Pacific Northwest
NATIONAL LABORATORY

Data-driven Scientific Discovery

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U.S. DEPARTMENT OF ENERGY BATTELLE

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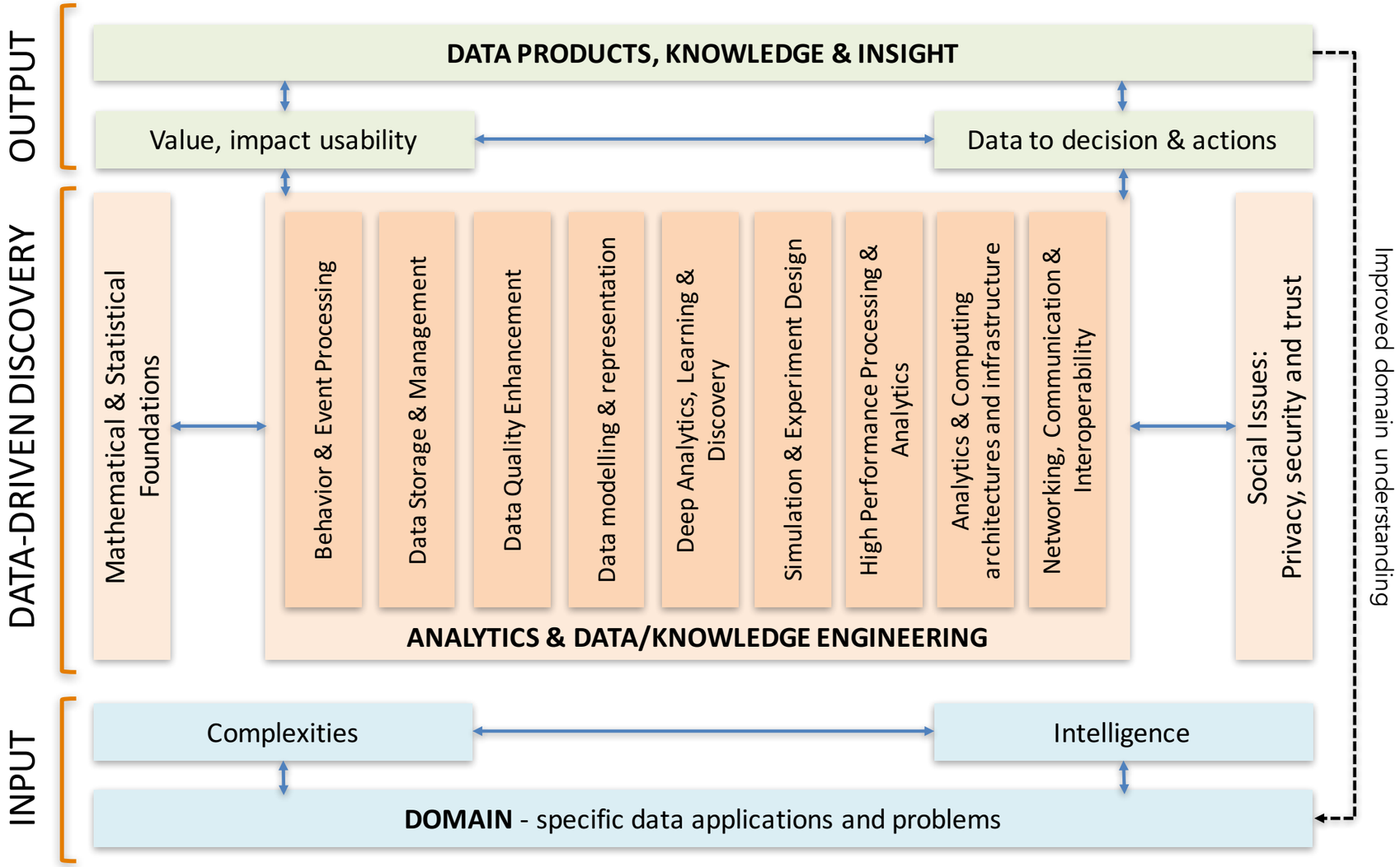
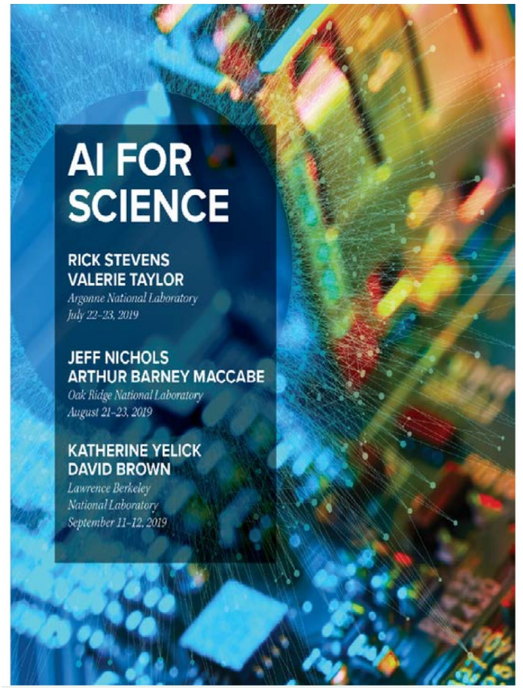
Data Science



Adapted from Cao, L. (2017). "Data Science: A Comprehensive Overview." ACM Comput. Surv. **50**(3): Article 43.

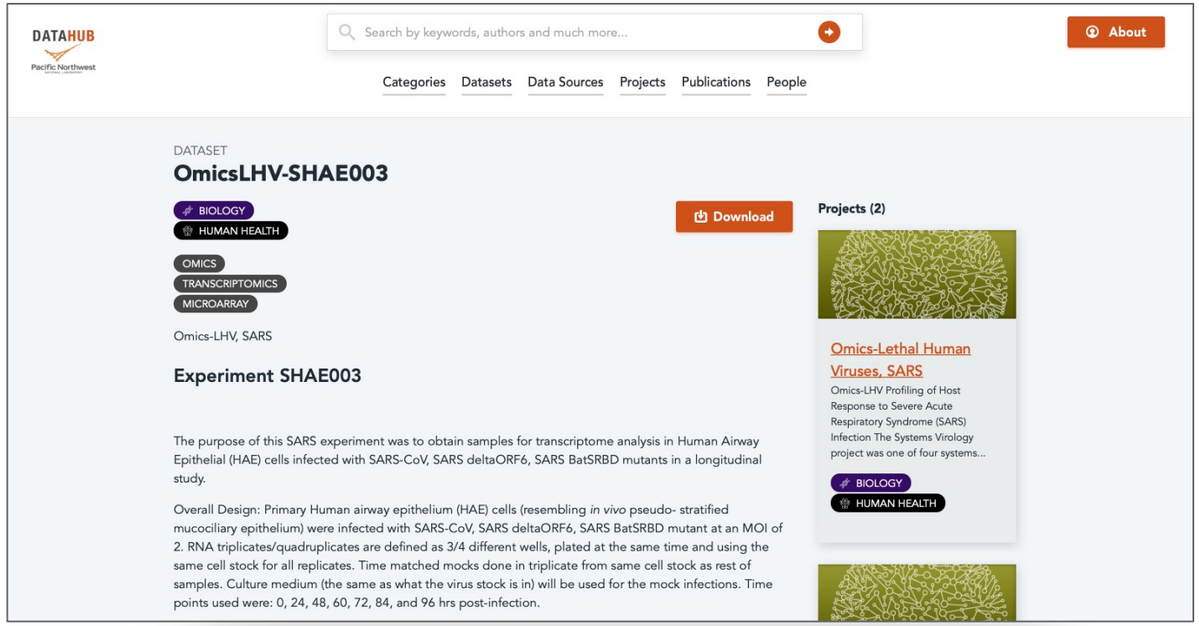
Scientific Machine Learning

- Machine Learning algorithms should be:
  - **Domain-aware**
  - Interpretable
  - Robust
  - Data-intensive
  - Scalable, deployable
- Machine Learning must contribute to:
  - Enhance current modeling and simulation
  - Automation and decision support



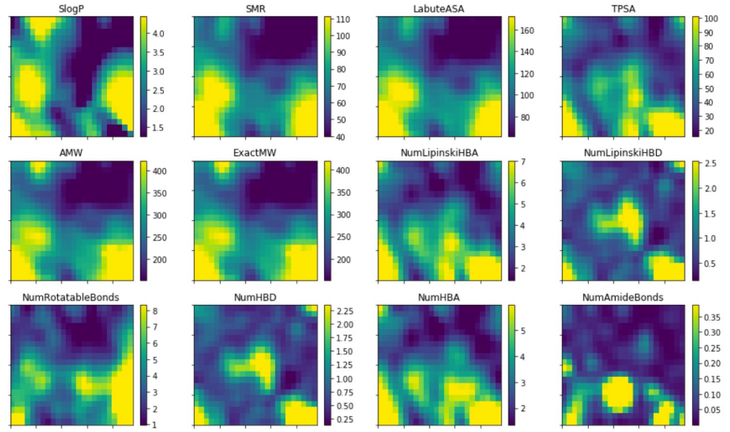
Data

- Data products
  - Beyond raw data
  - Models, workflows
- Data governance and data stewardship
  - Define process and procedures
  - Ensure compliance and security
  - Manages data, tools and processes
  - Comprehensive policies
- Data quality
  - Metrics
- Privacy preservation
  - Privacy-preserving analytics
  - Privacy-preserving AI/ML

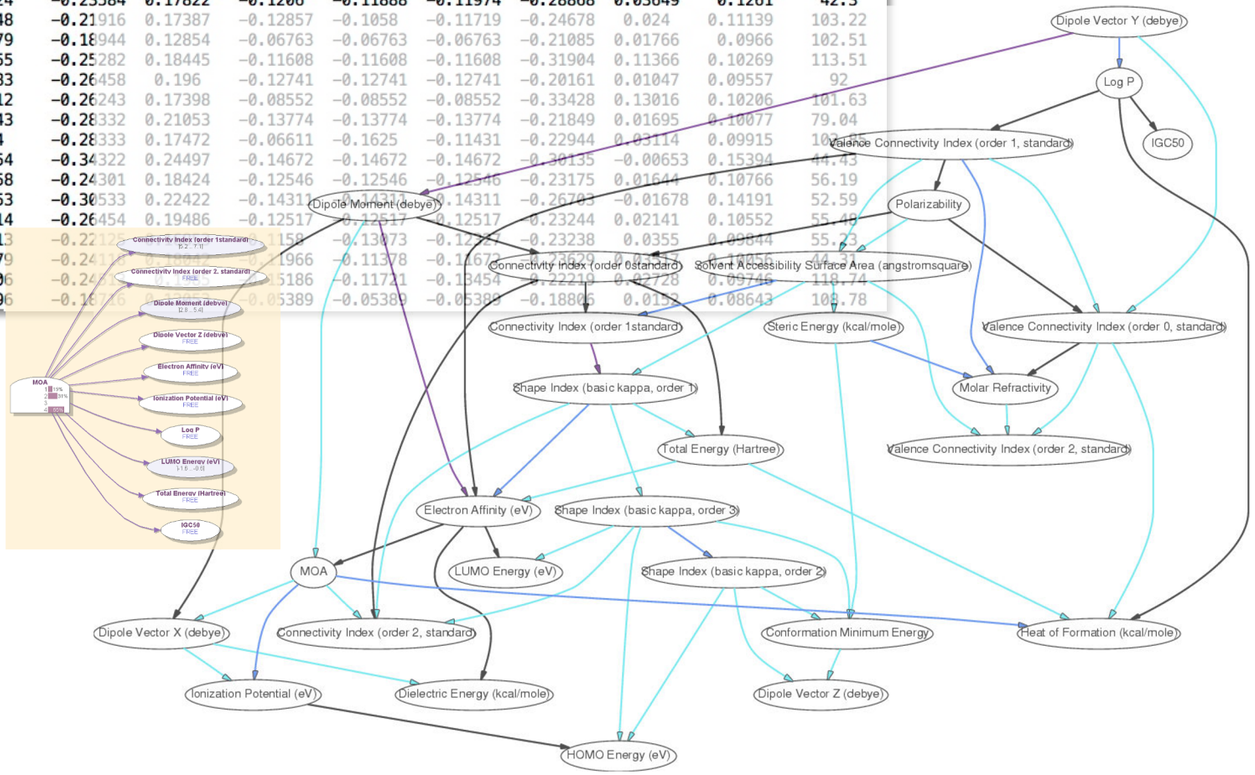


Data Representation

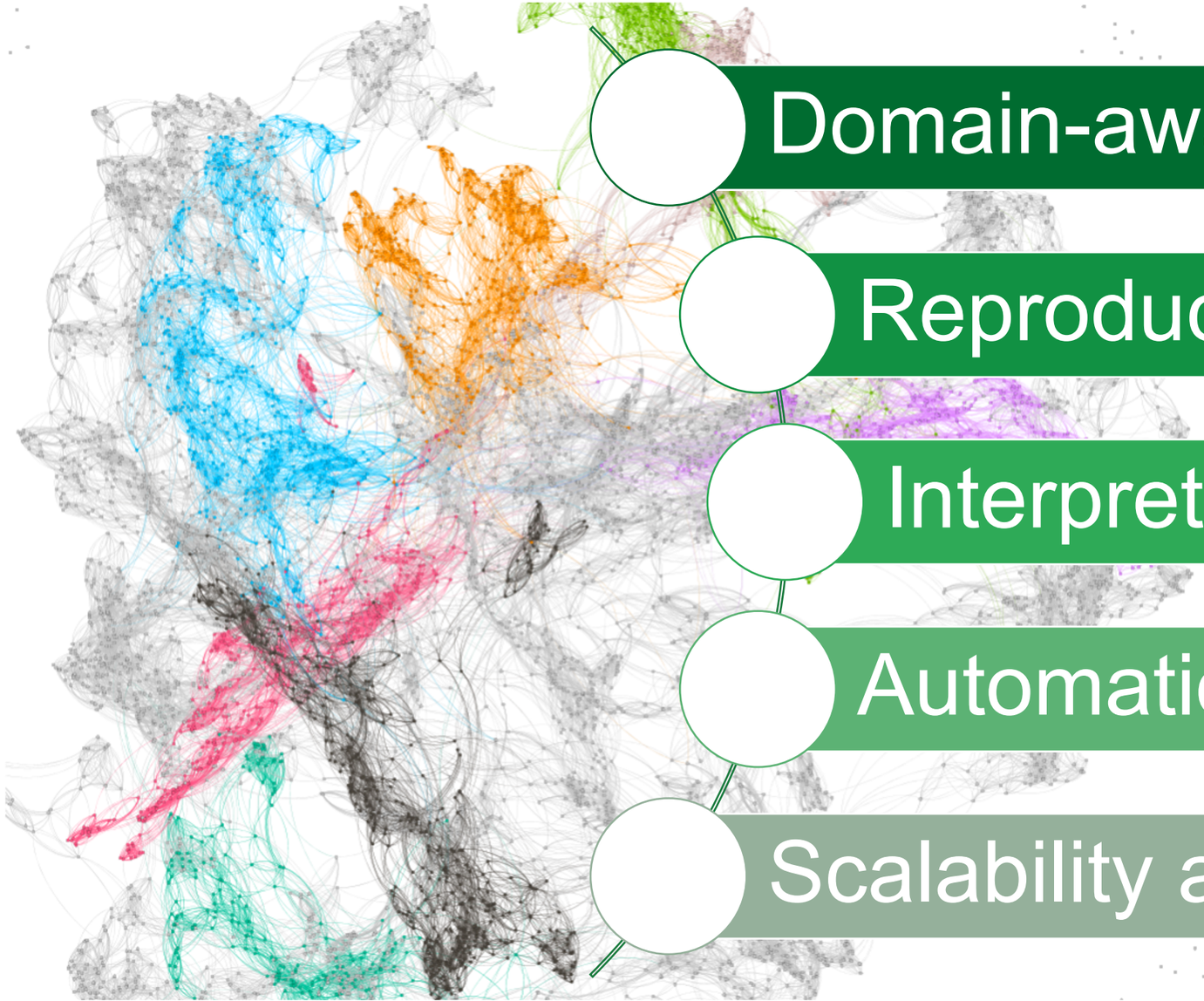
- Structured vs unstructured data
  - e.g., knowledge extraction from literature sources
- Efficient data structures
  - graphs
- Feature engineering
  - feature selection
  - feature synthesis
- **Representation learning**
  - interpretability



material	light_tox	dark_tox	HHOMO	LZELEHHO	LUMOA	LUMOB	ALZLUMO	MHOMOA	MLUMOA	QMELECT	Cp
Zn0	6.23	5.8	−0.22819	0.13198	−0.03576	−0.13869	−0.08723	−0.29251	0.04335	0.12458	40.25
Cu0	5.71	4.24	−0.23584	0.17822	−0.1206	−0.11888	−0.11974	−0.28868	0.03649	0.1261	42.3
V203	3.78	3.48	−0.21916	0.17387	−0.12857	−0.1058	−0.11719	−0.24678	0.024	0.11139	103.22
Y203	5.84	5.79	−0.18944	0.12854	−0.06763	−0.06763	−0.06763	−0.21085	0.01766	0.0966	102.51
Bi203	4.02	3.55	−0.25282	0.18445	−0.11608	−0.11608	−0.11608	−0.31904	0.11366	0.10269	113.51
In203	3.48	2.83	−0.26458	0.196	−0.12741	−0.12741	−0.12741	−0.20161	0.01047	0.09557	92
Sb203	3.66	3.12	−0.26243	0.17398	−0.08552	−0.08552	−0.08552	−0.33428	0.13016	0.10206	101.63
Al203	2.75	2.43	−0.28332	0.21053	−0.13774	−0.13774	−0.13774	−0.21849	0.01695	0.10077	79.04
Fe203	2.54	2.4	−0.28333	0.17472	−0.06611	−0.1625	−0.11431	−0.22944	0.03114	0.09915	10
Si02	2.92	2.54	−0.34322	0.24497	−0.14672	−0.14672	−0.14672	−0.30135	−0.00653	0.15394	44.43
Zr02	3.04	2.58	−0.24301	0.18424	−0.12546	−0.12546	−0.12546	−0.23175	0.01644	0.10766	56.19
Sn02	3.24	2.53	−0.30533	0.22422	−0.14311	−0.14311	−0.14311	−0.26703	−0.01678	0.14191	52.59
Ti02	4.68	2.14	−0.26454	0.19486	−0.12517	−0.12517	−0.12517	−0.23244	0.02141	0.10552	55.48
Co0	3.33	3.13	−0.22128		−0.1158	−0.13073	−0.12153	−0.23238	0.0355	0.09844	55.23
Ni0	3.87	3.79	−0.24		−0.11966	−0.11378	−0.11672	−0.25629	0.02425	0.10056	44.23
Cr203	2.06	2.06	−0.24		−0.15186	−0.11721	−0.13454	−0.22219	0.02728	0.09746	118.74
La203	5.56	4.96	−0.18		−0.05389	−0.05389	−0.05389	−0.18806	0.0153	0.08643	109.78



Opportunities for Accelerating Scientific Discovery with AI/ML



- Domain-awareness
- Reproducibility & Robustness
- Interpretability
- Automation
- Scalability and Deployment

Domain-awareness

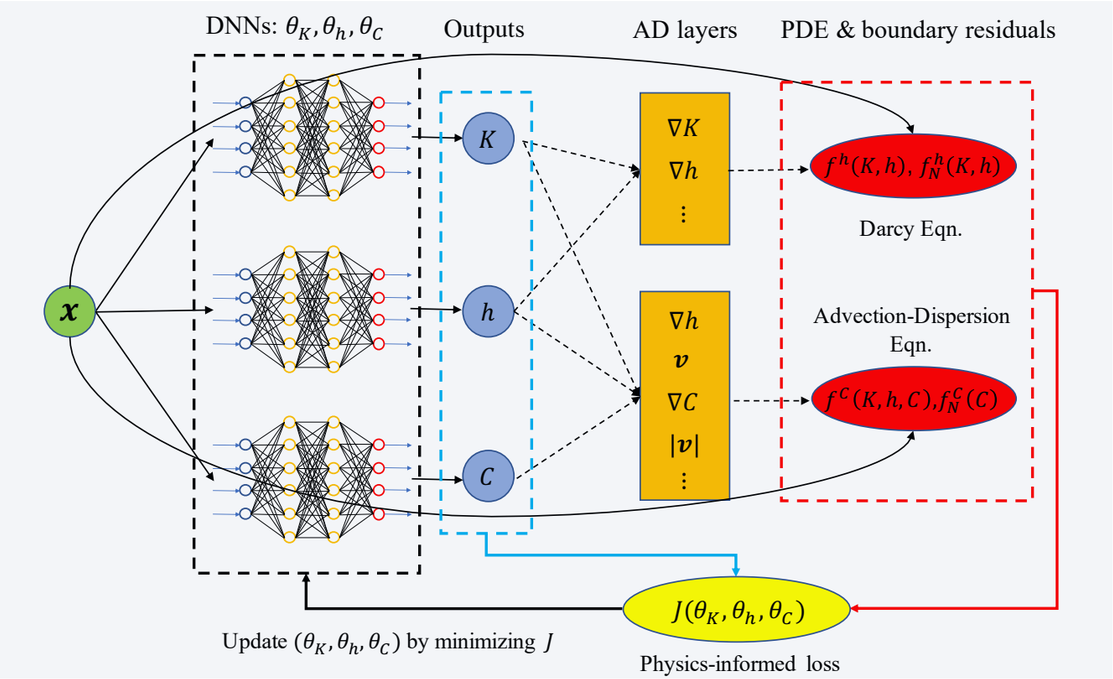
DATA

- Knowledge representations
  - Equations
  - Knowledge graphs
  - Causal models
  - Distributed knowledge models
- Domain-aware features

ALGORITHMS

- Knowledge embedding
  - Constraints
  - Loss function
  - Coupling with simulations
  - Model structure

Coupling limited experimental data with physics models improves accuracy and reduces the risk of model overfitting in subsurface transport modeling.

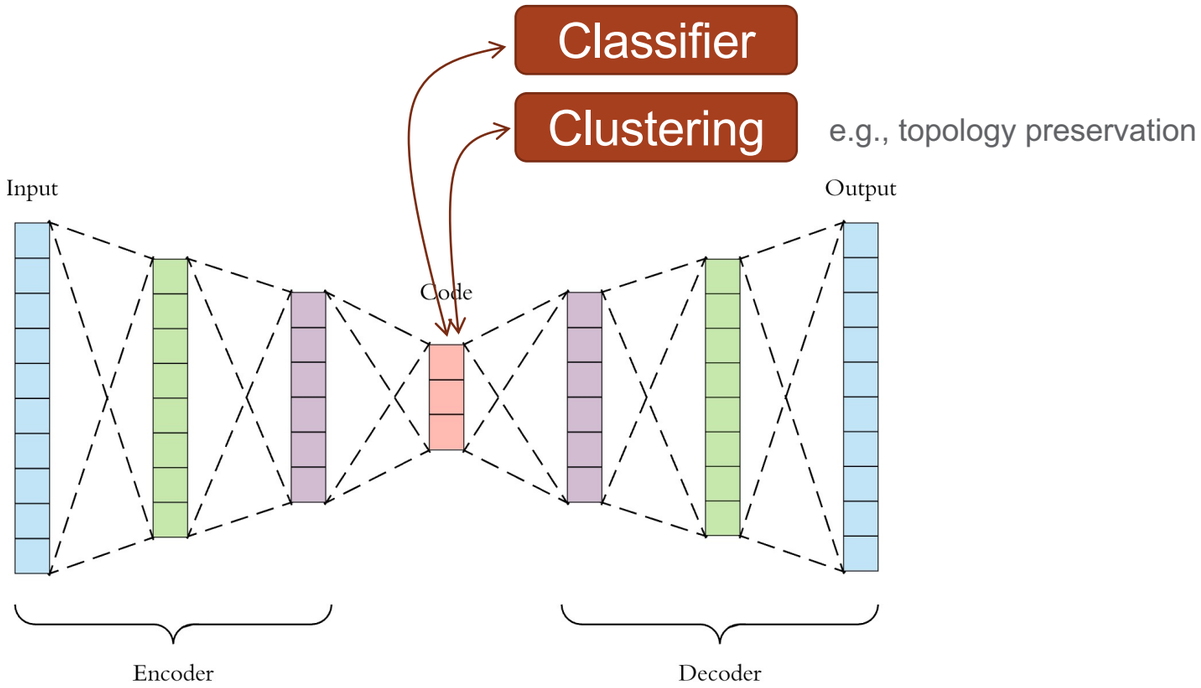


He Q et al.. 2020 Physics-informed neural networks for multi-physics data assimilation with application to subsurface transport. *Advances in Water Resources* (2020) 141.

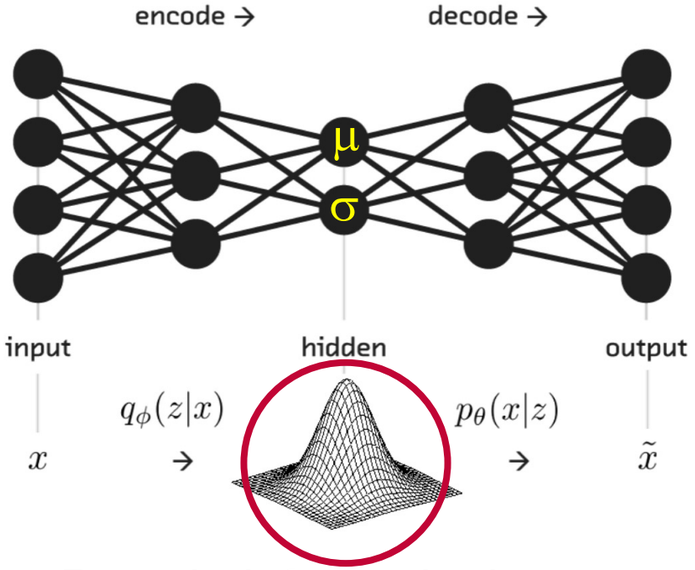
Domain-aware features

- Coupling autoencoders with:
  - Clustering algorithms
  - Classification algorithms

$$\mathcal{L}(x, \hat{x}) + \lambda_1 \sum_i |a_i| + \lambda_2 \mathcal{L}_{\substack{clustering \\ classifier}}$$

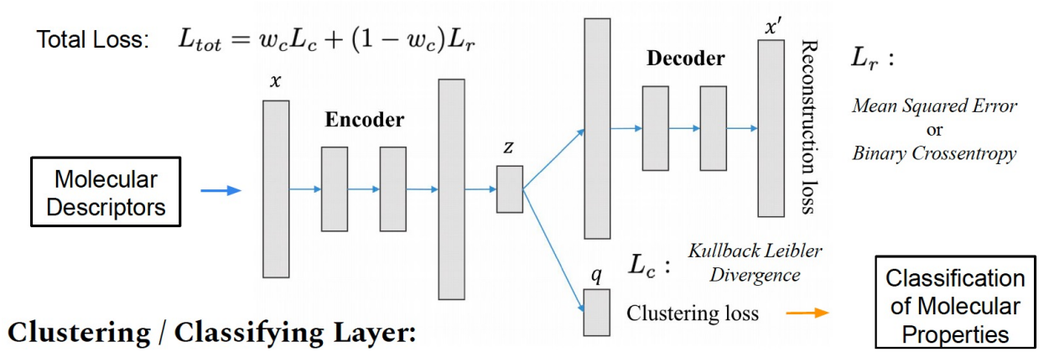


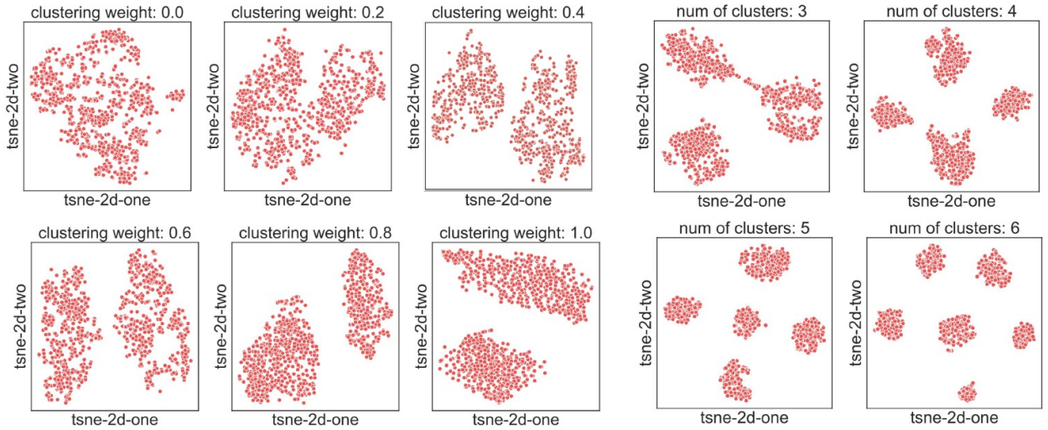
- Variational autoencoders with:
  - Predefined priors



- Domain-informed prior
- KL term in the loss function enforces the desired probability distribution

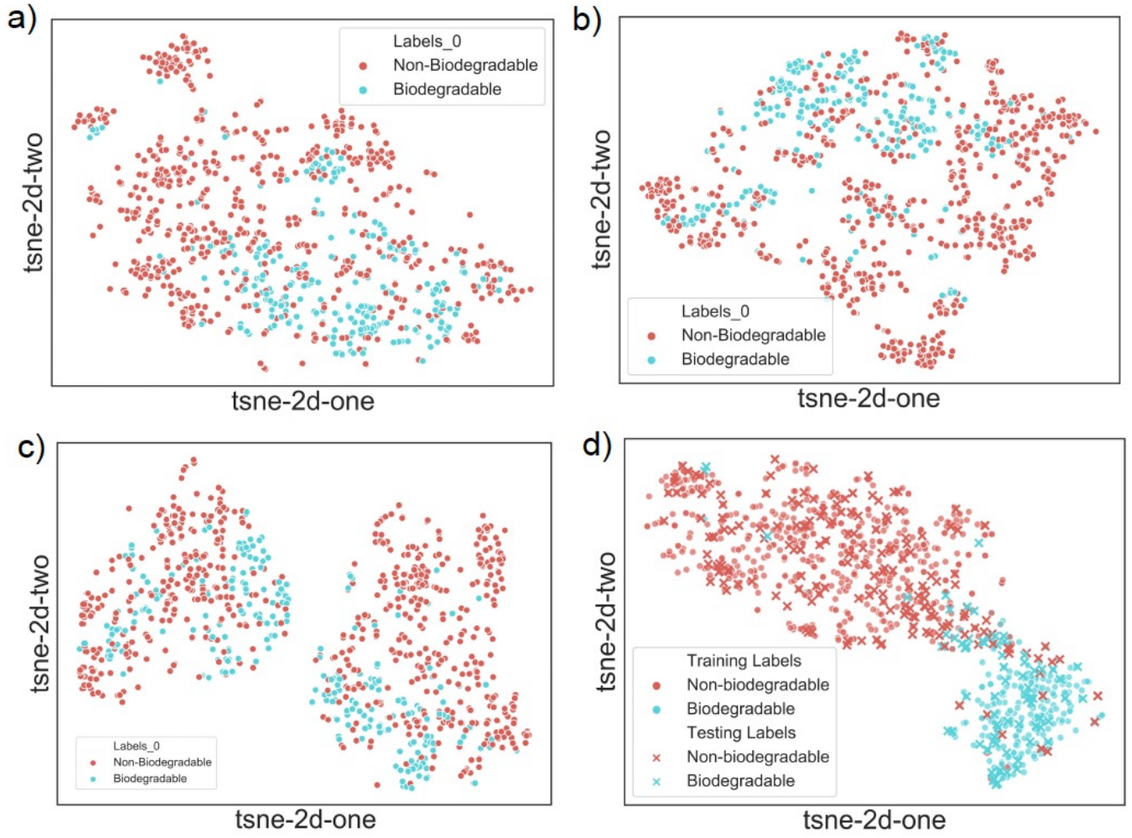
Biodegradability-aware embeddings





The 2-dimensional T-SNE projections of hidden layers, number of clusters = 2

The 2-dimensional T-SNE projections of hidden layers, clustering weights = 0.6

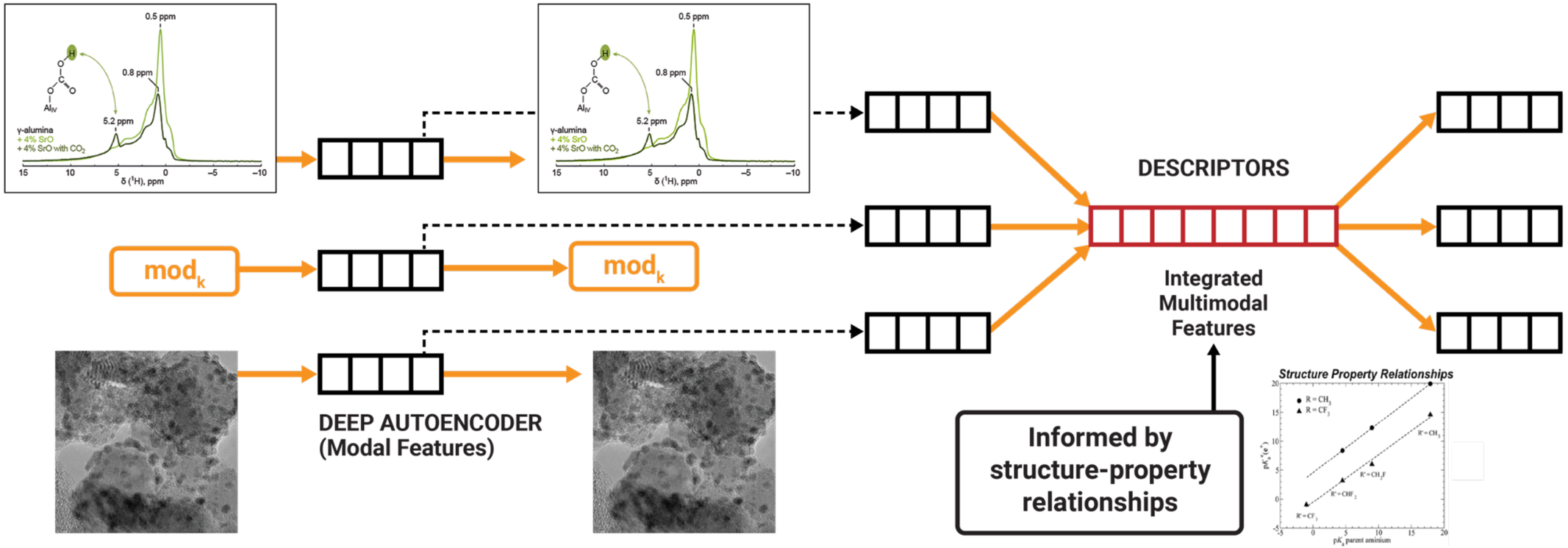


t-sne projection: (a) raw data; (b) autoencoder; (c) clustering ; (d) classification

H. Hu (UW), Y. Liu (UW), Y. Chen (UW), R. Rallo (PNNL)

Integrated multi-modal features

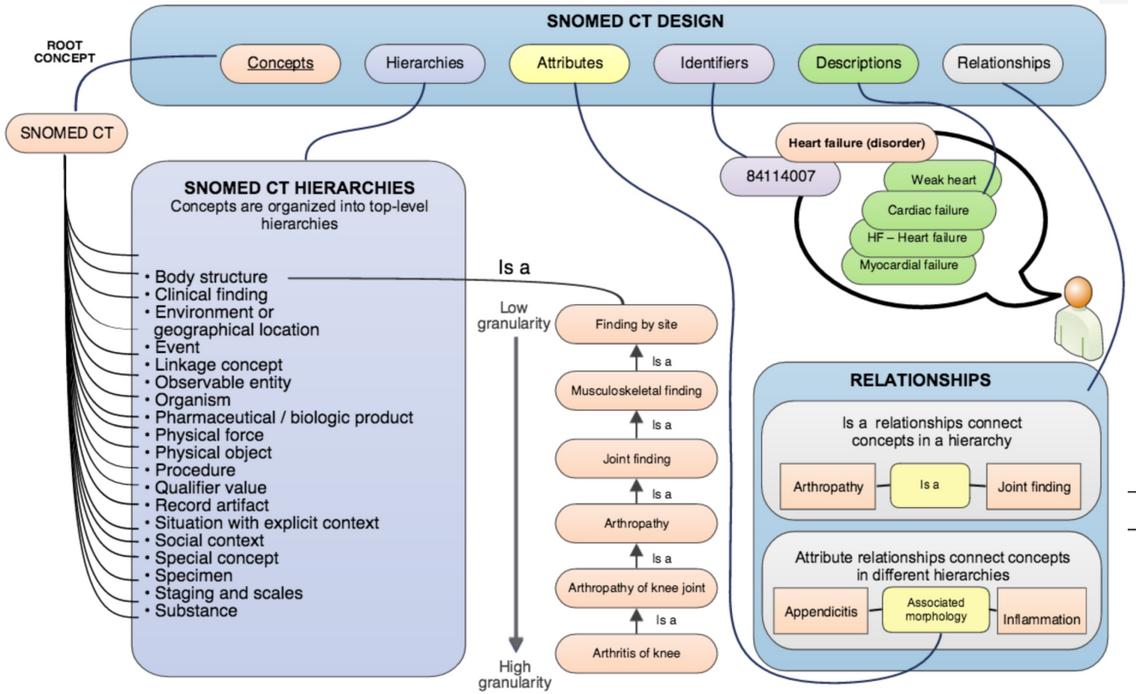
- Heterogeneous data
- Domain-informed stacked autoencoders → integrated features

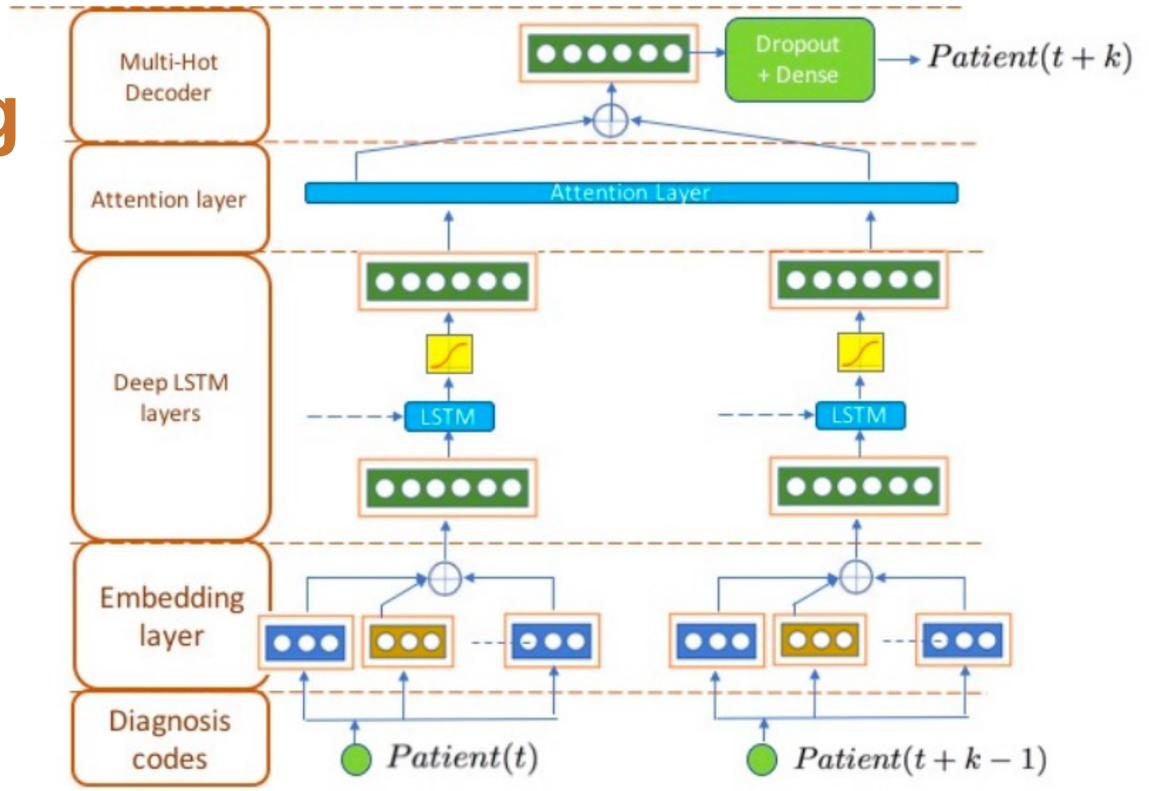


$$L = L_r + L_{SPR}$$

Knowledge embedding

- Medical knowledge / Knowledge graphs





	Node2vec	Metapath2vec	Poincare	CUI2vec	Med2vec
Node Classification	0.817	0.3287	**0.8579**	0.5685	0.0409
Link Prediction	**0.986**	0.3988	0.7135	0.7222	0.8665
Concept Similarity (D1)	**0.79**	0.3	0.7	0.16	NA
Concept Similarity (D3)	**0.90**	0.46	0.31	0.15	NA
Concept Similarity (D5)	**0.81**	-0.32	-0.06	-0.01	NA
Patient State Prediction (All Diagnosis)	0.3938	0.3359	**0.4197**	0.3948	0.3881
Patient State Prediction (Frequent 20)	0.8465	**0.9749**	0.85	0.8035	0.7980
Patient State Prediction (Rare 20)	0.018	0.001	**0.019**	**0.019**	0.011

K. Agarwal, T. Eftimov, R. Addanki, S. Choudhury, S. Tamang, R. Rallo, KDD – Workshop DSHealth, 2019 (https://arxiv.org/abs/1907.08650)

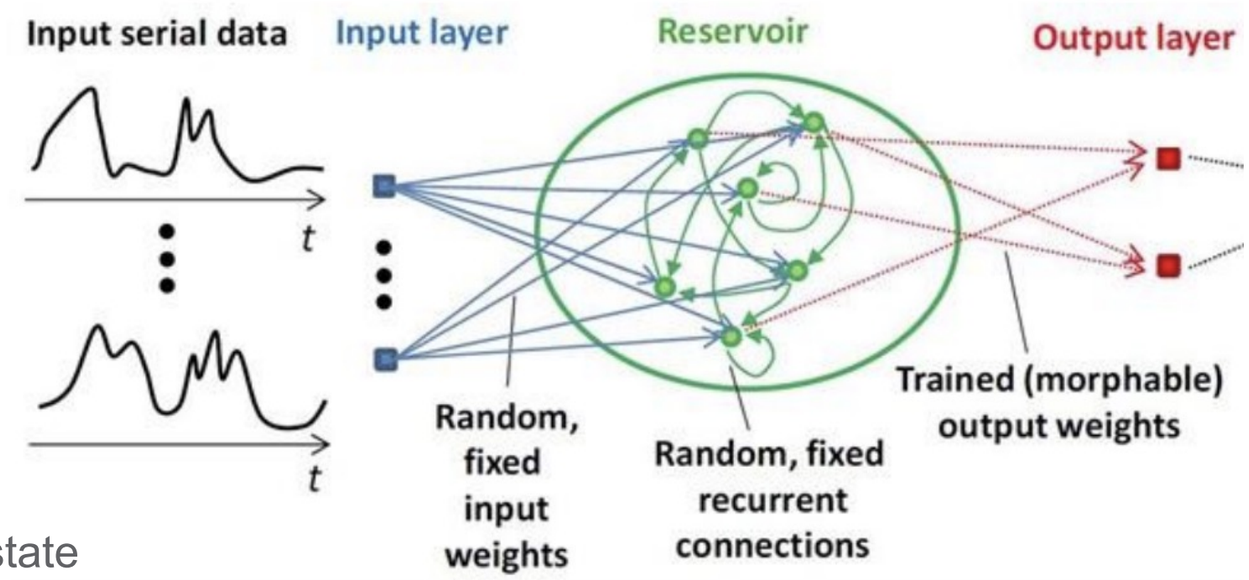
Model structure

- Reservoir computing
  - Generalization of recurrent neural networks
  - Dynamical systems
  - Maps inputs onto a high-dimensional space
  - Hardware implementation
- Elements
  - Input layer
    - ✓ random weights
  - Reservoir
    - ✓ Random sparse connectivity
    - ✓ Non-linear activation
  - Readout layer
    - ✓ Linear transformation of the reservoir state
    - ✓ Fast adaptation using ridge regression

Domain-awareness

Structured reservoir

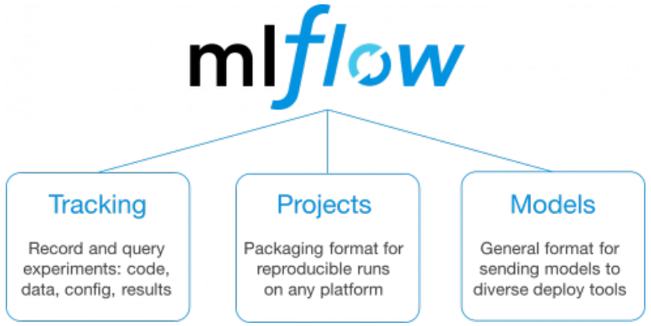
Graph analytics
Network Science

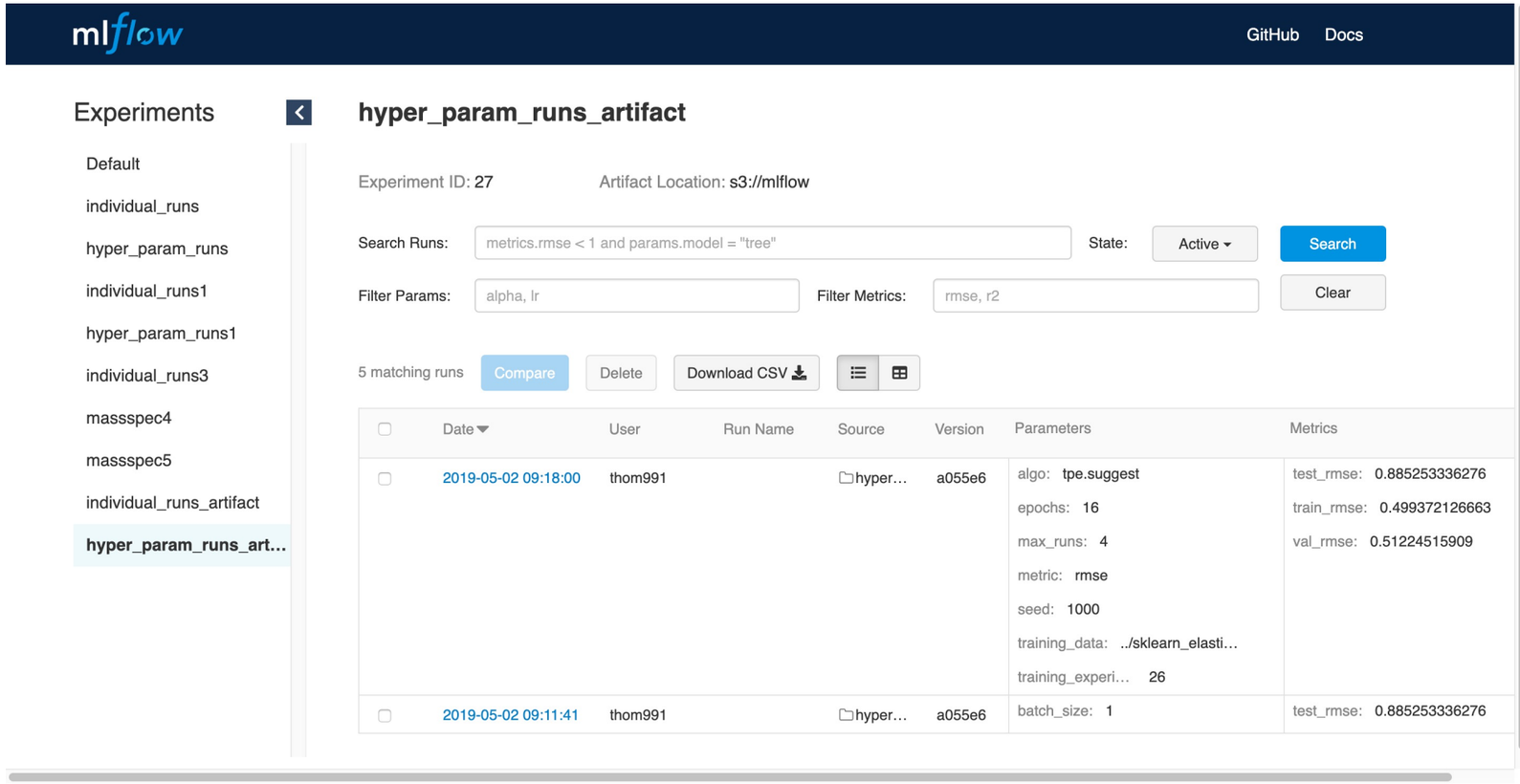


Reproducibility

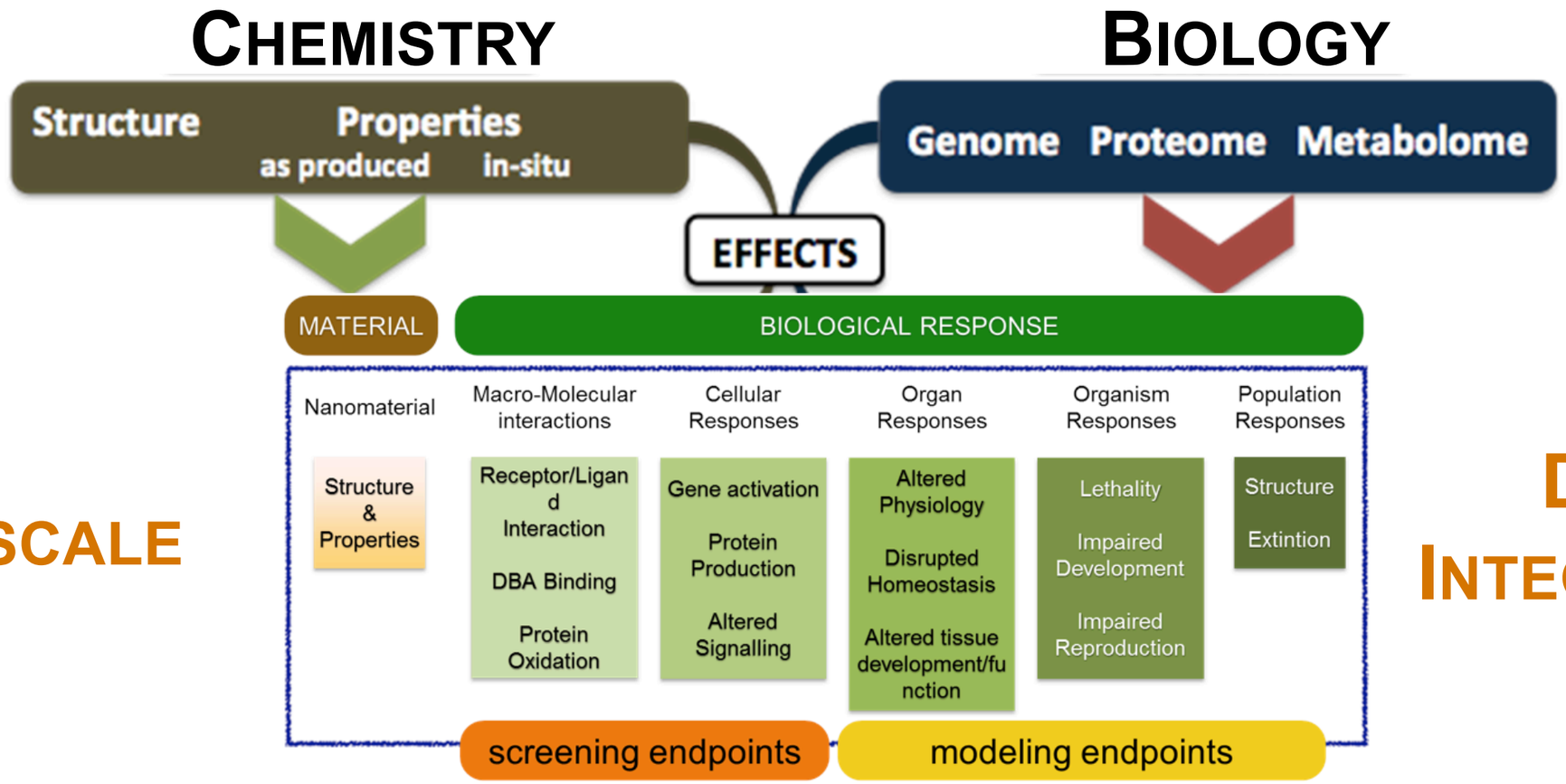
- Provenance tracking in AI/ML workflows

- Metadata on:
  - Task
  - Data
  - Algorithms
  - (Hyper)parameters
  - Performance
- Artifacts
- Packaging
- Deployment





Interpretability: Integrated Domain-informed frameworks



MULTISCALE

DATA INTEGRATION

Multiple levels of biological organization

Roca CP, Rallo R, Fernandez A, Giralt F. Nanoinformatics for Safe-by-Design Engineered Nanomaterials. In *Towards Efficient Designing of Safe Nanomaterials: Innovative Merge of Computational Approaches and Experimental Techniques*, Leszczynski J and Puzyn T (Eds.), 2012, RSC Publishing

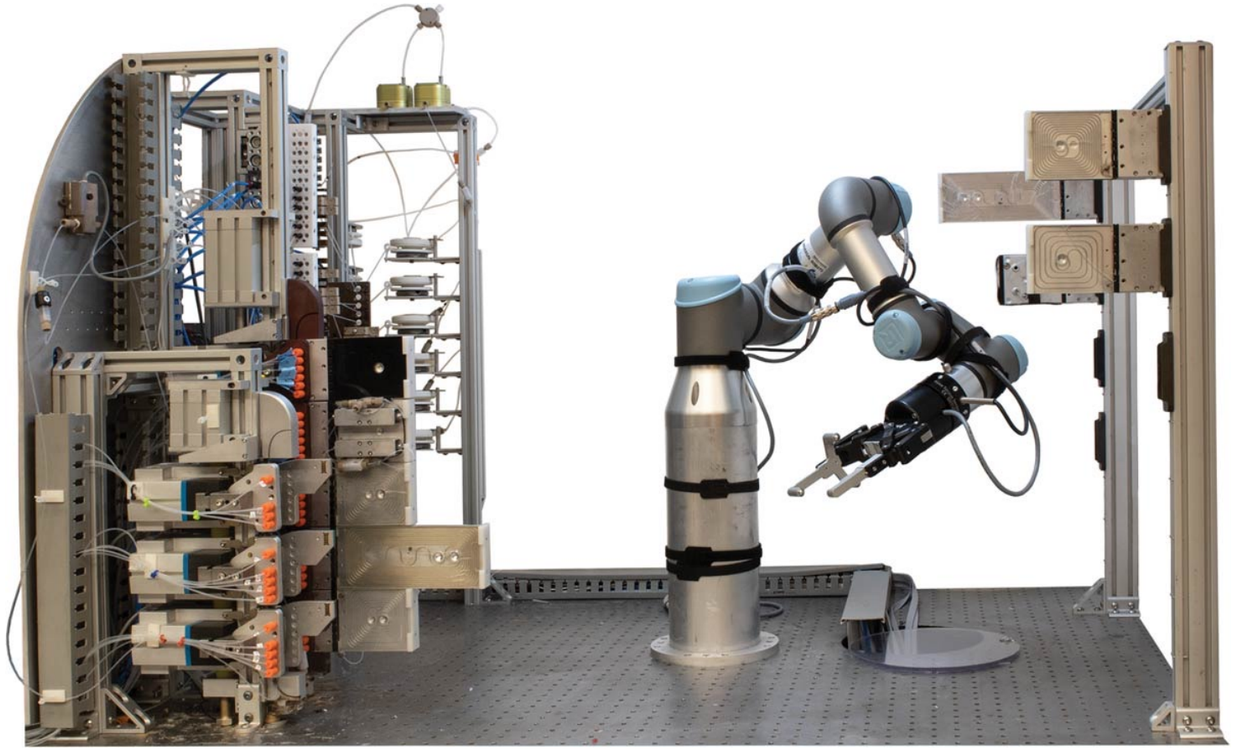
Automation

Interfacing with scientific instruments

- Edge computing for in-situ processing.
- Opportunity to leverage existing real-time control and optimization capabilities.
- Optimal exploration of large combinatorial spaces.

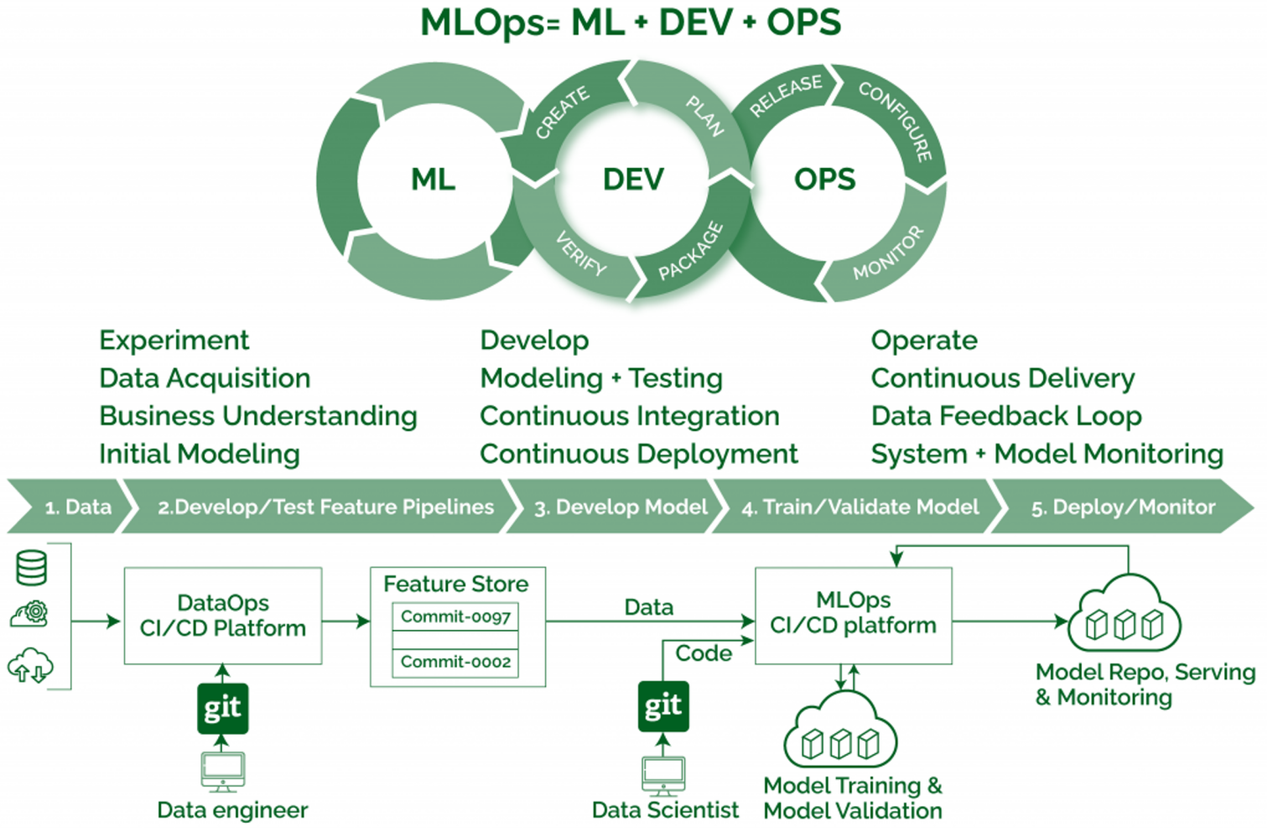
Beyond automation: autonomy

- Hypothesis generation, validation and refinement.
- From machine learning to machine reasoning



Scalability and Deployment

- Rethinking software engineering
  - Composable software systems
  - Heterogeneous computing
- Connecting “Software 1.0” with “Software 2.0”
- Managed and scalable deployment of AI/ML models
  - Lifecycle management
  - Reproducible results
  - Model governance
  - Monitoring and operational use



Adapted from:
[The fundaments of MLOps – The enabler of quality outcomes in production environments]

Summary

Better understanding of bio-nano interactions

Enhanced predictive capabilities

new hypothesis

DISTRIBUTED HIGH-THROUGHPUT COMPUTING

DATA GENERATION
- Synthesis
- Physicochemical characterization

Raw data

DATA MANAGEMENT
- Data Repositories
- Data annotation
- Data quality
- Ontologies
- Provenance
- Data governance

Curated data

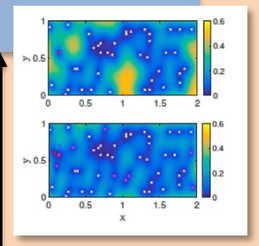
KNOWLEDGE EXTRACTION
- Data mining
- Hypothesis generation

new hypothesis

MATERIALS MODELS

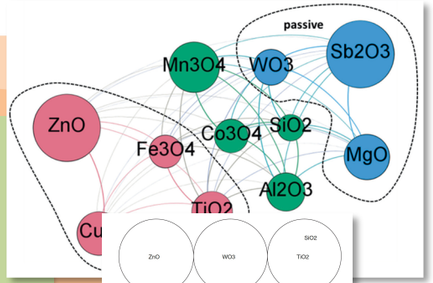
Data-driven
- Machine Learning
- Deep Learning

Simulation
- Multiscale/multiphys
- Multifidelity



Active learning

Optimal design of experiments



SCIENTIFIC COLLABORATION PLATFORM

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Thank you