Karlsruhe Institute of Technology

Information Theory as a Bridge Across the Geosciences and Modeling Sciences

Uwe Ehret (KIT) & Hoshin Gupta (UofA)

Introduction To The Workshop

Sept 11, 2023

Remember 2016 …

Remember 2016 …

Schedule

Day Zero (Sun April 24th): Arrival

Day One (Mon April 25th): WHAT IS INFORMATION THEORY AND WHY SHOULD WE CARE?

Morning session (chaired by Grey Nearing)

- 08:00 – 08:15 Coffee
- 08:15 – 08:30 Introduction (Hoshin Gupta, Grey Nearing, Uwe Ehret)
- 08:30 – 09:00 Group Introduction
- 09:00 – 10:00 **Knuth - On the reln. between Info Theory and Physics**
- 10:00 – 10:15 Coffee
- 10:15 – 10:45 **Branicki - On the reln. between Info Theory and Uncertainty**
- 10:45 – 11:30 Plenum Discussion

11:30 – 13:00 Lunch

Poster session (chaired by Florian Wellmann and Rohini Kumar)

- 13:00 – 13:45 Speed Presentations by Poster Presenters
- 13:45 – 15:30 Poster Session

Afternoon session (chaired by Ben Ruddell)

- 15:30 – 16:00 **Hoshin - On the reln. between Info Theory and Hyd. Science**
- 16:00 – 16:30 Plenum Discussion
- 16:30 – 18:00 Breakout Sessions: What are the core questions in the earth sciences and how can we inform these questions? 3 groups sessions (led by Kevin Knuth, Praveen Kumar, Jingfeng Wang)

18:00 - Dinner & Socializing

Day Two (Tue April 26th): INFORMATION IN DATA, MODELS AND SYSTEMS

Morning session (chaired by Steven Weijs)

- 08:00 – 08:15 Coffee
- 08:15 – 09:00 Reports from the 3 breakout sessions
- 09:00 – 09:30 Talk (Grey Nearing): On the Information Content in Data
- 09:30 – 10:00 **Gong - On Info in Models**
- 10:00 – 10:15 Coffee
- 10:15 – 10:45 **Ruddell - On Info in Networks**
- 10:45 – 11:30 Plenum Discussion

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Afternoon session (chaired by Uwe Ehret)

- 15:30 – 16:00 **Weijs - On Info & Complexity**
- 16:00 – 16:30 Plenum Discussion
- 16:30 – 18:00 Breakout Sessions: How can information theory help us understand the interface between models and data? 3 groups sessions (led by Michal Branicki, Wei Gong, Joon Kim)

18:00 - Dinner & Socializing

Day Three (Wed April 27th): PHYSICAL MODELS FROM AN INFORMATION PERSPECTIVE

Morning session (chaired by Bethanna Jackson)

- 08:00 – 08:15 Coffee
- 08:15 – 09:00 Reports from the 3 breakout sessions
- 09:00 – 09:30 **Wang – Maximum Entropy Production**
- 09:30 – 10:00 **Kumar & Goodwell – Info sharing in Eco-Hyd Systems**
- 10:00 – 10:15 Coffee
- 10:15 – 10:45 **Jackson – Info-based metrics to evaluate physical models**
- 10:45 – 11:30 Plenum Discussion

11:30 – 13:00 Lunch

13:00 – 16:30 Visit the research facilities of the Schneefernerhaus and the summit of the Zugspitze

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- 16:30 – 18:00 Group discussion, Workshop Conclusion, Future Planning, Paper Preparation

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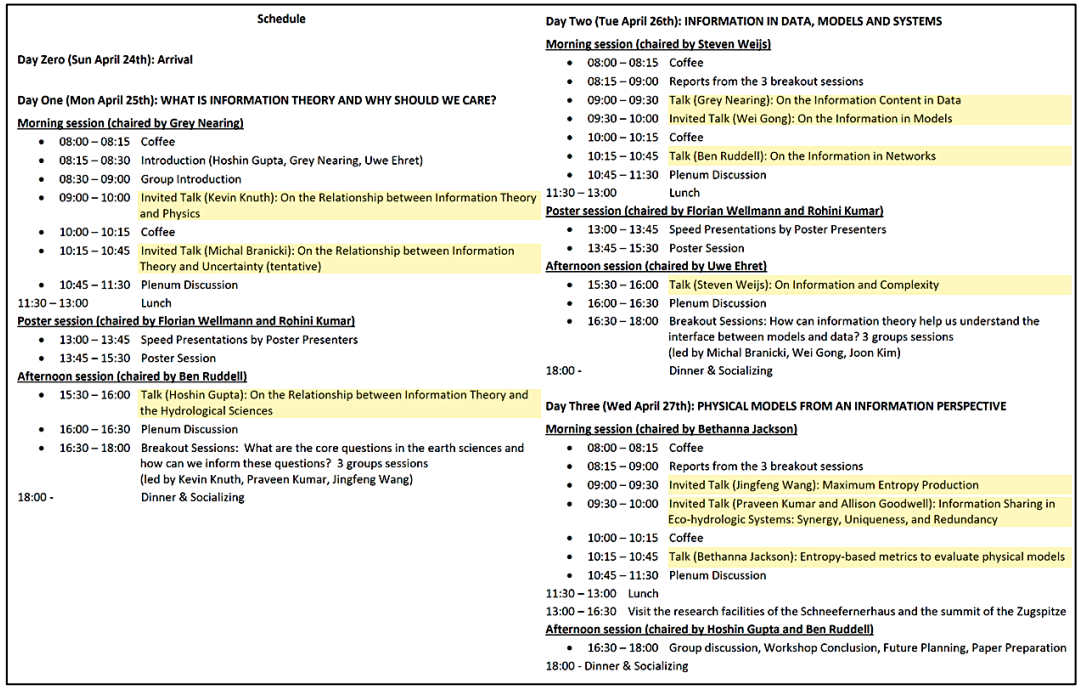
Remember 2016 … Fussball Champions

Since 2016 …

- Moved beyond "*Info ≡ Shannon Info*“
- Progress on *Causality* and *Transfer Entropy*
- No limits to applicability discovered (yet :-)
- *Information Bottleneck* as an inferential guideline
- The rise of ML
  - A broad *Representational Framework*
  - Sobering moments for *Theory-based modeling*
  - Better awareness of the tight integration of all inferential components



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- 09:30 – 10:00 Invited Talk (Praveen Kumar and Allison Goodwell): Information Sharing in Eco-hydrologic Systems: Synergy, Uniqueness, and Redundancy
- 10:00 – 10:15 Coffee
- 10:15 – 10:45 Talk (Bethanna Jackson): Entropy-based metrics to evaluate physical models
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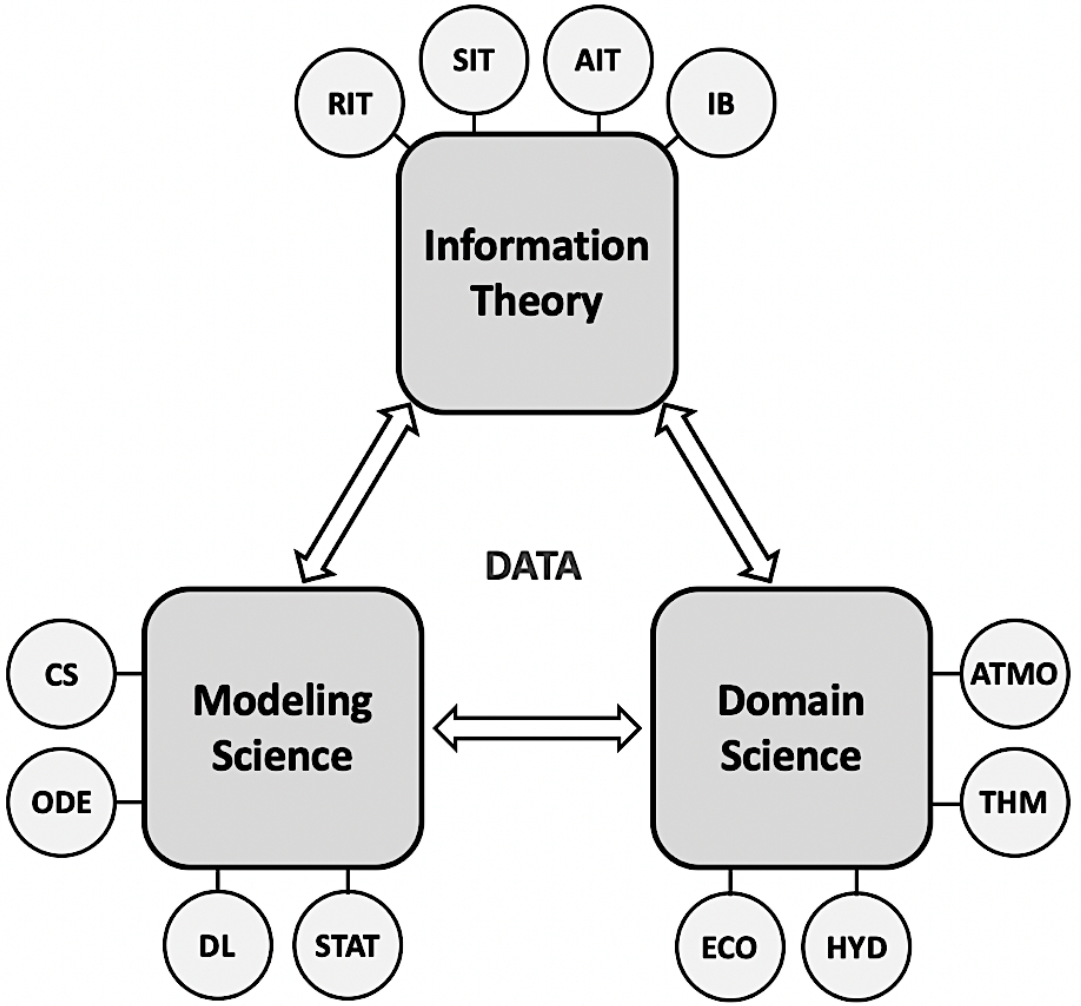
Of Course… Many Problems Still Remain to be Solved …

- *Theory-based (TB) models* are based on incomplete understanding of the world
  - (severely) *Lossy Compression* of *Data* due to overly strong (or wrong) constraints imposed by theory

- *Data-based (DB) models* outperform TB models on specific problems, but typically lack the hierarchical modularity of TB representations
  - This hampers *Interpretation, Reasoning, Transfer* (generalization across domains)

Workshop Focus

- **To Explore the Nexus of:**
  - *Information Theory (IT)*
  - *Modeling Sciences (MS)*
  - *Domain Relevant Theory (DRT)*
- **Goal**
  - To enhance the predictive capabilities of ESS models, and their suitability for *Reasoning* and *Understanding*
- **Approach**
  - Closer integration of the *Modeling* and *Domain Sciences*
  - A general framework with IT as a *conceptual* and *linguistic* foundation
  - Expanded understanding of the richness of how "*Information*" is expressed by *Models*



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Workshop Focus

- **To Explore the Nexus of:**
  - *Information Theory (IT)*
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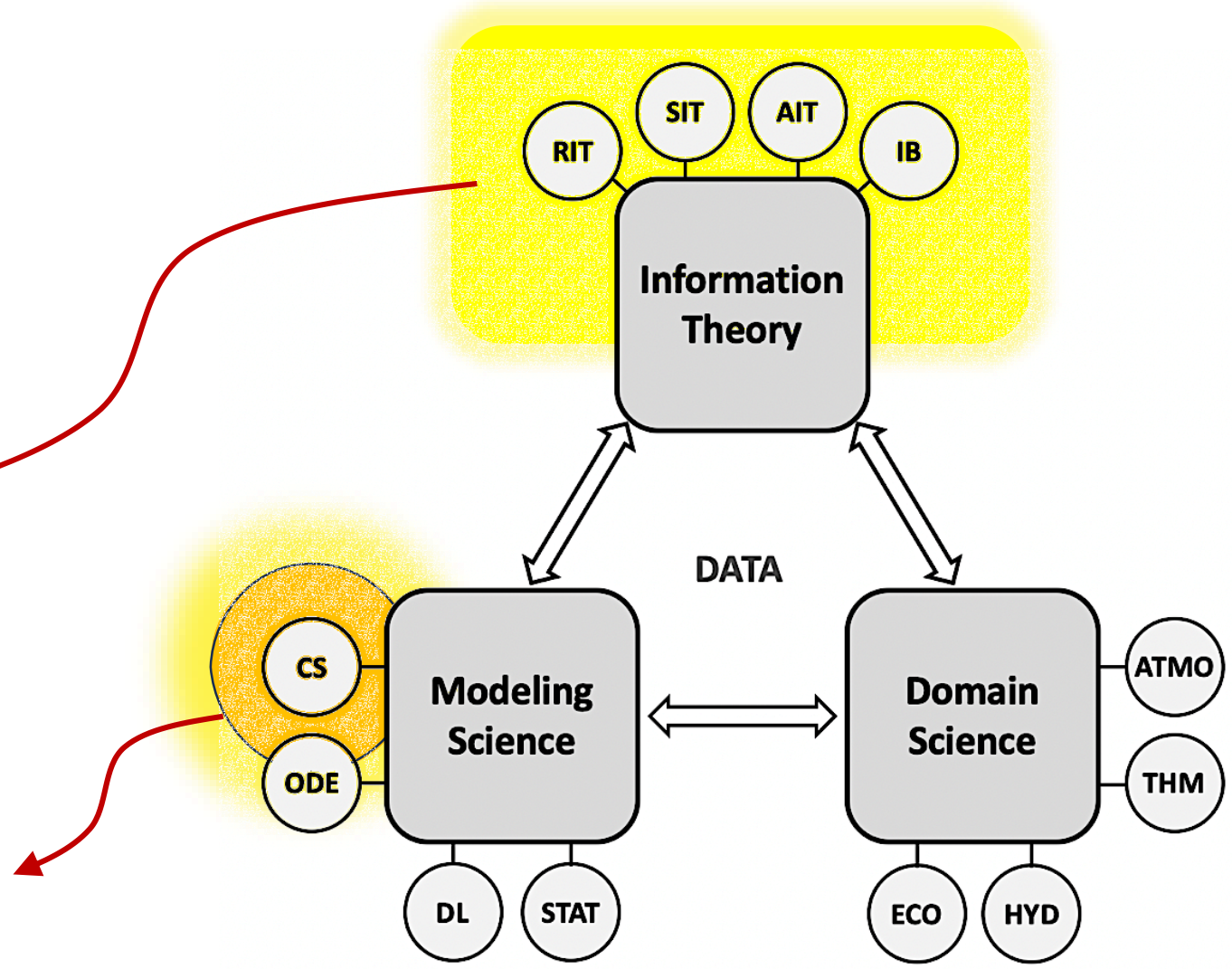
  - *Domain Relevant Theory (DRT)*

- ***Shannon (Statistical) Information***
- ***Algorithmic Information***
- ***Representational Information***

Theory of Computation

(Finite State Automata, Turing Machines, Chomsky Grammars)



Shannon versus ***Algorithmic*** Information

Shannon (Statistical) Information:

$$I_S(x) = \log_2\left(\frac{1}{p(x)}\right)$$ ***Code length of a Probabilistic Description***

- *Relates to **repeated events**/objects*
- *Characterizes the (expected/average) "surprise" associated with encountering such events*
- ***Description/Code Length after removing all Statistical Redundancy** (statistical compression)*

Algorithmic Information:

$$I_K(x) = K(x) = \log_2\left(\frac{1}{2^{-K(x)}}\right)$$ ***Code length of an Algorithmic Description***

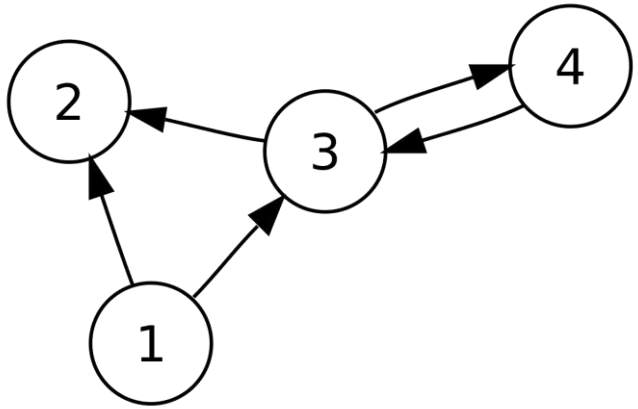
- *Relates to **individual events**/objects*
- *Characterizes the (expected/average) "surprise" associated with encountering such events*
- ***Description/Code Length after removing ALL Redundancy (statistical & non-statistical)** (structural compression)*

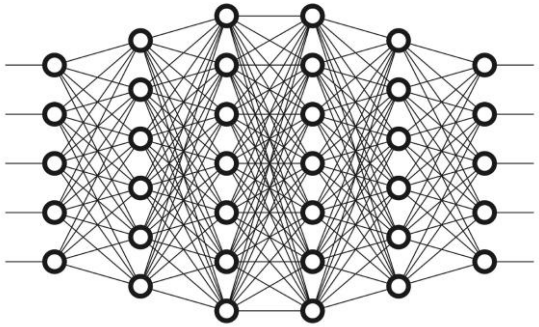
We are interested in
"Minimal" Description Lengths

But there is also Information bound up in ***Representations***

Representational Information for Building Dynamical Systems Models:

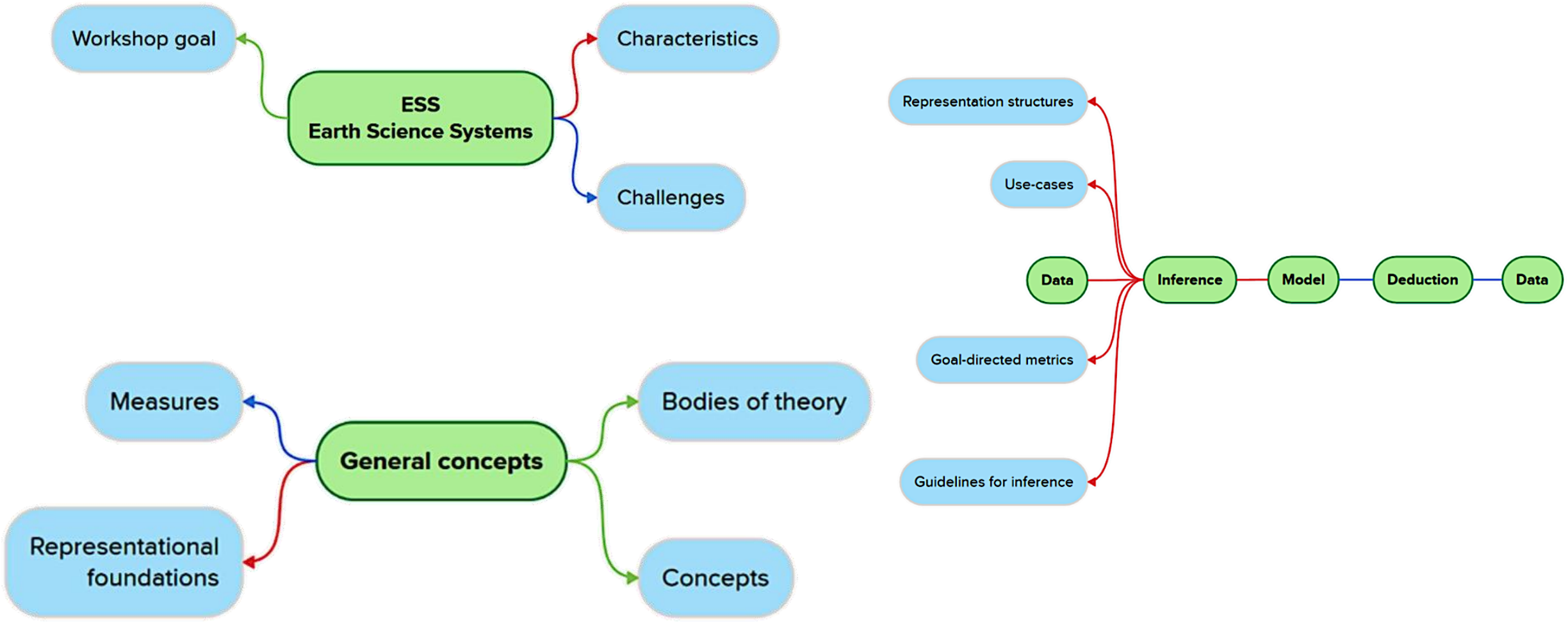
- *Symbols (Alphabet)*
- *Types of Objects (Dictionary … Features, States, Parameters, Mass Energy and Info Flows)*
- *Directed Graphs Structures (Nodes & Links, Associative Relationships, Short- & Long-term Memory)*





- *Relates to **Holoarchic Structural Organization of Systems***
- *Characterizes the (hypothesized) "generative/relational structure" underlying the generation of events*
- ***Description/Code Length after removing all Representational Redundancy** (representational compression)*
  - ***But also more than simply code length … the structure of the description is important***

Possible Conceptual Framework for our Discussions



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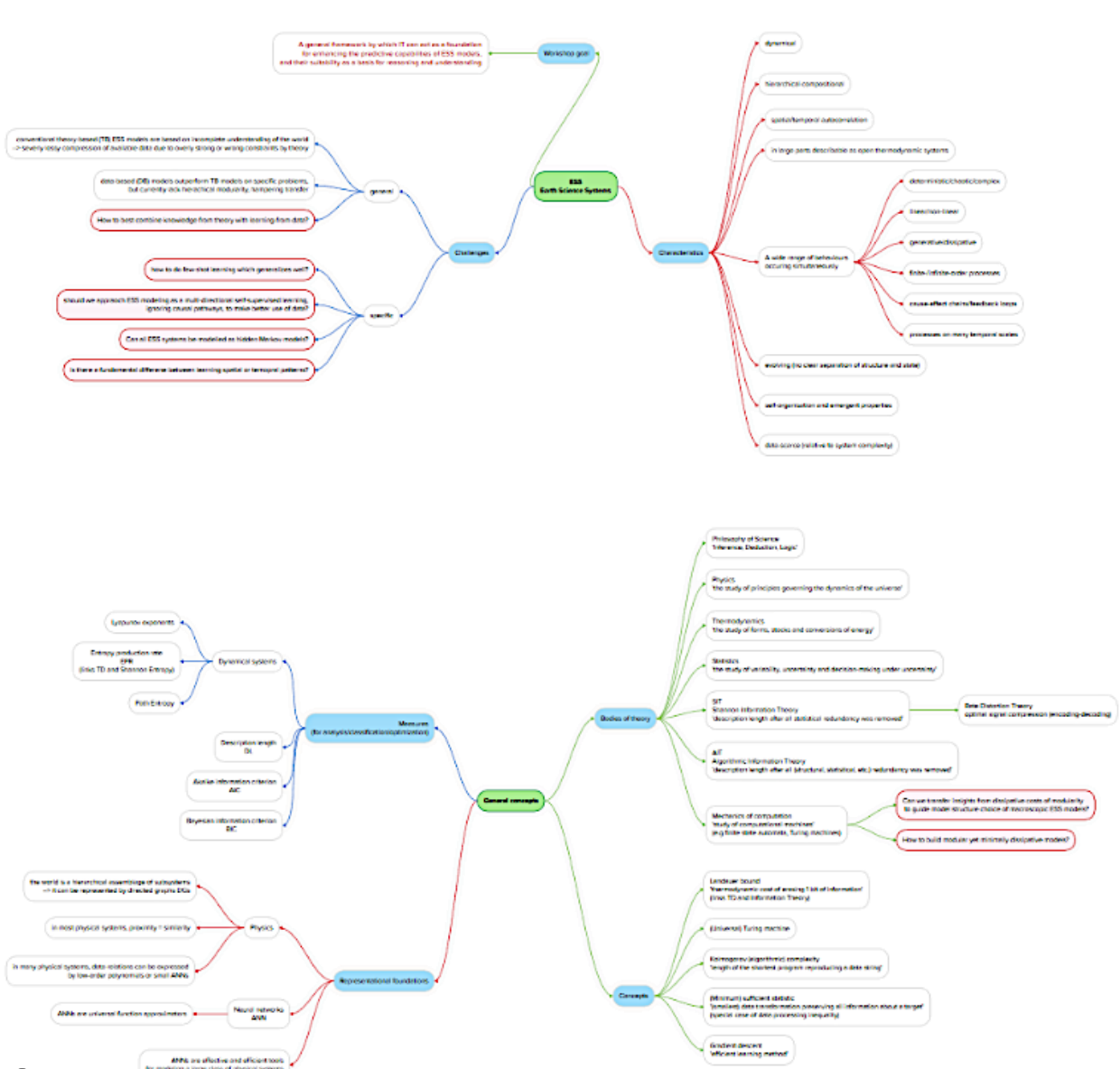
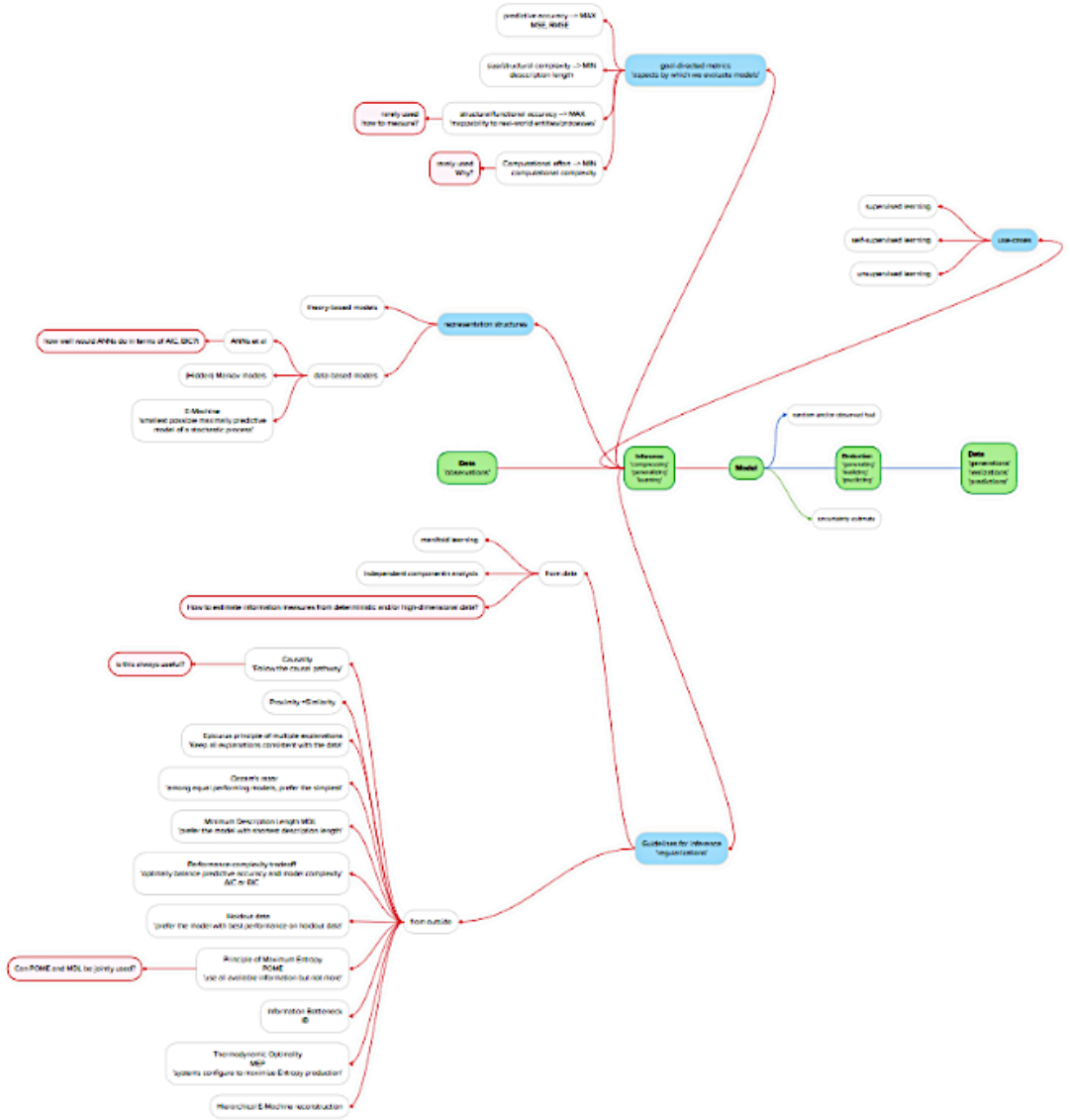
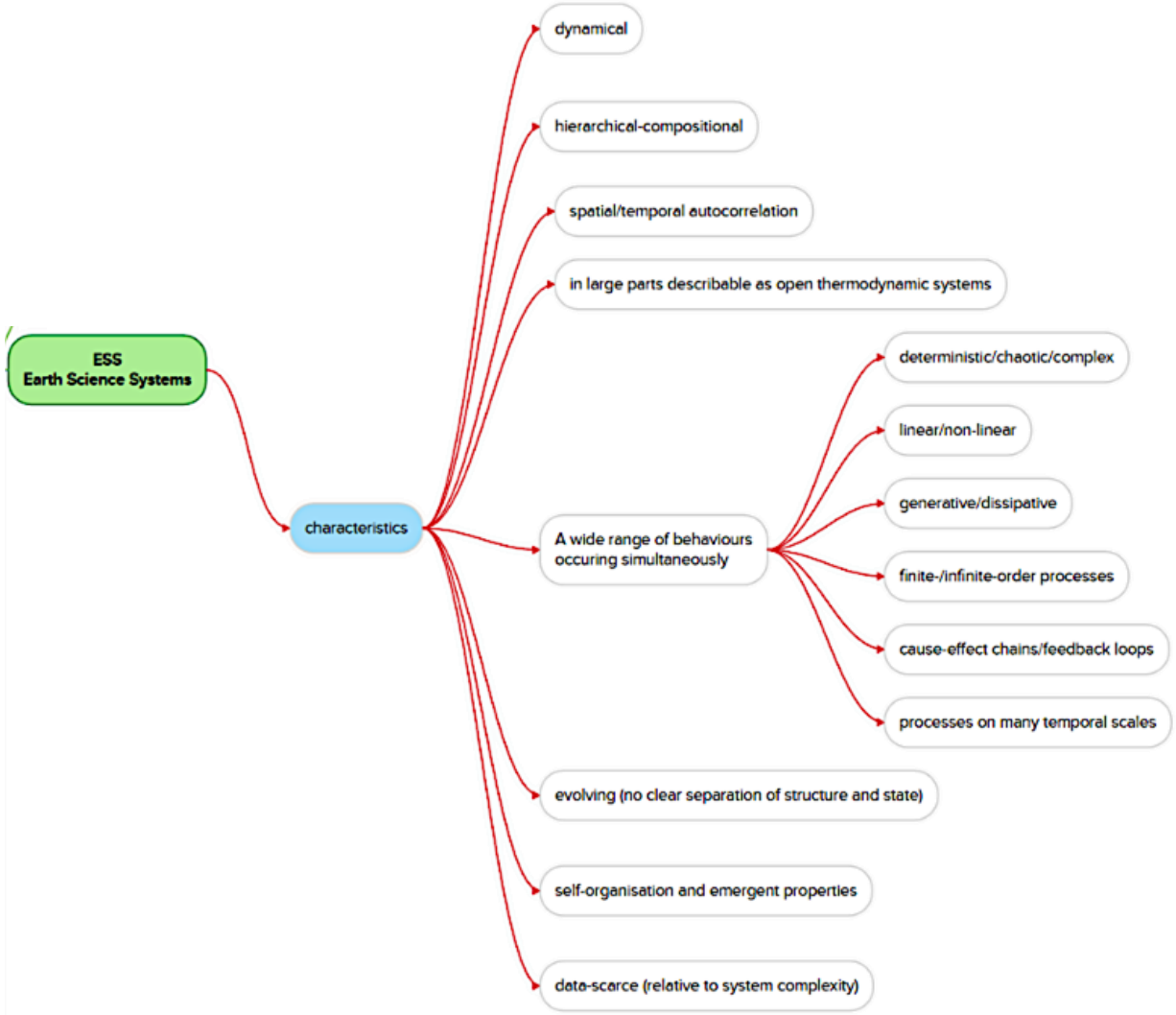
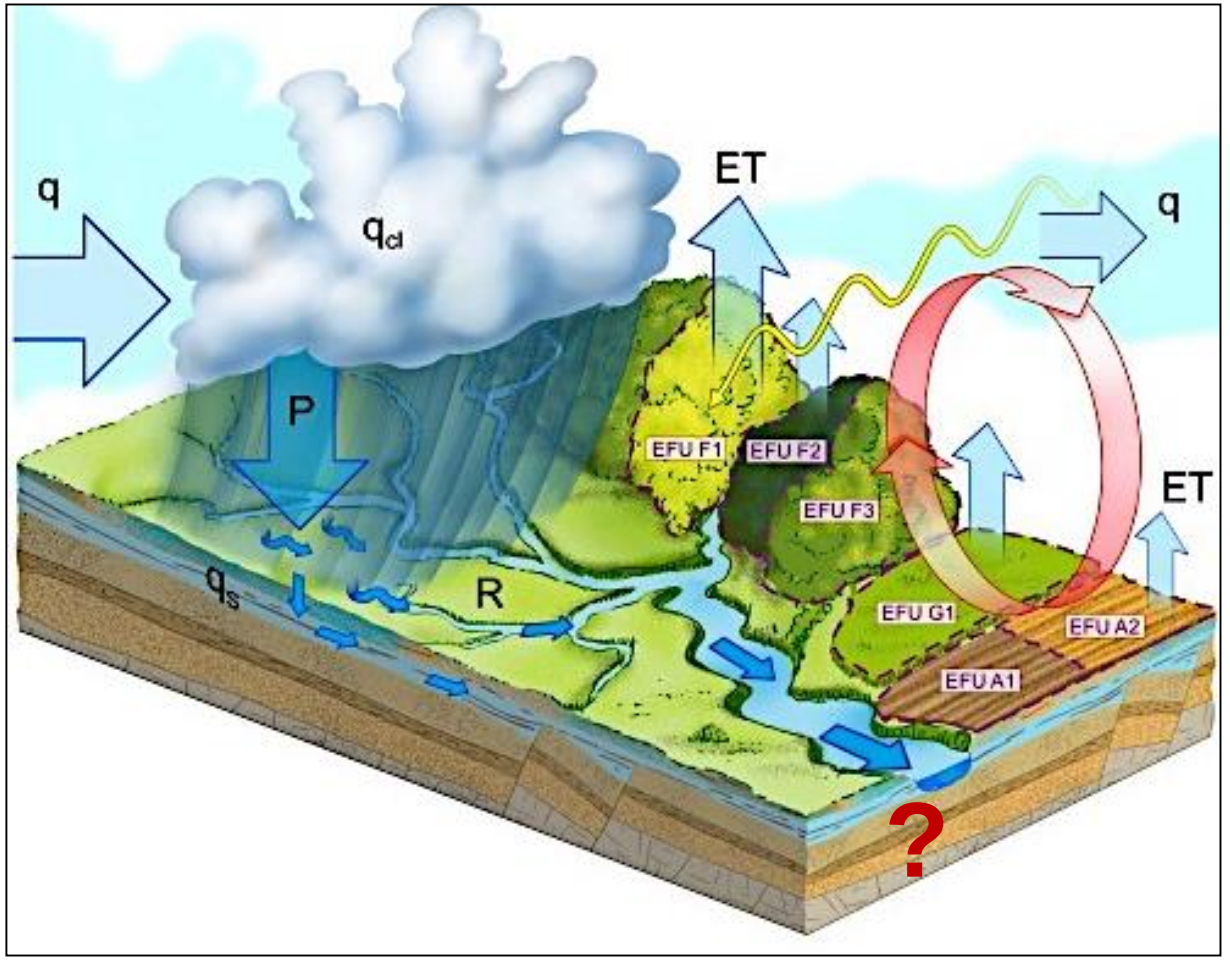


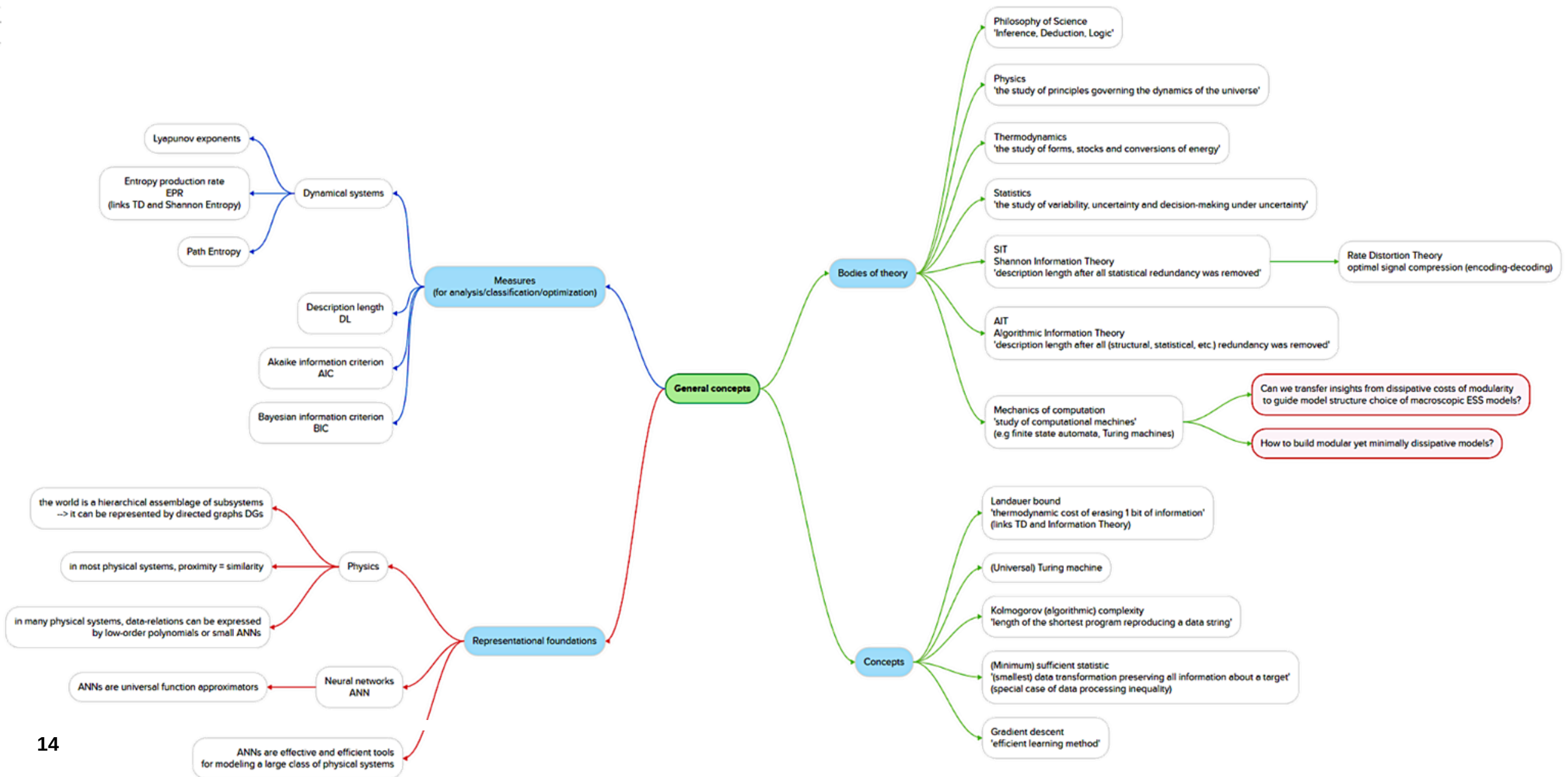


1. Earth Science Systems

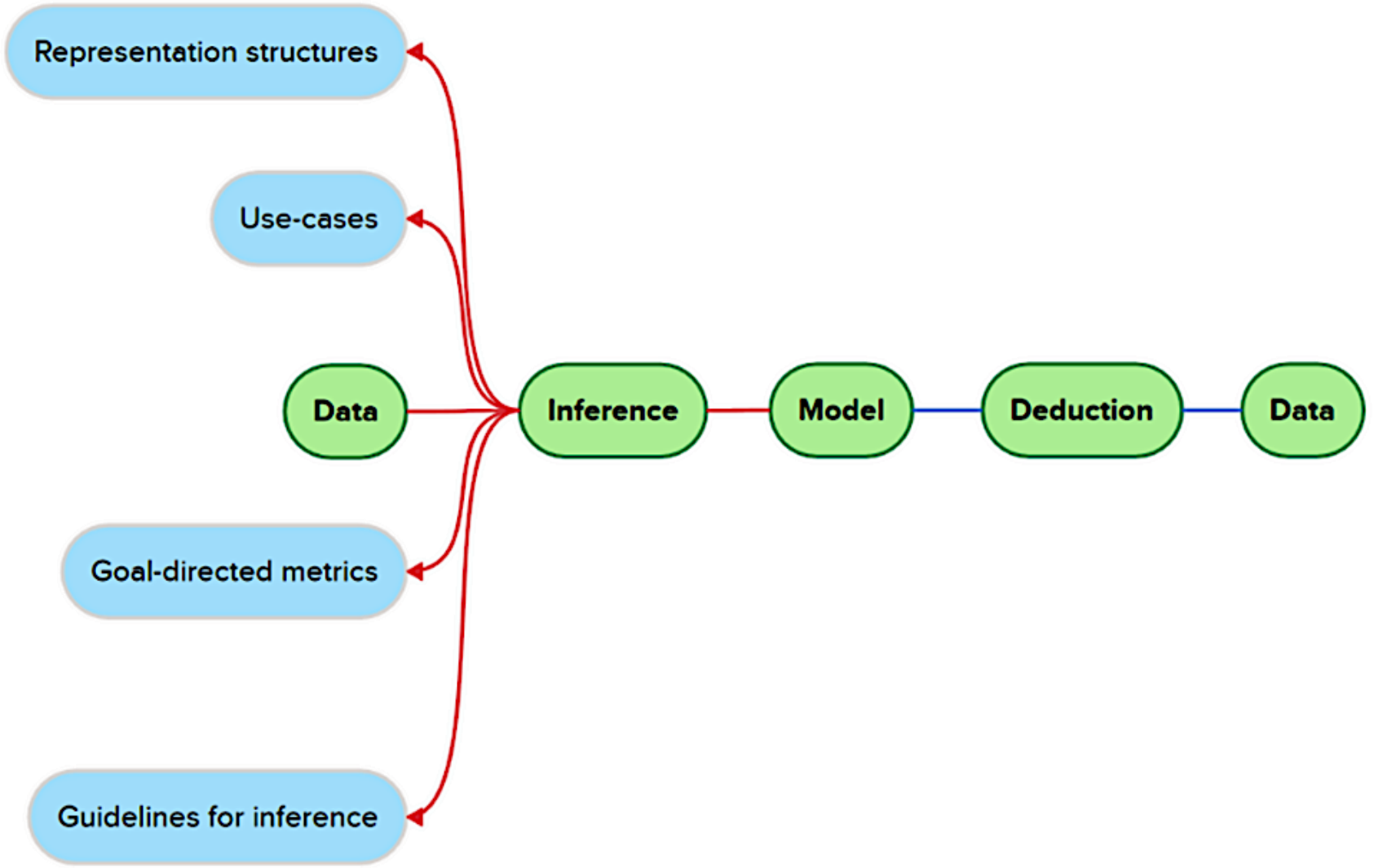




2. General Concepts

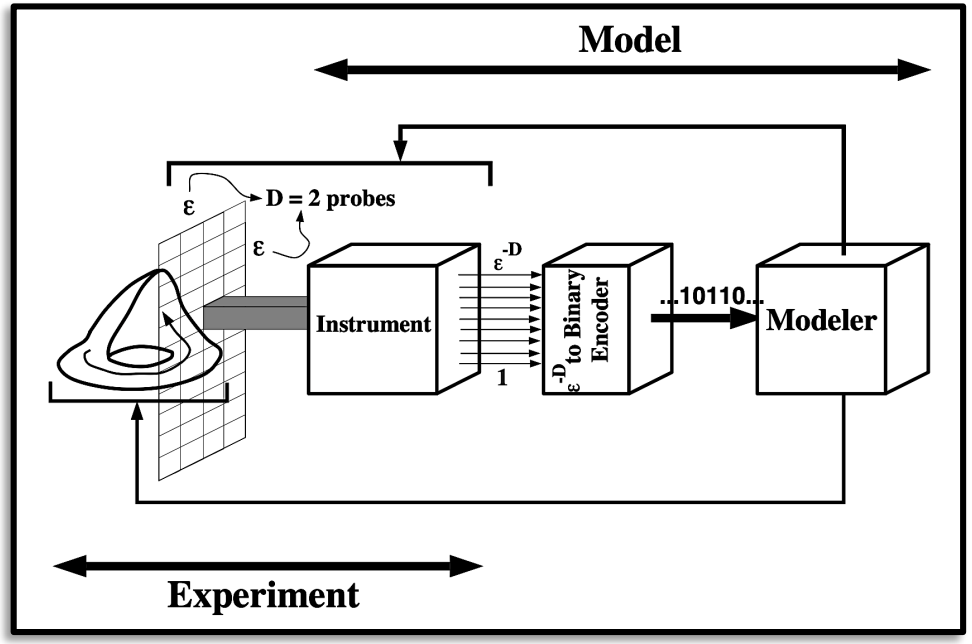


3. The Operational Pathway (Data → Inference → Deduction)



The Central Problem of Inference

Given an ***Instrument***, some number of ***Measurements***, and fixed ***Finite Inference Resources*** … ***how much Computational Structure in the underlying process can be extracted***?



On what sort of structure in the data stream should the models be based … given that:

- *Individual measurements are only indirect representations of the state*
- *The instrument may not supply data of quality sufficient to discover the true states*

So how can the process's "effective" states be accessed?

JP Crutchfield (1992) Knowledge and meaning… chaos and complexity

The "Info Theory" Persective on Model Development

Shannon's Coding Theorems

The *Capacity* (in bits) of the *Communication Channel* (instrument) between the *Process* and the *Modeler* larger than the *Entropy Generation Rate* of the Process.

Model

$\mathcal{X}_{t+\Delta t} = F(\mathcal{X}_t, \zeta_t, t)$

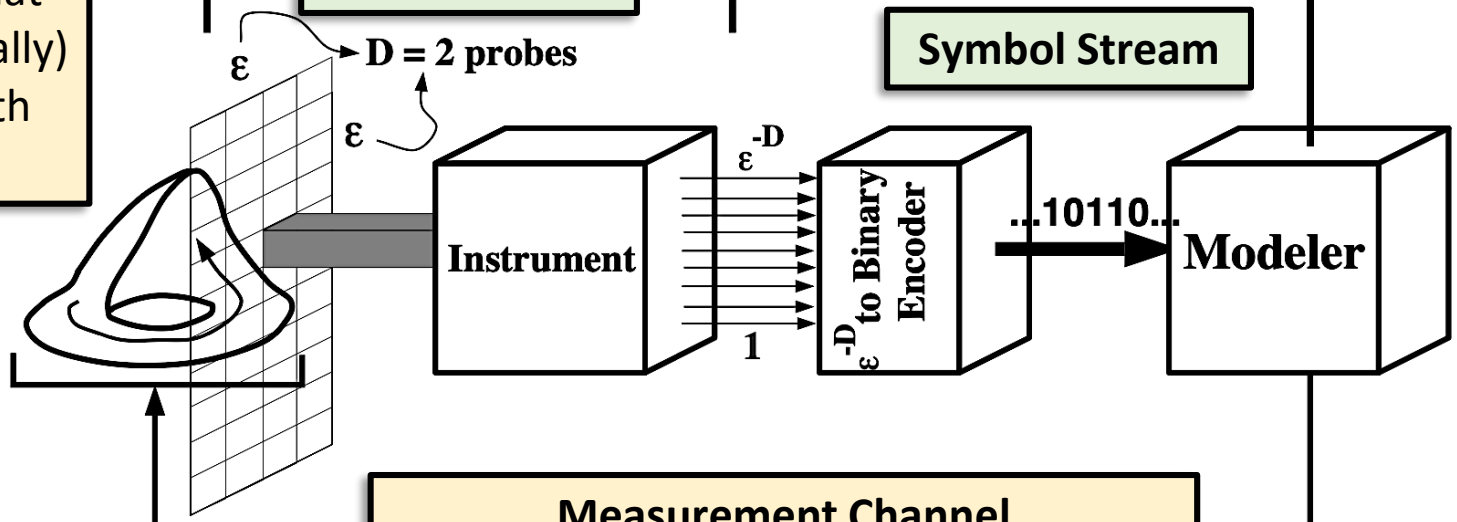
$X_{t+\Delta t} = f(X_t, \eta_t, t)$

Real-World System

Configurations that evolve (stochastically) through time with some *Entropy*

Measurement Space

Symbol Stream



Model/Representation

Effective States that evolve through *State Transitions*

Defined in terms of Available Resources

storage capacity, computational power, inferential efficacy, etc.

Effective Noise Level

Determined by the amount of data "unexplained" by the inferred model

Measurement Channel

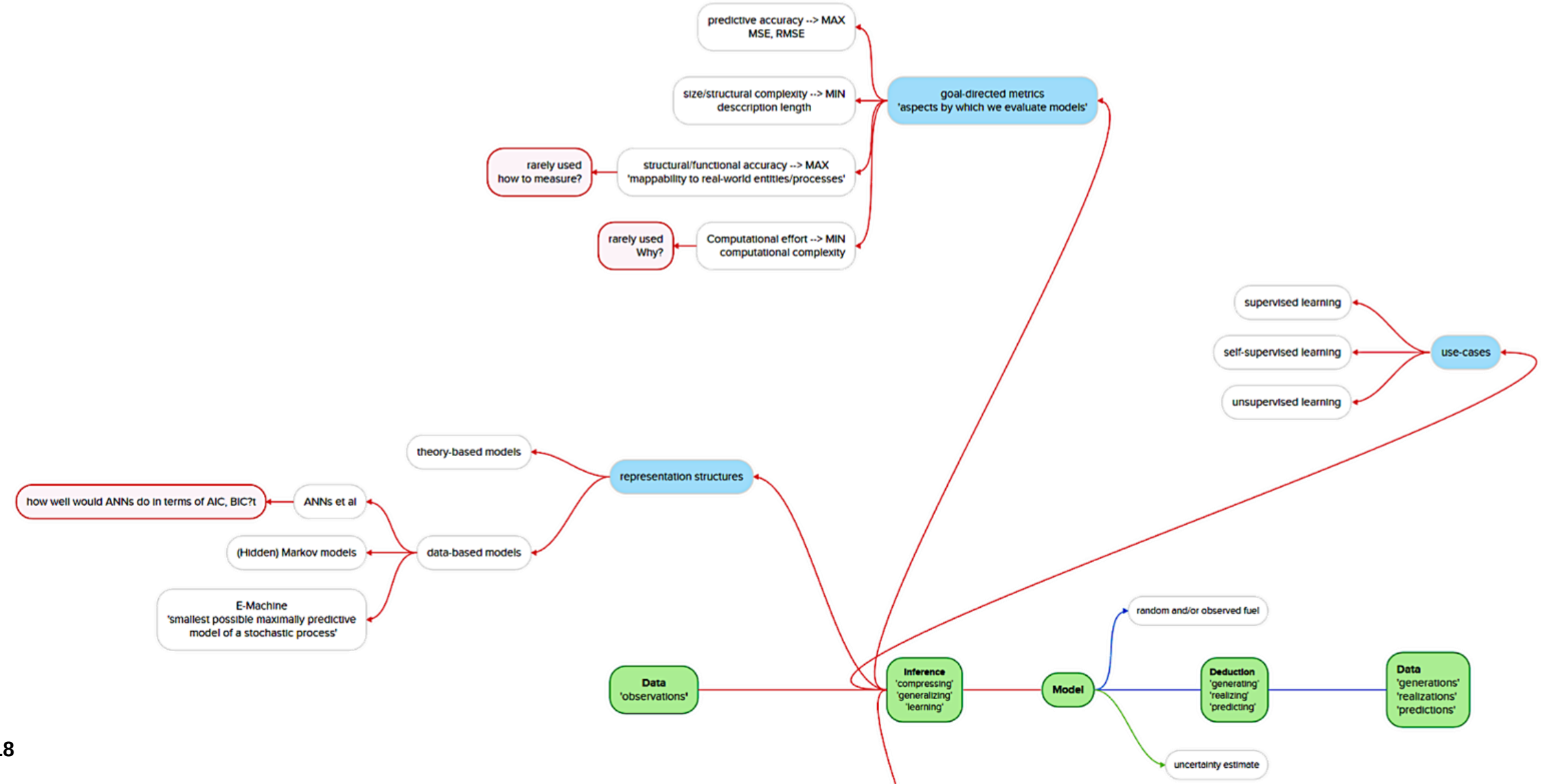
Transducer → ***Encoding of Information***

Maps $\mathcal{X}_t$ to some accessible states of Instrument $\mathcal{I}$

Exper

JP Crutchfield (1992) Knowledge and meaning… chaos and complexity

3. The Operational Pathway (Data → Inference → Deduction)



The Tension between Engineering & Science Perspectives

"The *Engineering* view of *Science* is that it is mere *Data Compression* … [but] *Scientists* seem to be *motivated by more than this*."

ENGINEERING: If a *representation is task-effective*, ***the engineer does not*** [necessarily] ***care what it implies about the underlying mechanisms*** *(although certainly concerned with minimizing implementation cost … representation size, compute time, storage, etc.).*

SCIENCE: ***To the scientist the implication makes all the difference in the world*** – the scientist presumes to be focused on *what the model means vis á vis natural laws*.

JP Crutchfield (1991) "Reconstructing language hierarchies," in Information Dynamics (HA Atmanspracher and H Scheingraber, eds.), (New York), p. 45, Plenum.

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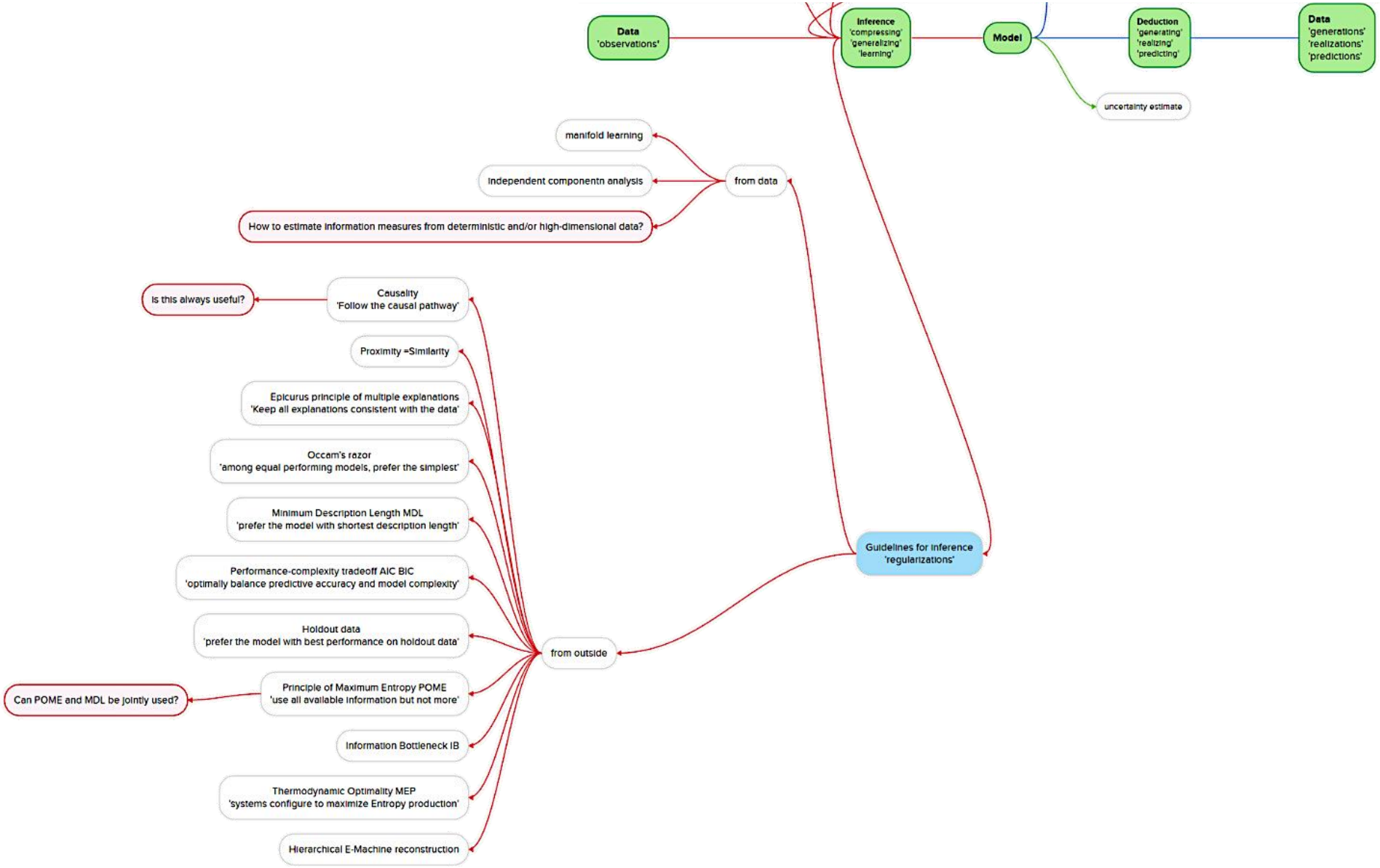
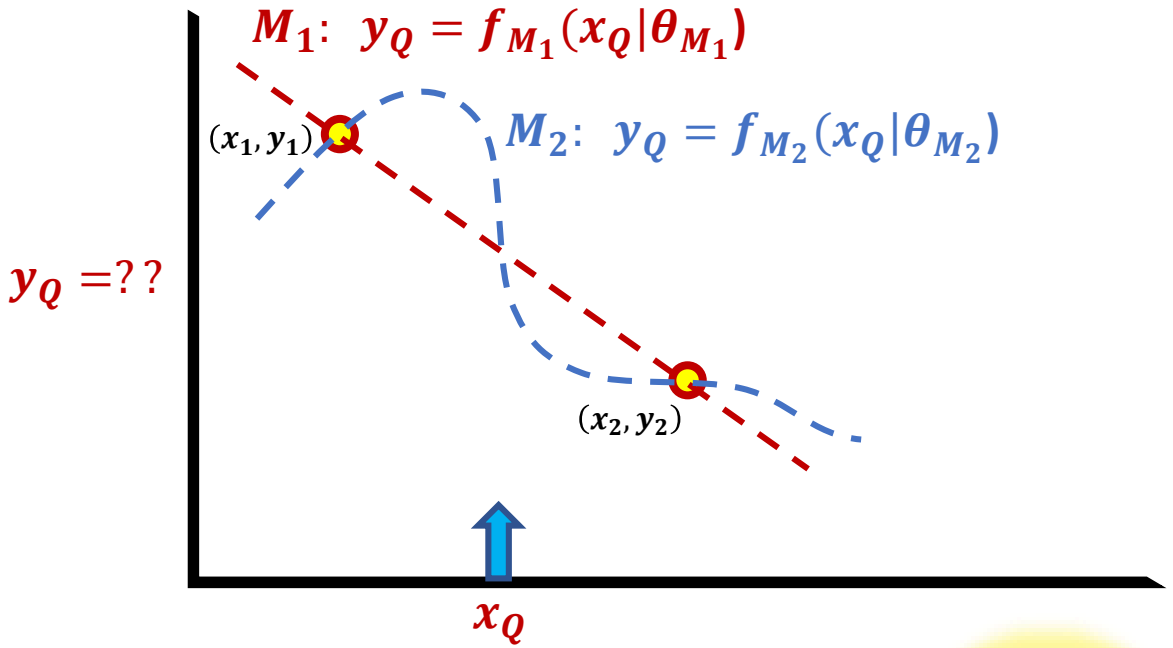
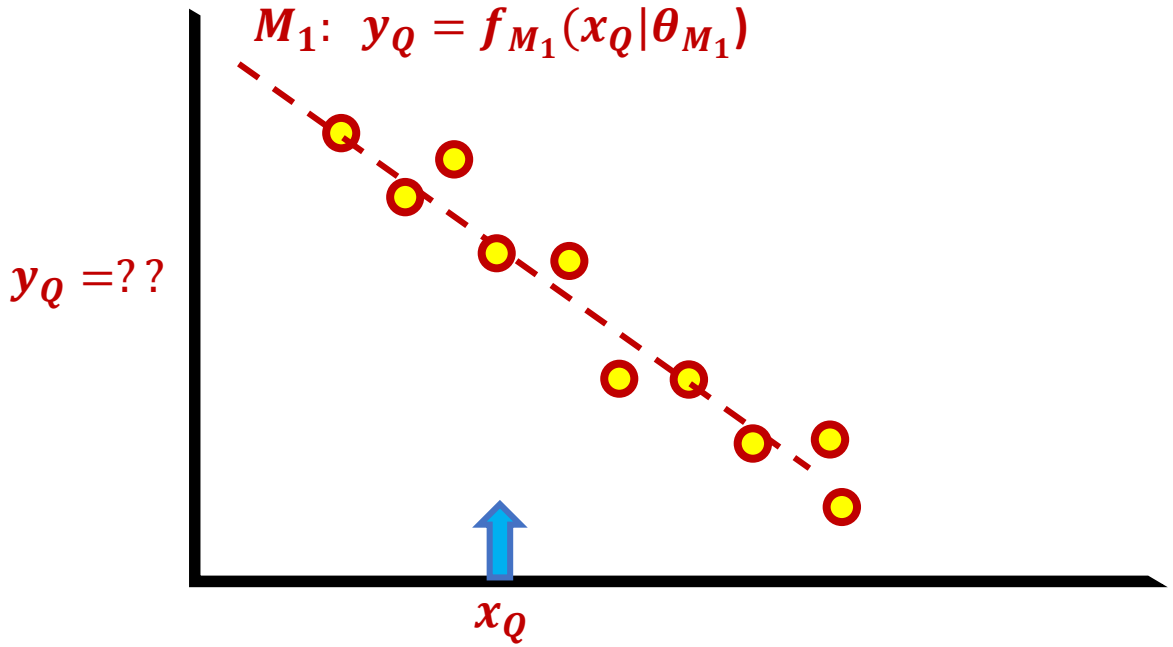


The Epistemological Problem of Inference

**"Have we *discovered something in our Data …*
… or *<u>have we projected the new-found structure</u>* onto it?"**





$$\mathbf{I}(y_Q|x_Q, Model, Data) \neq \mathbf{I}(y_Q|x_Q, Data) + \mathbf{I}(y_Q|x_Q, Model)$$

The Epistemological Problem of Inference

"Have we *discovered something in our Data …*
… or *have we projected the new-found structure* onto it?"

This was the main lesson of attempting to reconstruct equations of motion from a time series:

When it works, it works; when it doesn't, you don't know what to do; and in both cases it is ambiguous what you have learned.

Even though data was generated by well-behaved, smooth dynamical systems, there was an ***extreme sensitivity to the assumed model class*** that completely swamped "model order estimation".

Worse still there was ***no a priori way to select the class appropriate to the process*** (*In AI this is referred to as the "**representation problem**"*.

Despite representations to the contrary, … ***"model order estimation" does not address issues of class inappropriateness and what to do when confronted with failure***.

JP Crutchfield and BS McNamara (1987) Equations of motion from a data series," Complex Systems, vol. 1.

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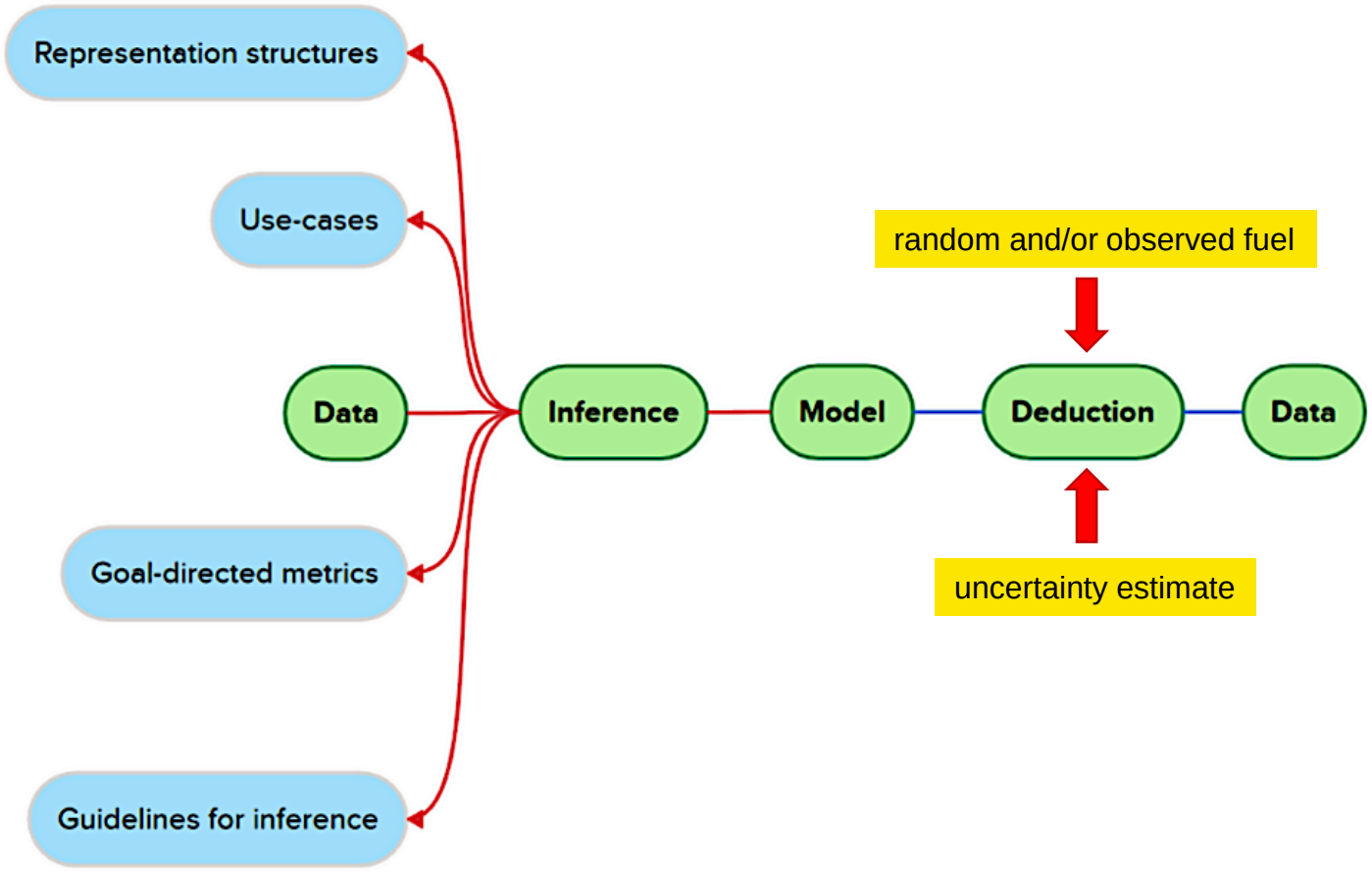
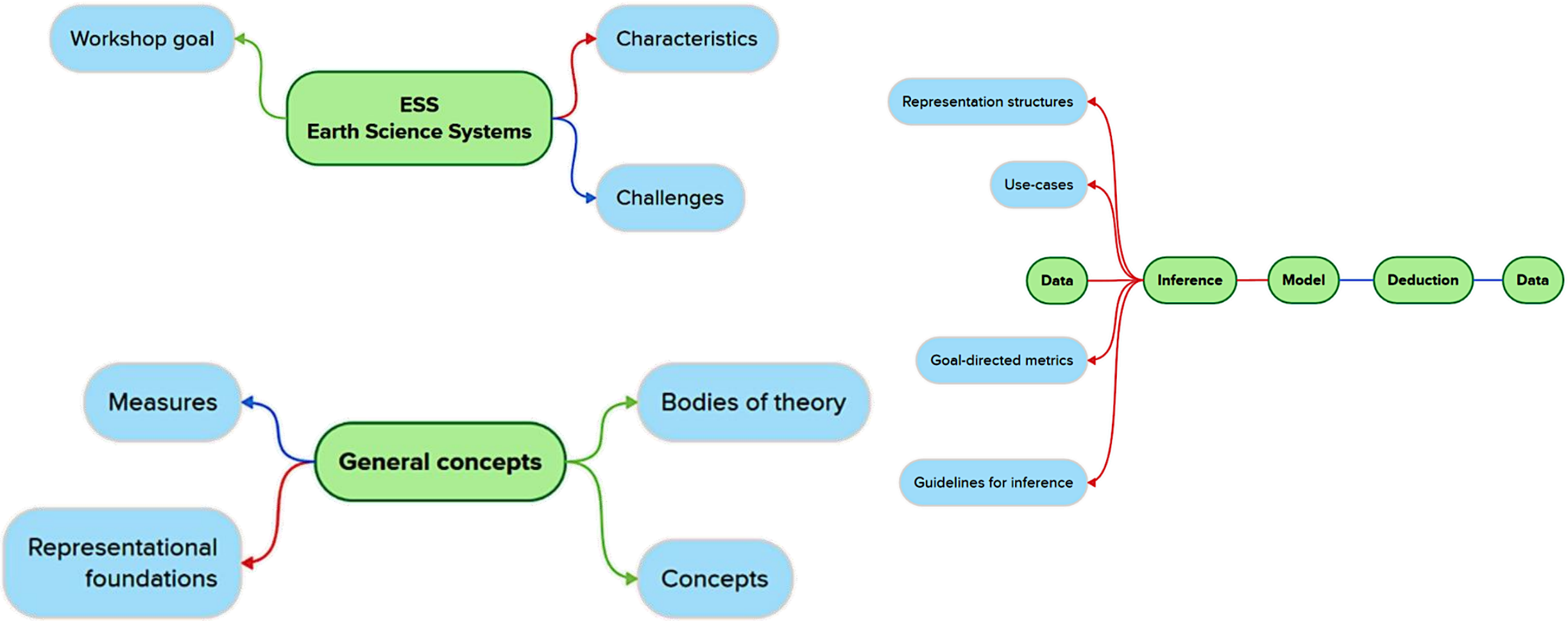


Please Contribute to the Mural



Schedule – Day One

Topical block I: Information Theory as a bridge

9:30-10:30 Invited talk 1 (45+15) A. Boyd
"Thermodynamic Overfitting: Limits on Complexity in Thermodynamic Learning"

10:30-11:30 Invited talk 2 (45+15) A. Jurgens
"Epsilon Machines and Randomness, Structure and Complexity: Predicting Complex Systems"

11:30-11:45 --- Break --- (15)

11:45-12:30 Plenum discussion (45)

12:30-14:00 --- Lunch --- (90)

Alexandra Jurgens

Epsilon Machines.
Intrinsic Randomness.
Structural Complexity.
Finite-state generators.
Statistical complexity dimension.
Minimal memory resources.

Alec Boyd

Max-Work corresponds to Thermodynamic Learning.
Requisite Complexity.
Information Engines.
Predictive Hidden Markov Models.
Overfitting.

Schedule – Day One

Topical block II: Data-based learning and modeling

14:00-14:45	Invited talk 3 (35+10)	R.
	"Decoding the Information Bottleneck in Self-Supervised Learni	
	Pathway to Optimal Representations and Semantic Alignment"	
14:45-15:30	Invited talk 4 (35+10)	A.
	"Probabilities are probably not enough"	
15:30-16:15	Invited talk 5 (35+10)	P.
	"Minimum Description Length, E-Values and Evidence: a brief in	
16:15-16:30	--- Break --- (15)	
16:30-17:30	Plenum discussion (60)	Al
17:30-18:30	Poster session I (60)	Al

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Peter Grünwald

Minimum Description Length
E-Values and Evidence.
Compression.
Optimal codes.
Combining data from different sources.

Ravid Schwartz-Ziv

Compression.
Self-Supervised IT Learning.
Information Bottleneck.
Minimal IT Statistics.
Information Plane.

Andreas Scheidegger

Good Predictions – versus --
Good Decisions.
Natural Systems.
Causal Inference.

Schedule – Day Two

Topical block III: Modeling in the Geosciences

8:00-8:45	Invited talk 6 (35+10) "Data Based Modeling at Scale"	G. Nea
8:45-9:30	Invited talk 7 (35+10) "Machine learning and mechanistic modeling in hydrology: successes and ongoing challenges"	L. Cond
9:30-10:15	Invited talk 8 (35+10) "Information theory in ecological system modelling"	H. Met
10:15-10:30	--- Break --- (15)	
10:30-11:30	Plenum discussion (60)	All

Holger Metzler

Ecological System Modelling.
Conserving (compartmental) systems.
Complexity measures for Dissipative systems.
Maximum Entropy principle.

Grey Nearing

Data Based Geoscientific Modeling at Scale.
Challenges in operational ML.
Relationship between academia and industry.

Laura Condon

Hydrological Systems.
Bridging ML & Physical Modeling.
ML for Model Emulation.
Accelerating simulation-based inference.

Schedule – Day Two

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9:30-10:15	Invited talk 8 (35+10) "Information theory in ecological system modelling"	H. Metzler
10:15-10:30	--- Break --- (15)	
10:30-11:30	Plenum discussion (60)	All

Topical block IV: Ways forward

11:30-12:30	Promises and challenges revisited (60) (identify forward-looking ideas for breakout groups)	All, M. Bassiouni, M. Höge
12:30-14:00	--- Lunch --- (90)	
14:00-15:30	Breakout groups	All
15:30-16:30	Poster session II (60)	All
16:30-18:00	Breakout group reports + discussion (90)	All
18:00-18:30	--- Break --- (30)	
18:30-19:30	--- Dinner ---	
20:00-21:30	--- Socializing / Games / Free Discussion ---	

Schedule – Day Three

Topical block V: Synthesis

8:00-8:30	Coffee (30)	
8:30-10:00	Synthesis group reports + discussion (90)	All, synthesis group members
10:00-10:45	Invited speaker reflections (45)	Invited speakers
10:45-11:00	--- Break --- (15)	
11:00-12:30	Plenum discussion and/or breakout groups (90)	All
12:30-14:00	--- Lunch --- (90)	
14:00-16:30	Guided tour to Schneeferner research facilities (2.5 h)	All
16:30-17:30	Conclusion / Outlook / Next steps (60)	All, H. Gupta, U. Ehret
17:30-18:30	--- Break --- (60)	
18:30-19:30	--- Dinner ---	
20:00-21:30	--- Socializing / Games / Free Discussion ---	

Potential Outcomes

- **Enhanced *Dialogue* and *Collaboration***
- **Community Progress towards *Development of a General Framework***
  (*rooted in the marriage of Information Theory, Modeling Science, and Domain Science*) **for:**
  - ***Constructing Task-Relevant Models that can Learn from Data***
  - ***While maintaining Interpretable Representational Structures consistent with physical understanding***
- **Joint/Collaborative *Papers* (or series)**
- **Other …**

We Invite Creative Suggestions

Discussion


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