Title: Solving physics many-body problems with deep learning

Speakers: Frank Noe

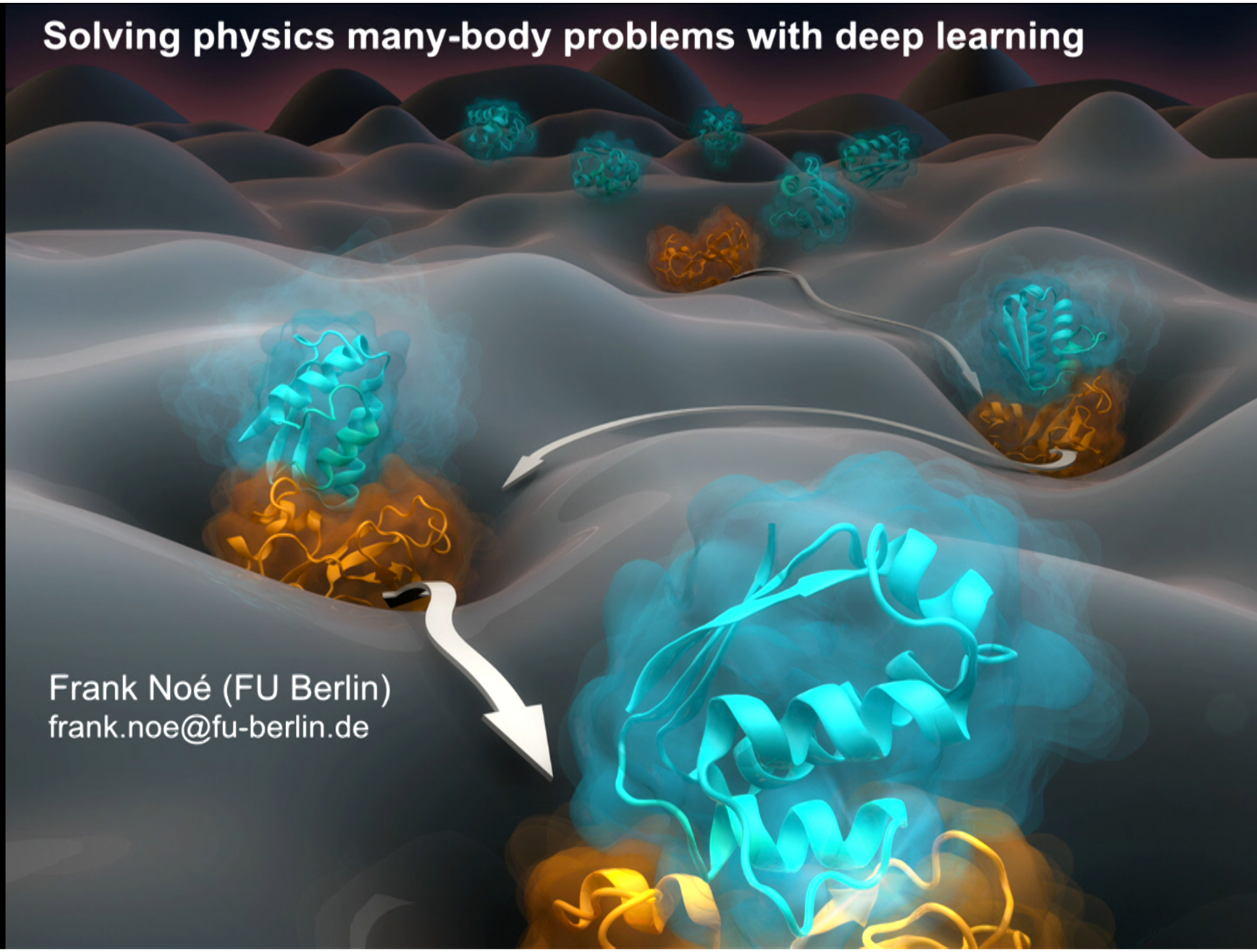
Series: Machine Learning Initiative

Date: November 12, 2019 - 1:00 PM

URL: http://pirsa.org/19110081

Abstract:

Solving classical and quantum physics many-body systems are amongst the hardest problems in the natural sciences, but also of fundamental importance for applications such as material and drug design. In this talk, I will give a an overview of fundamental physics problems at multiple time- and lengthscales and describe deep learning methods to address them: 1) solving the quantum-chemical electronic SchrÃ¶dinger equation with deep variational Monte Carlo, 2) learning to coarse-grain many-body systems, and 3) sampling equilibrium states of classical many-body systems with generative learning.


Solving physics many-body problems with deep learning
Frank Noé (FU Berlin)
frank.noe@fu-berlin.de

Statistical Mechanics

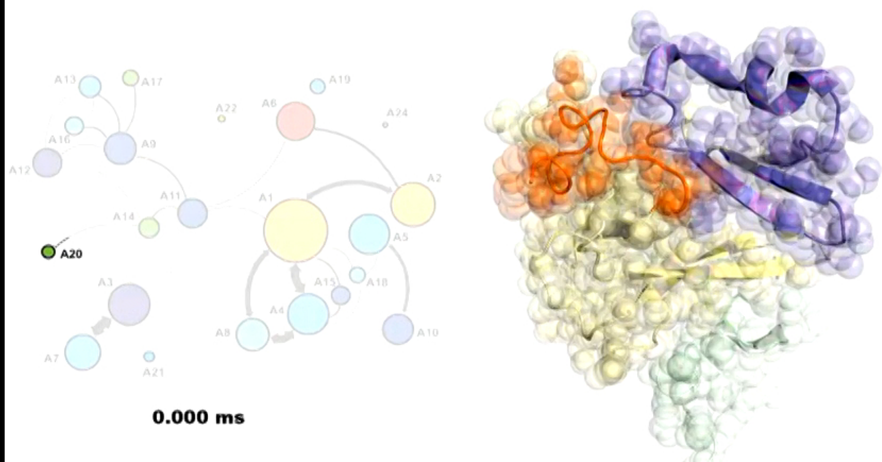
$$\mathbf{x} \sim \mathrm{e}^{-E(\mathbf{x}_1,\ldots,\mathbf{x}_N)}$$

Sampling problem

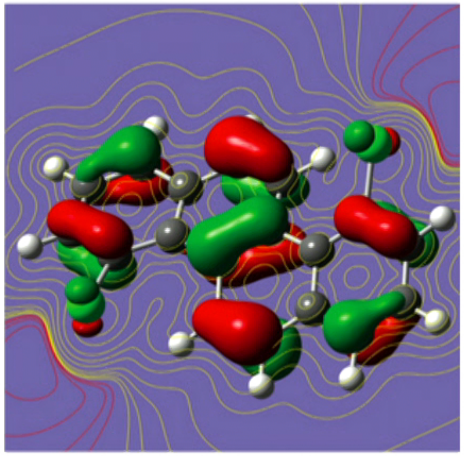
Quantum Mechanics

$$\hat{H}\psi = E_{\mathbf{x}}\psi$$

Electronic structure problem



Video from: Wiewora et al, eLife 8:e45403 (2019)



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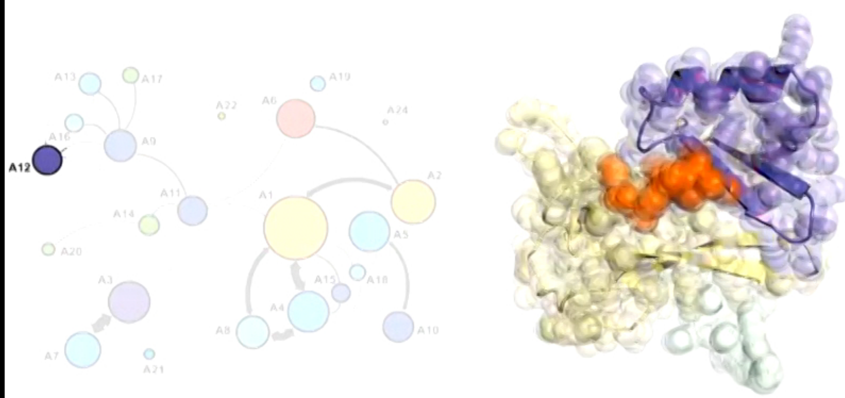

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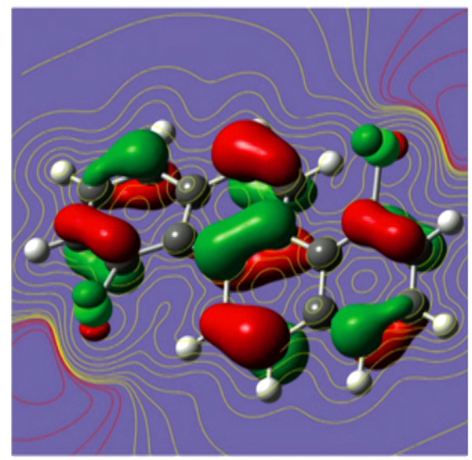

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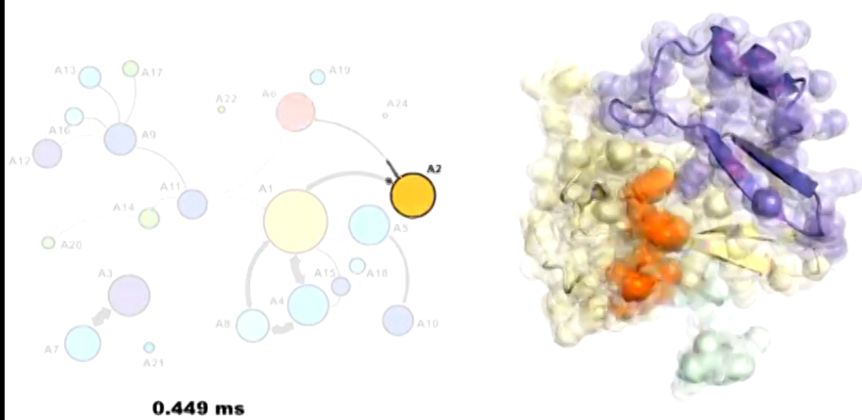

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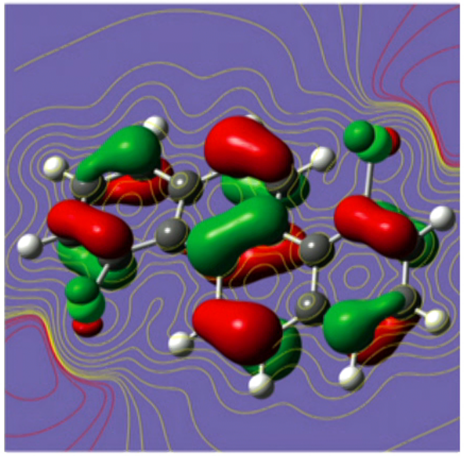

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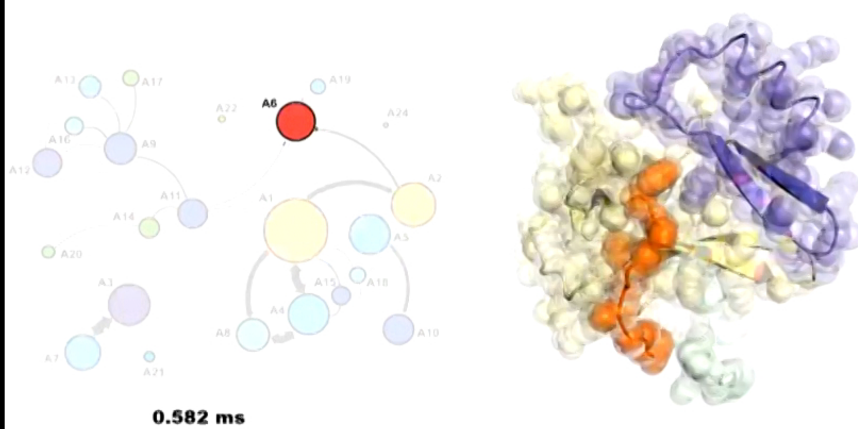

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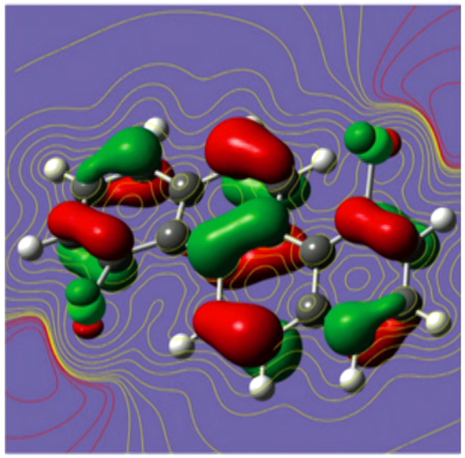
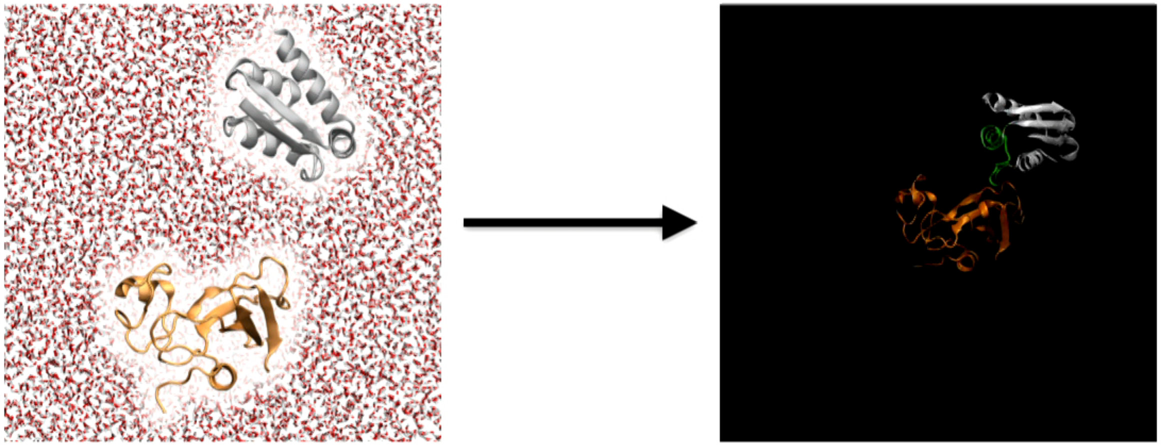


Samping problem of many-body physics systems



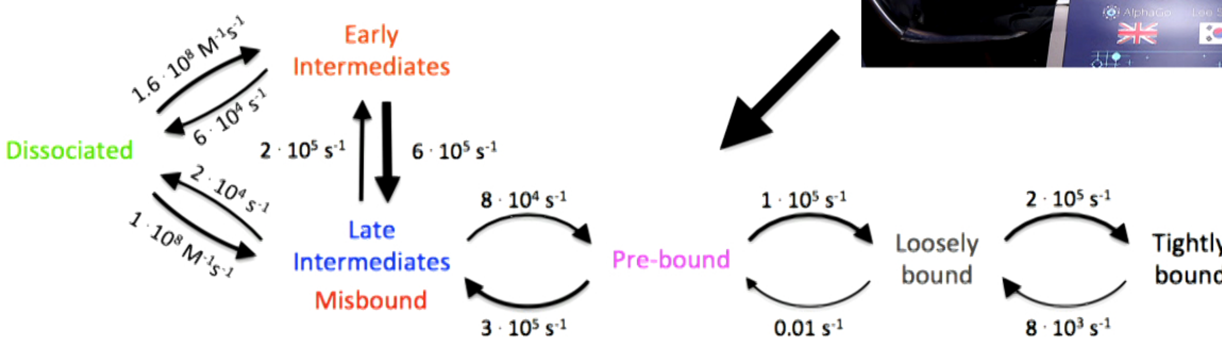
Microsecond
MD Trajectories

Samping problem of many-body physics systems

Plattner, Doerr, De Fabritiis, Noé
Nature Chemistry 9, 1005 (2017)

total 2 ms data

Reinforcement learning



Adaptive Markov State Model — **seconds to hours kinetics**

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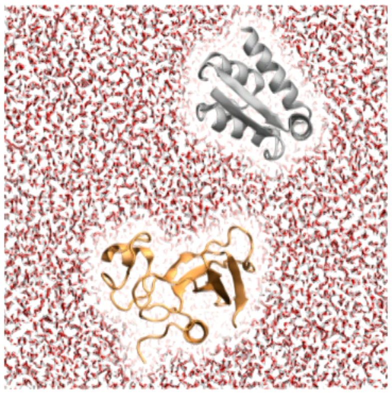
Samping problem of many-body physics systems

Standard simulation methods in molecular physics are INSANELY expensive

Current approach



very long time

a lot of energy

2 ms MD = 20,000 GPU days
500 gigajoule

PhD

1 non-transferable model

Burn a Saturn V rocket and deliver 50 ton payload to lunar orbit

1500 gigajoule

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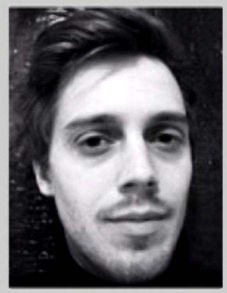
Thermodynamics **Sampling problem**

Boltzmann Generators
sampling equilibrium states of many-body systems with deep learning

Noé, Olsson, Köhler, Wu, **Science** 365: eaww1147 (2019)

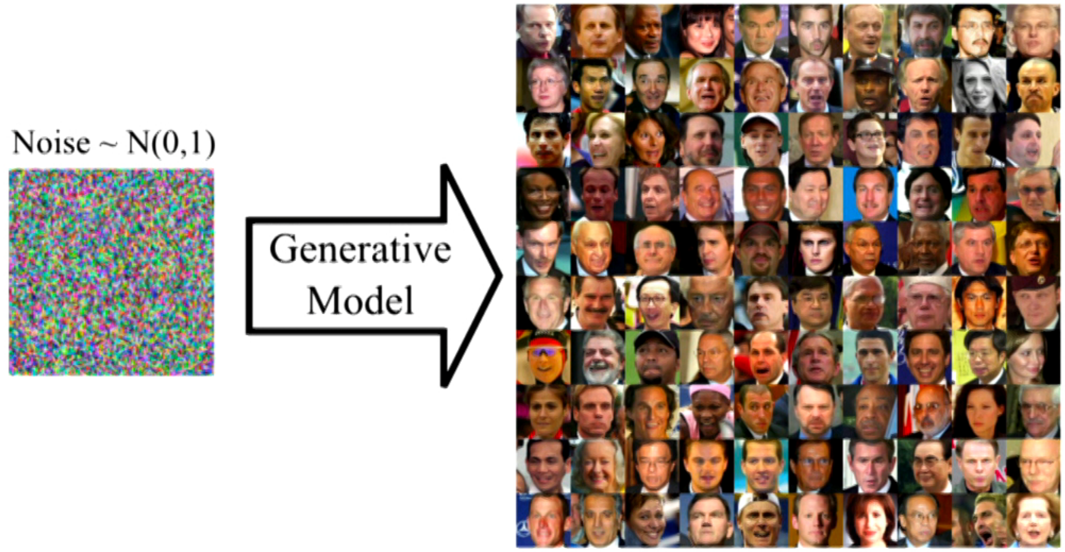
Simon Olsson



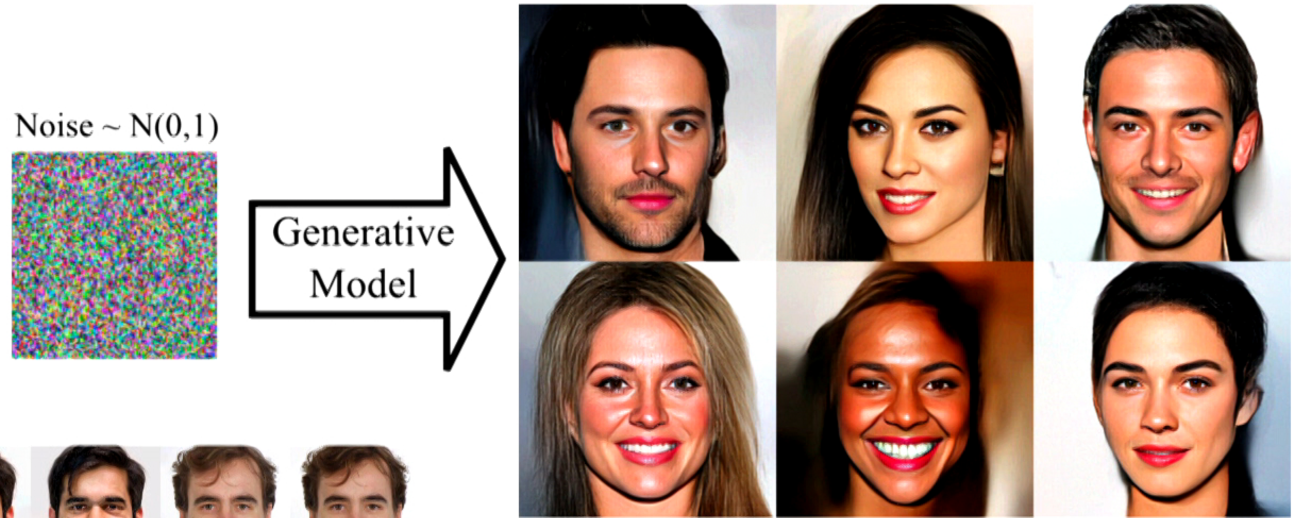
Jonas Köhler

Hao Wu

Directed generative models



Glow



Interpolations in latent space

Kingma, Dhariwal. Glow: Generative Flow with Invertible 1x1 Convolutions. NeurIPS 2018

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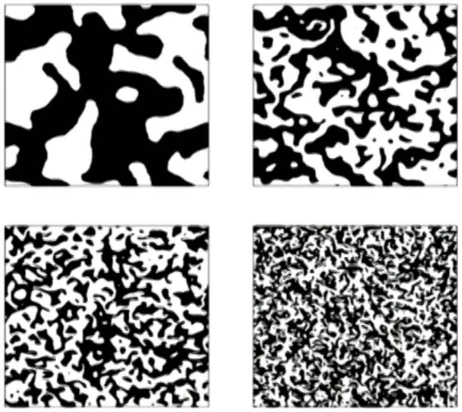
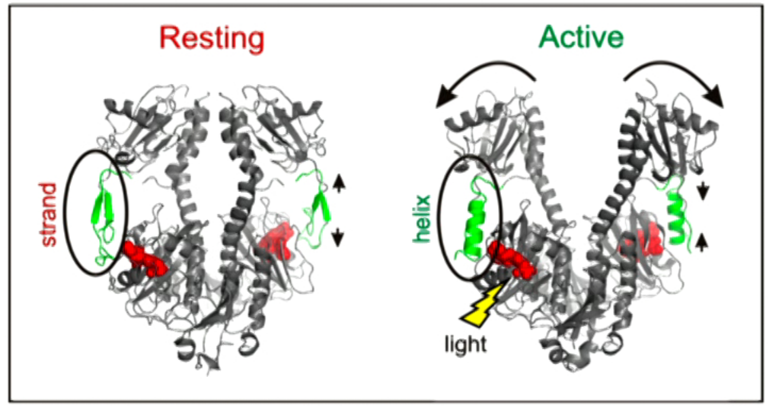
Boltzmann Generators





- **Input**: Reduced Potential Energy $u(\mathbf{x})$ in coordinates $\mathbf{x} \in \mathbb{R}^n$, e.g. $u(\mathbf{x}) = U(\mathbf{x})/k_B T$ (canonical ensemble).
- **Aim**: Generate *independent* Samples from Equilibrium Distribution.

$$\mu(\mathbf{x}) \propto \mathrm{e}^{-u(\mathbf{x})}$$

- **Problem**:
  - Direct MC (proposal for all n degrees of freedom + rejection or reweighting) not available.
  - Standard approach: MD/MCMC with local moves $\rightarrow$ sampling problem.

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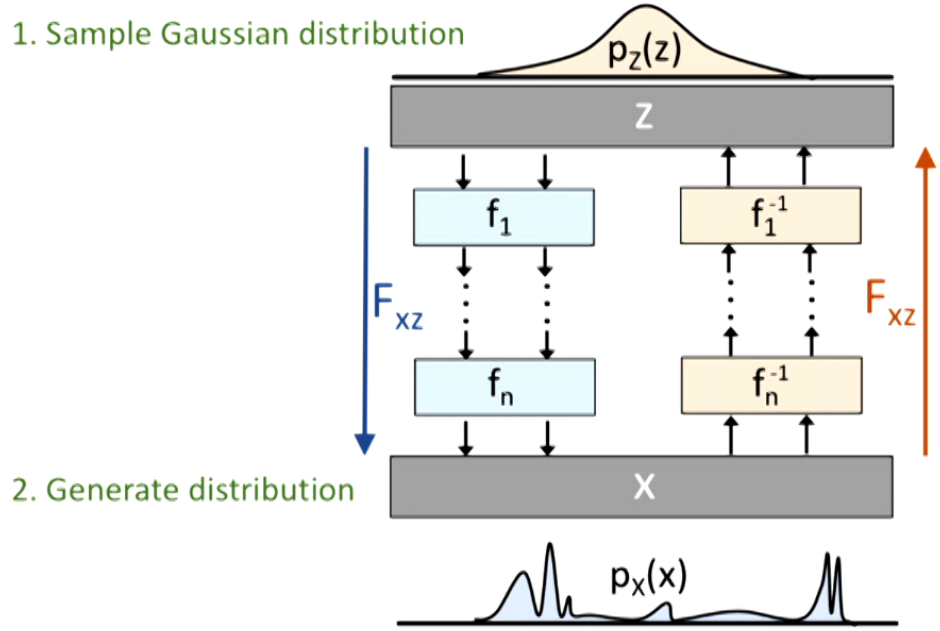
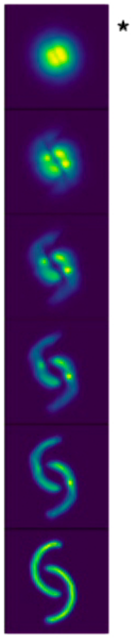
Flows and Normalizing Flows





Main idea: Transformation of random variables for bijective transformations:

$$p_X(\mathbf{x}) = p_Z(f(\mathbf{x})) \left| \frac{\partial f(\mathbf{x})}{\partial \mathbf{x}^\top} \right|$$

PDE Flows: Tabak, Vanden-Eijnden, Commun. Math. Sci. 2010
NICE: Dinh, Krueger, Y. Bengio, ICLR 2015
Normalizing Flows: Rezende, Mohamed, ICML 2015
RealNVP: Dinh, Sohl-Dickstein, S. Bengio, ICLR 2017
PixelRNN: van den Oord et al, ICML 2016
***Neural ODEs**: Chen et Al, NeurIPS 2018

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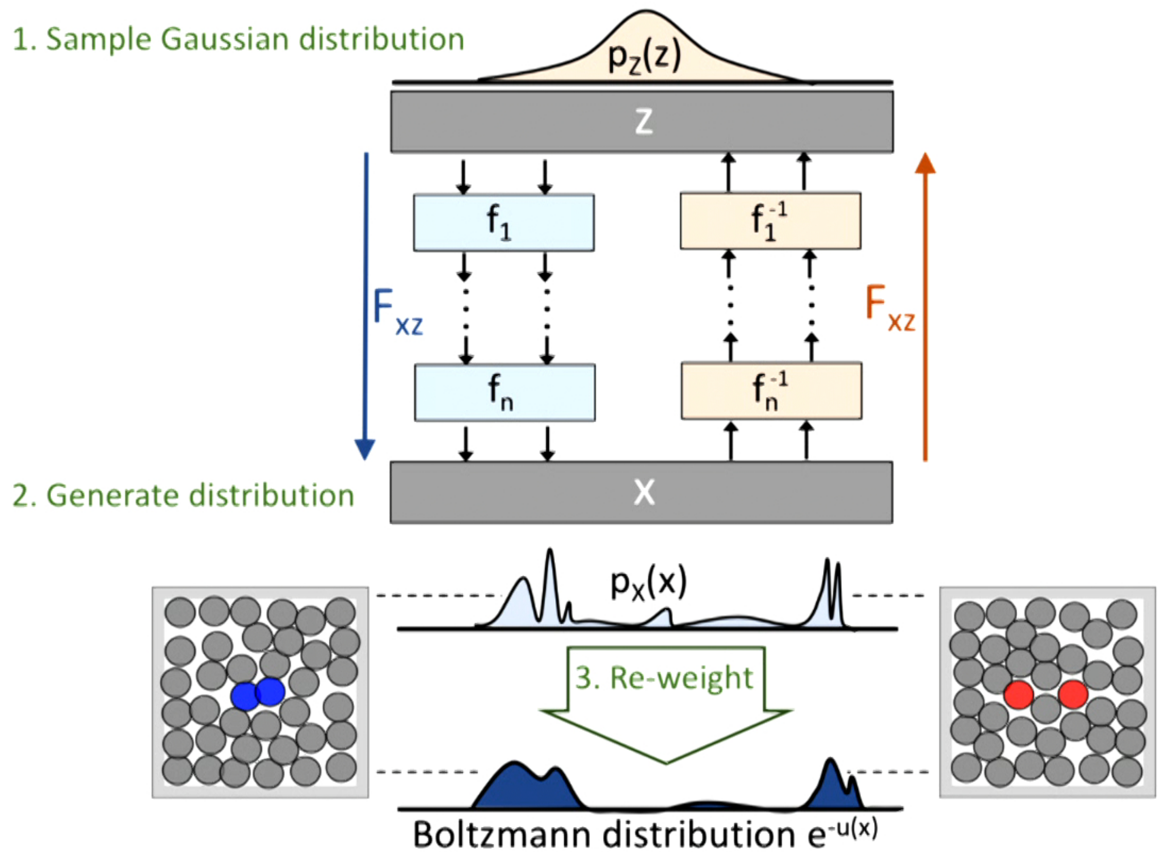
Boltzmann Generators: Exact probability generator + reweighting



Boltzmann Generators learn to generate **unbiased** samples from target distribution $e^{-u(\mathbf{x})}$

Noé, Olsson, Köhler, Wu, **Science** 365: eaww1147 (2019). arXiv:1812.01729

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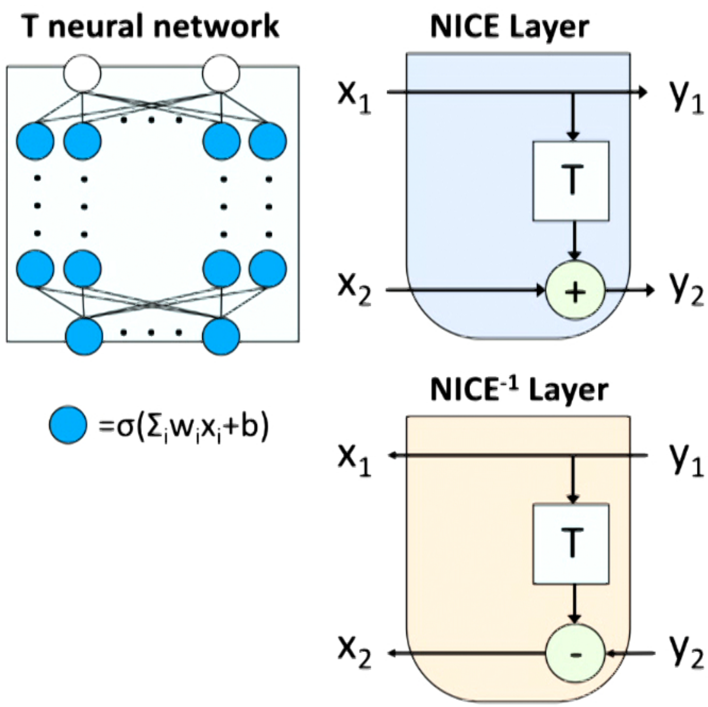
Invertible Networks



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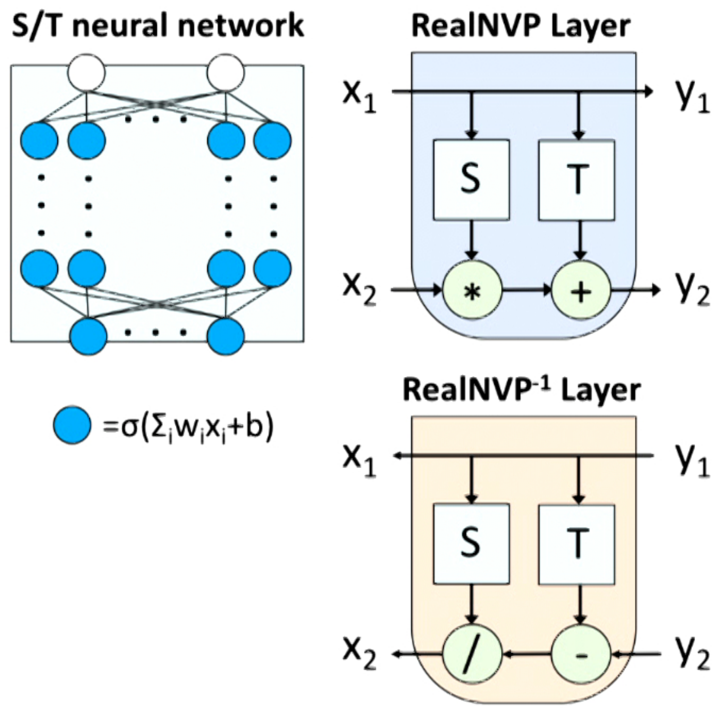

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*__Neural ODEs__: Chen et Al, NeurIPS 2018

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Boltzmann Generators: training with variational free energy

1. Train with **known** energy u(**x**)
   → Minimize KL divergence between generated and Boltzmann distribution

$$J_{KL} = \mathbb{E}_{\mathbf{z}\sim\mu_Z(\mathbf{z})}\left[u(F_{zx}(\mathbf{z};\theta)) - \log\left|\mathbf{J}_{zx}(\mathbf{z};\theta)\right|\right]$$

↑ Sample Gaussian — ↑ Energy of generated samples — ↑ Jacobian (Entropy) of generated samples

2. Maximum generator likelihood of training data **x**
   → Minimize KL divergence between latent and Gaussian distribution

$$\begin{aligned} J_{ML} &= -\mathbb{E}_{\mathbf{x}\sim\rho(\mathbf{x})}\left[\log p_X(\mathbf{x};\theta)\right] \\ &= \mathbb{E}_{\mathbf{x}\sim\rho(\mathbf{x})}\left[\frac{1}{\sigma^2}\left\|F_{xz}(\mathbf{x};\theta)\right\|^2 - \log\left|\mathbf{J}_{xz}(\mathbf{x};\theta)\right|\right] \end{aligned}$$

↑ Sample Data — ↑ Energy in Harmonic oscillator — ↑ Jacobian (Entropy) of data samples

Noé, Olsson, Köhler, Wu, **Science** 365: eaww1147 (2019). arXiv:1812.01729

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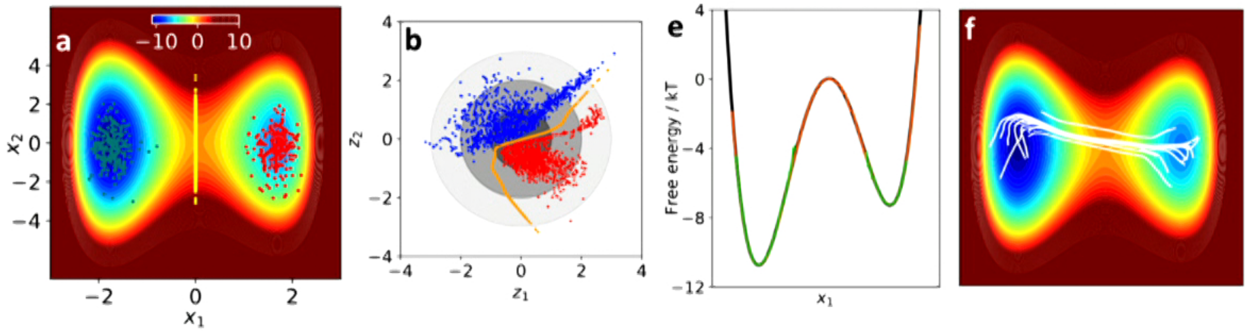
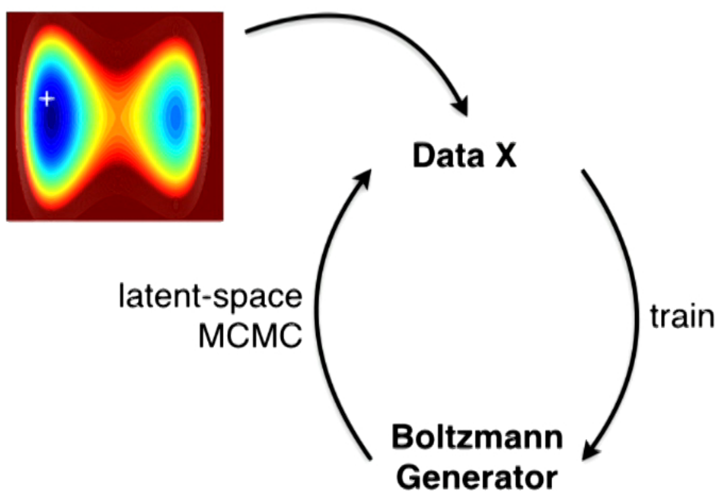
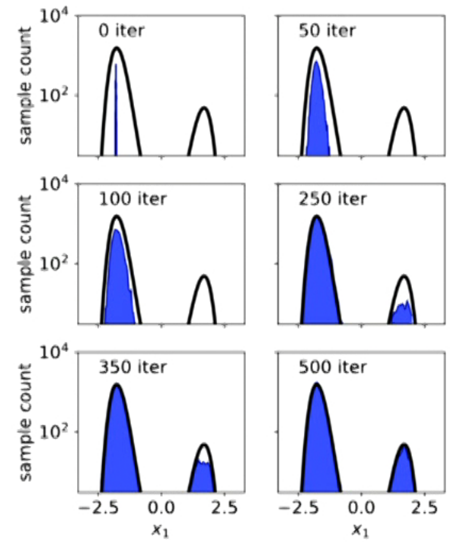
Boltzmann Generators: Double well

Train with data from multiple states:



Adaptive Exploration from one configuration:





Noé, Olsson, Köhler, Wu, **Science** 365: eaww1147 (2019). arXiv:1812.01729

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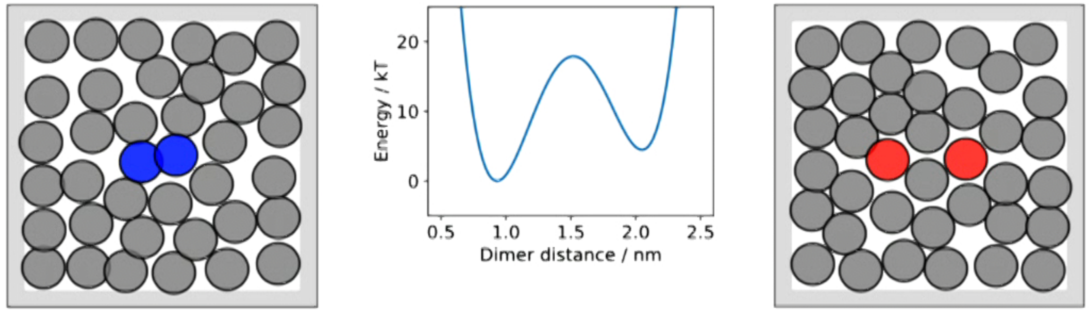
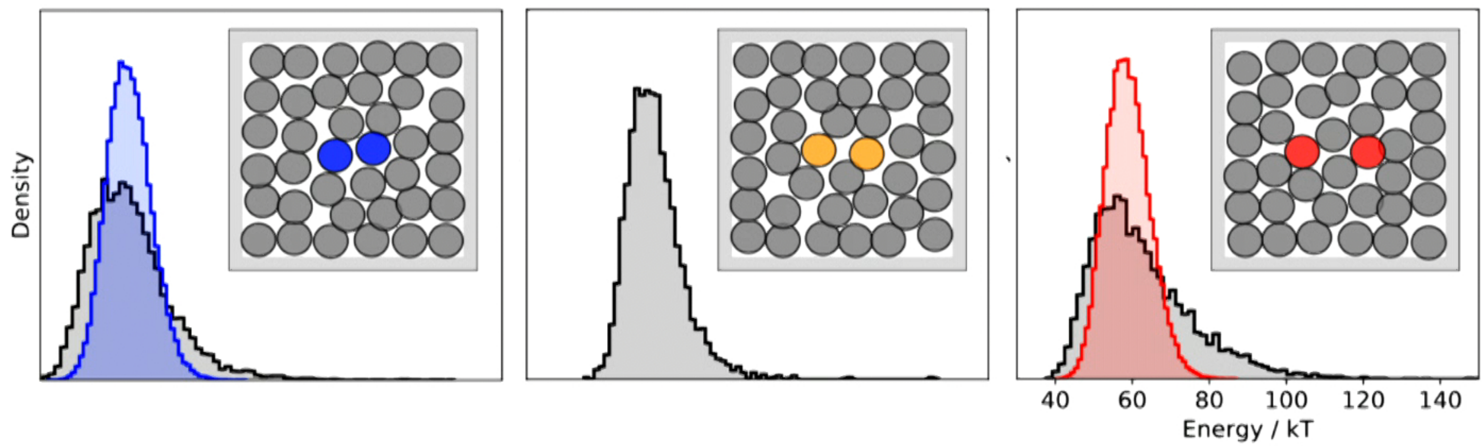
Boltzmann Generators: Bistable dimer in dense colloid solvent



Boltzmann-Generated samples:



Noé, Olsson, Köhler, Wu, **Science** 365: eaww1147 (2019). arXiv:1812.01729

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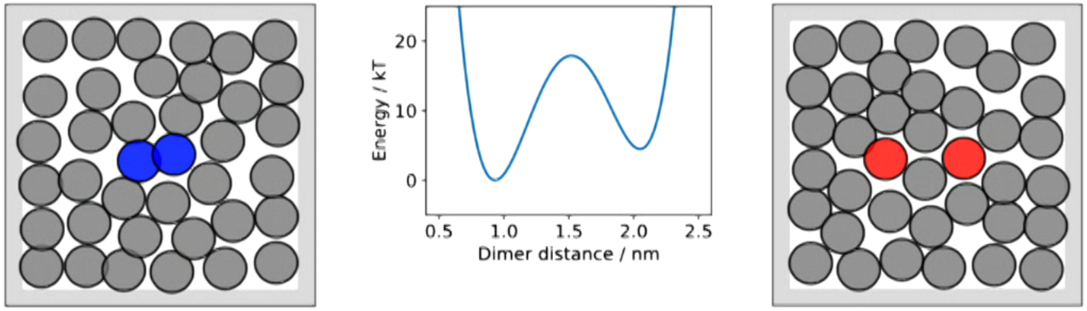
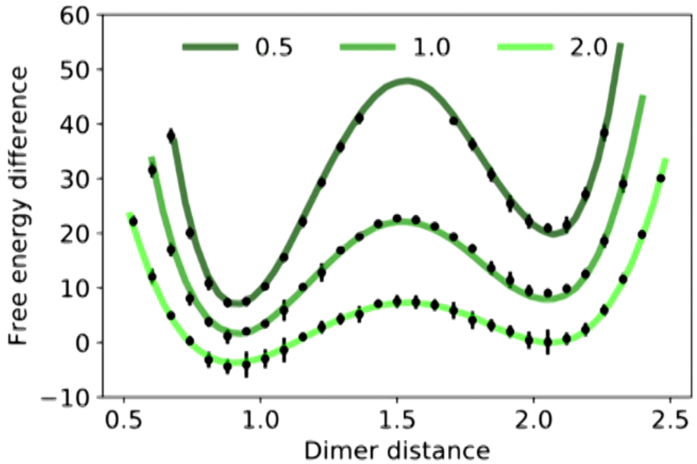
Boltzmann Generators: Bistable dimer in dense colloid solvent



Boltzmann-Generated free energy:



Noé, Olsson, Köhler, Wu, **Science** 365: eaww1147 (2019). arXiv:1812.01729

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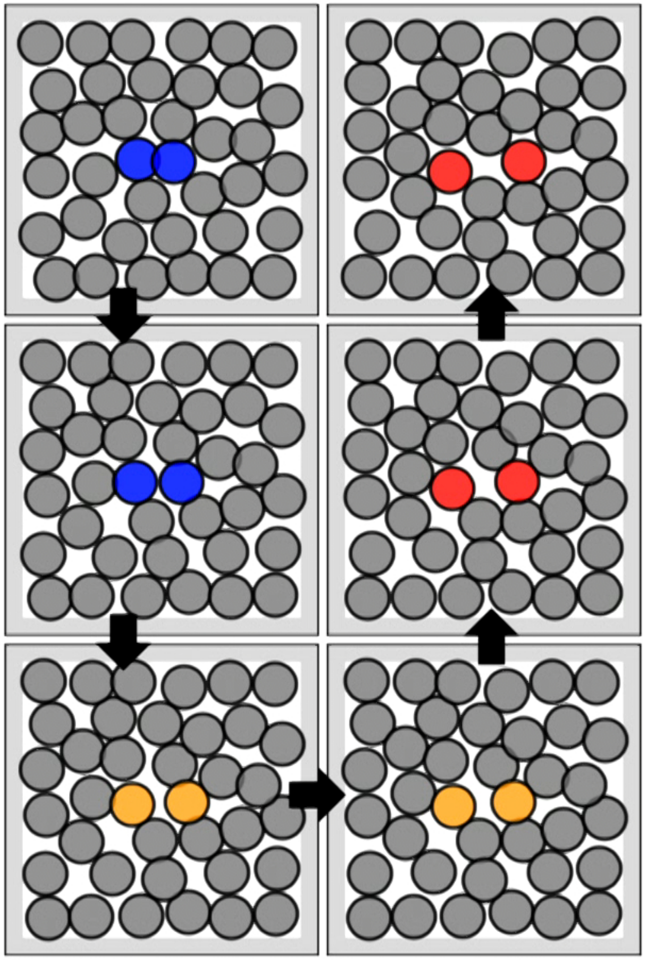
Boltzmann Generators: Bistable dimer in dense colloid solvent



Noé, Olsson, Köhler, Wu, **Science** 365: eaww1147 (2019). arXiv:1812.01729

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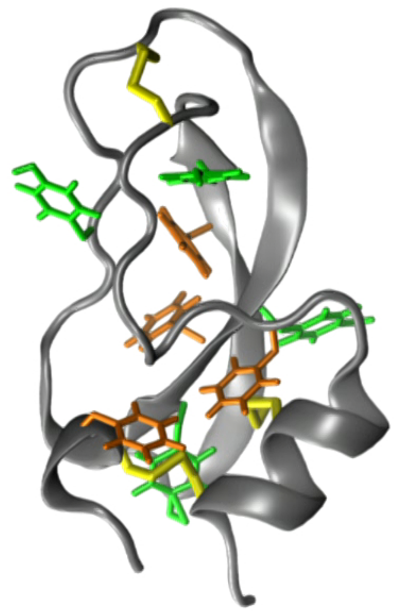
Boltzmann Generators: towards proteins



Noé, Olsson, Köhler, Wu, **Science** 365: eaww1147 (2019). arXiv:1812.01729

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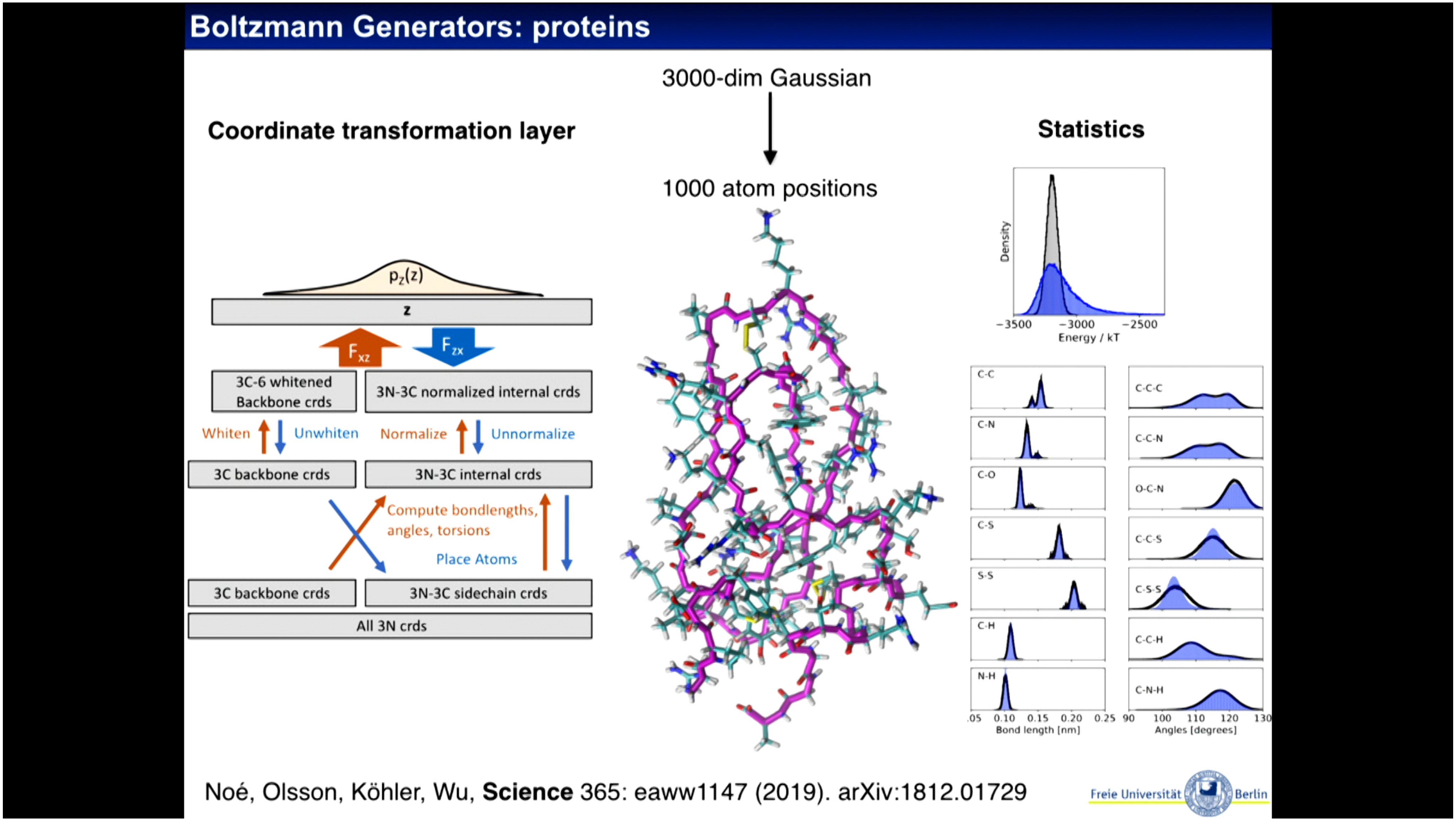

Boltzmann Generators: proteins
Coordinate transformation layer
$p_z(z)$
z
F_{xz}
F_{zx}
3C-6 whitened Backbone crds
3N-3C normalized internal crds
Whiten
Unwhiten
Normalize
Unnormalize
3C backbone crds
3N-3C internal crds
Compute bondlengths, angles, torsions
Place Atoms
3C backbone crds
3N-3C sidechain crds
All 3N crds
3000-dim Gaussian
1000 atom positions
Statistics
Density
Energy / kT
C-C
C-N
C-O
C-S
S-S
C-H
N-H
Bond length [nm]
C-C-C
C-C-N
O-C-N
C-C-S
C-S-S
C-C-H
C-N-H
Angles [degrees]
Noé, Olsson, Köhler, Wu, **Science** 365: eaww1147 (2019). arXiv:1812.01729
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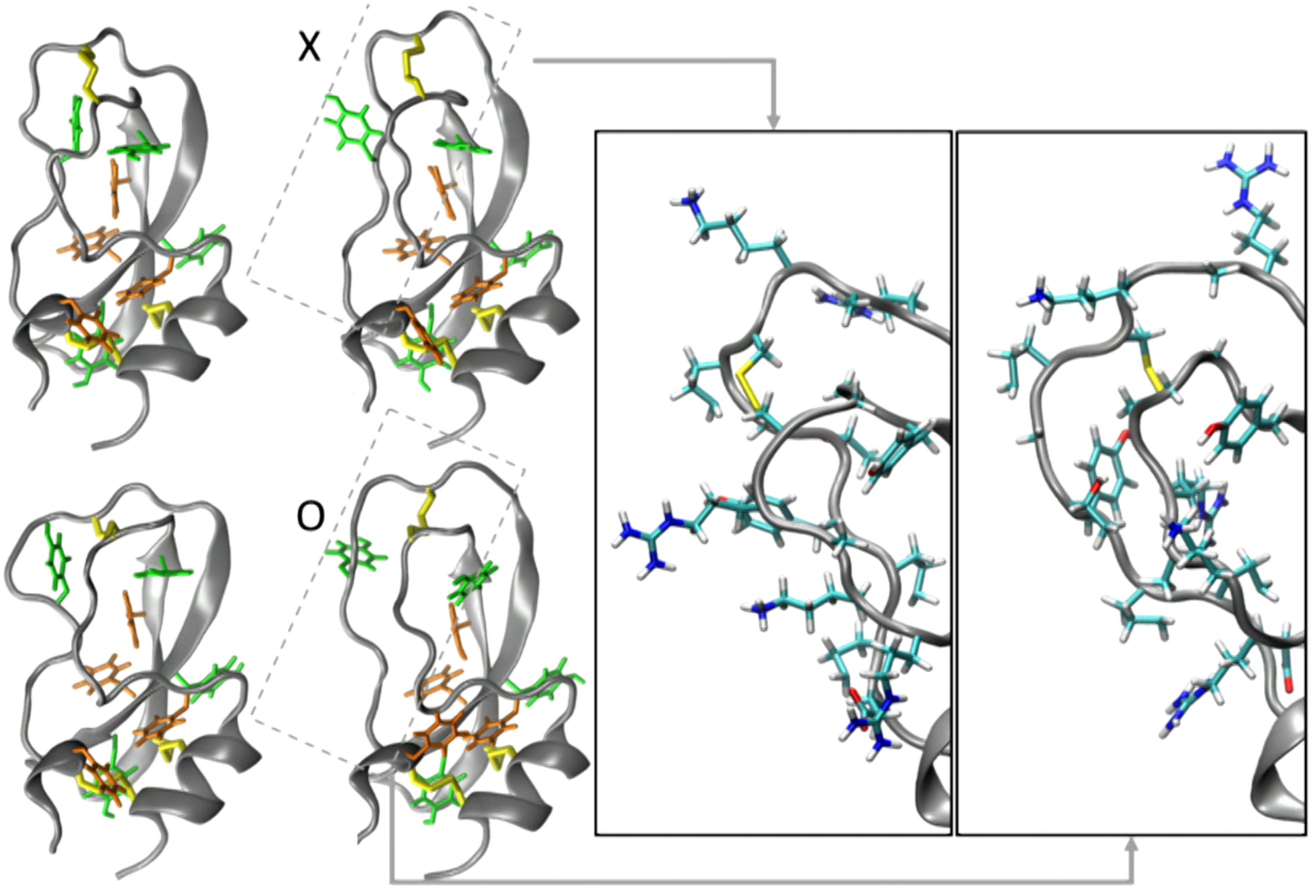
Boltzmann Generators: proteins



1 millisecond MD
= 1 year on Anton Supercomputer

Boltzmann Generator
5 hours training on 1 GPU

Noé, Olsson, Köhler, Wu, **Science** 365: eaww1147 (2019). arXiv:1812.01729

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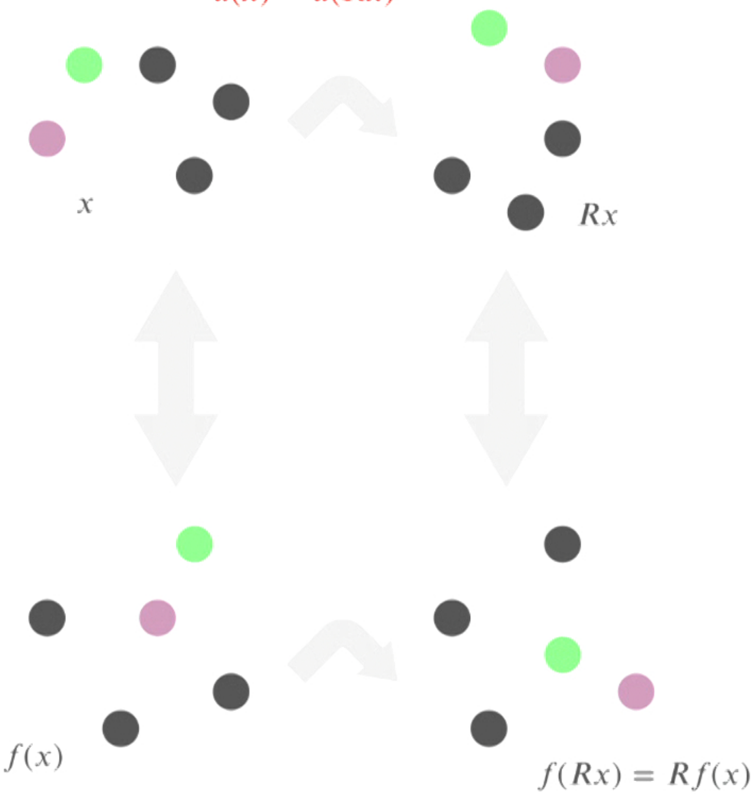
Equivariant Boltzmann Generators

$$u(x) = u(Rx)$$



$$\log p(f(x) = \log p(f(Rx)) = \log p(R(fx))$$

Köhler, Klein, Noé: NeurIPS workshop ML and the physical sciences, 2019

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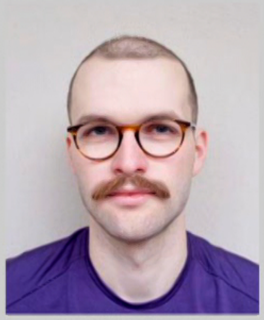
Quantum Mechanics **Electronic structure problem**

Deep neural network solution of the electronic Schrödinger Equation

Hermann, Schätzle, Noé, **arXiv** 1909.08423 (2019)



Jan Hermann

Zeno Schätzle

Electronic Schrödinger Equation

- **Electronic Schrödinger Equation**:

$$\hat{H}\psi(\mathbf{r}_1,\ldots,\mathbf{r}_N) = E\psi(\mathbf{r}_1,\ldots,\mathbf{r}_N)$$

  - $\mathbf{r} = (\mathbf{r}_1,\ldots,\mathbf{r}_N)^\top \in \mathbb{R}^{3N}$ spatial electron coordinates
  - E electronic energy, ψ electronic wave function.

- **Hamiltonian** operator:

$$\hat{H} := \sum_i \Big(-\tfrac{1}{2}\nabla^2_{\mathbf{r}_i} - \sum_I \frac{Z_I}{|\mathbf{r}_i - \mathbf{R}_I|} \Big) + \sum_{i<j} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}$$

  - Z_I nuclear charges
  - $\mathbf{R}_I$ fixed nuclear coordinates (Born--Oppenheimer approximation).

Electronic Schrödinger Equation - Antisymmetric wavefunctions

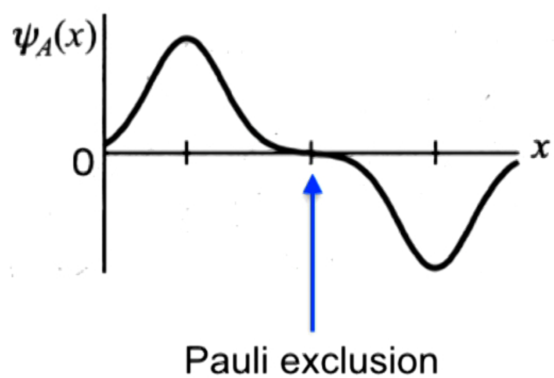
- **Electronic Schrödinger Equation**:

$$\hat{H}\psi(\mathbf{r}_1, \ldots, \mathbf{r}_N) = E\psi(\mathbf{r}_1, \ldots, \mathbf{r}_N)$$

  - $\mathbf{r} = (\mathbf{r}_1, \ldots, \mathbf{r}_N)^\top \in \mathbb{R}^{3N}$ spatial electron coordinates
  - E electronic energy, ψ electronic wave function.

- **Electronic spins** $s_i \in \{\uparrow, \downarrow\}$.
  ψ must be antisymmetric wrt exchange of equal-spin electrons

$$\psi(\ldots, \mathbf{r}_i, \ldots, \mathbf{r}_j, \ldots) = -\psi(\ldots, \mathbf{r}_j, \ldots, \mathbf{r}_i, \ldots)$$



Variational Approach — Keystone for machine learning

- **Variational Approach**

$$E_0 = \min_{\psi} E[\psi] \leq \min_{\theta} E[\psi(\mathbf{r};\theta)] \qquad E[\psi] = \int d\mathbf{r}\, \psi(\mathbf{r}) \hat{H} \psi(\mathbf{r})$$

Machine Learning loss function

Represent with neural network

Questions:

- Computation: How do we evaluate $E[\psi] = \int d\mathbf{r}\, \psi(\mathbf{r}) \hat{H} \psi(\mathbf{r})$?
- Representation: How do we build physics into $\psi(\mathbf{r})$?
  (antisymmetry, asymptotics, …)

Quantum Monte Carlo is the natural choice!

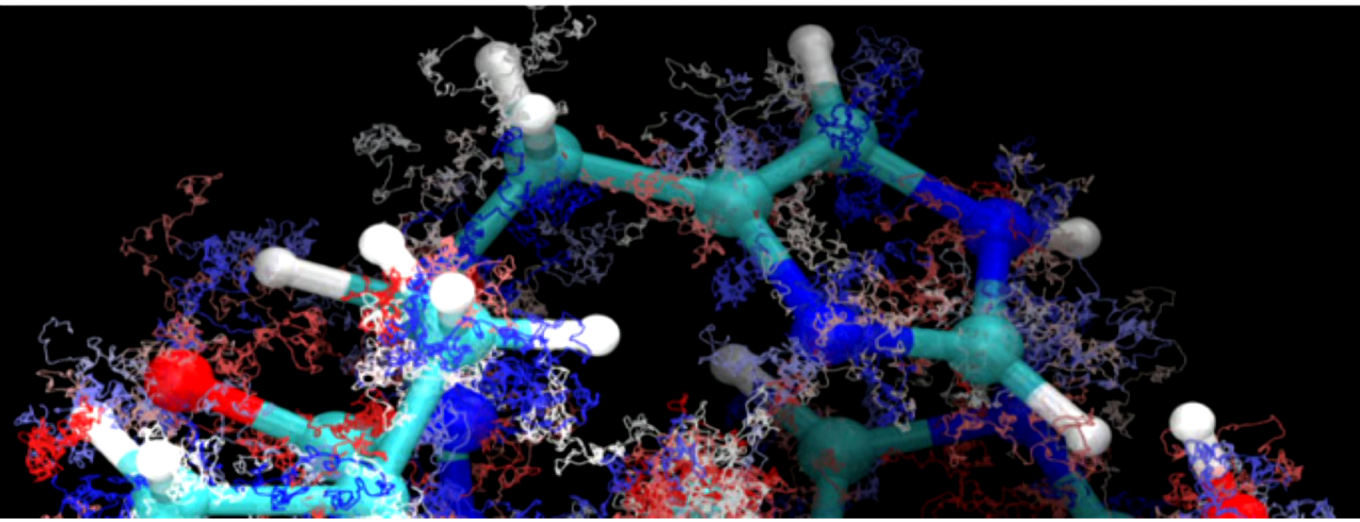
- **Variational Approach**

$$E_0 = \min_{\psi} E[\psi] \leq \min_{\theta} E[\psi(\mathbf{r};\theta)] \qquad E[\psi] = \int d\mathbf{r}\, \psi(\mathbf{r}) \hat{H} \psi(\mathbf{r})$$

- **VMC**: Variational Quantum Monte Carlo:

$$E[\psi;\theta] = \mathbb{E}_{\mathbf{r}\sim|\psi|^2}\left[E_{\text{loc}}[\psi](\mathbf{r};\theta)\right] \qquad E_{\text{loc}}[\psi](\mathbf{r};\theta) = \hat{H}\psi(\mathbf{r};\theta)/\psi(\mathbf{r};\theta)$$

Sample Minibatches



Why is Quantum Monte Carlo an accurate method?

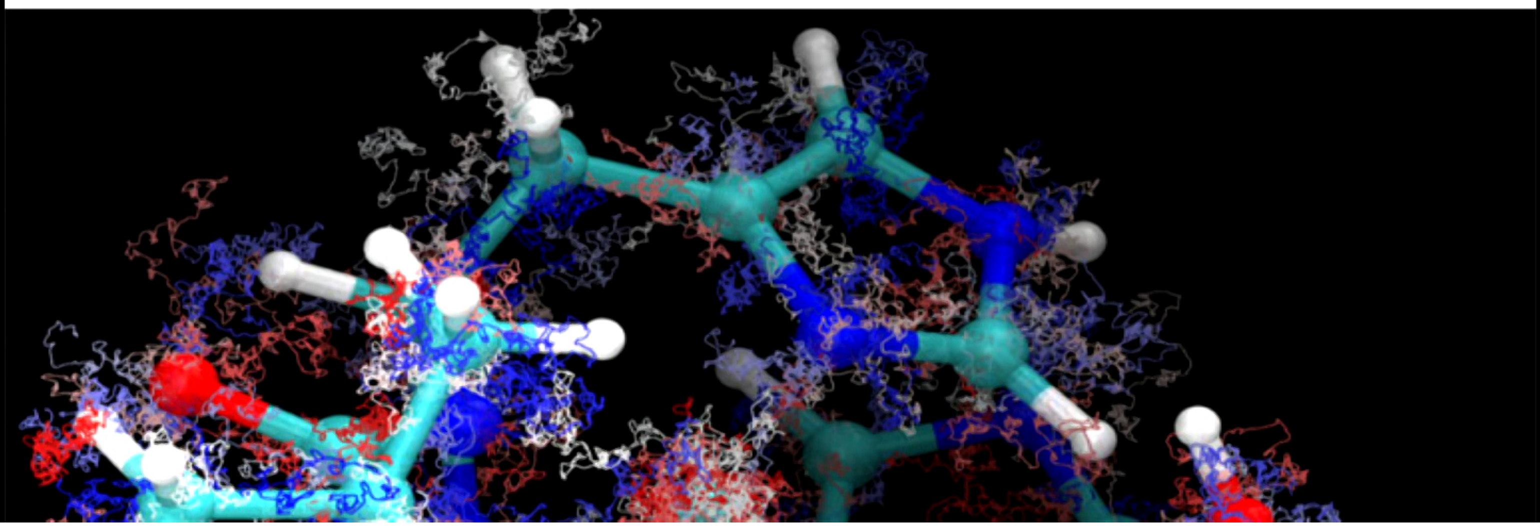
Monte Carlo converges slowly:

$$\mathrm{Var}\{E[\psi;\theta]\} = \frac{\mathrm{Var}_{\mathbf{r}}\{E_{\mathrm{loc}}[\psi](\mathbf{r};\theta)\}}{N_{\mathrm{sample}}}$$

But: **Variance** of local energy **decreases** during training

At the eigenstate: $E_{\mathrm{loc}}[\psi](\mathbf{r};\theta) = \hat{H}\psi(\mathbf{r};\theta)/\psi(\mathbf{r};\theta)$ = constant in **r** !

$\hat{H}\psi = E\psi$



Quantum Monte Carlo + Neural Networks

- **Variational Approach**

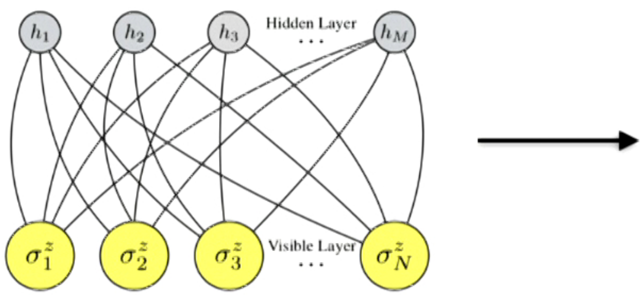
$$E_0 = \min_{\psi} E[\psi] \le \min_{\theta} E[\psi(\mathbf{r};\theta)] \qquad E[\psi] = \int d\mathbf{r}\, \psi(\mathbf{r}) \hat{H} \psi(\mathbf{r})$$

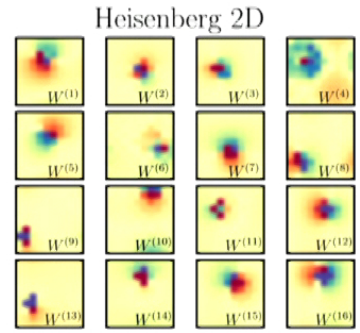
- **VMC**: Variational Quantum Monte Carlo:

$$E[\psi;\theta] = \mathbb{E}_{\mathbf{r}\sim|\psi|^2}\left[E_{\text{loc}}[\psi](\mathbf{r};\theta)\right] \qquad E_{\text{loc}}[\psi](\mathbf{r};\theta) = \hat{H}\psi(\mathbf{r};\theta)/\psi(\mathbf{r};\theta)$$

QMC with Restricted Boltzmann Machines:

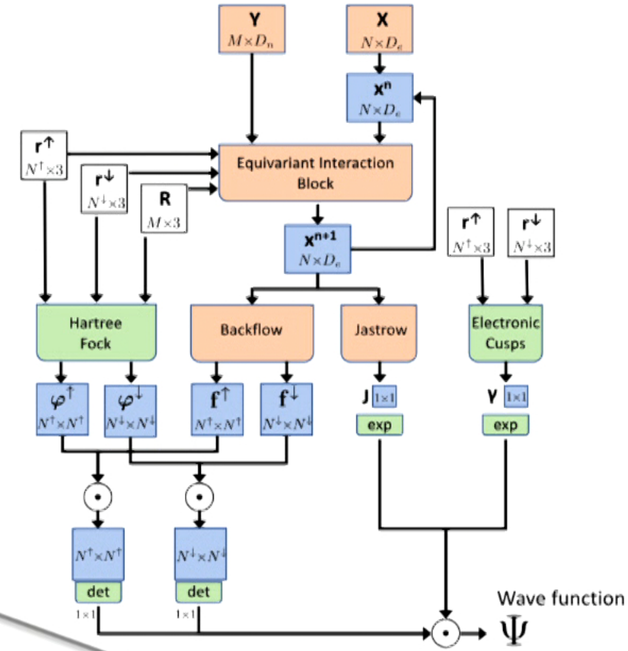
Carleo, Troyer: Solving the Quantum Many-Body Problem with Artificial Neural Networks, Science 355: 602-606 (2011)



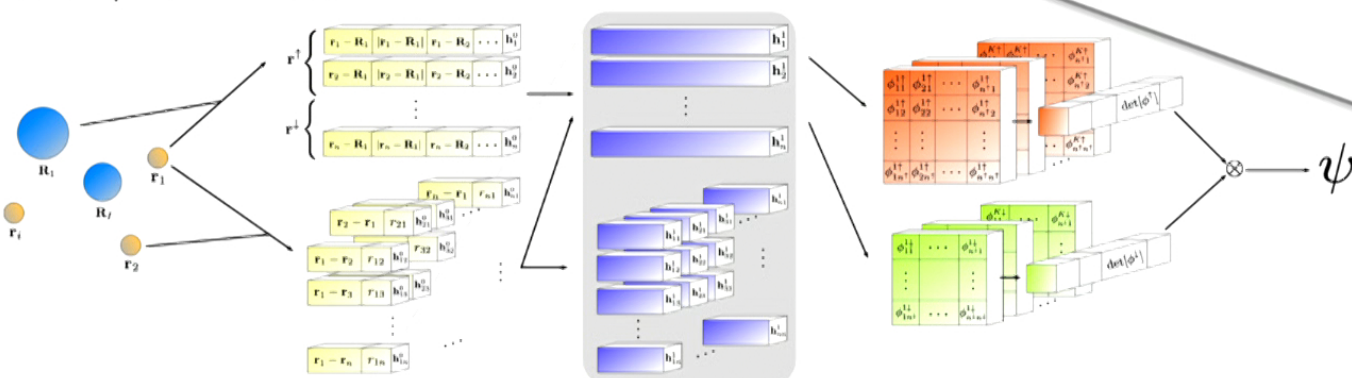


Quantum Chemistry Approaches (both Sept 2019)

PauliNet: (this work)
Hermann, Schätzle, Noé: **arXiv**:1909.08423
Deep neural network solution of the electronic Schrödinger equation



FermiNet
Pfau, Spencer, Matthews, Foulkes: **arXiv**:1909.02487
Ab-Initio Solution of the Many-Electron Schrödinger Equation with Deep Neural Networks



PauliNet Wavefunction

$$\psi(\mathbf{r};\theta) = \det[\varphi_\mu(\mathbf{r}_i^\uparrow) f_{\mu i}(\mathbf{r};\theta)] \det[\varphi_\mu(\mathbf{r}_i^\downarrow) f_{\mu i}(\mathbf{r};\theta)] \mathrm{e}^{\gamma(\mathbf{r})+J(\mathbf{r};\theta)}$$

Incorporating Physics

1) Enforce Antisymmetry
⟶ Backflow

2) Baseline Performance
⟶ Hartree Fock Input

3) Correlation Energy
⟶ Slater-Jastrow Backflow

4) Asymptotics
⟶ Cusp conditions

PauliNet Wavefunction

$$\psi(\mathbf{r};\theta) = \det[\varphi_\mu(\mathbf{r}_i^\uparrow) f_{\mu i}(\mathbf{r};\theta)] \det[\varphi_\mu(\mathbf{r}_i^\downarrow) f_{\mu i}(\mathbf{r};\theta)] \mathrm{e}^{\gamma(\mathbf{r})+J(\mathbf{r};\theta)}$$

spin-up electrons spin-down electrons

Assignment to spin-groups avoids spin coordinates

PauliNet Wavefunction

$$\psi(\mathbf{r};\theta) = \det[\varphi_\mu(\mathbf{r}_i^\uparrow) f_{\mu i}(\mathbf{r};\theta)] \det[\varphi_\mu(\mathbf{r}_i^\downarrow) f_{\mu i}(\mathbf{r};\theta)] \mathrm{e}^{\gamma(\mathbf{r}) + J(\mathbf{r};\theta)}$$

antisymmetric part

1) Enforcing antisymmetry: Standard QM approach

- **Antisymmetry** for **single-electron** functions: Slater determinants.

$$\psi_{\mathrm{HF}}(\mathbf{r}) := \det[\varphi_\mu(\mathbf{r}_i^\uparrow)] \det[\varphi_\mu(\mathbf{r}_i^\downarrow)]$$

$$\det[\varphi_\mu(\mathbf{r}_i^\uparrow)] = \begin{vmatrix} \varphi_1(\mathbf{r}_1^\uparrow) & \varphi_2(\mathbf{r}_1^\uparrow) & \cdots & \varphi_N(\mathbf{r}_1^\uparrow) \\ \varphi_1(\mathbf{r}_2^\uparrow) & \varphi_2(\mathbf{r}_2^\uparrow) & \cdots & \varphi_N(\mathbf{r}_2^\uparrow) \\ \vdots & \vdots & & \vdots \\ \varphi_1(\mathbf{r}_N^\uparrow) & \varphi_2(\mathbf{r}_N^\uparrow) & \cdots & \varphi_N(\mathbf{r}_N^\uparrow) \end{vmatrix}$$

→ Limited representative power

→ Many Slater determinants needed for high accuracy (CI)

PauliNet Wavefunction

$$\psi(\mathbf{r};\theta) = \det[\varphi_\mu(\mathbf{r}_i^\uparrow) f_{\mu i}(\mathbf{r};\theta)] \det[\varphi_\mu(\mathbf{r}_i^\downarrow) f_{\mu i}(\mathbf{r};\theta)] e^{\gamma(\mathbf{r}) + J(\mathbf{r};\theta)}$$

antisymmetric part

1) Enforcing antisymmetry in PauliNet: Backflow

- **Antisymmetry** for **many-electron** functions $\varphi_\mu(\mathbf{r}_i) \to \varphi_{\mu i}(\mathbf{r})$ holds if $\varphi_{\mu i}(\mathbf{r})$ is equivariant wrt exchange $\mathscr{P}$ of same-spin electrons[1],[2]

$$\varphi_\mu(\mathbf{r}_i) \to \varphi_{\mu i}(\mathbf{r}),$$
$$\mathscr{P}\varphi_{\mu i}(\mathbf{r}) = \varphi_{\mu i}(\mathscr{P}\mathbf{r})$$

- **PauliNet**: $\varphi_{\mu i}(\mathbf{r}) = \varphi_\mu(\mathbf{r}_i^\uparrow) f_{\mu i}(\mathbf{r};\theta)$, $f_{\mu i}$ equivariant – SchNet[3].

→ Greater representative power

→ Hope: few or one Slater determinant give high accuracy

[1] P. López Ríos et al, *Phys. Rev. E*, 74:066701(2006)
[2] D. Luo, B. K. Clark. *Phys. Rev. Lett.* 122:226401 (2019)
[3] K. T. Schütt et al., *J. Chem. Phys.* 148:241722 (2018)

PauliNet Wavefunction

$$\psi(\mathbf{r};\theta) = \det[\varphi_\mu(\mathbf{r}_i^\uparrow) f_{\mu i}(\mathbf{r};\theta)] \det[\varphi_\mu(\mathbf{r}_i^\downarrow) f_{\mu i}(\mathbf{r};\theta)] e^{\gamma(\mathbf{r})+J(\mathbf{r};\theta)}$$

2) Baseline Performance: Hartree-Fock

- Use fixed Hartree-Fock (HF) orbitals $\varphi_\mu(\mathbf{r}_i^\uparrow)$
- Pro: HF fast, captures physics of atoms and molecules qualitatively
- Con: poor quantitative predictions, no electron-electron correlations.

PauliNet Wavefunction

$$\psi(\mathbf{r};\theta) = \det[\varphi_\mu(\mathbf{r}_i^\uparrow) f_{\mu i}(\mathbf{r};\theta)] \det[\varphi_\mu(\mathbf{r}_i^\downarrow) f_{\mu i}(\mathbf{r};\theta)] e^{\gamma(\mathbf{r}) + J(\mathbf{r};\theta)}$$

3) **Correlation Energy** (beyond Hartree-Fock): **deep learning**

- **Jastrow factor**[4] $J(\mathbf{r};\theta)$: Antisymmetric part is multiplied by nonnegative symmetric function $e^{J(\mathbf{r};\theta)}$. Can capture complex electron correlations but not change the nodal surface.
- **Backflow**[5,6] $\mathbf{f}(\mathbf{r};\theta)$: Generalize one-electron orbitals $\varphi_\mu(\mathbf{r}_i)$ to many-electron orbitals $\varphi_{\mu i}(\mathbf{r})$. Can change the nodal surface.

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[4] N. D. Drummond et al. *Phys. Rev. B* 70:235119 (2004)
[5] P. López Ríos et al, *Phys. Rev. E*, 74:066701(2006)
[6] D. Luo, B. K. Clark. *Phys. Rev. Lett.* 122:226401 (2019)

PauliNet Wavefunction

$$\psi(\mathbf{r};\theta) = \det[\varphi_\mu(\mathbf{r}_i^\uparrow) f_{\mu i}(\mathbf{r};\theta)] \det[\varphi_\mu(\mathbf{r}_i^\downarrow) f_{\mu i}(\mathbf{r};\theta)] e^{\gamma(\mathbf{r})+J(\mathbf{r};\theta)}$$

4) Asymptotics

- **Cusp conditions**:

$$\frac{1}{\psi_0}\frac{\partial \psi_0}{\partial|\mathbf{r}_i - \mathbf{R}_I|}\bigg|_{\mathbf{r}_i=\mathbf{R}_I} = -Z_I \qquad \frac{1}{\psi_0}\frac{\partial \psi_0}{\partial|\mathbf{r}_i - \mathbf{r}_j|}\bigg|_{\mathbf{r}_i=\mathbf{r}_j} = \begin{cases} \frac{1}{4} & s_i = s_j \\ \frac{1}{2} & s_i \neq s_j \end{cases}$$

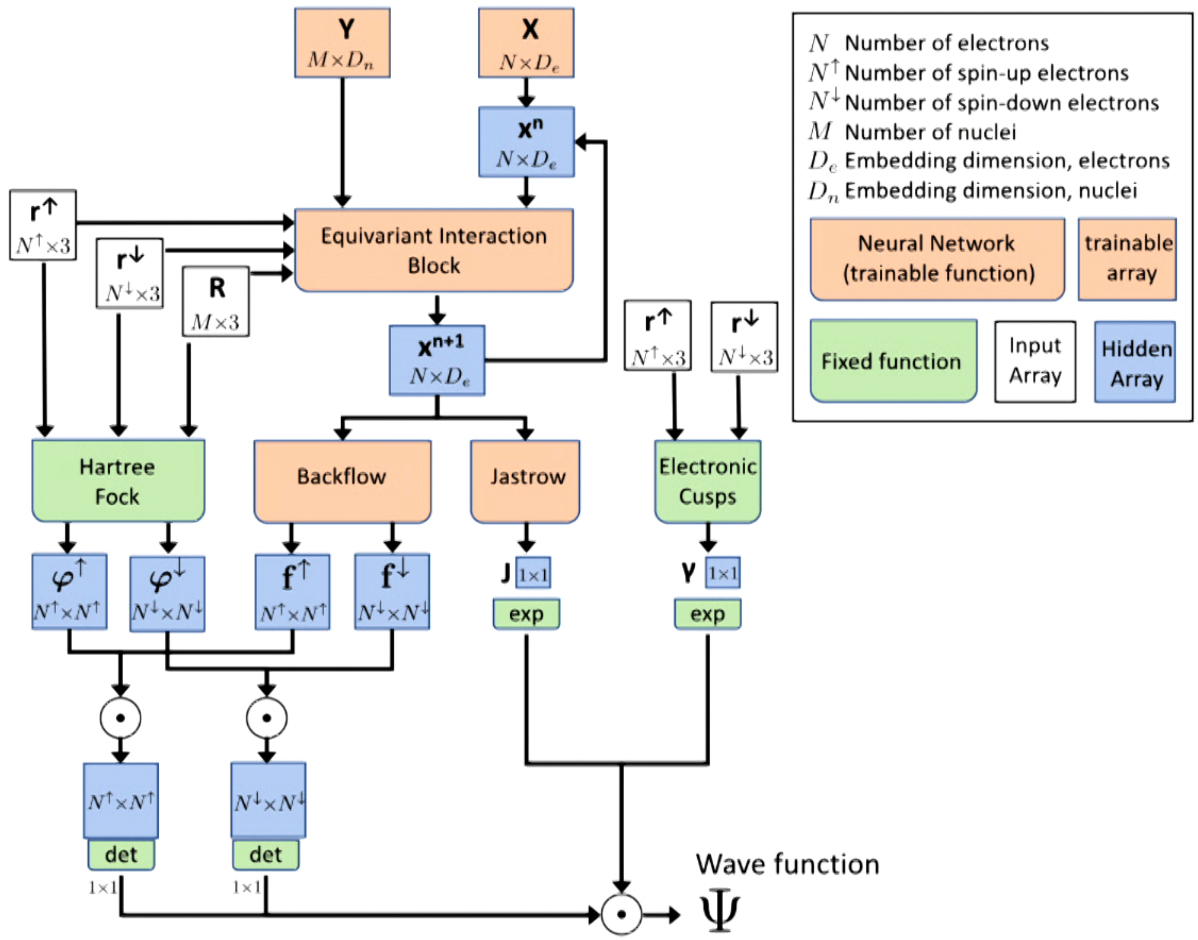
- **PauliNet**:
  - Nuclear cusps are built into $\varphi_\mu(\mathbf{r}_i)$[7].
  - Electronic cusps: use asymptotic function

$$\gamma(\mathbf{r}) := \sum_{i<j} -\frac{c_{ij}}{1+|\mathbf{r}_i - \mathbf{r}_j|} \qquad c_{ij} = \begin{cases} \frac{1}{4} & s_i = s_j \\ \frac{1}{2} & s_i \neq s_j \end{cases}$$

  - Backflow and Jastrow networks are cuspless by construction:

[7] A. Ma et al: J. Chem. Phys. 122:224322 (2005)

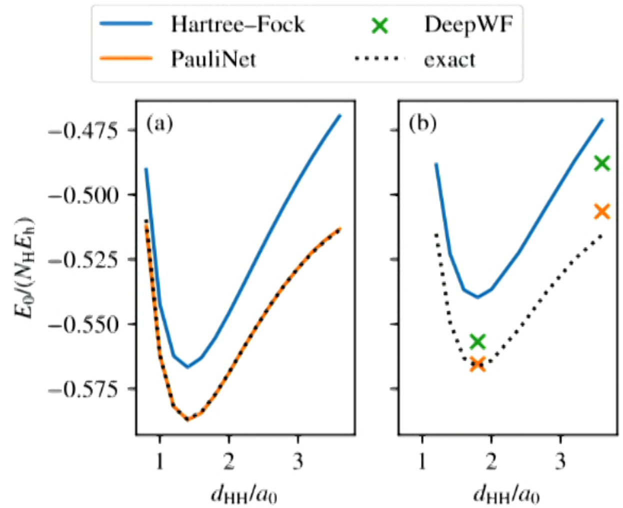
PauliNet



Y
$M \times D_n$
X
$N \times D_e$
x^n
$N \times D_e$
r↑
$N^\uparrow \times 3$
r↓
$N^\downarrow \times 3$
R
$M \times 3$
Equivariant Interaction Block
x^{n+1}
$N \times D_e$
r↑
$N^\uparrow \times 3$
r↓
$N^\downarrow \times 3$
Hartree Fock
Backflow
Jastrow
Electronic Cusps
$\varphi^\uparrow$
$N^\uparrow \times N^\uparrow$
$\varphi^\downarrow$
$N^\downarrow \times N^\downarrow$
$f^\uparrow$
$N^\uparrow \times N^\uparrow$
$f^\downarrow$
$N^\downarrow \times N^\downarrow$
J 1×1
exp
γ 1×1
exp
$N^\uparrow \times N^\uparrow$
det
1×1
$N^\downarrow \times N^\downarrow$
det
1×1
Wave function
Ψ
N Number of electrons
$N^\uparrow$ Number of spin-up electrons
$N^\downarrow$ Number of spin-down electrons
M Number of nuclei
D_e Embedding dimension, electrons
D_n Embedding dimension, nuclei
Neural Network (trainable function)
trainable array
Fixed function
Input Array
Hidden Array

PauliNet: Results

system[a]	E_0/E_h (% E_{corr}) VMC		DMC		DeepWF		PauliNet	
H_2^b					−1.1738	98.4%	−1.174 37(6)	99.7%
LiH[c]	−8.0635[f]	91.5%	−8.0703[f]	99.7%	−7.8732	[g]	−8.0690(3)	98.1%
Be[d]	−14.6311[d]	61.6%	−14.6572[d]	89.2%	−14.6141	43.6%	−14.6546(7)	86.5%
B[d]	−24.6056[d]	60.0%	−24.6398[d]	88.3%	−24.2124	[g]	−24.634(2)	83.5%
H_{10}^e					−5.5685	63.8%	−5.655(2)	96.0%



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