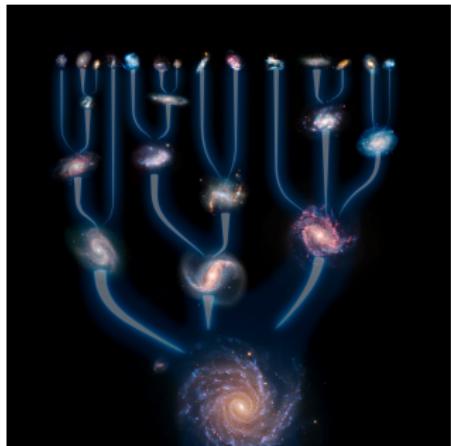


Unveiling the Milky Way's Formation History: Resolving Chemo-Dynamical Substructures in APOGEE and GALAH

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Galactic Archaeology's Motivation



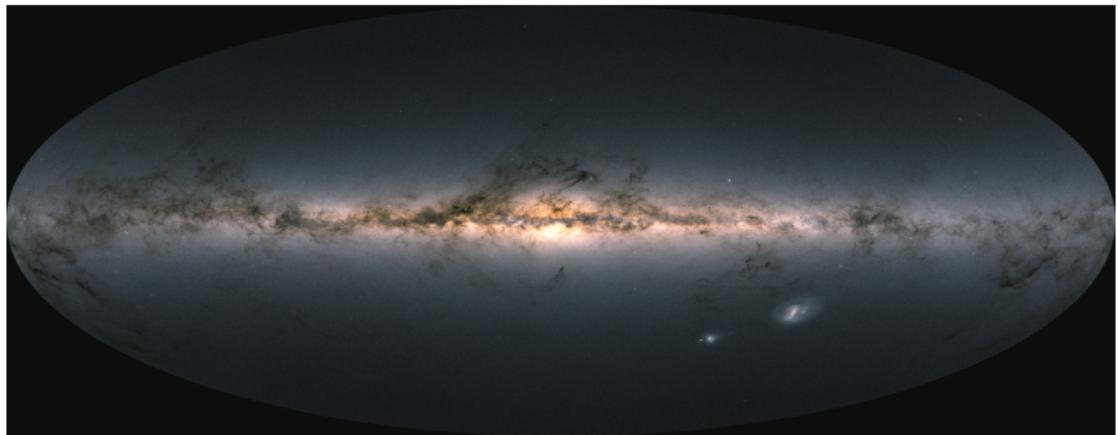
Credit: ESO/L. Calçada

- ▶ Uncovering hierarchical galaxy formation.
- ▶ Complements higher redshift galaxy formation surveys.
- ▶ Probe the Λ CDM model and dark matter distribution.

Merger Type	Number	Mass Ratio
Minor Mergers	~30	1:3 – 1:100
Major Mergers	~3	>1:3

N-Body Simulations from Fakhouri et al. (2010)

The Era of ‘Big Data Astronomy’



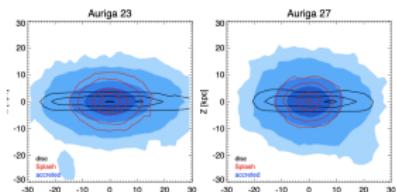
Credit: ESA/Gaia/DPAC, A. Moitinho.

Survey	Gaia EDR3	APOGEE	GALAH
Focus	Astrometry, Photometry	IR spectroscopy	Optical spectroscopy
Sources	$\sim 1.4 \times 10^9$	$\sim 734,000$	$\sim 918,000$

The Evolving Picture

Splash

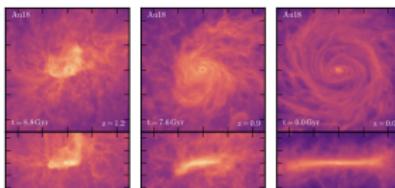
- ▶ Proto-disk population (pre-GS/E)
- ▶ Gravitational perturbations of orbits



Credit: V. Belokurov et al. (2020)

Eos

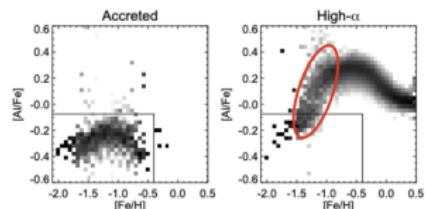
- ▶ GS/E triggered star formation
- ▶ Gas from thick disk and GS/E polluted gas
- ▶ Evolves into outer thin disk



Credit: R. Grand et al. (2020)

Aurora

- ▶ Near isotropic velocity distribution
- ▶ Ancient pre-disk/ spin-up population
- ▶ Rapid star formation/ self-enrichment



Credit: Belokurov et al. (2022)

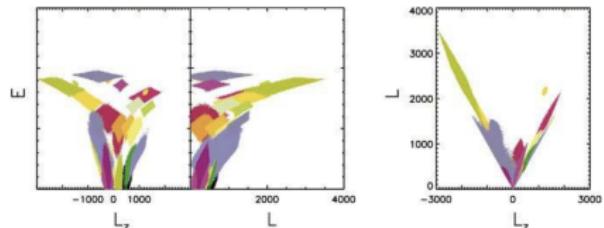
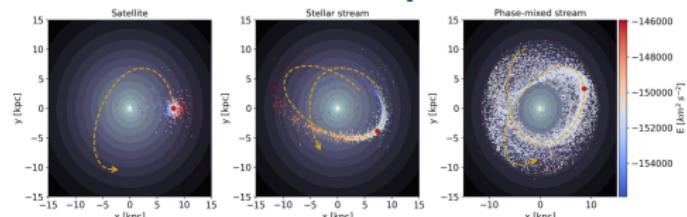
Unbiased Detection of Halo Substructures

Goal:

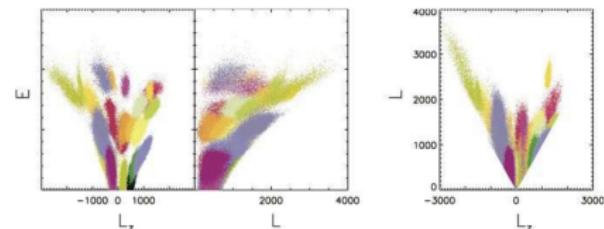
- ▶ Unbiased Decomposition of the Milky Way's Halo's (stellar neighbourhood) Substructures.
- ▶ **Approach:**
 - ▶ Ensure the reproducibility of Myeong et al. (2022).
 - ▶ Apply dimensionality reduction to provide insights into clustering stability.
 - ▶ Alternative clustering approaches to improve the convergence and computational efficiency.

Integral of Motion Space

Traditional 6D Phase Space:



(a) Initial distribution of simulated merger events



(b) Distribution after 12 Gyr (with observational errors)

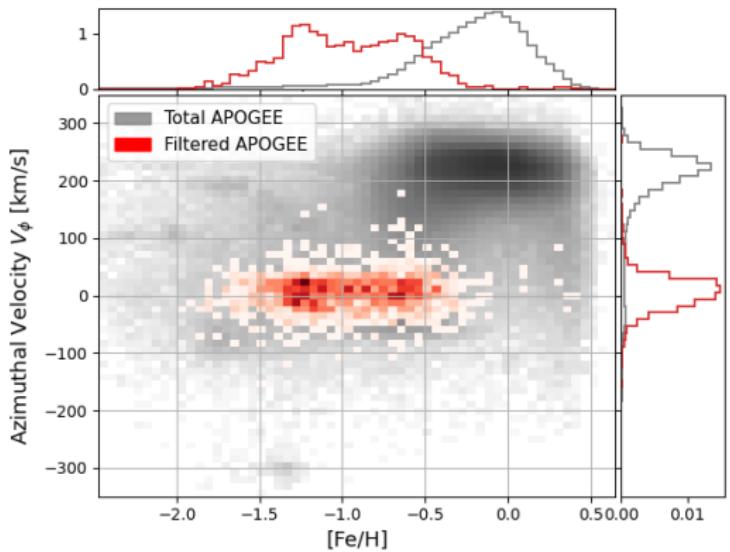
Credit: Helmi et al. (2000)

- Adiabatic invariant
- \approx constant over evolution

For axisymmetric potentials:

Symbol	Description
E	Orbital energy
L_z	Angular momentum (along z -axis)
L	Angular momentum (Total, quasi-conserved)

Biases of Halo Selection

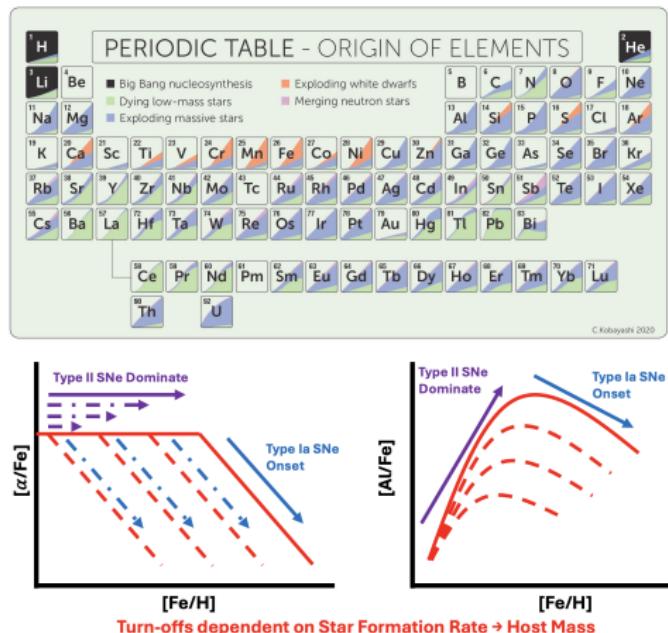


Dynamical Cuts:

- ▶ Eccentricity, $e > 0.85$
- ▶ Apocenter, $> 5\text{kpc}$
- ▶ Energy, $< 0\text{km}^2\text{s}^{-2}$

Chemical Tagging

Credit: Kobayashi et al. (2020)



Insights from Chemical Abundances

- ▶ Probe star formation environment (ISM)
- ▶ Trace nucleosynthetic sources (e.g. SNe, AGB)
- ▶ Reflect rates of:
 - ▶ Star formation
 - ▶ Self-enrichment
- ▶ Link to host galaxy mass (IMF)

Data Acquisition

APOGEE

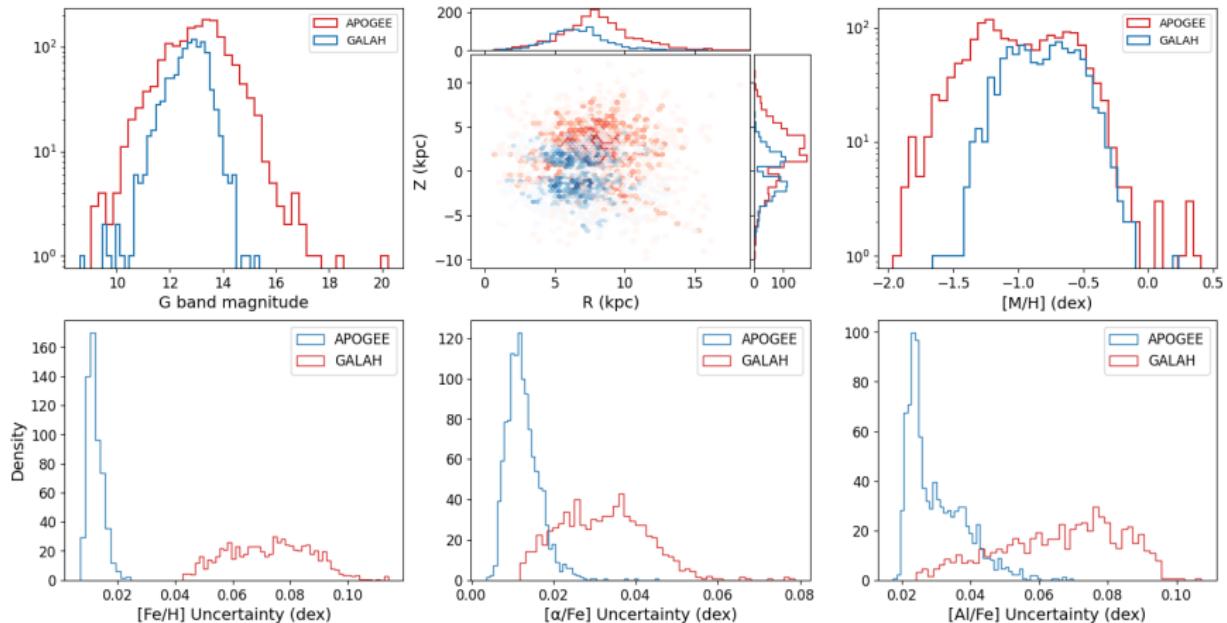
- ▶ **Sample Size:** 1612
- ▶ **Dimensions:** Energy, [Fe/H], [α /Fe], [Al/Fe], [Ce/Fe], [Mg/Mn]

GALAH

- ▶ **Sample Size:** 1061
- ▶ **Dimensions:** Energy, [Fe/H], [α /Fe], [Na/Fe], [Al/Fe], [Mn/Fe], [Y/Fe], [Ba/Fe], [Eu/Fe], [Mg/Cu], [Mg/Mn], [Ba/Eu]

Group	Elements	Traces
Iron-peak	Fe, Mn, Ni	Overall Metallicity - Type Ia and II SNe
α -elements	Mg, Si, Ca, Ti	Core-collapse (Type II) SNe
Odd-Z elements	Na, Al	Similar Core-collapse (Type II) SNe
s-process	Y, Ba, Ce	Slow neutron capture - AGB stars
r-process	Eu	Neutron star mergers/ Rare CC-SNe

Dataset Comparison



Extreme Deconvolution

The latent distribution of true values \mathbf{v} is modeled as a mixture of K Gaussians:

$$p(\mathbf{v}) = \sum_{j=1}^K \alpha_j \mathcal{N}(\mathbf{v} | \mathbf{m}_j, \mathbf{V}_j), \quad (1)$$

Likelihoods of noisy observations \mathbf{w}_i are computed by marginalising over \mathbf{v} :

$$p(\mathbf{w}_i | \theta) = \sum_j \int d\mathbf{v} p(\mathbf{w}_i | \mathbf{v}) p(\mathbf{v}|j, \theta) p(j|\theta). \quad (2)$$

Where:

$$p(\mathbf{w}_i | \mathbf{v}) = \mathcal{N}(\mathbf{w}_i | \mathbf{v}, \mathbf{S}_i), \quad (3)$$

$$p(\mathbf{v}|j, \theta) = \mathcal{N}(\mathbf{v} | \mathbf{m}_j, \mathbf{V}_j), \quad (4)$$

$$p(j|\theta) = \alpha_j. \quad (5)$$

Credit: Bovy et al (2011)

- ▶ \mathbf{w}_i : observed (noisy) data point
- ▶ \mathbf{v} : latent true value
- ▶ \mathbf{S}_i : noise covariance of \mathbf{w}_i
- ▶ α_j : mixture weight for component j
- ▶ \mathbf{m}_j : mean of Gaussian component j
- ▶ \mathbf{V}_j : covariance of component j

Extreme Deconvolution

As a result, the total likelihood of \mathbf{w}_i simplifies to another mixture of Gaussians:

$$p(\mathbf{w}_i | \theta) = \sum_j \alpha_j \mathcal{N}(\mathbf{w}_i | \mathbf{m}_j, \mathbf{T}_{ij}), \quad (6)$$

where the effective covariance \mathbf{T}_{ij} accounts for both the Gaussian component and the measurement uncertainty:

$$\mathbf{T}_{ij} = \mathbf{V}_j + \mathbf{S}_i. \quad (7)$$

The log-likelihood across all N data points becomes:

$$\phi = \sum_i \ln p(\mathbf{w}_i | \theta) = \sum_i \ln \sum_{j=1}^K \alpha_j \mathcal{N}(\mathbf{w}_i | \mathbf{m}_j, \mathbf{T}_{ij}). \quad (8)$$

Credit: Bovy et al (2011)

Extreme Deconvolution Pipeline

1. Unbiased component optimisation (AIC/BIC):

$$\text{AIC} = 2k - 2 \ln \mathcal{L}, \quad \text{BIC} = k \ln n - 2 \ln \mathcal{L}$$

where:

- ▶ k : number of free parameters
- ▶ n : number of data points
- ▶ \mathcal{L} : maximum likelihood

2. Scaling schemes:

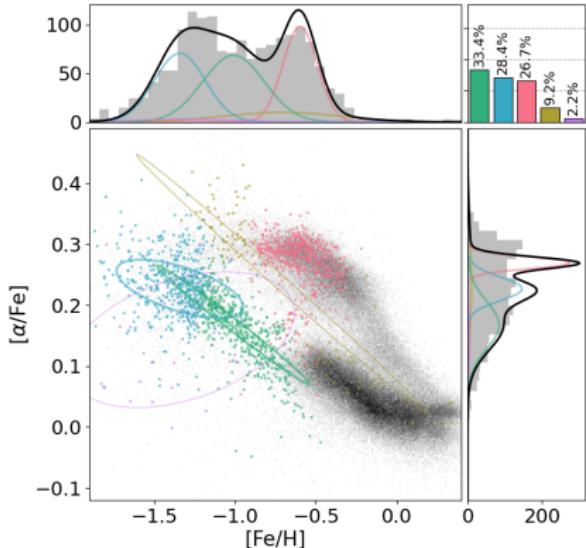
- 2.1 Rescale energy by 10^5 to match other dimensions
- 2.2 Standard normal scaling applied to all features

3. Added functionality to XD:

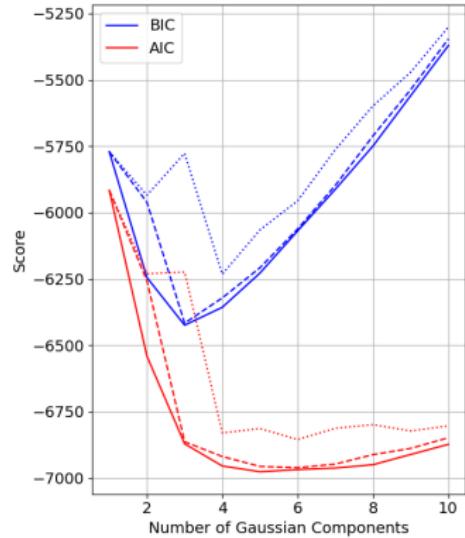
- ▶ Automatic probabilistic assignment
- ▶ Automated model selection and initialisation convergence via AIC/BIC

Extreme Deconvolution Pipeline

Motivation of Scaling Scheme

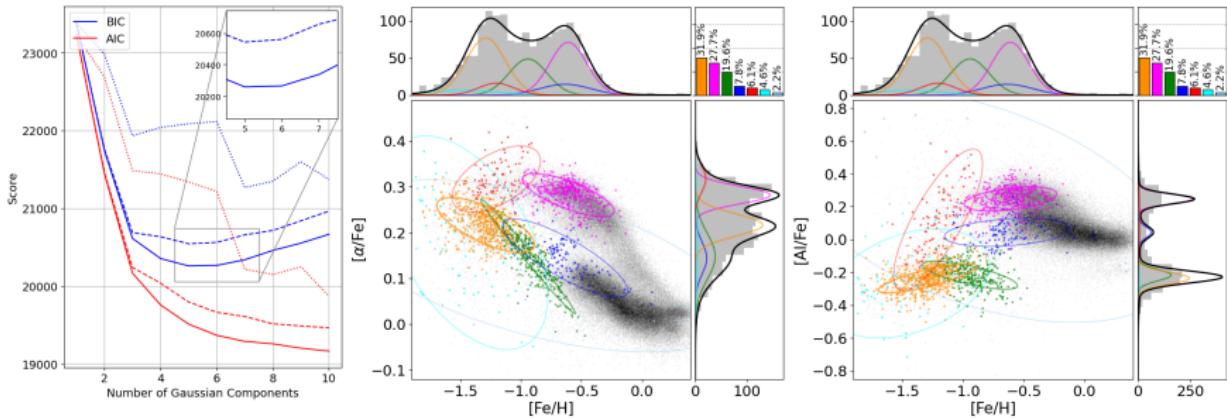


Unscaled XD Clustering Results in $[Fe/H]$ -
 $[\alpha/Fe]$ Plane



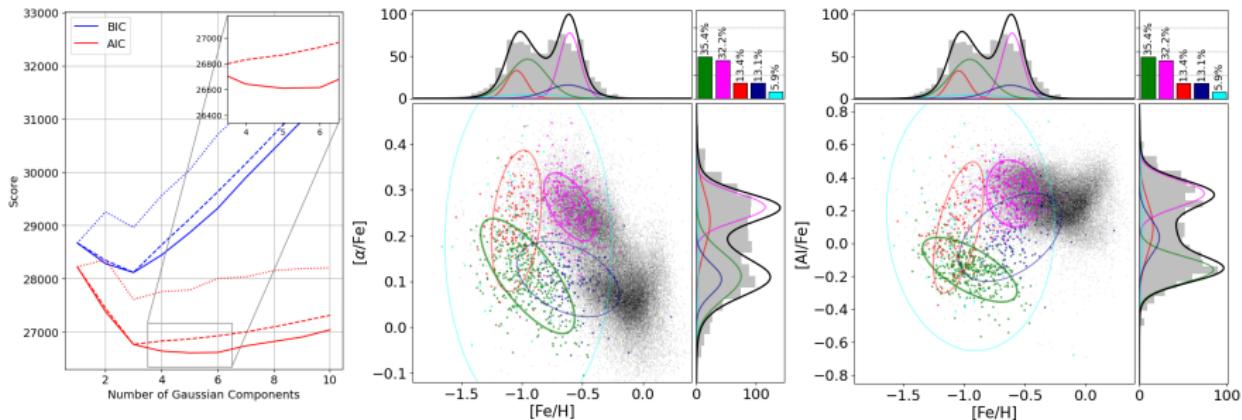
Unscaled XD Clustering
Quantitative Model Comparison

Extreme Deconvolution - APOGEE



- Subtle BIC Discrepancy with original work (favouring 5 over 7)
- ‘Loss’ of Aurora (Red) Detection in 5 Component Model
- Trivial differences between GS/E (Green/Orange) split

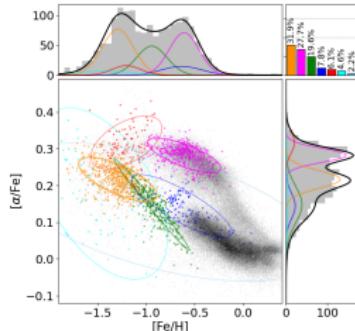
Extreme Deconvolution - GALAH



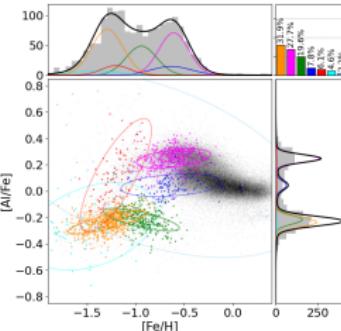
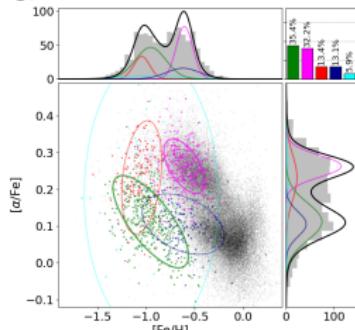
- ▶ AIC providing correct isolation of 5 gaussian components
- ▶ ‘Exact’ agreement with original work

Key Scientific Recoveries: GS/E Merger

APOGEE



GALAH



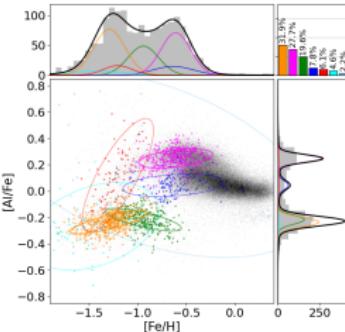
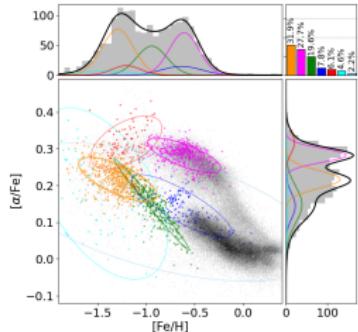
Singular Accreted Component

- ▶ Early α knee turnoff
- ▶ Low [Al/Fe] turning point
- ▶ Trends resembles low mass/ SFR progenitor
- ▶ Fractional weighting 51%
→ consistent with
V. Belokurov et al
2018
- ▶ GALAH's high metallicity limit → smaller weighting
and lack of plateau split

GS/E Eos Aurora Splash

Key Scientific Recoveries: Splash

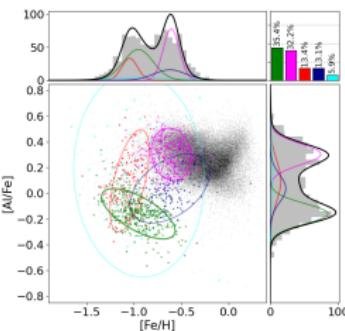
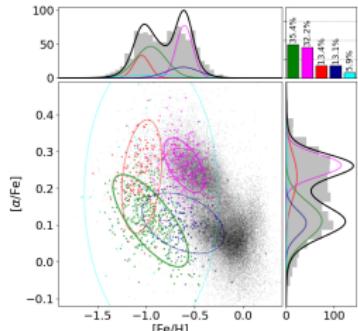
APOGEE



Splash

- ▶ Dominant metal rich component ($[Fe/H] \approx -0.7$)
- ▶ Thick disk like chemistry
- ▶ 'Splashed' out proto-disk from GS/E

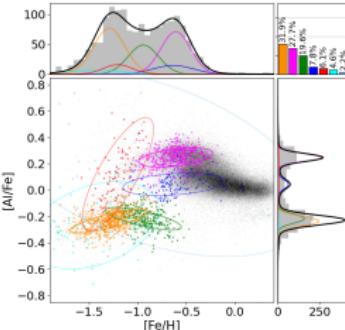
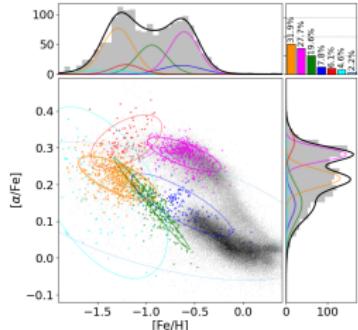
GALAH



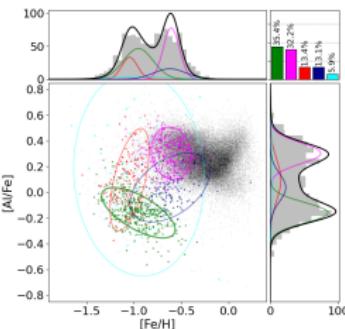
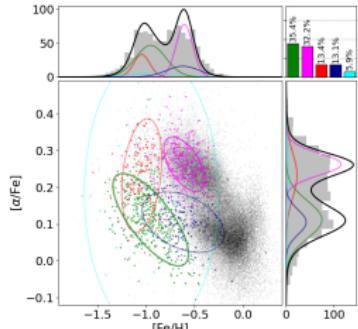
◀ GS/E □ Eos ▢ Aurora ▨ Splash

Key Scientific Recoveries: Aurora

APOGEE



GALAH

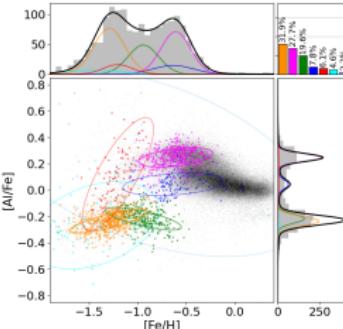
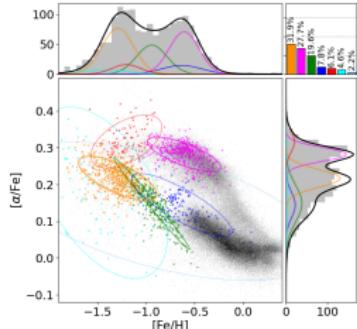


Aurora

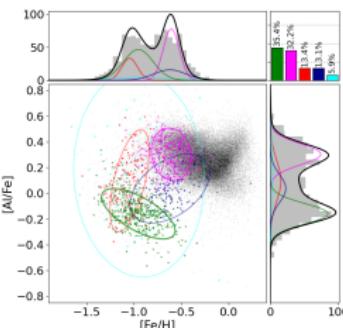
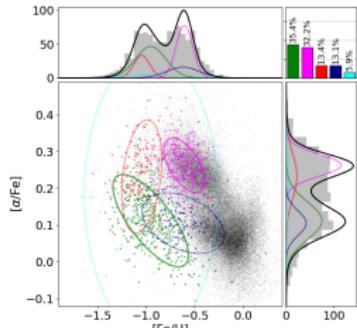
- ▶ Highly correlated planes: $[\alpha/\text{Fe}]\text{-}[\text{Fe}/\text{H}]$ and $[\text{Al}/\text{Fe}]\text{-}[\text{Fe}/\text{H}]$
- ▶ Ancient rapidly enriching population - early life in a large mass system
- ▶ Early pre-disk MW population

Key Scientific Recoveries: Eos

APOGEE



GALAH



Eos

- ▶ Chemically residing between the GS/E population and thin disk
- ▶ Born in gas polluted by GS/E merger and thick disk
- ▶ Evolves into the thin outer disk

Dimensionality Reduction

Goals:

- ▶ Investigate the cohesion and isolation of the substructures identified during high-dimensional clustering
- ▶ Understand sensitivity of Aurora's detection.

Dimensionality Reduction

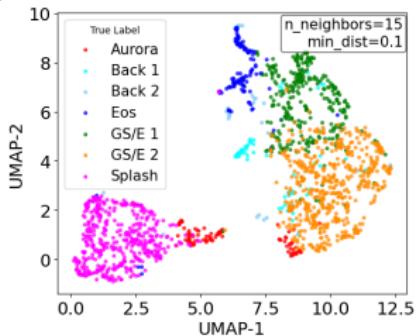
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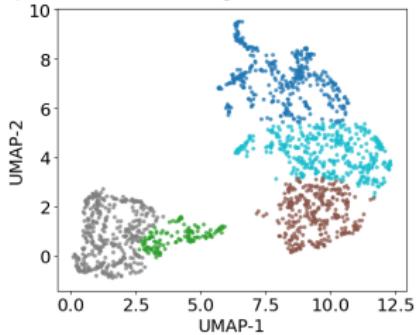
UMAP:

- ▶ Non-Linear dimensionality reduction
- ▶ Advantages over T-SNE:
 - ▶ Increased speed
 - ▶ Better preservation of global structure
- ▶ Hyperparameters:
 - ▶ `n_neighbours`: Balance of the local and global structure
 - ▶ `min_dist`: Controls lower dimensional projection

UMAP - 6D APOGEE



a) Colors based on High Dimensional XD



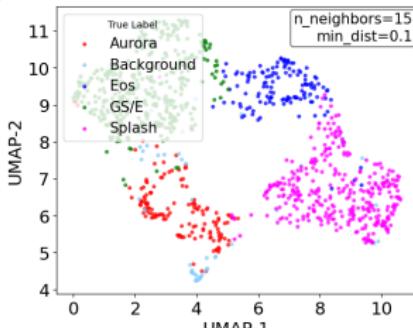
b) Colors based on GMM recovery

GS/E Eos Aurora Splash

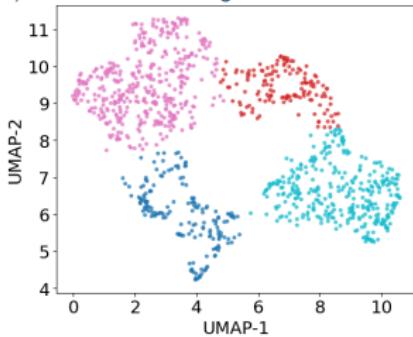
Key Results:

- ▶ Proof of concept
- ▶ A split in Aurora?
- ▶ GMM used to demonstrate cohesion and isolation
- ▶ Caveated:
 - ▶ Non-Linear Reduction: GMM has no probabilistic foundation.

UMAP - 12D GALAH



a) Colors based on High Dimensional XD



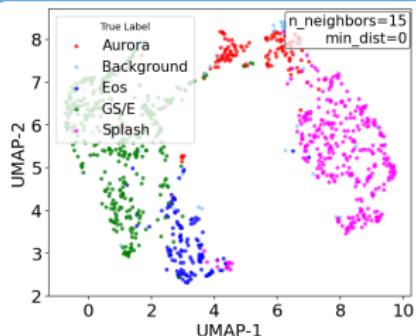
b) Colors based on GMM recovery

GS/E Eos Aurora Splash

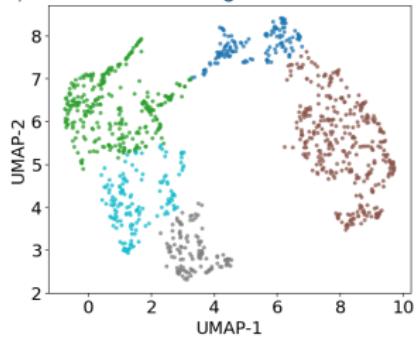
Key Results:

- ▶ Near ‘perfect’ GMM recovery
- ▶ Greater Cohesion and Isolation:
 - ▶ 12D → Nucleosynthetic discrimination
 - ▶ Is this the only reason ?

UMAP - 6D GALAH



a) Colors based on High Dimensional XD



b) Colors based on GMM recovery

GS/E Eos Aurora Splash

Key Results:

- ▶ Still Greater Cohesion and Isolation
- ▶ Attributed to:
 - ▶ Exclusion of low metalicity
 - ▶ Region of 'confusion' with GS/E

Scalable Methodologies

A Low-Dimensional Pipeline:

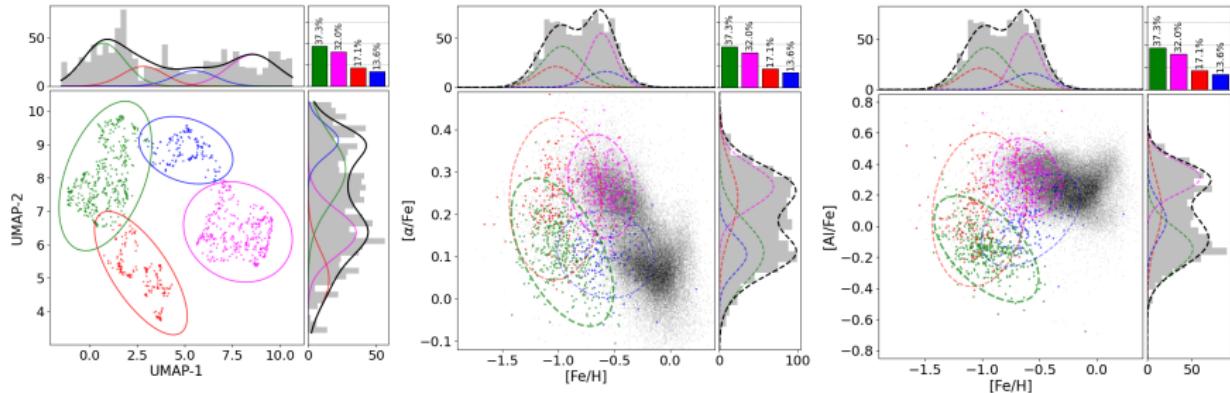
1. Dimensionality Reduction
2. Clustering in Embedding Space
3. Re-projection back into Original Space

Caveat:

- ▶ Lack uncertainties in embedding space → Traditional GMM
- ▶ Approximate De-convolution of Variances:

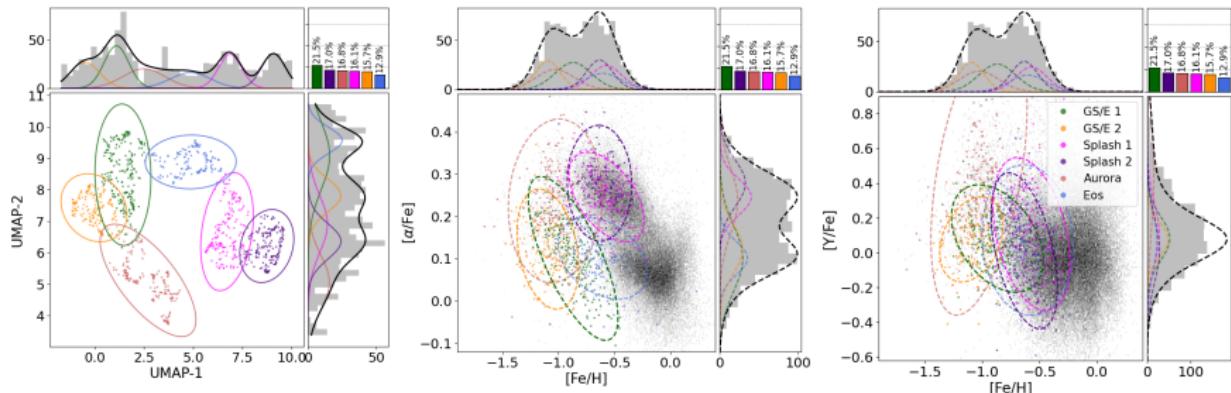
$$\boldsymbol{\Sigma}_{\text{intr}} = \boldsymbol{\Sigma}_{\text{obs}} - \langle \boldsymbol{\Delta} \rangle \quad (9)$$

4 Component Re-identification



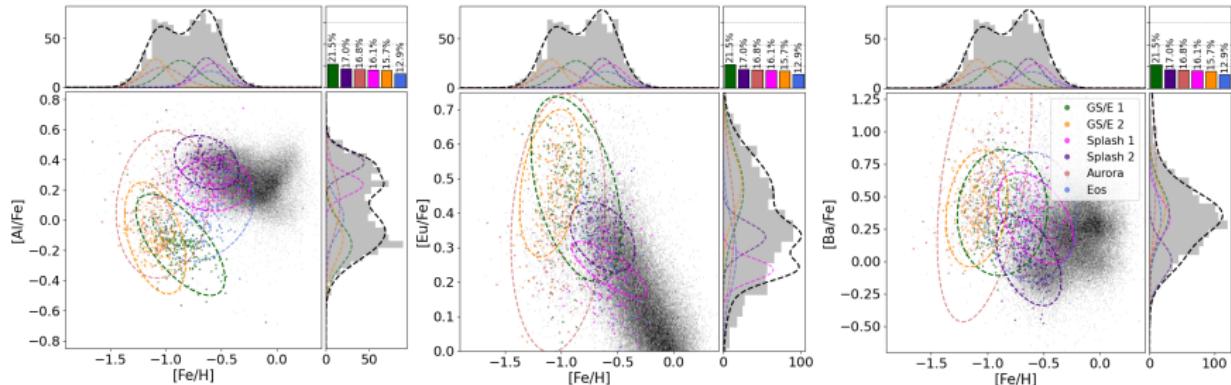
- ▶ 4.7 hours → 7 seconds ($2500 \times$ Speed-Up)
- ▶ Entirely Consistent Results
- ▶ 29.3% Increase in Uncertainties

6 Component Re-identification



- ▶ A rough recovery of the GS/E Split
- ▶ Not achievable in high dimensional clustering

6 Component Re-identification



- ▶ A potential split in splash?
- ▶ A simple division of a large components in embedding space
- ▶ Or ... an astrophysical distinction

Key Results

1. **Recovered key populations:** Confirming objectivity and reproducibility.
2. **GALAH's higher dimensionality:** Provides greater halo substructure separation despite higher uncertainties.
3. **Clustering in Embedding space:**
 - ▶ Near-identical results to high-dimensional analysis
 - ▶ Achieved in 0.04% of the time (29% higher uncertainty)
 - ▶ A future stable and scalable alternative

Future Work

1. **Aurora's Split:** Test for bimodality in Aurora structure
2. **Splash's Split:** Explore physical basis for two Splash subpopulations (simulations)
3. **Hybrid Pipeline:**
 - ▶ Fast (low-D) clustering for initial grouping
 - ▶ Uncertainty-aware (high-D) clustering for accuracy

Questions

Thank you for your attention!

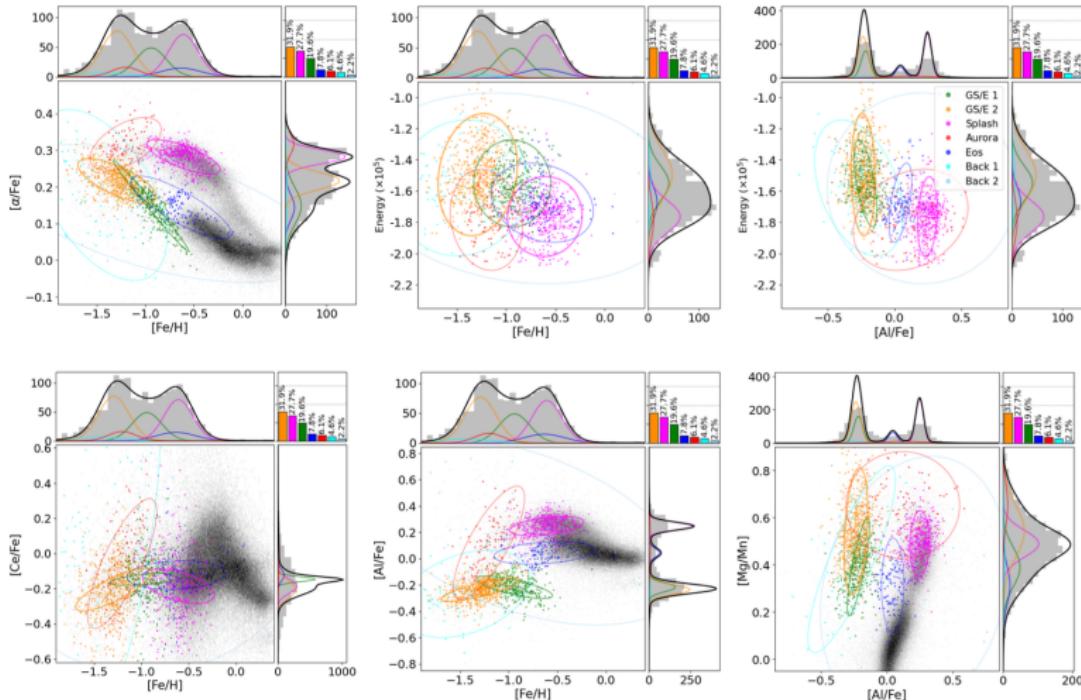
Jacob Tutt

Department of Physics, University of Cambridge

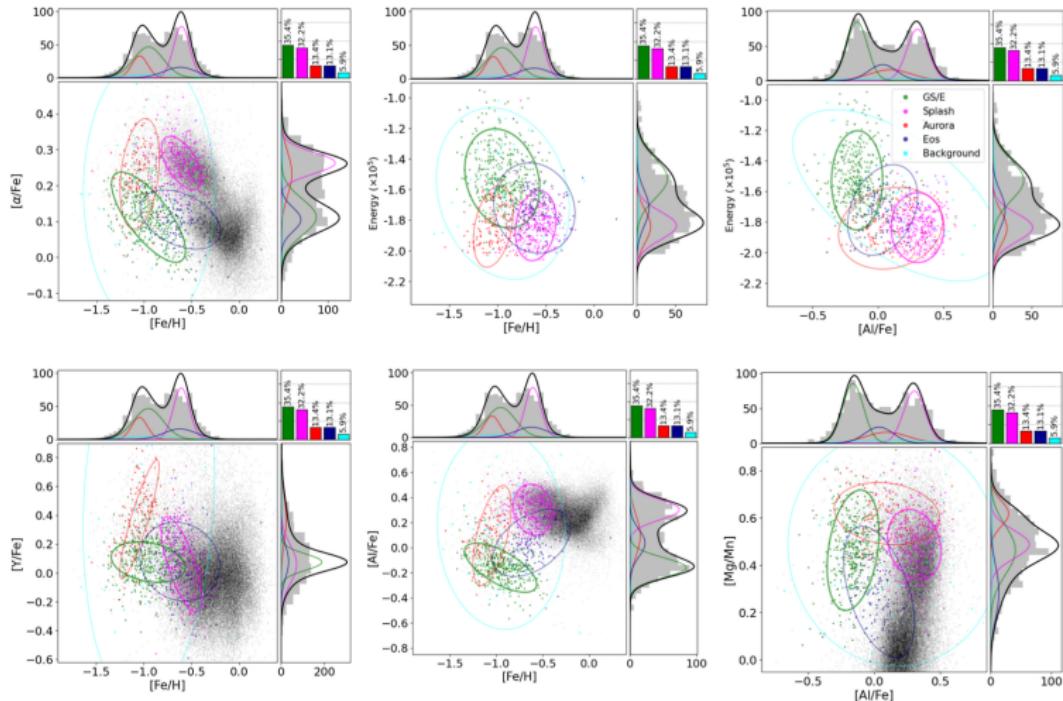
jlt67@cam.ac.uk

<https://github.com/jacbtutt>

APOGEE Results



GALAH Results



Extreme Deconvolution

Expectation-step

$$q_{ij} = \frac{\alpha_j \mathcal{N}(\mathbf{w}_i | \mathbf{m}_j, \mathbf{T}_{ij})}{\sum_k \alpha_k \mathcal{N}(\mathbf{w}_i | \mathbf{m}_k, \mathbf{T}_{ik})} \quad (10)$$

Maximisation-step

$$\alpha_j = \frac{1}{N} \sum_i q_{ij} \quad (13)$$

$$\mathbf{b}_{ij} = \mathbf{m}_j + \mathbf{V}_j \mathbf{T}_{ij}^{-1} (\mathbf{w}_i - \mathbf{m}_j) \quad (11)$$

$$\mathbf{m}_j = \frac{1}{q_j} \sum_i q_{ij} \mathbf{b}_{ij} \quad (14)$$

$$\mathbf{B}_{ij} = \mathbf{V}_j - \mathbf{V}_j \mathbf{T}_{ij}^{-1} \mathbf{V}_j \quad (12)$$

$$\mathbf{V}_j = \frac{1}{q_j} \sum_i q_{ij} \left[(\mathbf{m}_j - \mathbf{b}_{ij})(\mathbf{m}_j - \mathbf{b}_{ij})^\top + \mathbf{B}_{ij} \right] \quad (15)$$

Model Comparison

Akaike Information Criterion

- ▶ Favors models with best predictive accuracy

Bayesian Information Criterion

- ▶ Favors models with best overall fit

$$\text{AIC} = 2k - 2 \ln \mathcal{L},$$

$$\text{BIC} = k \ln n - 2 \ln \mathcal{L},$$

where:

- ▶ k : number of free parameters,
- ▶ n : number of data points,
- ▶ \mathcal{L} : maximum likelihood of the model.

UMAP Algorithm:

1. Compute local distances

- ▶ For each point, find distance to the n-th nearest neighbor
(`n_neighbours`)

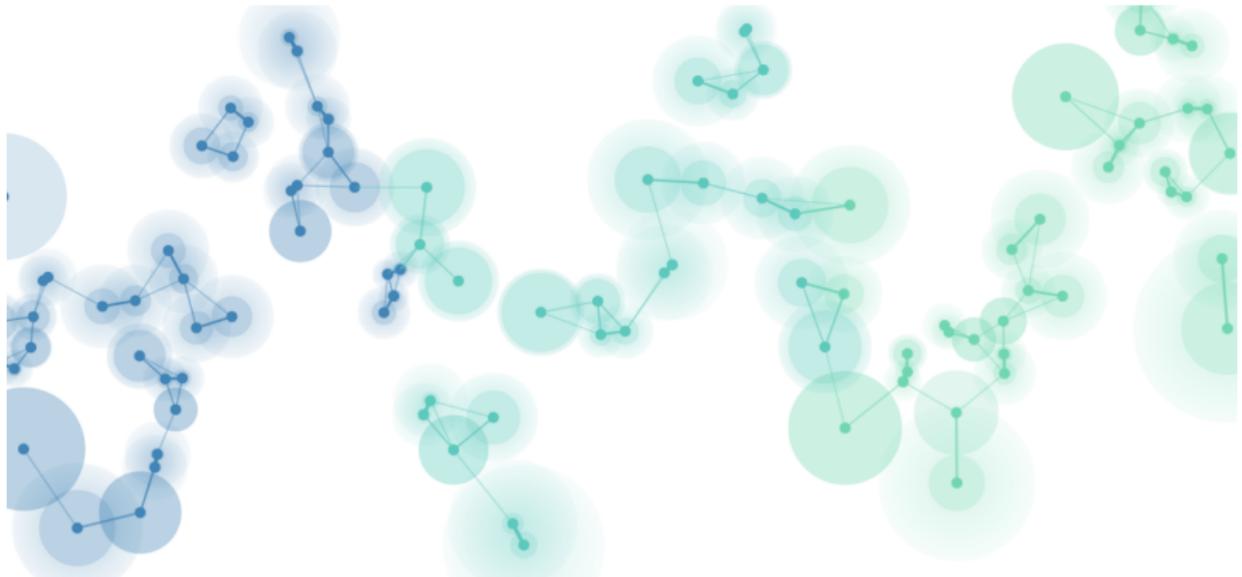
2. Construct Representation

- ▶ Build a weighted graph representing connection probabilities
- ▶ Done using local radii (scaled by nth nearest neighbor)
- ▶ Ensures mutual relationships are captured

3. Optimise low-dimensional embedding

- ▶ Initialise points in low-dimensional space (`min_dist`)

UMAP Visualisation



Splash Decomposition

Feature	Splash 1	Splash 2	Tracer
Colour	Magenta	Purple	
Fraction	16.1%	17.0%	
[Eu/Fe]	Lower	Higher	r-process
[Al/Fe]	Lower	Higher	Core-collapse SN
[Ba/Fe]	Higher	Lower	s-process (AGB)

Table: Comparison of chemical properties between Splash 1 and Splash 2 populations.