Taming nuclear complexity with deep neural networks

R.-D. Lasseri[1], D. Regnier[2]

[1]ESNT, CEA, IRFU, DPhN, Université Paris Saclay, F-91191 Gif-sur-Yvette
[2]CMLA, CNRS, ENS Paris-Saclay, Université Paris-Saclay, 94235, Cachan cedex, France

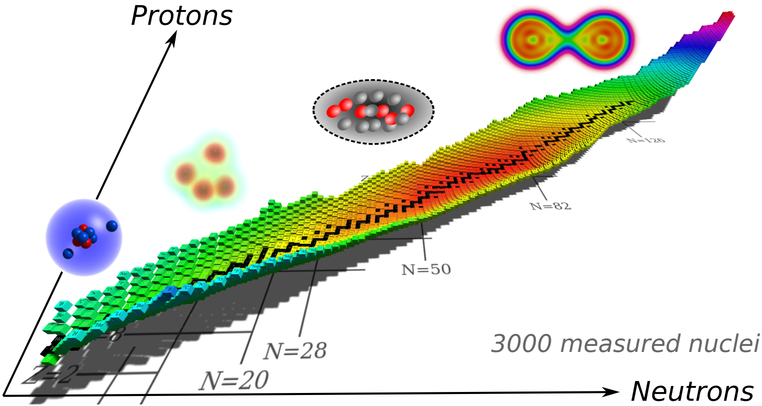
The nuclear complexity

Why so complex ?

- Three fundamental interactions
- Non elementary fermions
- Mesoscopic many-body problem

Some open questions

- Properties of exotic matter ?
- Mechanism of nucleosynthesis ?
- Super-heavy island of stability ?



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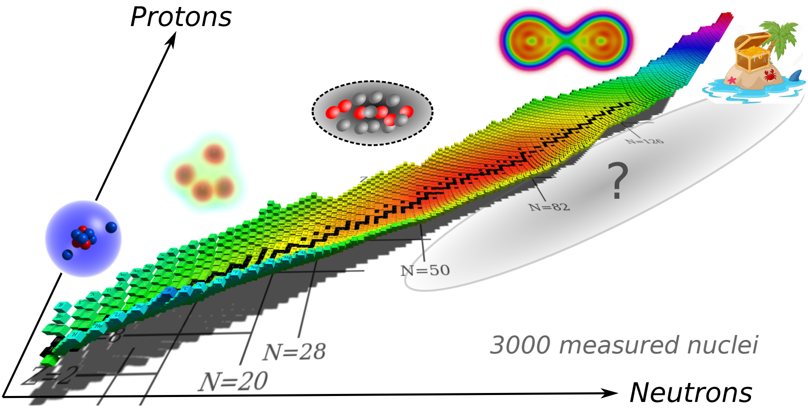
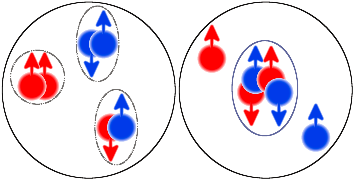


When complexity leads to diversity – Superfluidities

Fermions in presence of an attractive interaction[1]

- Pairing
- Quartetting



Questions:

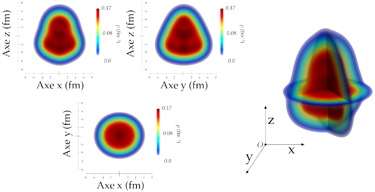
- Spatial properties of pairs/quartets
- BEC/BCS Transitions

[1] Lasseri, Ebran, Khan, Sandulescu Phys. Rev. C 98, 014310 (2018)

When complexity leads to diversity – Deformation and Clustering

Emerging phenomena[2 3 4 5]

- Anisotropy: Deformation
- Inhomogeneities: Clusters



Questions:

- Cluster localization
- Quantum Phase Transitions
- Alpha/Cluster Radioactivity

[2] Le Bars, Guerlin, Lasseri *et al* Phys. Rev. D 95, 075026 (2017)
[3] Ebran, Khan, Lasseri, Vretenar Phys. Rev. C 97, 061301 (2018)
[4] Ebran, Khan, Lasseri Submitted to PRC (2019)
[5] Ebran, Girdo, Khan, Lasseri, Schuck Submitted to PRC (2019)

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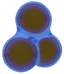

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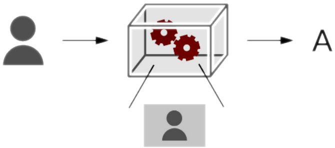
Representations

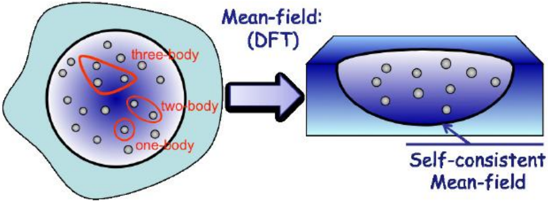
Transparent + Explicit

- Arithmetics
- ◇ Reductionism



The nuclear energy density functional framework (EDF)

Classical or covariant "microscopic" approach capable of predictions over the whole nuclear chart[6] [7]



Many implementations:

- Symmetry breaking/restoration: Multi-Reference EDF
- Linear response: RPA, QRPA
- Time dependency: TDHFB, TDGCM...
- Perturbation Theories: MBPT, BMBPT

Limitations

- Numerical cost
- No link with the bare n-n interaction
- Double counting, spuriosities

[6] Perez, Schunck, Lasseri, Zhang, J.Sarich Comp. Phys. Comm (2017)
[7] Arthuis, Duguet, Tichai, Lasseri, Ebran Comp. Phys. Comm (2018)

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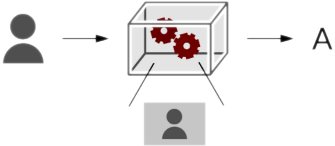
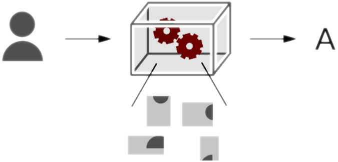


Transparent + Implicit

- Encrypted messages
- ◇ Emergentism



Quantum mechanics is a theory about the physical ***description*** *of physical systems* ***relative*** *to other systems, and this is a complete description of the world*[8] *– Carlo Rovelli*

[8] International Journal of Theoretical Physics August 1996, Volume 35, Issue 8, pp 1637?1678

How can we leverage machine learning in nuclear theory ?

Progress of machine learning:

- Image classification:
  cancer detection, particle detection
- Generative AI:
  turbulence
- Inverse problems:
  cosmology
- Many body problem:
  spin systems, bosons

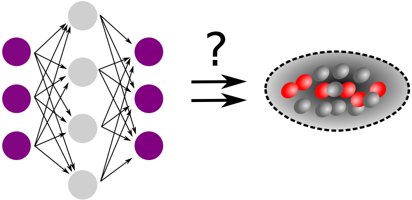
A review:

G. Carleo *et. al.*, arXiv:1903.10563 (2019)

In nuclear theory:

- Machine learning for experimental nuclear masses or radii tables
- Acceleration of EDF calculations

$\Longrightarrow$ An unexplored territory



Question (march 2019)...

Can we teach an artificial intelligence (AI) to predict nuclear structure ?

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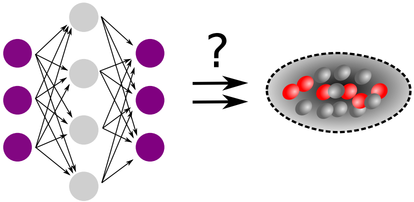

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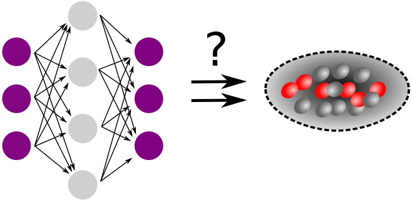

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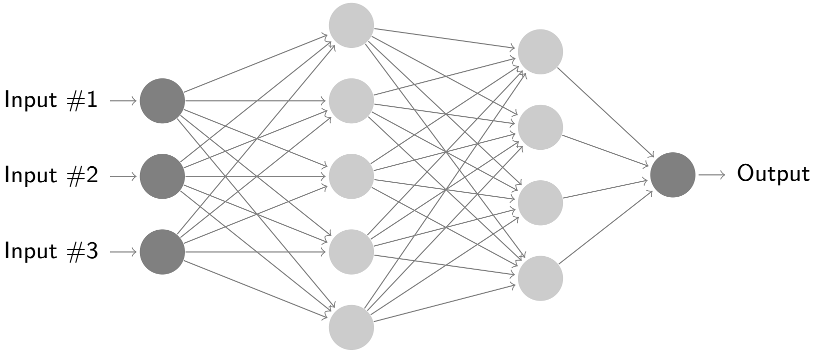

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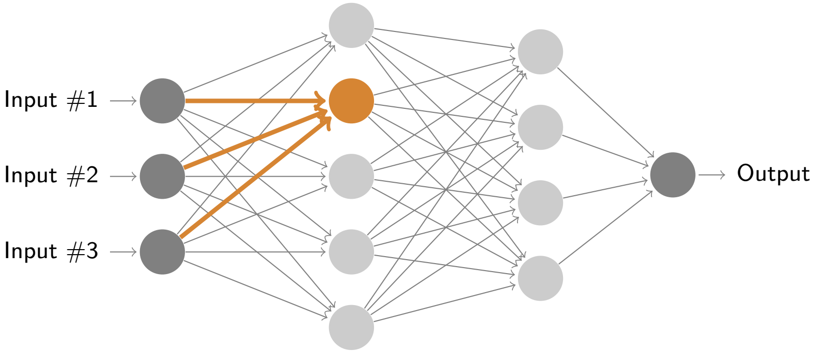

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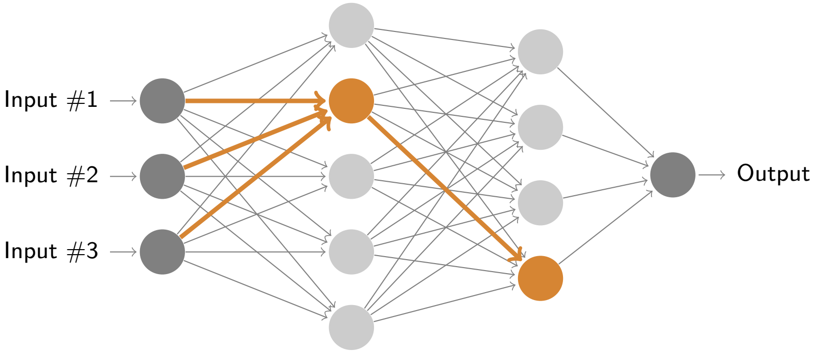

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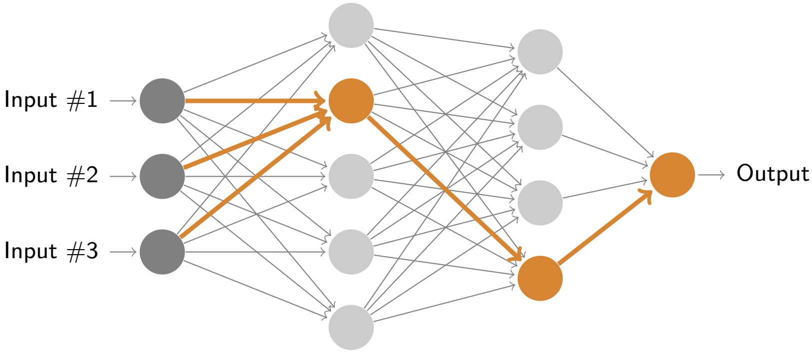

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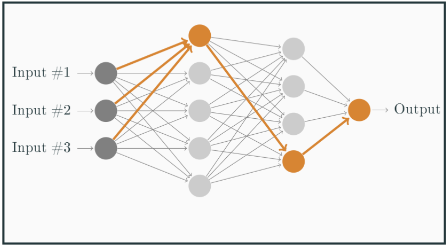

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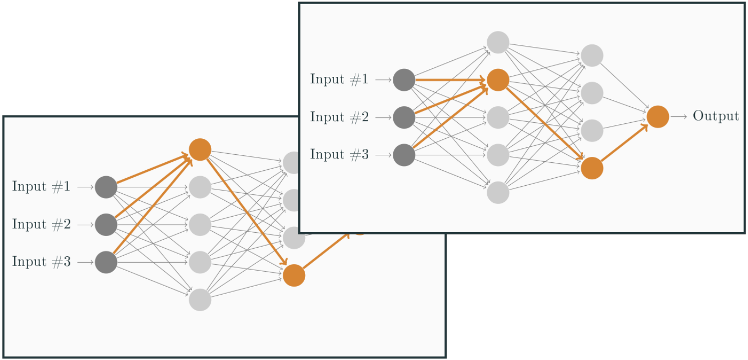

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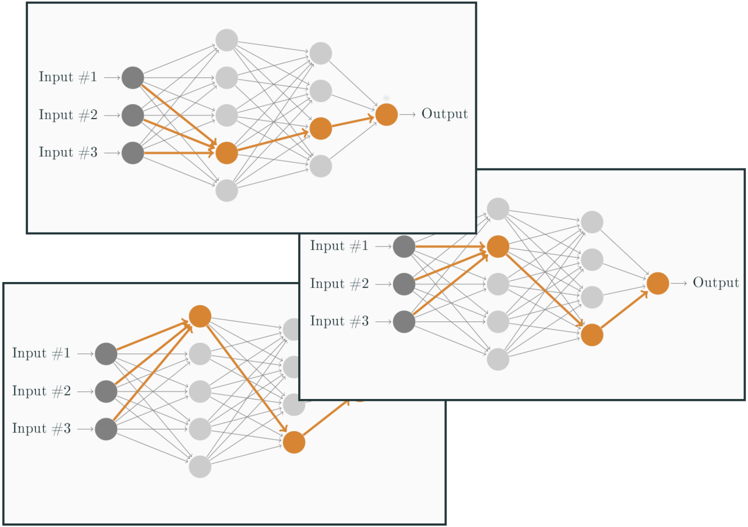
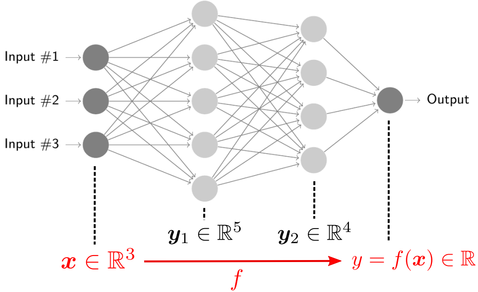
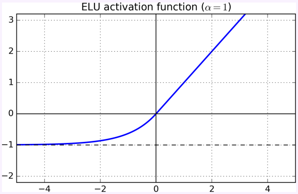


The mathematical picture



$$
\begin{aligned}
\boldsymbol{y}_1 &= f_1(\boldsymbol{x}) &&= A_1(W_1 \cdot \boldsymbol{x} + \boldsymbol{b}_1) \\
\boldsymbol{y}_2 &= f_2(\boldsymbol{y}_1) &&= A_2(W_2 \cdot \boldsymbol{y}_1 + \boldsymbol{b}_1) \\
y &= f_3(\boldsymbol{y}_2) &&= A_3(W_3 \cdot \boldsymbol{y}_2 + \boldsymbol{b}_2) \\
y &= f(\boldsymbol{x}) &&= f_3 \circ f_2 \circ f_1(\boldsymbol{x})
\end{aligned}
$$

$A_1, A_2, A_3 =$ non-linear functions.



$W_1, W_2, W_3 =$ matrices,
$\boldsymbol{b}_1, \boldsymbol{b}_2, \boldsymbol{b}_3 =$ vectors.

We fit these parameters so to reproduce some training data $(\boldsymbol{x}^i, y^i), i \in [0, N]$.

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State of the art

Neural networks, Bayesian Neural Net. and Gaussian Processes were used to:

Fit nuclear masses

- Athanassopoulos *et. al.* NPA 743 (2004)
  RMS = 950 keV
- Utama *et. al.* PRC 96 (2017)
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  RMS decreased by 40%
- Zhang *et. al.* J Phys. G (2017)
  Drip-lines predictions
- Neufcourt *et. al.* PRC 98 (2018)
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  Estimation of uncertainties

Fit nuclear radii

- Akkoyun *et. al.* J. Phys. G: NPP 40 (2013)
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Current limitations

- AI trained on 80% of an experimental dataset, i.e $>$ 1800 nuclei
- Only trained to capture one observable

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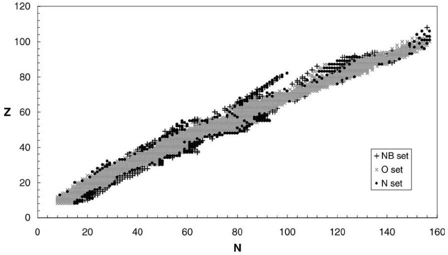

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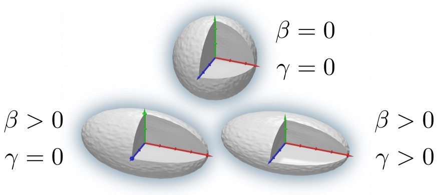
Structure from the 5D collective Hamiltonian 1/2

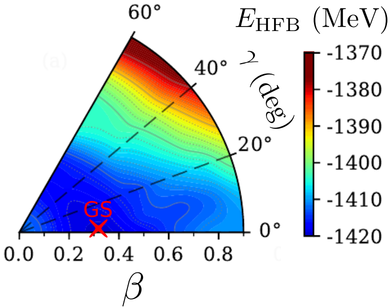
Building the collective Hamiltonian

1. Define collective variables:
   - β, γ: quadrupol deformation
   - $\mathbf{\Omega}$: Euler angles
2. Generate a manifold of constrained Hartree-Fock-Bogoliubov states
3. Compute:
   - the potential energy
   - the inertia



$\Longrightarrow$ Eight functions of (β, γ)

$$E_{\mathrm{HFB}}, \Delta V$$
$$\boldsymbol{B}_{00}, \boldsymbol{B}_{01}, \boldsymbol{B}_{11},$$
$$\mathcal{I}_k \; (k = 1, 2, 3)$$



Cost $>$ 16 h.cpu / nucleus

Structure from the 5D collective Hamiltonian 2/2

Solving the collective Hamiltonian

$$\left(\hat{\mathcal{H}}_{K,rot} + \hat{\mathcal{H}}_{K,vib} + \hat{\mathcal{H}}_{V}\right) g(\beta,\gamma,\mathbf{\Omega}) = E\, g(\beta,\gamma,\mathbf{\Omega}). \tag{1}$$

with:

$$\hat{\mathcal{H}}_{K,rot} = \frac{1}{2}\sum_{k=1}^{3}\frac{\hat{I}_k^2}{\mathcal{I}_k(\beta,\gamma)}, \qquad \mathcal{H}_V = E_{\text{HFB}}(\beta,\gamma) - \Delta V(\beta,\gamma),$$

$$\hat{\mathcal{H}}_{K,vib} = \frac{1}{2}\sum_{\substack{q=\beta,\gamma\\ p=\beta,\gamma}} \frac{1}{D^{1/2}}\frac{\partial}{\partial q} D^{1/2} \boldsymbol{B}^{-1}_{i_q i_p}(\beta,\gamma)\frac{\partial}{\partial p}.$$

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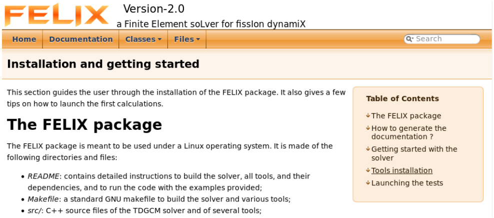
Discretization:

- Ω: Wigner rotation basis
- β,γ: Finite elements

Eigen solver:

- Krylov (SLEPc)

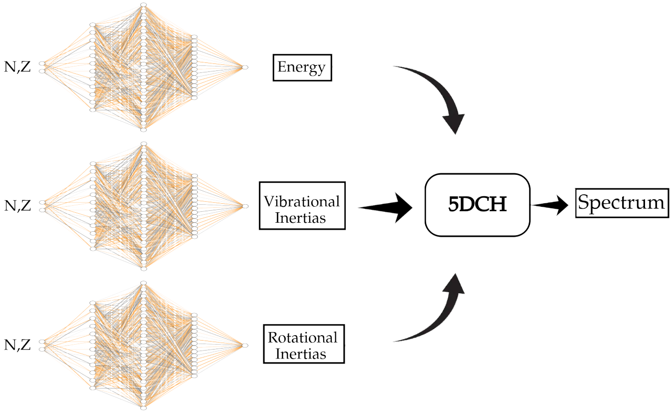
Cost $\simeq$ 5 min.cpu / nucleus



D. Regnier *et. al.*, CPC **225** (2018)

Replacing the time consuming part by a neural network

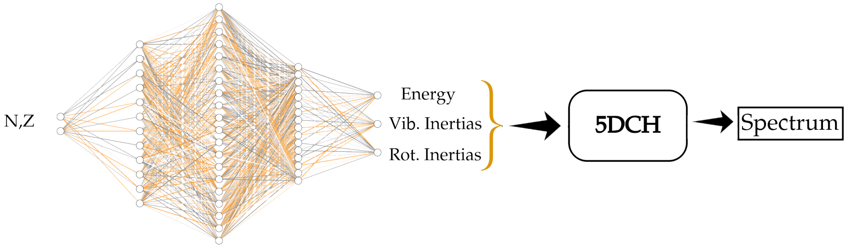
Single task learning



- Good individual features *RMS*

Multi-tasking: more than just a fit

Multi task Learning



- Similar individual RMS
- Better correlated *RMS* for the spectrum

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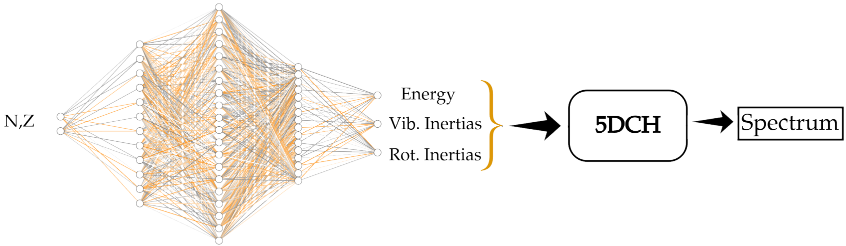

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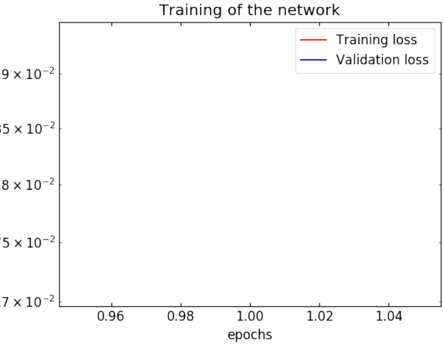
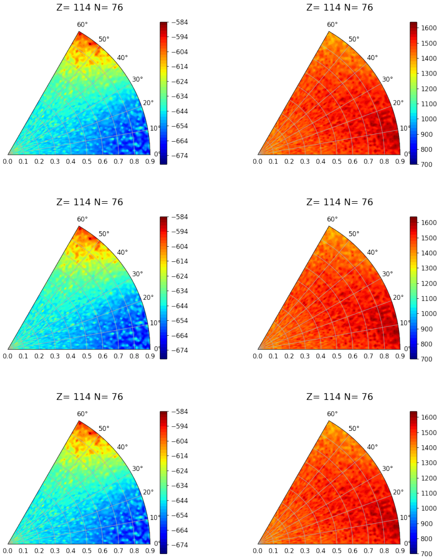
Emergence of the topology



Energy Vib. Inertia



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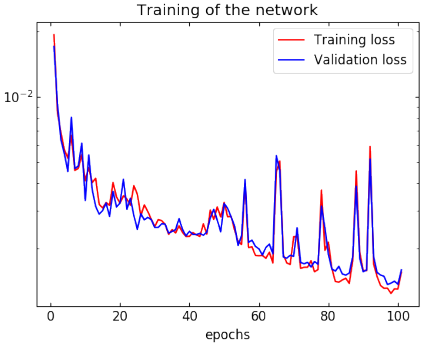

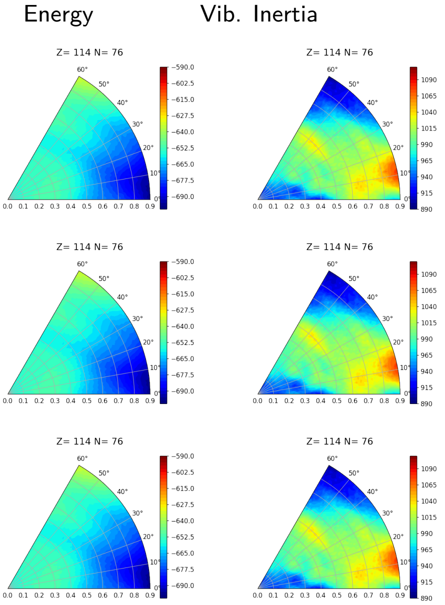

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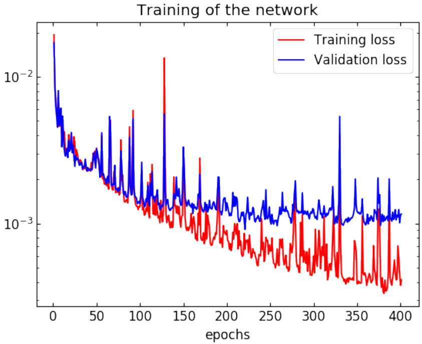

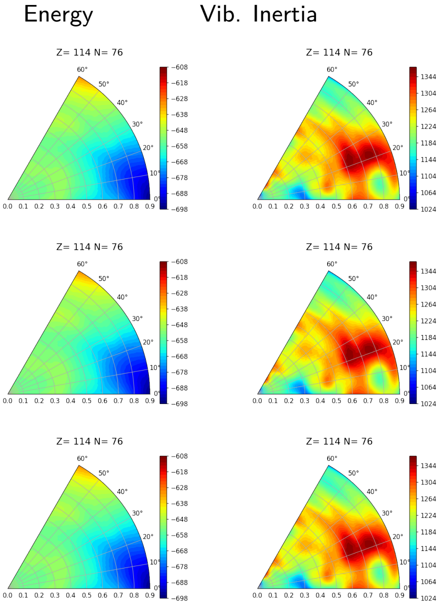

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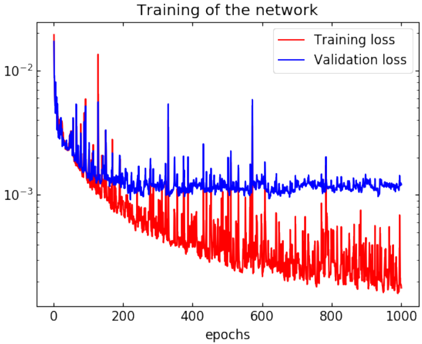

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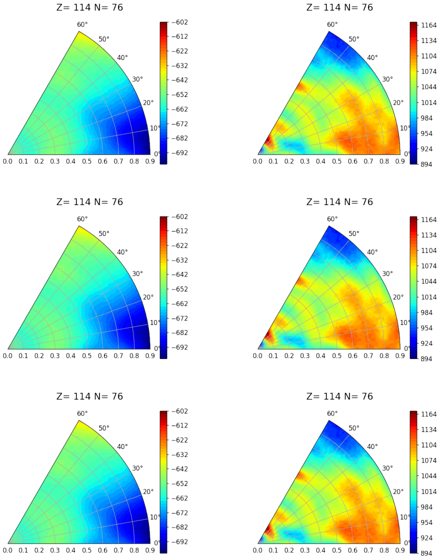
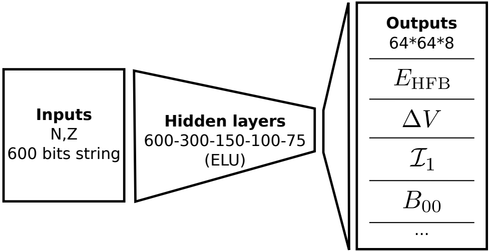


Building the neural network

Architecture:



Implementation:

- Keras/TensorFlow
- Fast GPU execution

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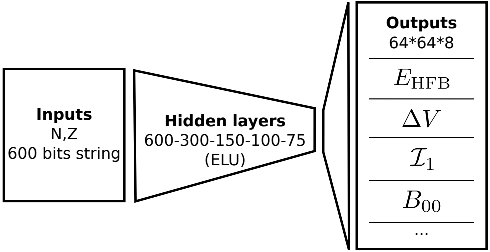

Implementation:

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Training:

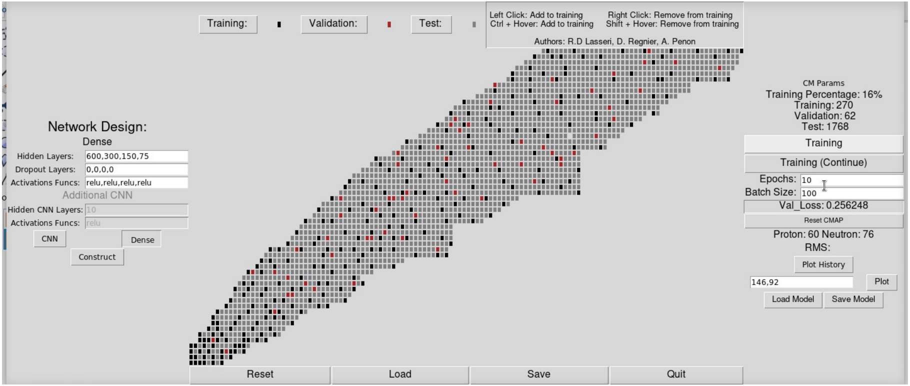
- Training set: sample from 2100 even-even nuclei, Gogny D1S functional
- Loss function based on a weighted sum of:

$$\mathcal{L}_t(N,Z) = \frac{6}{\pi B^2} \int_{\beta,\gamma} \left| t_{\mathrm{AI}}(\beta,\gamma) - t_{\mathrm{HFB}}(\beta,\gamma) \right|^2 \mathrm{d}\beta\beta\mathrm{d}\gamma, \qquad (2)$$

with $t = E_{HFB}, \Delta V, \mathcal{I}_1, \dots$.

Optimal training set: the story of a tradeoff

Physicist Knowledge through a Graphical Interface.



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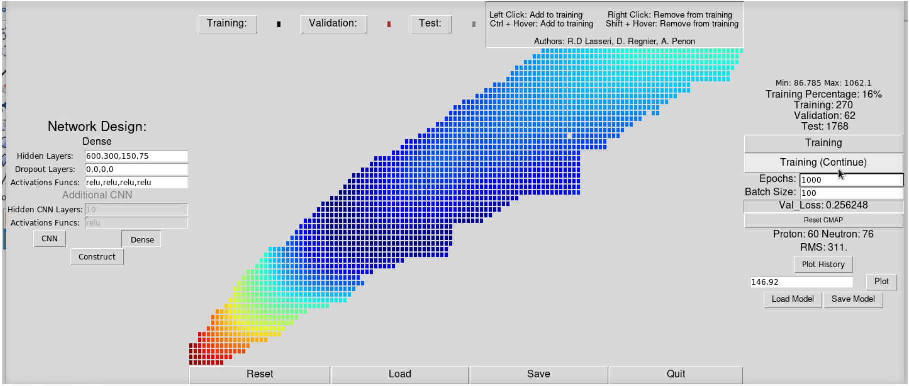

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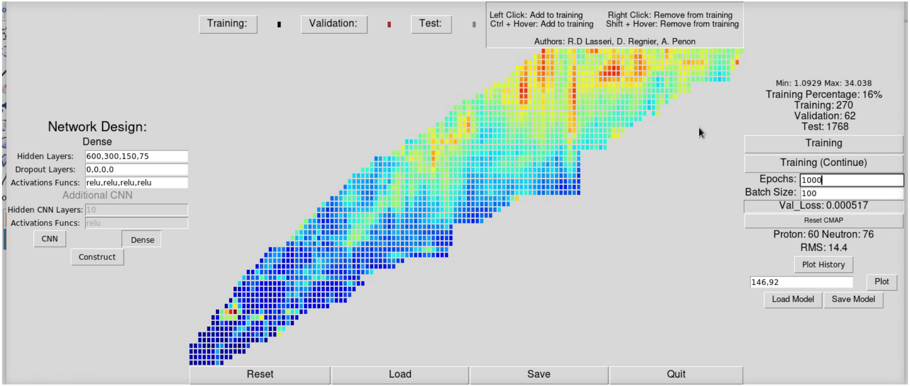
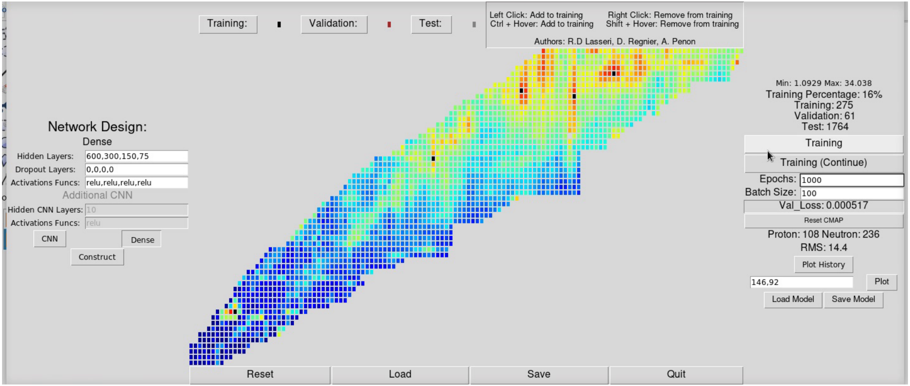


Optimal training set: the story of a tradeoff

Physicist Knowledge through a Graphical Interface. *(Schematic)*



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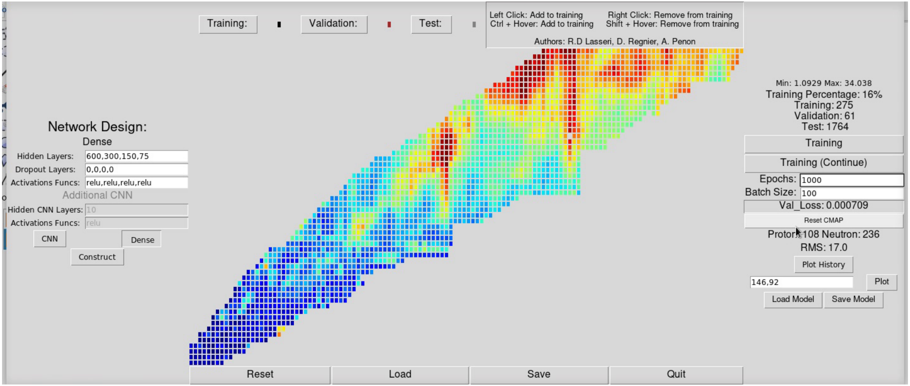
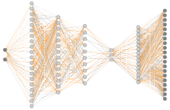
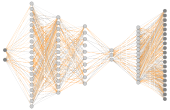
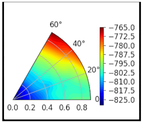
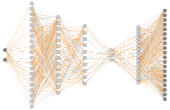


Query by committee

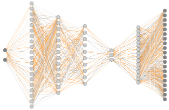
Committee	"Query"	Candidate
	825	
	821	^{100}Sn 
	828	

Benefits of a committee

- Less sensitive to the random initialization
- Estimation of uncertainty

Query by committee

Committee | "Query" | Candidate



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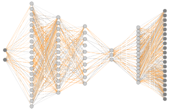

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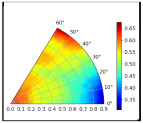
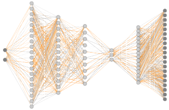
^{318}Uuh





698

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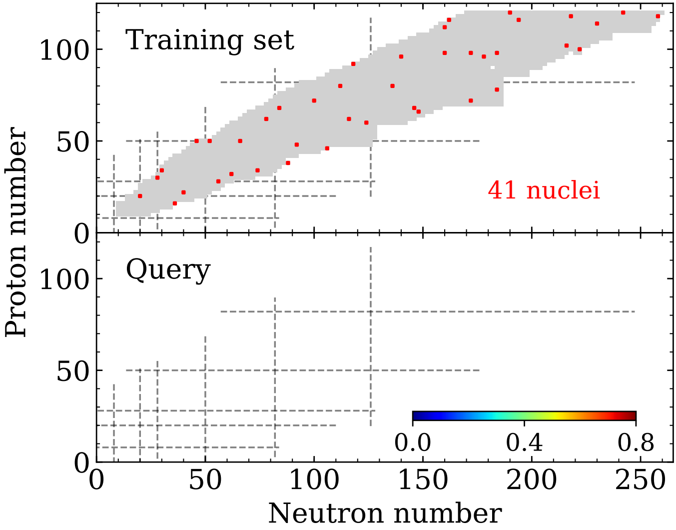
Active learning

- An incremental and automatic choice of training nuclei (5 nuclei/step)
- Query $\simeq$ standard deviation between the committee members



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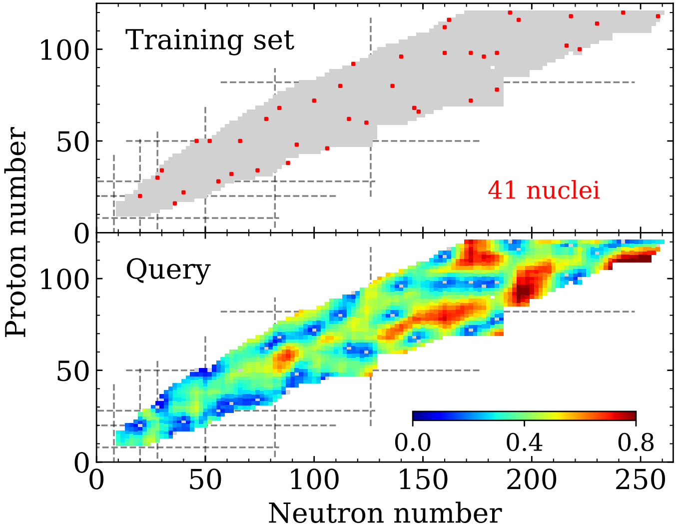

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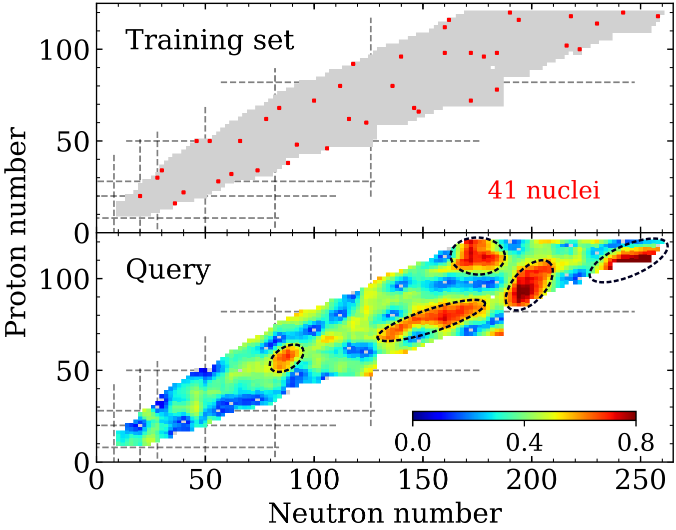

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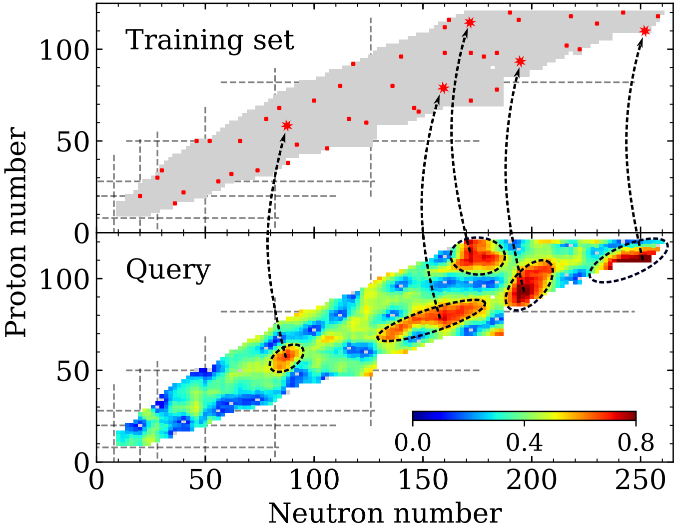

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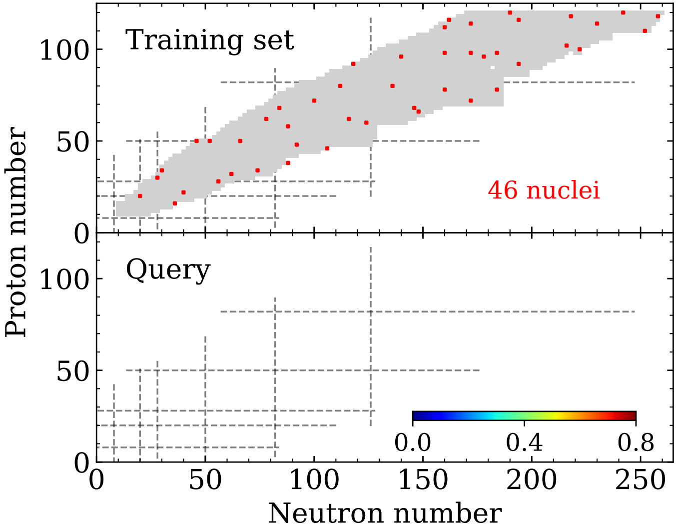

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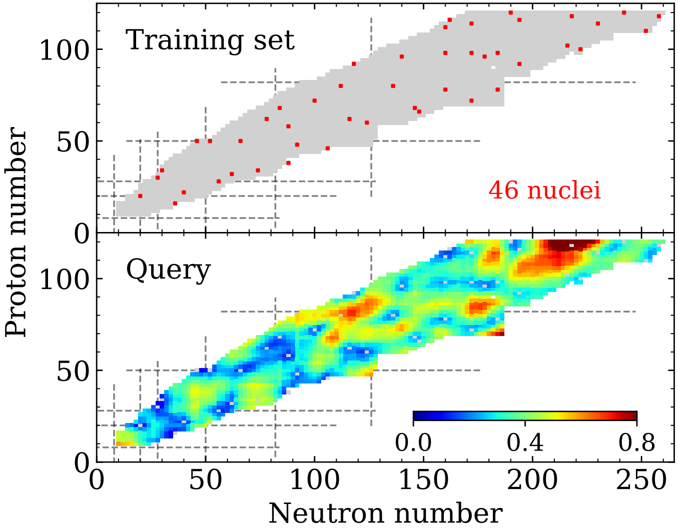

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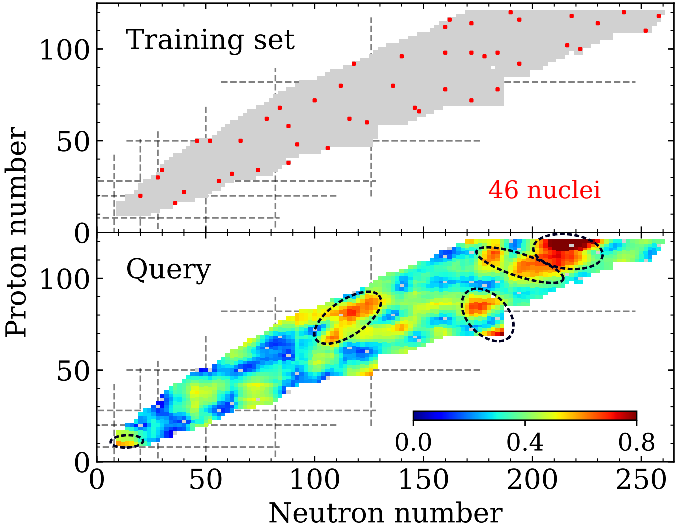

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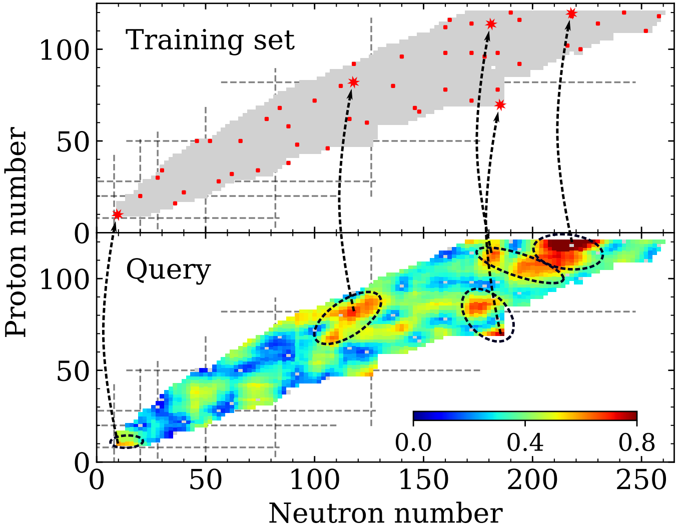

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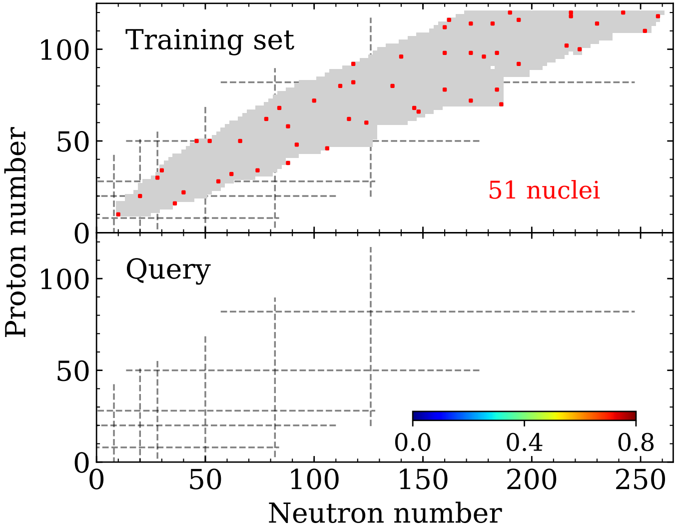
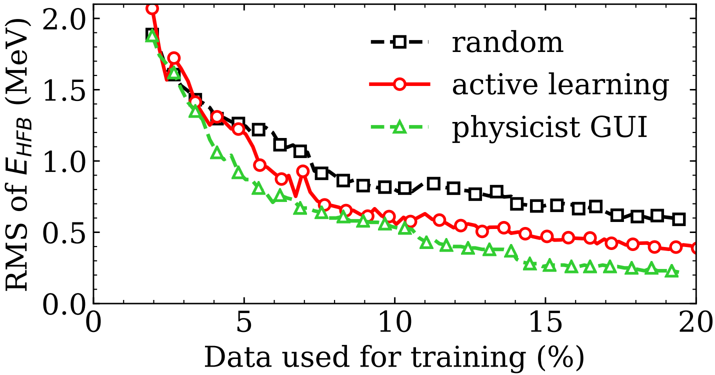


Root Mean Square error (RMS) of the potential energy

Test RMS $=$ on the nuclei not in the training set



Root Mean Square error (RMS) of all outputs

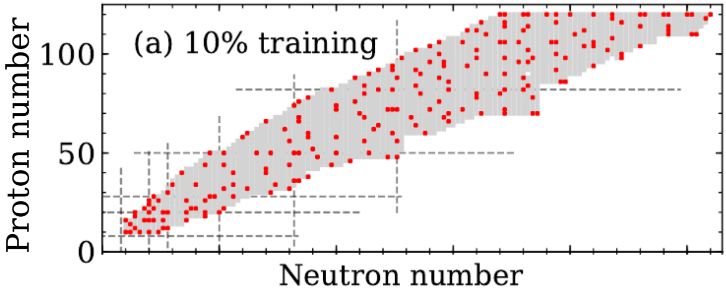
Train %	E_{HFB} (keV)	ΔV	$\mathcal{I}_1$ ($\hbar^2\times\mathrm{MeV}^{-1}$)	$\mathcal{I}_2$	$\mathcal{I}_3$	$\boldsymbol{B}_{00}$ (MeV^{-1})	$\boldsymbol{B}_{01}$	$\boldsymbol{B}_{11}$	E_{GS} (keV)
5	1190	417	1.84	2.80	0.97	13.8	12.0	28.2	1325
10	**557**	**312**	**1.40**	**2.25**	**0.76**	**11.7**	**10.2**	**23.9**	**716**
15	471	247	1.25	2.02	0.69	10.6	9.4	21.9	655
20	388	202	1.22	1.96	0.68	10.2	9.1	21.2	518

The first column contains the size of the training set in % of the AMEDEE database while the others highlight the RMS of the outputs of the AI. The last column contains the RMS associated to the correlated ground state energy E_{GS}.

Keep in mind:

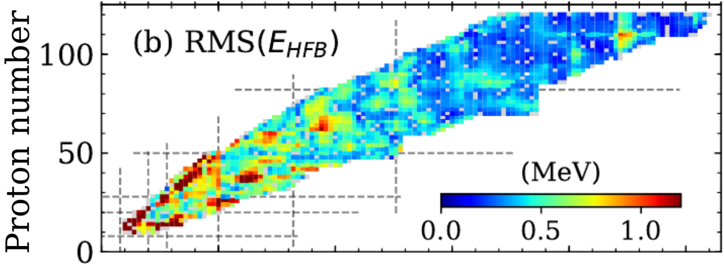
- RMS= 950 keV: Athanassopoulos *et. al* (2004), fitted on 1800 nuclei
- RMS= 790 keV: Gogny D1M S. Hilaire and M. Girod, (2007)

Repartition of the precision



- ✓ Automatic refinement in the light sector
- ✗ $N = Z$ line
- ✗ Shell closures

Repartition of the precision



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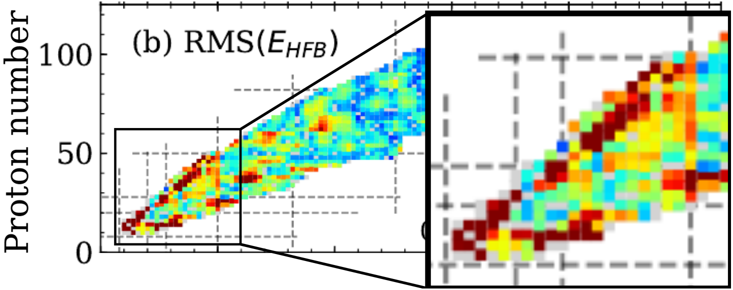

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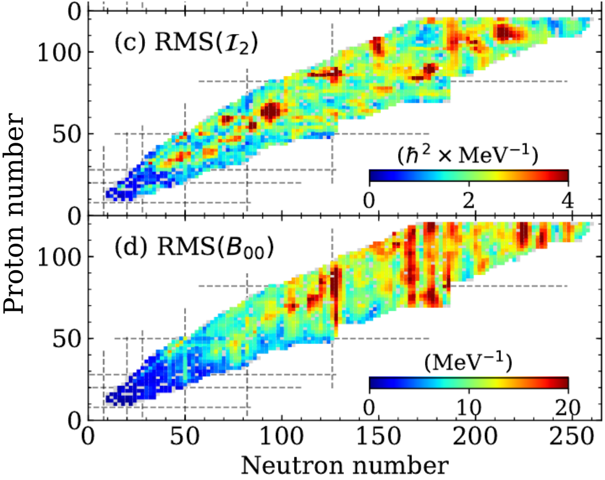

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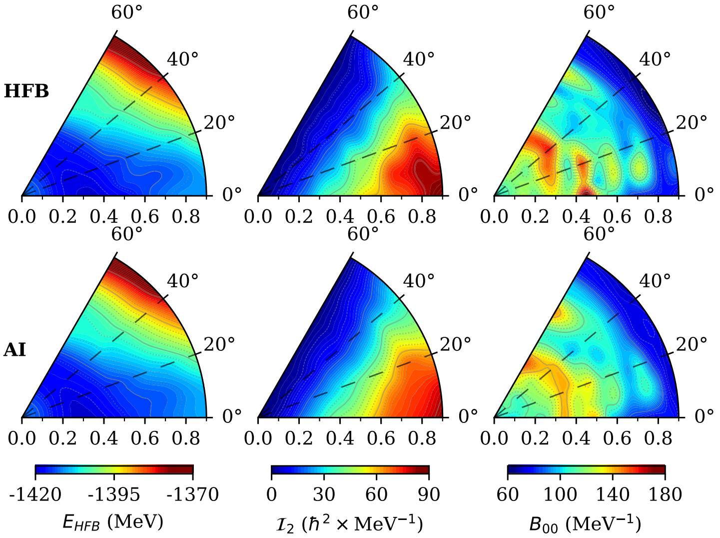
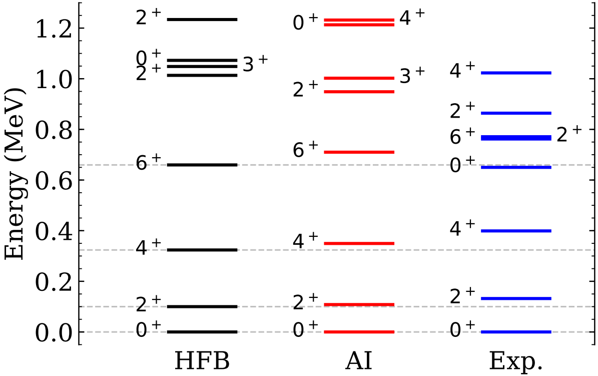
Example of ^{178}Os

- RMS(E_{HFB}) $\simeq$ median RMS on the 1800 test nuclei
- Closest trained nucleus: +4 neutrons, -2 protons



Excitation spectrum of ^{178}Os

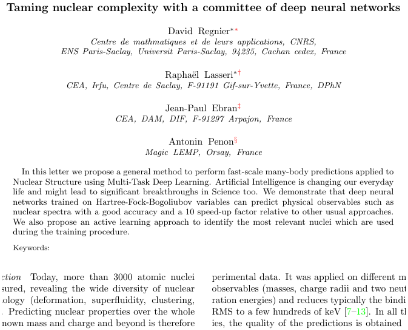


- Correlated ground state: $|E_{GS}^{AI} - E_{GS}^{HFB}| = 150$ keV
- Rotational states reproduced within 8%
- First vibrational state within 13%

To conclude on AI + 5D collective Hamiltonian

Results

- First AI predicting multiple observables
- State of the art accuracy when trained only on 210 nuclei
- Still room for improvement



Taming nuclear complexity with a committee of deep neural networks

David Regnier*[*]
Centre de mathmatiques et de leurs applications, CNRS, ENS Paris-Saclay, Universit Paris-Saclay, 94235, Cachan cedex, France

Raphaël Lasseri*[†]
CEA, Irfu, Centre de Saclay, F-91191 Gif-sur-Yvette, France, DPhN

Jean-Paul Ebran[‡]
CEA, DAM, DIF, F-91297 Arpajon, France

Antonin Penon[§]
Magic LEMP, Orsay, France

In this letter we propose a general method to perform fast-scale many-body predictions applied to Nuclear Structure using Multi-Task Deep Learning. Artificial Intelligence is changing our everyday life and might lead to significant breakthroughs in Science too. We demonstrate that deep neural networks trained on Hartree-Fock-Bogoliubov variables can predict physical observables such as nuclear spectra with a good accuracy and a 10 speed-up factor relative to other usual approaches. We also propose an active learning approach to identify the most relevant nuclei which are used during the training procedure.

Keywords:

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arXiv:1910.04132 (2019)

And Submitted to PRL $\simeq$ 2 Months Ago...

What for ?

- Fast estimation of global properties from one density functional
- Fit new functionals beyond mean field ?

Can we go beyond ?

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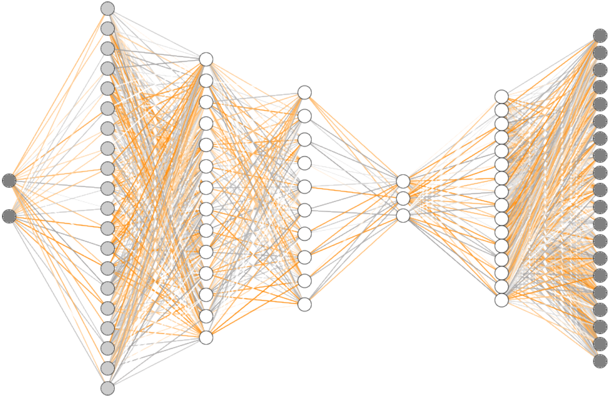

Can we get insights from the internal representation ?

Paper on materials discovery ?

Work in progress...

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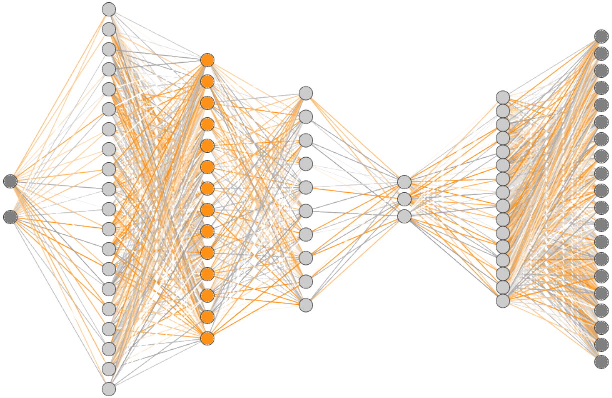

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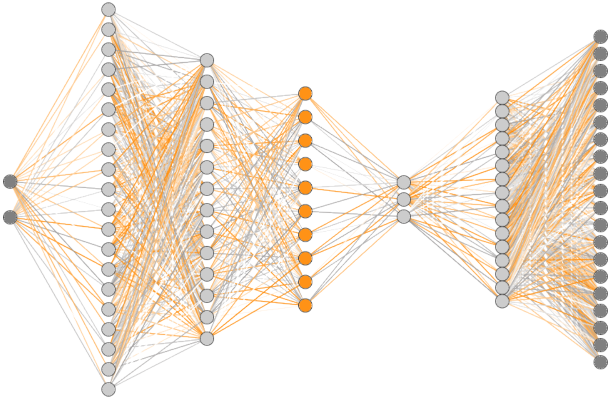

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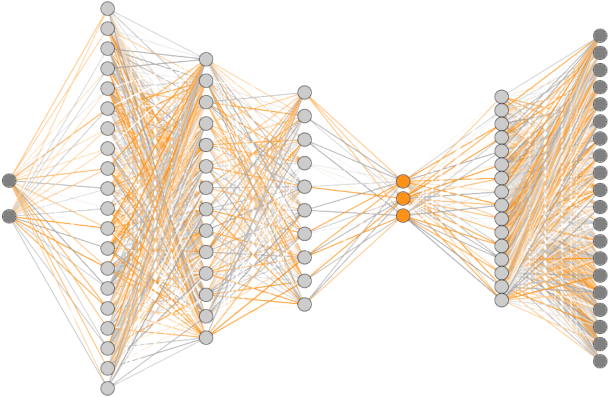

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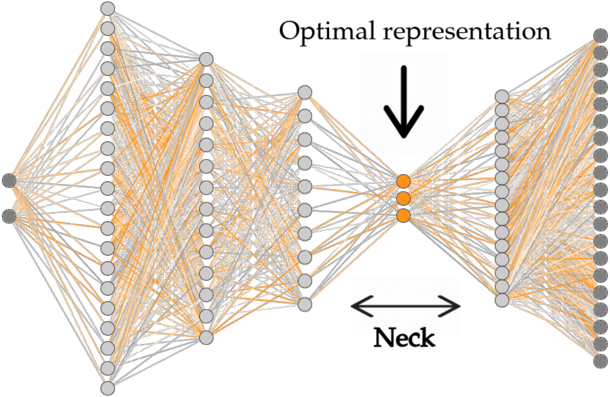

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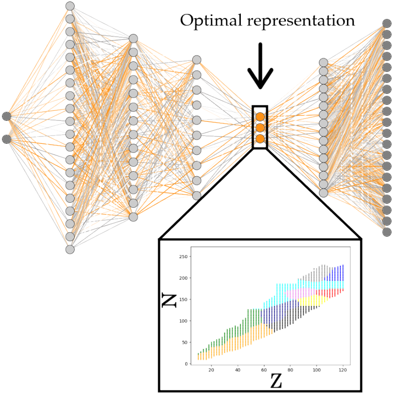

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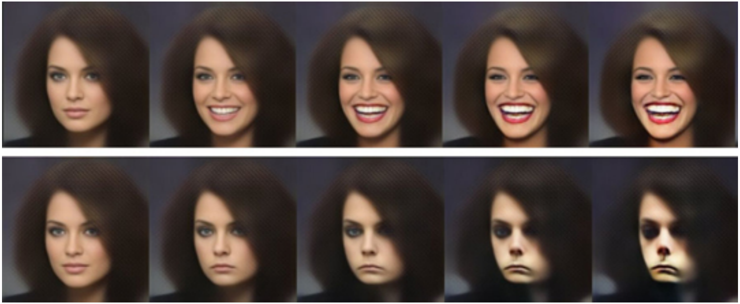
Generative AI: building manifolds of many-body states

Generative Adversarial Networks, Variational Auto Encoders: capacity to

1. Reduce information to a small optimal latent space (neck)
2. Generate a continuous outputs from the latent space

Example: the smile vector (T. White, Victoria Univ. of Wellington)



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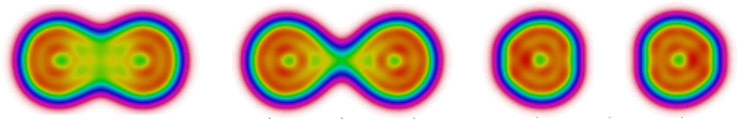
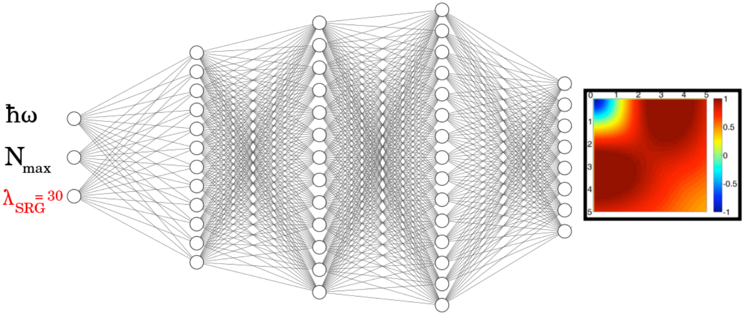
Project: continuous manifolds of Hartree-Fock-Bogoliubov states



A new way to include the diabatic effects in our description of fission ?

Ab-initio

- From the bare to the dressed interaction:
- And back...
- Applications to perturbation theory
- NN as ansatz for Many-Body problems
- Many more...



◇ SRG data ◇ Natural scale separation

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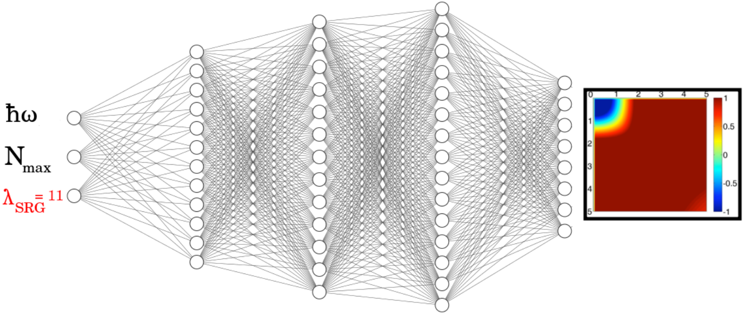

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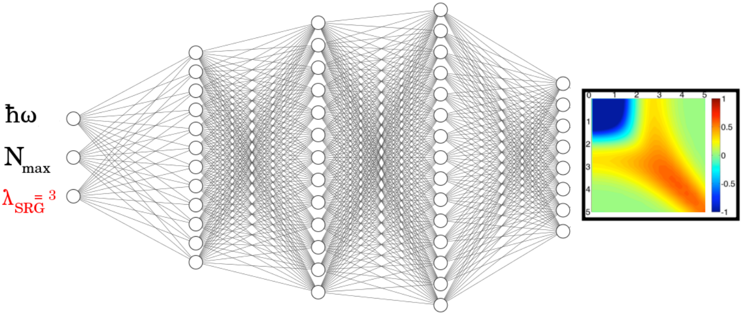

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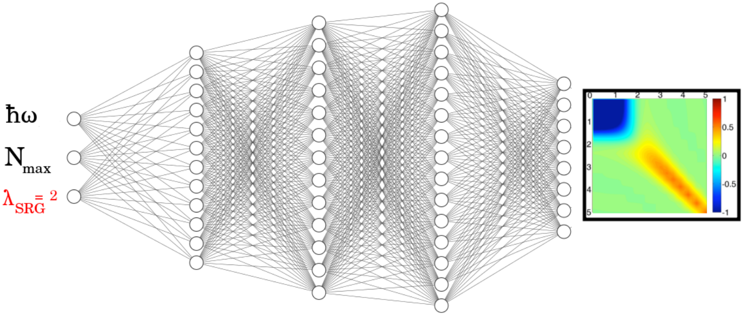

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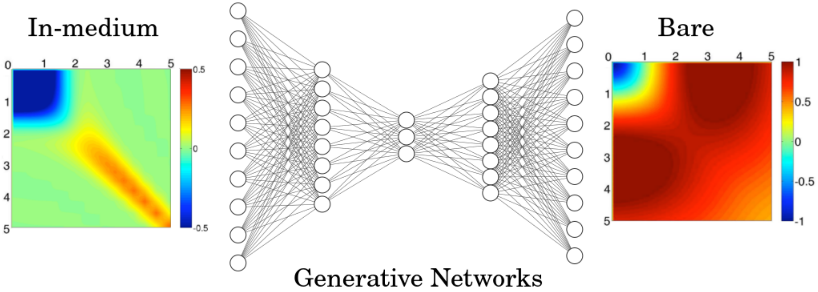

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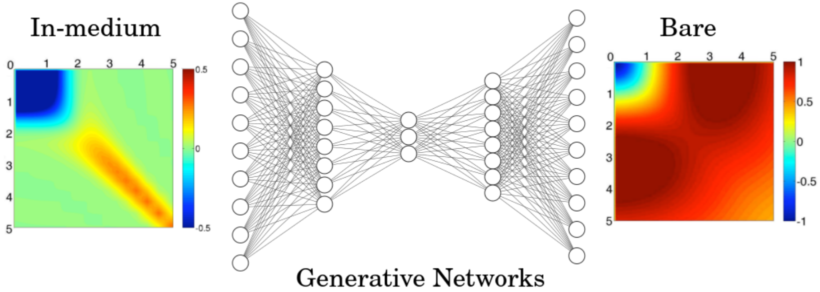

Also applied to Gogny or RMF ?

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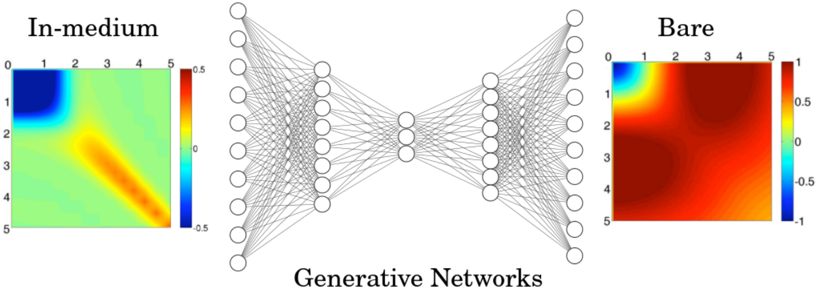

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Graph Neural Networks

Ab-initio

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$$\hat{H}\,|\Psi\rangle = E|\Psi\rangle$$

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Collaborators:

- G. Hupin, CNRS, IPNO
- A. Penon, Magic Lemp
- J-P. Ebran, CEA, DAM
- S. Hilaire, CEA, DAM

Key dates:

- ✓ GDR Resanet GT5, 29-30 Oct. 2019: Machine Learning & Physique Nucléaire
- Workshop ESNT, Feb-Mar. 2020: Can an Artificial Intelligence do Science ?

Support:

- NVIDIA GPU Grant Program: $2\times$ Titan V GPU

Thank you for your attention !

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