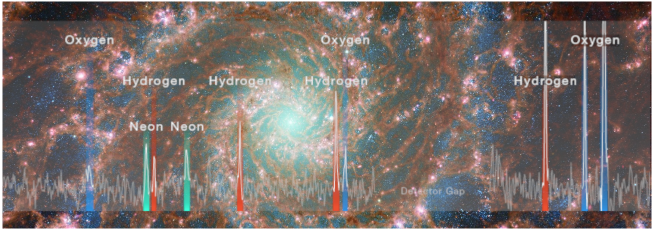
Multiline models of galaxies

Overview of modeling strategies using nearby galaxies as references

Vianney Lebouteiller (CNRS/AIM @CEA Saclay), prepared with Lise Ramambason (Univ. of Heidelberg)



△ Disclaimers

- Wide topic (like others) potentially related to many astrophysical questions
  - Despite my efforts, there will be some bias toward dwarf galaxies, low-metallicity, infrared spectroscopy, Bayesian statistics, and `Cloudy` models. . . !
- Not about ISM models per se particularly adapted to a given physical object/process within galaxies (e.g., PDR, molecular cloud etc. . . ; see presentations by B. Godard and P. Lesaffre) but about how to model multiple galactic components and processes
  - Mostly about models to match variety of lines & processes in large-scale/integrated observations
- Not about simulations, but about galaxy models that can be compared to individual, specific galaxies (and as a result also samples of galaxies)

△ Disclaimers

- Goal: provide some background and recent advances in order to
  - Be aware of biases and existing strategies/codes before choosing the modelling approach
  - Have a critical thinking of the results when reading papers or interpreting own results

- Some references/techniques presented here, but far from exhaustive

Outline

- General considerations and motivating questions
  - What are we trying to model?
  - Why are nearby galaxies useful
  - What physical processes to consider
  - What constraints
- Common diagnostics
- Modelling full galaxies, accounting for complexity of ISM and sources
  - Using 1D models
  - (BREAK?)
  - Evidence of mixing/smearing issues
  - Using >1D models & n x 1D models
  - Some results and ongoing works
- Statistical framework
  - Samplers
  - Model comparisons / decision tree
- Concluding remarks

Outline

- General considerations and motivating questions
  - What are we trying to model?

Galaxies are complex objects!

- Various kinds (dwarfs, spirals, Seyfert, mergers etc. . .)
  - What the object is when we observe it: result of integrated history of star-formation, active nuclear phases, interactions, gas exchange with CGM and IGM. . .
  - What we see: snapshot, often limited number of tracers due to incomplete wavelength coverage, extinction, signal-to-noise etc. . .

What is the object we are trying to model?

Not always easy to define a galaxy as a well-identified/circumscribed object, we limit ourselves to the object as it appears in some specific tracers or to sub-components $\Rightarrow$ Hard guess from unresolved observations

Fig.: *M82 galactic outflow observed with HST, Spitzer & Chandra.*

Fig.: *Extended UV & radio disk of M83 observed with GALEX & VLA.*

Physical processes act on various spatial scales

Observing in different tracers (e.g., Hα, CO, HI...) illustrate the complex ISM structure. Not always easy to link regions with a given excitation source

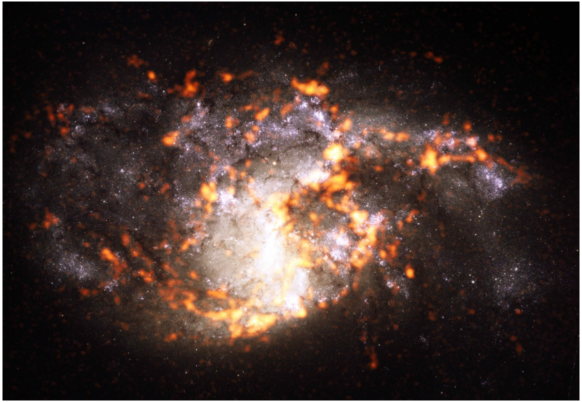


***Fig.**: NGC1385 with ALMA and HST (PHANGS; NRAO).*

Limited information

Distant galaxies are difficult to resolve (e.g., even with JWST), galaxy spectra are often spatially- and spectrally-unresolved

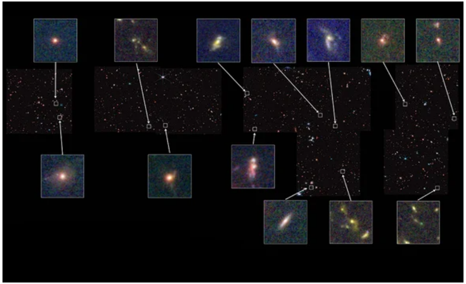
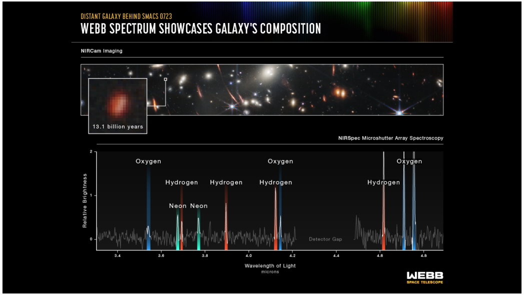


***Fig.**: JWST/NIRcam CEERS field. Credit: NASA/STScI/CEERS/TACC/S. Finkelstein/M. Bagley/Z. Levay; NASA/STScI/CEERS/TACC/S. Finkelstein/M. Bagley/J. Kartaltepe.*



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  - What are we trying to model?
  - Why are nearby galaxies useful

Why study nearby galaxies?

External galaxies in general

- Galaxy evolution (SFR, Z, M*, AGNs. . .) *(e.g., Kewley+ 2019)*
  - Mass-metallicity-SFR relation *(e.g., Nakajima+ 2023)*
  - Looking for metal-free gas in the reionization epoch *(e.g., Vanzella+ 2023)*
  - (see presentations by D. Dale, K. Sandström, B. Groves)
- Multiline modeling also tackles the specific role of ISM in galaxy evolution (e.g., SF)
  - e.g., role of H_2 in SF, tracers of H_2. . . *(e.g., Madden+ 2020)*
  - Cosmic evolution of the ISM as an astrophysical object like stars and compact objects

Nearby galaxies

- Great opportunity to understand extragalactic ISM in ≠ environments and to design relevant models
- Some galaxies nearby enough to spatially disentangle physical components
  - Modelling sum of individual regions vs. full galaxy? Do results change with spatial scale considered?

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Why study nearby galaxies: tracers!

- Some galaxies nearby enough to detect many tracers arising from different phases/physical processes
  - Observed tracers are signatures that reflect the complexity of the galaxy
  - Inversely: the complexity of the model physical representation of the galaxy needs to reflect these signatures (and hopefully those we don't observe)
  - What useful information from limited amount of tracers, do results change with choice of tracers? Should we consider simple models (despite unrealistic) when signatures are available?

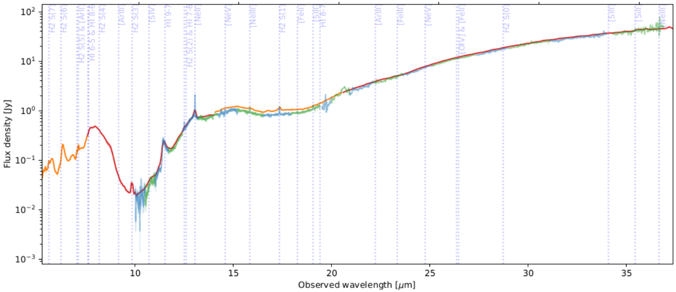

Fig.: *Arp 220 with Spitzer/IRS.*

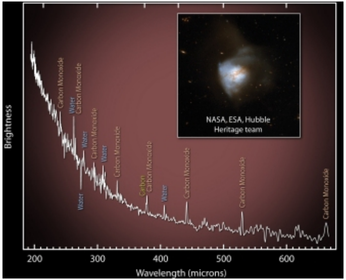

Fig.: *Arp 220 with Herschel/SPIRE (ESA).*

Why study nearby galaxies: we have interesting neighbors

- Some nearby galaxies probe quite different environments compared to MW (Z, SSCs, AGNs. . .)
  - Need some specific prescriptions (e.g., abundance patterns, D/G. . .)

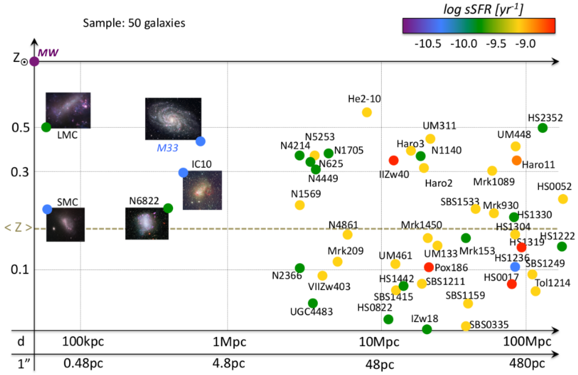

Fig.: Metallicity vs. distance for the Dwarf Galaxy Survey (Madden+ 2013; Cormier+ 2019).

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  - What are we trying to model?
  - Why are nearby galaxies useful
  - What physical processes to consider

Physical processes at work

Typical model parameters to distinguish

- Parameters that describe the matter (gas, dust, composition, spatial distribution. . .)
- Parameters that control the excitation of matter (radiative / mechanical energy)
- Parameters that link both (e.g., ionization parameter U = ionizing photon flux / nc = $Q(\mathrm{H})/4nc\pi r^2$)

Variety of radiative and mechanical feedback processes

- Ionization and heating of the various ISM phases (ionized, neutral atomic, neutral molecular)
- Young stars (UV, X-rays), WR, AGNs, X-ray binaries. . .
- Cosmic rays
- Turbulence and shocks
- Magnetic field
- Molecule formation/destruction. . .

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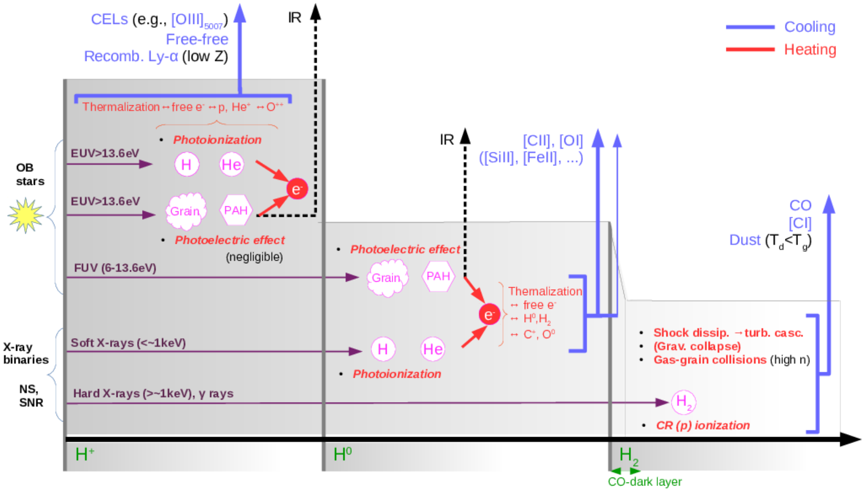
Illustration: 1D model



Some approximations

Assuming local conditions and snapshot

- Difficult to do everything right: turbulence, magnetic field, time evolution, chemical network. . .
  - Often relying on specific galaxy regions or galaxies dominated by some process

- Typical timescale problems: disconnection between radiative phases of AGNs or X-ray binaries (state transitions) and observed ISM tracers
  - Non-isotropic emission, light propagation, heating & cooling timescales. . .
  - For simplicity: inferred properties of transient objects reflect conditions seen by the matter when it cools down and not those inferred from the compact object itself

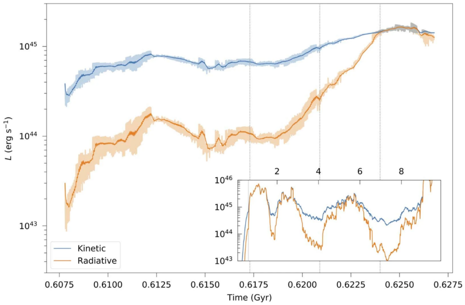


***Fig.**: Evolution of AGN feedback luminosity in zoom-in simulations for a varying SMBH accretion rate (Qiu+ 2020).*

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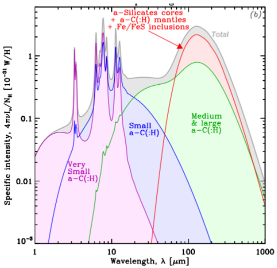
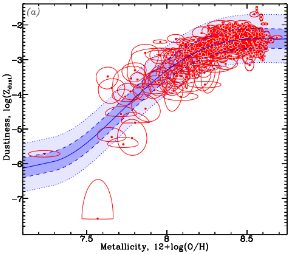
What constraints?

Dust

- Dust essential ingredient of models (Presentation by N. Ysard)
- Dust SED holds much information
  - Local physical conditions, $T_{\rm dust}$, $M_{\rm dust}$, $M_{\rm gas}$ through D/G. . . *(e.g., Galliano+ 2021)*
- Difficult to disentangle ISM phases (e.g., those associated or not with SF), especially in integrated galaxy spectra

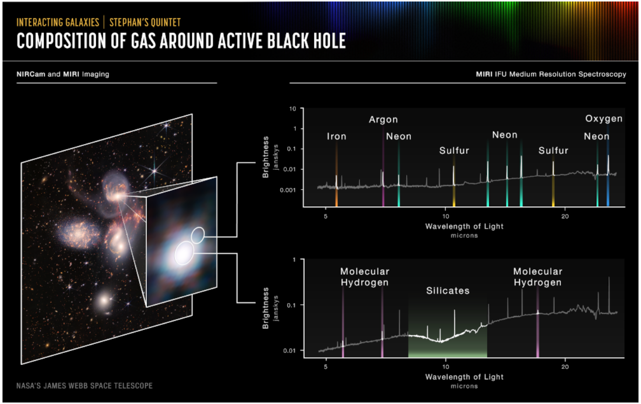




What constraints?

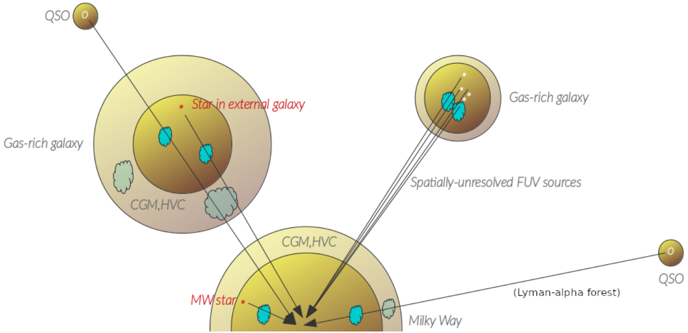
Line spectroscopy

- Gas tracers may constrain:
  - Specific phases: hydrogen (H^+, H^0, H_2), metal ionization (e.g., (OIII)/(OII)...), density (e.g., (SII), (SIII)),
  - Specific excitation mechanisms (X-rays, shocks... e.g., (NeV))
  - Sometimes in a single spectrum



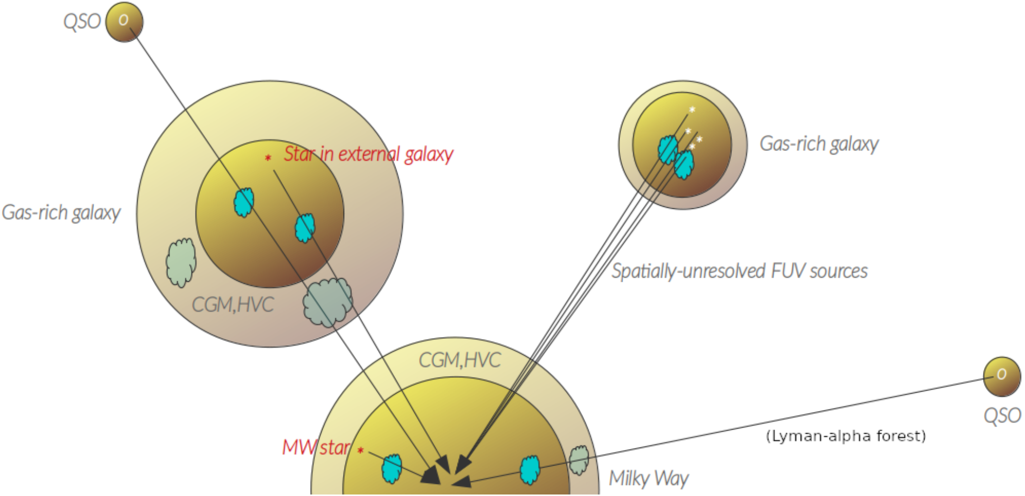
Absorption spectroscopy

- Absorption spectroscopy is very useful for chemical composition, D/H, depletion patterns, cooling rates, molecular gas fraction, even CO-dark H_2 *(Balashev+ 2017, 2020, 2022)*
  - But limited to single line of sight (LOS) or LOS averages (for which there is mixing)
  - Comparison absorption/emission not straightforward *(e.g., Arabsalmani+2023, Wilson+ 2023)*
  - $\approx 5^{+5}_{-0}$ US presidents in the future: HabWorlds Observatory for LOS mapping



- Will focus on emission lines here, it's complicated enough

Absorption spectroscopy



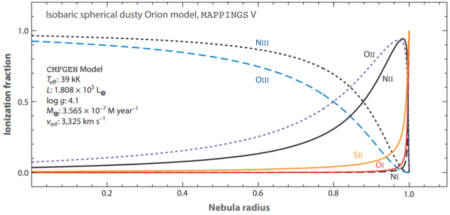
Worth noting. . .

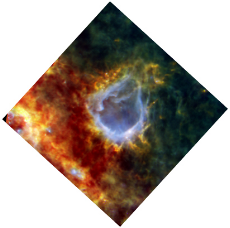
It's obvious but. . . we model what we can see. . .

- Diagnostics are valid only for the regions that are emitting!
- Results may thus be biased by selection effects of emitting components, by extinction
  - As much as possible, such effects need to be accounted for a priori or within models
- What are the possible processes (model ingredients) that can contribute to what we see?
  - We may limit ourselves to assumptions based on current knowledge, but useful to explore a priori unexpected processes as well

. . . and emission arises from different regions. . .

- For instance, the (SII) optical line ratio diagnostic is indicative of density around ionization fronts





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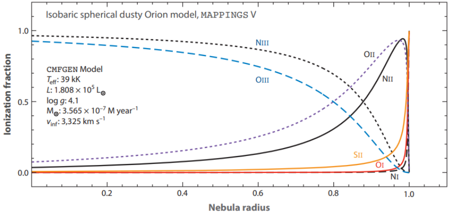

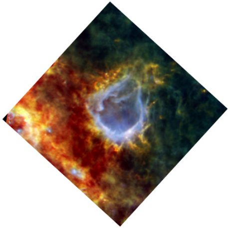

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Typical empirical diagnostics using emission lines

Many signatures potentially available to constrain galactic parameters and physical processes

- Primary ingredients of models may be the ultimate goal (e.g., gas density n, metallicity Z)
- Or other physical parameters can be deduced if the "right" processes have been considered
  - either in a relatively trivial way: e.g., SFR, $M(\mathrm{H}^+)$, AGN fraction...
  - or not: f_{esc}, $M(\mathrm{H}_2)$...

Many, many potential diagnostics through spectroscopy of galaxies

- Historically, long-slit or integrated spectroscopy of galaxies used to probe average physical conditions / chemical composition / dominant excitation sources :
  - Gas (electron) density & pressure, ionization parameter from line ratios *(e.g., Kewley+ 2019)*
  - Chemical composition (abundances, metallicity, depletion patterns) *(e.g., Dopita+ 2016)*
  - SFR (e.g., Hα, far-IR lines, 24 μm...) *(e.g., de Looze+ 2017)*
  - BPT (Baldwin–Phillips–Terlevich) & AGN fraction (excitation diagram) vs. mass, vs. z
- Coronal lines indicating unambiguous AGN activity *(e.g., CLASS survey, Reefe+ 2022)*
- UV ($\sim$1400-1900Å) diagnostics to distinguish SF, AGN, and shocks *(e.g., CLASSY survey, Mingozzi+ 2023)*

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Illustrations: electron/gas density diagnostics

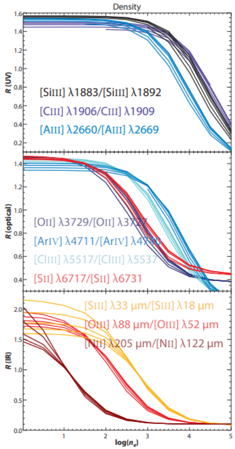

***Fig.**: Density diagnostics for UV, optical, and IR line ratios (Kewley+ 2019).*

Illustrations: excitation mechanisms

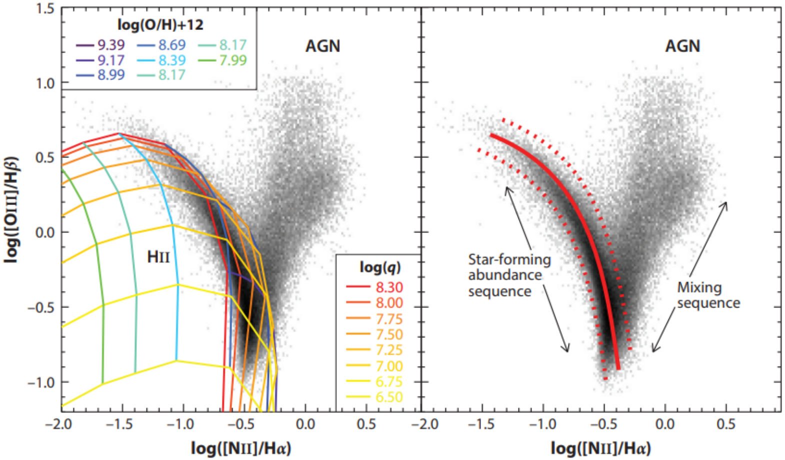

***Fig.**: BPT diagram with optical lines (Kewley+ 2019).*

Illustrations: AGN fraction

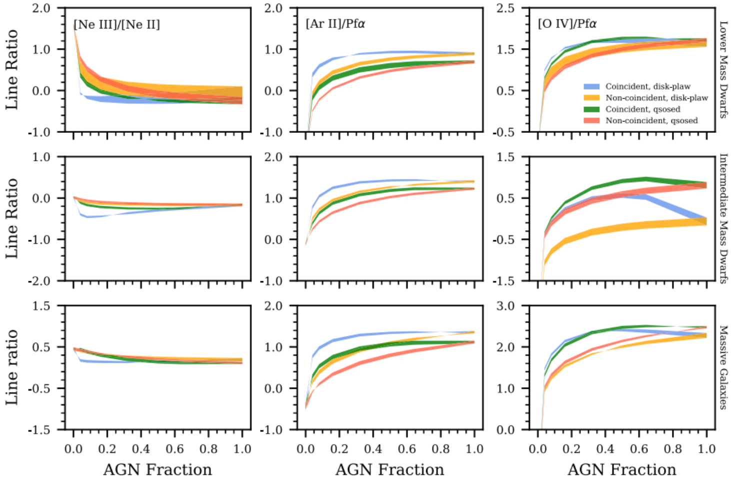

***Fig.**: JWST MIRI line ratios vs. AGN fraction for a given BH mass and for various geometries (Richardson+ 2022).*

Illustrations: AGN activity

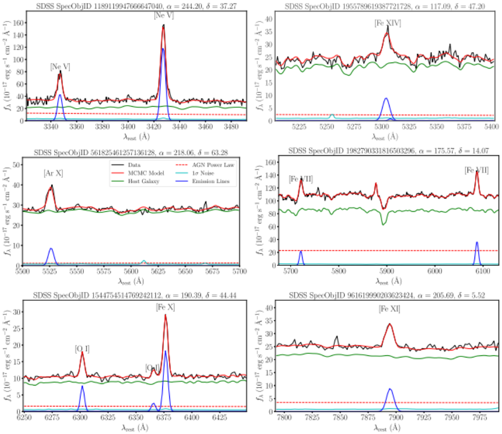

Fig.: Coronal lines in SDSS probe the relatively harder BH spectrum in low-mass galaxies and probe AGN activity where optical diagnostics suggest SF (Reefe+ 2022).

Illustrations: disentangling excitation mechanisms

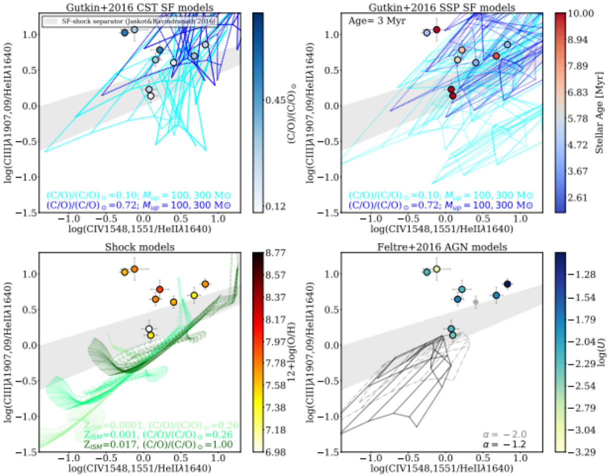

Fig.: *UV diagnostics to distinguish SF, AGN, and shocks (Mingozzi+ 2023).*

Spectroscopic diagnostics have a bright future

Wide-field/all-sky optical and near-IR spectroscopic surveys

- SDSS-V 2020-, Euclid 2023-2030, Rubin 2024-2033, Roman 2026-2032, SPHEREx >2025
- Millions of spatially-resolved and integrated spectra, including mostly dwarf galaxies as well as low-surface brightness galaxies for a wide redshift range

IR spectroscopy

- JWST is observing much fainter IR lines compared to *Spitzer* $\Rightarrow$ new diagnostics
- Mid/far-IR spectra @z=0 mostly not resolved with *Spitzer*, *Herschel*, same for a potential future IR NASA probe-class mission (waiting for IR space interferometry. . .)

High-z spectroscopy

- JWST is providing optical diagnostics at very high-z, spatially unresolved $\rightarrow$ ELT
- Exciting JWST+ALMA synergies, ALMA high-z galaxies already show multi-phase ISM *(e.g., Fujimoto+ 2022)*
- UV diagnostics shift to NIRspec when optical ones shift to MIRI *(CLASSY; Mingozzi+ 2023)*

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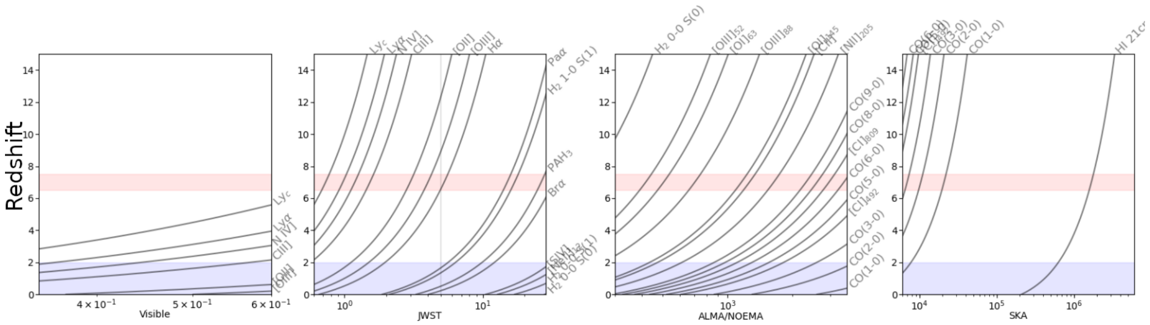
Tracers vs. z



- Sweet spot $z \lesssim 2$ (UV → opt., opt. → NIRspec, near-IR → MIRI, CO ladder with ALMA)
- Sweet spot $z \sim 7$ (UV → NIRspec, far-IR → ALMA, CO → SKA)
- Far-IR diagnostics will remain unvailable at z∼0 until potentially PRIMA
- Mid-IR diagnostics will remain unavailable at z∼2-10 until potentially PRIMA

Same diagnostics with integral field spectroscopy (IFS)

Some instruments and surveys

- SDSS-IV MaNGA, VLT/MUSE, GTC/MEGARA, JWST/MIRI MRS. . .
- Local Universe: SAURON *(de Zeeuw+ 2002)*, ATLAS3D *(Cappellari+ 2011)*, CALIFA *(Sánchez+ 2012)*, SAMI *(Croom+ 2012)*, MaNGA *(Bundy+ 2015)*, PHANGS-MUSE *(Emsellem+ 2021)*. . .
- High-redshift: KMOS3D *(Wisnioski+ 2015)*, SINS/zC-SINF *(Förster Schreiber+ 2018)*. . .
- Future: VLT/BlueMUSE, SDSS-V Local Volume Mapper, ELT/METIS,HARMONI. . .

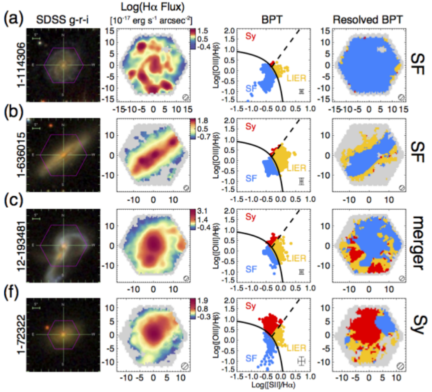
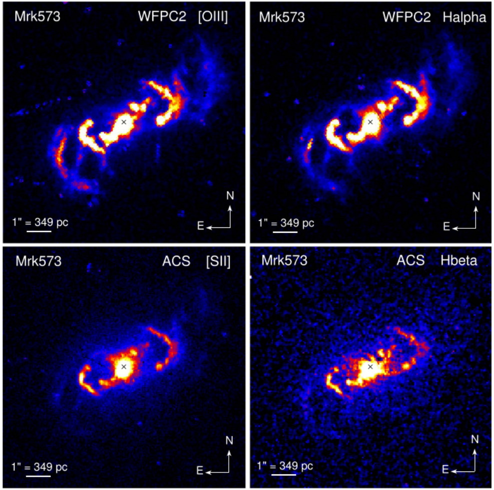


Fig.: Spatially resolved excitation properties of the ionized gas with SDSS/MaNGA (Belfiore+ 2016). LIER component in SF galaxies ∼ DIG.

Narrow-band imaging



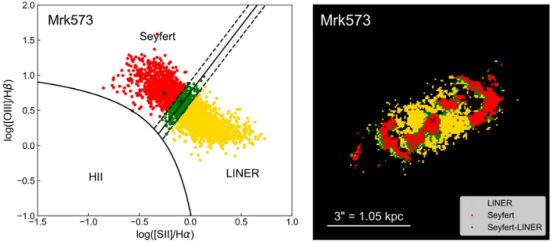


***Fig.**: Spatially resolved BPT mapping of the extended narrow-line regions of nearby Seyfert 2 galaxies with HST (Ma+ 2021).*

How to make the best of existing and future observations

Empirical diagnostics

- We need to understand potential biases, selection effects, and the meaning of average quantities
- We need to design new empirical diagnostics for future observatories with the help of state-of-the-art models

Some complex parameters require full-on models

- Masses (H^+, H^0, H_2...)
- Tracers of $M(H_2)$: (CII) 158 μm, (OI) 63 μm, OH, HD...
- ISM structure (clump distribution, escape fraction of ionizing photons...)
- Multi-phase observations in general
- Ideally at any redshift!

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- We need to design new empirical diagnostics for future observatories with the help of state-of-the-art models

Some complex parameters require full-on models

- Masses (H^+, H^0, H_2...)
- Tracers of $M(H_2)$: (CII) 158 μm, (OI) 63 μm, OH, HD...
- ISM structure (clump distribution, escape fraction of ionizing photons...)
- Multi-phase observations in general
- Ideally at any redshift!

Outline

- General considerations and motivating questions
  - What are we trying to model?
  - Why are nearby galaxies useful
  - What physical processes to consider
  - What constraints
- Common diagnostics
- Modelling full galaxies, accounting for complexity of ISM and sources
  - Using 1D models
  - Evidence of mixing/smearing issues
  - Using >1D models & n x 1D models
  - Some results and ongoing works
- Statistical framework
  - Samplers
  - Model comparisons / decision tree
- Concluding remarks

Outline

- General considerations and motivating questions
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Some specific "favorable" cases (still complicated!)

Favorable geometries

- Spatially-resolved individual regions (single HII region, single molecular cloud)
- HII galaxies, AGN-dominated galaxies. . . ⇒ single ionizing source

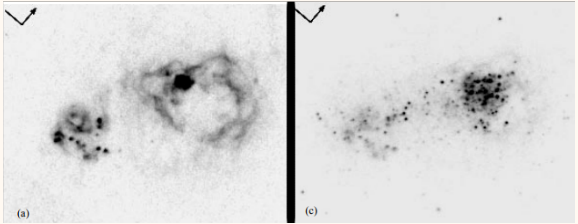

***Fig.**: Ionized gas filaments surrounding a young stellar cluster in the dwarf SF galaxy IZw18, very favorable geometry for models! (Cannon+ 2004).*

- 1D model with spherical geometry or full 3D model can be envisioned (e.g., `Cloudy 3D`, M^3)

Messenger Interface Monte Carlo MAPPINGS V (M^3; *Jin+ 2022*)

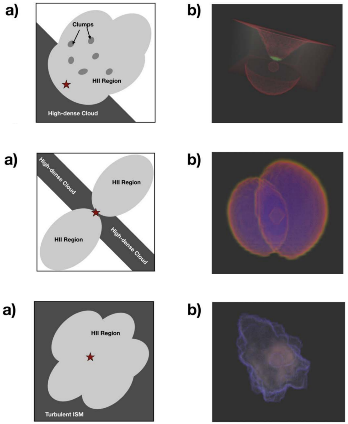

***Fig.**: Modeling nebulae with arbitrary 3D geometries (Jin+ 2022).*

Cloudy 3D/pyCloudy *(Morisset+ 2013)* and PyCROSS *(Fitzgerald+ 2020)*

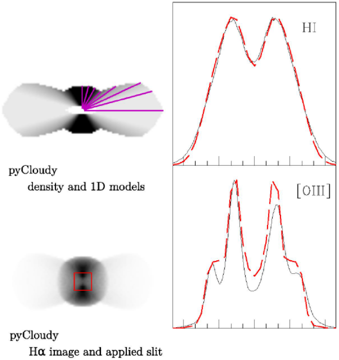

Fig.: *Pseudo-3D models: set of n 1D models following angular laws, populating emissivity cube and projecting (Morisset+ 2013; PN application in Gesicki+ 2016).*

Modeling full galaxies with single 1D models: some codes

1D (or 2D) line and dust RT models

- RADEX *(van der Tak+ 2007)*, RADMC *(Dullemond and Dominik 2004)*. . .
- With LTE or simple non-LTE approximations (such as escape probability or Large velocity gradient - LVG methods)
- No photoionization and no chemistry
- Potentially spherically symmetric
- ⇒ Constraints on physical conditions such as N, n, and T through generation of synthetic spectra & grids

1D photoionization and photochemistry steady-state models

- Cloudy *(Ferland+ 2017)*, MAPPINGS V *(Binette+ 1985, Sutherland+. 2018)*, Meudon PDR *(Le Petit+2006, Bron+ 2016)*. . .
- ⇒ long to run! (e.g., OTF MCMC is difficult)
- Main focus in this presentation

Modeling full galaxies with single 1D models: some codes

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Modeling full galaxies with single 1D models: applications

Applications

- Useful to link observables to "average" physical conditions
- Physical conditions may be interesting by themselves (n, U...) but we're also eventually interested in other resulting parameters (mass of gas, SFR, f_{esc}...)
  - Some codes provide plenty of interesting output quantities from which we can examine things like the formation pathways of H_2, X-ray photoionization etc...

- Single 1D: assuming co-spatial excitation sources (all stellar clusters, potentially AGN – i.e., with coincident mixing)

Prescriptions for photoionization/photodissociation codes

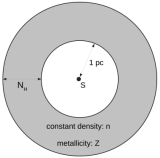
Required prescriptions for models

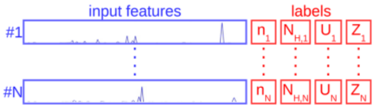
- Abundance patterns, D/G, dust properties. . .
- Equation of state
  - Constant pressure (e.g., Orion, but also for diffuse and translucent clouds; *van Dishoeck and Black 1986*)
  - High densities quickly reached and not well adapted to average galaxy properties. Some alternatives: density scaling with N(H), magnetic field pressure term, pseudo constant pressure. . .
- Shocks: complicated, can use a mechanical heating term (e.g., from SNe rate) flat or not with depth
- CR: nearby starbursts and ULIRGs all suggest MW-like range values $10^{-16,-13}$ s^{-1} with higher values in nuclei and regions with intense SF *(Indriolo+ 2012, 2018; Oka+ 2019; van der Tak+ 2016; Holdship+ 2022; Gonzalez-Alfonso+ 2018)*
- Heavy dependence on stellar atmospheres: BPASS, new versions to test each time. . .

- Extremely low Z: little knowledge on dust opacity curves, CR, stellar atmospheres

Examples: machine learning (ML) techniques

- Supervised ML technique with GAME (GAlaxy Machine learning for Emission lines; *Ucci+ 2017*)





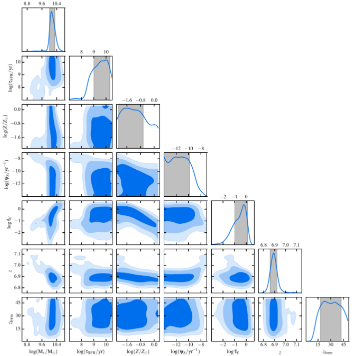
Details

- Library of synthetic spectra assuming very simple, single, 1D models (spherical geometry)
- Z, U, $N(\mathrm{H})$ predictions from an arbitrary suite of emission lines
- Great performance for a large number of tracers (better than Bayesian techniques in that regard)
- Possible application to IFS observations *(Ucci+ 2019)*

Examples: probablistic methods

Going Bayesian with BEAGLE (BayEsian Analysis of GaLaxy sEds; *Chevallard and Charlot 2016*)

- Using *Gutkin+ (2016)* models that combine stellar population synthesis and photoionization codes to describe an ensemble of HII regions and diffuse gas ionized by young stars
- Effective HII region: all HII regions and DIG ionized by a single stellar generation with a set of effective parameters
  - Strong – though classic – assumption
  - Collection of isolated HII regions currently being investigated
- Geometry accounted for by dust attenuation for stellar+nebular emission (inclination, disk, bulge)
- Powerful algorithm including instrumental effects
- Using nested sampling techniques to account for multi-modal posterior distributions

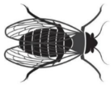


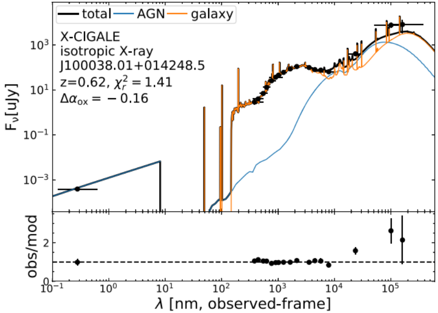
Examples: probablistic methods

Going Bayesian with the Code Investigating GALaxy Emission (`CIGALE`; *Burgarella+ 2005*)

- Relying on energy balance principle (absorption by dust in UV-optical vs. re-emission in IR)
- Using geometry templates for dust attenuation
- Detailed treatment of X-ray sources: `X-CIGALE` *(Yang+ 2022)*
- Nebular emission treated *(Boquien+ 2019)* to decontaminate broadband photometry
  - Line predictions for HII region + PDR under development

- ⇒ Hands-on project @GISM2

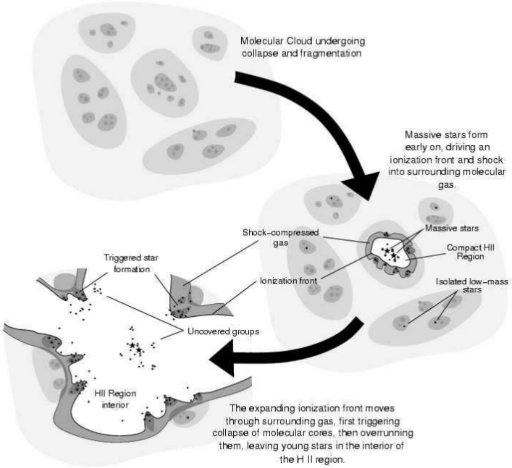




Limitations of single 1D models

- Like all static nD models, cannot capture the complex and dynamic structure of the ISM along with all of the relevant, time-varying star formation and feedback
- 1D models assume co-spatial sources / effective galactic-wide parameters
- Like all parameterized models: wide range of theoretically allowed parameters
- Distribution/geometry of gas is difficult to implement (e.g., HII region, PDR, molecular cloud)

Limitations of single 1D models



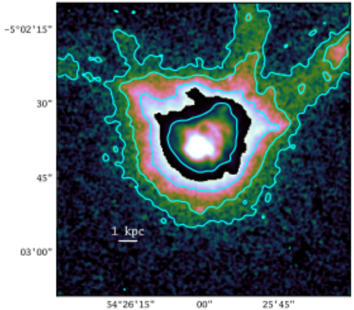
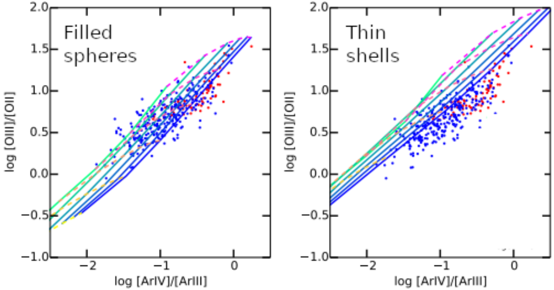


Fig.: *Left: evolution of HII regions (Hester and Desch 2005). Right: Escaping photons channels through (OIII) with MUSE (Herenz+ 2020).*

Possible tweaks to single 1D model approaches

- Accounting for different (spherical) geometries
- Accounting for holes and/or matter-bounded (aka density-bounded) models
- Accounting for time evolution

Assumption of geometry



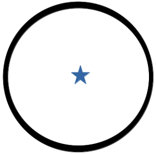


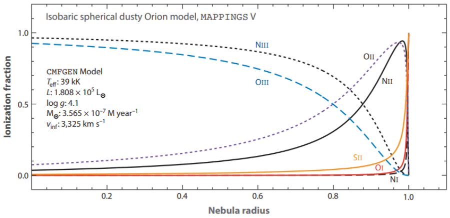
***Fig.**: Line ratio diagnostic line assuming different spherical geometries (Stasinska+ 2015).*

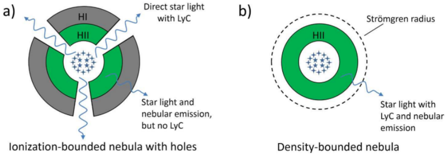
- Playing with geometry not enough to reproduce low values of (OI)/(OIII) in LyC-leaking galaxies or (CII)/(OIII) in high-z galaxies

Accounting for holes and/or matter-bounded models

BPT-like diagnostics & metallicity diagnostics

- Matter-bounded nebula produce the "normal" amount of (OIII) close to the stars, but some H RL-emitting regions are missing further out ⇒ (OIII)/Hβ $\nearrow$
- Matter-bounded nebula lack low-ionization lines (e.g., (NII), (SII)) emitting regions





Escape fraction of ionizing photons

- As a result, weak low-ionization lines may be used to identify potential leakers (e.g., Wang+ 2020, 2021, Zackrisson+2013, Ramambason+ 2020, 2022)

Accounting for holes and/or matter-bounded models

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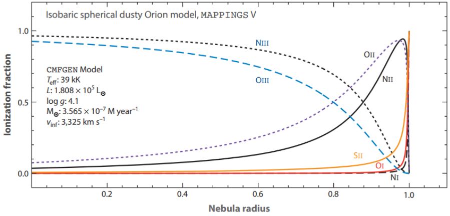
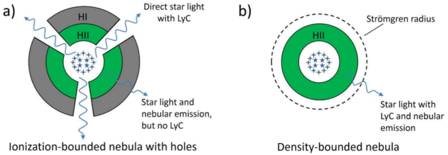




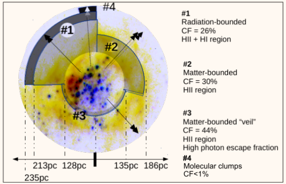
Escape fraction of ionizing photons

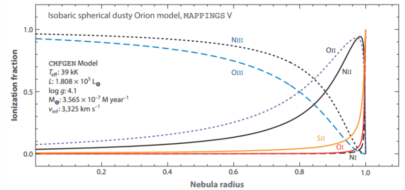
- As a result, weak low-ionization lines may be used to identify potential leakers *(e.g.,, Wang+ 2020, 2021, Zackrisson+2013, Ramambason+ 2020, 2022)*

Accounting for matter-bounded models

Once upon a time

- Long-standing high T_e([OIII]) problem in dwarf galaxy IZw18: extra heating due to stellar winds, SNe, shocks?
  - T_e constrained by [OIII]λ4363Å/([OIII]λ5007Å+[OIII]λ4959Å) and depends on local density
  - Density from [SII] is not representative of the ionized nebula





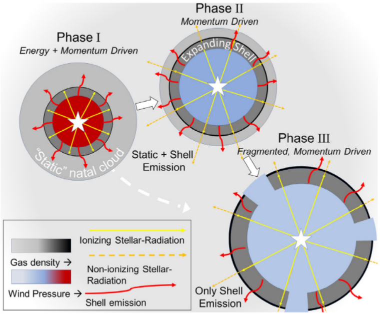
- *Péquignot (2008)*: radiation-bounded shells embedded in a matter-bounded medium produces a lower mean density and higher $T_e \Rightarrow$ photoionization by (non-population III) hot stars is enough!
- Introducing "topological models", i.e., combination of 1D models

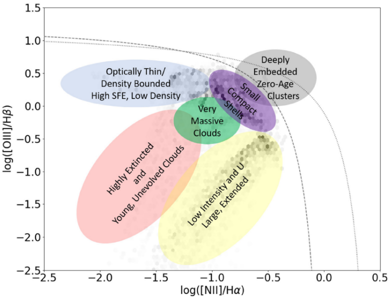
Accounting for time evolution of single HII region + PDR

△ Requiring coupling with time-dependent models

1D spherical with time-evolution

- WARPFIELD-EMP *(Pellegrini+ 2020)* couples the 1D stellar feedback code WARPFIELD with the Cloudy HII region/PDR code and the POLARIS line and continuum RT code, in order to make detailed predictions for the time-dependent emission arising from the HII region and PDR surrounding an evolving star cluster





Break

- Questions
- Take a good breath
- (Wake up?)

Outline

- General considerations and motivating questions
  - What are we trying to model?
  - Why are nearby galaxies useful
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- Common diagnostics
- Modelling full galaxies, accounting for complexity of ISM and sources
  - Using 1D models
  - Evidence of mixing/smearing issues

Mixing

- Eventual goal: build a comprehensive model able to explain the multi-phase signatures and able to account for complex ISM/source geometries
  - Unresolved spectroscopy is often inevitable (e.g., high-z galaxies, some specific wavelength domains)

Components

- Galaxies in general do include:
  - A collection of HII regions following some luminosity function, some leaking ionizing photons – possibly super-stellar clusters as well ⇒ Q, U mixing
  - A distribution of gas following some density PDF related to turbulence, self-gravitation, and rotational support *(e.g., Khullar+ 2021)* ⇒ n, P mixing (biases depend on critical densities)
  - A collection of molecular clouds, some associated with recent SF
  - WR stars, high-mass X-ray binaries and possibly AGN

Mixing: distributions

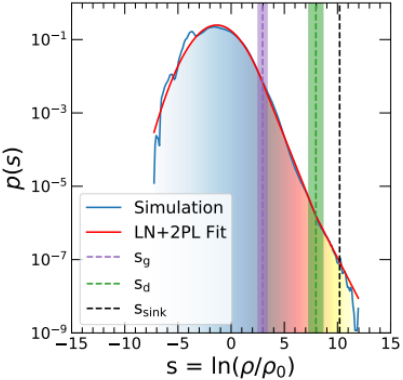


***Fig.**: Density PDF from simulations with 3 regimes associated with turbulence, self-gravitation, and disc/rotation (Khullar+ 2021).*

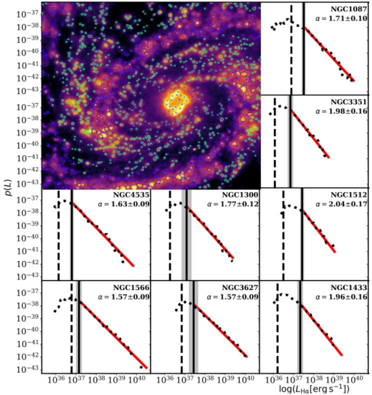
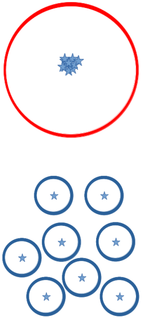


***Fig.**: HII region luminosity function in PHANGS-MUSE galaxies (Santoro+ 2022).*

Mixing: effective HII region vs. collection of HII regions

- Stellar population radiation field (BPASS), potential X-ray source, fixing all but *U* and SED shape (age)
- (Don't read too much into this, depends a lot on how models are designed)



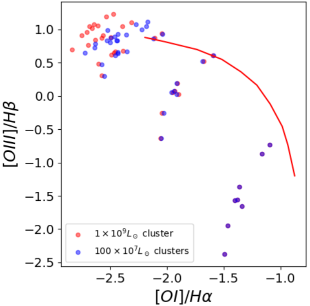


***Fig.**: Globally high-density regime, same volume. But same parameters lead to different line fluxes for high U values (thinnest nebulae; dust absorption).*

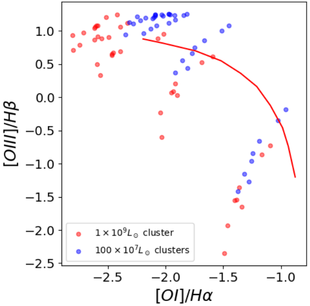
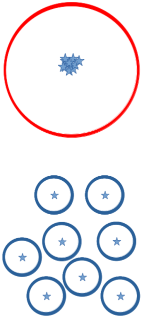


***Fig.**: Absorption of X-rays doesn't follow the same "rules" as UV photons. Line ratios cannot be recovered even choosing a different U value, this is a geometry effect.*

Mixing: effective HII region vs. collection of HII regions

- PDR diagnostics (no X-ray source)



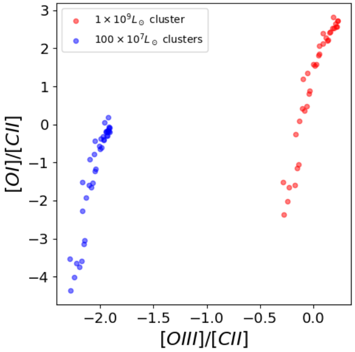


Fig.: *The effective region model would need a much lower density to match better with collection of models.*

Mixing: (non-)coincident AGN/SF mixing

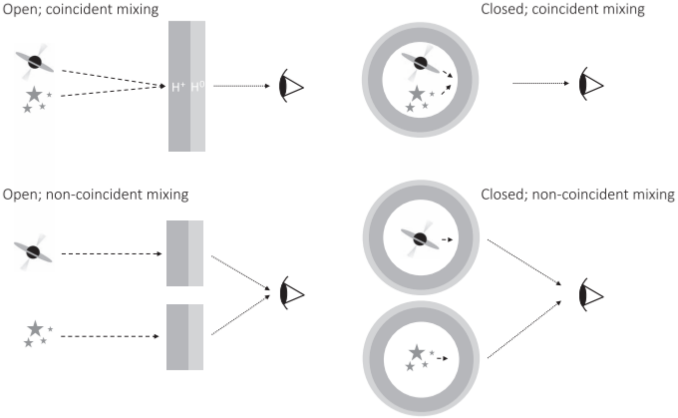
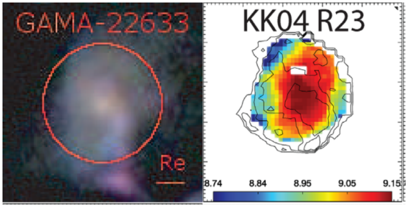


Fig.: *Different geometries for AGN and SF excitation (Richardson+ 2022).*

Evidence of inhomogeneities

- IFS observations reveal the mixing, AGN contribution, metallicity variations. . . within galaxies. This should be kept in mind when modelling a spatially-unresolved galaxy
- Kewley+ (2019): *"For example, the global metallicity of a high-redshift galaxy may not be the true mean metallicity but may be weighted toward specific HII regions with certain sets of properties."*



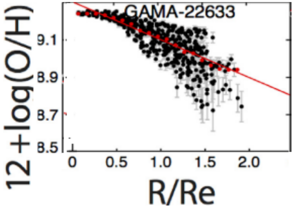


***Fig.**: Metallicity gradient and dispersion in SAMI galaxies (SF face-on spirals; Poetrodjojo+ 2018).*

Biases due to smearing and selection effects

IFS results

- M* can be severely underestimated (factors up to 5) using the integrated SED due to the bias of young stars dominating the SED *(Sorba and Sawicki 2015, 2018)*
  - See also *Galliano+ (2011)* for dust mass estimates vs. spatial resolution in LMC
- Detailed study of biases due to beam smearing for spectroscopic diagnostics still limited (e.g., Z, SFR, $M(\mathrm{H}^+)\ldots$)
  - Note that a single 1D component always imply some kind of bias for a single pixel in IFS observations (e.g., SAMI, MUSE. . .) ⇒ Longitudinal mixing and spatial disconnection between excitation source and matter that may lie in different pixels

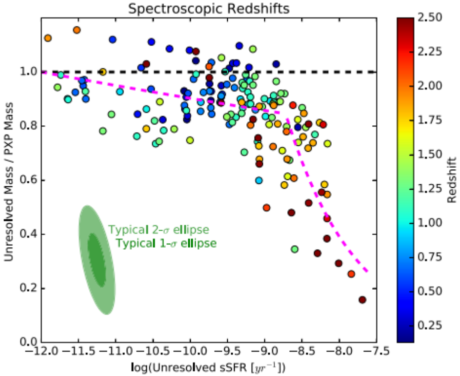
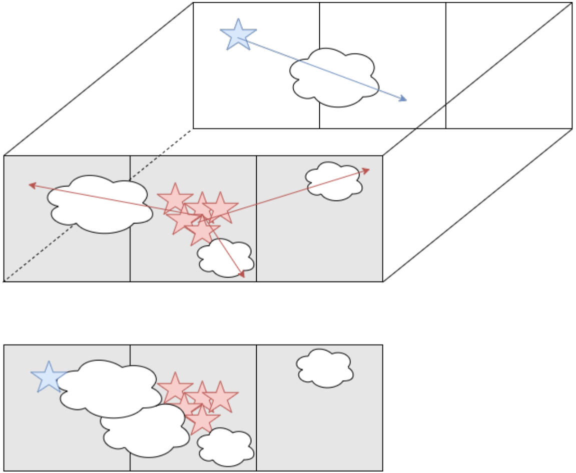


***Fig.**: Missing mass for high sSFR galaxies (Sorba and Sawicki 2018)*

Beam smearing and LOS mixing in IFS observations



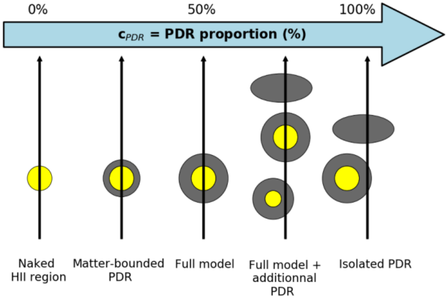


***Fig.**: Line of sight mixing (Lambert-Huyghe+ 2022).*

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Beyond single 1D models: options (and difficulties)

- Combination of 1D models
  - Pseudo 3D
  - Combination of independent 1D models representing galaxy components
- Full 3D RT
- Simulations

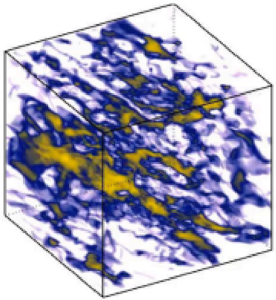
(Focus on nebular emission, for panchromatic SED models, see, e.g., *Conroy+ 2013; Baes+ 2019*)

Simulations

Simulations

- Include dynamical effects, a realistic/consistent ISM structure and distribution of sources
  - Chemistry is numerically expensive (most simulations do not include any form of non-equilibrium metal chemistry)
  - Need to rely on subgrid models to account for the physics on sub-pc scales (including resolving the ionization fronts)

- Post-processing: feed numerical simulations to photoionization codes or chemical networks in order to measure the metal ionization states and their relevant emission after the simulation has been run *(e.g., Jonsson+ 2010, Melekh+ 2015, Vandenbroucke and Wood 2019)*
  - See Hirschmann+ (2017, 2019, 2022,2023) for post-processing with `Cloudy` (photoionization) and `MAPPINGS V` (fast radiative shocks)



Simulations with large chemical networks

Simulations

- Solving a large chemical network within a 3D simulation, e.g., combination of thermochemical network PRISM with on-the-fly radiation hydrodynamics code RAMSES−RTZ
  - Full 3D cosmological or isolated galaxy simulations *(e.g., Katz+ 2022)*
- Study of cooling and heating processes in the ISM, synthetical observations. . .
- Prescriptions usually limited to general properties rather than individual objects or even samples, exploration of large regions of parameter space remains difficult
- Ideally: grids of 1000s-100,000s simulations with varied parameters to produce synthetic library of spectra to compare to observations! (can heat entire labs in the winter. . .)

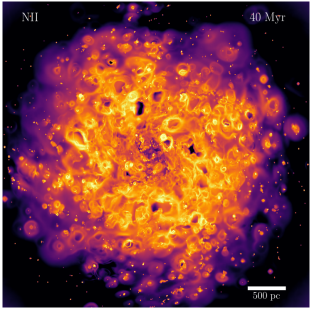


***Fig.**: SMC-like simulated galaxy, N^{+} column density (Katz+ 2022).*

Simulations with large chemical networks

Simulations

- Very useful to test "unmixing" techniques or spatial-resolution biases!
  - Known distributions of density, metallicity…
  - We would like to reproduce the average parameters and their dispersion

- △ Comparison of intrinsic parameter average values or variations in simulations vs. parameters derived from emitting regions is not trivial
  - Not all cells in simulations lead to emitting species
  - Biases due to instrumental uncertainties
  - What internal distributions should be used in models?

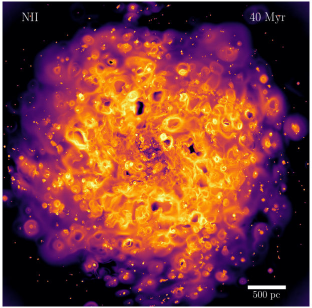


***Fig.**: SMC-like simulated galaxy, N^+ columndensity (Katz + 2022).*

Full 3D RT (w/o photoionization)

Full 3D RT

- Adapted to objects with known (potentially complex) geometries
- 3D Monte-Carlo RT codes can handle complex geometries and density structures
  - e.g.: `RADMC-3D` *(Dullemond+ 2012)*, `SKIRT` *(Baes+ 2003, 2011)*: produce synthetic images/spectra from an arbitrary distribution of stars, dust, and gas density distribution from 1- to 3-D
  - Applications often limited to stellar populations and dust-heating processes *(e.g., de Looze+ 2014)*
- Future is fully self-consistent 3D RT models, which will allow detailed dust and gas distributions to be embedded within the photoionized nebula with arbitrary T, n, and dust distributions
  - Promising avenues with `SKIRT+Cloudy` *(Romero+ 2023)*

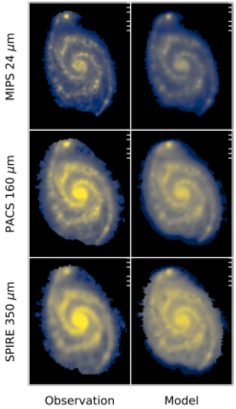
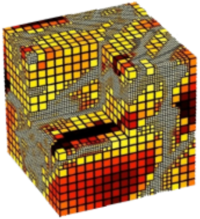


***Fig.**: Comparison simulated/observed images for M51 (Nersesian+ 2020).*

Full 3D RT (w/ photoionization)

Full 3D RT

- Full 3D photoionization is great but expensive (MOCASSIN, TORUS−3DPDR, SOC/LOC, RASCAS, ART2, M^3...)
  - Need to know the distribution of matter and sources (geometry is not a free parameter)
  - Particularly adapted to PNe, bipolar HII regions, fractal HII regions...



Overall pros and cons of 3D methods

- Great to treat the transfer and deal with projection effects
- Great to test the impact of geometry or model specific objects
- So far impractical to explore large parameter space
- Still cannot capture the complex and dynamic structure of the ISM along with all of the relevant, time-varying star formation and feedback

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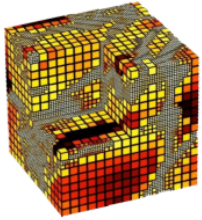

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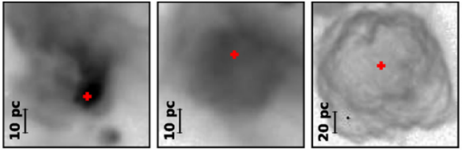
Back to 1D: combination of independent 1D models

Principle

- Integrated spectrum of a galaxy ∼ sum of many emitting stars+ISM components that are correlated or that may even share similar properties (not a new idea)

Example: ensemble averages of aging HII regions *(Dopita+ 2006; Groves+ 2008)*

- Removing the (single) age parameter
- Continuous formation of stellar clusters (each cluster forming stars coevally) ⇒ Evolutionary track of an HII region with given parameter sets
- Flux-averaged spectra along this track



Combination of independent 1D models

Locally optimally emitting cloud (LOC; *Ferguson+ 1997; Richardson+ 2016*)

- Assumes that the cumulative observed emission from each individual emission-line galaxy is the result of selection effects stemming from various emission lines optimally emitted by a large number of gas clouds spanning a large range in physical conditions
  - Fully parameterized, useful for non trivial components like AGNs
  - Potentially >100s of models

$$L_{line} = \underbrace{\int ... \int}_{\mathrm{n}} L(p_1, ..., p_n)\psi(p_1, ..., p_n)dp_i...dp_n \qquad \psi = U^{\alpha_U} n^{\alpha_n}...$$

General model "architecture": topological models

- Linear combination of independent 1D models
  - "Topology" vs. geometry: the exact way in which the components are distributed doesn't matter
  - Many models (grids) but less computationally intensive than simulations or full 3D models

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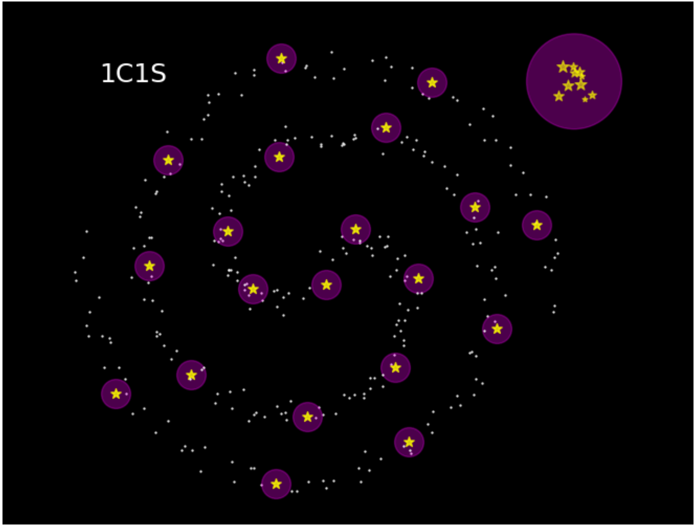
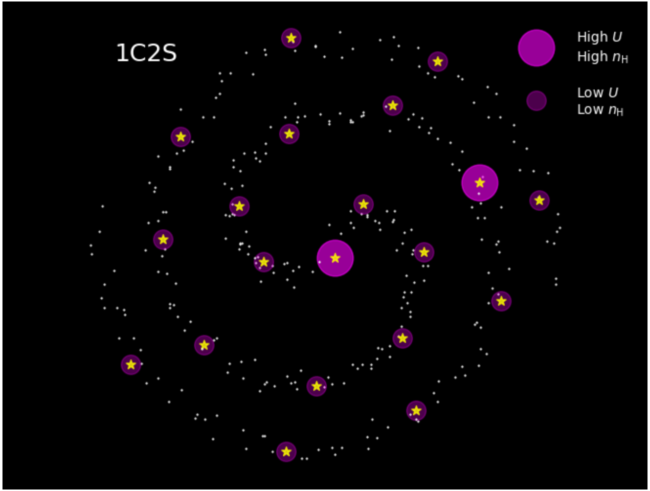
Single effective representative cluster, single ISM component

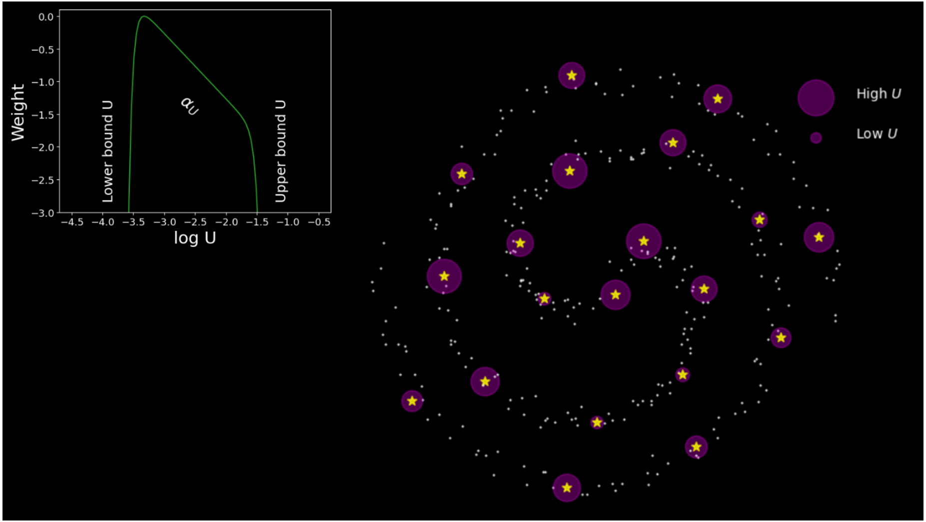


Single effective representative cluster, two ISM components

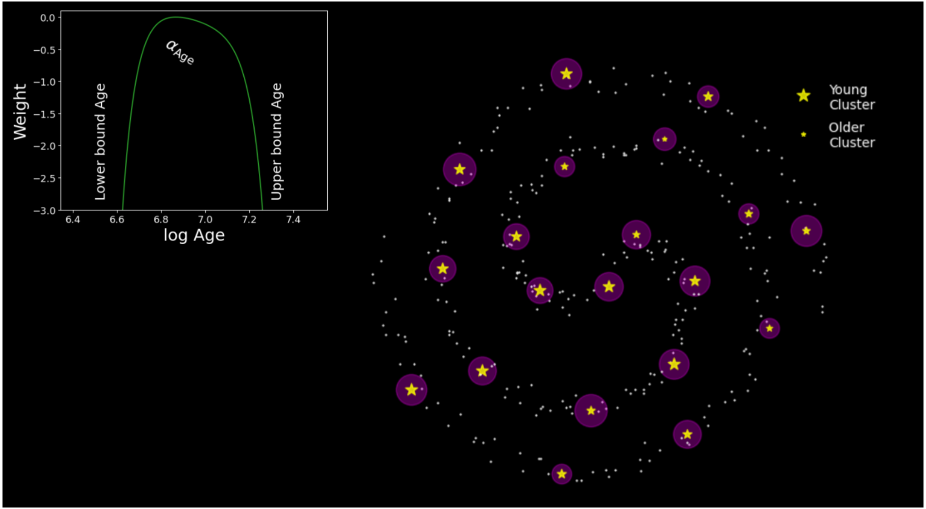


Each component is described by a single value, this doesn’t sound very realistic. . .

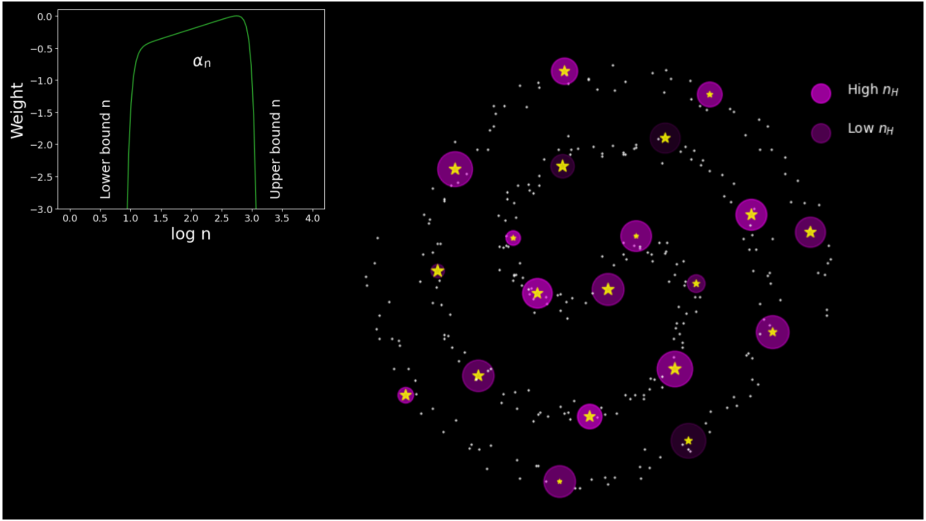
Single effective representative cluster, U distribution



U & age distribution

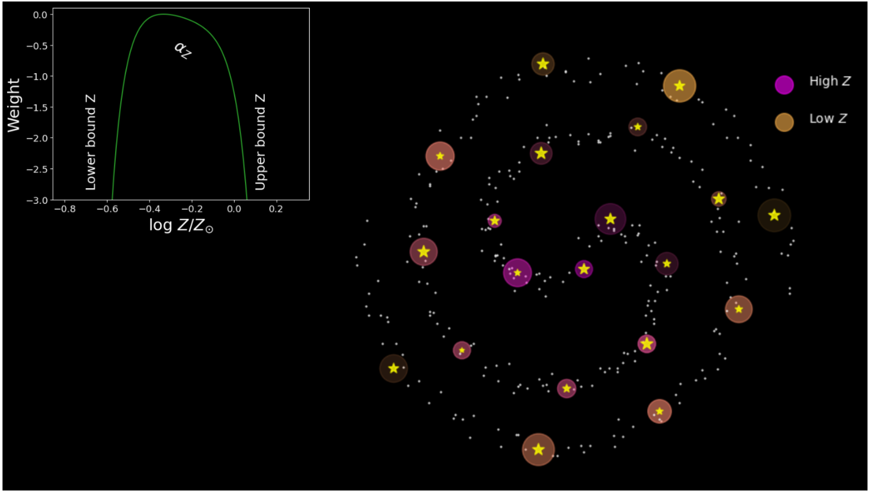


U & age & n distribution

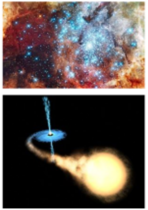


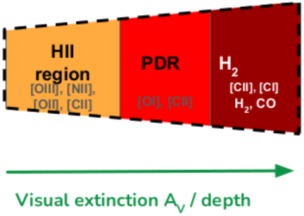
U & age & n & Z distribution

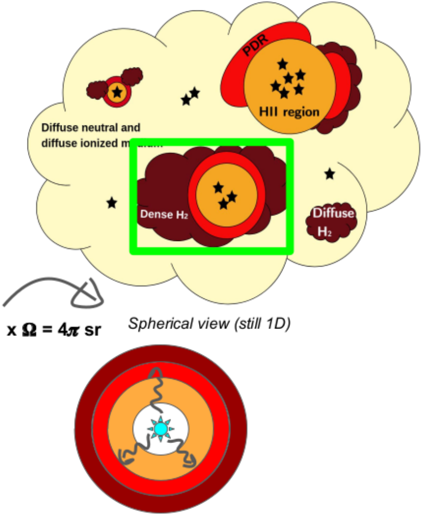
(Actual spatial distribution is not important)



Accounting for physical depth of clouds







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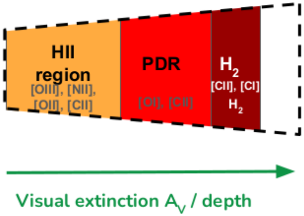

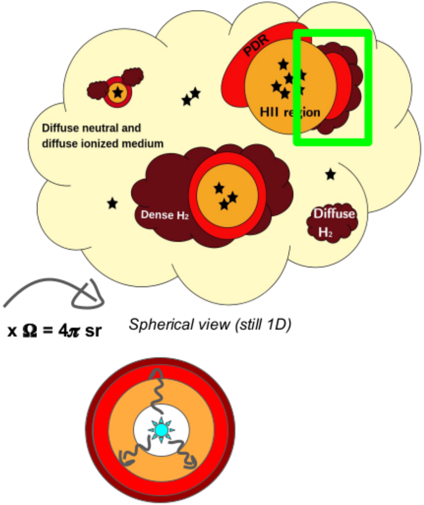

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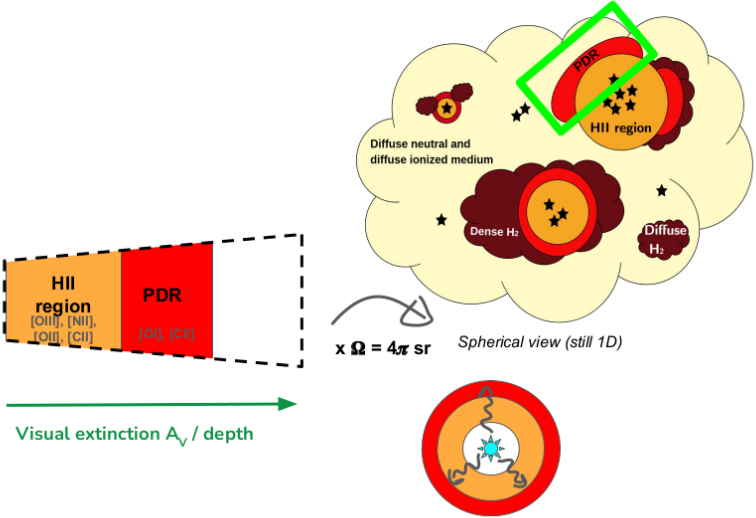

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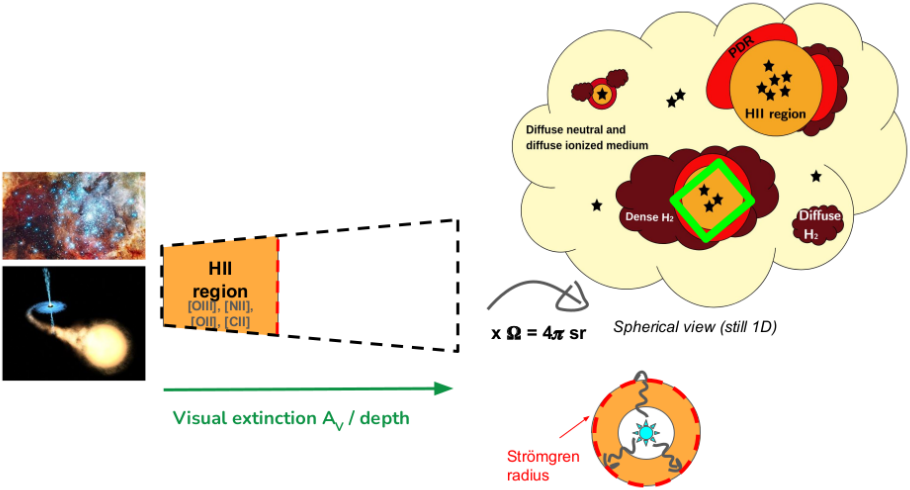

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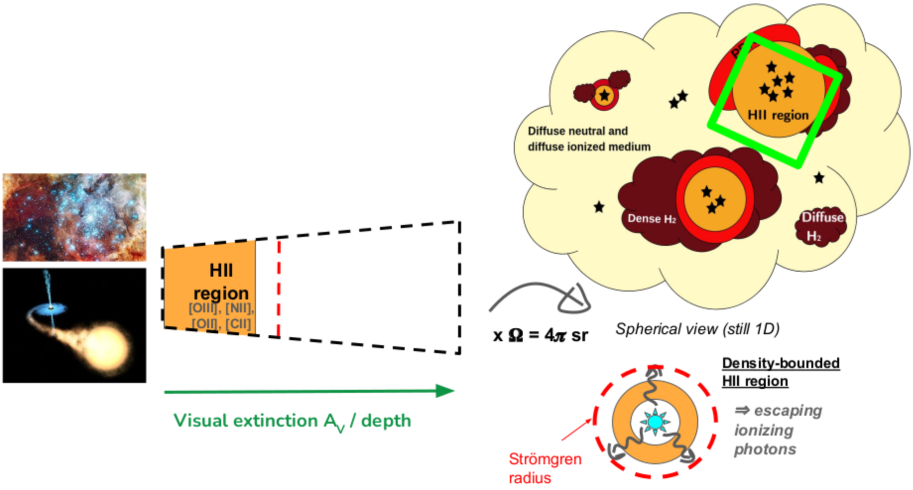

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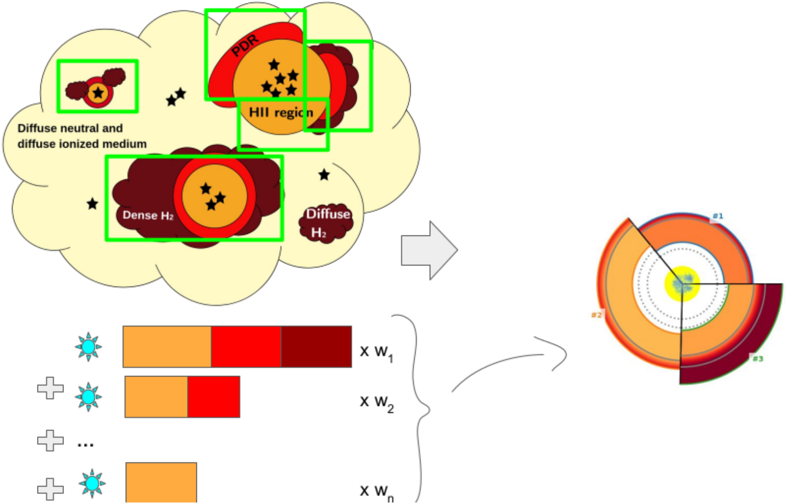


Iterations of (simple) combinations

IZw18
(Lebouteiller+ 2017)

3 & 4-sector radiation- or matter-bounded
CFs tailored
Specific model

Haro 11
(Cormier+ 2012)

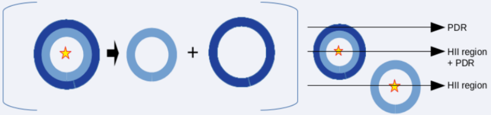
HII region + PDR CF scaled a posteriori

Diffuse ionized gas

IC10
(Polles 2017; Polles+ 2019)

Radiation-bounded or matter-bounded

SMC/LMC SF regions
(Lambert-Huyghe+ 2022)



Combination of HII region + PDR from single radiation-bounded sector

DGS
(Cormier+ 2019)

2 radiation-bounded sectors, Only dense HII region has a PDR CFs from grid

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  - Some results and ongoing works

Combinations of 1D models for nearby galaxies: flash results

Matching suite of lines

- Reproducing T_e([OIII]) in IZw18 *(Péquignot 2008)*
- Matching many IR and optical lines (PDR+HII region) at once in an unresolved galaxy *(Cormier+ 2012)*

PDR and CO-dark gas

- PDR "covering factor" ↘ when Z ↘ *(Cormier+ 2019)*
- CO-dark gas fraction is a function of Z and geometry *(Ramambason+ in prep.)*
- Origin of [CII] in the neutral atomic gas and influence of X-ray sources in ISM heating *(Lebouteiller+ 2017)*
- Evidence of wide range of PDR fractions in spatially-resolved SF regions *(Lambert-Huyghe+ 2022)*

Escape fraction of ionizing photons

- Fraction of escaping photons ↘ when integrating larger spatial scales *(Polles+ 2017, 2019)*
- Fraction of escaping photons ↗ when Z ↘ *(Ramambason+ 2022)*

Illustration of ongoing works: LOC models

- (Testing phase!) Comparing (single) parameter values from single 1D models to average LOC parameters: single 1D model captures well the average *U* and *n*, not so good for age (i.e., stellar population SED shape) and *Z*

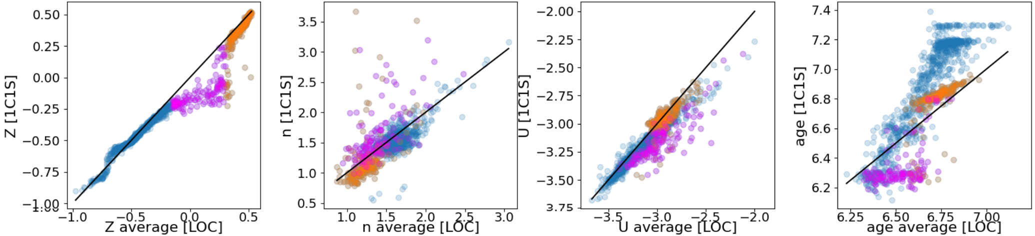
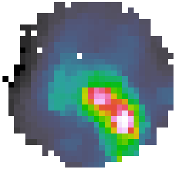
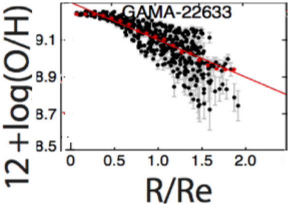
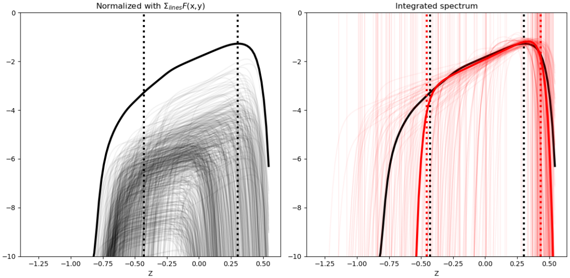


Illustration of ongoing works: recovering internal variations

- (Testing phase!) Each IFS pixel is a distribution, can we recover the internal variations from the integrated map?







Applications to high-z galaxies

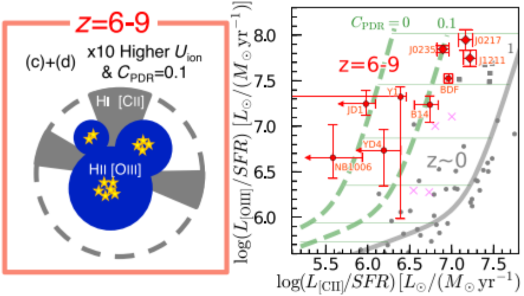


Fig.: *Considering HII region + PDR components in high-z galaxies to explain high (OIII)/(CII) observed with ALMA (Harikane+ 2020).*

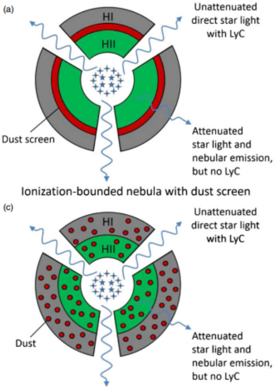


Fig.: *Considering different dust distributions for EoR galaxies (Zackrisson+ 2013).*

Caveats of combination of 1D models

- △Still 1D models: static, components don't talk to each other
- △Projection effects are difficult to handle
  - Better adapted to optically thin tracers and dust-poor ISM
- △Still parameterized models: potentially too wide allowed parameter space
  - Considered models combinations may be matching observations but may lead to parameter distributions that are unrealistic or not motivated/confirmed by self-consistent simulations
  - Unless priors are explicitly introduced

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Statistical framework

- How do we handle this many tracers and/or such complex combinations?

Deterministic methods

- Focus on selection of "best-fitting" parameters rather than on the uncertainties associated with these parameters, e.g., χ^2 method
  - Limited capabilities with interpolation, outliers, upper limits, more complex topology, confidence intervals, use of priors. . .

Probabilistic methods

- Bayesian inference with state-of-the-art posterior sampling techniques, such as the Markov Chain Monte-Carlo (MCMC) has become a standard practice
- Probabilistic approach also introduces priors, nuisance variables, and may allow a finer scan of the parameter space

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Bayesian inference

- Single models too long to run at each iteration ⇒ fine grid and/or interpolation techniques

Inference on grids including pre-computed geometry

- `NebulaBayes` *(Thomas+ 2016)* (some caveats with line normalization hypothesis)
  - Agnostic to model grid used so desired topology can be pre-computed/tabulated in grid
  - "Brute force" Bayesian likelihood calculations
- `MULTIGRIS` *(Lebouteiller+ 2022)*: same as `NebulaBayes` but with a sampler
  - + RVs controlling combination of models and any nuisance variables (e.g., extinction, systematic uncertainties. . .)

Random walkers (i.e., one or a few "chains")

- High dimensionality is common ⇒ slow parameter space exploration
- ISM model grids are highly multi-modal, worse if combination of models. . .
  - Can get stuck in local likelihood maximum
  - Stochasticity: different solutions from different starting points
  - Difficult to probe the entire parameter space (⇒ difficult to compute marginal likelihood)

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General principle

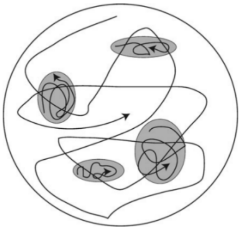
- $p(\theta|\mathbf{O},\mathcal{M}) = \frac{p(\mathbf{O}|\theta,\mathcal{M})p(\theta|\mathcal{M})}{p(\mathbf{O}|\mathcal{M})} \propto p(\mathbf{O}|\theta,\mathcal{M})p(\theta|\mathcal{M})$
- $posterior = \frac{likelihood \times prior}{marginalization}$ (for a given model)

Multi-modal posteriors

- Nested sampling techniques (e.g., BEAGLE)
- Sequential Monte-Carlo (e.g., MULTIGRIS): Markov kernels used to rejuvenate particle using IMH or HMC kernels
- Genetic algorithms. . .

Example: particle filtering techniques (e.g., SMC)

- Tempered likelihood *(Ching and Chen 2007, Mison+ 2013)*
  - Parallel runs varying the "temperature" of (many) particles through the index β
  - $p(\theta|\mathbf{O},\mathcal{M})_\beta \propto p(\mathbf{O}|\theta,\mathcal{M})^\beta p(\theta|\mathcal{M})$



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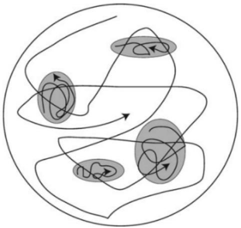
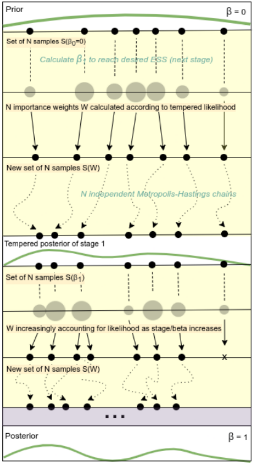


Illustration (SMC)



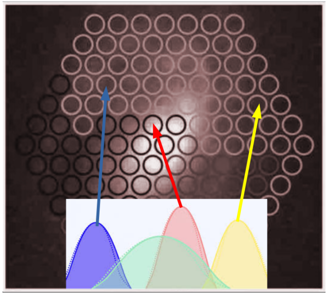
- Makes it possible to evaluate the entire parameter space if well sampled
  - Marginal likelihood can be estimated

Illustrations (see accompanying .odp file)

- No U-turn Sampler (Hamiltonian MC sampler)
- SMC

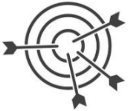
Hierarchical method

- Sample of galaxies
- Sample of galaxy regions
- Pixels in IFS observations $\Rightarrow$ spatial regularization / smoothing
- Still very recent for spectroscopic diagnostics



The power of statistics

- We usually don't know the geometry a priori: assumed geometry and infer parameters
- Usually assuming simple geometries when few tracers are available, and increase complexity with additional tracers (*"Don't use more parameters than tracers"*)
- BUT more complex (i.e., realistic) geometries can still be explored/evaluated!
  - Is it better to knowingly use an unrealistic geometry and infer inaccurate (possibly precise) measurements? Or use a realistic geometry and infer an accurate (possibly imprecise) measurement?
- My 2 cents: accept imprecision due to unknown/unconstrained geometry and in the future rely on hierarchical methods to gain as much precision as possible

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Model comparison: evaluating the hypotheses

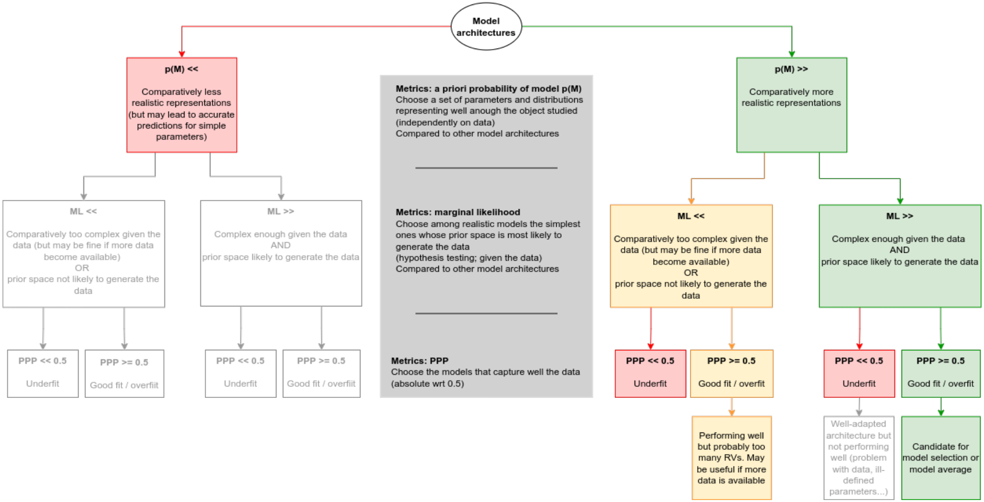
$$\begin{cases} R_{\text{bayes}} = \dfrac{p(\mathcal{M}_1|\vec{O})}{p(\mathcal{M}_2|\vec{O})} \\ R_{\text{bayes}} \propto \dfrac{p(\vec{O}|\mathcal{M}_1)}{p(\vec{O}|\mathcal{M}_2)} \dfrac{p(\mathcal{M}_1)}{p(\mathcal{M}_2)} \end{cases}$$

MARGINAL LIKELIHOOD

PRIOR PROBABILITY OF THE MODEL

- Marginal likelihood: hypothesis testing, i.e., how likely the prior space may generate the data
  - $p(\mathbf{O}|\mathcal{M}) = \int_\theta p(\mathbf{O}|\theta, \mathcal{M}) p(\theta|\mathcal{M}) d\theta$
  - (integration on the whole parameter space of likelihoods × priors on θ)
- Prior probability of the model: how likely the model is, independently on the data
  - i.e., how likely the architecture, choice of parameters, is
  - Quite arbitrary! For instance: a single 1D model has a "low" $p(\mathcal{M})$

Model decision tree



Implications

- A simple architecture (e.g., 2 components sharing the same radiation field) may produce great metrics, even marginal likelihood
  - But single parameter values are fine tuned to match observations, it doesn't make it realistic
- LOC models include thousands of models but linked through very few parameters
  - We may loose in some metrics because the architecture is less flexible than n-component models
  - But we gain in realism (i.e., prior probability of the model)

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Some prospective

Future modeling

- Short term: bridge the gap between models with complex geometries and simulations
  - Static nD models can be combined within complex, parameterized geometries but are not fully self-consistent ⇒ Needs calibration (IFS, simulations. . .)
  - Simulations rapidly improve the chemistry network, photoionization treatment etc. . .
- Long term: probabilistic methods applied to big data
  - Run dynamic simulations on the spot with specific parameters and/or make grids of simulations ⇒ ML techniques
  - Use full static 3D models with parameterized geometries / ingredients
- Dust and gas, orientation of models. . .
- Multi-wavelength resolved observations are essential

End of presentation

Modelling a full galaxy and its suite of lines

Geometry

- It may be apparently simpler to consider a single spectrum but we have to consider that the spectrum is the result of strong selection effects (a simple spectrum doesn't imply a simple model)
- Sources: is the galaxy dominated by a single or a couple of excitation mechanisms (e.g., AGN, HII galaxies) or by a "standard" distribution of HII regions?
- ISM: physical conditions are highly inhomogeneous but follow some physically-motivated distributions
- X-rays and/or PDRs complicate everything and require complex geometries

Model ingredients

- Stellar populations: need to be systematically explored and tested
- Cosmic rays, magnetic field: rely on poorly constrained prescriptions until new tracers become available and/or new knowledge of dependency with environment
- Turbulence: exists in Cloudy for line transfer purposes
- Shocks: high-spectral resolution is key until shocks are self-consistently integrated in photoionization codes

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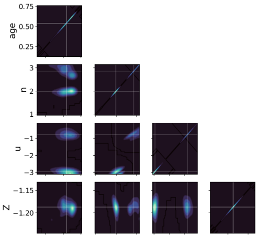
Illustration: MULTIGRIS *(Lebouteiller Ramambason 2022)*

- Grid of predicted fluxes (+ interpolation function)
- Model $\mathcal{M}$ ("architecture"): components, mixing weights, parameters θ, priors...
- Data d: observed emission lines / bands (incl. upper limits)

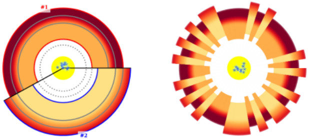
PyMC

- Sampling: draw from the likelihood with a given step algorithm
  - $\mathcal{L} = p(\mathbf{O}|\theta) = \prod_{i=0}^{N} \mathcal{N}(\mu = O_i, \sigma^2 = U_i^2)$

- Use Bayes theorem to obtain posterior probability density functions (PDFs)
  - $p(\theta|\mathbf{O}, \mathcal{M}) \propto \frac{p(\mathbf{O}|\theta,\mathcal{M})p(\theta|\mathcal{M})}{p(\mathbf{O}|\mathcal{M})}$



2D representation of a 3D object modeled with 1D code



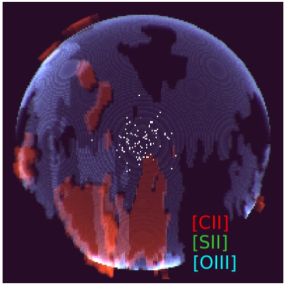
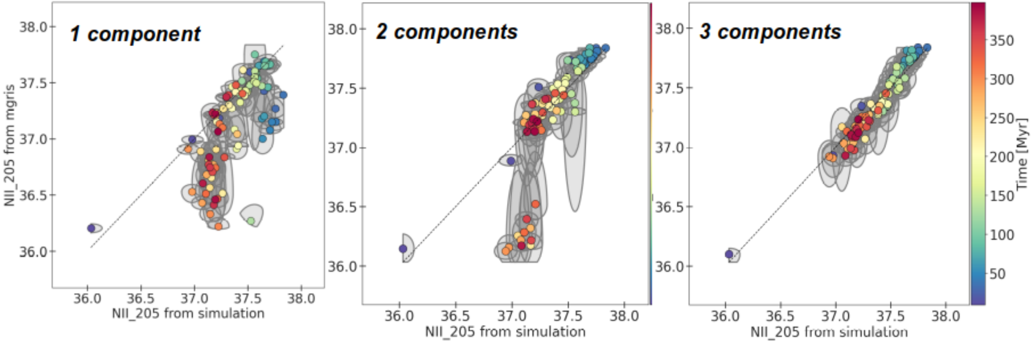


Illustration of ongoing works: comparison with simulations

- (Testing phase!) Calibrating combinations of 1D models to match PRISM simulations. Some lines are particularly difficult to reproduce with a single component.



Why is the probabilistic approach best

- BUT this doesn't mean that more complex (i.e., realistic) geometries shouldn't be explored/evaluated!
  - Even if few tracers used, that doesn't mean the real geometry is simple. It means we don't have enough constraints to constrain a complex geometry $\Rightarrow$ Are the parameters derived from a simple architecture meaningful? Depends on the parameter. . . !
  - For instance, we have only 3 lines (e.g., ALMA high-z) and we wanna know the mass of HI or $f_{\rm esc}$. Is it better to knowingly use an unrealistic geometry and infer inaccurate (possibly precise) measurements? Or use a realistic geometry and infer an accurate (possibly imprecise) measurement?
  - My 2 cents: accept imprecision due to unknown/unconstrained geometry and in the future rely on hierarchical methods to gain as much precision as possible

△ Terminology

- Model: physical nD model (typically RT) usually adapted to given physical object within a galaxy
- Model "architecture": pompous way to refer to a galaxy model, i.e., ways to consider galaxy components, i.e., how do we build a galaxy, i.e., model of models