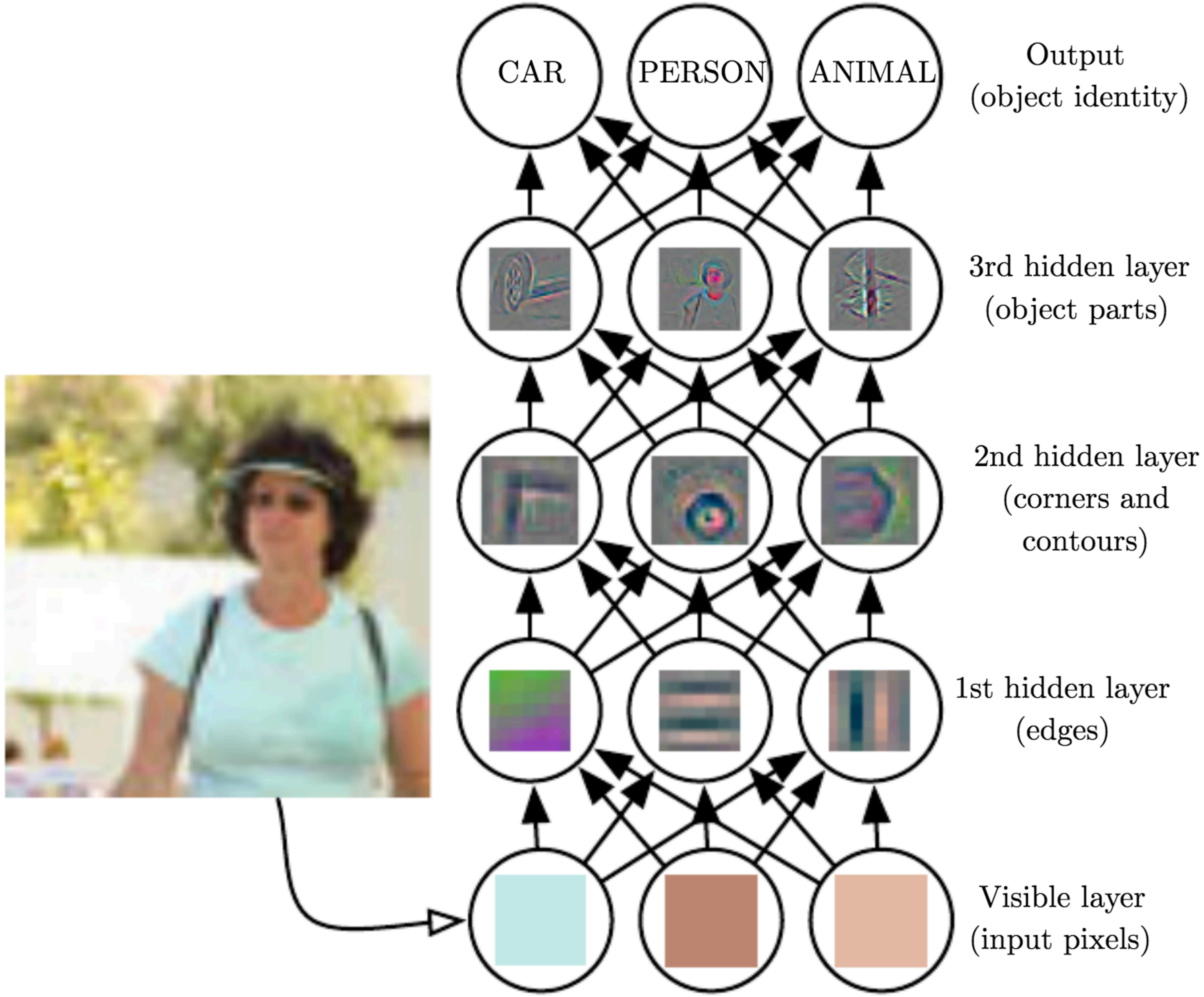


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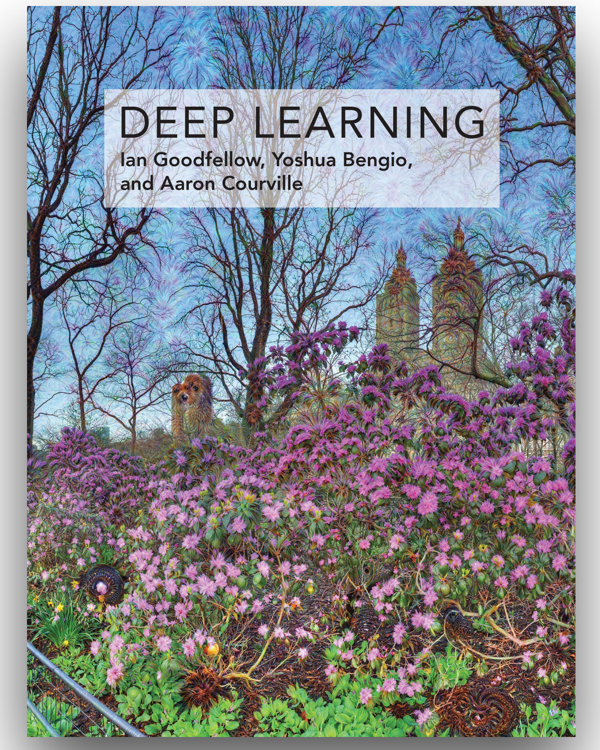
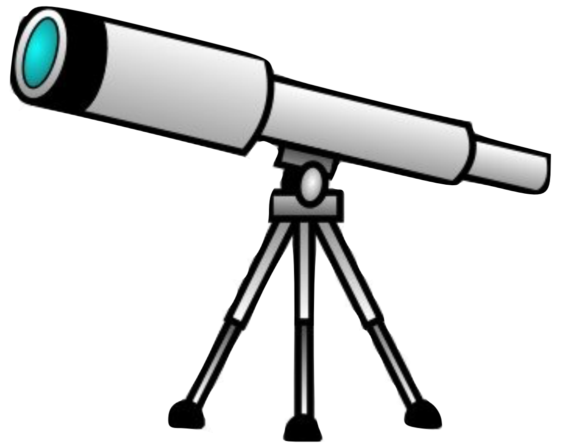
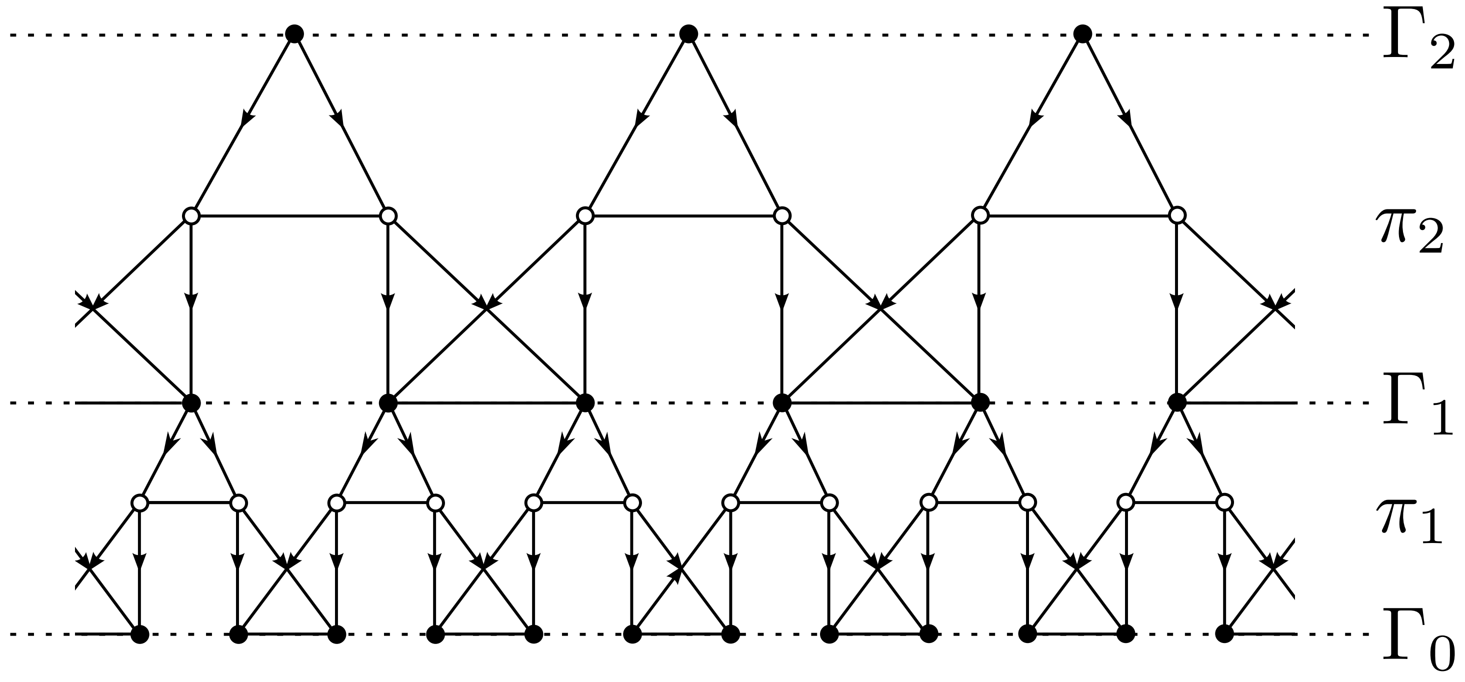
Figure 1.2



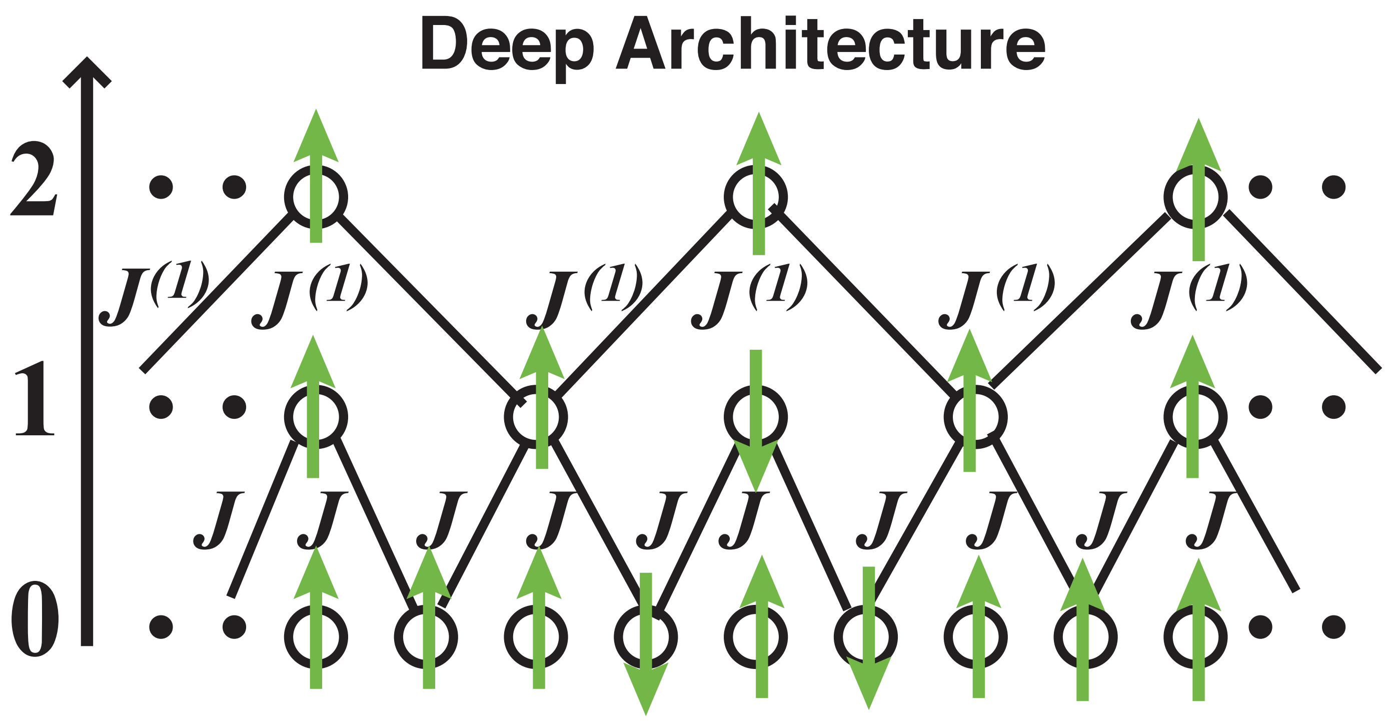
Goodfellow, Bengio, Courville, http://www.deeplearningbook.org/



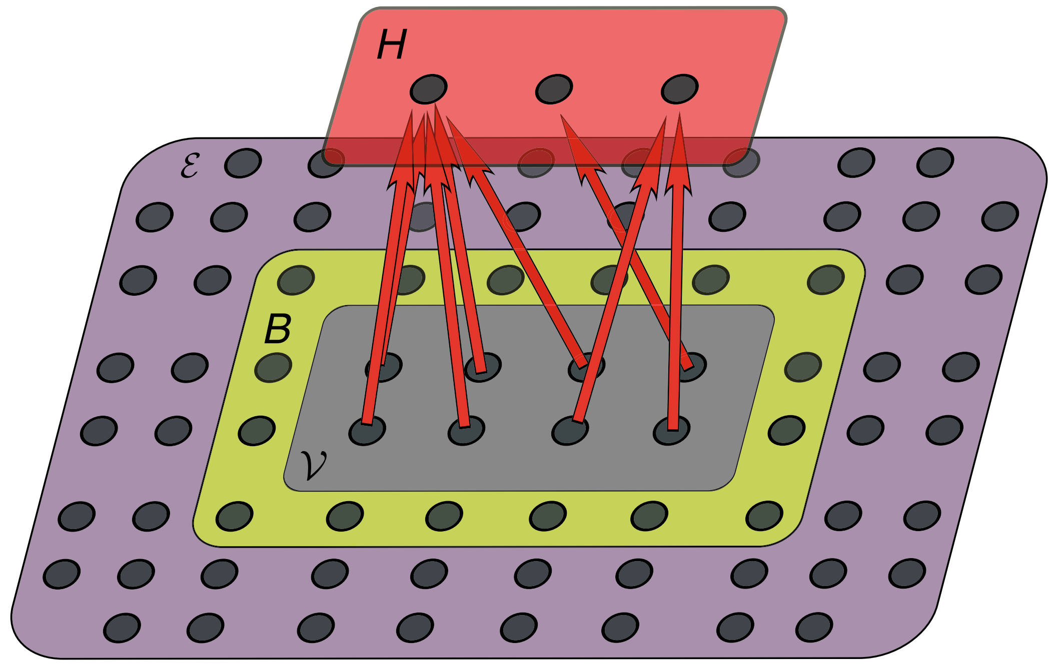
RG and Deep Learning



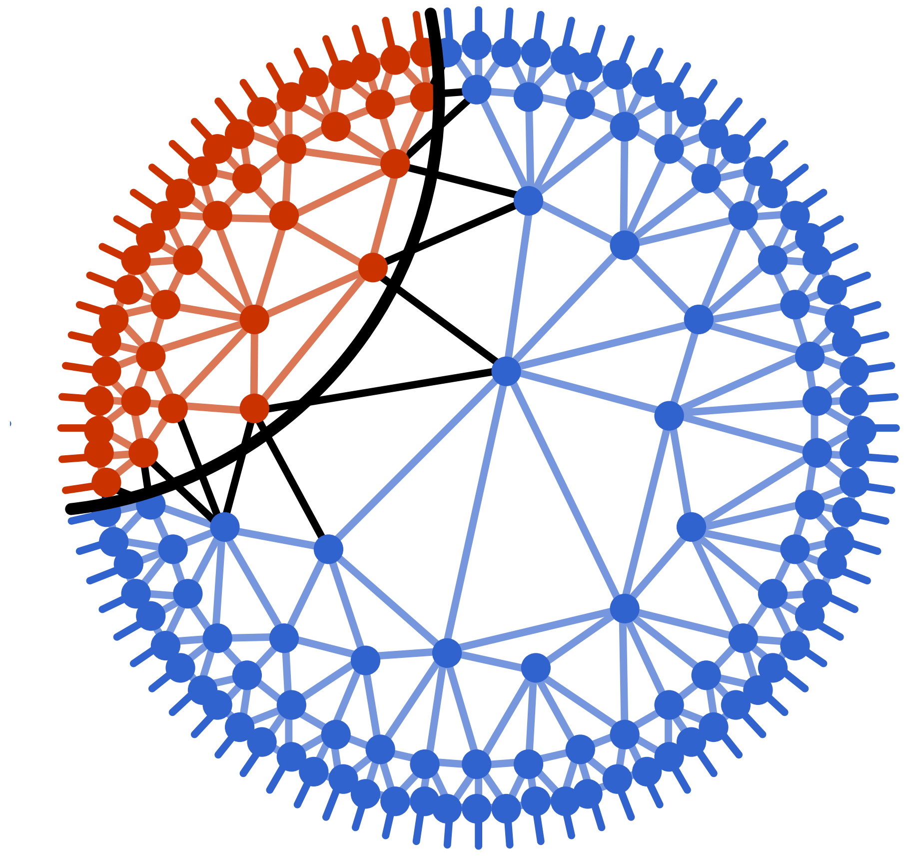
Bény, 1301.3124



Mehta and Schwab, 1410.3831



Koch-Janusz and Ringel, 1704.06279

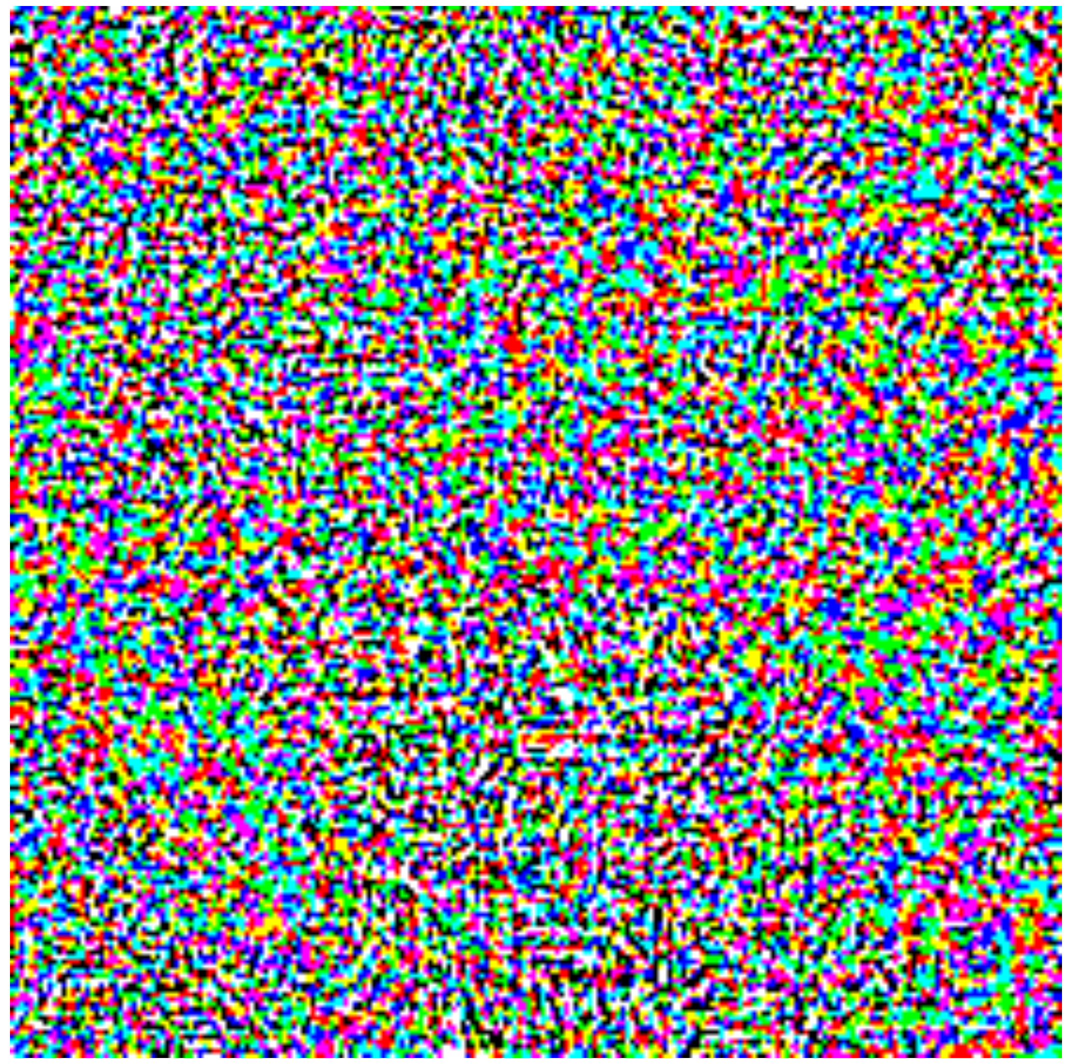


You, Yang, Qi, 1709.01223

and more…

RG and Deep Learning

$+ .007 \times$



$=$

Panda
58% confidence

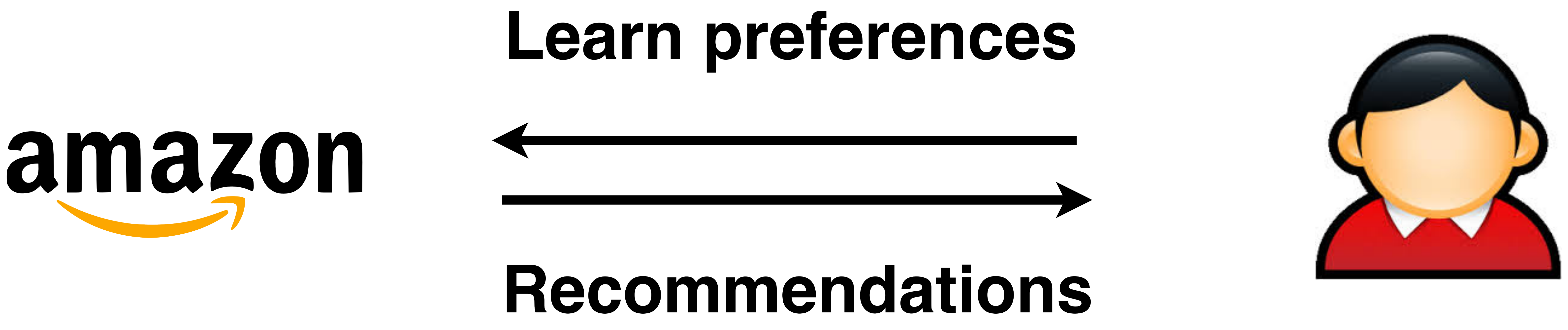
Goodfellow et al, 2014

Gibbon
99% confidence

Vulnerability of deep learning, Kenway, 1803.06111 & 1803.10995

and more…

Monte Carlo update proposals using Boltzmann Machines

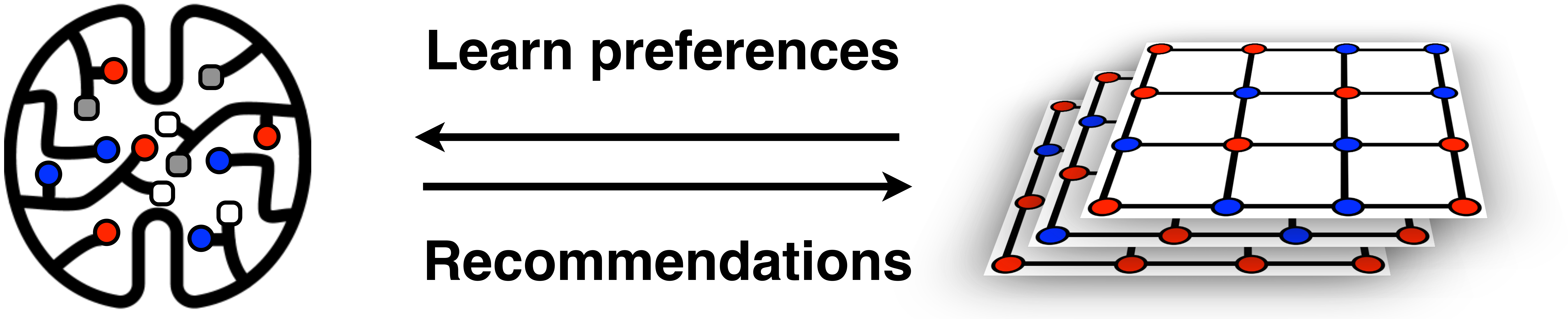


- Use Boltzmann Machines as recommender systems for Monte Carlo simulation of physical problems

Li Huang and LW, 1610.02746

Liu, Qi, Meng, Fu, 1610.03137

Monte Carlo update proposals using Boltzmann Machines



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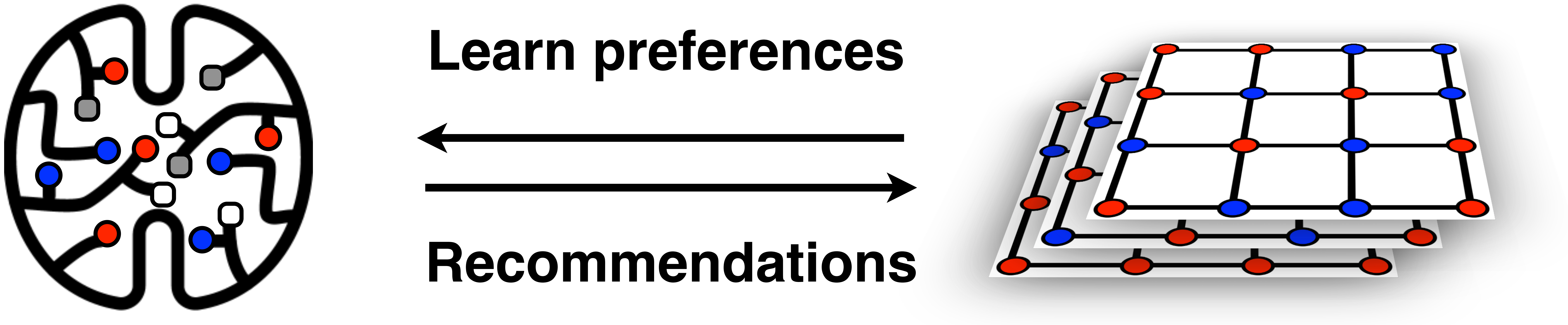
Monte Carlo update proposals using Boltzmann Machines



- Use Boltzmann Machines as recommender systems for Monte Carlo simulation of physical problems

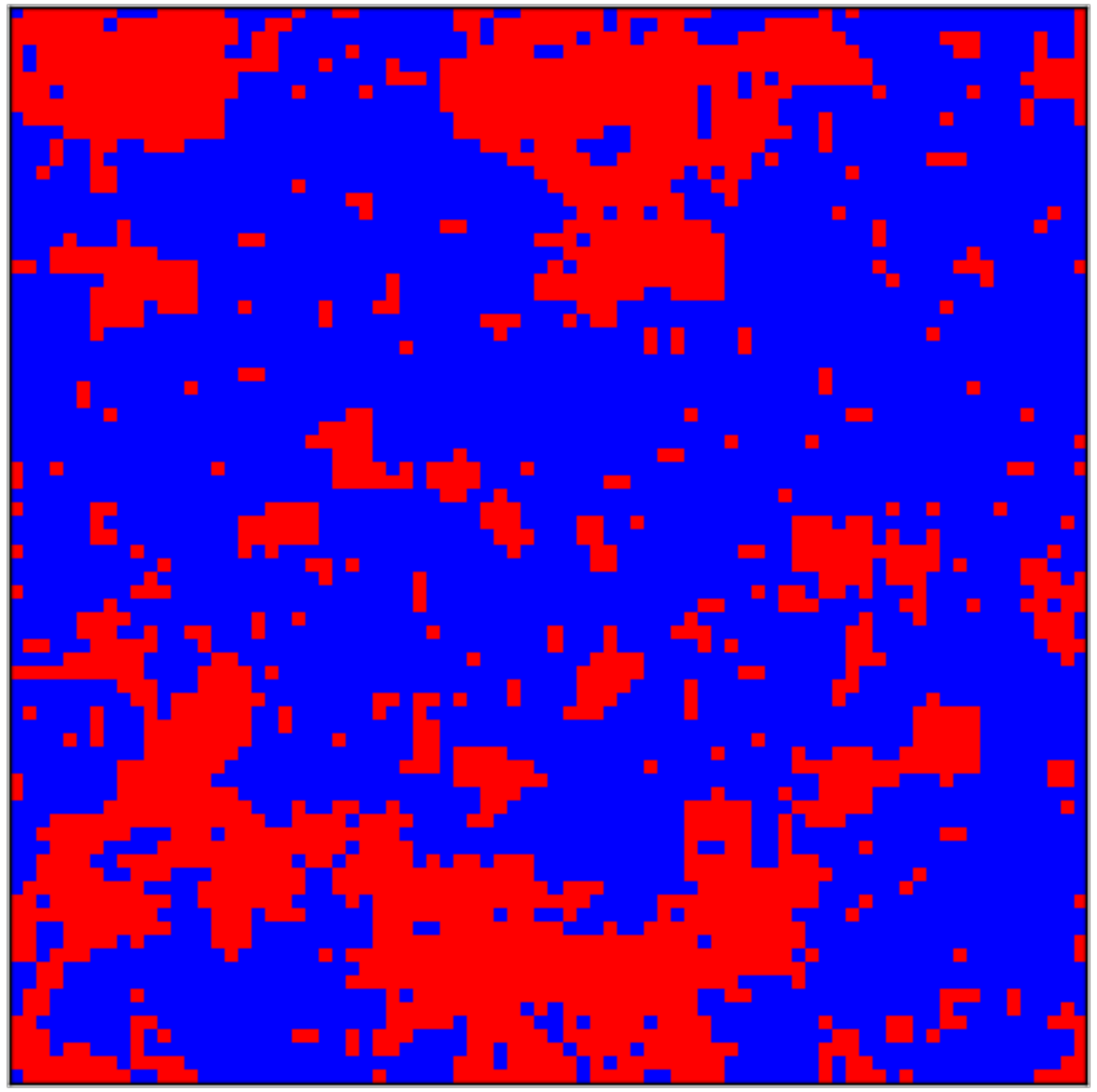
Li Huang and LW, 1610.02746

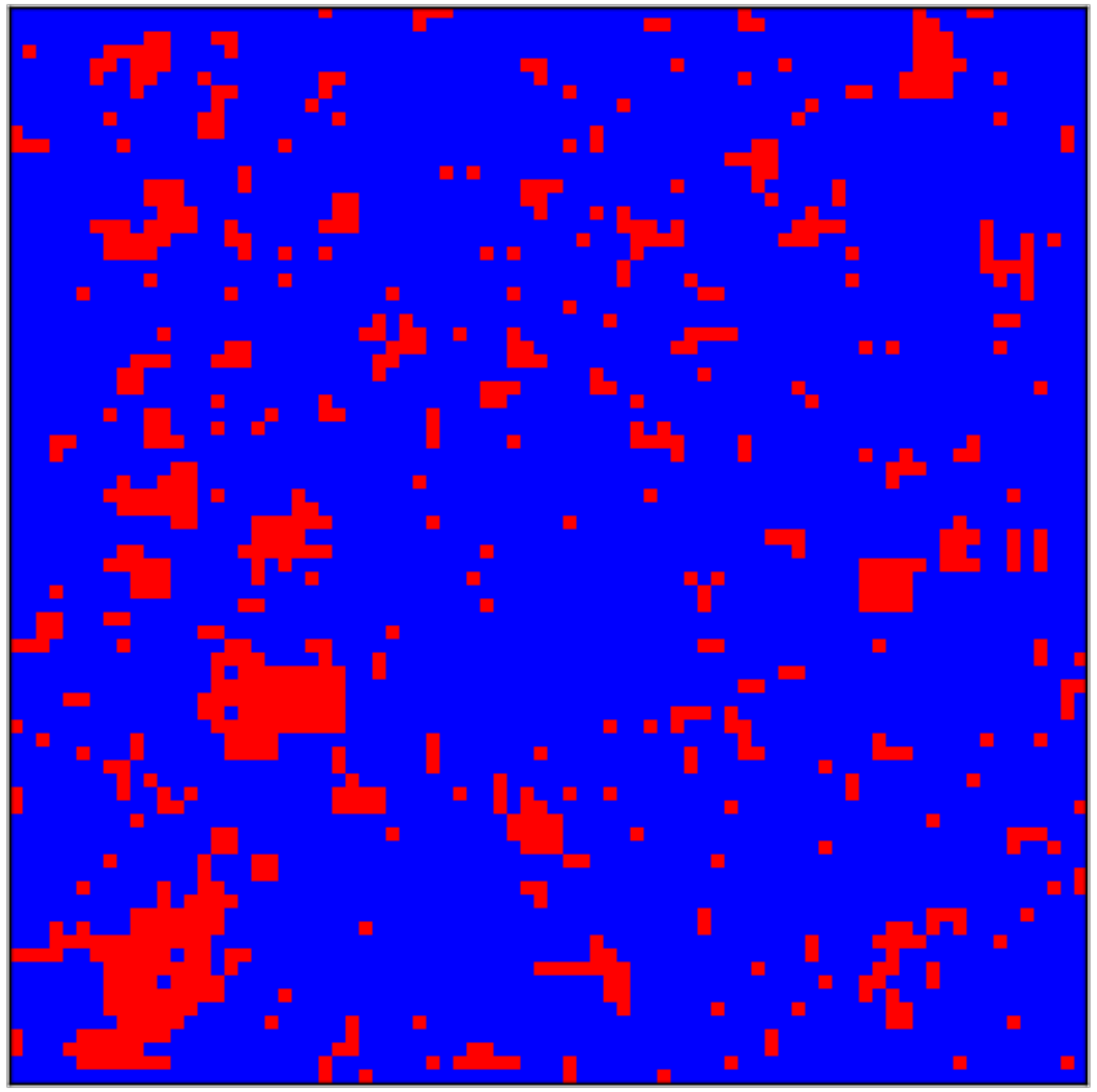
Liu, Qi, Meng, Fu, 1610.03137

- Moreover, BM parametrizes Monte Carlo policies and can explore novel algorithms!

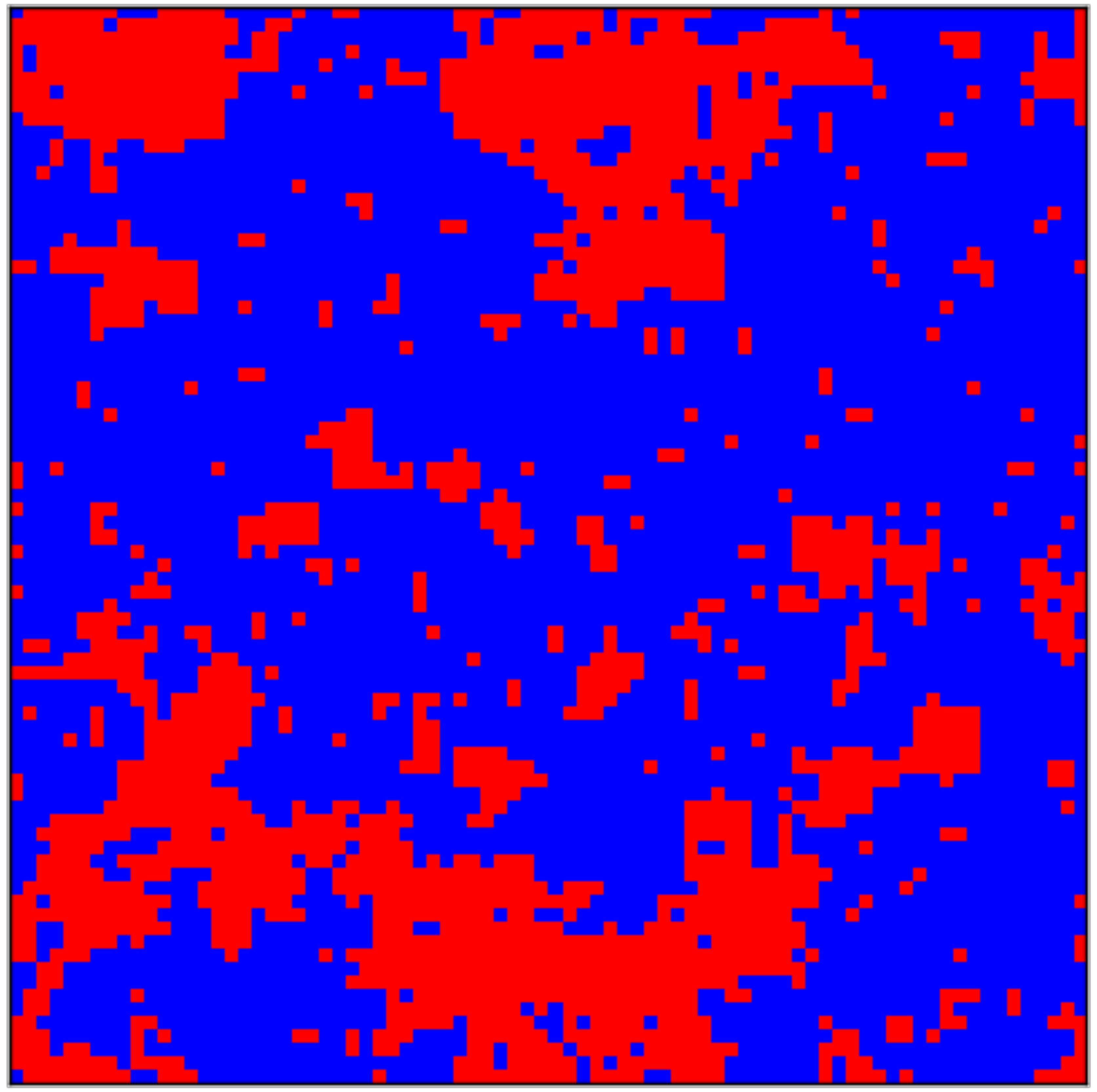
LW, 1702.08586

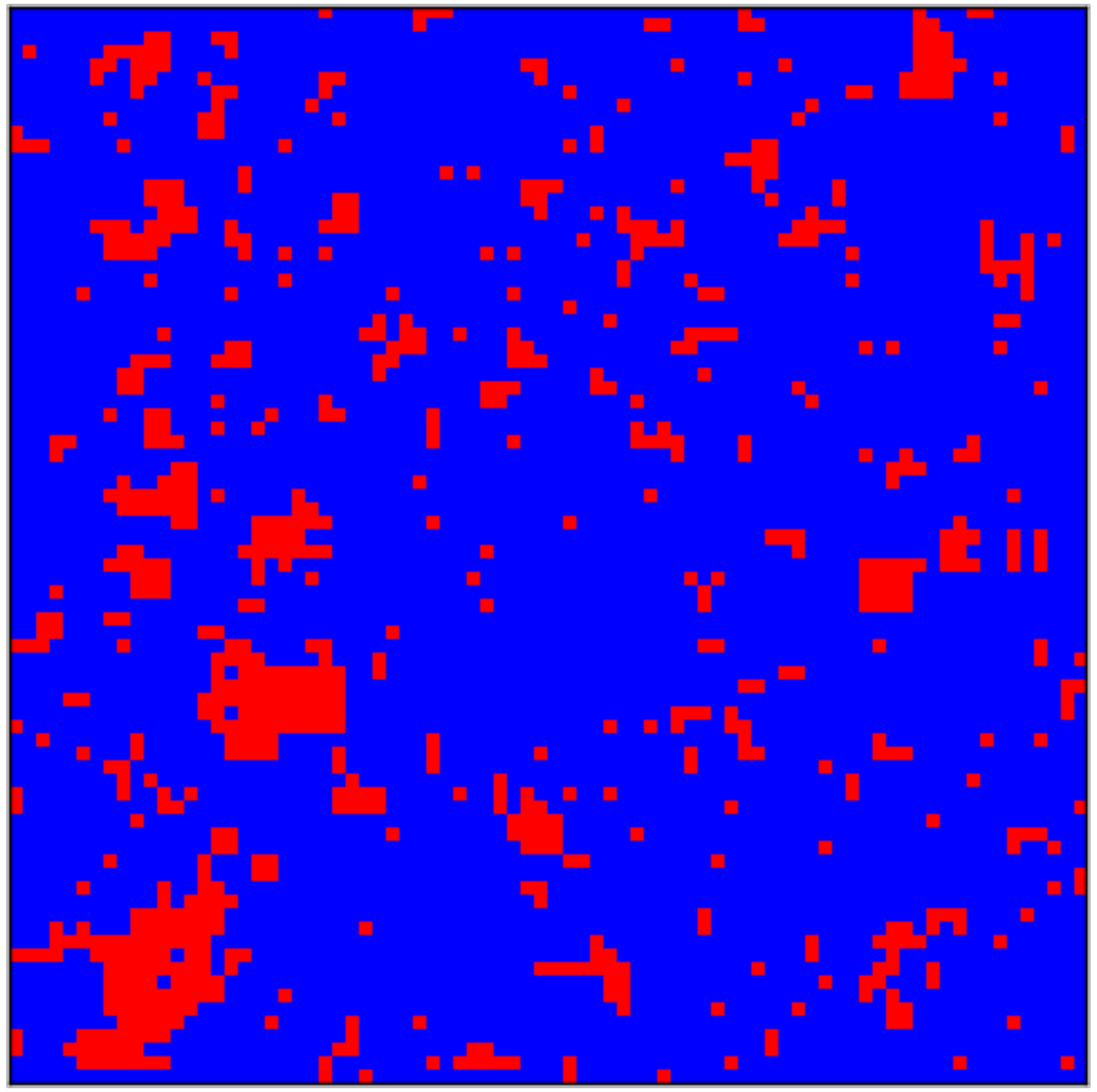
Local vs Cluster update polices



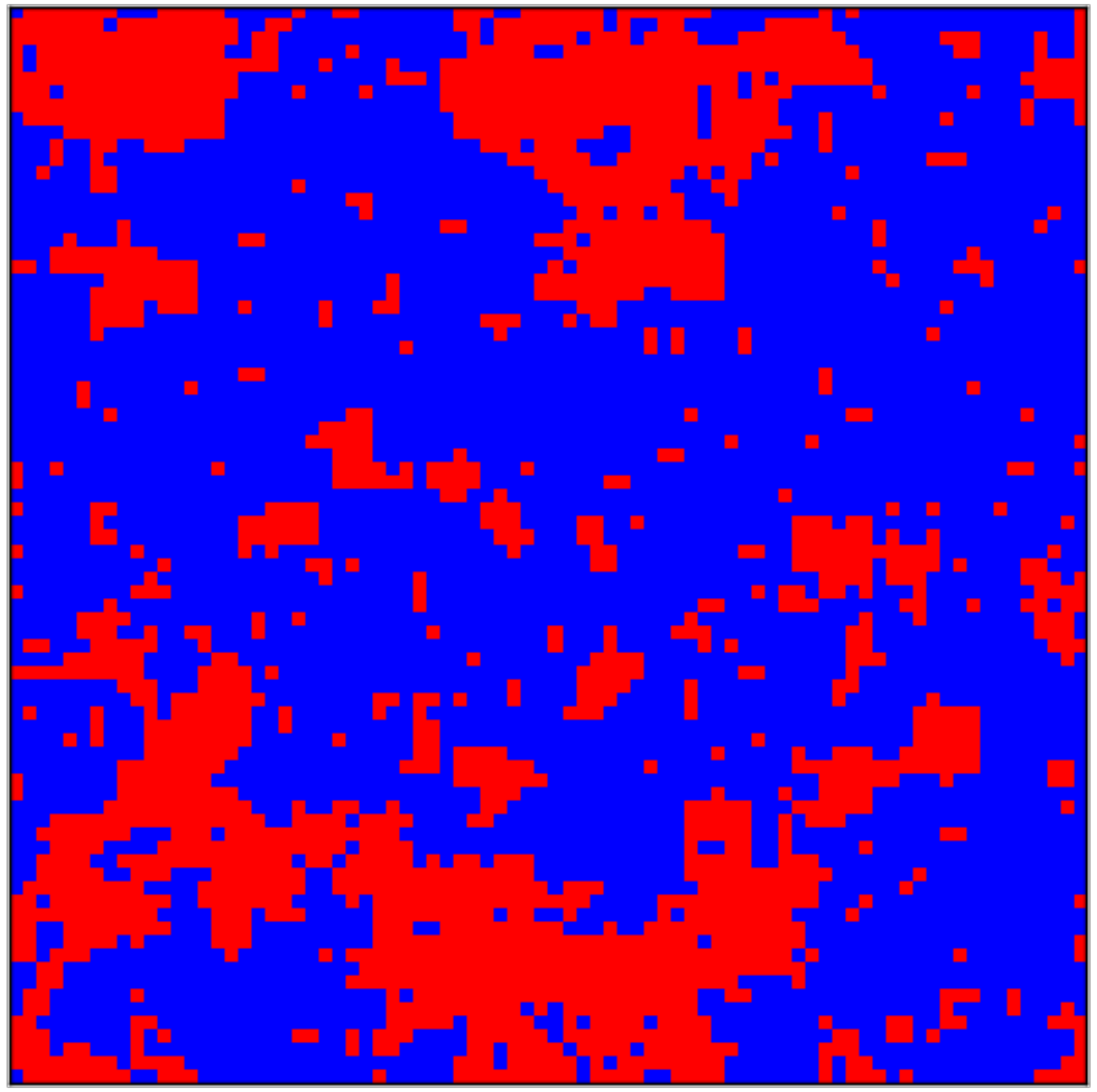


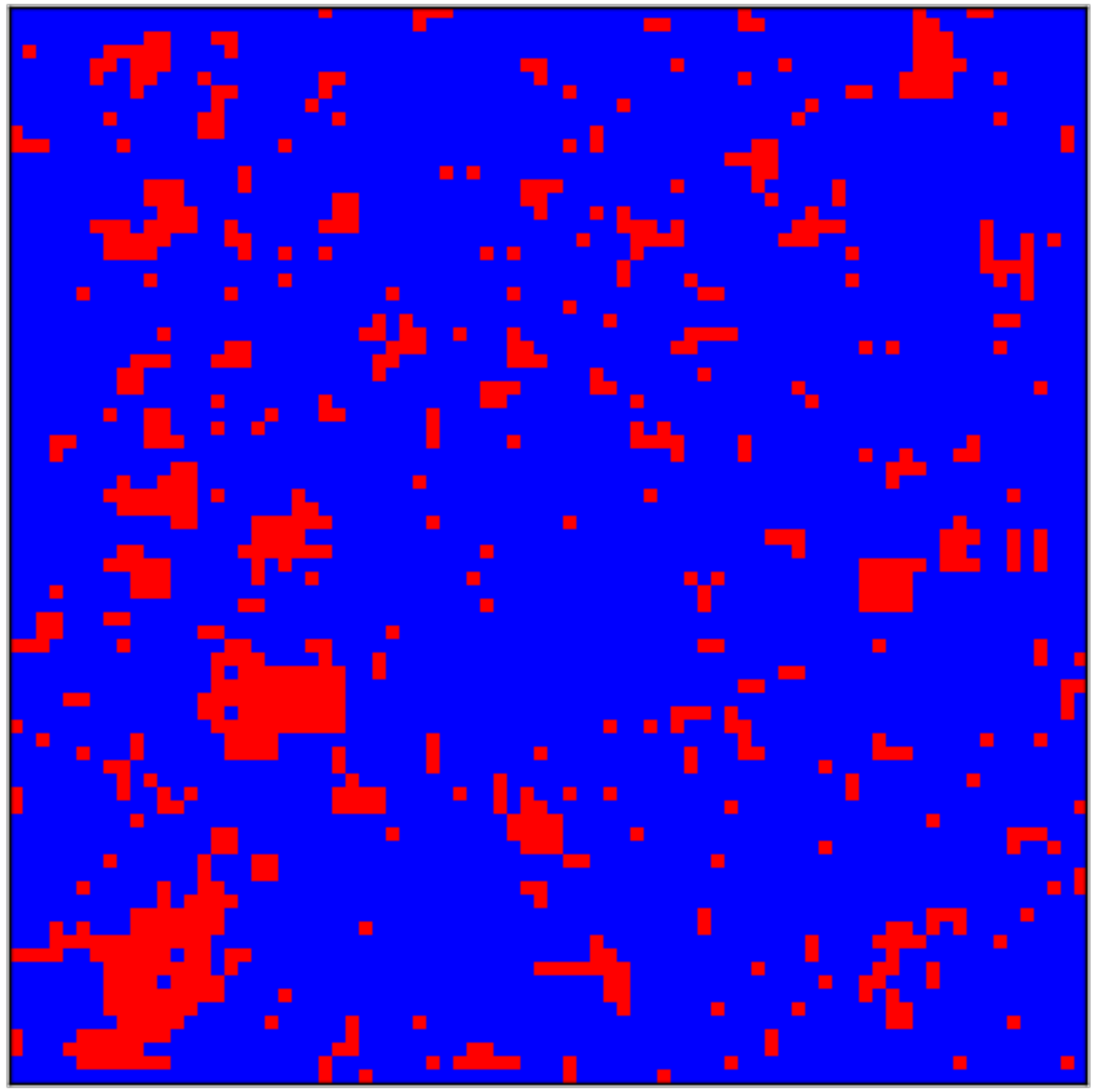
Local vs Cluster update polices



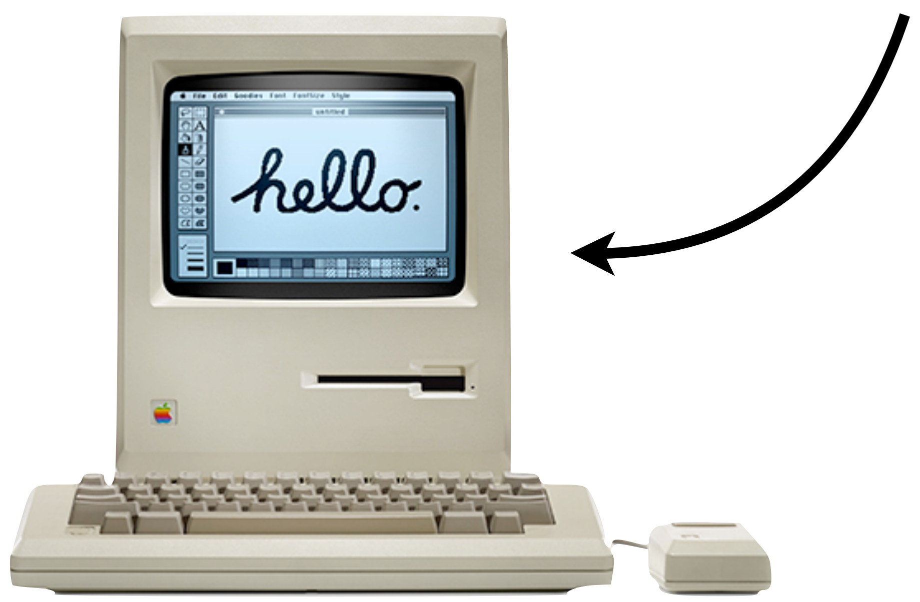


Local vs Cluster update polices

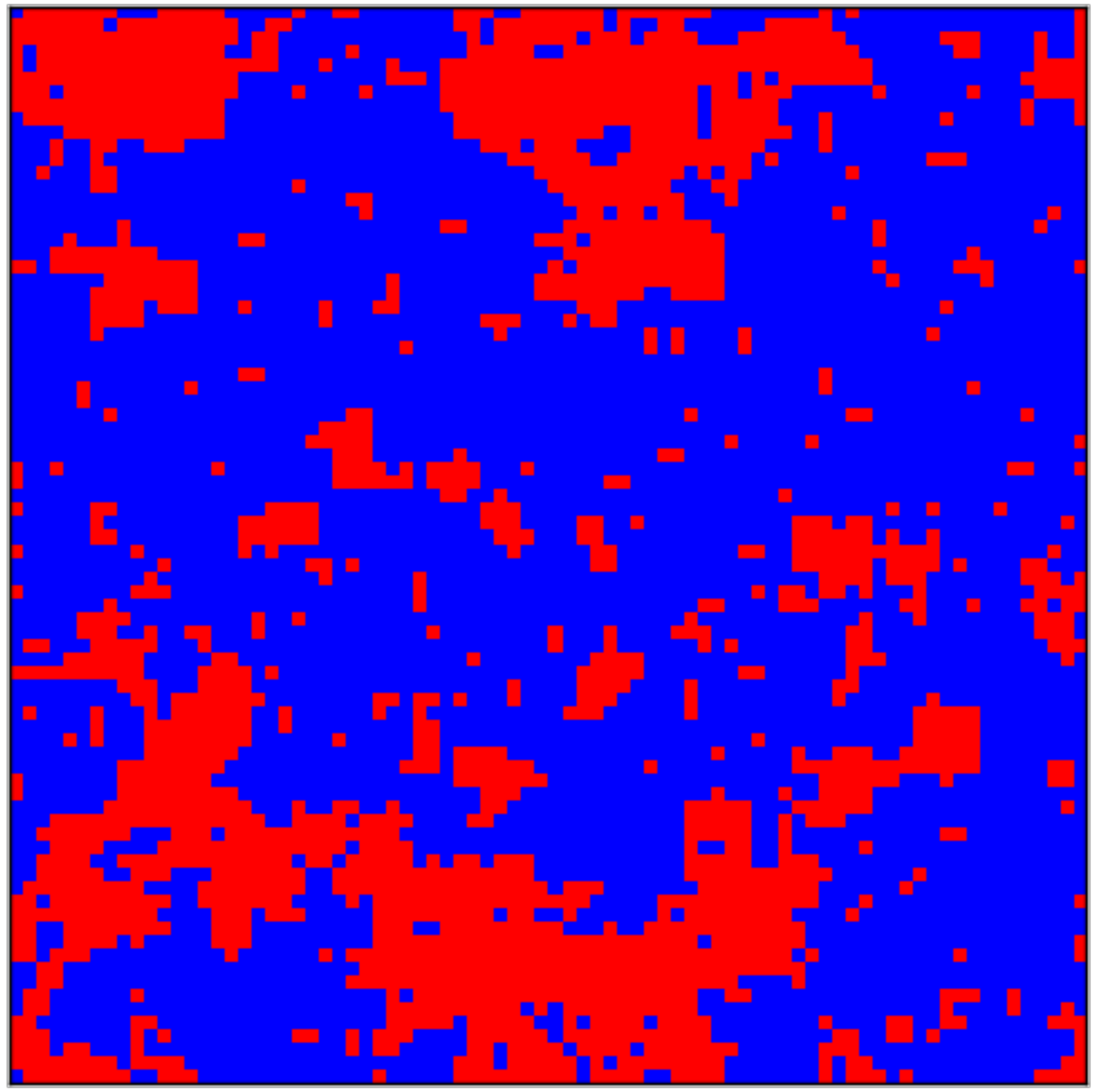


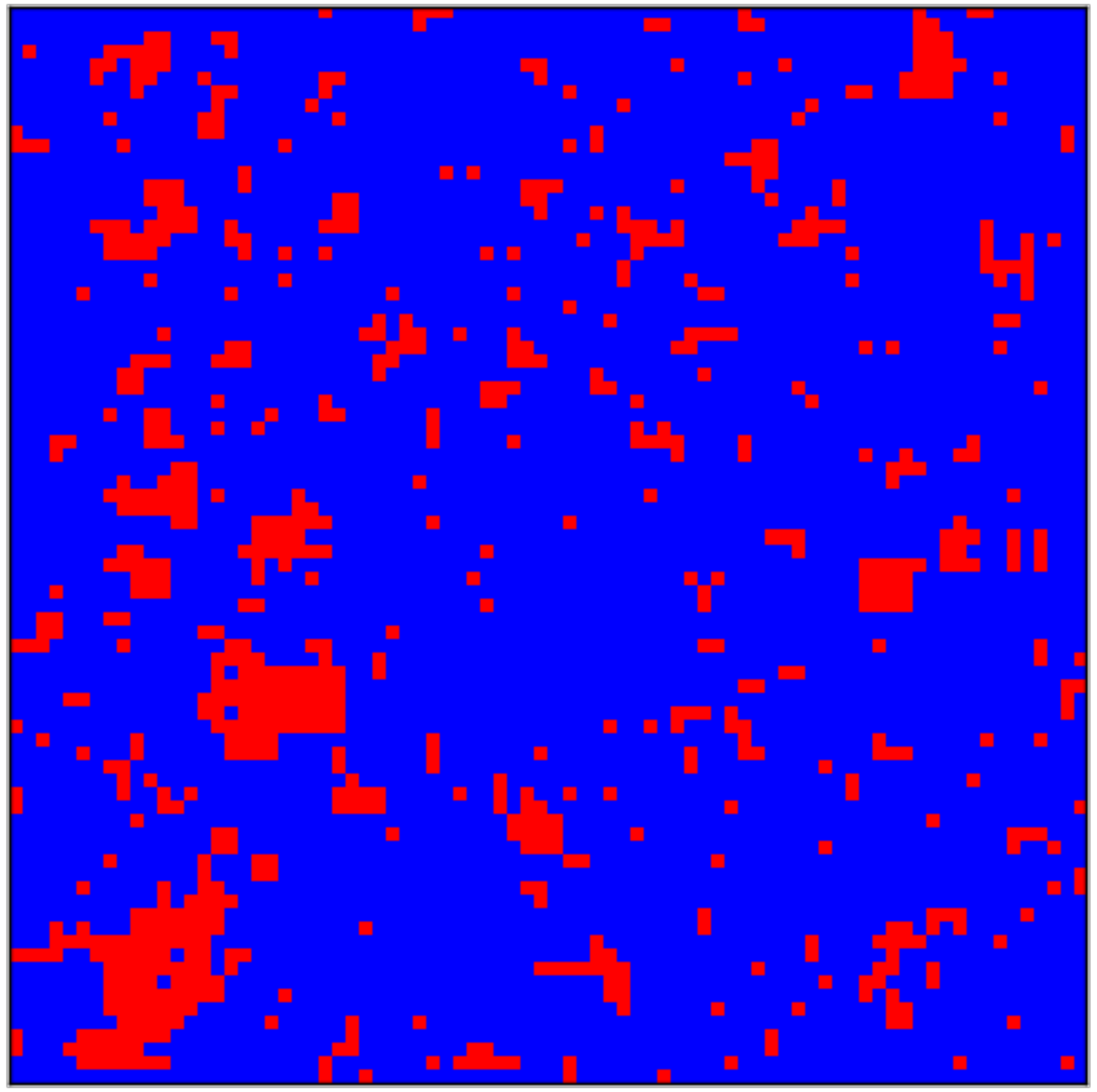


is slower than



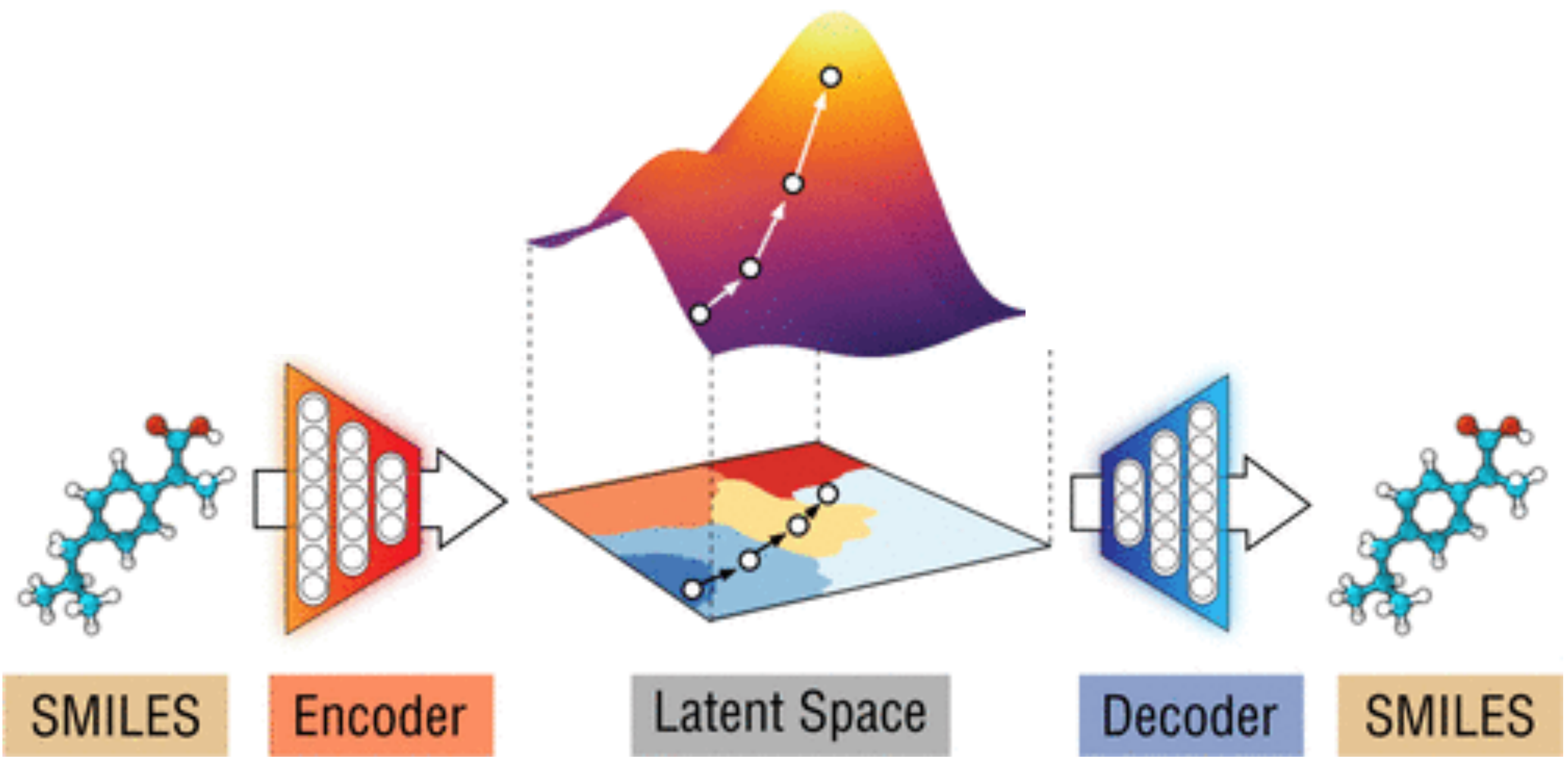
Local vs Cluster update polices



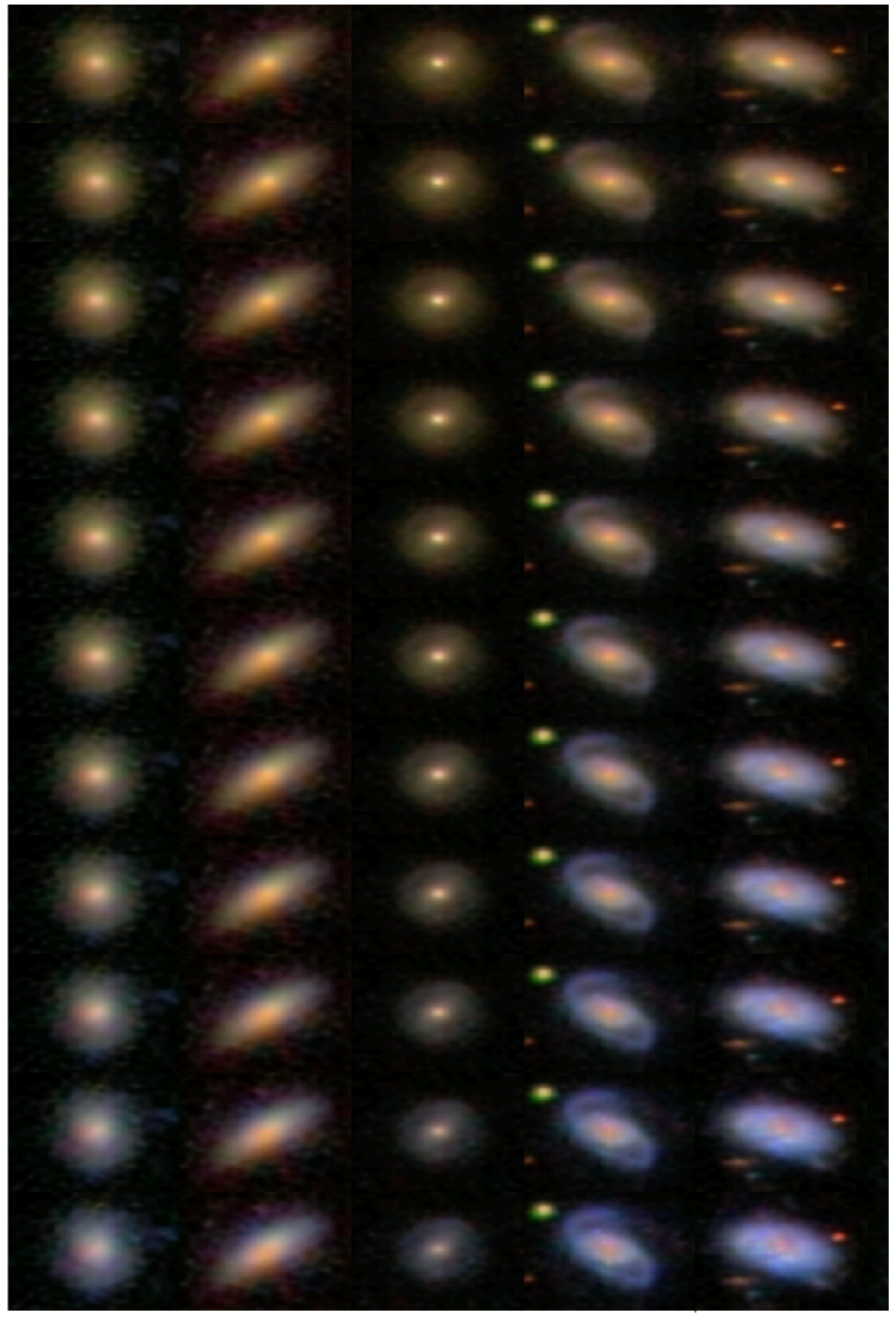


Algorithmic innovation outperforms Moore's law!

And more…

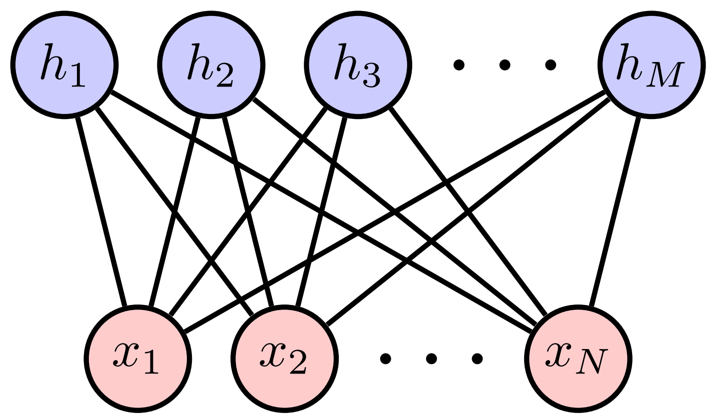


Automatic chemical design
Gomez-Bombarelli et al,1610.02415



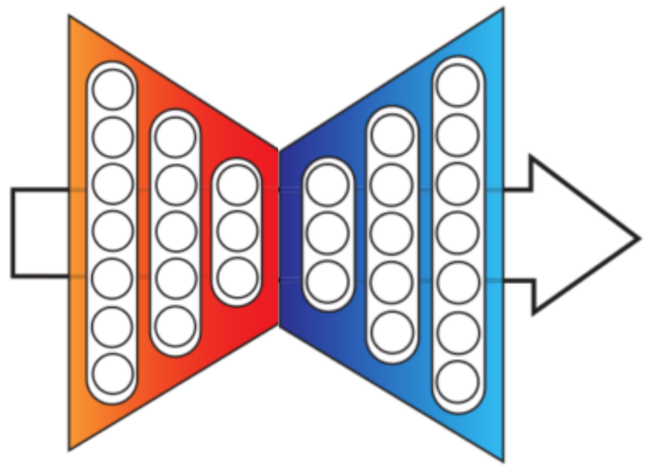
Galaxy evolution
Schawinski et al, unpublished

Timeline of Generative Models



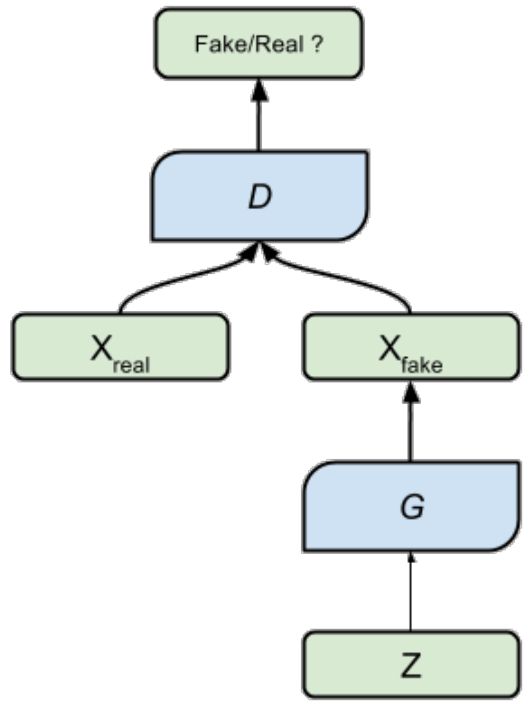
Boltzmann Machines

1980s



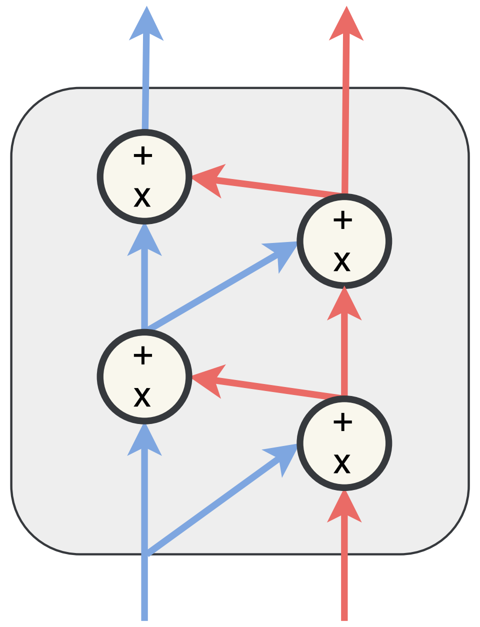
Variational Autoendoer

2013



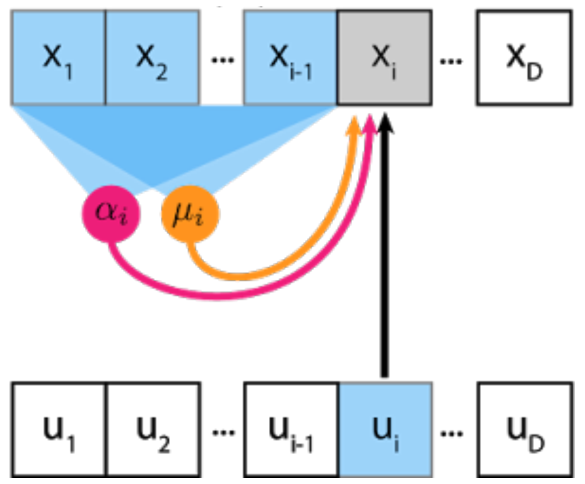
Adversarial Network

2014



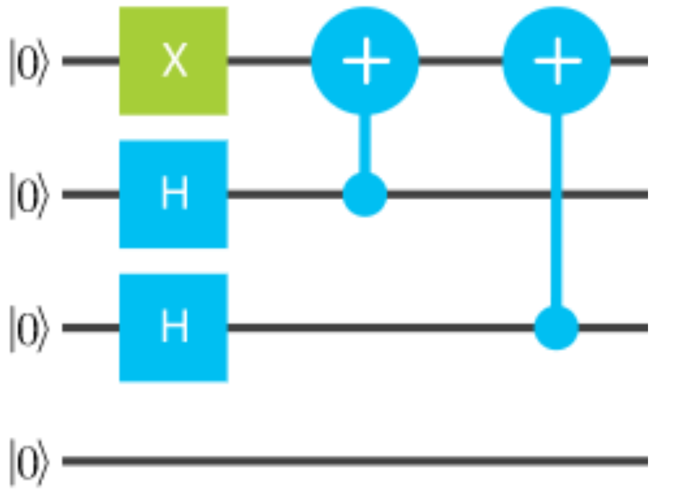
Normalizing Flows

2015



Autoregressive Flows

2016



Born Machines

2017

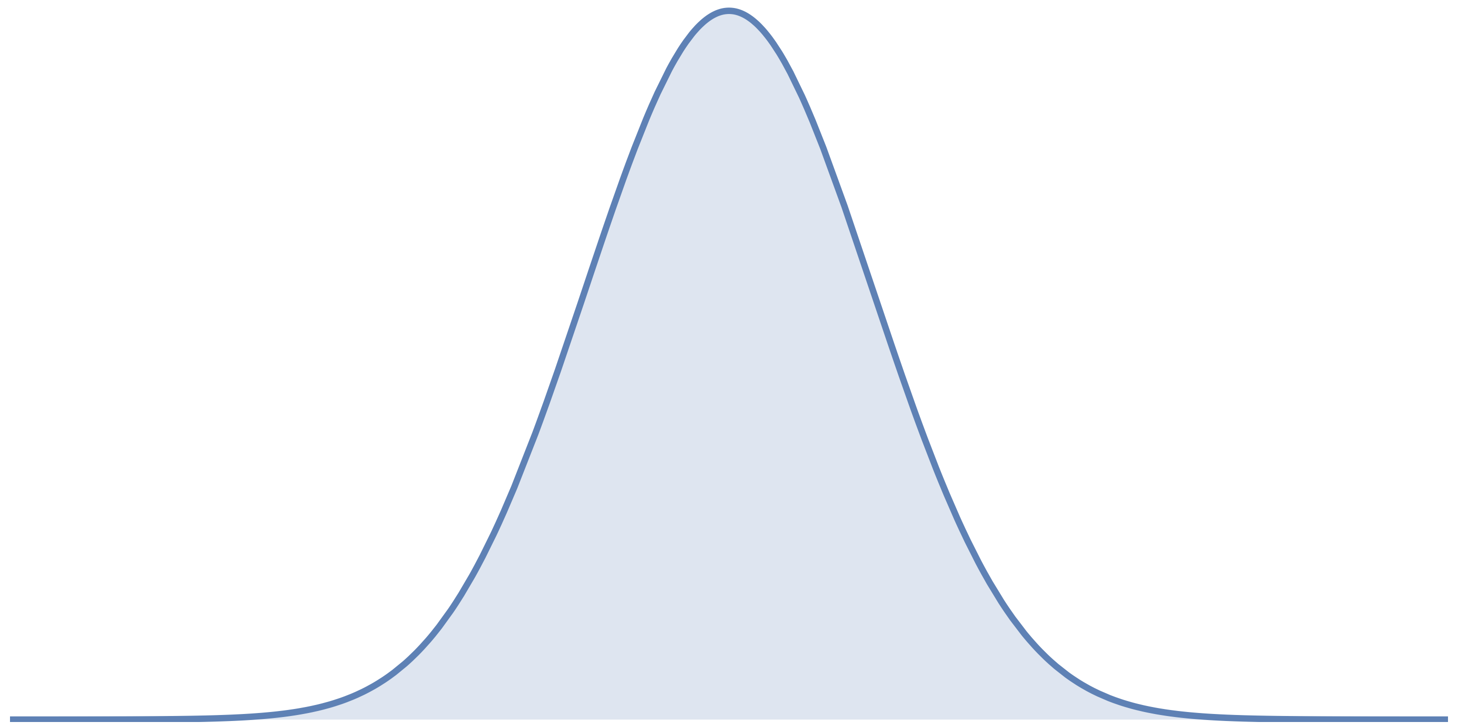
1. **Leverage the power of modern generative models for physics**
2. **Statistical, quantum, and fluid physics inspired generative models**

DL as a fluid control problem

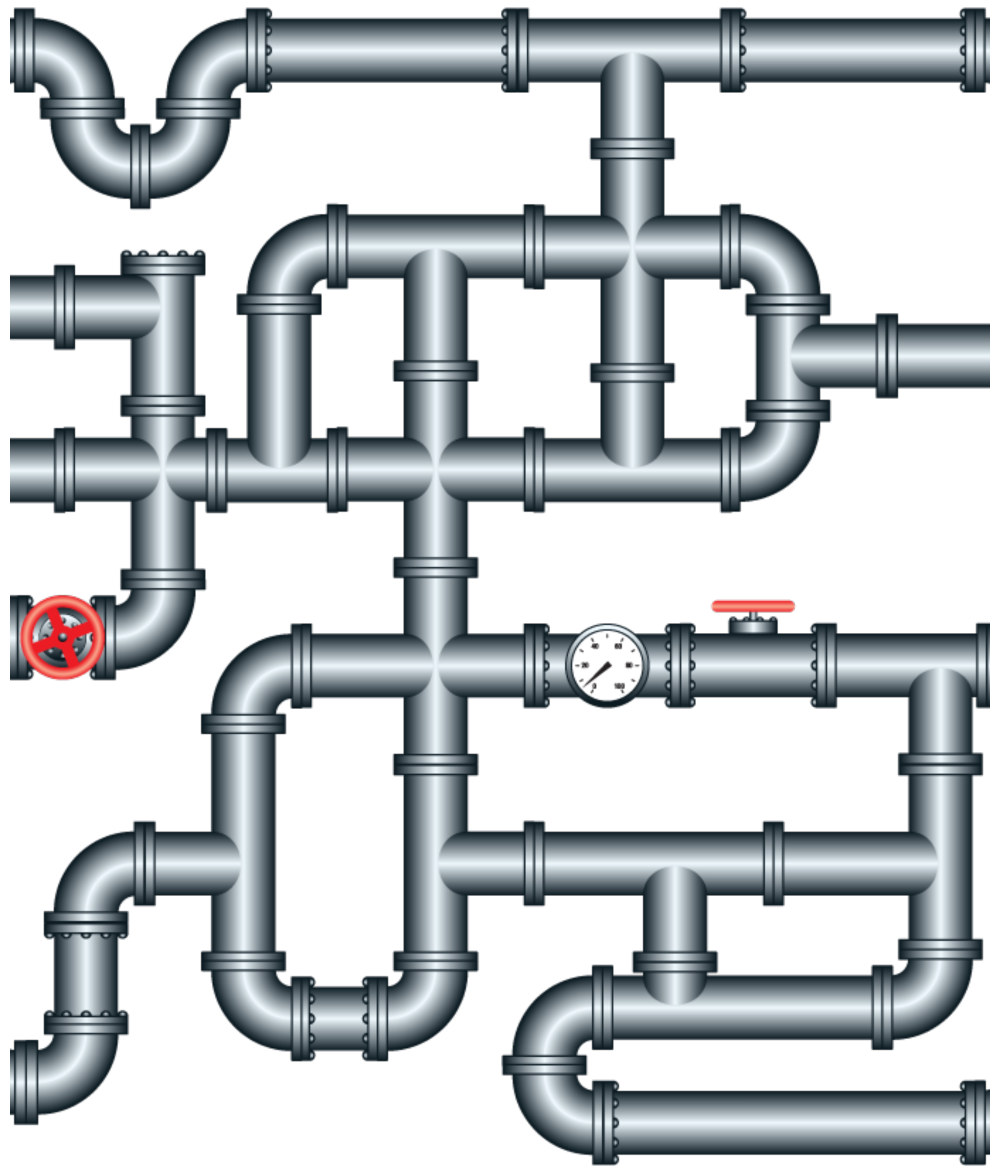
$$\frac{p(\boldsymbol{z})}{q(\nabla u(\boldsymbol{z}))} = \det\left(\frac{\partial^2 u}{\partial z_i \partial z_j}\right) \xrightarrow[u(\boldsymbol{z}) = |\boldsymbol{z}|^2/2 + \epsilon\varphi(\boldsymbol{z})]{\text{Continuous-time limit}} \frac{\partial p(\boldsymbol{x},t)}{\partial t} + \nabla \cdot \left[p(\boldsymbol{x},t)\nabla\varphi\right] = 0$$

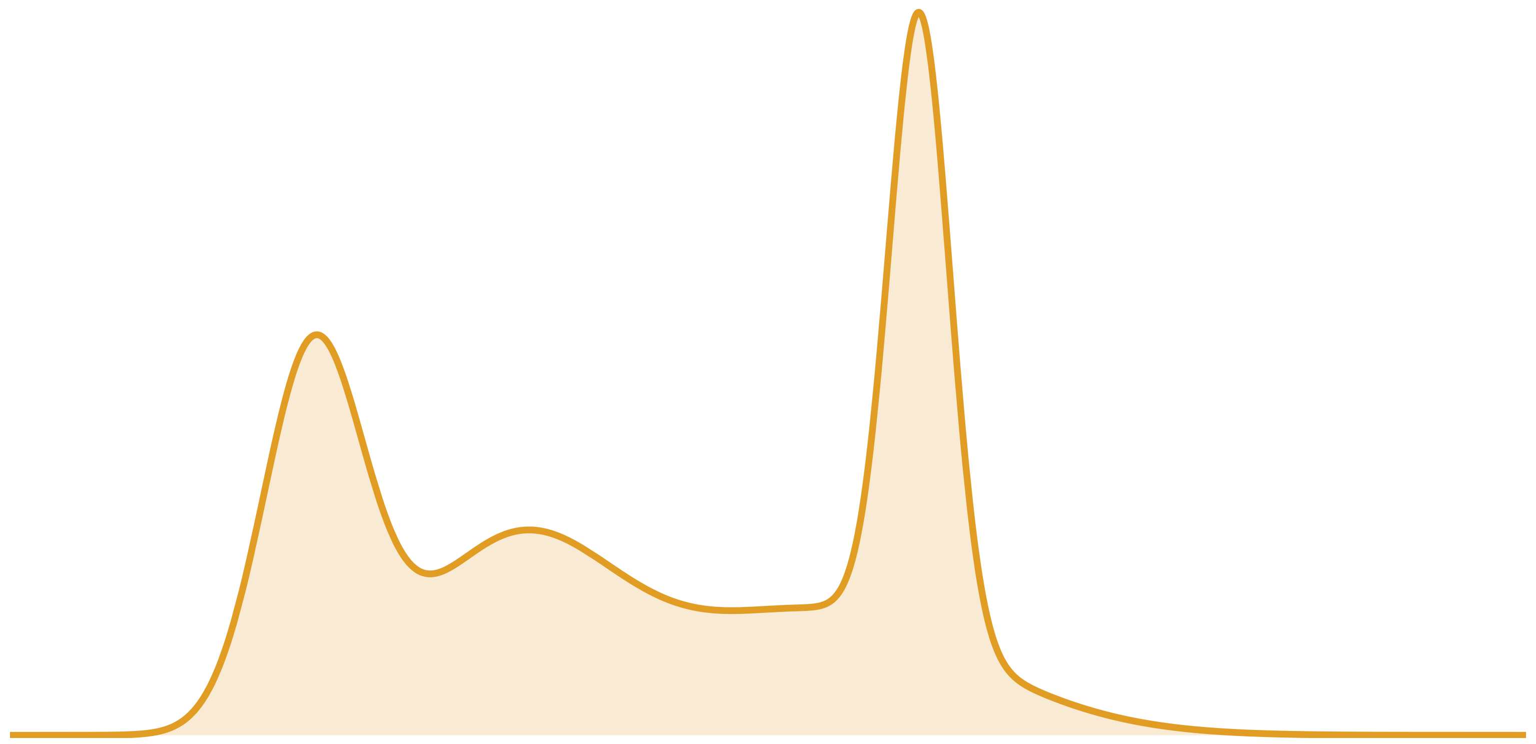
Monge-Ampère equation
optimal transport theory

Continuity equation of
compressible fluids



Simple density





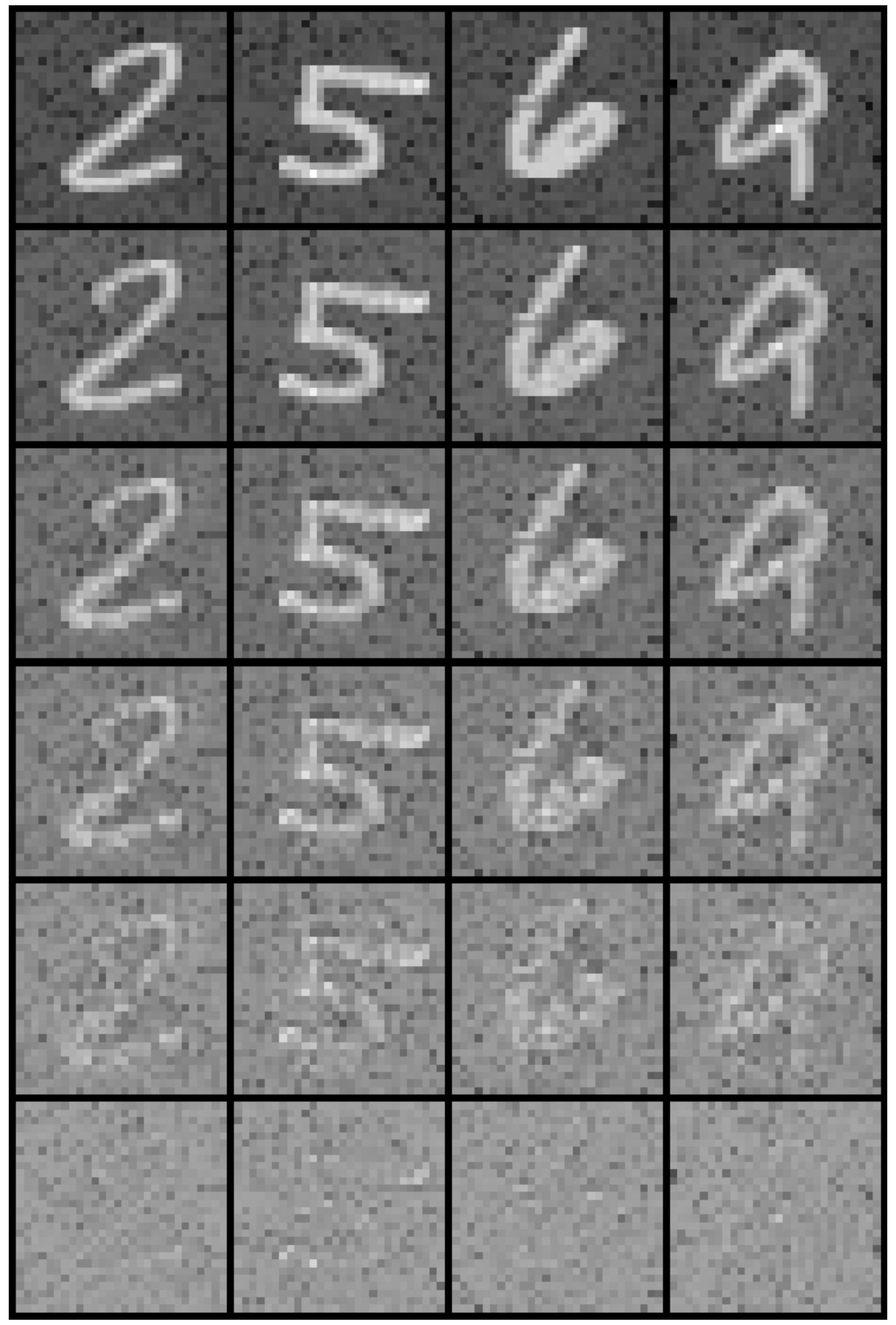
Complex density

Zhang, E, LW, 1809.10188
c.f. Neural ODE, 1806.07366

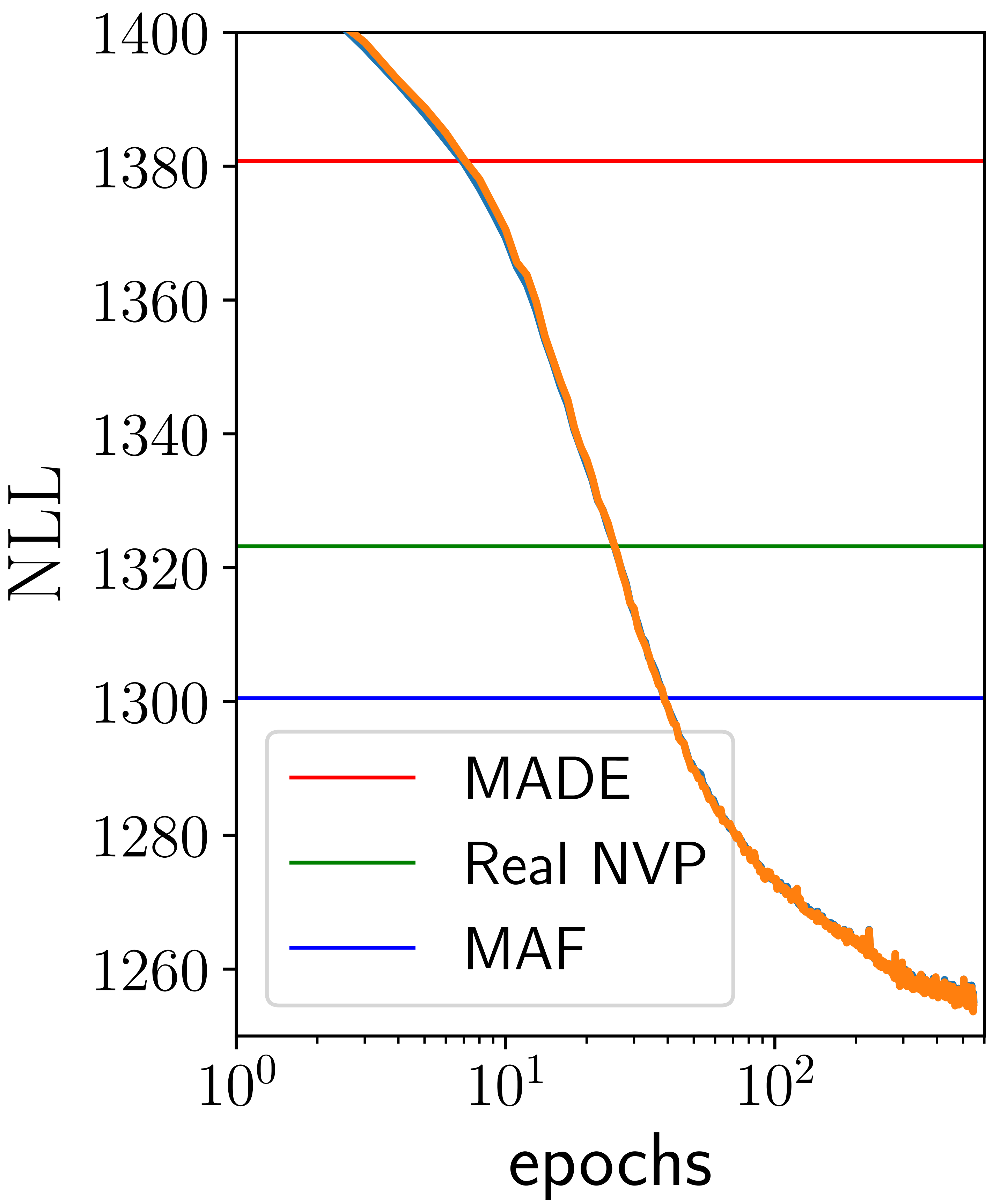
Density estimation of hand-written digits

A standard benchmark for generative models, lower is better

Data space



Latent space



'15

'16

'17

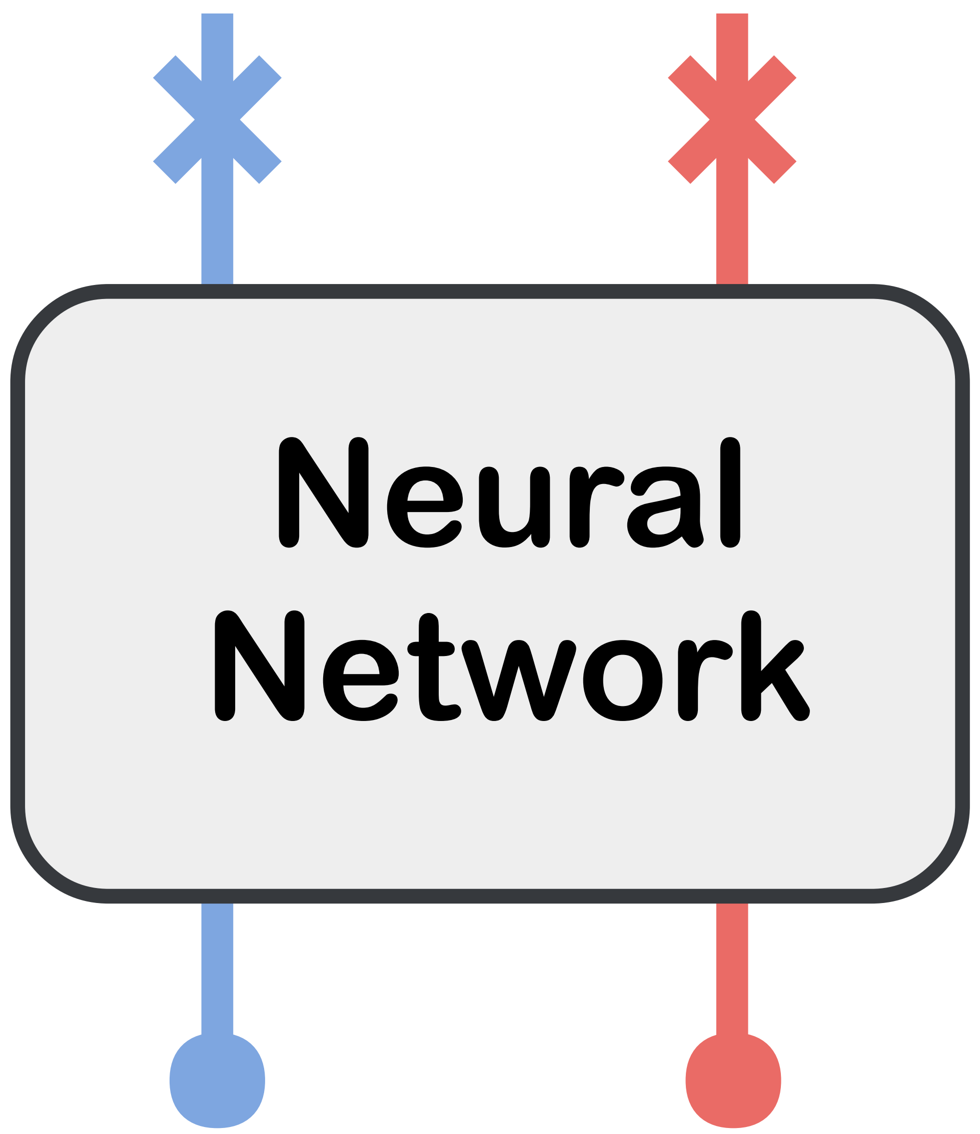
'18 Our Result

① **State-of-the-art performance in unstructured density estimation**

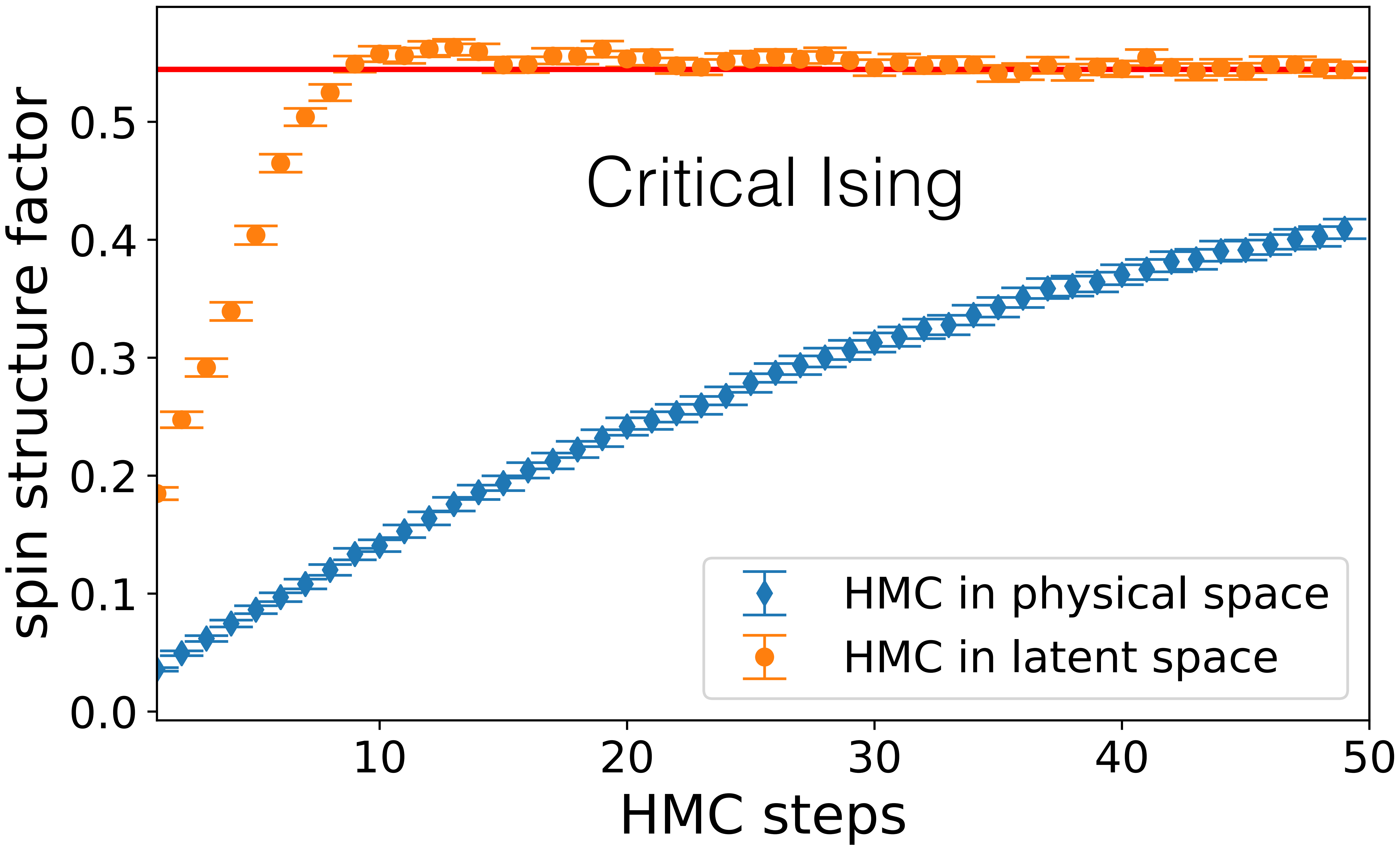
MC update in the latent space

Latent space energy function

$$E_{\text{eff}}(z) = E(g(z)) + \ln q(g(z)) - \ln p(z)$$



Physical energy function $E(\boldsymbol{x})$



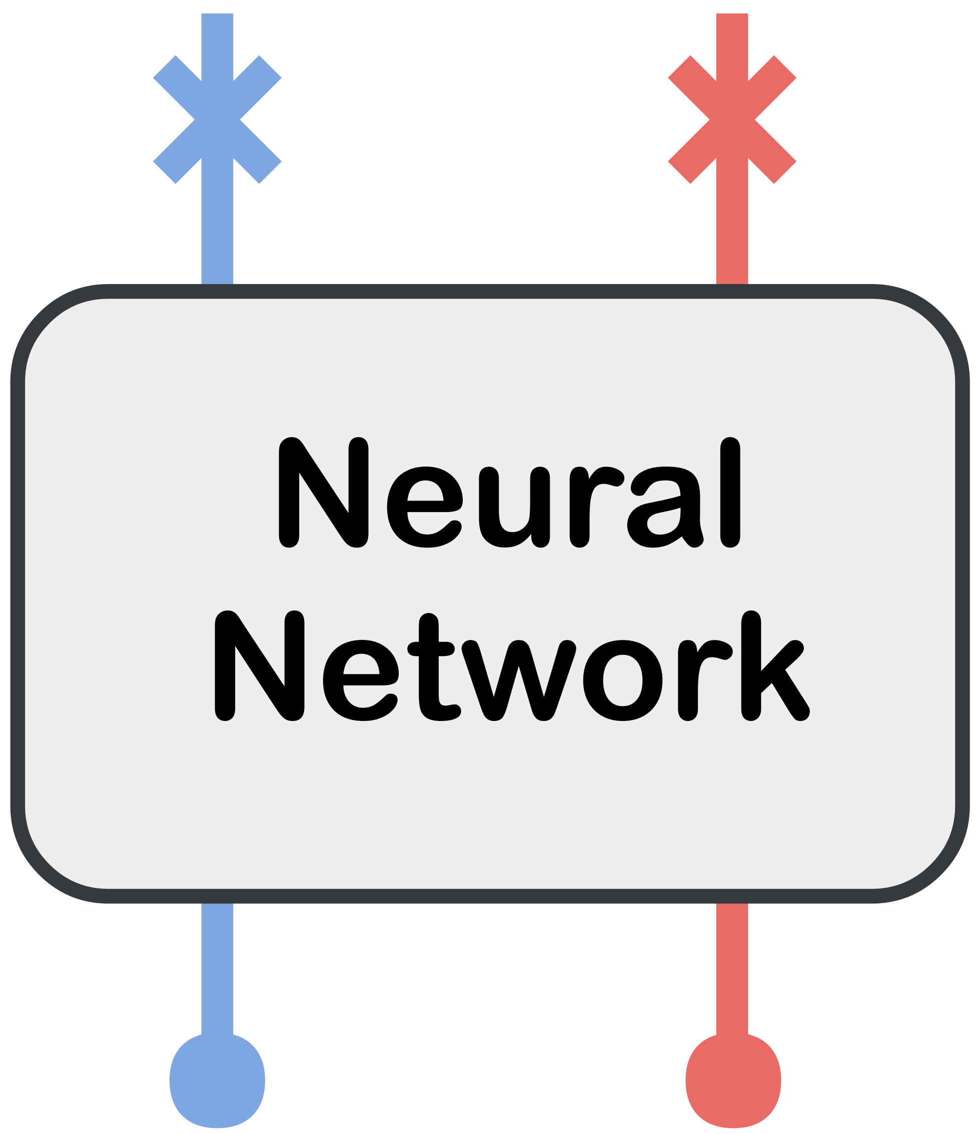
2 **Fast thermalization in the latent space;**

Local move in the latent space => nonlocal move in the physical space

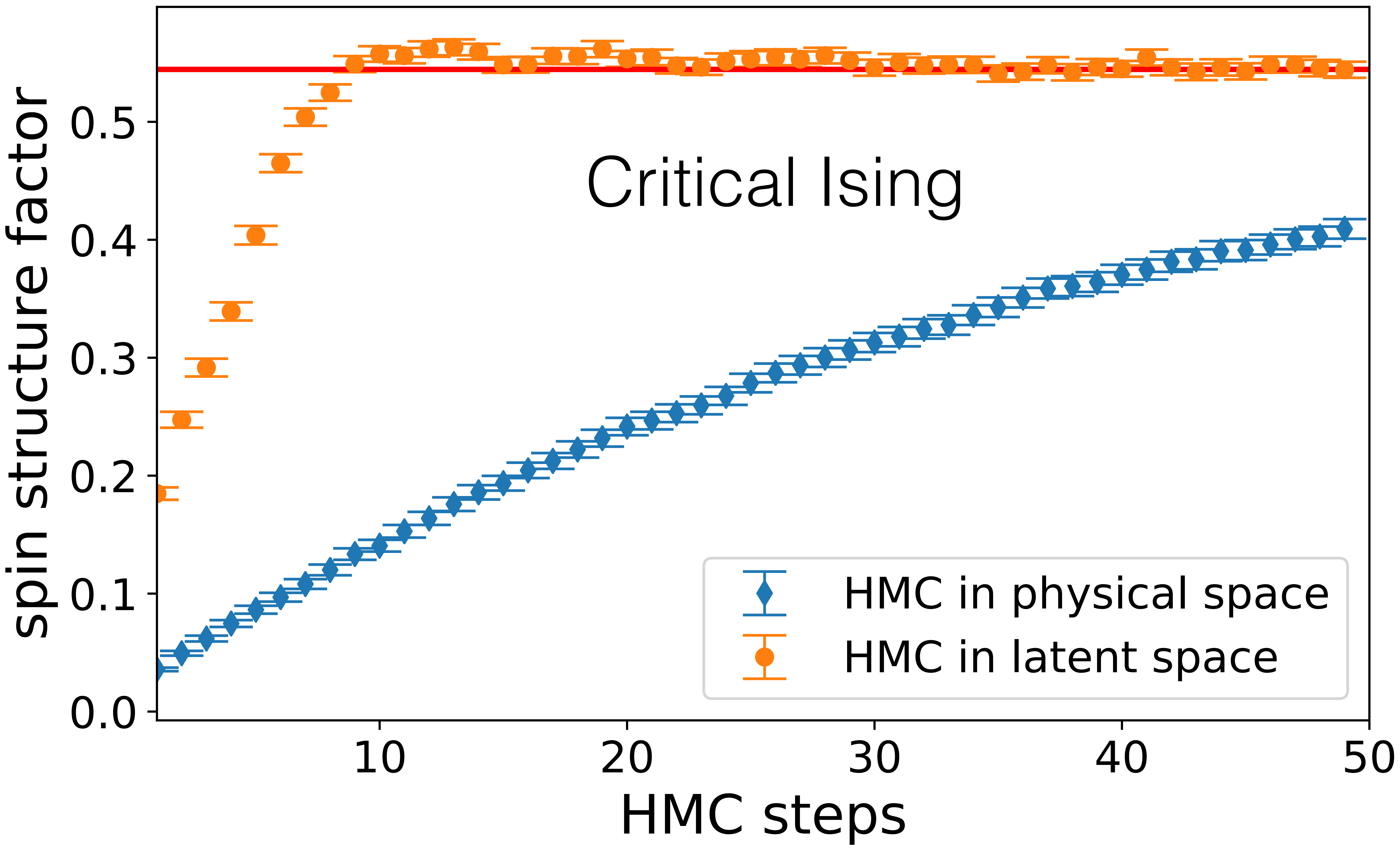
MC update in the latent space

Latent space energy function

$$E_{\text{eff}}(z) = E(g(z)) + \ln q(g(z)) - \ln p(z)$$



Physical energy function $E(\boldsymbol{x})$



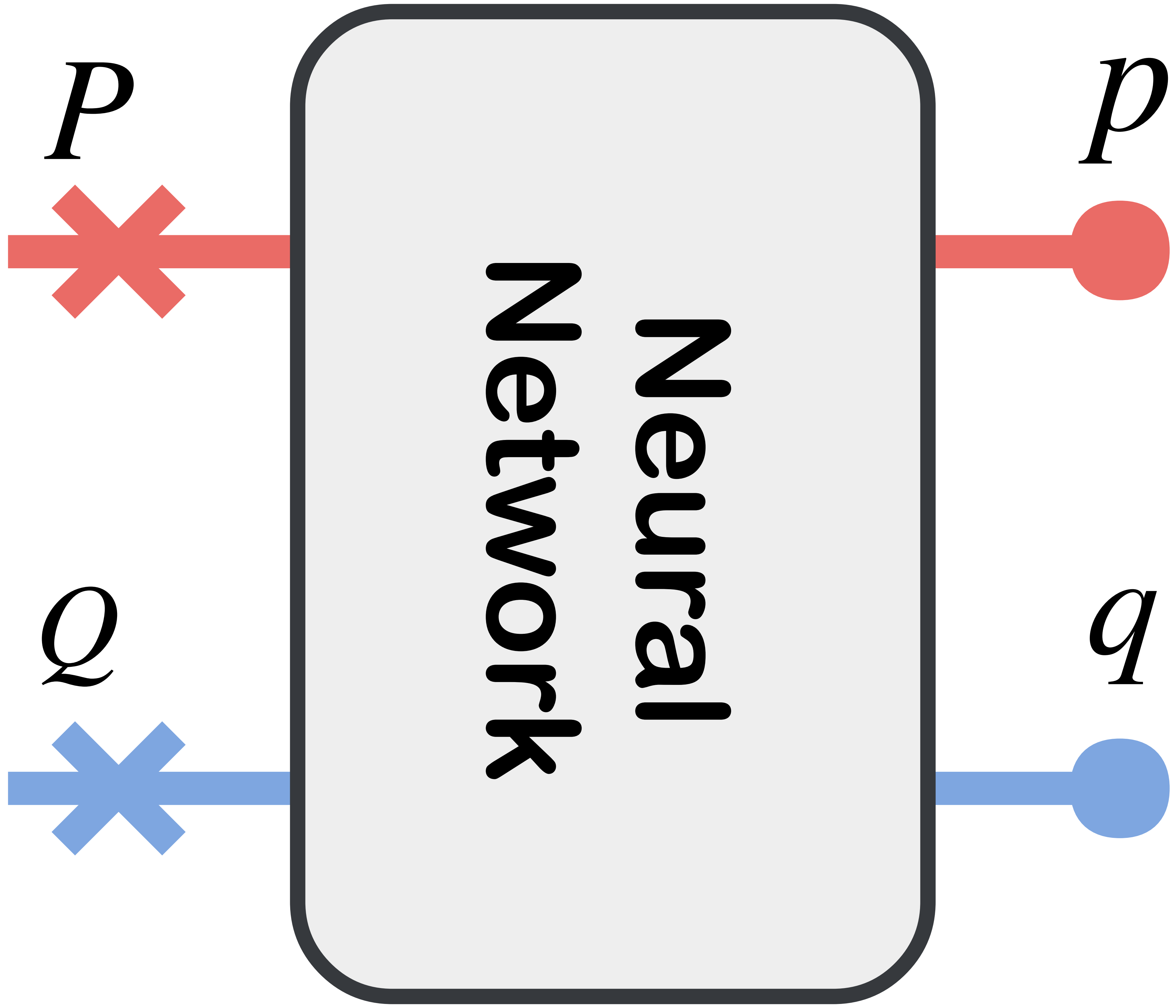
❷ **Fast thermalization in the latent space;**

Local move in the latent space => nonlocal move in the physical space

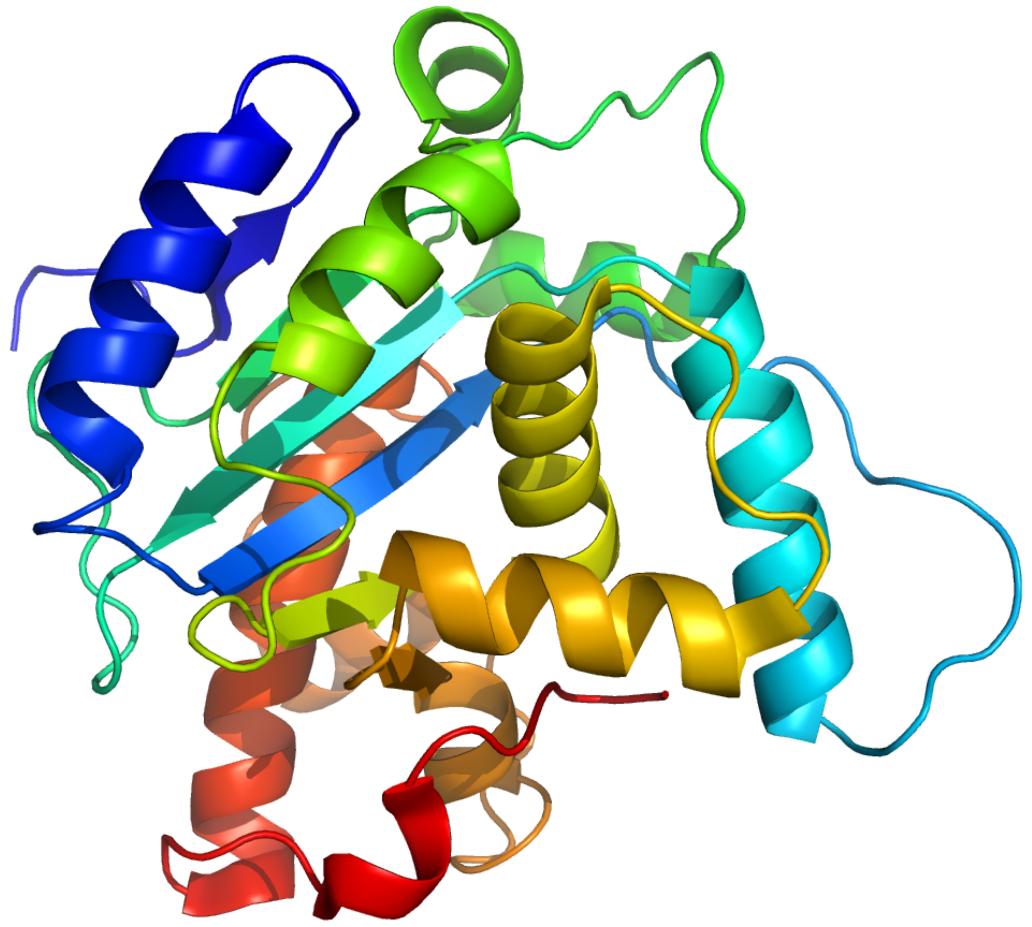
Neural Canonical Transformations

Incompressible symplectic flow in phase space

$H(P,Q) = (P^2 + Q^2)/2$



$H(p,q)$

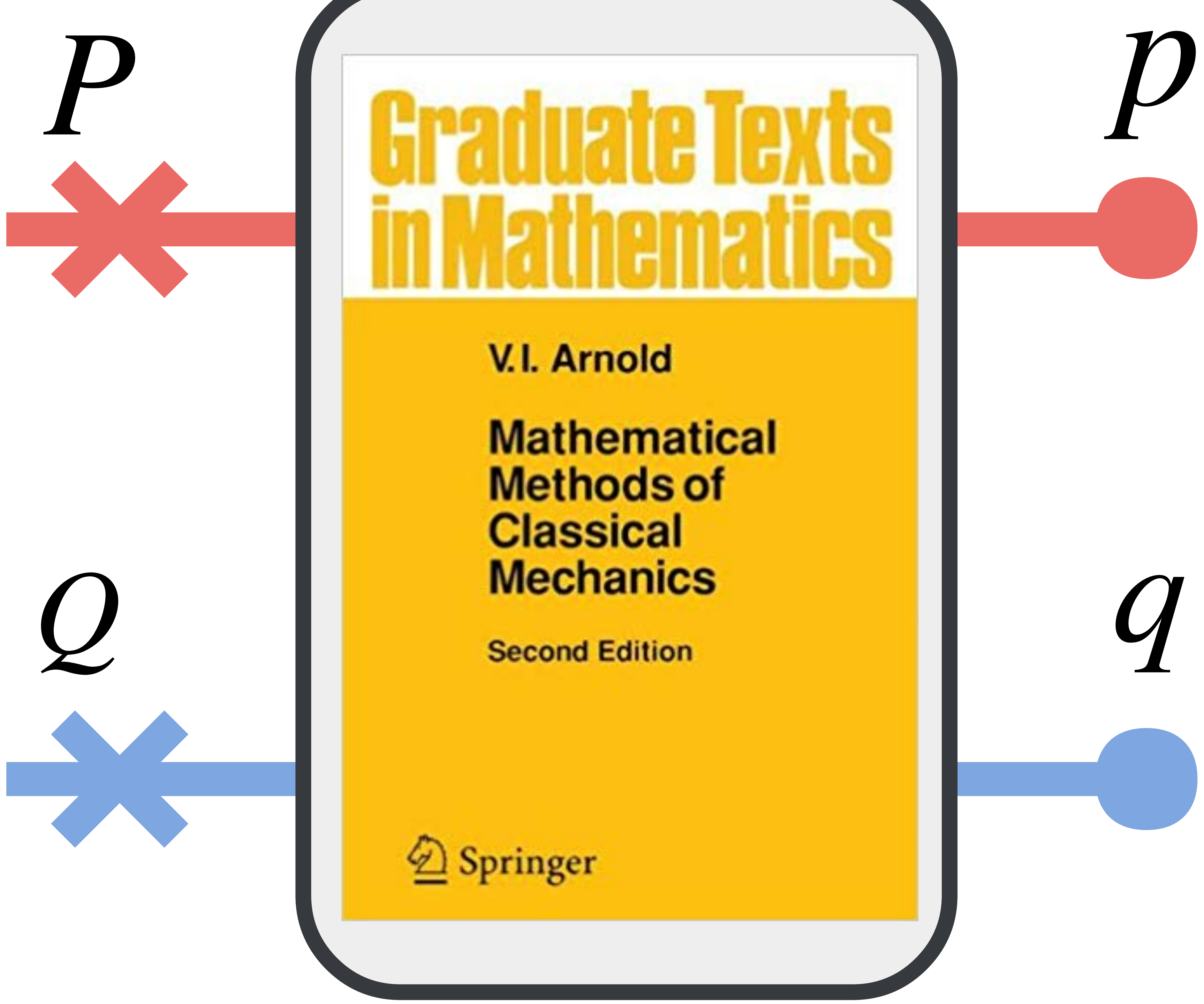


③ Identifying mutually independent collective modes for molecular simulations (MD, PIMD), and effective field theory

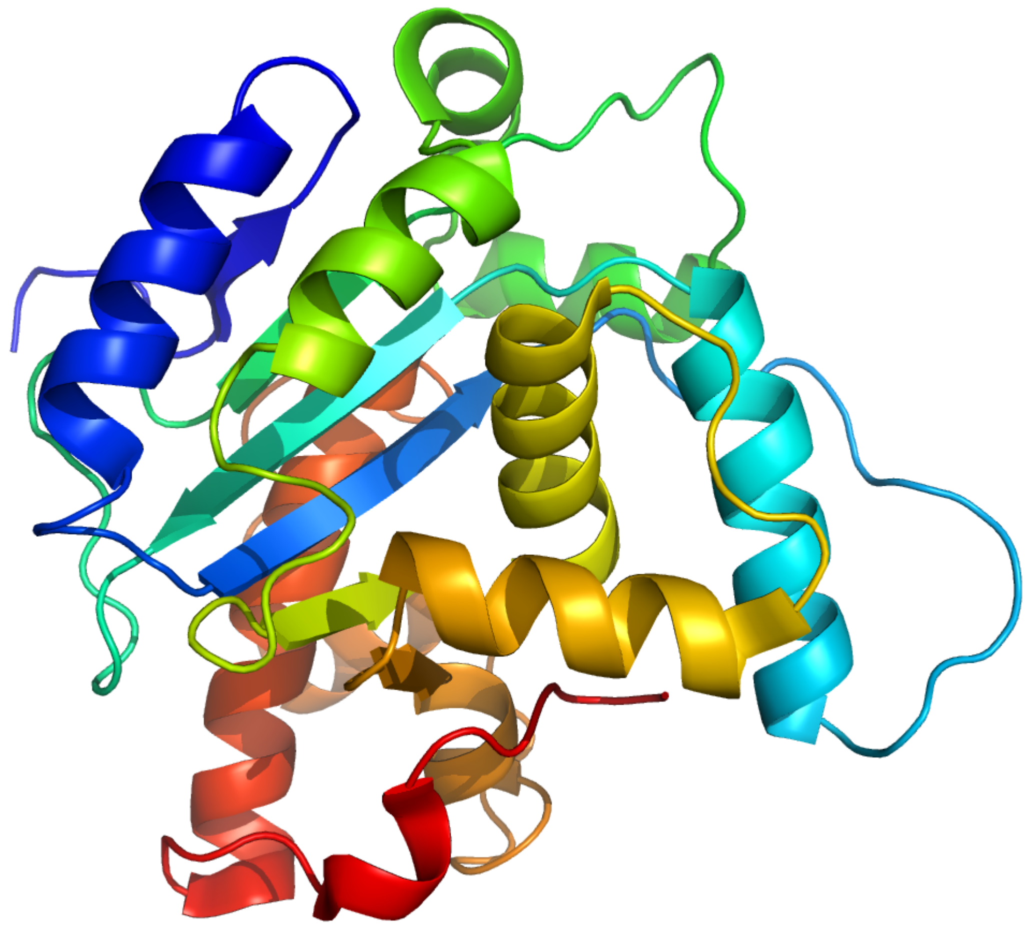
Neural Canonical Transformations

Incompressible symplectic flow in phase space

$H(P, Q) = (P^2 + Q^2)/2$



$H(p, q)$

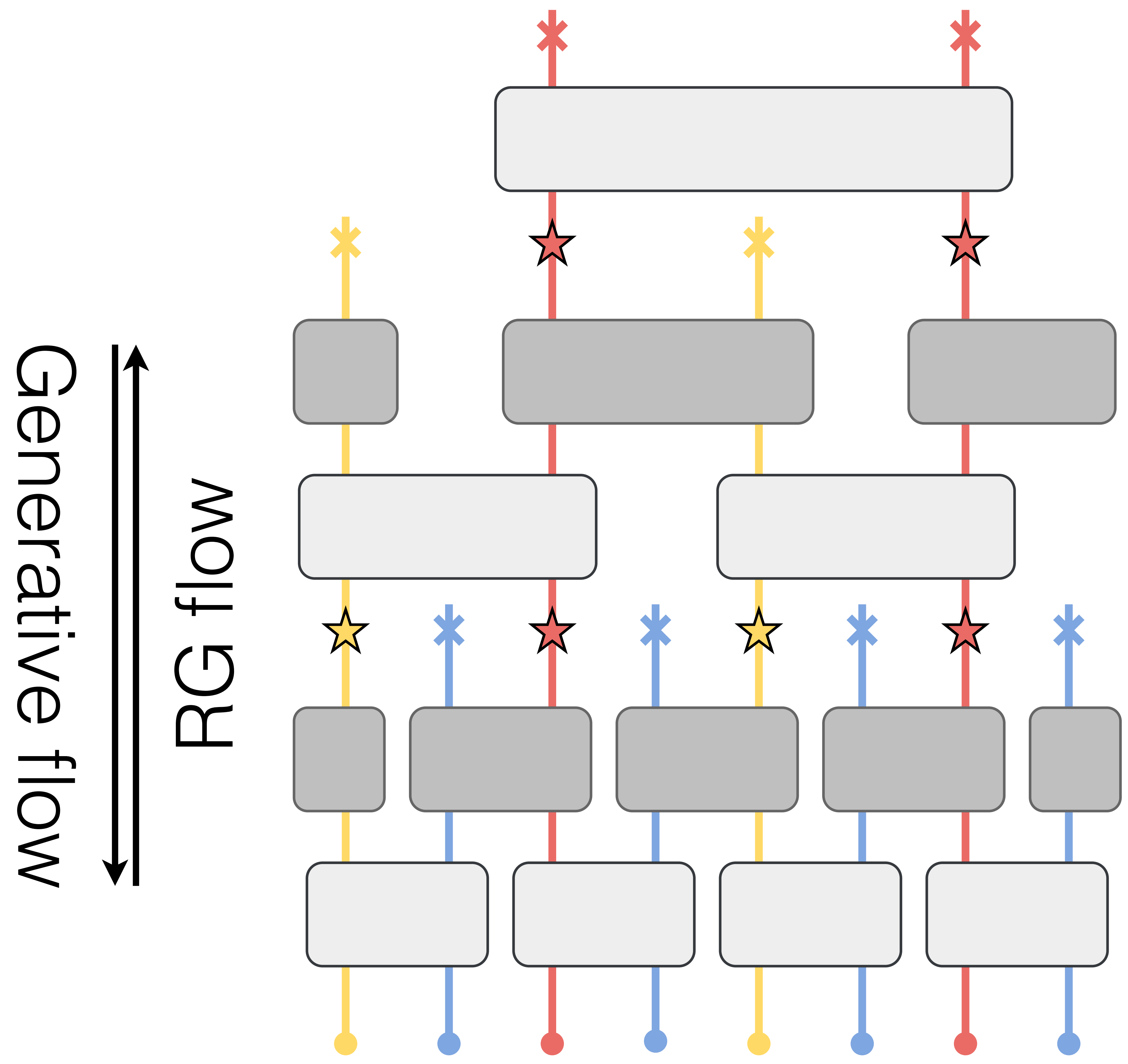


3

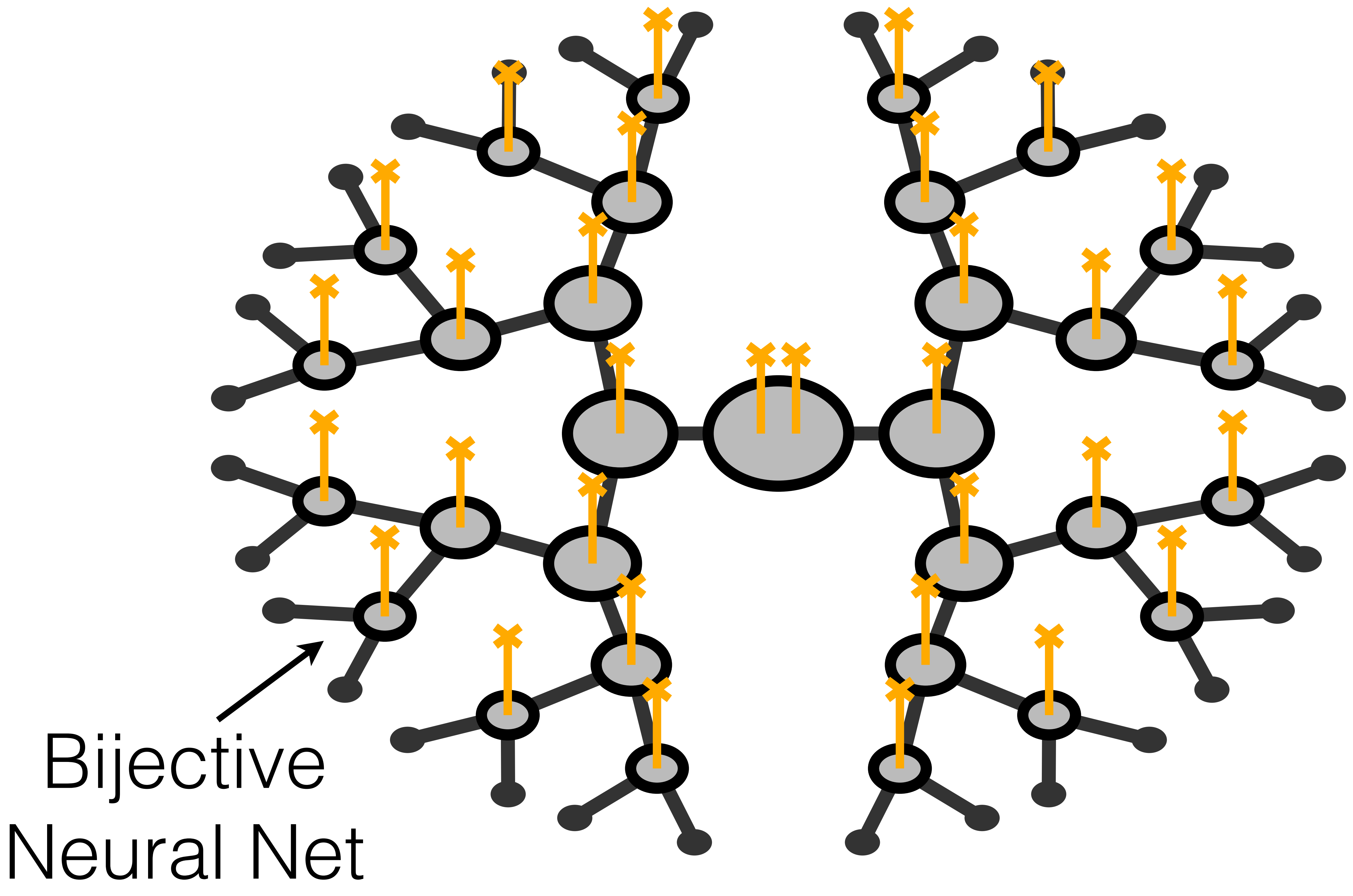
Identifying mutually independent collective modes for molecular simulations (MD, PIMD), and effective field theory

Neural Renormalization Group Flow

Normalizing flow with multiscale network structures



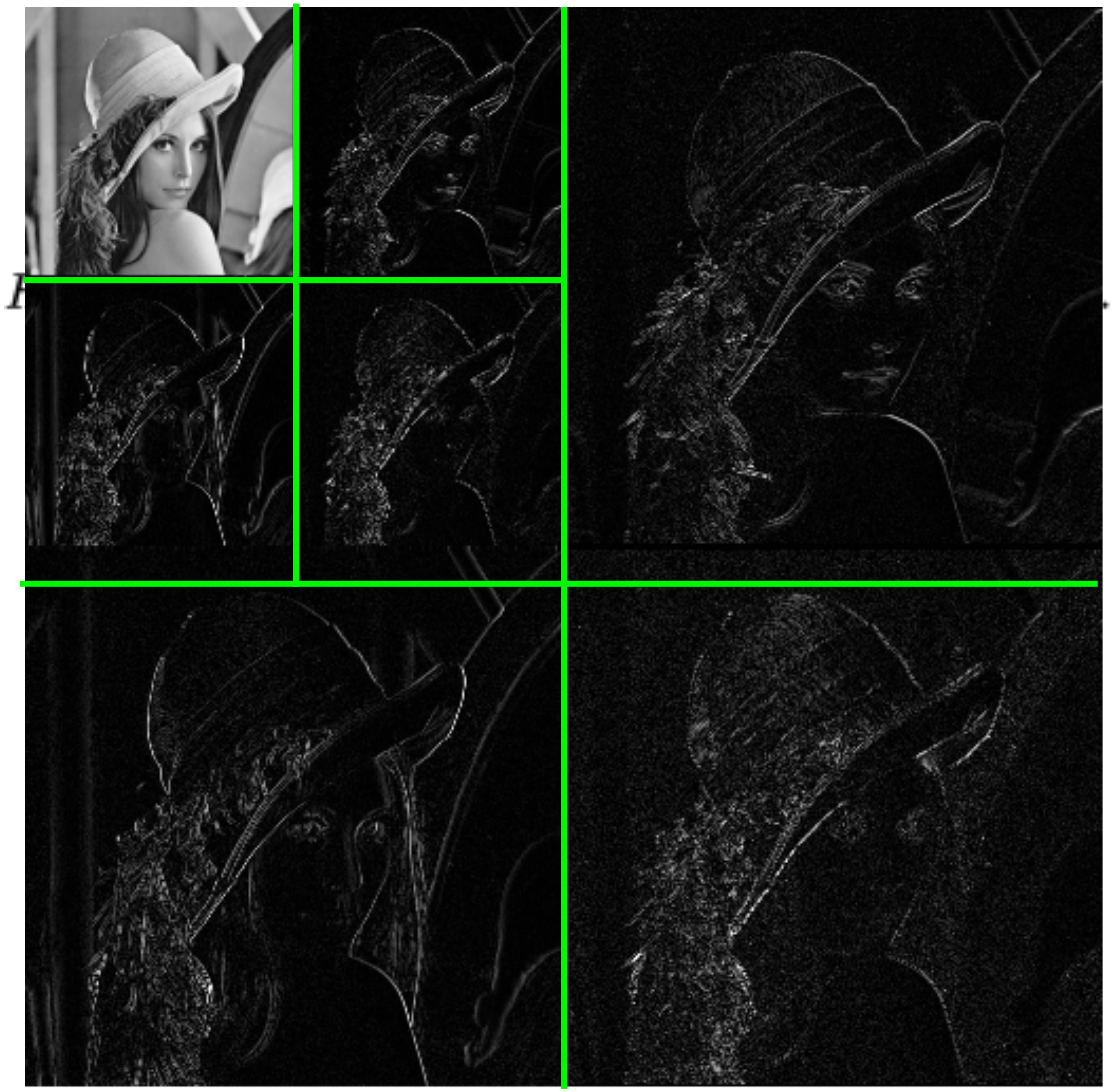
Swingle 0905.1317, Qi 1309.6282 and more

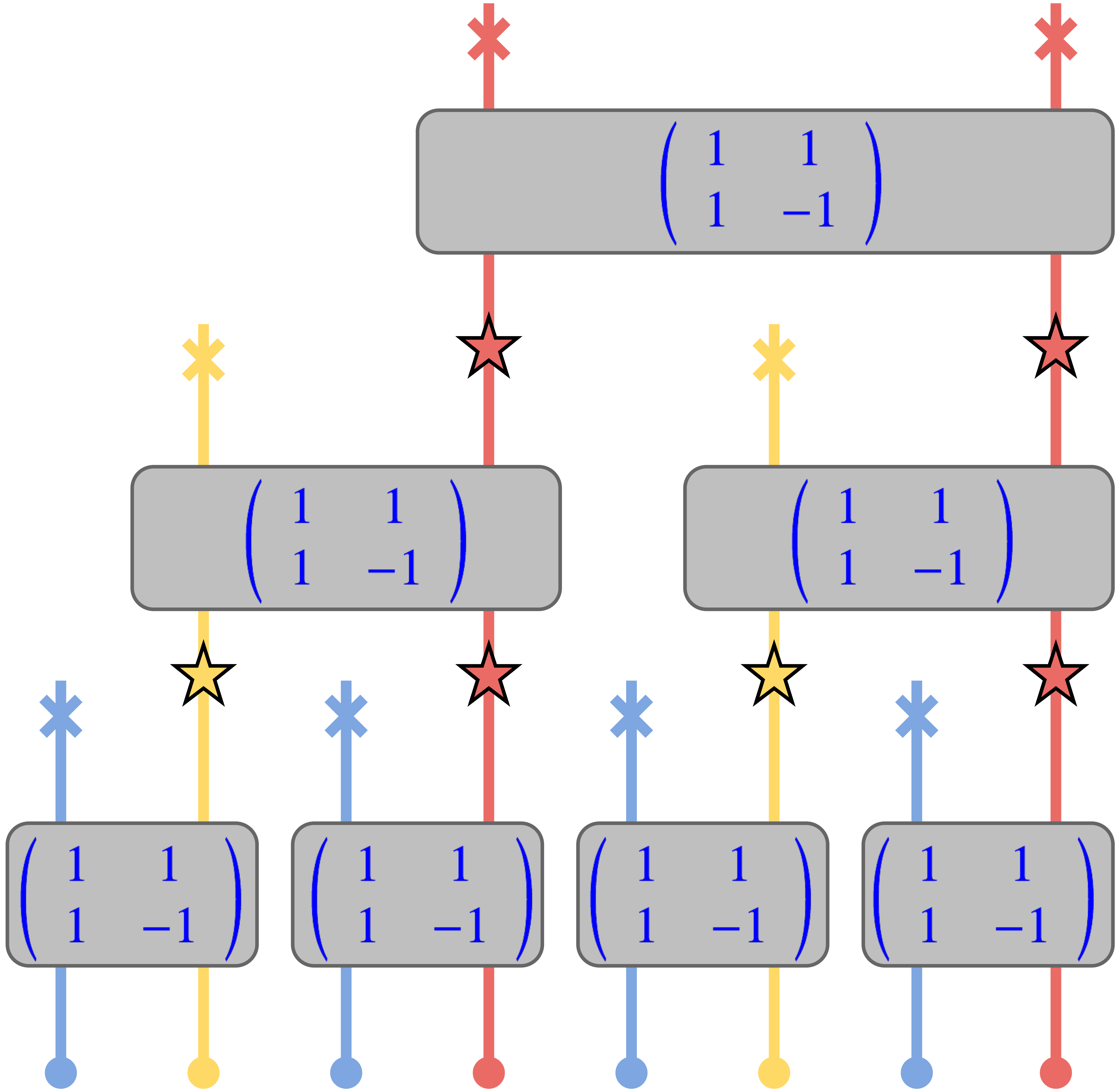


④ **A fresh approach for holographic duality**

Li and LW
[arXiv:1802.02840](https://arxiv.org/abs/1802.02840)

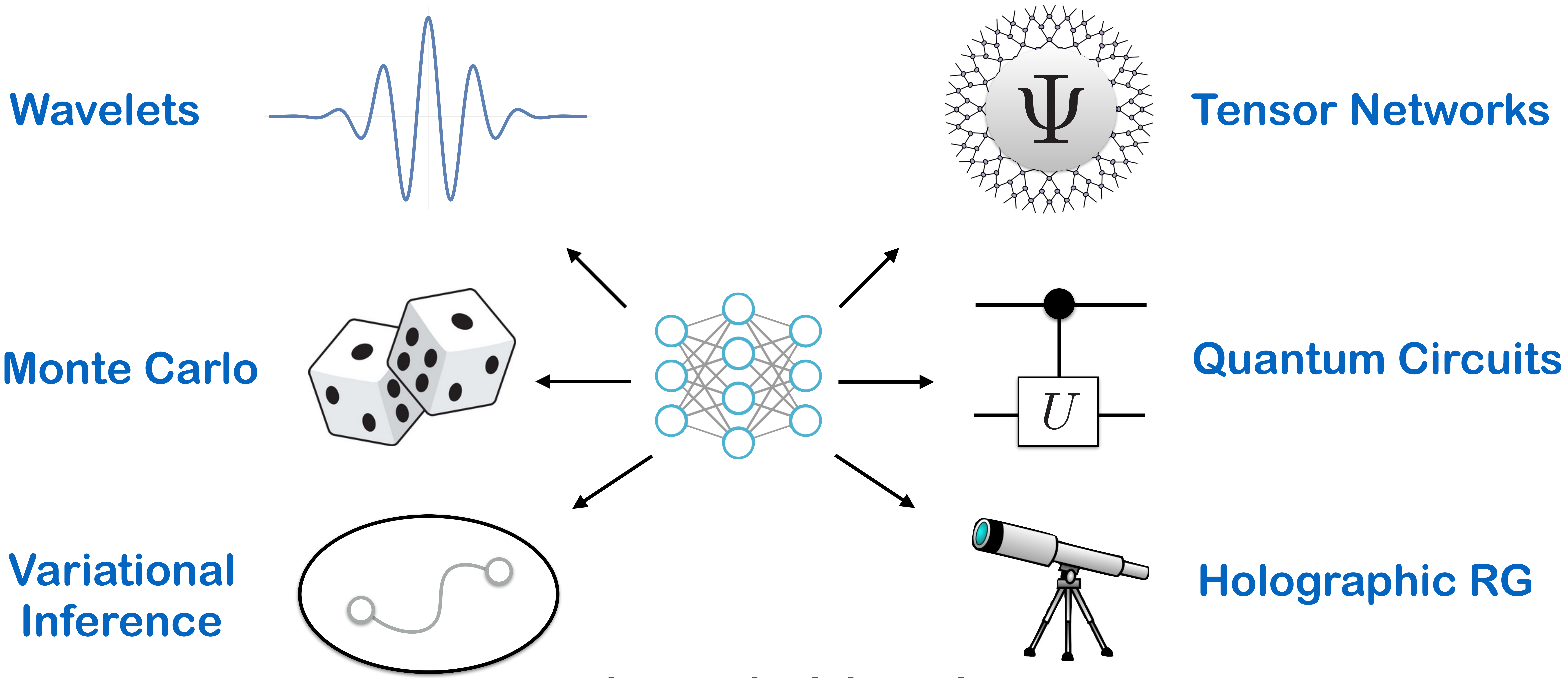
Learned collective representation





⑤ **Nonlinear & adaptive generalizations of wavelets**

Guy, Wavelets & RG1999+ White, Evenbly, Qi, Wavelets, MERA, and holographic mapping 2013+



Thank You!

Shuo-Hui Li
Jin-Guo Liu

Linfeng Zhang
Weinan E

Pan Zhang

Yi-Zhuang You