Unsupervised Machine Learning Based on Non-negative Tensor Factorization for Analysis of Filed Data and Simulation Outputs

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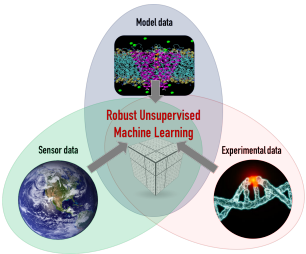

Why unsupervised Machine Learning (ML)?

- **Supervised** ML: requires prior categorization (knowledge) of the processed data **random forest**, **neural networks**, **active**, **reinforcement** learning, ...

  Example: Recognize images of cats and dogs after extensive training; but cannot recognize horses if not trained

- **Unsupervised** ML: extracts hidden features (signals) in the processed data without any prior information (**exploratory analysis** for **data-driven science**)

  Example: Identify features that distinguish images of animals (e.g., cats, dogs, horses, etc.); without prior information or training

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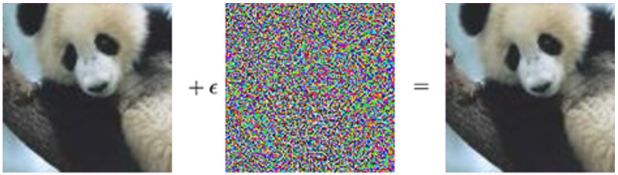
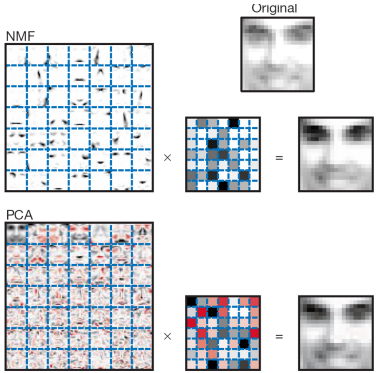
Supervised vs. Unsupervised

Supervised



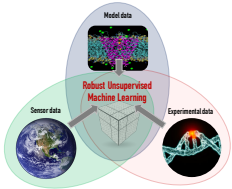
An adversarial input, overlaid on a typical image, can cause a classifier to miscategorize a panda as a gibbon.

Unsupervised

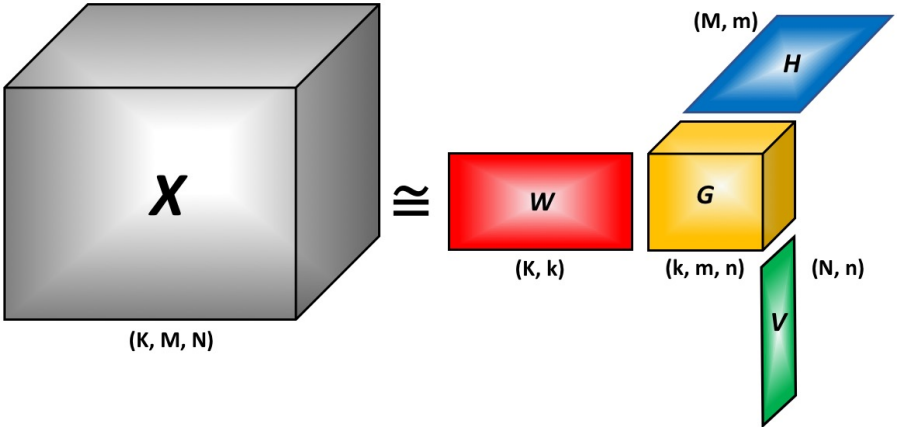


Our Unsupervised Machine Learning Methodology

- We have developed a series of novel Unsupervised Machine Learning methods based on Nonnegative Factorization (Matrix and Tensor) + custom clustering (NMFk / NTFk) that
  - identify **the number of features** (related to the tensor rank) in the data
  - extract **robust features** representing the data
  - extracted features are parts of the data allowing for **intuitive** interpretations
  - applicable to a wide-range of real-world problems (not limited to hydrology)



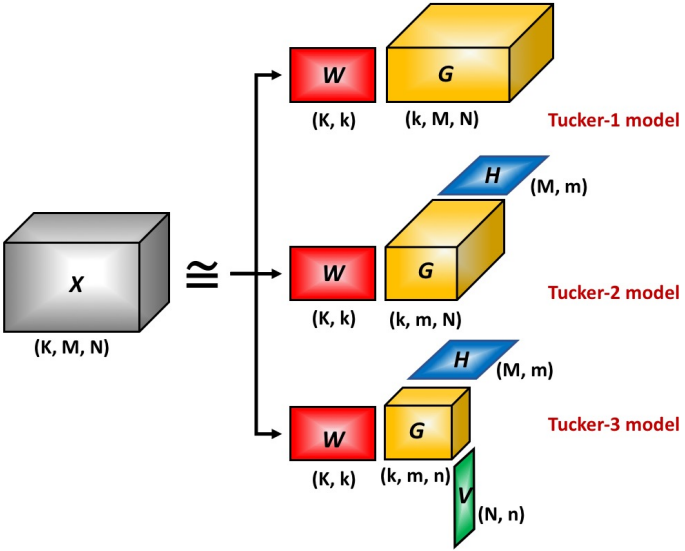
Nonnegative Tucker Tensor factorization (3D Tucker-3)



$X = G \times_k W \times_m H \times_n V$ **Constraints**: G, W, H, V elements ≥ 0

$(K \times M \times N) \rightarrow (k \times m \times n)$ where $K > k$, $M > m$, $N > n$

Nonnegative Tucker Tensor factorization (3D alternatives)



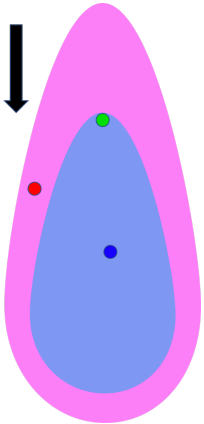
Nonnegative Tensor Factorization (NTFk) Analyses

- **Field Data**: Groundwater contaminant sources ♣ (paper submitted)
- **Lab Data**: X-ray Spectroscopy (paper submitted)
- **Lab Data**: Fluorescence Spectroscopy
- **Model Data**: Reactive mixing $A + B \rightarrow C$ ♣ (paper submitted)
- **Model Data**: Phase separation of co-polymers (paper in preparation)
- **Model Data**: Molecular dynamics of lipids (paper in preparation)
- **Model Data**: Climate model of Europe

Our Recent ML Publications

- Stanev, Vesselinov, Kusne, Antoszewski, Takeuchi, Alexandrov, Unsupervised Phase Mapping of X-ray Diffraction Data by Nonnegative Matrix Factorization Integrated with Custom Clustering, **Nature Computational Materials**, (submitted), 2018.
- Vesselinov, Munuduru, Karra, O'Maley, Alexandrov, Unsupervised Machine Learning Based on Non-Negative Tensor Factorization for Analyzing Reactive-Mixing, **Journal of Computational Physics**, (submitted), 2018.
- Vesselinov, O'Malley, Alexandrov, Nonnegative Tensor Factorization for Contaminant Source Identification, **Journal of Contaminant Hydrology**, (submitted), 2018.
- O'Malley, Vesselinov, Alexandrov, Alexandrov, Nonnegative/binary matrix factorization with a D-Wave quantum annealer, **PLOS ONE**, (submitted), 2018.
- Vesselinov, O'Malley, Alexandrov, Contaminant source identification using semi-supervised machine learning, **Journal of Contaminant Hydrology**, 10.1016/j.jconhyd.2017.11.002, 2017.
- Alexandrov, Vesselinov, Blind source separation for groundwater level analysis based on nonnegative matrix factorization, **WRR**, 10.1002/2013WR015037, 2014.

Geochemistry: ML for extracting contaminant plumes



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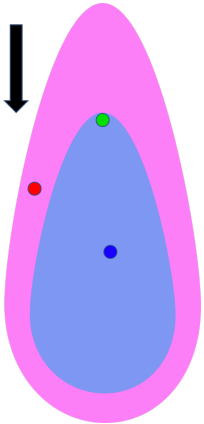

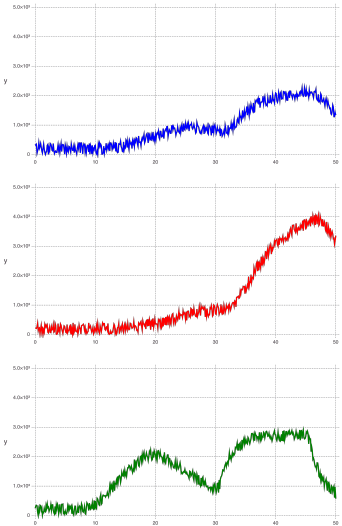

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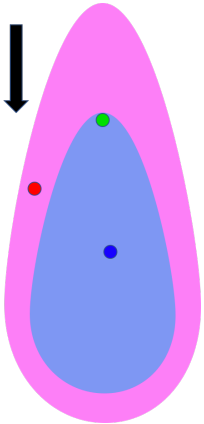
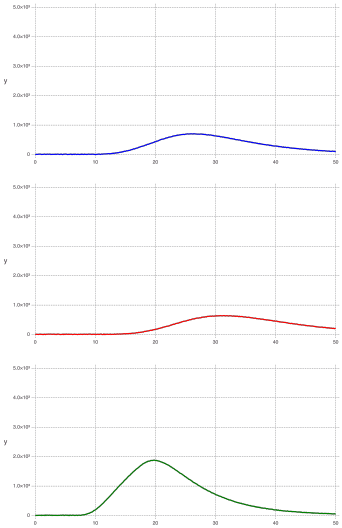
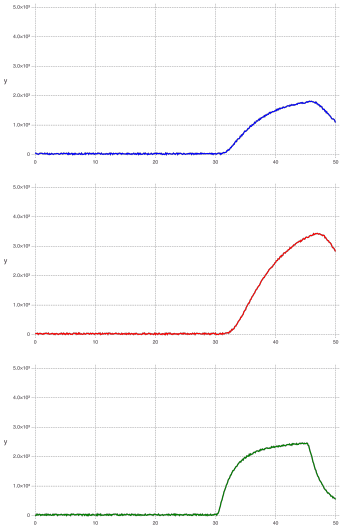
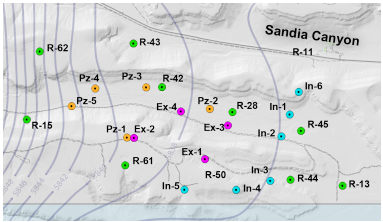


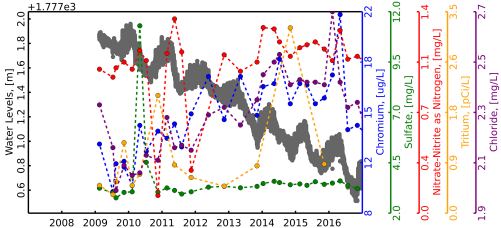




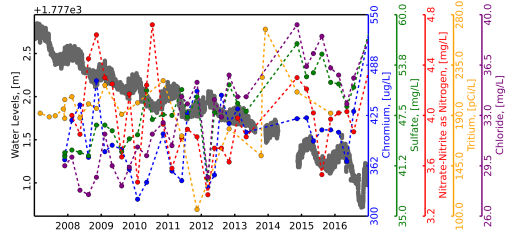
Geochemistry: LANL hydrogeochemical dataset



R-44#1



R-28



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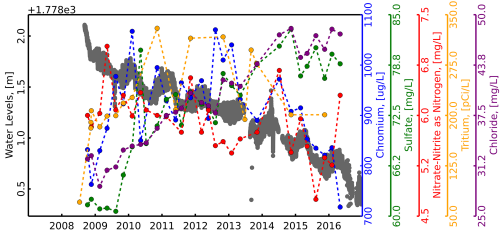
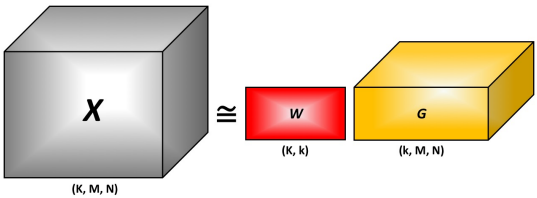


(18 × 8 × 12) tensor ($wells \times species \times years$)

Geochemistry: Nonnegative Tensor Factorization based on Tucker-1 decomposition



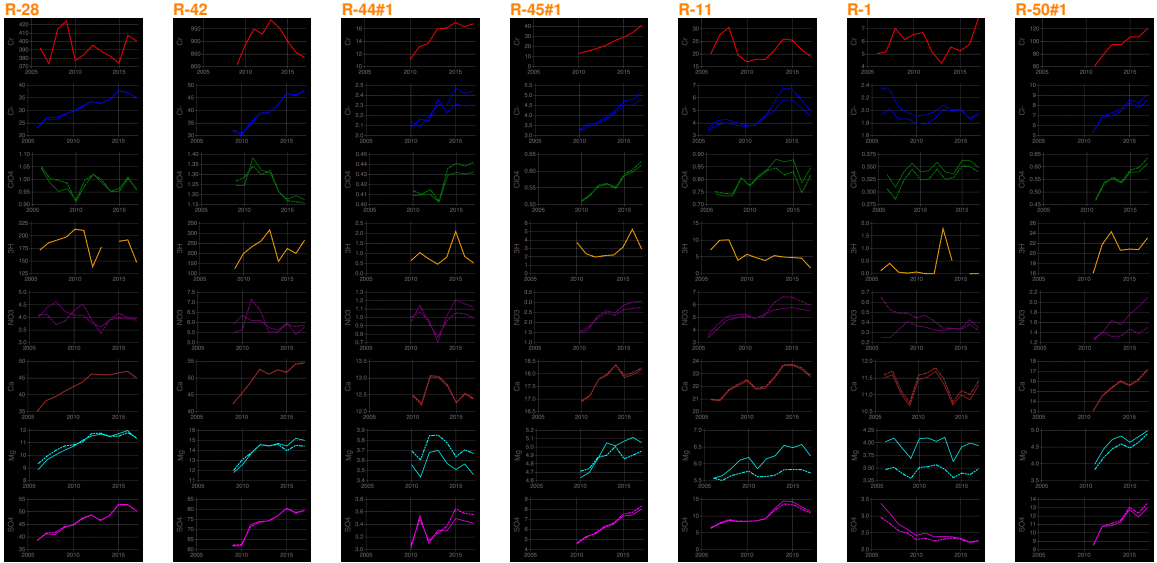
- **X**: data tensor
- **W**: source (groundwater type) matrix (**unknown**)
- **G**: mixing tensor (**unknown**)

- **M**: number of observation points (wells; 18)
- **N**: number of observation times (12: 2005, 2006, ..., 2017)
- **K**: number of geochemical species observed (8: Cr^{6+}, SO_4^{2+}, NO_3^-, etc.)
- **k**: number of **unknown** groundwater types mixed at each well
- **Constraints**:
  all tensor/matrix elements ≥ 0
  $$\sum_{i=1}^{k} G_{i,j,t} = 1 \; \forall j, t$$

NTFk analysis estimated 7 groundwater types

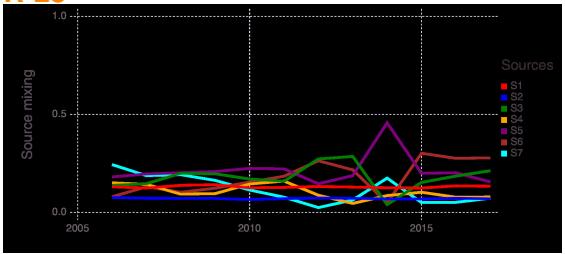
Sources	Cr $(\mu g/L)$	Cl^- (mg/L)	ClO_4 $(\mu g/L)$	^3H (pCi/L)	NO_3 (mg/L)	Ca (mg/L)	Mg (mg/L)	SO_4 (mg/L)
S1	**2970.00**	**63.00**	0.00	0.00	**14.00**	**73.00**	**25.00**	**170.00**
S5	**21.00**	**51.00**	0.00	**950.00**	2.40	**67.00**	15.00	**50.00**
S6	1.50	**64.00**	0.00	0.00	2.80	51.00	10.00	**68.00**
S2	0.79	0.35	**14.00**	0.00	0.50	5.30	1.70	0.60
S4	0.50	0.14	0.00	0.00	**10.00**	21.00	5.00	10.00
S3 (**B**)	0.25	**3.60**	0.00	0.00	0.01	**41.00**	**11.00**	0.06
S7 (**B**)	0.10	0.03	0.00	0.00	0.01	0.40	0.80	0.90

NTFk estimated concentrations at various wells



NTFk estimated time-dependent mixing of 7 groundwater types at various wells

R-28



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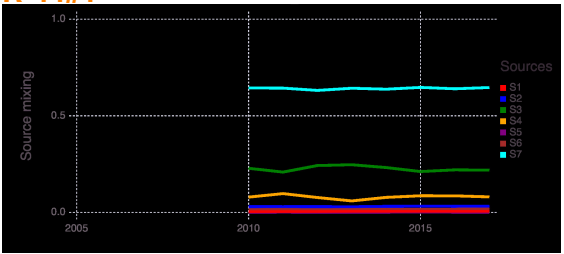
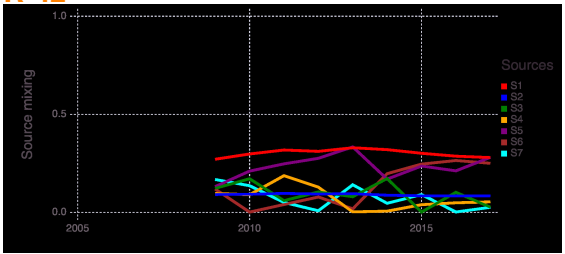


R-42



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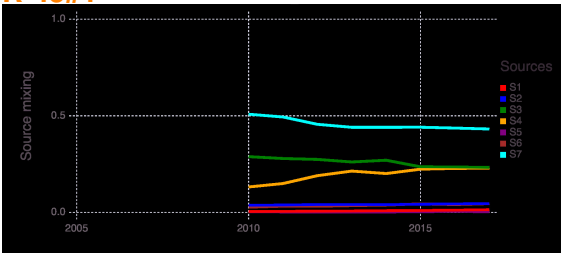
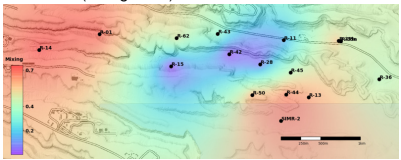
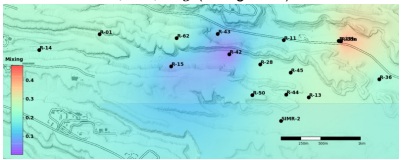


NTFk identified sources (groundwater types) Jan-Dec 2016

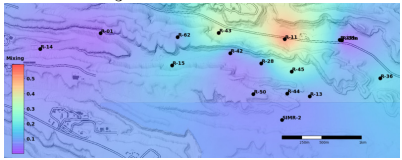
Source 7: (background)



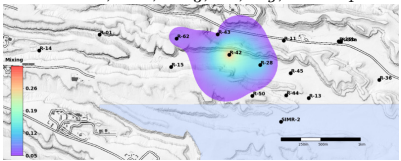
Source 3: Cl^-, Ca, Mg (background)



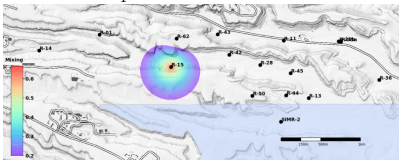
Source 4: NO_3



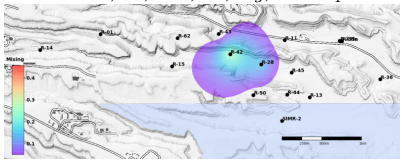
Source 1: Cr, Cl^-, NO_3, Ca, Mg, and SO_4



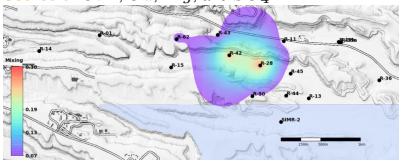
Source 2: ClO_4



Source 5: ^3H, Cr, Cl^-, Ca, Mg, and SO_4

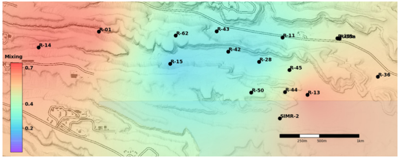


Source 6: Cl^-, Ca, Mg, and SO_4

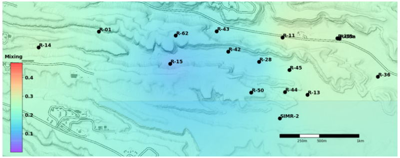


NTFk identified sources (groundwater types) Jan-Dec 2005

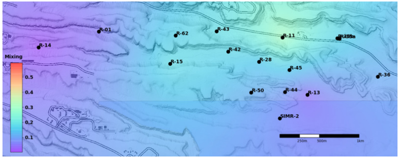
Source 7: (background)



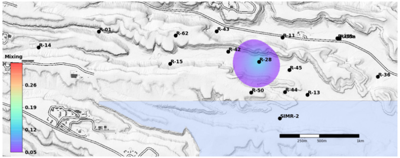
Source 3: Cl^-, Ca, Mg (background)



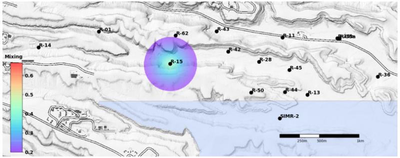
Source 4: NO_3



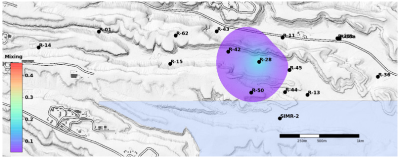
Source 1: Cr, Cl^-, NO_3, Ca, Mg, and SO_4



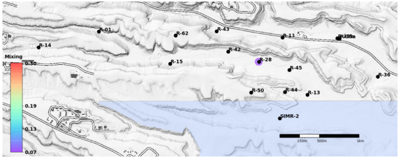
Source 2: ClO_4



Source 5: ^3H, Cr, Cl^-, Ca, Mg, and SO_4



Source 6: Cl^-, Ca, Mg, and SO_4



NTFk identified sources (groundwater types) Jan-Dec 2006

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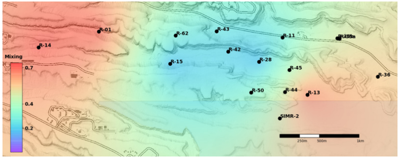
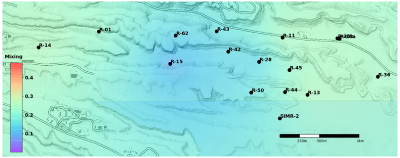
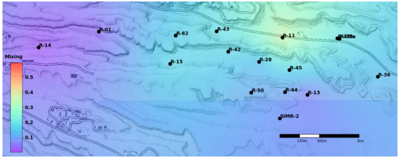


Source 3: Cl^-, Ca, Mg (background)



Source 4: NO_3



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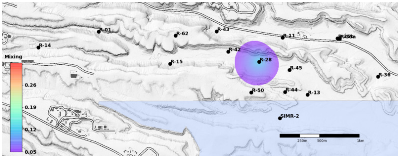
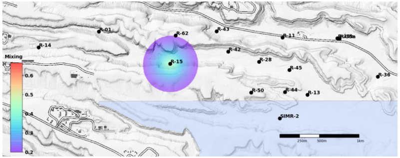
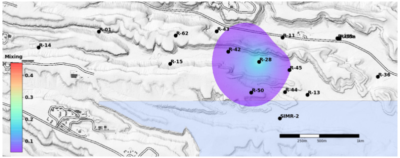


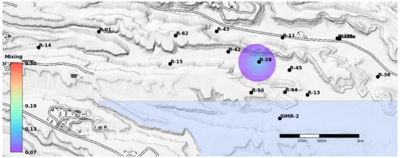
Source 2: ClO_4



Source 5: ^3H, Cr, Cl^-, Ca, Mg, and SO_4

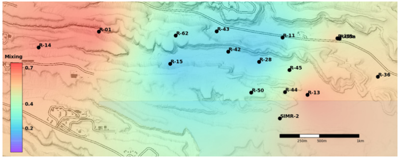


Source 6: Cl^-, Ca, Mg, and SO_4

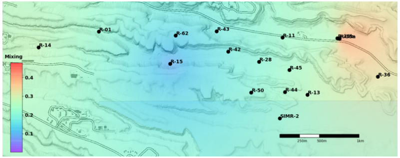


NTFk identified sources (groundwater types) Jan-Dec 2007

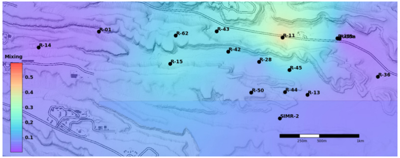
Source 7: (background)



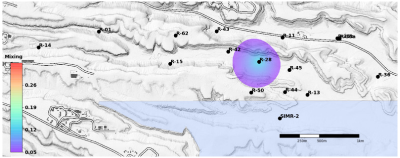
Source 3: Cl^-, Ca, Mg (background)



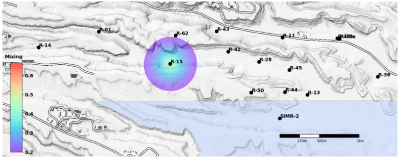
Source 4: NO_3



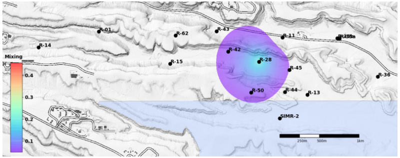
Source 1: Cr, Cl^-, NO_3, Ca, Mg, and SO_4



Source 2: ClO_4



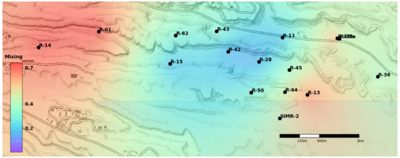
Source 5: ^3H, Cr, Cl^-, Ca, Mg, and SO_4



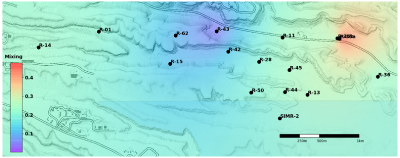
Source 6: Cl^-, Ca, Mg, and SO_4

NTFk identified sources (groundwater types) Jan-Dec 2008

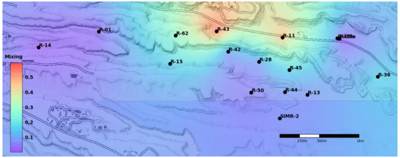
Source 7: (background)



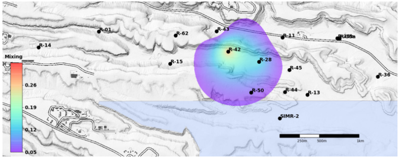
Source 3: Cl^-, Ca, Mg (background)



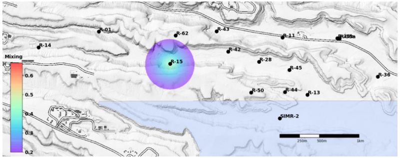
Source 4: NO_3



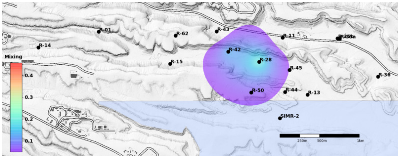
Source 1: Cr, Cl^-, NO_3, Ca, Mg, and SO_4



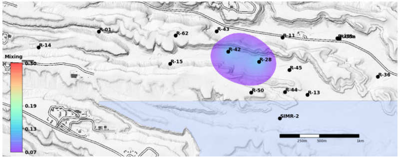
Source 2: ClO_4



Source 5: ^3H, Cr, Cl^-, Ca, Mg, and SO_4

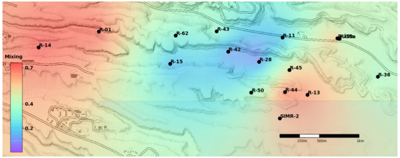


Source 6: Cl^-, Ca, Mg, and SO_4

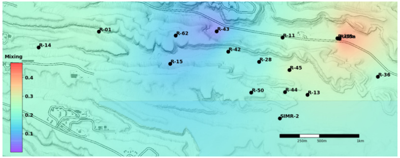


NTFk identified sources (groundwater types) Jan-Dec 2009

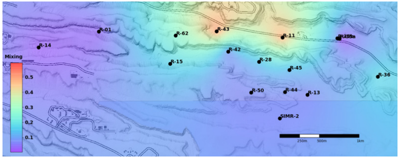
Source 7: (background)



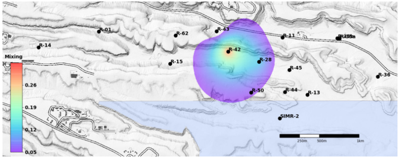
Source 3: Cl^-, Ca, Mg (background)



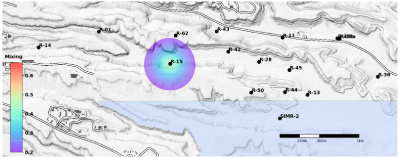
Source 4: NO_3



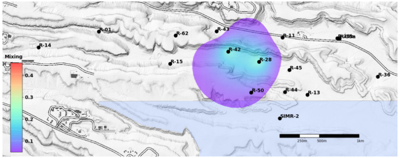
Source 1: Cr, Cl^-, NO_3, Ca, Mg, and SO_4



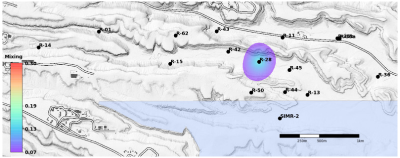
Source 2: ClO_4



Source 5: ^3H, Cr, Cl^-, Ca, Mg, and SO_4

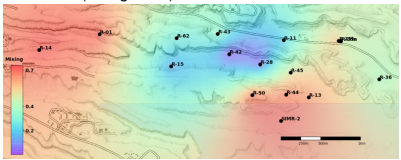


Source 6: Cl^-, Ca, Mg, and SO_4

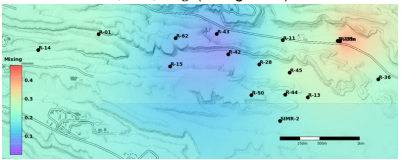


NTFk identified sources (groundwater types) Jan-Dec 2010

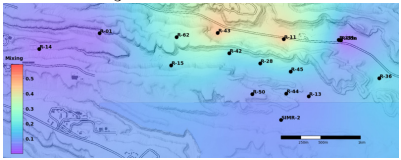
Source 7: (background)



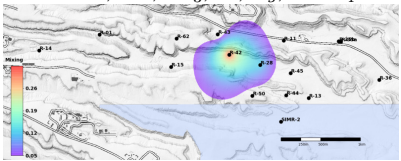
Source 3: Cl^-, Ca, Mg (background)



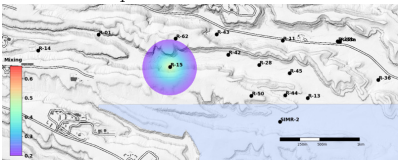
Source 4: NO_3



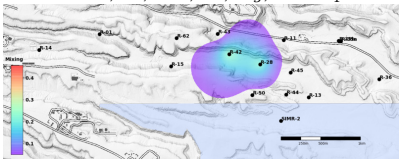
Source 1: Cr, Cl^-, NO_3, Ca, Mg, and SO_4



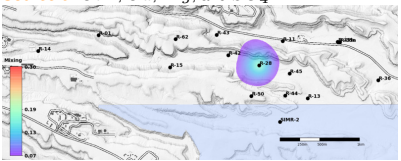
Source 2: ClO_4



Source 5: $^3H, Cr, Cl^-, Ca, Mg$, and SO_4

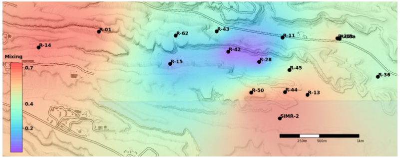


Source 6: Cl^-, Ca, Mg, and SO_4

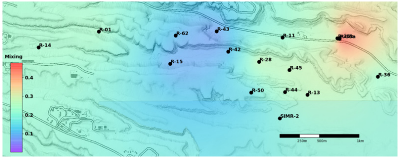


NTFk identified sources (groundwater types) Jan-Dec 2011

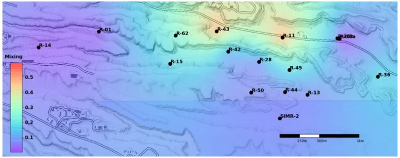
Source 7: (background)



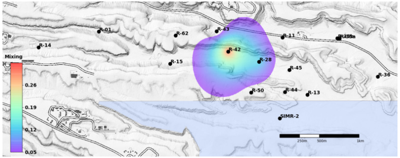
Source 3: Cl^{-}, Ca, Mg (background)



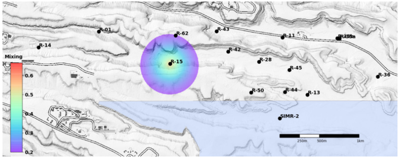
Source 4: NO_3



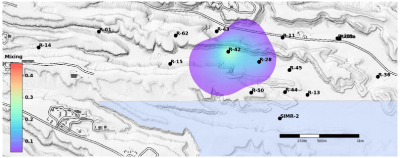
Source 1: Cr, Cl^{-}, NO_3, Ca, Mg, and SO_4



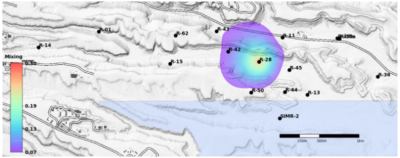
Source 2: ClO_4



Source 5: ^3H, Cr, Cl^{-}, Ca, Mg, and SO_4

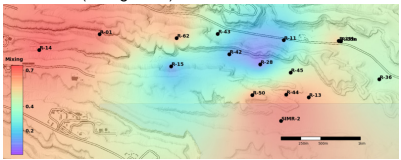


Source 6: Cl^{-}, Ca, Mg, and SO_4

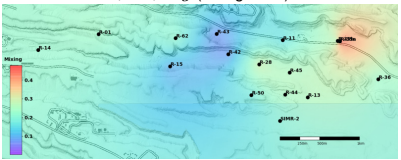


NTFk identified sources (groundwater types) Jan-Dec 2012

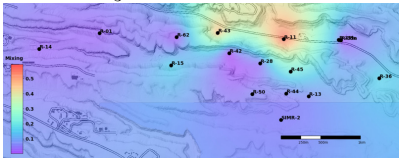
Source 7: (background)



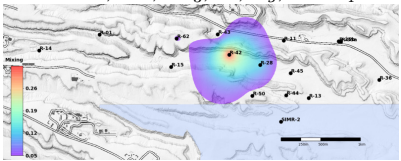
Source 3: Cl^-, Ca, Mg (background)



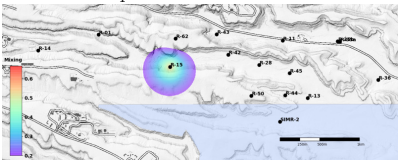
Source 4: NO_3



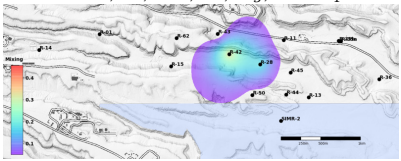
Source 1: Cr, Cl^-, NO_3, Ca, Mg, and SO_4



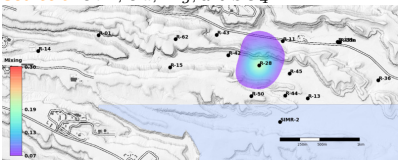
Source 2: ClO_4



Source 5: $^3H, Cr, Cl^-, Ca, Mg$, and SO_4

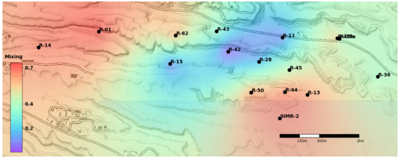


Source 6: Cl^-, Ca, Mg, and SO_4

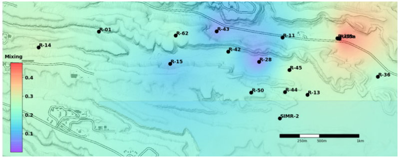


NTFk identified sources (groundwater types) Jan-Dec 2013

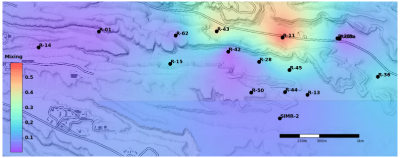
Source 7: (background)



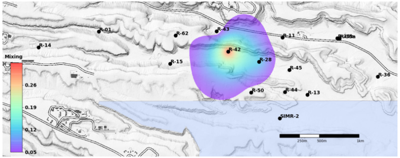
Source 3: Cl^-, Ca, Mg (background)



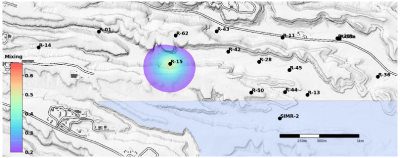
Source 4: NO_3



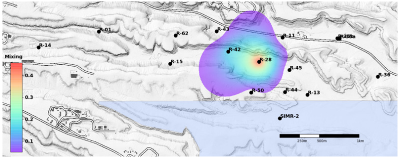
Source 1: Cr, Cl^-, NO_3, Ca, Mg, and SO_4



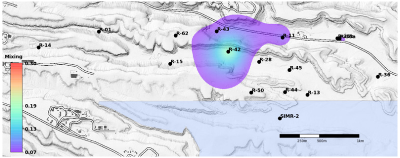
Source 2: ClO_4



Source 5: ^3H, Cr, Cl^-, Ca, Mg, and SO_4

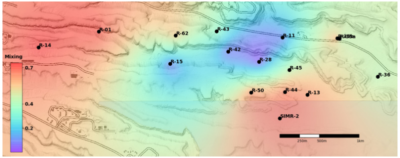


Source 6: Cl^-, Ca, Mg, and SO_4

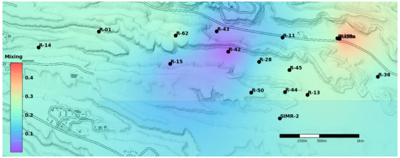


NTFk identified sources (groundwater types) Jan-Dec 2014

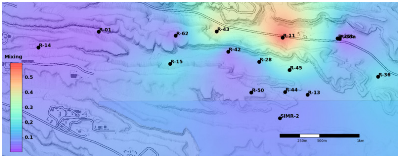
Source 7: (background)



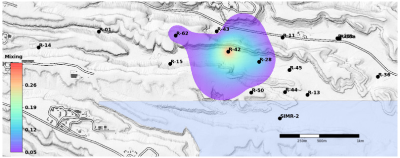
Source 3: Cl^-, Ca, Mg (background)



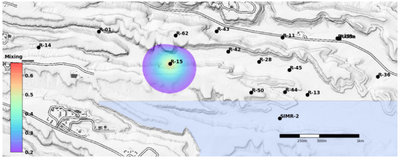
Source 4: NO_3



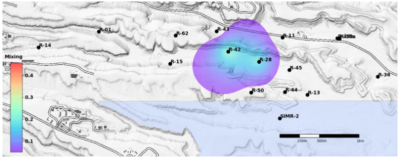
Source 1: Cr, Cl^-, NO_3, Ca, Mg, and SO_4



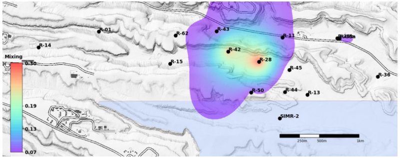
Source 2: ClO_4



Source 5: ^3H, Cr, Cl^-, Ca, Mg, and SO_4

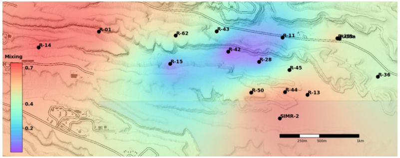


Source 6: Cl^-, Ca, Mg, and SO_4

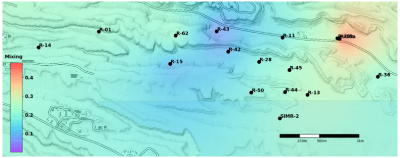


NTFk identified sources (groundwater types) Jan-Dec 2015

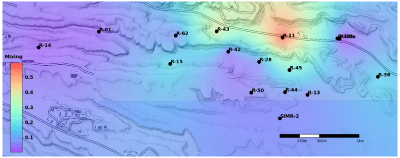
Source 7: (background)



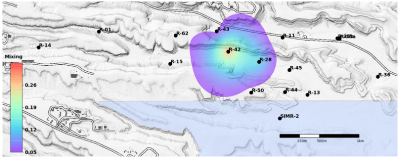
Source 3: Cl^-, Ca, Mg (background)



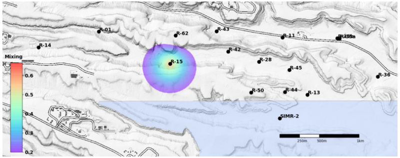
Source 4: NO_3



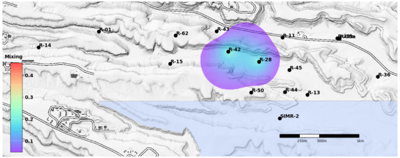
Source 1: Cr, Cl^-, NO_3, Ca, Mg, and SO_4



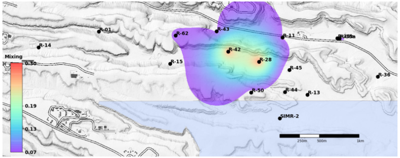
Source 2: ClO_4



Source 5: ^3H, Cr, Cl^-, Ca, Mg, and SO_4

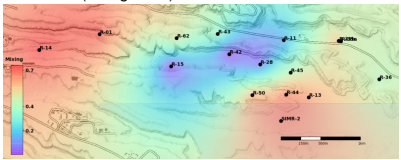


Source 6: Cl^-, Ca, Mg, and SO_4

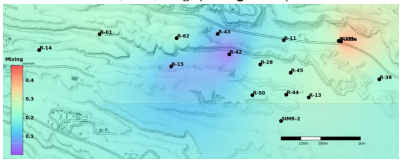


NTFk identified sources (groundwater types) Jan-Dec 2016

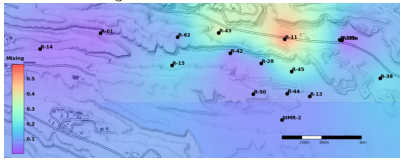
Source 7: (background)



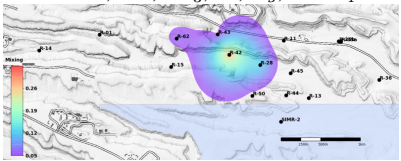
Source 3: Cl^-, Ca, Mg (background)



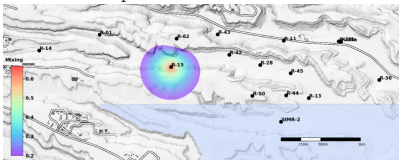
Source 4: NO_3



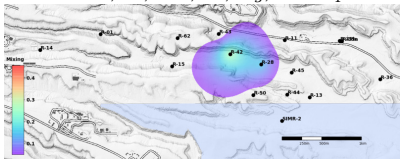
Source 1: Cr, Cl^-, NO_3, Ca, Mg, and SO_4



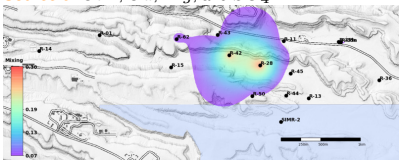
Source 2: ClO_4



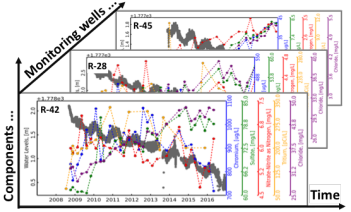
Source 5: ^3H, Cr, Cl^-, Ca, Mg, and SO_4



Source 6: Cl^-, Ca, Mg, and SO_4

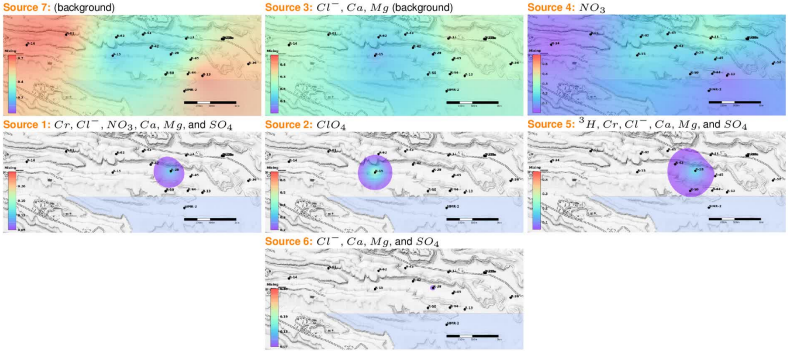


NTFk analysis of LANL hydrogeochemical datasets

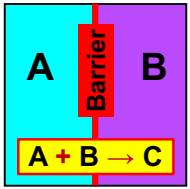


$(18 \times 8 \times 12)$ tensor
$(wells \times species \times years)$

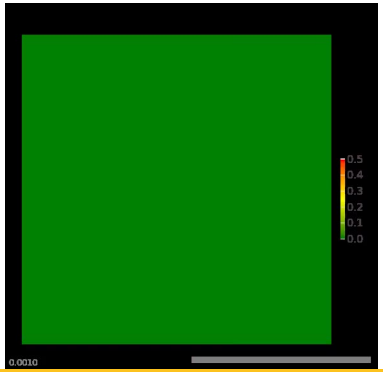
January 2005 – December 2005

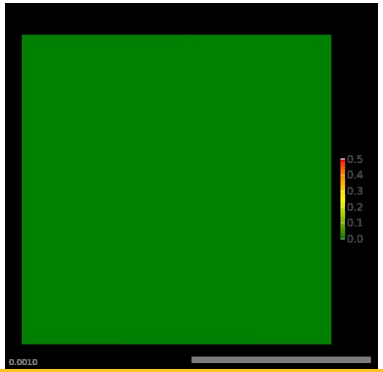


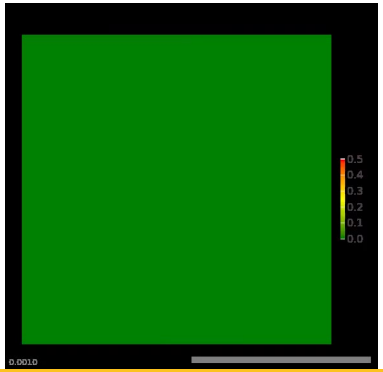
Reactive mixing



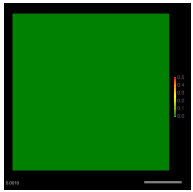
- > 2000 simulations of C concentrations in time/space with varying model inputs representing reactive mixing (5 input model parameters)
- **NTF**k identifies physics processes impacting C concentrations and their relationship to model inputs



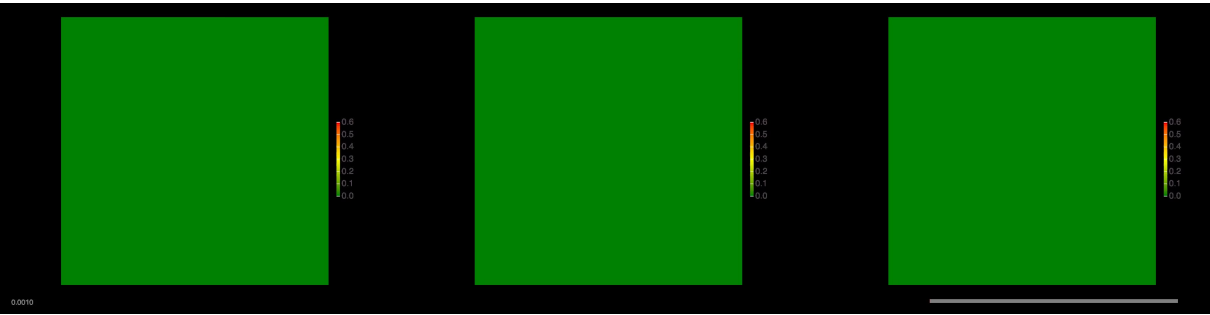




Reactive mixing: NTFk results

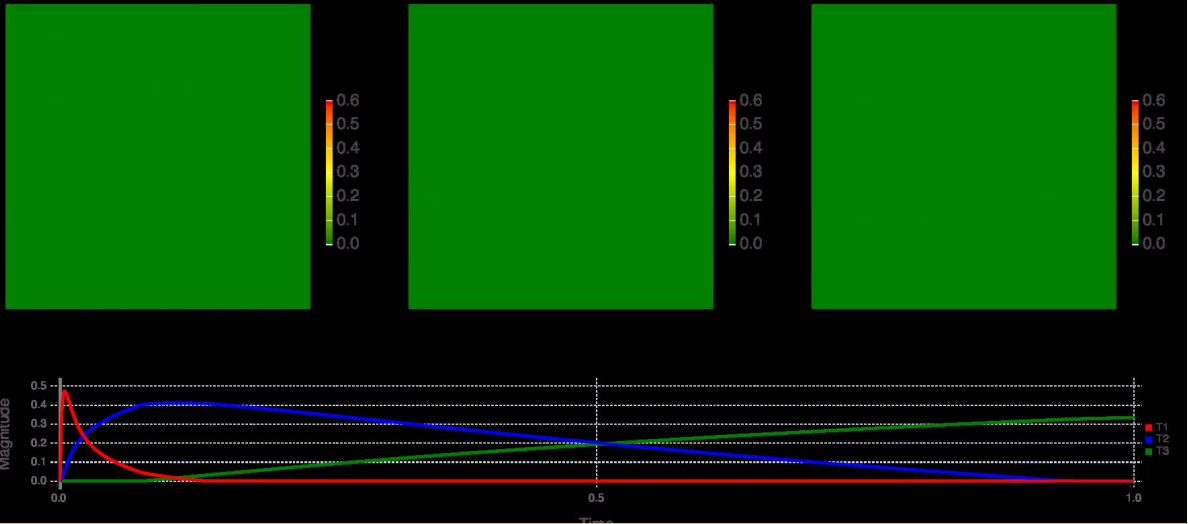


- NTFk extracts the dominant time/space features (**processes** / **vortices**) and compresses the model outputs
- Compression: > 200GB $\rightarrow \sim 70$MB (ratio ~ 3000
  Here, $(1000 \times 81 \times 81) \rightarrow (3 \times 12 \times 13)$ $(time \times rows \times columns)$



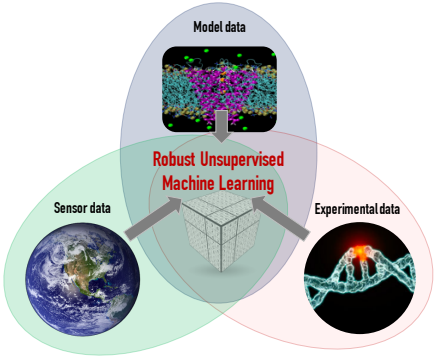
Advection **Dispersion** **Diffusion**

Reactive mixing: NTFk results



Summary

- Developed **novel** unsupervised ML methods and computational tools based on Nonnegative Factorization (Matrices/Tensors)
- Our ML methods have been used to solve various real-world problems (brought breakthrough discoveries related to human cancer research)
- Our goal is to extend the ML methods and tools to solve big ($>$ terabyte-scale) high-dimensional (> 5) data



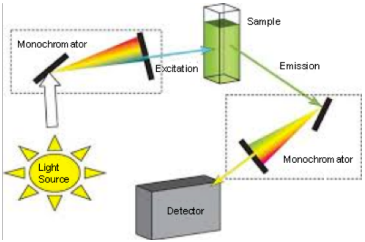
Machine Learning (ML) Algorithms / Codes developed by our team

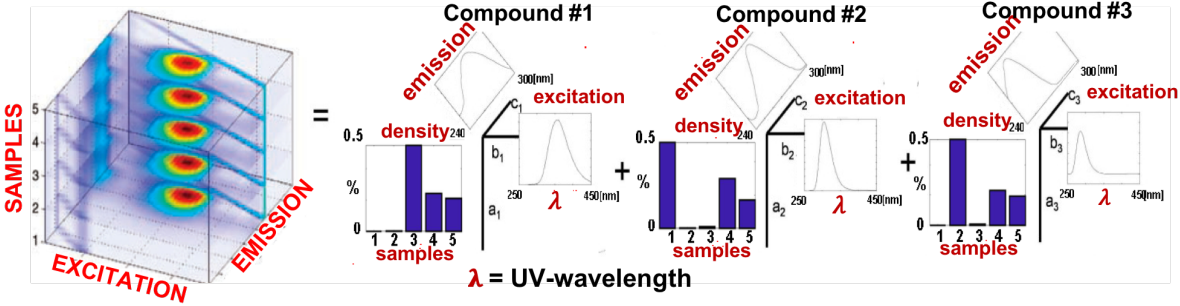
- NMFk + ShiftNMFk + GreenNMFk **(patent)**
- NTFk **(copyright disclosure)**
- NBMF: Quantum machine learning using **D-Wave** **(paper in review)**
- MADS: Model-Analyses & Decision Support
  open-source, version-controlled, high-performance computational framework
  `http://mads.lanl.gov` `http://madsjulia.github.io/Mads.jl`

- Blind Source Separation examples:
  `http://madsjulia.github.io/Mads.jl/Examples/blind_source_separation`

Fluorescence Spectroscopy

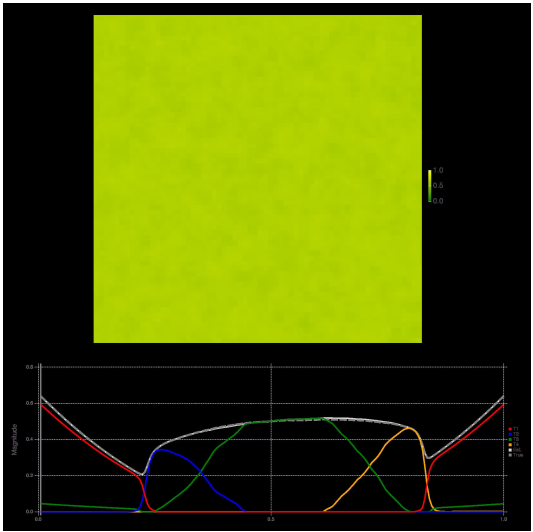
- 5 cuvettes (samples) with unknown mixtures of 3 unknown compounds
- Emissions and excitations measured ($5 \times 250 \times 200$ tensor)
- **NTF**k identifies the mixing ratios of the compounds and their characteristic spectra





Polymer-chain folding

- polymer transitions between different states
- **NTF**k extracts phase-transition stages
- $(201 \times 64 \times 64 \times 3) \rightarrow (5 \times 12 \times 12 \times 1)$
  $(state \times rows \times columns \times phases)$



« Play/Pause