AHEAD 2020

Definition of Equity (by K. Marx): "**From each according to his ability, to each according to his needs**"

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Advanced Tools for Data Analysis

(Work-Package 14 in AHEAD2020)

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Participating Institutes/Countries:

Italian National Institute of Astrophysics (INAF, Italy)
Cantambria Institute of Physics (IFCA, Spain)
University of Turku (UTurku, Finland)
University of Tartu (UTARTU, Estonia)
University of Amsterdan (UVA, Netherlands)
Netherlands Institute for Space Research (SRON, Netherlands)
National Observatory of Athens (NOA, Greece)
University of Tor Vergata (UniTorV, Italy)
University of Roma-Tre (UniRM3, Italy)
University of Leicester (ULEIC, UK)
Spanish National Research Council (CSIC, Spain)
French Atomic and Alternative Energy Commission (CEA, France)

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Advanced Tools for Data Analysis

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Optimize science output from next generation X-ray observatories

(Athena, XRISM, LEM, Arcus, HUBS, eROSITA, eXTP, Einstein Probe, HERMES, etc) by designing and developing appropriate tools for the new capabilities offered by those missions, and support the community for best data exploitation.

- XRISM and Athena/X-IFU micro-calorimeters will provide in the next decades spectra with unprecedented energy resolution in the X-ray band. Furthermore, X-IFU will be the first X-ray integral field instrument with a number of pixels similar to current optical/NIR IFU
- eROSITA and Athena/WFI are and will revolutionize the field of X-ray surveys, opening new large discovery spaces on this field.
- Einstein Probe and eXTP are/will give(ing) access to unprecedented timing of galactic and extragalactic sources
- SVOM, HERMES, and many others will join the multi-messenger revolution

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Tasks/Tools/Models

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- Advanced background modelling (INAF)
- Instrument effective-area cross calibrations (UTurku, INAF)
- Machine learning techniques for micro-calorimeter data-reduction (IFCA)
- Multi-dimensional source detection, Bayesian source detection, automatic redshift determination (NOA, IFCA)
- Extraction and identification of line features from high-res. spectra (INAF)
- Physical Models for high resolution spectral/timing (INAF, UVA, SRON)
- Hyperspectral imaging and fitting & advanced analysis of extended sources (INAF, UniTorV, UniRM3)
- Blind source separation/reconstruction in extended sources (CEA)
- Lobster-eye advanced triggering processes (ULEIC)

Advanced Tools for Data Analysis: impact

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- Six post doc funded with AHEAD2020 support
- So far **>50** publications produced exploiting AHEAD2020 support, involving >200 scientists
- First workshop on inputs from the community Feb 21st 2022: http://ahead2020-advanced-da.oats.inaf.it; emphasis on:
  - Advanced tools for transient-triggering and temporal study (e.g. STATiX, NOA)
  - Bayesan models for the analysis of cluster of galaxies (INAF)
  - 3D (Imaging – X,Y – Energy, E) analysis of extended sources through Morphological Component Analysis (CEA)
  - Physical models for high resolution spectroscopy in view of XRISM and Athena (e.g. TEPID – INAF – TPHOT – SRON)

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Advanced Tools for Data Analysis:
Time-Evolving Photoionization Models

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- Time-Evolving-Photoionization modeling and analysis tools. Carried out by two teams: TPHOT (optically-thin gas only; SRON) and TEPID (also optically-thick cases; INAF), for application to different astrophysical contexts (Ionized winds from AGNs and compact sources, ISM of external galaxies flashed by transients, etc)
- Compute the ionization and energy balance in the gas and follow its evolution in time with the varying flux (TPHOT and TEPID), transferring the radiation throughout the cloud with approximated radiative-transfer equations (TEPID)
- Link the evolving ionization balance to atomic databases, compute opacities and emerging spectra as function of time, density and column density of the gas.

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Time-Evolving Photoionization

AGN outflows
Transients & ISM

A. Luminari, A.L. Thakur, R. Serafinelli

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Why Bothering?

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- Baryons in the Universe lie in the surroundings or ionizing sources or are embedded in photon fields

- The intensity of light that baryons feel varies with time, on different timescales
  - AGNs or XRBs vary on timescales from s to days or even years
  - IGM density decreases as universe expands and so does the metagalactic photon flux they experience on Hubble timescale
  - Stars form and die on timescales of million to billion years and affect the physical state of the ISM of star-forming regions
  - When star explodes their transient phenomena (Supernovae, GRBs, Kilonovae) strongly modify the ionization state of the ISM they leave in, on timescales from seconds to weeks

- In all these cases photoionization-equillibrium models are not accurate and provide wrong diagnostics
- Time-evolving photoionization depends on n_e ➔ removes the n_e–R degeneracy intinsic in the ionization parameter definition

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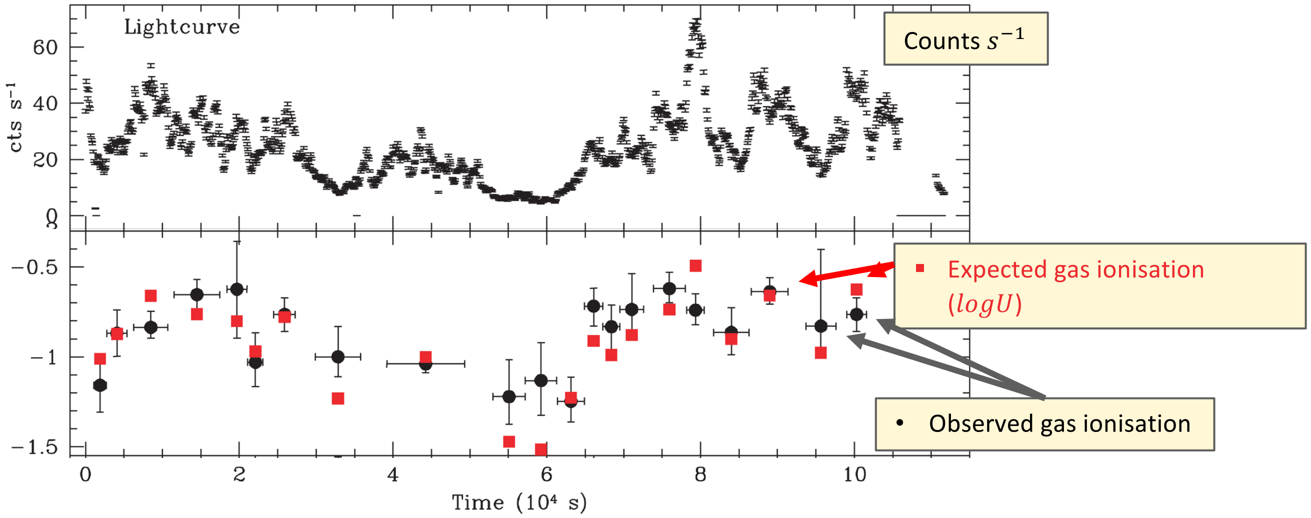
Can we always assume the gas to be in **ionisation** equilibrium?

NGC4051 – Krongold, Nicastro+07



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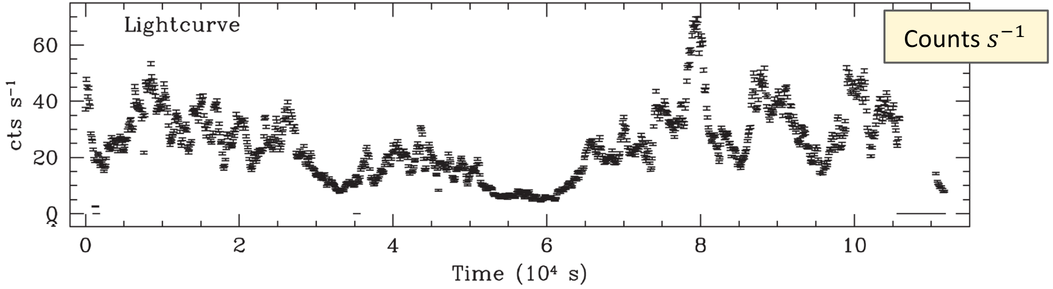
Can we always assume the gas to be in **ionisation** equilibrium?

NGC4051 – Krongold, Nicastro+07



…no!

The equilibrium timescale is: $$t_{eq} \approx 1 \Big/ \left(\alpha_{rec}^{X^i} \cdot n_e\right)\left(1 + \frac{\alpha_{rec}^{X^{i-1}}}{\alpha_{rec}^{X^i}} + \frac{n_{X^{i+1}}}{n_{X^i}}\right)$$ Nicastro+99

<u>Low density</u>: longer t_{eq} , ionisation equilibrium not granted

<u>High density</u>: smaller t_{eq} , closer to the ionisation equilibrium limit

→ time-evolving ionisation breaks the density degeneracy!

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TEPID:

Time-Evolving PhotoIonisation Device

Non-equilibrium gas ionisation and time-resolved transmitted spectrum from optical to X-ray

Funded by the Horizon 2020 Framework Program of the European Union Grant Agreement No. 871158

Time Evolving Photo Ionisation Device (TEPID): A novel code for out-of-equilibrium gas ionisation

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ABSTRACT

Context. Photoionisation is one of the main mechanisms at work in the gaseous environment of bright astrophysical sources. A great deal of information on the gas physics, chemistry and kinematics, and on the ionising source itself, can be gathered through optical to X-ray spectroscopy. While several public time equilibrium photoionisation codes are readily available and can be used to infer average gas properties at equilibrium, time-evolving photoionisation models have only very recently started to become available. They are needed when the ionising source varies faster than the typical gas equilibration timescale. Using equilibrium models to analyse spectra of non-equilibrium photoionised gas may lead to inaccurate results, and prevents a solid assessment of gas density, physics, and geometry.

Aims. Our main objective is to present and make available the Time-Evolving PhotoIonisation Device (TEPID), a new code that self-consistently solves time evolving photoionisation equations (both thermal and ionisation balance) and accurately follows the response of the gas to changes in the ionising source.

Methods. TEPID self-consistently follows the gas temperature and ionisation in time by including all the main ionisation/recombination and heating/cooling mechanisms. The code takes in input the ionising light curve and spectral energy distribution and solves the time-evolving equations as a function of gas electron density and of time. The running time is intelligently optimised by an internal algorithm that initially scans the input light curve to set a time-dependent integration frequency. The code is built in a modular way, can be applied to a variety of astrophysical scenarios and produces time-resolved gas absorption spectra to fit the data.

Results. To describe the structure and main features of the code, we present two applications of TEPID to two dramatically different astrophysical scenarios: the typical ionised absorbers observed in the X-ray spectra of active galactic nuclei (e.g. warm absorbers and ultra-fast outflows), and the circumburst environment of a gamma-ray burst. For both cases we show how the gas energy and ionisation balances vary as a function of time, gas density and distance from the ionising source. We show that time-evolving photoionisation leads to unique ionisation patterns that cannot be reproduced by stationary photoionisation codes when the gas is out of equilibrium. This demonstrates the need for codes such as TEPID in view of the unprecedented capabilities that will be offered by the upcoming high-resolution X-ray spectrometers on board missions like XRISM or Athena.

Diffusive Models

e.g. Hidrogen Photo-Ionization

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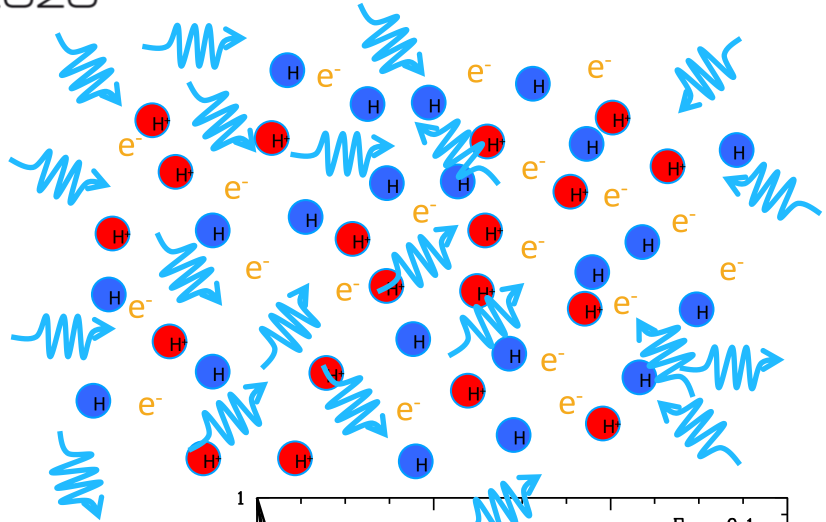

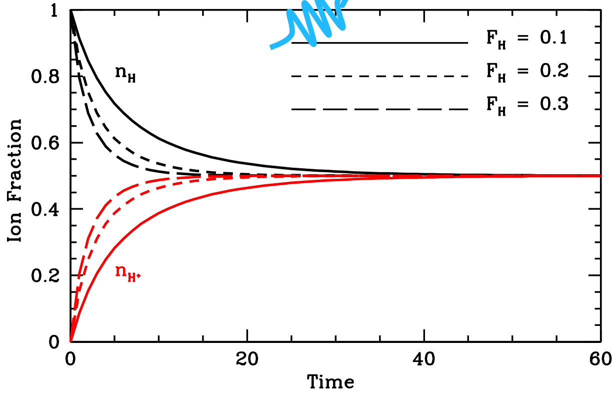

$H + \gamma \rightarrow H^+$

$H^+ + e^- \rightarrow H$

$$\begin{cases} \frac{dn_H}{dt} = -F_H n_H + \alpha n_{e^-} n_{H^+} = -F_H n_H + \alpha n_{H^+}^2 \\ n_H + n_{H^+} = 1 \end{cases}$$

$$\int_{n_H^0}^{n_H} \frac{dn'_H}{\alpha n'_H[(F_H/\alpha) + n'_H]} = \int_0^t dt'$$

$$n_H(t) = \frac{\gamma}{1 - \varsigma_0 e^{-F_H t}}$$, Logistic with:

$$\gamma = \frac{F_H}{\alpha}, \quad \varsigma_0 = \frac{n_H^0 - \gamma}{n_H^0}$$

Simple Epidemic Diffusion Diagram

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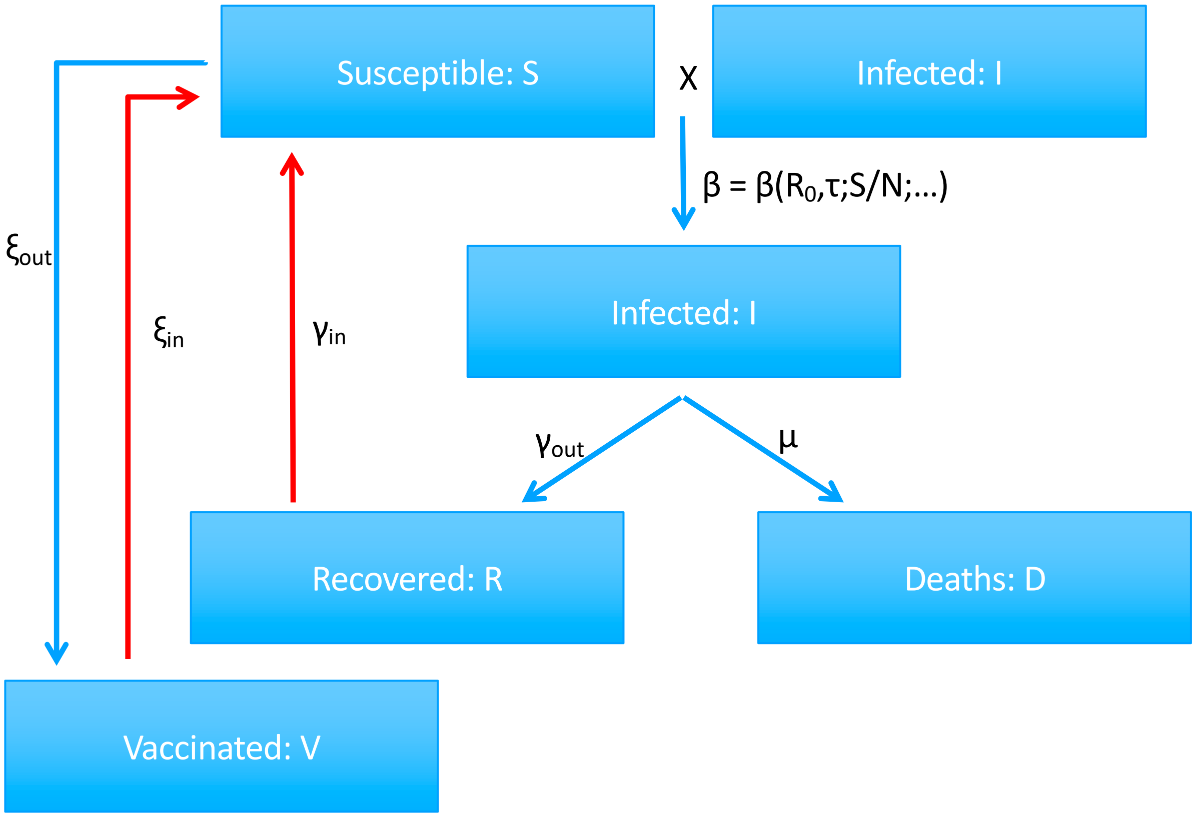

Seasonality of Respiratory Diseases

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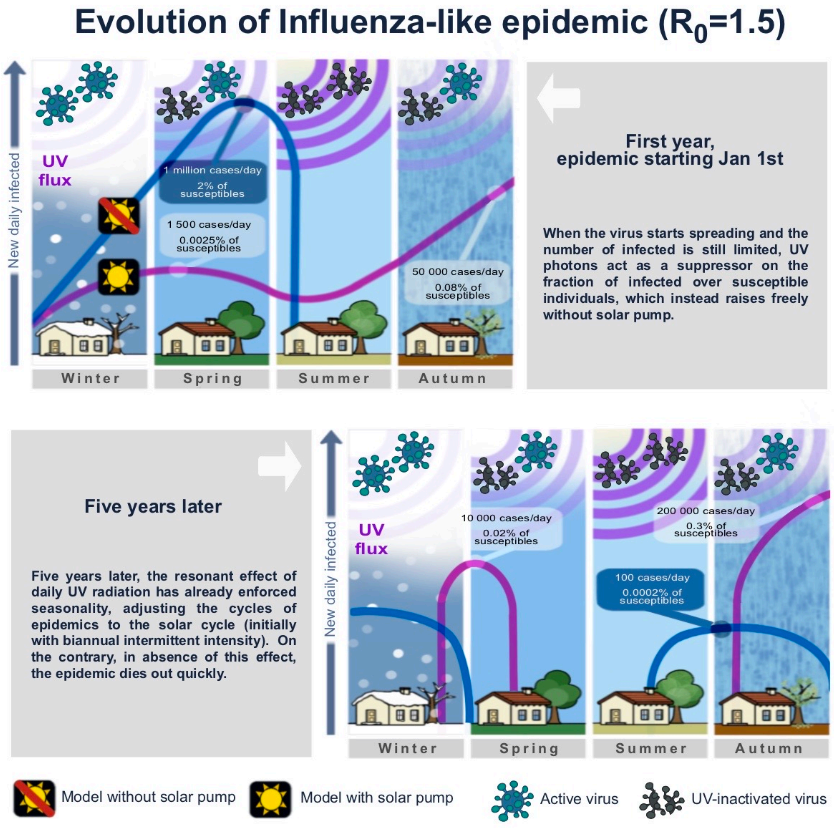

Nicastro et al., 2020, iScience, 23, 10, 102695:

Time-evolving Equations

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The driving parameters are:

1. the ionising flux $F_{ion} \propto \frac{Q_{ion}}{r^2}$
2. the gas density n_e

Sets the energy transferred to the gas (→ 1)

Sets the gas timescale: Ionisation rates and heating (→ 2)

Ionic abundances

$$\frac{dn_{X^i}}{dt} = -\left[F_{X^i} + \alpha_{rec}^{X^i} n_e\right] n_{X^i} + F_{X^{i-1}}\, n_{X^{i-1}} + \alpha_{rec}^{X^{i+1}} n_e n_{X^{i+1}}$$

Charge conservation

$$n_e = n_{HII} + n_{HeI} + 2n_{HeII} + \ \ldots$$

Temperature

$$\frac{dT}{dt} = \Sigma_{X,i}[\Gamma - \Lambda] + \Theta$$

Radiative Transfer

$$F' = F_0 e^{-\tau} + \phi_{rrc}$$

Dependence on n_e breaks the distance-density degeneracy intrinsic in equilibrium photoionisation

Linearly depends on F_{ion}

Linearly depends on n_e

TEPID vs Cloudy @ eq: gas emission

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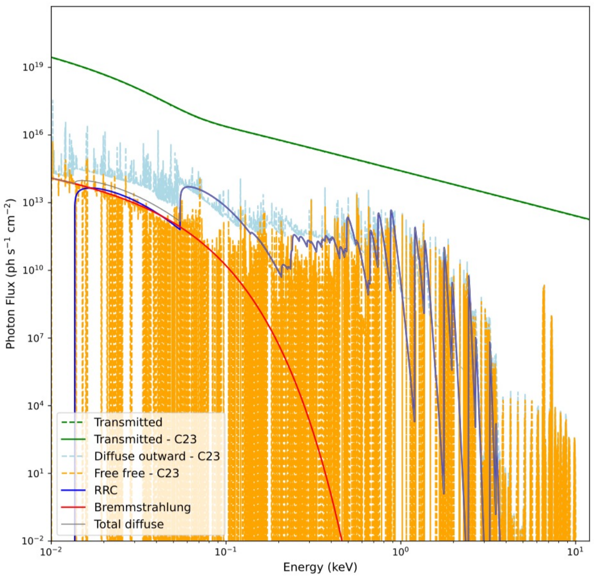
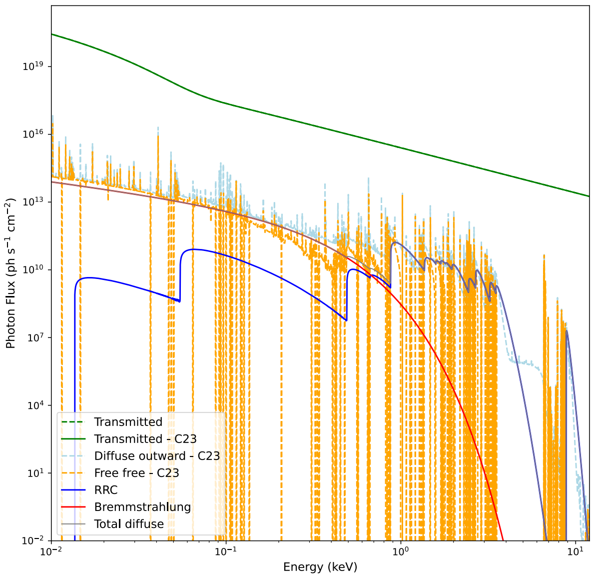
logU=0.5, logN_H=20 (opt. thin)



logU=1.5, logN_H=20 (opt. thin)



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TEPID vs Cloudy/XSTAR @eq

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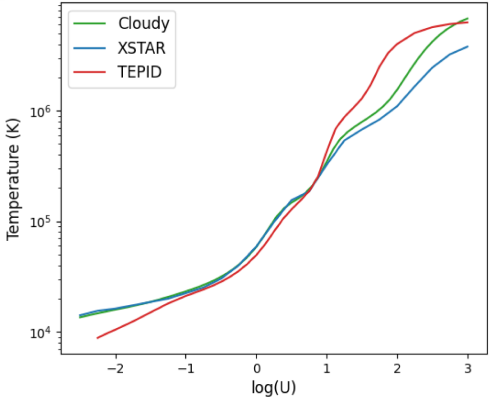
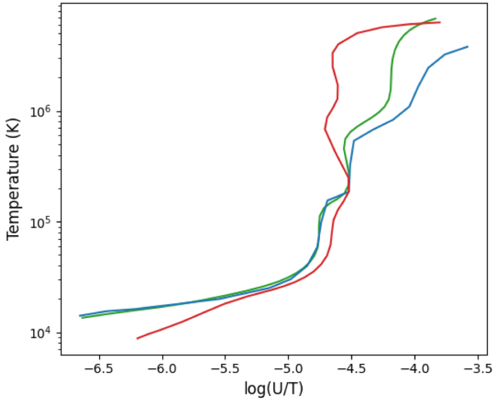
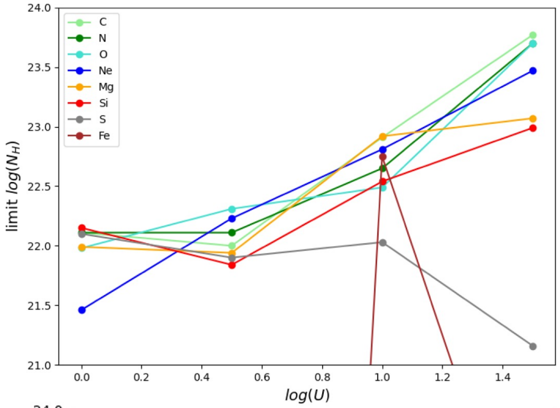
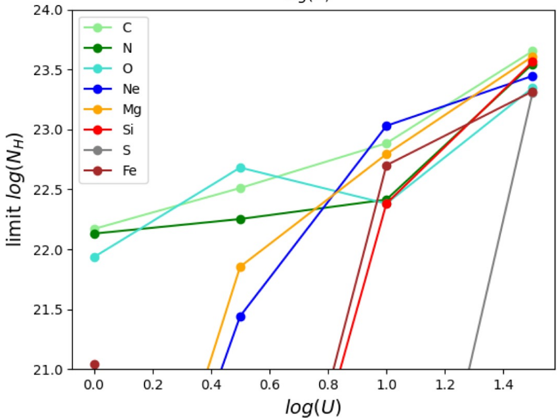
T vs U





Rad.-Transf





AHEAD 2020 TEPID

Evolution of gas temperature and ionisation

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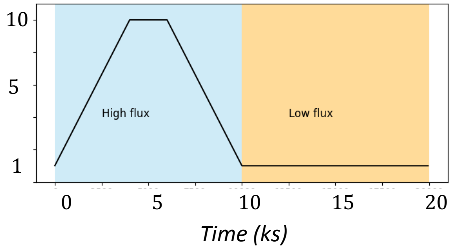
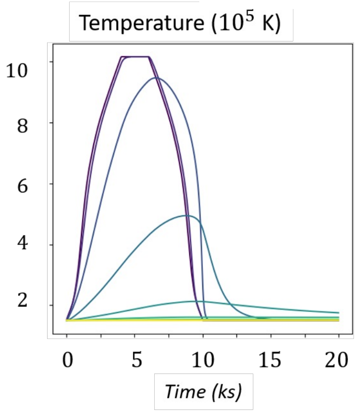


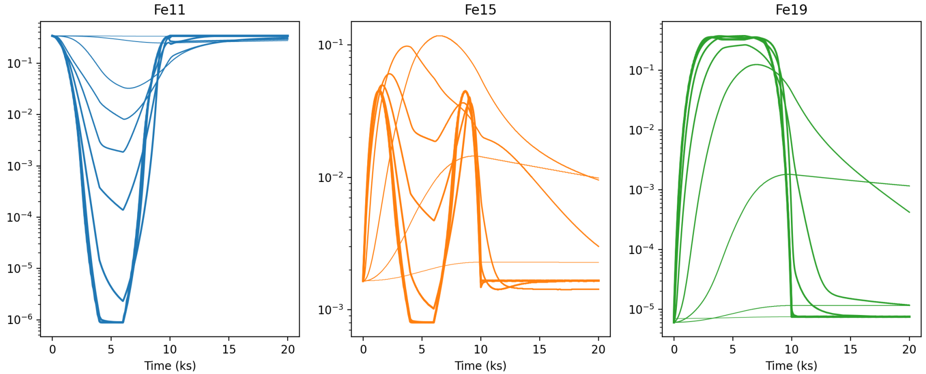


$n_e = 10^{12} cm^{-3}$: *instantaneous response (ionisation equilibrium)*

$n_e = 10^{8} cm^{-3}$: *damped and delayed response*

$n_e = 10^{4} cm^{-3}$: *always out of equilibrium (no gas response)*

Iron ion abundances (ratio)



Time-Resolved spectra

AHEAD 2020 *TEPID*

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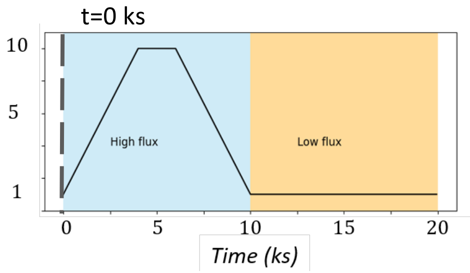
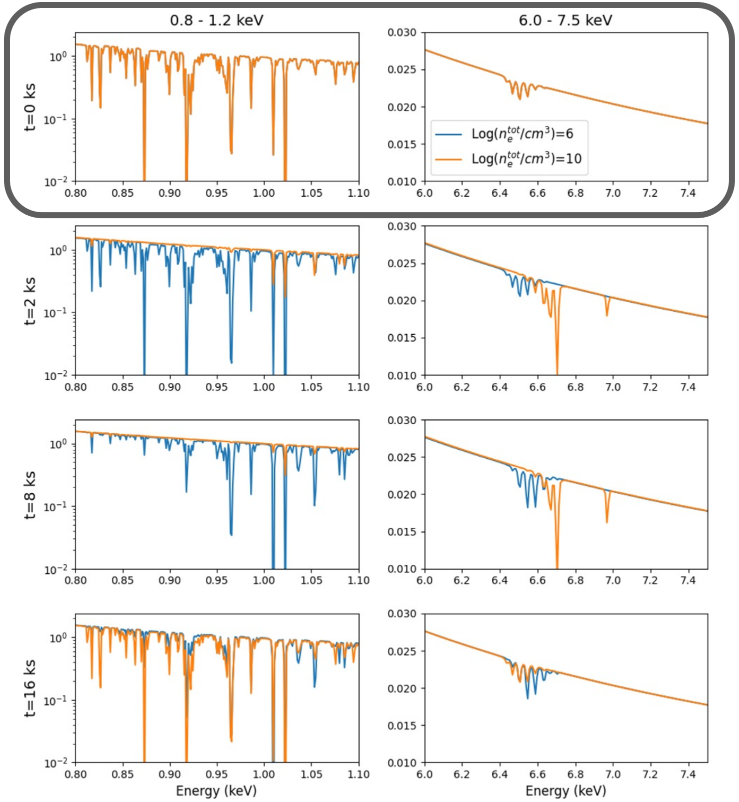
$\log(n_e/cm^3) = 6$

$\log(n_e/cm^3) = 10$

t=0 ks. Gas in equilibrium, $\log(U) = 1.5$

→ Spectra are identical by construction





Time-Resolved spectra

AHEAD 2020 *TEPID*

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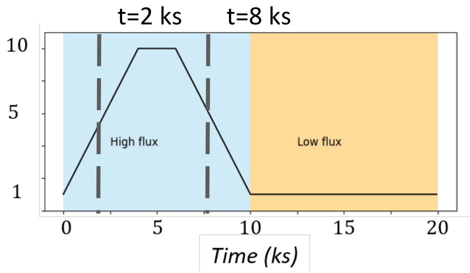
Blue line: $\log(n_e/cm^3) = 6$

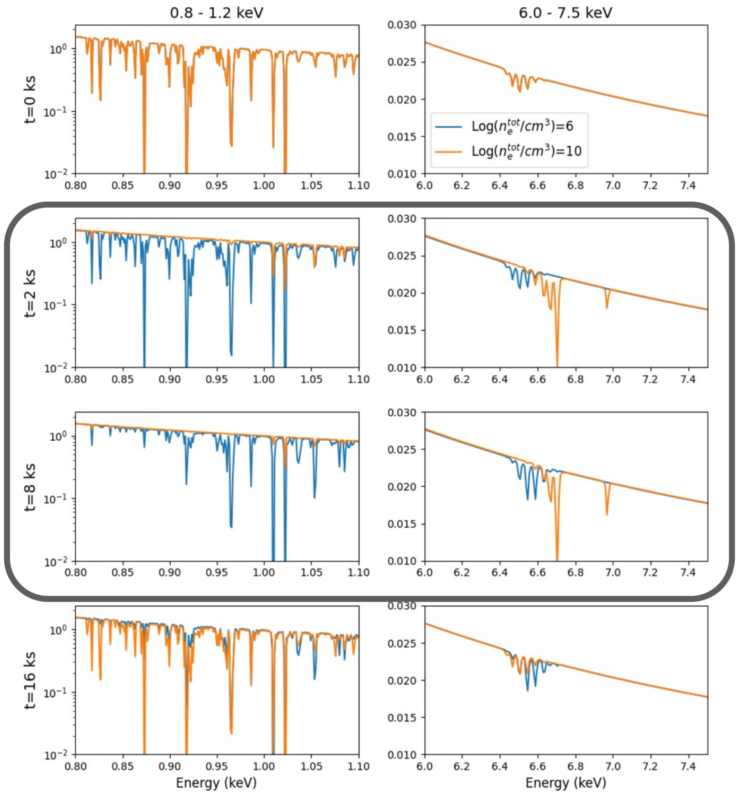
Orange line: $\log(n_e/cm^3) = 10$

t=0 ks. Gas in equilibrium, $\log(U) = 1.5$
→ Spectra are identical by construction

t=2,8 ks. Mid-time of the rise and decay phase (<u>same flux</u>):

- $n_e = 10^{10}$: gas in equilibrium → same opacity
- $n_e = 10^6$: gas is overionised → *lower opacity at t=8 ks!*





Time-Resolved spectra

AHEAD 2020 *TEPID*

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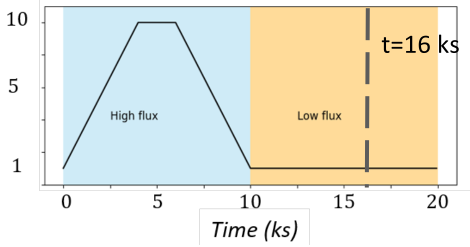
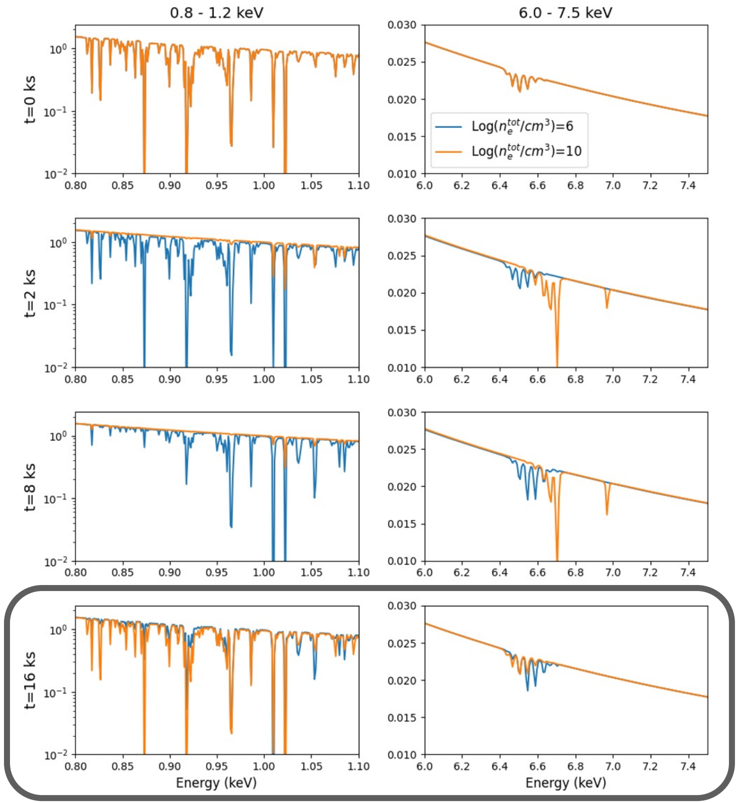
$\log(n_e/cm^3) = 6$
$\log(n_e/cm^3) = 10$

t=0 ks. Gas in equilibrium, $\log(U) = 1.5$
→ Spectra are identical by construction

t=2,8 ks. Mid-time of the rise and decay phase (same flux):
- $n_e = 10^{10}$: gas in equilibrium → same opacity
- $n_e = 10^6$: gas is overionised → *lower opacity at t=8 ks!*

t=16 ks. Same flux as t=0.
- $n_e = 10^{10}$: spectrum equal to T=0 ks
- $n_e = 10^6$: overionised spectrum





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Work in progress: NGC 4051

R. Serafinelli, F. Nicastro, Y. Krongold, R. Middei, in prep.

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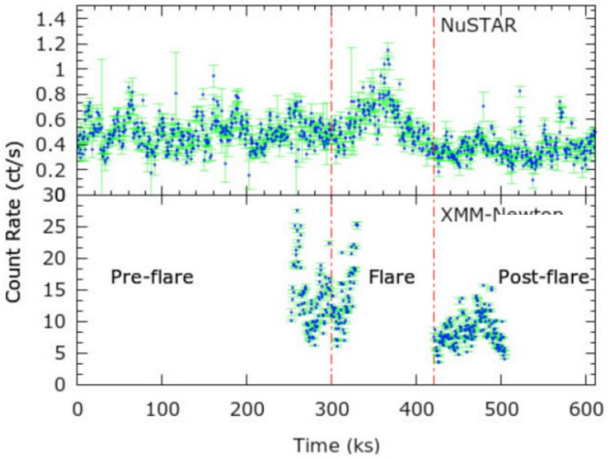
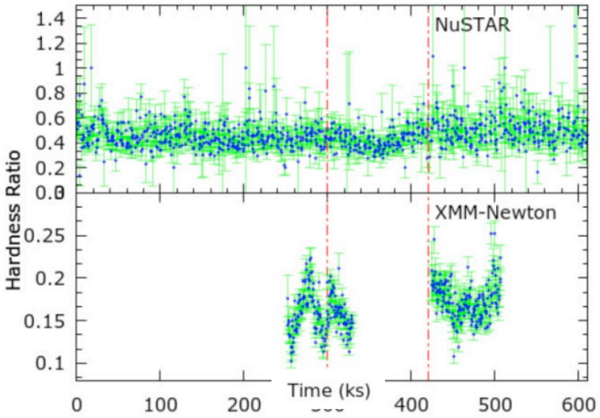
Fit of *XMM-Newton* time-resolved spectra of the Narrow-Line Sy1 NGC 4051

A simultaneous NuSTAR+XMM-Newton observation (taken in 2018) displaying both flux and shape variability:





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Gamma Ray Bursts

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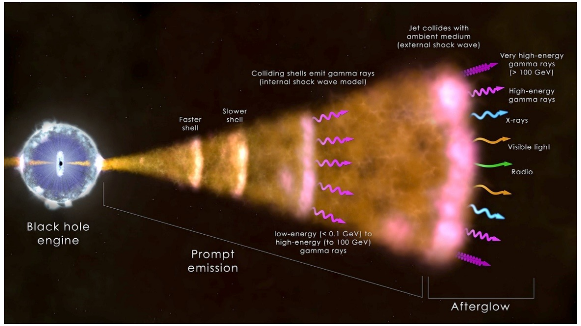
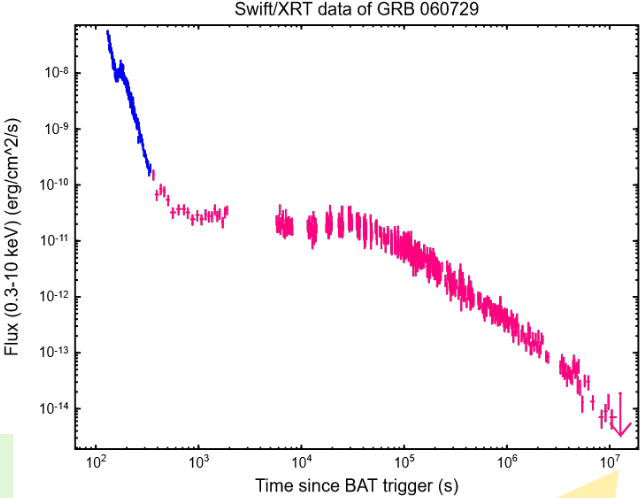
GRB are intrinsically transient,
non-equilibrium sources:





GRB are ideal probes to illuminate surrounding environment and shed light on <u>density, metallicity, volume</u> of Star Forming Regions and host galaxies… but:

Illuminated ambient gas is out of photoionisation equilibrium:
Need for time-evolving modelling!

Piro+02, D’Elia+09 , Krongold+13, Heintz+18

AHEAD 2020 GRBs

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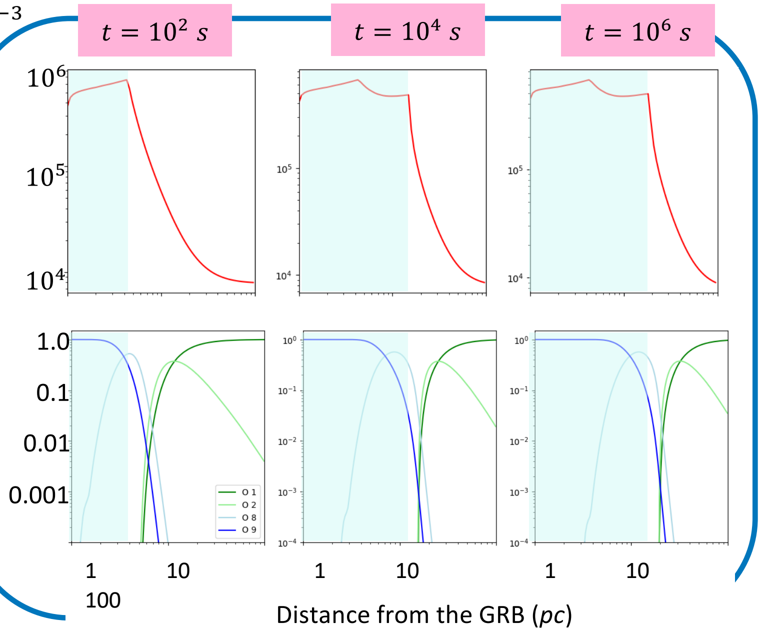
2. Time evolving computation

$n_e = 10^1\ cm^{-3}$

Temperature (Kelvin)

Oxygen ion abundances



The ionisation front moves outward for increasing time after the burst

O 9 (fully stripped)
O 8
O 2
O 1 (neutral)

2. Time evolving computation

AHEAD 2020 GRBs

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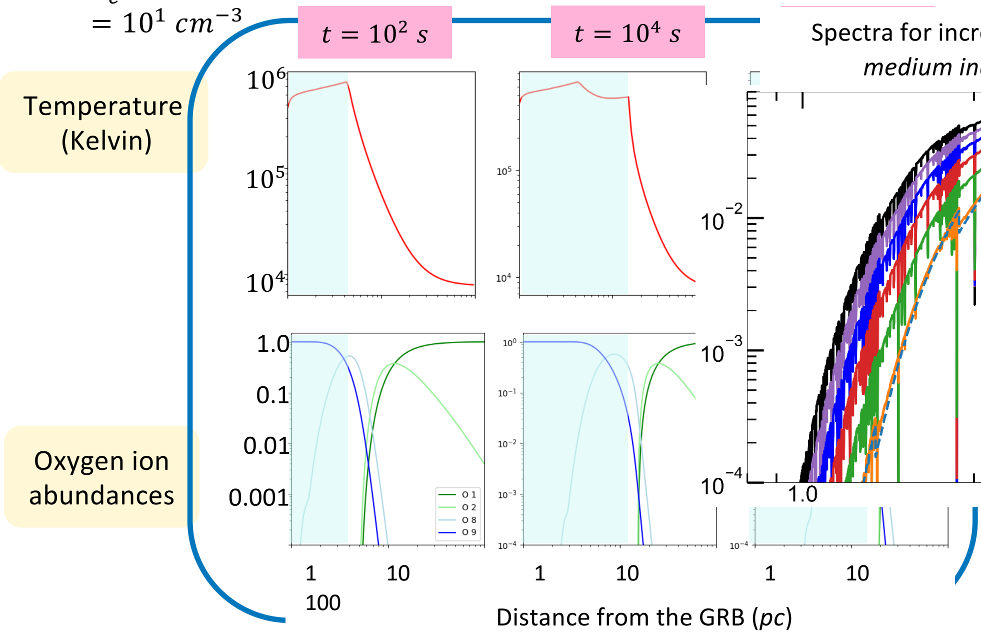
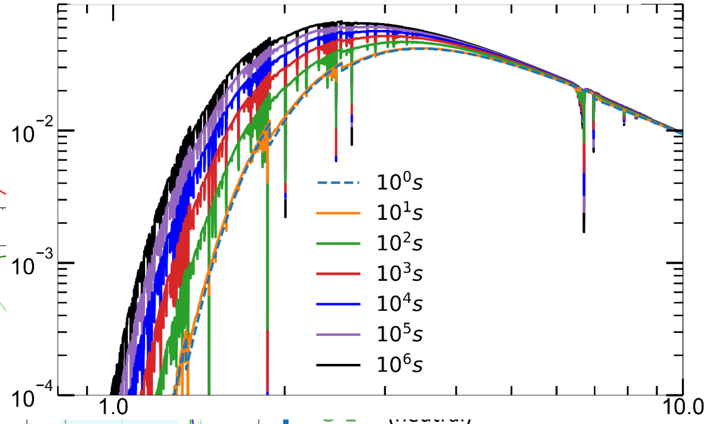
$n_e = 10^1\ cm^{-3}$



Spectra for increasing time after the burst:
medium increasingly transparent



AHEAD 2020 GRBs

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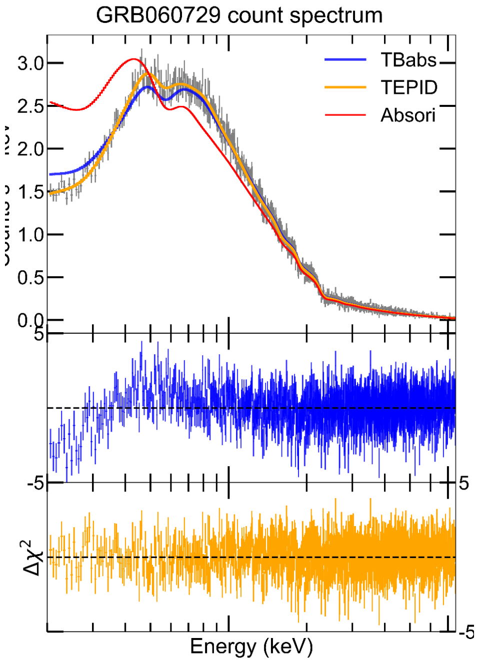

X-ray afterglow spectra are usually fitted phenomenologically through a layer cold absorber (Tbabs model in xspec).

However, proper time-evolving ionisation of the circumburst environment with TEPID gives a much better fit!

XMM-Newton GRB Golden-Sample

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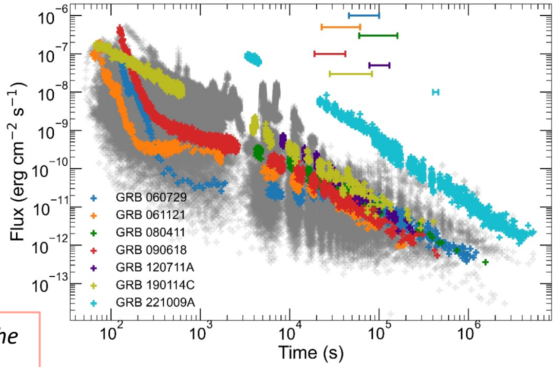
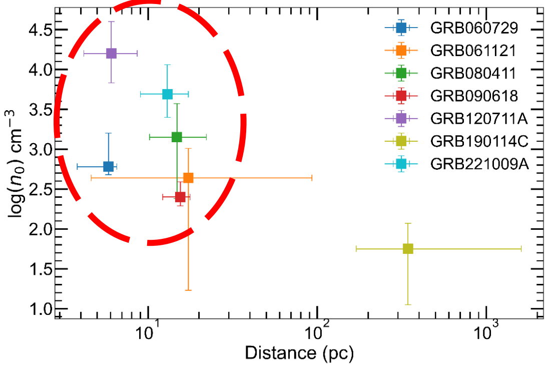
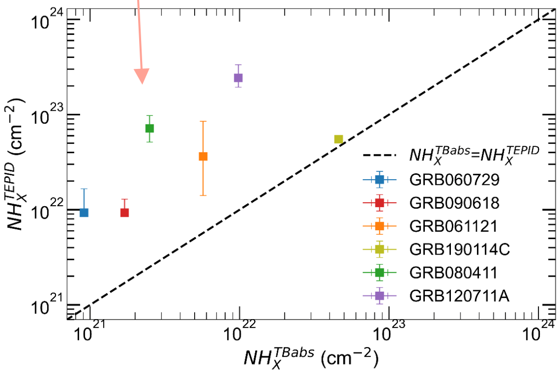
Fit of *XMM-Newton* spectra of high-flux GRB afterglows



TEPID reveals Star Forming Region-like overdensities around GRBs with $\approx 10\ pc$ *radii*

A fit with a TBabs neutral screen underpredicts the N_H *by up to a factor* 10





A. Thakur, L. Piro, A. Luminari, F. Nicastro et al, *to be submitted soon*

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Conclusions

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- AHEAD2020 activitites have been extremely productives over the past four years
  - many novel powerful tools for advanced data-analysis and modeling for current and new X-ray observatories have been realized, tested and delivered
  - For some of these tools and models the work will keep going (within the perimiter of the project and beyond that) towards continuous upgrades and updates (i.e. time-evolving photoionization tools, STATiX, 2D of ICM inhomogeneities, etc.) in close synergy with the continuous improvement and refinement of the atomic database.
  - TEPID Time-Evolving Photoionization Device is already available for absorption and continuum-emission spectral studies (not yet publicly, but please contact us), will “soon” (12-24 months) include level-population and so line-emission and be made publicly abailable via a GUI