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# Towards new approaches to cluster detection for cosmology

#### Vincent Reverdy

[vincent.reverdy@lapp.in2p3.fr]

Researcher in Computer Science and Numerical Cosmology CNRS - French National Centre for Scientific Research LAPP - Laboratoire d'Annecy de Physique des Particules

November 18th, 2022







	Clusters and computers	MCTS and AlphaZero	A clustering game	Conclusions
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Galaxy clusters					

# Galaxy clusters

Clusters and computers

# Game trees

- MCTS and AlphaZero
- A clustering game

# Conclusions

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Galaxy clusters	Clusters and computers		MCTS and AlphaZero	A clustering game	Conclusions
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Halos in simulations					



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Galaxy clusters	in observations				



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## Observational cosmology using galaxy clusters

Galaxy clusters as building blocks of cosmological analyses.

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Galaxy clusters in observations	
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## Observational cosmology using galaxy clusters

Galaxy clusters as building blocks of cosmological analyses.

## Main problem of this presentation in the context of LSST

How to detect galaxy clusters?

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Galaxy cluster of	detection				

### Clusters in simulations

Input: particles

#### Simulation cluster detectors

- Spherical Over Density (SOD)
- Friends-of-Friends (FoF)
- ....

## Clusters in observations

Input: sources/galaxies

#### Observational cluster detectors for LSST

- redMaPPer (Rykoff et al. 2013)
- WaZP (Benoist 2014)
- ...

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Galaxy clusters	Clusters and computers	Game trees	MCTS and AlphaZero	A clustering game	Conclusions
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Galaxy cluster	detection				



#### Improving cluster detection for observational cosmology

Can we use machine-learning to improve cluster detection for observational cosmology?

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Clusters and co	mputers			

# Galaxy clusters

# Clusters and computers

# Game trees

- MCTS and AlphaZero
- A clustering game

# Conclusions

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Galaxy clusters	Clusters and computers	Game trees	MCTS and AlphaZero	A clustering game	Conclusions		
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Using deep neural networks to detect galaxy clusters							



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Using deep	neural networks to de	etect galaxy clu	isters		



- Ultra large images
- More than 3 colors

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Galaxy clusters	Clusters and computers	Game trees	MCTS and AlphaZero	A clustering game	Conclusions
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Using deen	neural networks to de	etect galaxy clu	isters		



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## Scientific problems

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## Scientific problems

 Training phase: implicit dependency on cluster detection algorithm used in simulations (FoF)

Galaxy clusters	Clusters and computers	Game trees	MCTS and AlphaZero	A clustering game	Conclusions
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Using deen	neural networks to de	etect galaxy clu	isters		



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## Scientific problems

- Training phase: implicit dependency on cluster detection algorithm used in simulations (FoF)
- Performance depends on image rescaling / color treatment

Galaxy clusters	Clusters and computers	Game trees	MCTS and AlphaZero	A clustering game	Conclusions
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Using deep r	neural networks to de	etect galaxy clu	isters		



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#### Scientific problems

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- Blackbox effect: hard to understand, interpret, and adjust performance

Galaxy clusters	Clusters and computers	Game trees	MCTS and AlphaZero	A clustering game	Conclusions
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Using deep r	neural networks to de	etect galaxy clu	isters		



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- Risk of circular dependency: may just learn how to invert semi-analytical prescription

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#### Direction of investigation

Physics-guided machine-learning?

	Clusters and computers	MCTS and AlphaZero	A clustering game	Conclusions
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A problem of de	efinition			

### The fundamental problem of clusters

- No universal definition: many definitions and parameterization accross simulations and observations
- Computers require definitions: implicit or explicit parameterization in algorithms
- Algorithms  $\Leftrightarrow$  Definitions

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	Clusters and computers	MCTS and AlphaZero	A clustering game	Conclusions
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A problem of de	efinition			

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#### Physics-based definitions

- Physical distance
- Gravitational potential
- Virialized structures
- ...

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- Physical distance
- Gravitational potential
- Virialized structures
- ...

#### Example of FoF: linking-length







# Cluster dendrograms

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## A universal representation

- Traditional galaxy cluster finders  $\Rightarrow$  3-level trees (root/clusters/sources)
- With subhalo finders  $\Rightarrow$  4-level trees (root/clusters/subclusters/sources)
- Hierarchical finders  $\Rightarrow$  N-level trees (root/supersuperclusters/superclusters/clusters/.../sources)

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Graph as a num	nerical representatior	of the cosmic	web		







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Graph as a num	erical representation	of the cosmic	web		







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### Representing the cosmic web as a graph

- Vertices: particles, sources
- Edges: physical parameterization (physical distance...)
- Going beyond: fuzzy graphs to take into account error bars

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A computer	science perspective	on galaxy clust	ering: graphs and tr	ees			
Reframing of the galaxy clustering problem							
• Cosmic web $\Leftrightarrow$ Graph							

• Galaxy clustering  $\Leftrightarrow$  Trees

 
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 A computer science perspective on galaxy clustering: graphs and trees

#### Reframing of the galaxy clustering problem

- $\blacksquare Cosmic web \Leftrightarrow Graph$
- Galaxy clustering  $\Leftrightarrow$  Trees

#### Computer science perspective

 $\mathsf{Galaxy}\ \mathsf{clustering}\ \mathsf{problem}\ \Leftrightarrow\ \mathsf{Computing}\ \mathsf{Trees}\ \mathsf{on}\ \mathsf{Graphs}$ 

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A computer science perspective on galaxy clustering: graphs and trees							
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Galaxy clusters	Clusters and computers	Game trees	MCTS and AlphaZero	A clustering game	Conclusions		

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#### Computer science perspective

 $\mathsf{Galaxy}\ \mathsf{clustering}\ \mathsf{problem}\ \Leftrightarrow\ \mathsf{Computing}\ \mathsf{Trees}\ \mathsf{on}\ \mathsf{Graphs}$ 

#### Discrete vs continuous mathematics

- $\blacksquare$  Comparison of galaxy clustering algorithms  $\Rightarrow$  comparison of trees
- Computer science related problem: tree metric and distances

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 A clustering game 0000
 Conclusions 000

 A computer science perspective on galaxy clustering: graphs and trees

#### Reframing of the galaxy clustering problem

- $\blacksquare Cosmic web \Leftrightarrow Graph$
- Galaxy clustering ⇔ Trees

#### Computer science perspective

 $\mathsf{Galaxy\ clustering\ problem} \Leftrightarrow \mathsf{Computing\ Trees\ on\ Graphs}$ 

#### Discrete vs continuous mathematics

- $\blacksquare$  Comparison of galaxy clustering algorithms  $\Rightarrow$  comparison of trees
- Computer science related problem: tree metric and distances

#### Research direction

Playing games on the cosmic web: computing galaxy clustering trees on the cosmic web graph

- Well-framed computer science problem
- Bridge between numerical cosmology, computer science, and discrete mathematics
- Computer science tools available

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Game trees					

- Galaxy clusters
- Clusters and computers

- MCTS and AlphaZero
- A clustering game

# Conclusions

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Galaxy clusters	Clusters and computers	Game trees	MCTS and AlphaZero	A clustering game	Conclusions		
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Game trees: starting with Tic-Tac-Toe							



A universal way to represent sequential *N*-player(s) games with perfect information.

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#### Game trees

A universal way to represent sequential *N*-player(s) games with perfect information.

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Game trees: starting with Tic-Tac-Toe							
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A universal way to represent sequential *N*-player(s) games with perfect information.

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A universal way to represent sequential *N*-player(s) games with perfect information.

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A universal way to represent sequential *N*-player(s) games with perfect information.

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Game complexi	ty				







#### Tic-Tac-Toe

- Board size  $\Rightarrow 3^2 = 9$
- Average game length  $\Rightarrow 9$
- $\blacksquare$  Average branching factor  $\Rightarrow 4$
- Number of games  $\Rightarrow 255168$

### Chess

- Board size  $\Rightarrow 8^2 = 64$
- $\blacksquare$  Average game length  $\Rightarrow 70$
- Average branching factor  $\Rightarrow 35$
- Complexity  $\Rightarrow 35^{70} \approx 10^{64}$

#### Go

- Board size  $\Rightarrow 19^2 = 361$
- Average game length  $\Rightarrow 150$
- Average branching factor  $\Rightarrow 250$
- Complexity  $\Rightarrow 250^{150} \approx 10^{360}$

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	Clusters and computers	Game trees	MCTS and AlphaZero	A clustering game	Conclusions
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Playing ches	s algorithmically				





# Brute-forcing

Game tree still tractable: average depth d = 70, average branching factor b = 35

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The problem wi	th the game of Go				

### Intractability

Go's game tree average depth d = 150, average branching factor b = 250

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The problem	with the game of G	0			

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Go's game tree average depth d = 150, average branching factor b = 250

# Deepmind's AlphaGo/AlphaZero



	Clusters and computers	MCTS and AlphaZero	A clustering game	Conclusions
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MCTS and Alp	haZero			

- Galaxy clusters
- Clusters and computers
- Game trees
- MCTS and AlphaZero
- A clustering game
- Conclusions

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	Clusters and computers		MCTS and AlphaZero	A clustering game	Conclusions
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Monte-Carlo	p-Tree-Search (MCTS	S) overview			



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Monte-Carlo-T	ree-Search (MCTS) o	overview			



Select a leaf node.

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Select a leaf node.

#### Expansion

Create one or more children nodes and select one of them.

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	Clusters and computers		MCTS and AlphaZero	A clustering game	Conclusions
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Monte-Carlo-T	ree-Search (MCTS) o	overview			



Select a leaf node.

### Expansion

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## Simulation

Complete a full random playout from the selected child.

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	Clusters and computers		MCTS and AlphaZero	A clustering game	Conclusions			
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Monte-Carlo-Tree-Search (MCTS) overview								



Select a leaf node.

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Complete a full random playout from the selected child.

## Backpropagation

Backpropagate the result of the simulation back to the root.

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	Clusters and computers		MCTS and AlphaZero	A clustering game	Conclusions		
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Galaxy clusters	Clusters and computers	Game trees	MCTS and AlphaZero	A clustering game	Conclusions
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Monte-Carlo-Tr	ee-Search (MCTS) re	efinements			

- $\blacksquare$  To get a distribution of results,  $N_s$  simulations can be performed at each step
- Simulated playouts can be done in a better way than using random moves

Galaxy clusters	Clusters and computers	Game trees	MCTS and AlphaZero	A clustering game	Conclusions
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#### Selection: exploitation vs exploration

Example of the UCT (Upper Confidence Bound 1 applied to Trees) policy:

$$\max_{x} \left( \frac{w_{i}\left(x\right)}{n_{i}\left(x\right)} + c \sqrt{\frac{\log\left(N_{i}\left(x\right)\right)}{n_{i}\left(x\right)}} \right)$$

Galaxy clusters	Clusters and computers	Game trees	MCTS and AlphaZero	A clustering game	Conclusions
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•  $w_i \Rightarrow$  number of wins for the node x after the *i*-th move

Galaxy clusters	Clusters and computers	Game trees	MCTS and AlphaZero	A clustering game	Conclusions
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- $w_i \Rightarrow$  number of wins for the node x after the i-th move
- $n_i \Rightarrow$  number of simulations for the node x after the i-th move

Galaxy clusters	Clusters and computers	Game trees	MCTS and AlphaZero	A clustering game	Conclusions
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Monte-Carlo-Tr	ee-Search (MCTS) re	efinements			

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- $w_i \Rightarrow$  number of wins for the node x after the i-th move
- $n_i \Rightarrow$  number of simulations for the node x after the *i*-th move
- $N_i \Rightarrow$  total number of simulations for the parent node of x after the *i*-th move

Galaxy clusters	Clusters and computers	Game trees	MCTS and AlphaZero	A clustering game	Conclusions
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Monte-Carlo-Tr	ee-Search (MCTS) re				

- $\blacksquare$  To get a distribution of results,  $N_s$  simulations can be performed at each step
- Simulated playouts can be done in a better way than using random moves

### Selection: exploitation vs exploration

Example of the UCT (Upper Confidence Bound 1 applied to Trees) policy:

$$\max_{x} \left( \frac{w_{i}\left(x\right)}{n_{i}\left(x\right)} + c \sqrt{\frac{\log\left(N_{i}\left(x\right)\right)}{n_{i}\left(x\right)}} \right)$$

- $w_i \Rightarrow$  number of wins for the node x after the i-th move
- $n_i \Rightarrow$  number of simulations for the node x after the *i*-th move
- $N_i \Rightarrow$  total number of simulations for the parent node of x after the *i*-th move
- $c \Rightarrow$  exploration coefficient ( $c = \sqrt{2}$ )

Galaxy clusters 0000	Clusters and computers	Game trees 00000	MCTS and AlphaZero 000●	A clustering game	Conclusions 000			
AlphaZero = Monte-Carlo-Tree-Search + Deep Neural Networks								
Monte-Ca	rlo-Tree-Search (MCTS)							
Selection	tion		Simulation					

Backpropagation

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Expansion

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AlphaZero = Monte-Carlo-Tree-Search + Deep Neural Networks	Galaxy clusters	Clusters and computers	Game trees	MCTS and AlphaZero	A clustering game	Conclusions	
AlphaZero = Monte-Carlo-Tree-Search + Deep Neural Networks	0000	000000	00000	0000	0000	000	
	AlphaZero = Monte-Carlo-Tree-Search + Deep Neural Networks						

Monte-Carlo-Tree-Search (MCTS)	
Selection	Simulation
Expansion	<ul> <li>Backpropagation</li> </ul>

### Policy deep neural network

- Input: *s*, the current state of the board (+ optionally previous states)
- Output: *p*, to select the most probable/promising moves
- General idea: reduce the breadth of the tree search

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AlphaZero = Monte-Carlo-Tree-Search + Deep Neural Networks						
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Galaxy clusters	Clusters and computers	Game trees	MCTS and AlphaZero	A clustering game	Conclusions	

Monte-Carlo-Tree-Search (MCTS)	
<ul> <li>Selection</li> </ul>	Simulation
Expansion	<ul> <li>Backpropagation</li> </ul>

### Policy deep neural network

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### Value deep neural network

- Input: s, the current state of the board (+ optionally previous states)
- Output: v, the probability to win
- General idea: reduce the depth of the tree search

Galaxy clusters	Clusters and computers	Game trees	MCTS and AlphaZero	A clustering game	Conclusions		
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AlphaZero = I	AlphaZero = Monte-Carlo-Tree-Search $+$ Deep Neural Networks						

Monte-Carlo-Tree-Search (MCTS)	
<ul> <li>Selection</li> </ul>	Simulation
Expansion	Backpropagation

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### Value deep neural network

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- Output: v, the probability to win
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## $\mathsf{AlphaZero} = \mathsf{MCTS} + \mathsf{Policy} \ \mathsf{Net} + \mathsf{Value} \ \mathsf{Net}$

Tree search guided by "intuition" and "expert-knowledge".

	Clusters and computers		MCTS and AlphaZero	A clustering game	Conclusions	
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A clustering game						

- Galaxy clusters
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- Game trees
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- A clustering game
- Conclusions

Galaxy clusters	Clusters and computers	Game trees	MCTS and AlphaZero	A clustering game	Conclusions
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Game's board

The cosmic-web graph

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## Game's board

The cosmic-web graph

Game's goal

Extracting a clustering tree from the graph

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### Game's board

The cosmic-web graph

Game's goal

Extracting a clustering tree from the graph

### Game's move

Create a link between a particle and its best neighbouring candidate

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Galaxy clusters	Clusters and computers	Game trees	MCTS and AlphaZero	A clustering game	Conclusions
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Using MCTS a	and Neural Nets to	play the clust	ering game		

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Galaxy clusters	Clusters and computers	Game trees	MCTS and AlphaZero	A clustering game	Conclusions
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Using MCTS a	nd Neural Nets to pla	ay the clusterir	ng game		

 $\blacksquare$  Compute the cosmic-web graph  ${\cal G}$ 

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Galaxy clusters	Clusters and computers	Game trees	MCTS and AlphaZero	A clustering game	Conclusions
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Using MCTS ar	nd Neural Nets to pla	w the clusterin	g game		

- Compute the cosmic-web graph  $\mathcal G$
- Compute a reference tree  $\mathcal{T}_0$  using a physics-based criteria  $\phi$  (distance, gravitational potential, ...)

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Galaxy clusters	Clusters and computers	Game trees	MCTS and AlphaZero	A clustering game	Conclusions
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Galaxy clusters	Clusters and computers	Game trees	MCTS and AlphaZero	A clustering game	Conclusions
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### Training phase

Galaxy clusters and computers Game trees MCTS and AlphaZero 0000 Coole 00000 Coole 0000 Coole 0000

#### Preparation using simulations

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### Training phase

 $\blacksquare$  Play the 1-player game using MCTS + Neural Nets to extract a tree  ${\cal T}$  from the graph  ${\cal G}$ 

Galaxy clusters	Clusters and computers	Game trees	MCTS and AlphaZero	A clustering game	Conclusions
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Using MCTS and Neural Nets to play the clustering game					

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## Training phase

- Play the 1-player game using MCTS + Neural Nets to extract a tree  ${\cal T}$  from the graph  ${\cal G}$
- For each-move use only the information of  $\vec{x} = (x_0, x_1, x_2, \cdots, x_{n-1})$
| Galaxy clusters | Clusters and computers | Game trees       | MCTS and AlphaZero | A clustering game | Conclusions |
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| Using MCTS a    | nd Neural Nets to pla  | av the clusterin | g game             |                   |             |

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	Clusters and computers		MCTS and AlphaZero	A clustering game	Conclusions
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Using MCTS a	nd Neural Nets to pl	av the clusterin	ig game		

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#### Playing phase

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## Playing phase

Play the 1-player game using MCTS + Neural Nets on real observations using  $\vec{x} = (x_0, x_1, x_2, \cdots, x_{n-1})$ 

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#### Preparation using simulations

- Compute the cosmic-web graph  $\mathcal G$
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- Extract observational data from simulation:  $\vec{x} = (x_0, x_1, x_2, \cdots, x_{n-1})$  (RA, DEC, redshift with error bars, simulated images, ...)

#### Training phase

- $\blacksquare$  Play the 1-player game using MCTS + Neural Nets to extract a tree  ${\cal T}$  from the graph  ${\cal G}$
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- Compute the reward as a tree-distance d between  $\mathcal{T}$  and  $\mathcal{T}_0$ :  $d = f(\mathcal{T}, \mathcal{T}_0) \in [0, 1]$

#### Playing phase

- Play the 1-player game using MCTS + Neural Nets on real observations using  $\vec{x} = (x_0, x_1, x_2, \cdots, x_{n-1})$
- $\blacksquare$  No need of observational data on  $\phi$

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	Clusters and computers		MCTS and AlphaZero	A clustering game	Conclusions
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Combining the	best of both worlds				

## Physics-guided machine-learning approach

- Works for any physics-based criteria  $\phi$  and observational data  $\vec{x}$  (including images and error bars)
- Builds an "intuition" on  $\phi$  using simulations ( $\phi \Leftrightarrow$  How does the game board looks like?)
- No black-box effect anymore

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	Clusters and computers	MCTS and AlphaZero	A clustering game	Conclusions
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Combining the	best of both worlds			

## Physics-guided machine-learning approach

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- No black-box effect anymore

#### Possible cluster definitions based on $\phi$

- Physical distance
- Matter density
- Gravitational potential
- Virialization
- Linear combination of all of the above
- **.**..

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Galaxy clusters	Clusters and computers	Game trees	MCTS and AlphaZero	A clustering game	Conclusions
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Conclusions					

- Galaxy clusters
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# Conclusions

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Galaxy clusters	Clusters and computers	Game trees	MCTS and AlphaZero	A clustering game	Conclusions
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Towards the ult	imate definition?				

- In  $t = +\infty \Rightarrow$  isolated clusters
- All definitions are equivalent

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Galaxy clusters	Clusters and computers	Game trees	MCTS and AlphaZero	A clustering game	Conclusions
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# Simulating the end of time

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# Simulating the end of time

Let simulations run far into the future

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Galaxy clusters	Clusters and computers	Game trees	MCTS and AlphaZero	A clustering game	Conclusions
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Towards the ult	timate definition?				

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# Simulating the end of time

- Let simulations run far into the future
- Detect clusters

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Towards the ult	timate definition?				

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# Simulating the end of time

- Let simulations run far into the future
- Detect clusters
- Go back in time to z = 0 tracking particles

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Galaxy clusters	Clusters and computers	Game trees	MCTS and AlphaZero	A clustering game	Conclusions
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- $\blacksquare$  Use this knowledge to build a reference tree  ${\mathcal T}$

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Galaxy clusters	Clusters and computers	Game trees	MCTS and AlphaZero	A clustering game	Conclusions
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Galaxy clusters	Clusters and computers	Game trees	MCTS and AlphaZero	A clustering game	Conclusions			
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## Analysis

- Play the game using this criterion
- Use computer science and discrete mathematics to compare  $T_i = f(\phi_i)$

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	Clusters and computers	MCTS and AlphaZero	A clustering game	Conclusions
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Conclusions				

#### Limitations of machine-learning approaches

- Black-box approaches, hard to interpret and adjust in terms of physics
- Risk of circular definitions

# Cluster detection as a computer science problem

- Cosmic-web  $\Leftrightarrow$  Graph
- Clusters ⇔ Trees
- Galaxy clustering problem ⇔ Computing Trees on Graphs

## The game of cluster detection

- MCTS + Deep Neural Networks = physics-guided machine-learning approach
- Work with arbitrary physics criterion  $\phi$  and observational data  $\vec{x}$

## A starting project!

Reach out if you're interested: vincent.reverdy@lapp.in2p3.fr