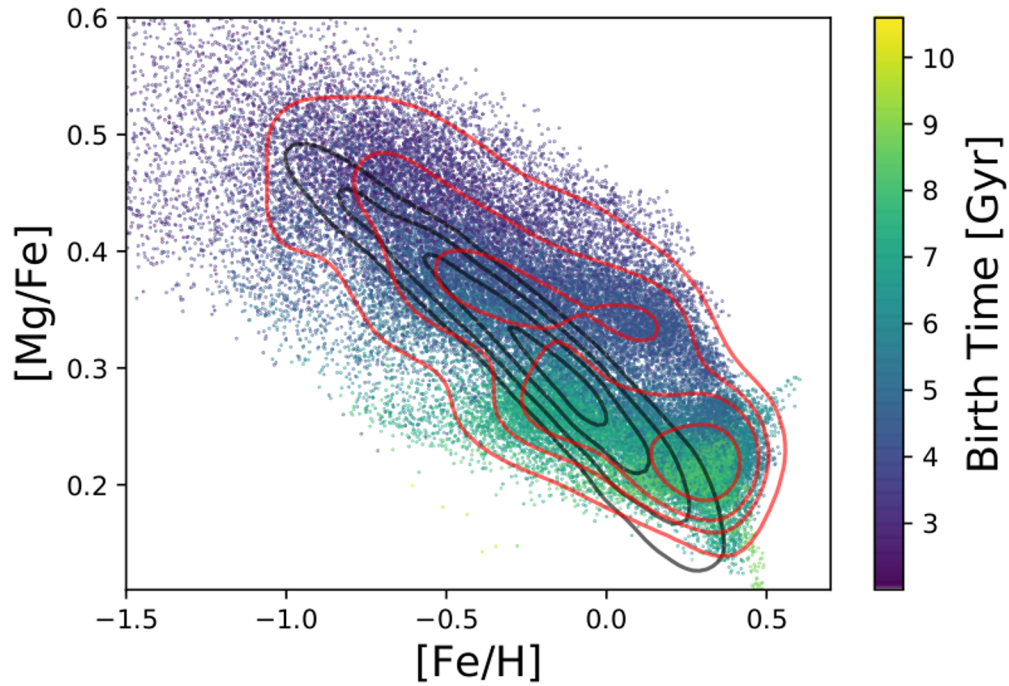
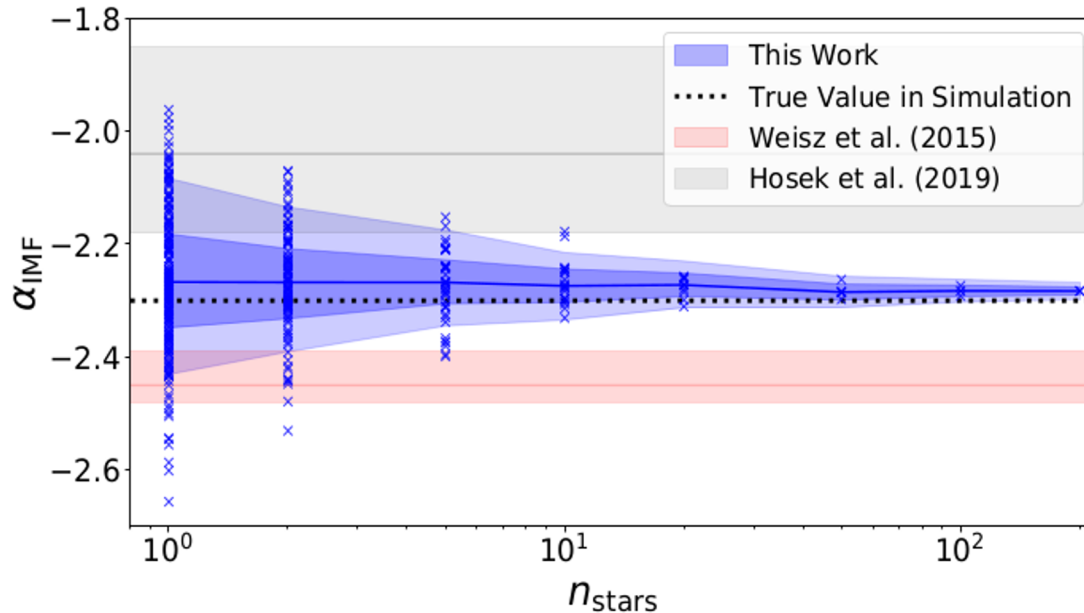


CHEMISTRY



PHYSICS



# Inferring Galactic Parameters from Chemical Abundances

OLIVER PHILCOX (PRINCETON)

with:

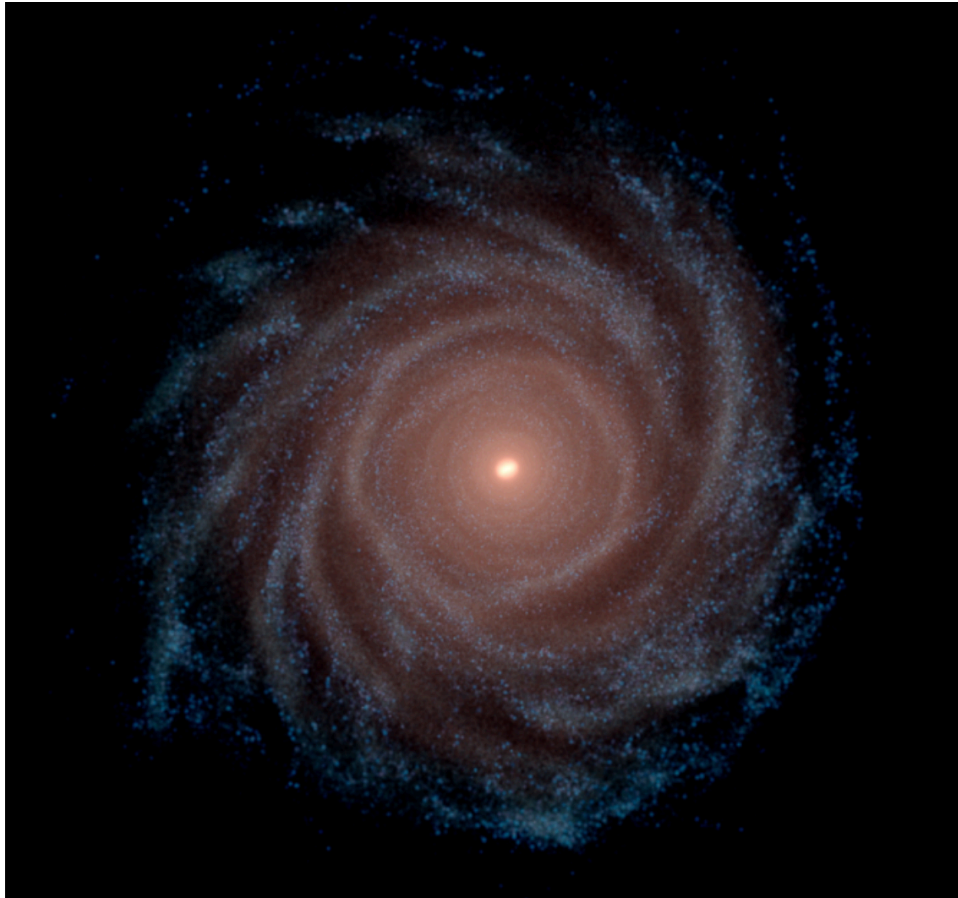
Jan Rybizki (MPIA, Heidelberg)

JOINT STATISTICAL MEETING

Aug 5<sup>th</sup> 2020

arXiv: 1909.00812

# Simulating Galaxies



**Mock Galaxy**  
*(Auriga Simulations)*

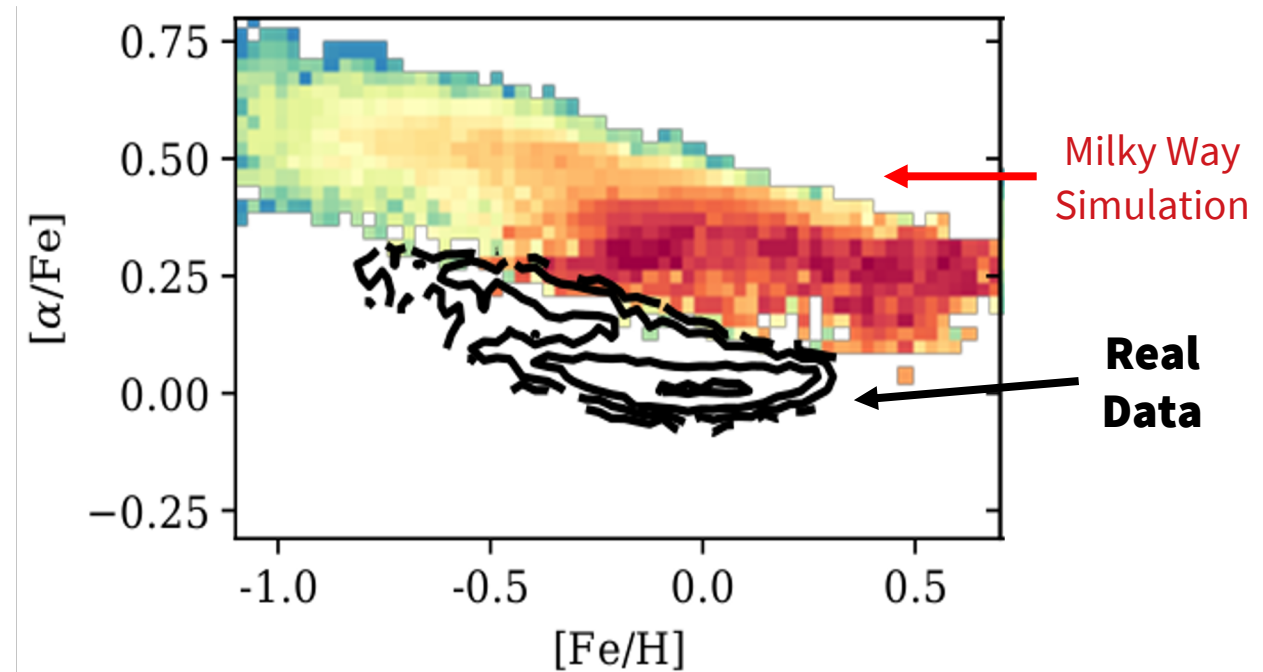
*Are these  
consistent?*

**Real Galaxy**  
*(M101)*



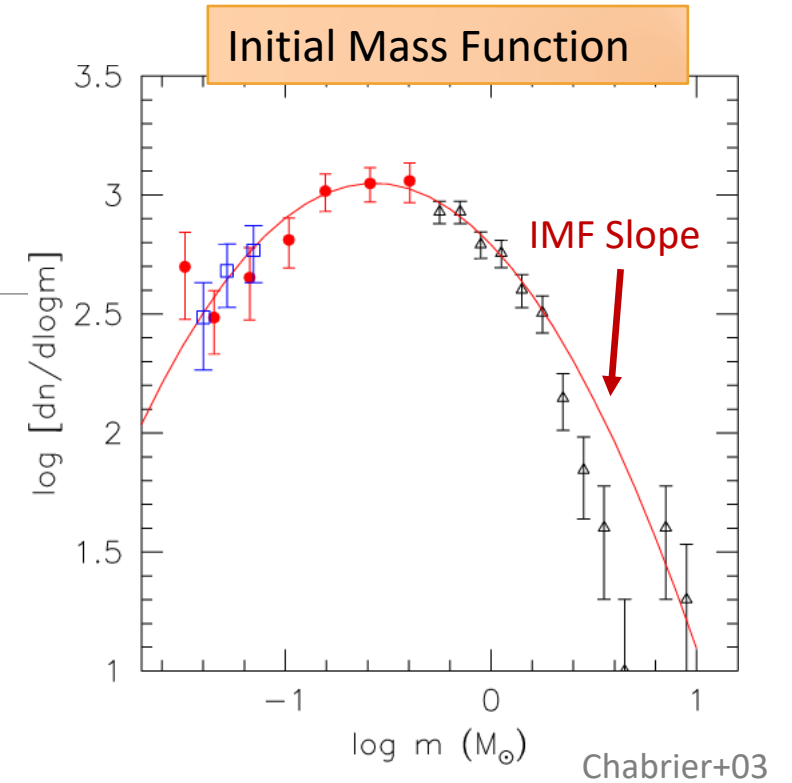
# Are our Simulations Accurate?

- Simulations of galaxies do **not** match the Milky Way
- **Chemical evolution** is wrong
- They depend on **poorly constrained** parameters

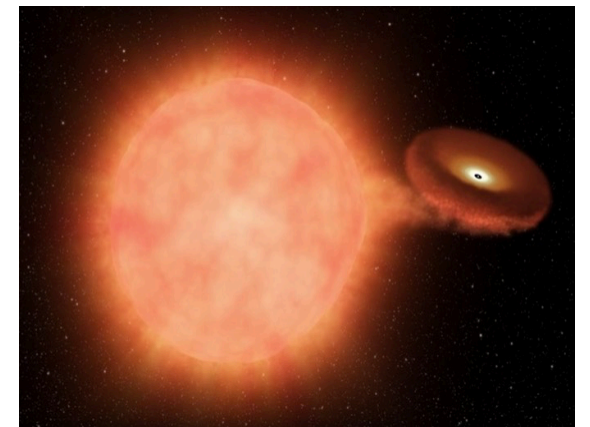


# Parametrizing the Galaxy

- What are these parameters?
  - The slope of the **Initial Mass Function (IMF)**
    - Controls stellar **mass distribution**
  - The number of **Type Ia Supernovae**
    - Removes **gas** from galaxies and spreads metals
- And many more...



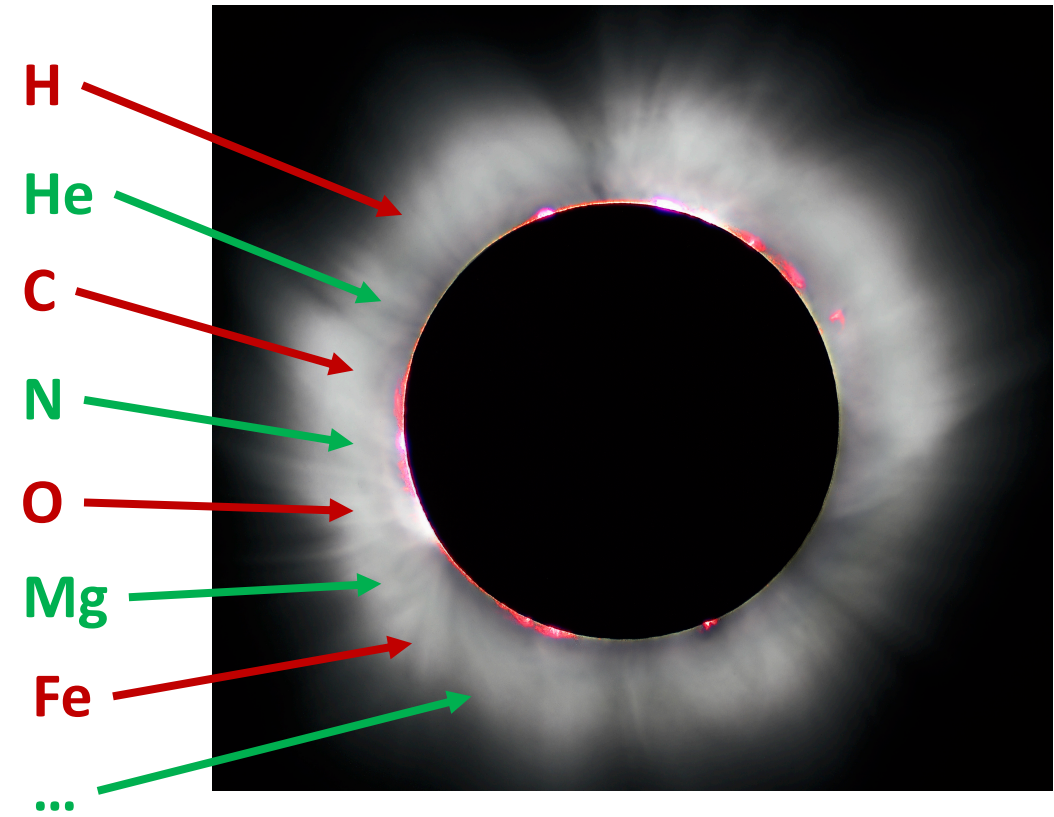
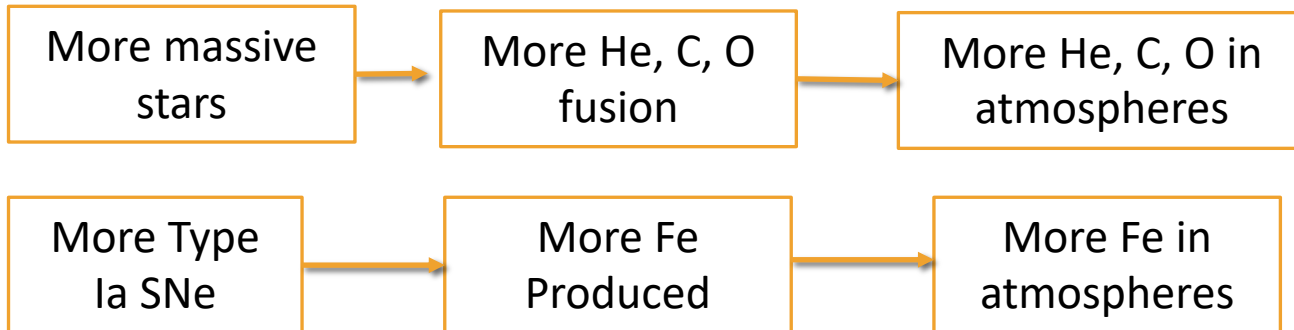
Type Ia Supernovae





# Chemistry from Stellar Atmospheres

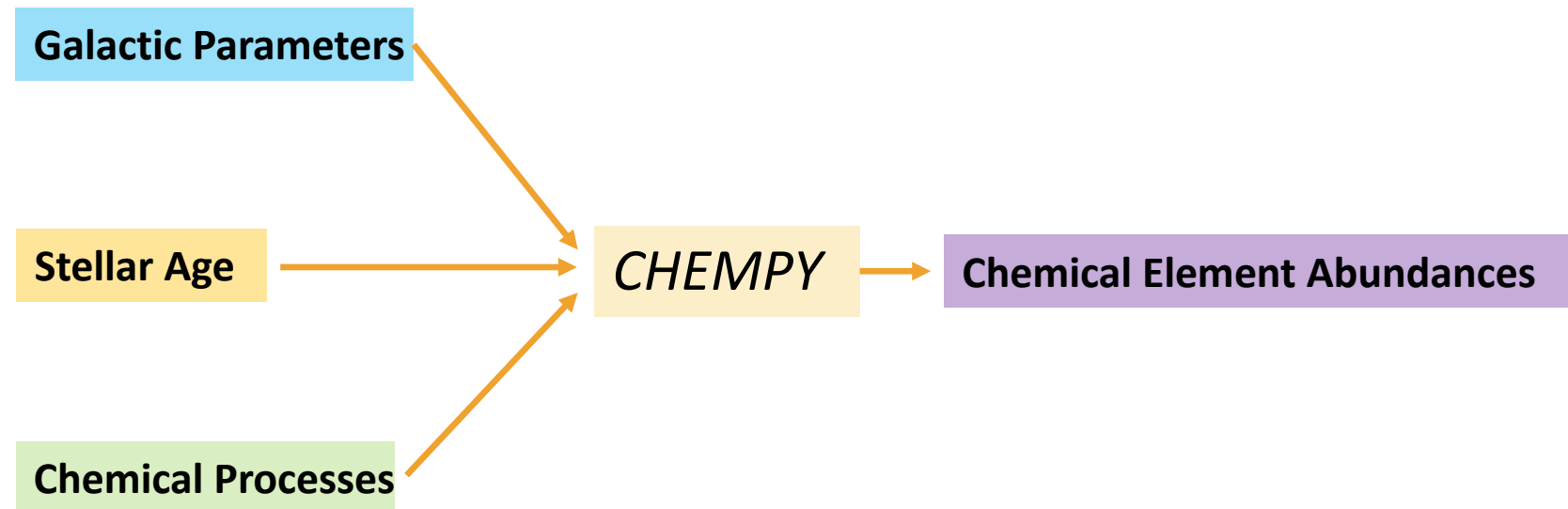
- Stars **explode** and enrich the **interstellar medium**
- Stellar atmospheres encode chemical **abundances** of the interstellar medium
- These depend on **galactic parameters**, e.g.,



# Modeling Chemical Evolution

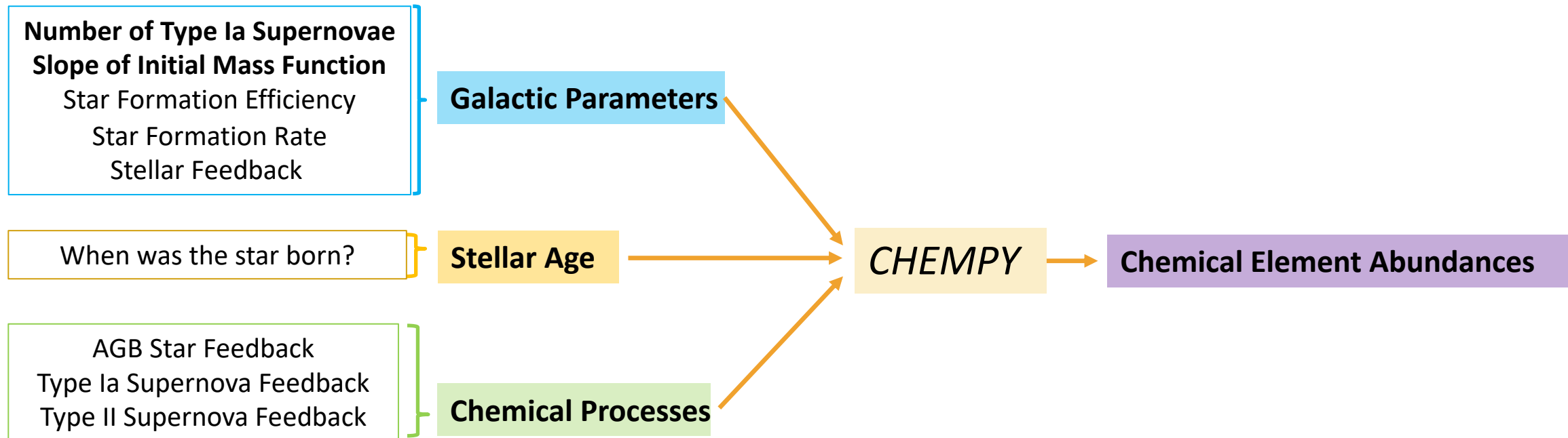
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- Given **galactic parameters** we can model the **element abundances** in stellar atmospheres
- We need a **fast** and **flexible** model: *Chempy*



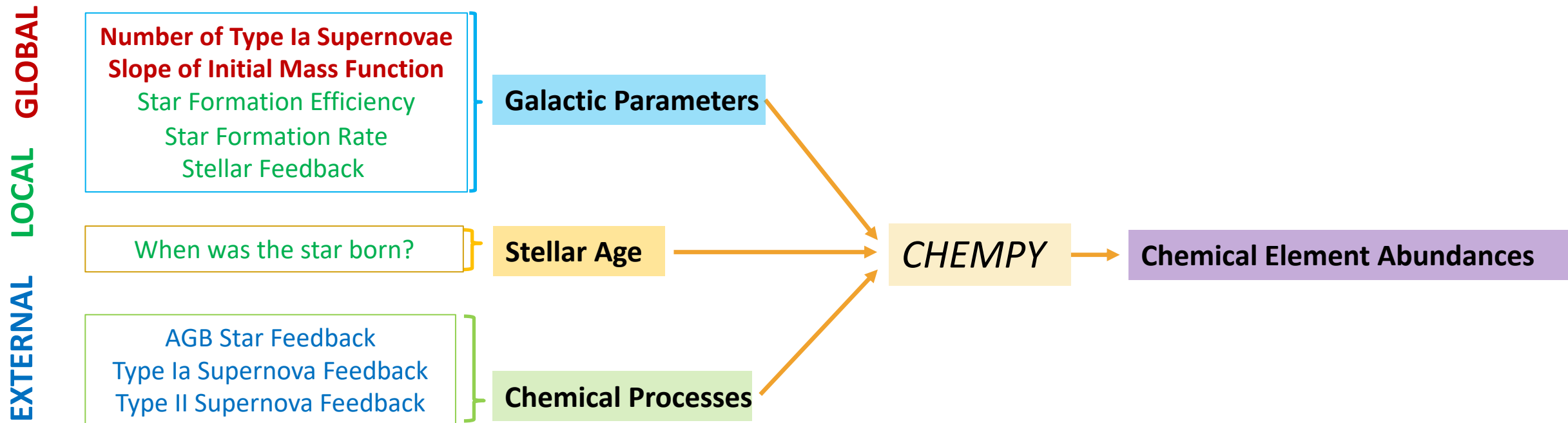
# Modeling Chemical Evolution

- Given **galactic parameters** we can model the **element abundances** in stellar atmospheres
- We need a **fast** and **flexible** model: *Chempy*



# Modeling Chemical Evolution

- Given **galactic parameters** we can model the **element abundances** in stellar atmospheres
- We need a **fast** and **flexible** model: *Chempy*





# A Bayesian Framework

---

- From a set of **stellar chemical abundances** we can infer **galactic parameters**,  $\Lambda$

- Via Bayes' theorem:

$$P(\Lambda|\text{Data}) \sim \int d\Theta dT \underbrace{P(\text{Data}|\Lambda, \Theta, T)}_{\text{Likelihood}} \underbrace{p(\Lambda)p(\Theta)p(T)}_{\text{Priors}}$$

integrating over local parameters  $\Theta$  and the age of the star,  $T$  with priors  $p$ .

- We can extend this to **multiple stars**

$$P(\Lambda|\text{Data}) \sim p(\Lambda) \prod_{i=1}^{n_{\text{stars}}} \int d\Theta_i dT_i \underbrace{P(\text{Data}_i|\Lambda, \Theta_i, T_i)}_{i^{\text{th}} \text{ star likelihood}} \underbrace{p(\Theta_i)p_i(T_i)}_{\text{Priors}}$$

# A Bayesian Framework

---

- We can extend this to **multiple stars**

$$P(\Lambda|\text{Data}) \sim p(\Lambda) \prod_{i=1}^{n_{\text{stars}}} \int d\Theta_i dT_i \underbrace{P(\text{Data}_i|\Lambda, \Theta_i, T_i)}_{i^{\text{th}} \text{ star likelihood}} \underbrace{p(\Theta_i)p_i(T_i)}_{\text{Priors}}$$

- What about inadequacies in our model?
  - Add free **model error** parameters,  $\sigma_{\text{model}}$  (one per chemical element)
  - These will **downweight** constraints from poorly modeled elements

$$P(\Lambda|\text{Data}) \sim p(\Lambda) \int d\sigma_{\text{model}} p(\sigma_{\text{model}}) \prod_{i=1}^{n_{\text{stars}}} \int d\Theta_i dT_i \underbrace{P(\text{Data}_i|\Lambda, \Theta_i, T_i, \sigma_{\text{model}})}_{i^{\text{th}} \text{ star likelihood}} \underbrace{p(\Theta_i)p_i(T_i)}_{\text{Priors}}$$

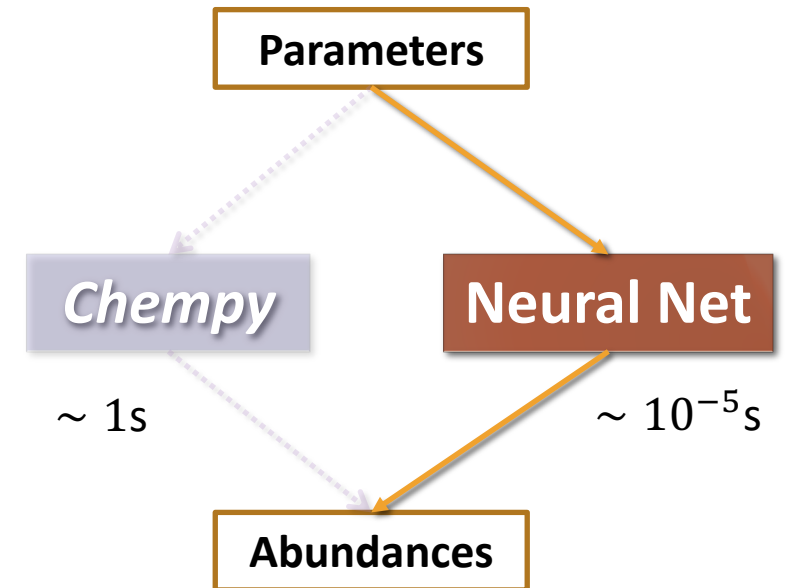
# 21<sup>st</sup> Century Statistics

---

- Our model for the two **global** galactic parameters depends on:
  - 3 local **star formation** parameters per star
  - 1 **age** parameter per star
  - 1 **error** parameter per element.

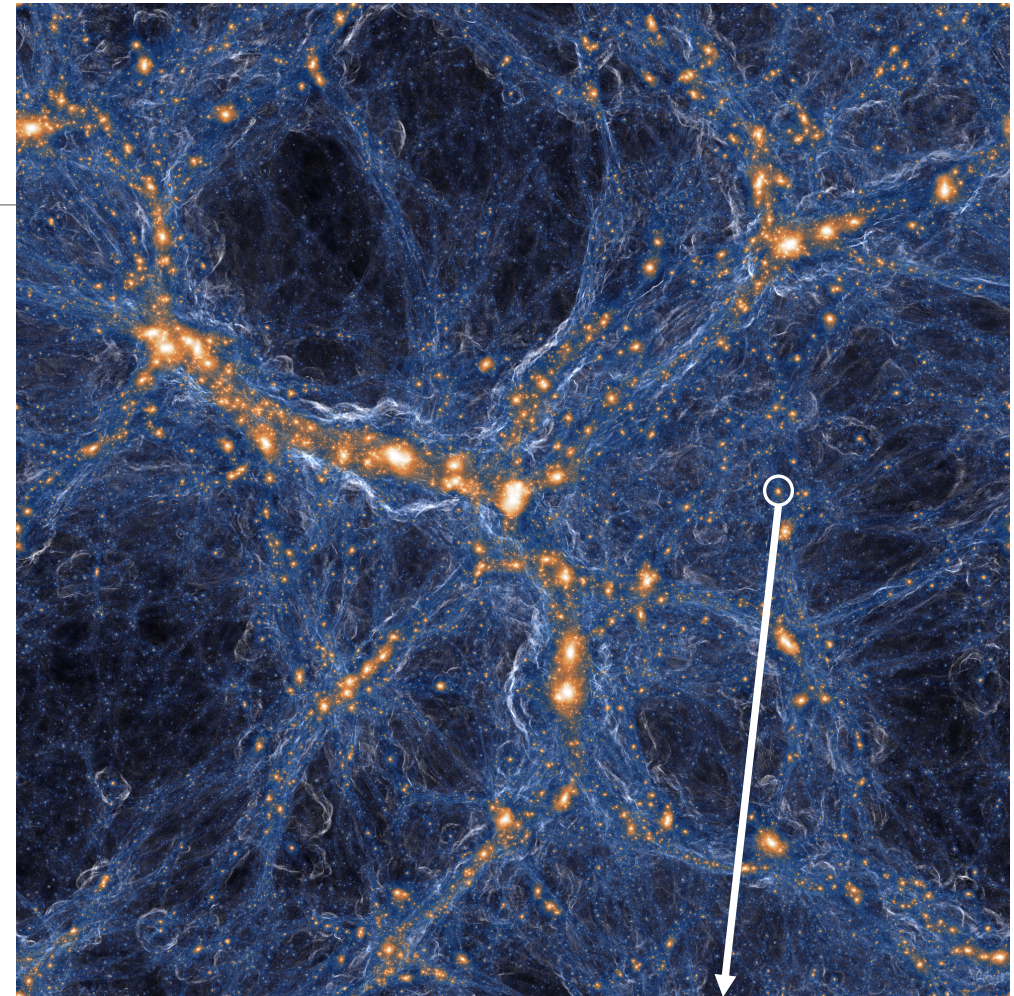
For 100 stars with 8 elements, this gives **408** free parameters!

- We need **modern methods** for efficient sampling:
  - 1. Replace the **slow** *Chempy* model with a (differentiable) trained **neural network**
  - 2. Use **Hamiltonian Monte Carlo** with **No U-Turn Sampling** (NUTS)



# Mock Data

- Use the **IllustrisTNG-100** simulation
  - Has **much** more complex physics than *Chempy*!
- Extract  $\sim 200$  ‘**stellar particles**’ from a **Milky Way**-like galaxy each with:
  - **Stellar ages**
  - **Abundances** of H, He, C, N, O, Mg, Si, Ne, Fe
- Supplement these with realistic observational **errors**

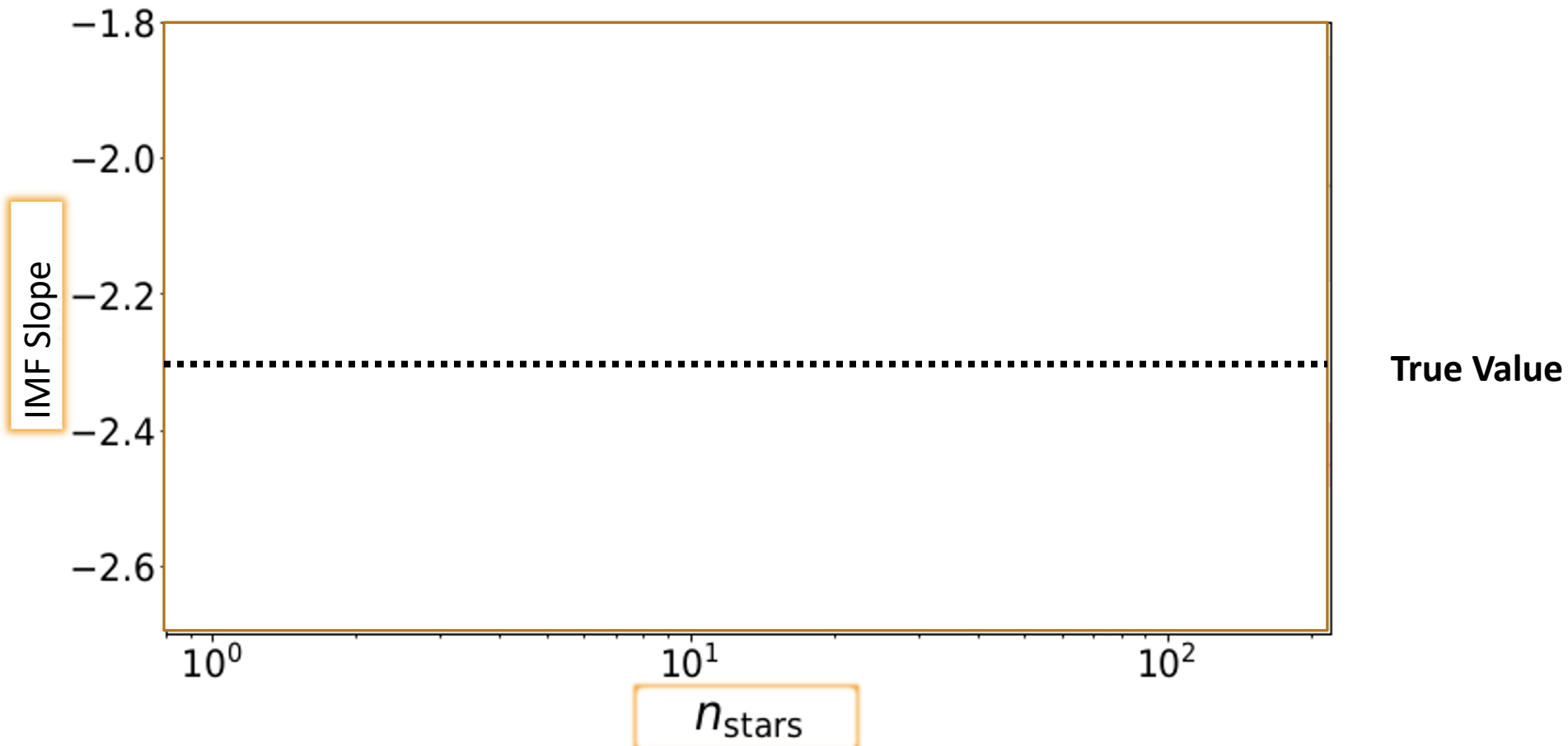


Milky Way v2.0



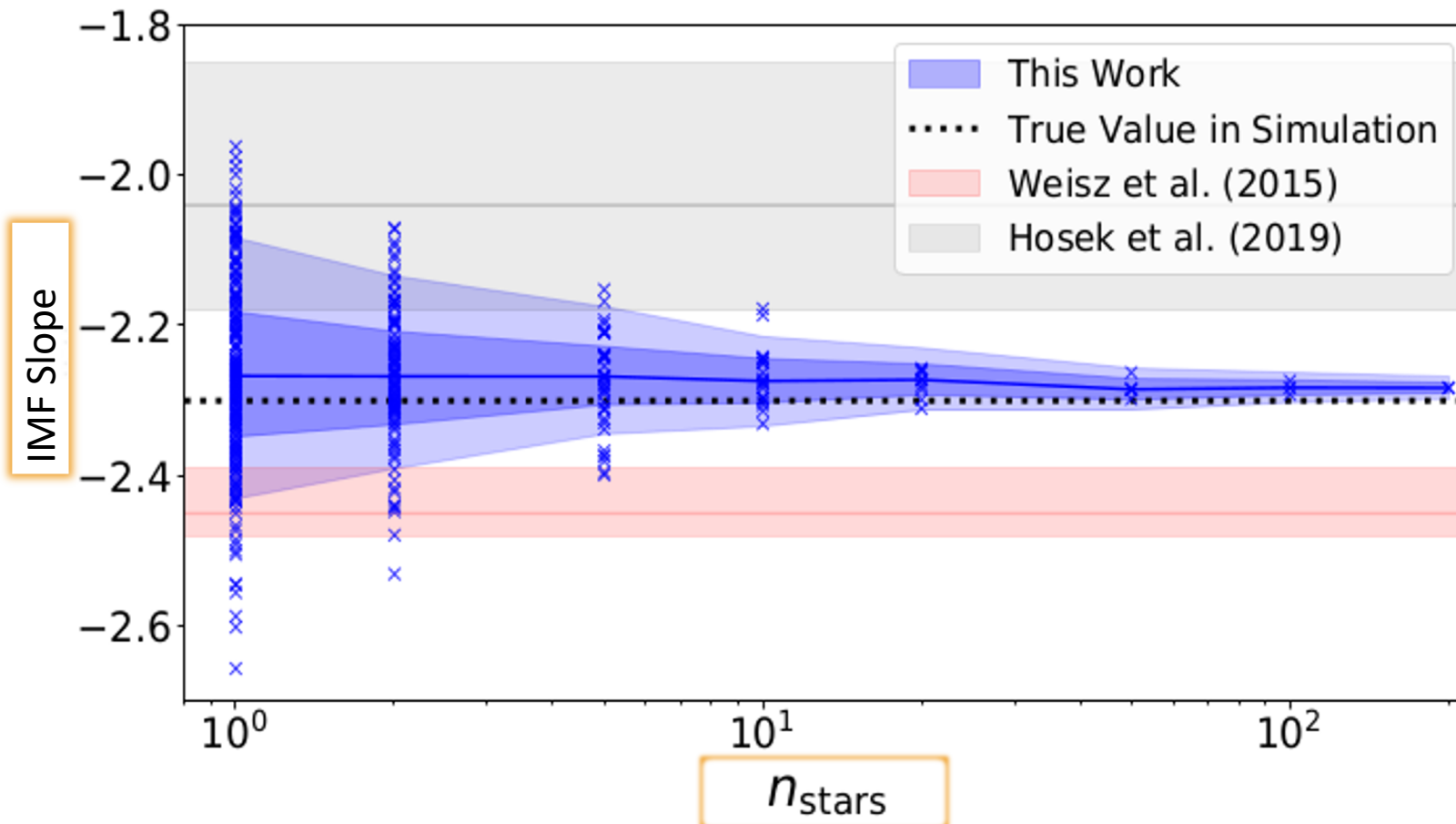
# How well do we do?

- Compare our parameter inference with the true values in the simulation



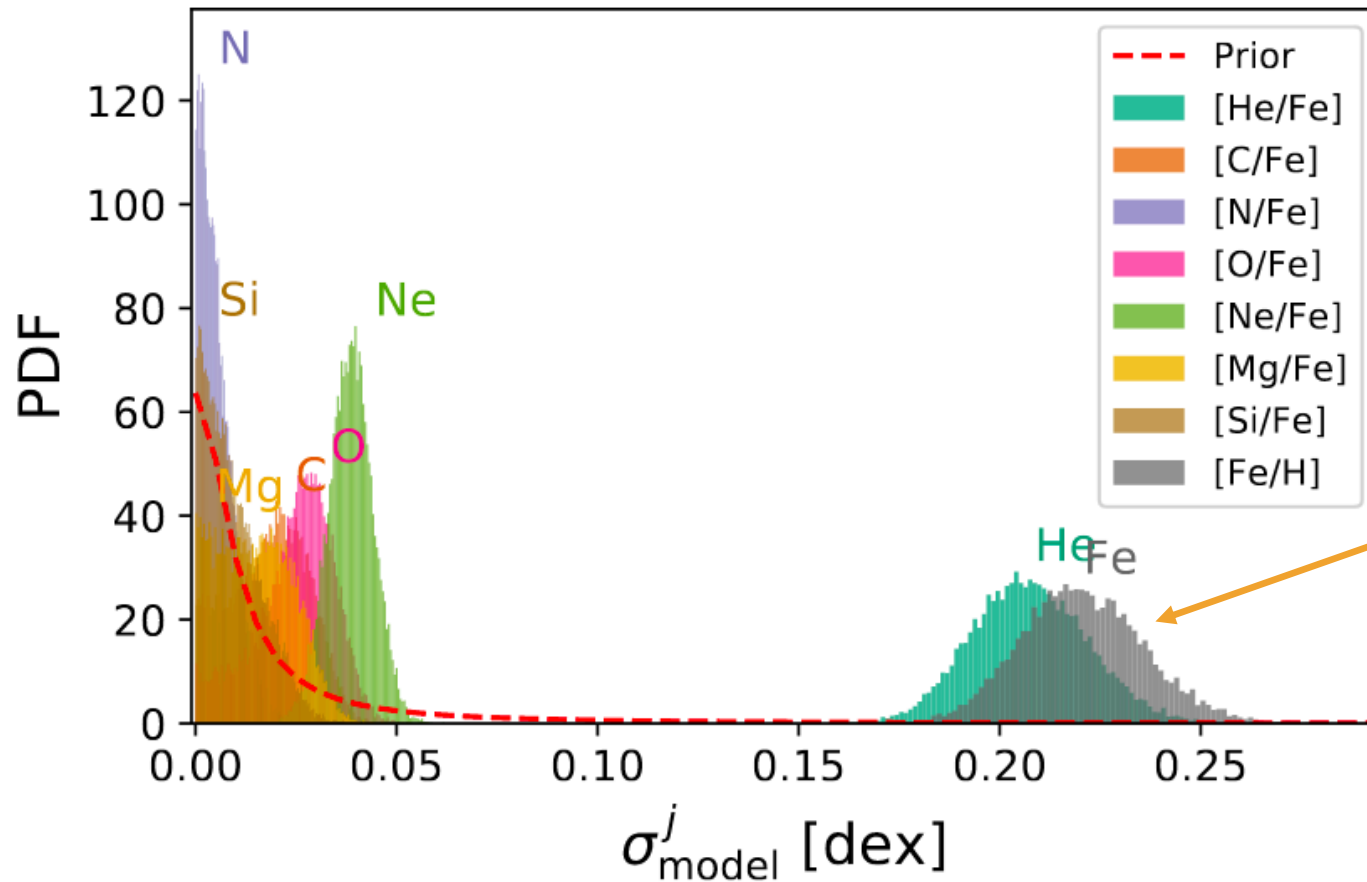
# How well do we do?

- Compare our parameter inference with the true values in the simulation



- A strong measurement of galactic parameters
- Tightens with more stars

# How well do we do?



Model error posteriors

Absolute metallicity is **poorly predicted** but **metal line ratios** are useful

# Summary

- We can use measure **galactic evolution** parameters from **stellar atmospheres** using:
  - A **simple** chemical evolution model (*Chempy*)
  - **Modern** statistical methods
- This has other applications e.g. ;
  - **Application** to real data
  - **Optimizing** hydrodynamical simulation parameters
  - **Constraining** stellar nucleosynthesis

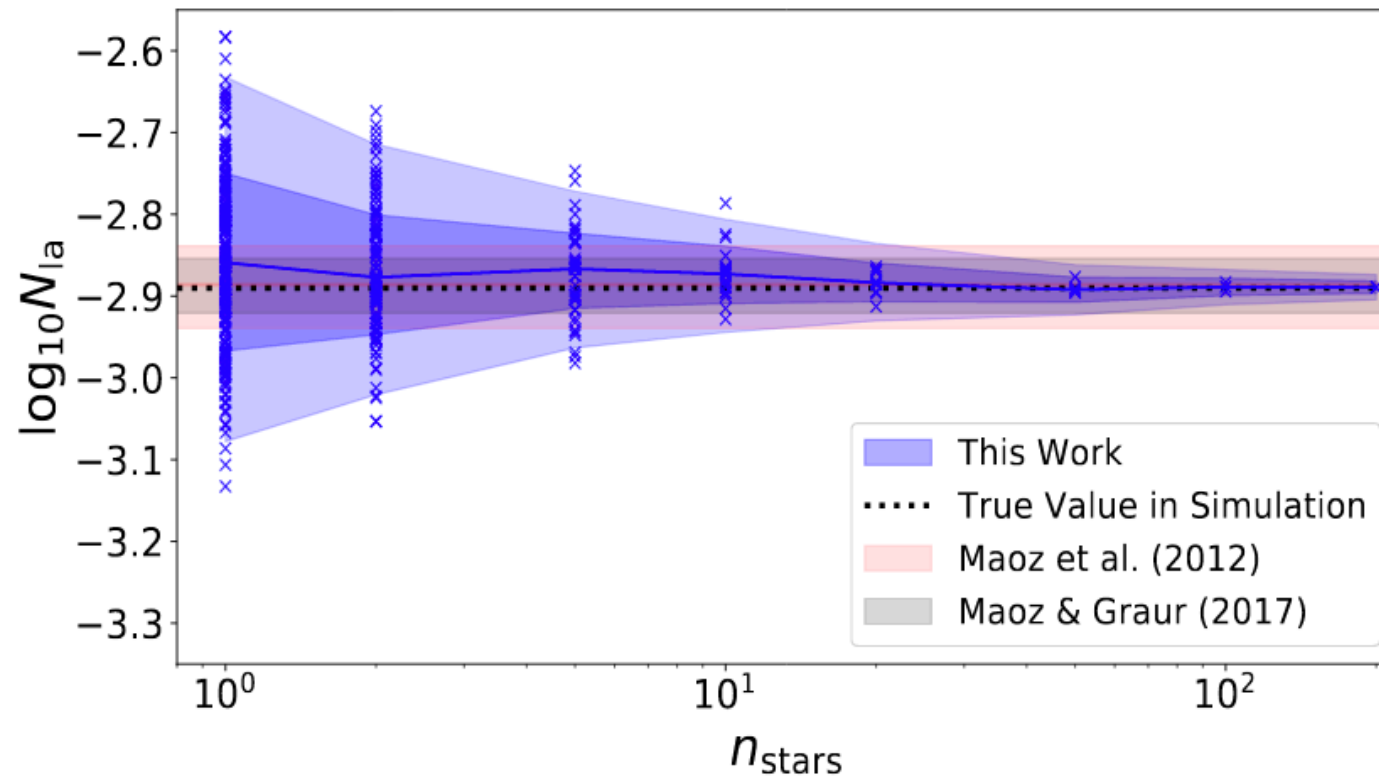
Further Questions?

[ophilcox@princeton.edu](mailto:ophilcox@princeton.edu)



# Type Ia Supernova Constraints

- Compare our parameter inference with the true values in the simulation



# Neural Networks

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- ❑ Evaluation of the *Chempy* function is slow ( $\sim 1s$ )
- ❑ Use neural networks to **predict** output chemical elements from input parameters.
- ❑ This acts as a **fast, non-linear** interpolator, which is **differentiable**.

Diagram illustrating the structure of a neural network layer:

Hidden Layer  $\longrightarrow \mathbf{h} = \mathbf{W}_0 \cdot \mathbf{x} + \mathbf{b}_0$

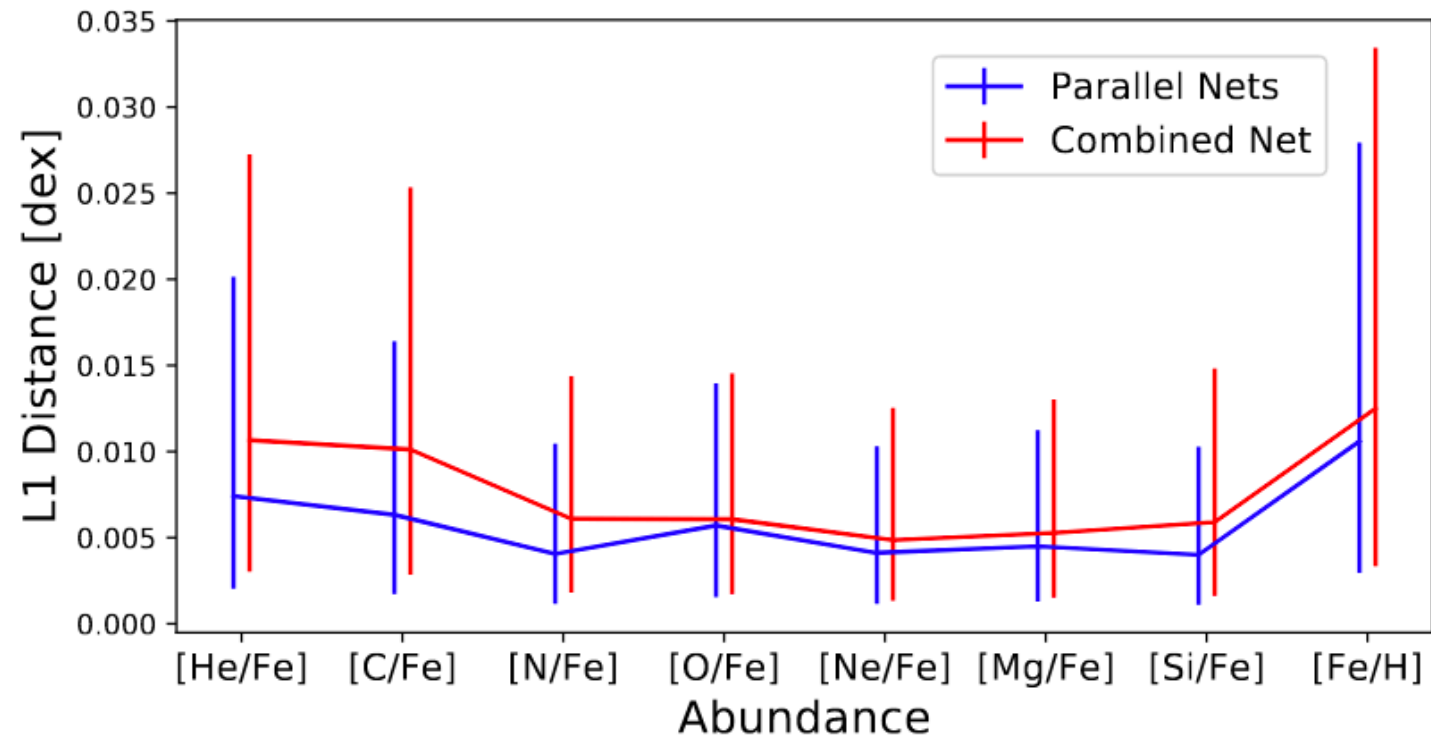
Output  $\longrightarrow \mathbf{y} = \mathbf{W}_1 \cdot f(\mathbf{h}) + \mathbf{b}_1$

Annotations:

- An orange arrow labeled "Input" points to  $\mathbf{x}$  in the hidden layer equation.
- An orange arrow labeled "Non-Linearity" points to  $f(\mathbf{h})$  in the output equation.

# Neural Networks

- This is trained by running *Chempy* on  $\sim 10^4$  points in parameter space.



**Errors are much below observational error  $\sim 0.05$  dex**

# Hamiltonian Monte Carlo (HMC)

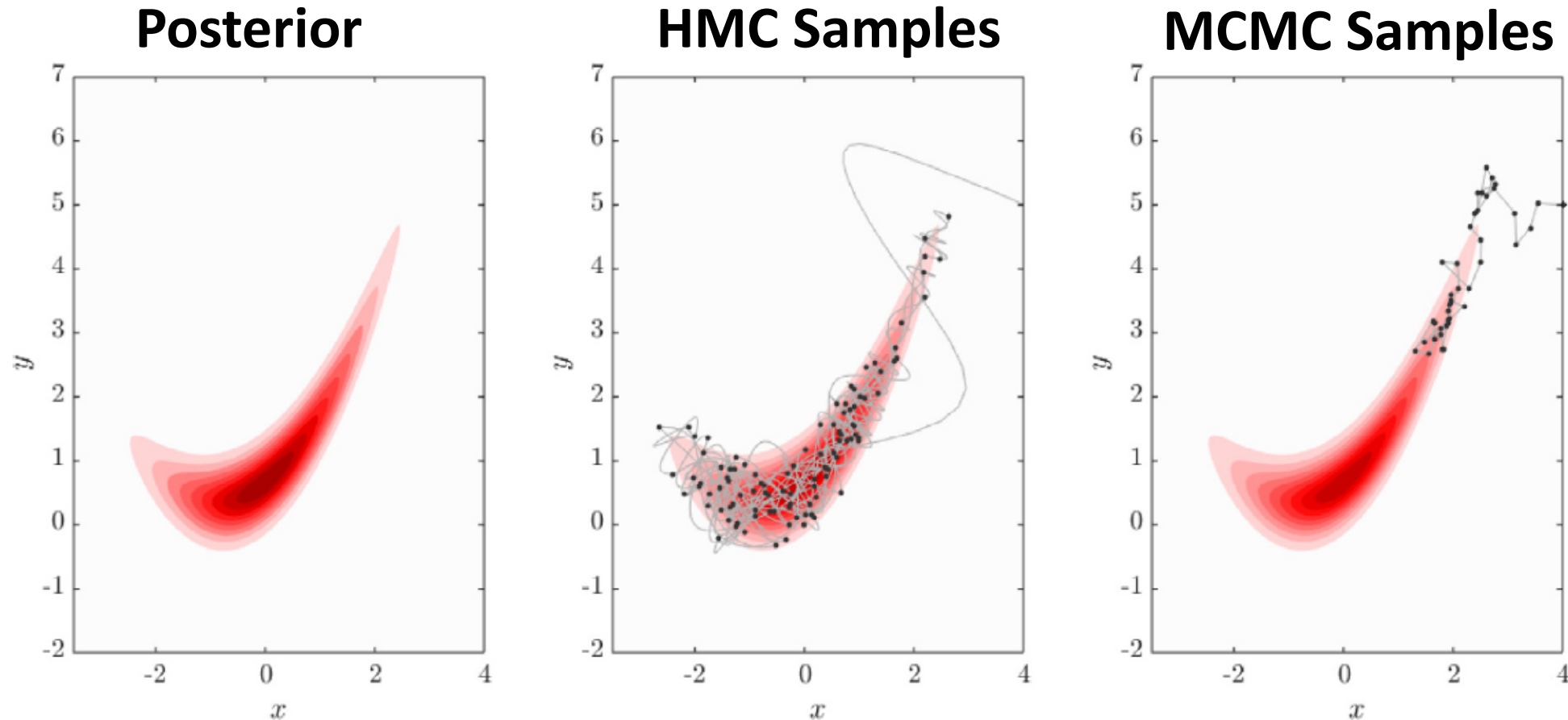
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- ❑ Markov Chain Monte Carlo (MCMC) is **slow** and **unsuitable** for high-dimensional problems.
- ❑ MCMC works by jumping between points in parameter space at random.
- ❑ HMC preferentially samples where the posterior is **large**.
- ❑ It's **much more efficient** but requires a **differentiable** model.



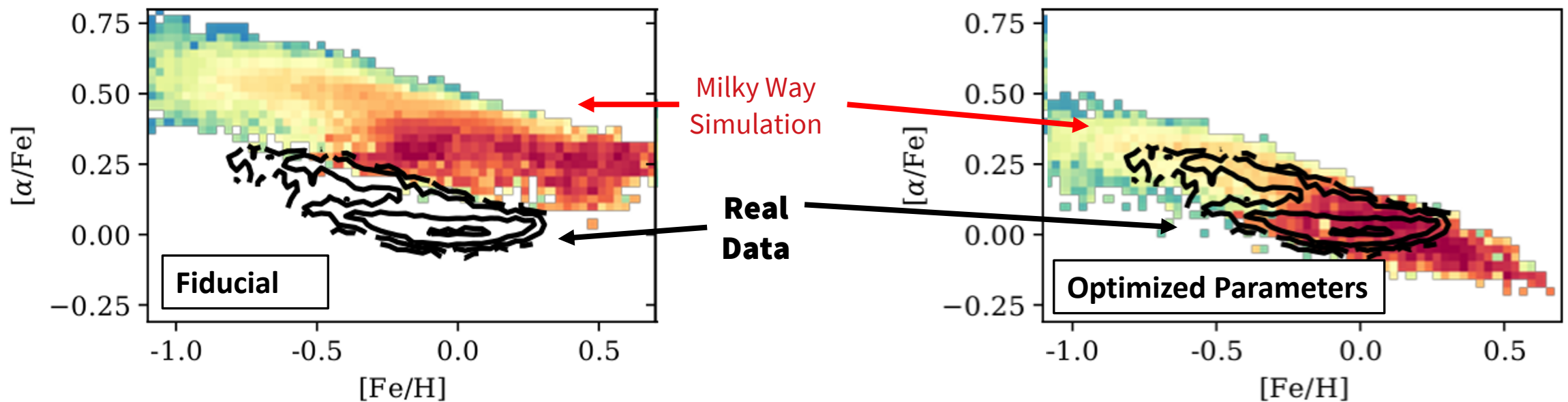
# Hamiltonian Monte Carlo (HMC)

□ HMC preferentially samples where the posterior is **large**.



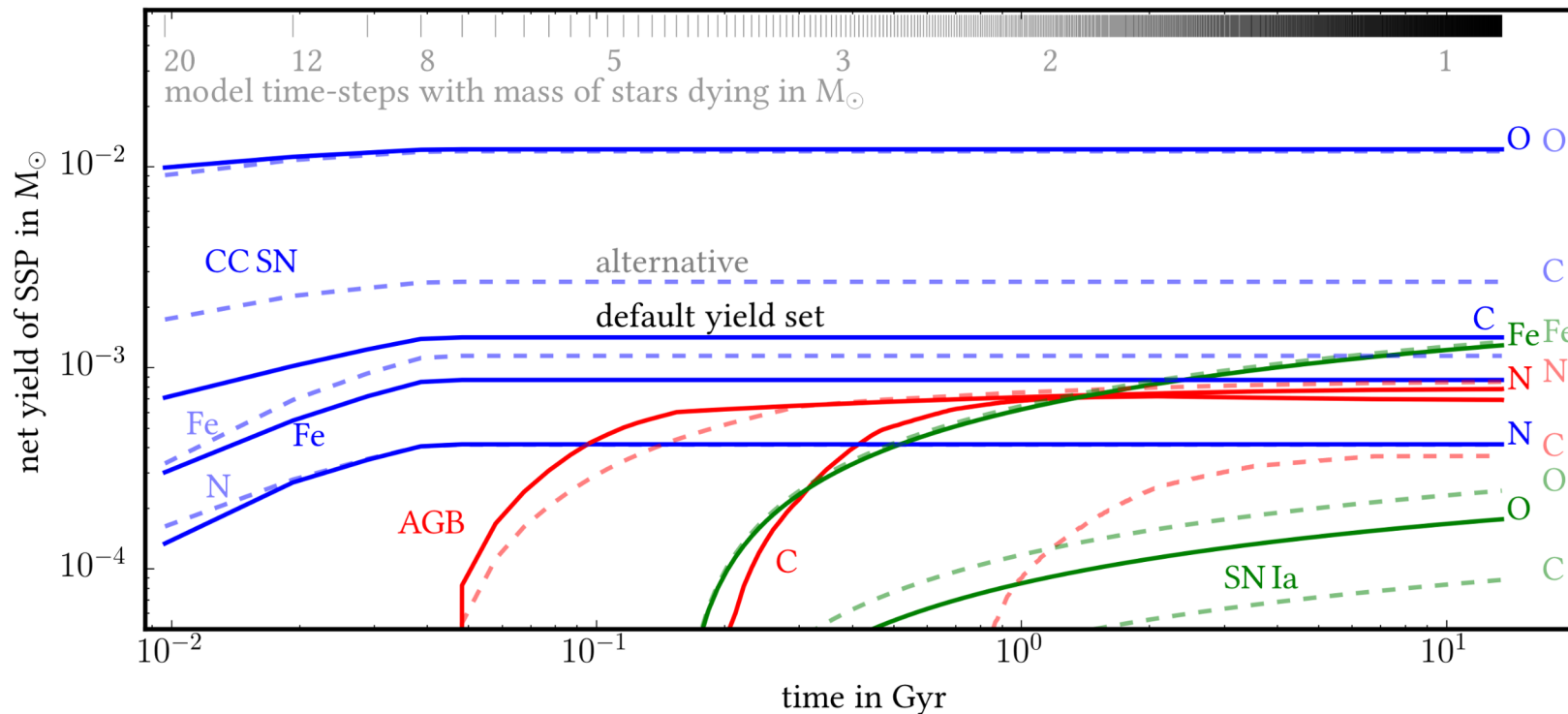
# Optimizing Simulations

- ❑ *Chempy* can be combined with **solar abundances** to measure parameters.
- ❑ This is done via **MCMC** or more advanced methods
- ❑ To test, we can put our **best-fit parameters** into a cosmological simulation
  - ❑ Do we get a more realistic galaxy simulation?



# Building a Fast and Flexible GCE: *Chempy*

- *Chempy* (including **chemical yields**, and **SSP** parameters):
  - **IMF** integrated, metallicity-dependent yield over time



**SSP = Simple Stellar Population**  
(A group of stars born at the same time in the same environment)

**IMF = Initial Mass Function**  
(Contribution of stars born in a certain mass range to total mass)

# How do we measure ISM Abundances?

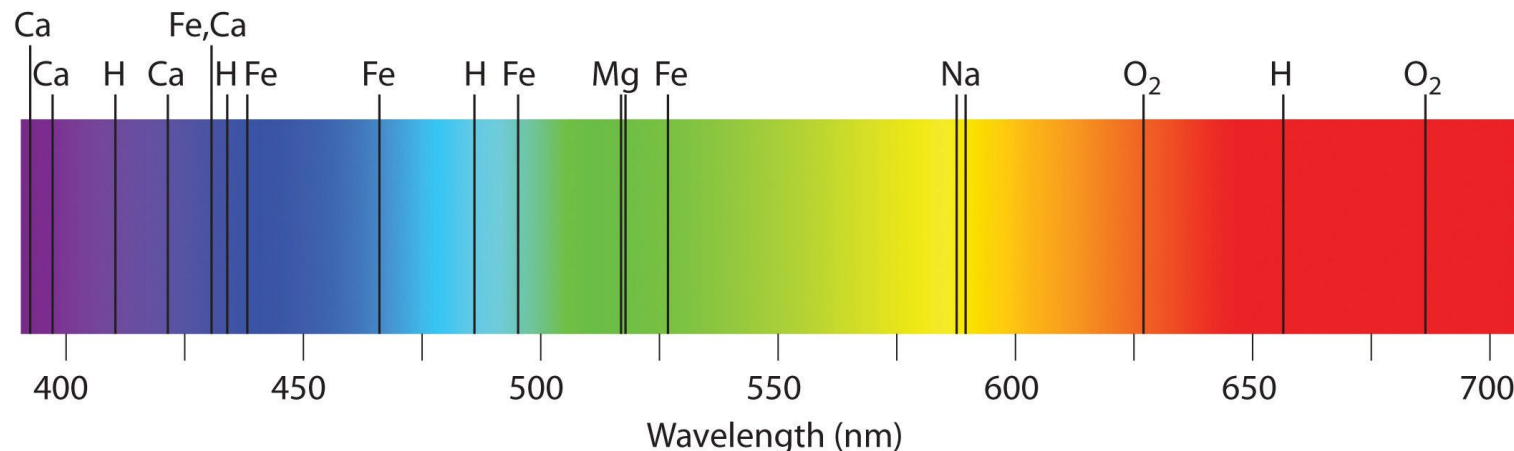
## Option 1: Spectroscopy of the ISM

- Difficult
- Depends on the ISM temperature and density

## Option 2: Stellar Atmospheres

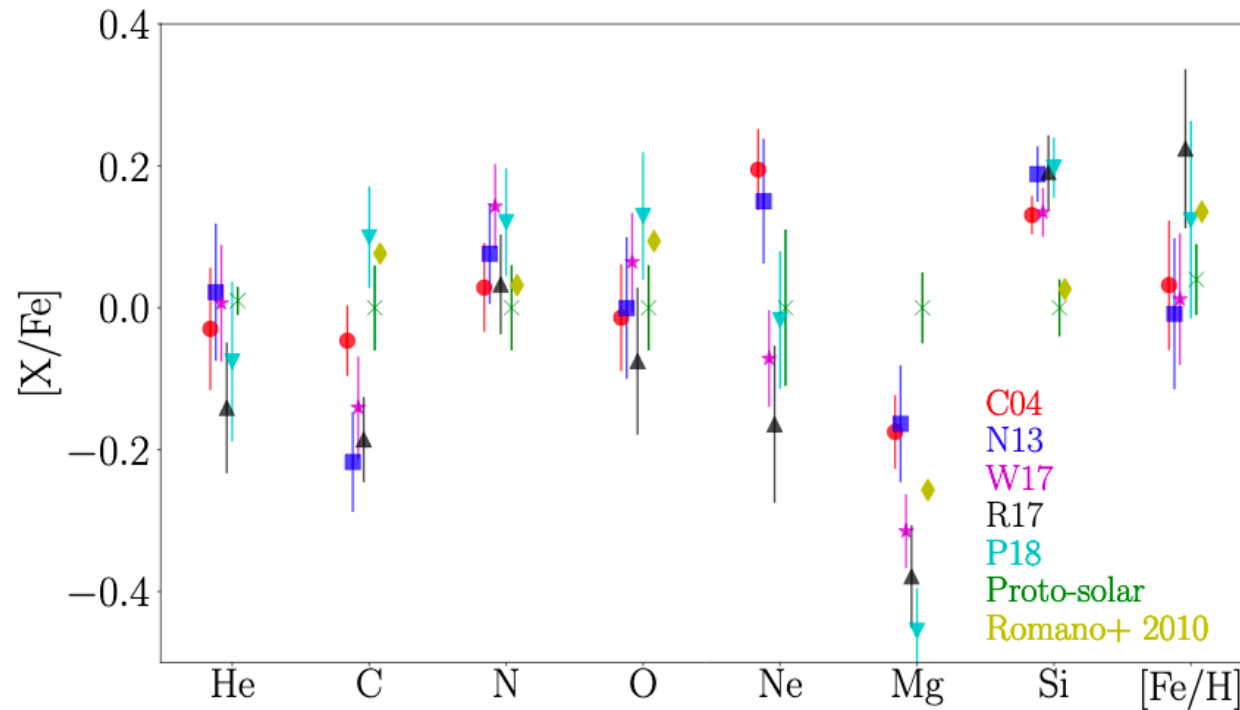
- Can observe stellar chemistry in **absorption lines**
- Many data catalogs exist, e.g. APOGEE
- Metal lines have little contamination

**To Begin:** Use a *single* star – the **Sun** with 28 elements



# Yield Table Scoring

- Different Yield Tables predict **very different** proto-Solar abundances



# Yield Table Scoring

---

## ❑ Method:

- ❑ Compare *Chempy* observations to **proto-Solar** abundances
- ❑ **Marginalize** over SSP and ISM parameters
- ❑ Include **model error** to account for modeling inaccuracies

## ❑ Model Comparison Statistics:

- ❑ Bayes Factor
  - ❑  $B \sim \int d\Theta \text{Posterior}(\Theta | \text{Data})$
- ❑ Cross-Validation
  - ❑ Use  $n - 1$  elements to predict  $n$ -th element



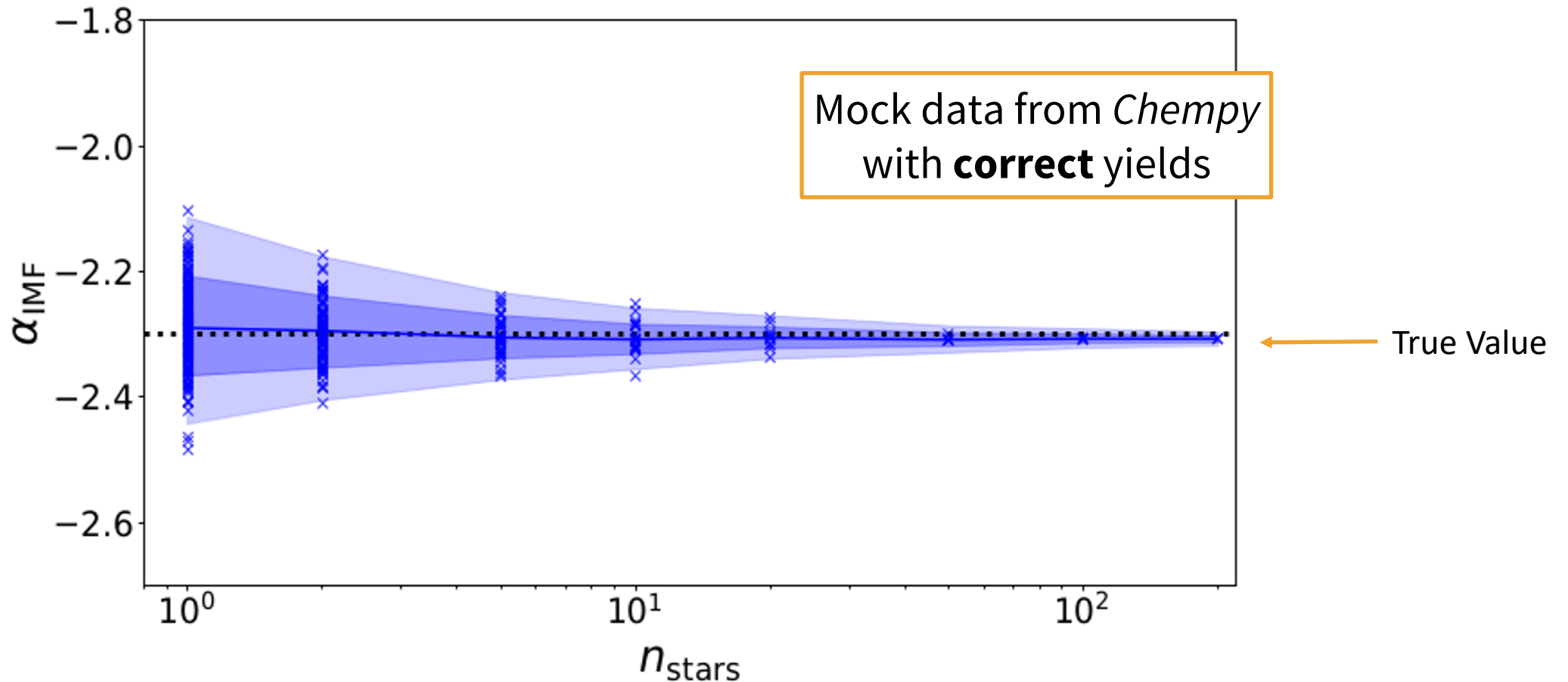
# Yield Table Scoring

Comparing Core-Collapse Supernovae Yield Tables using 28 Elements

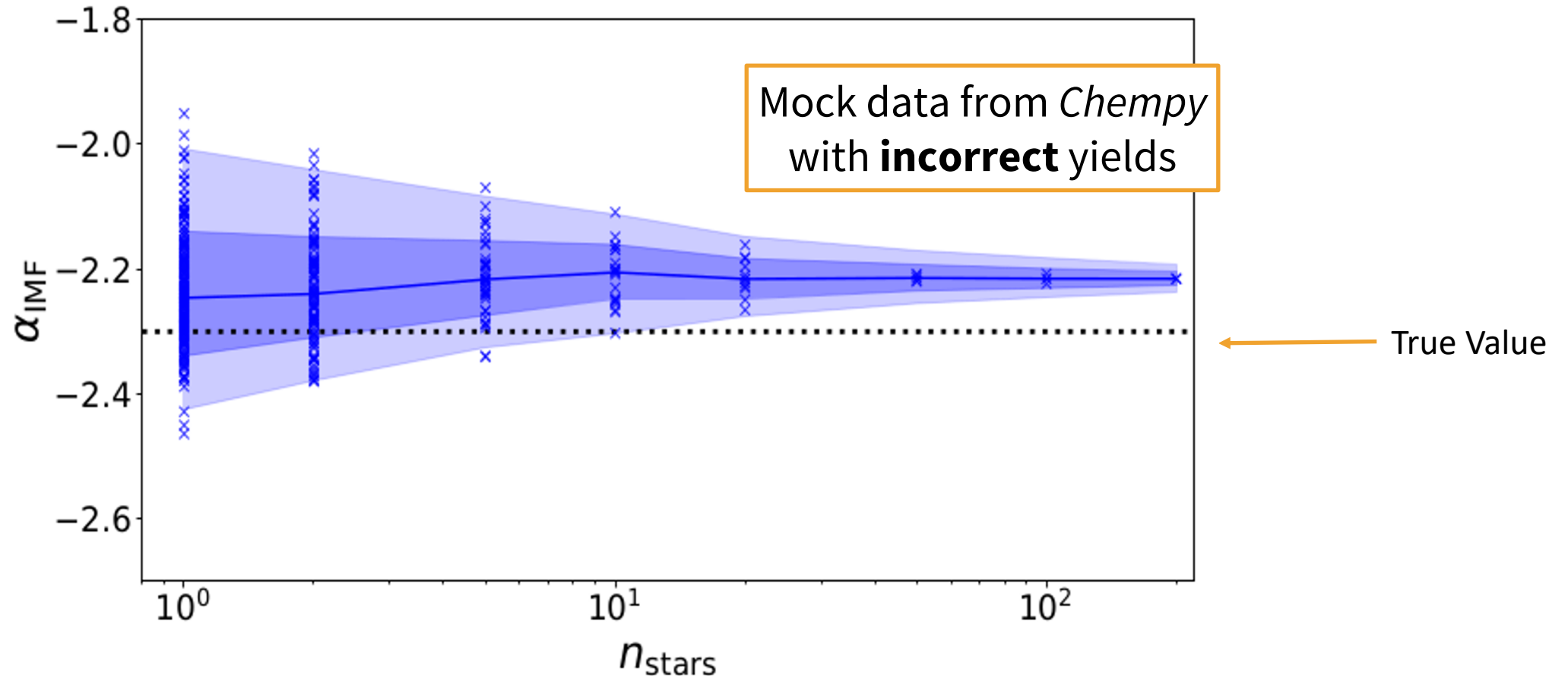
Yield Set	Bayes Score
C04	-1.21
N13	-5.69
W17	-0.78
R17	-6.11
P18	0.86

Nikos Prantzos' yields perform best here!

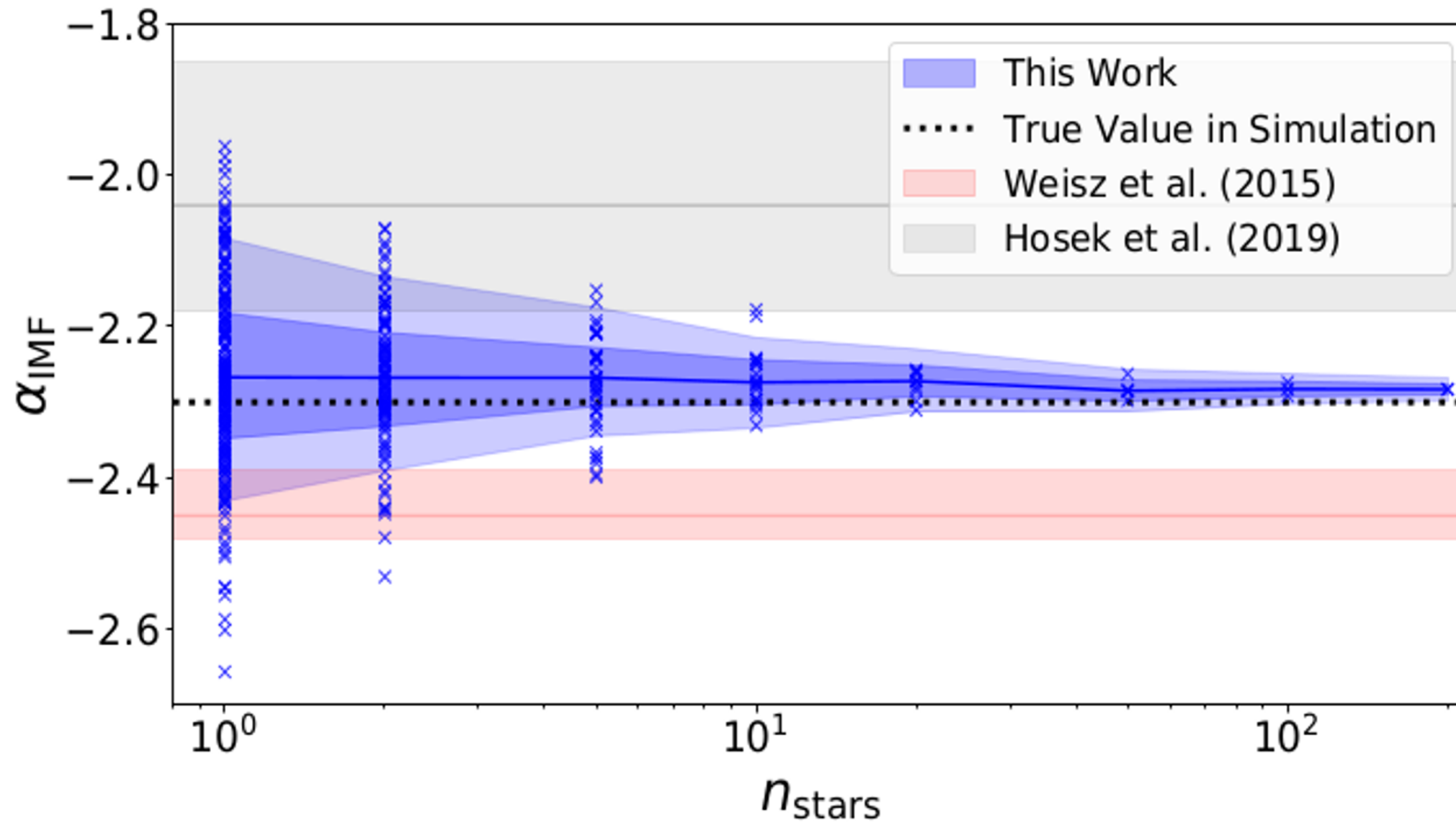
# Multi-Star Inference with *Chempy*



# Multi-Star Inference with *Chempy*



# Multi-Star Inference with *Chempy*

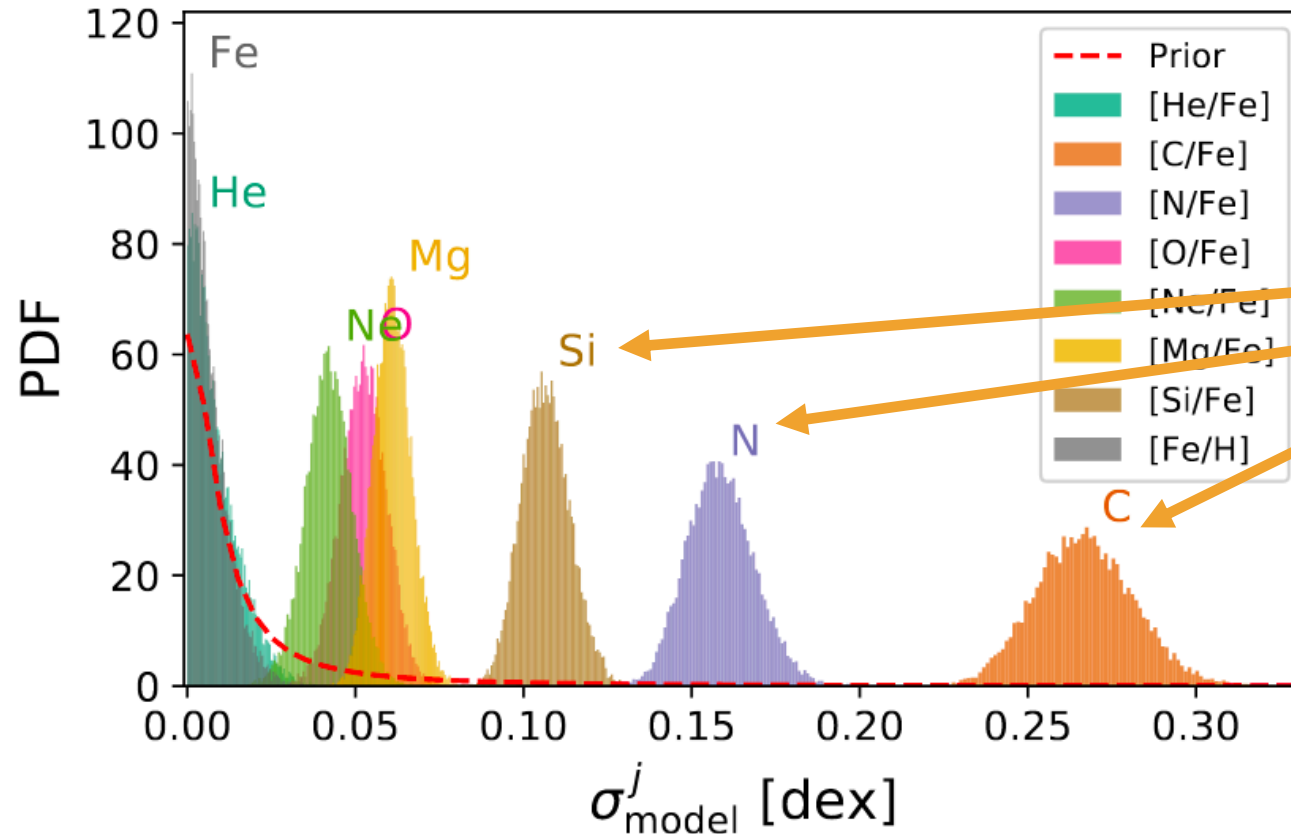


Mock data from **IllustrisTNG** with **correct** yields

# Multi-Star Inference with *Chempy*

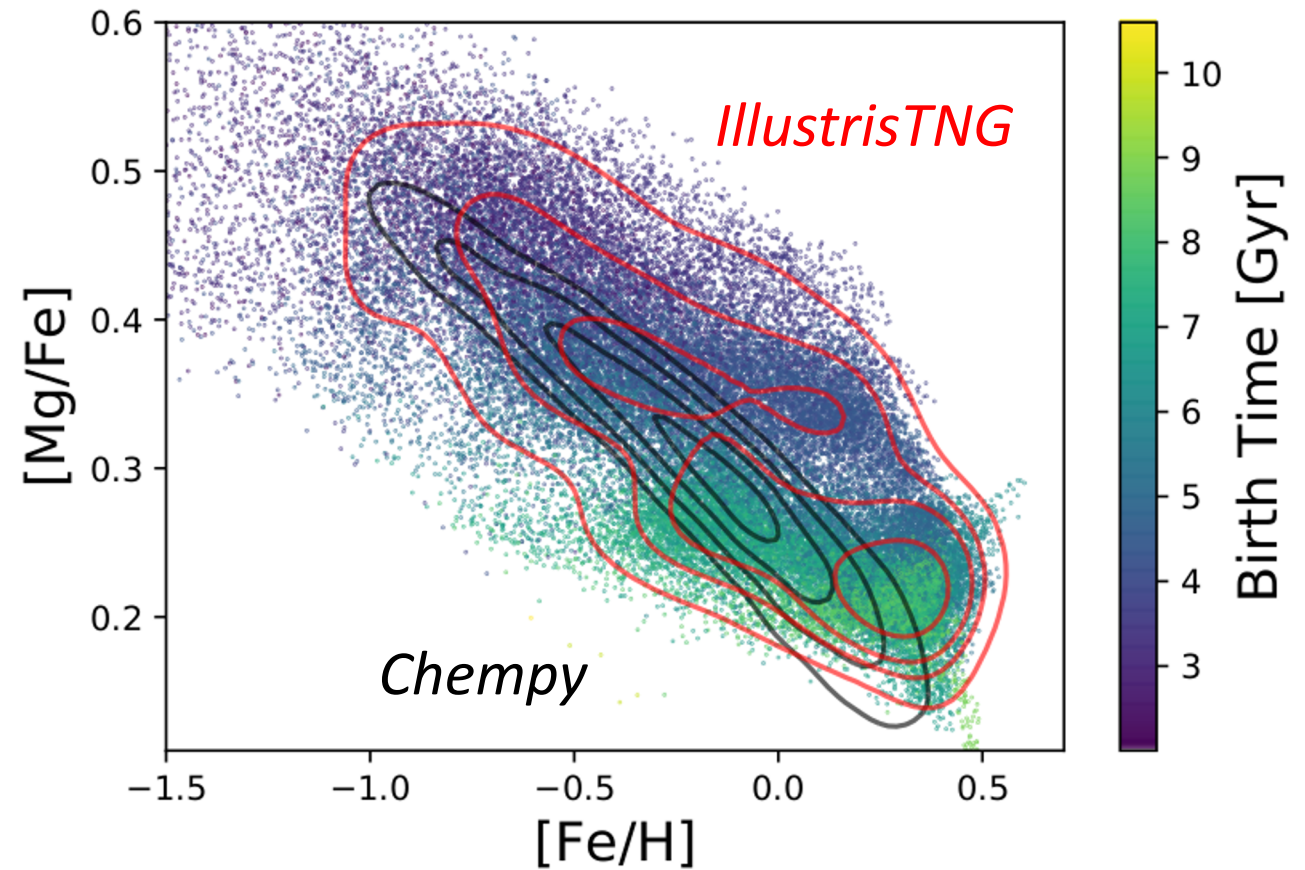
- ❑ **Model errors** indicate errors in our yield tables.

Model Error Distributions for analysis with **incorrect** yield set



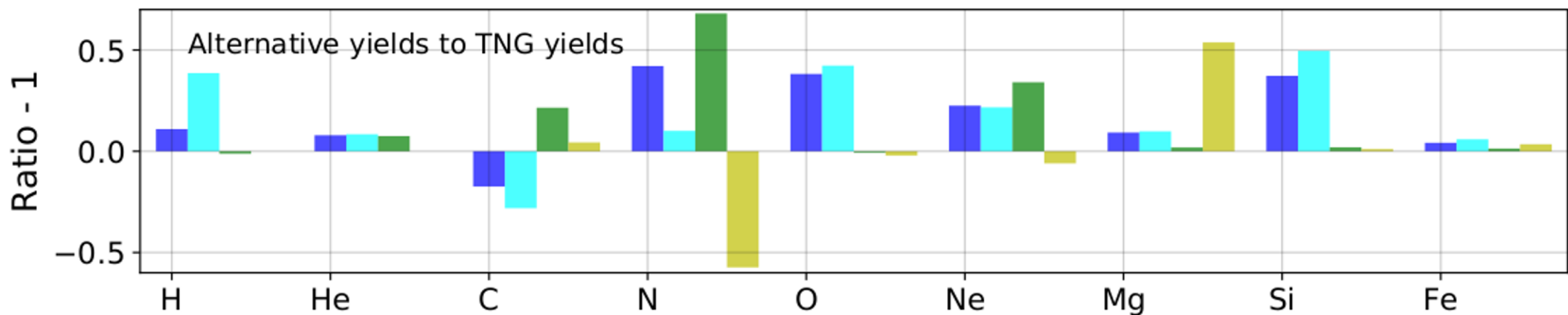
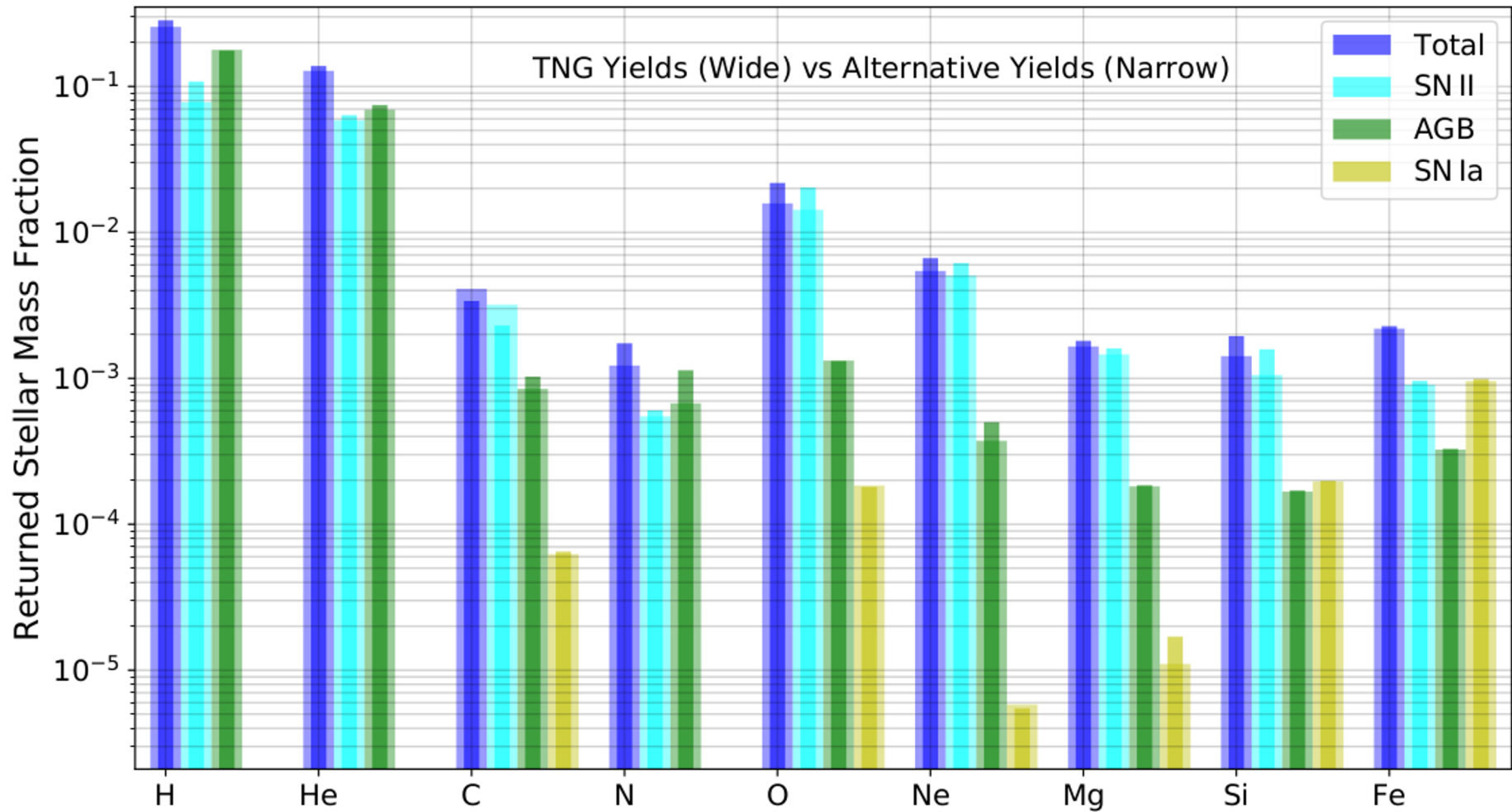
*Si, N and C are the most discrepant elements between our yield sets!*

# Abundance Diagrams

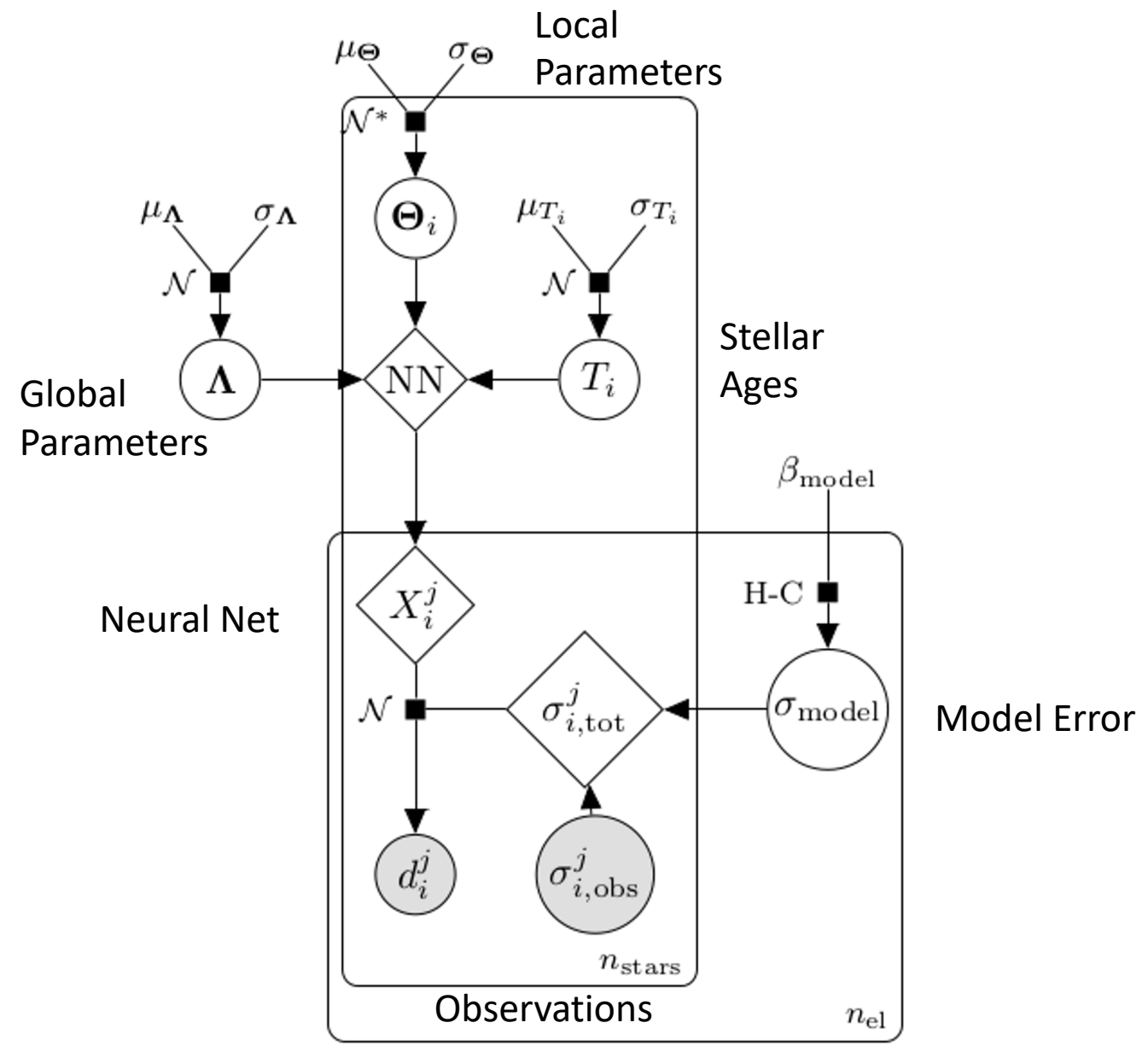




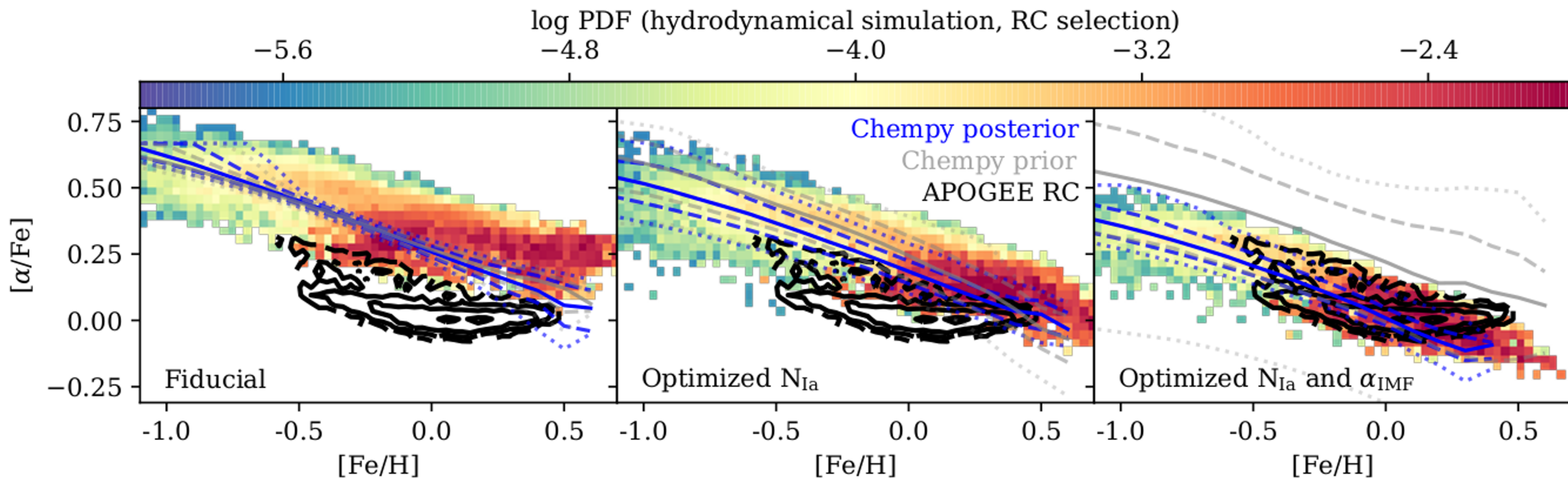
# Default and Alternative Yields



# ChempyMulti Architecture



# Full Hydrodynamical Simulation Optimization



# Full Corner Plot

