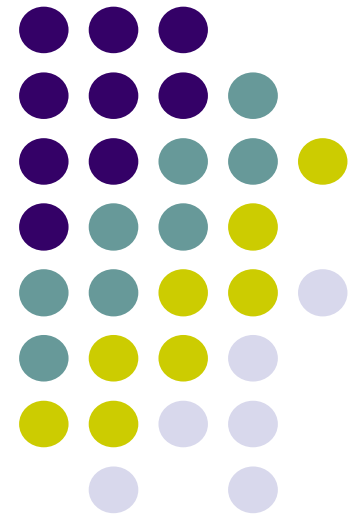# Development of theoretical databases with TITAN
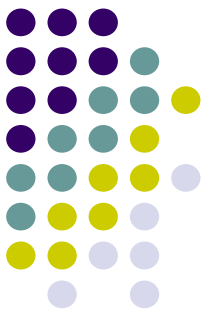
*Anabela C. Gonçalves*

LUTh, Observatoire de Paris

# Paris Observatory Numerical Gate

Its mission…

- To list, to promote, and to optimize the use of **numerical tools and codes (modeling and simulation)** developed at Paris Observatory

- By providing an easy access to the codes and related information

- By offering a "computation structure" for running the codes: provides both memory/hard disk space and support to the User

- To implement interface tools between the codes and the User, and between the different codes (workflow efforts)

- To build, to release, and give support to **databases of theoretical models** computed with those codes

- Census: 29 codes presently listed at Paris Observatory
  Test case: **PDR code** insertion progressing well (F. LePetit, F. Roy)
  To do next (in priority list): **TITAN code**

Paris Observatory Numerical Gate
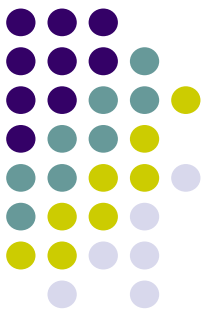
Grids' projects: computing the grids of results, plus developing the interface and exploitation tools

- Three grids' projects are presently contemplated:

  - Database of diluted clouds' models: **PDR code** (MIS team, LUTh)
    Project phase: stand by

  - Database of collapsing clouds' models: **Ramses/MHD codes** (PI: P. Hennebelle, LERMA)
    Project phase: computation, validation, documentation

  - Database of models for photoionized media in pressure equilibrium: **TITAN code** (PI: A. C. Gonçalves, LUTh)
    Project phase: tests were validated => larger grid computation, validation, automation, documentation

- Applications to large projects/space missions: ALMA, *Chandra, XMM-Newton, Simbol-X,…*
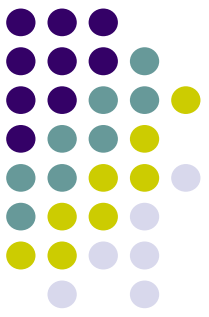
The TITAN code

Transfer−photoionization code for dense, warm, and optically thick/thin media irradiated by X-ray continuum

- Provides: ionization, temperature, and density structures for media in constant density, constant gas pressure, or **constant total pressure**

- Also: outward, transmitted and reflected **spectra** in multiple directions

- **Scientific applications:** theoretical modeling of Active Galactic Nuclei (AGN), X-ray binaries, Ultraluminous X-ray sources (ULXs), …

- **Observational applications:** interpretation of high-quality X-ray data from *Chandra, XMM-Newton, Suzaku*, …

- **Instrumental applications:** preparation of future X-ray missions (*Constellation-X*, **Simbol-X***, XEUS,…*), data simulation
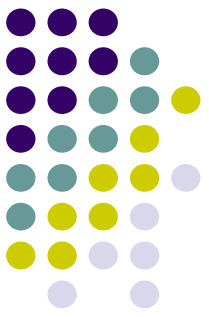
The need for TITAN databases

## TITAN unique modeling capabilities required by a growing community working on X-ray spectra

- TITAN models compute the exact transfer for ~1000 lines and the continuum **=> longer computation times** (~30h for constant P_{tot})

- TITAN allows for the modeling of regions in total pressure equilibrium, solves the thermal instabilities **=> complex models, hand-check** for convergence, choice of stable solutions

- Several domains of applicability: physical parameters can vary over a large range **=> needs quick, first-order estimation** of the physical parameters prior to complete modeling

- To compare TITAN physical modeling with other tools, to model and to simulate X-ray data in XSPEC => needs `table` **FITS models**
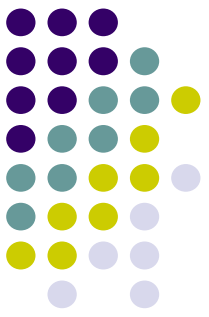
Grids of models benchmark

Focused on a TITAN particularity: constant P_{tot} models

- Started by a small number of varying parameters characterizing the ionized medium: ξ, N_H, and Γ

- Parameters covered by the first test grids:
  - Ionization parameter $1000 \leq \xi \leq 4000$ erg cm s^{-1}
  - Incident continuum (a power-law) photon index: $2.1 \leq \Gamma \leq 3.3$
  - Ionised medium column density: $10^{22} \leq N_H \leq 10^{23}$ cm^{-2}

- Computed multiple sets of grids, for different resolutions
  - Absorption grid
  - Emission grids in multiple directions (~7'−37.5°, 37.5−60°, 60−83.5°)
  - Reflection grids in multiple directions (same angles)
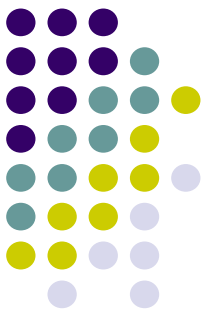
TITAN interface: XSPEC, Web

● **Confrontation of grids of results with the data: first order estimation**

● **Input parameters in Web interface => full model computation**

Utilisateur

ξ N_H Γ

profils de température, densité,
et ionisation, spectres, etc.

Portail Numérique

x^2

XSPEC

Grilles de modèles
théoriques TITAN

Estimation
de premier
ordre

Interface Web
Code de photoionisation
TITAN

Résultats
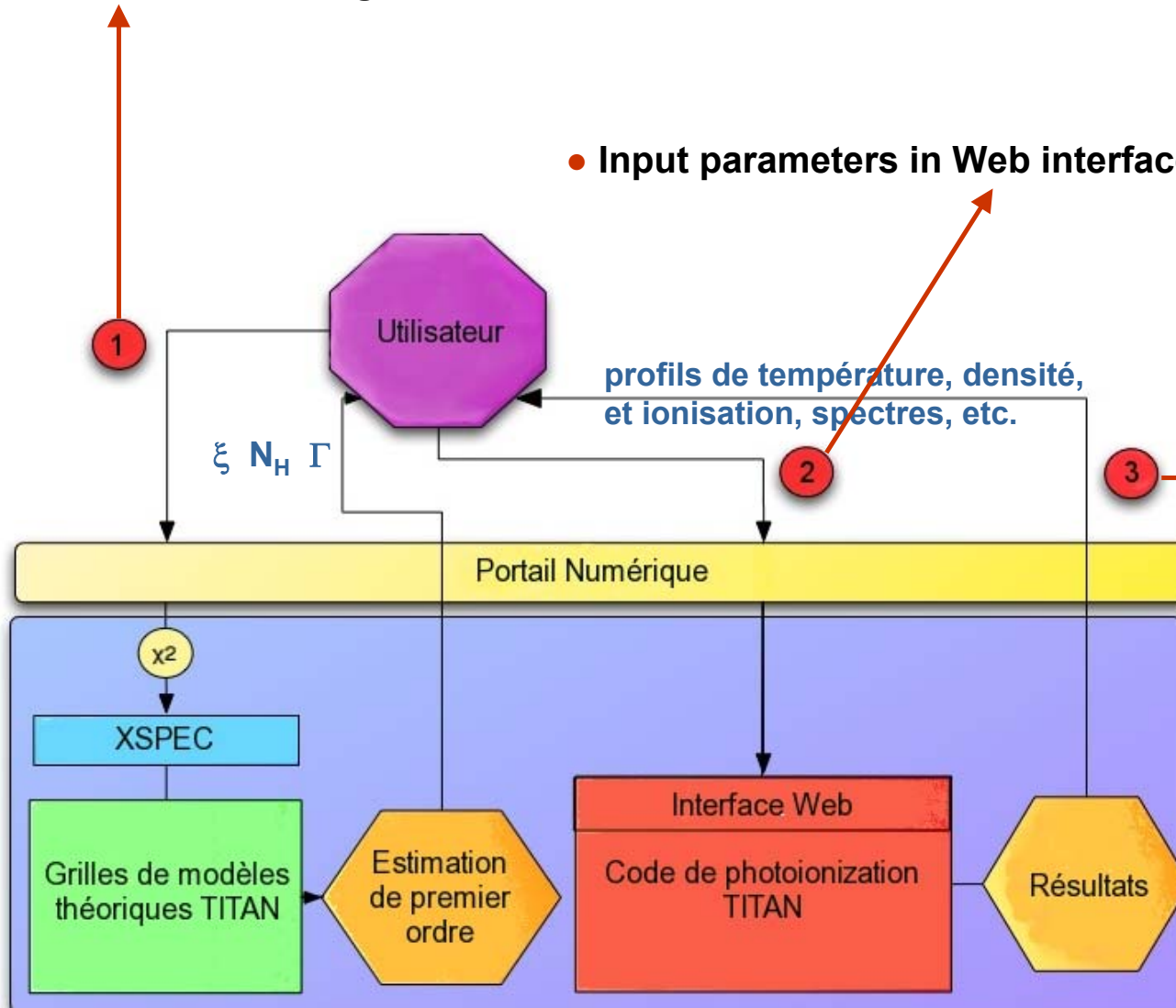
● **Interface tools development**

● **Complete database of results
(Temperature, Density, Ionic column
density, Pressure, …)**

● **At all stages (1, 2, and 3):** provide
User's support ('Service modeling')
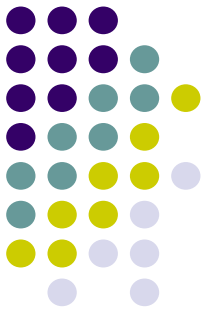
TITAN interface: XSPEC

Header and body format, specific to XSPEC

TITAN interface: Web

First tests will be replaced by a similar interface as the PDR code

- TITAN final Web interface will be addressed after the PDR code

- Similar interface (homogeneity)

- Will offer different levels of expertise (more or less visible parameters)
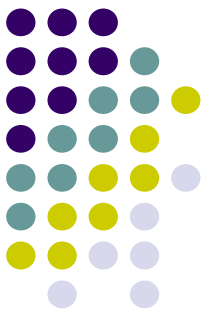
Perspectives and future work

TITAN photoionization models available to all

- Extend varying parameter's range to ~1000 models:
  - Ionization parameter $10 \leq \xi \leq 10^5$
  - Incident continuum (power-law) photon index: $1.2 \leq \Gamma \leq 3.6$
  - Ionised medium column density: $10^{20} \leq N_H \leq 10^{24.5}$
  - Storage needs ~1 Ko/model (R=300), computation time $\leq$ 30 h/model

- Extend energy range (and resolutions):
  - TITAN as stand-alone code: E < 25 keV
  - TITAN + NOAR (Compton heating/cooling): 25 < E < 100 keV

- Automation and documentation effort:
  - Interface tools between TITAN, other codes, XSPEC, and the User
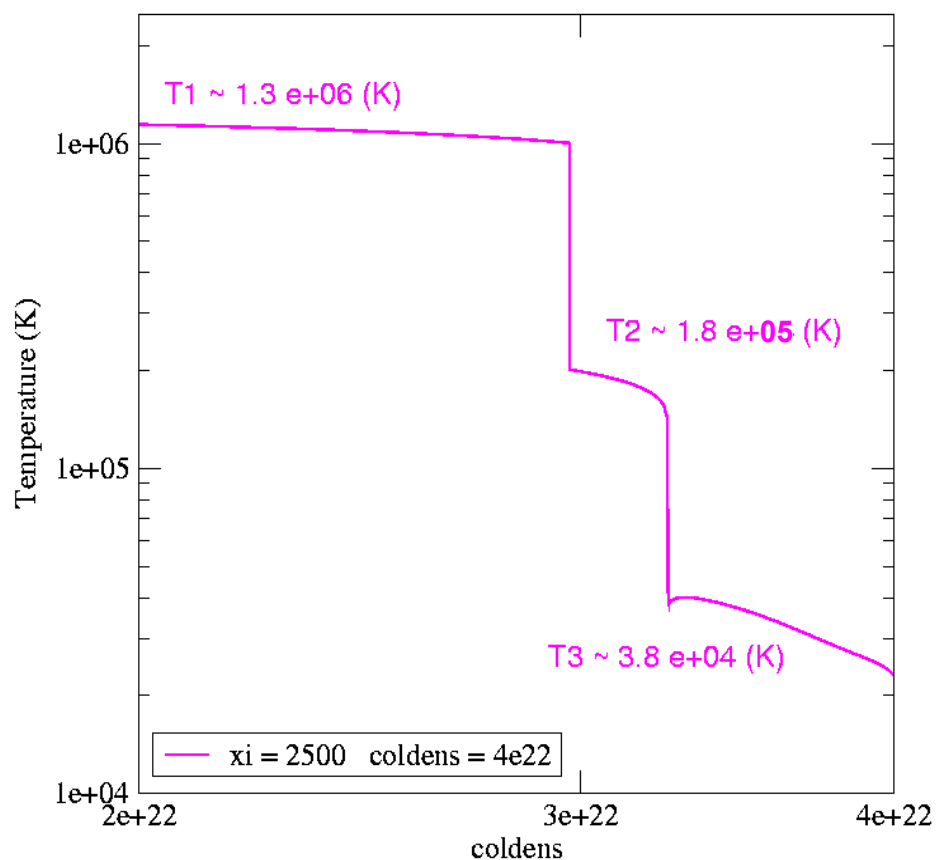 - Databases for other information produced by the code (T, ions, …)

Application to *Chandra* data

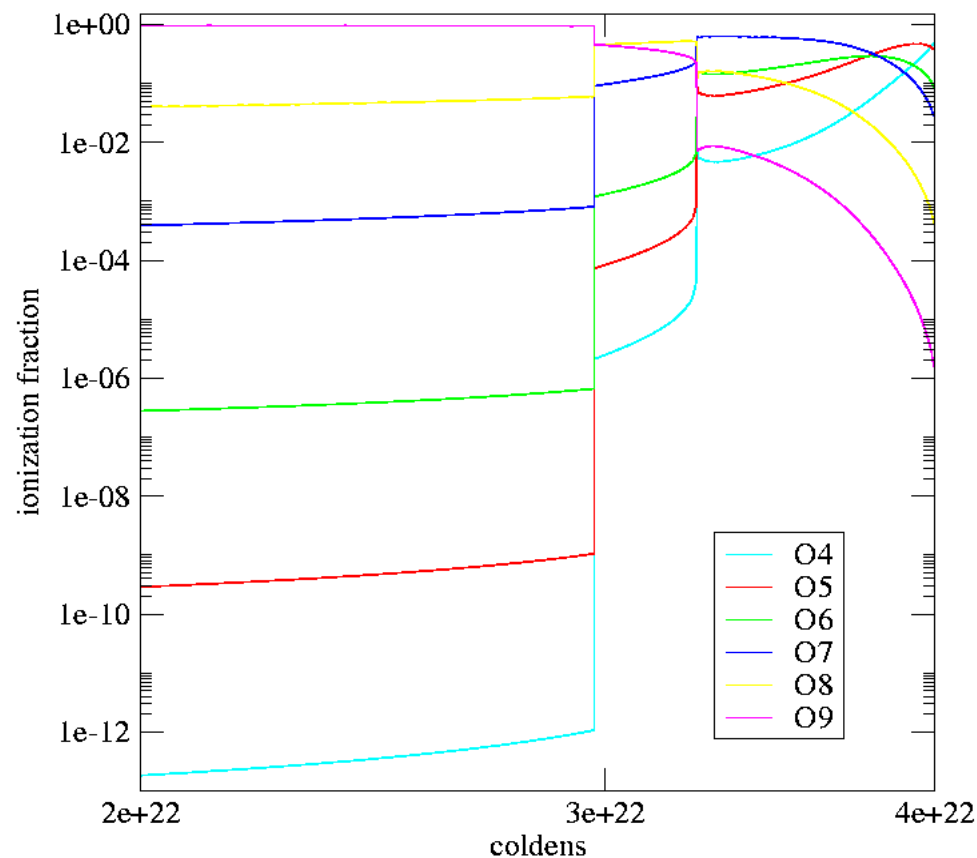## Modeling the Warm Absorber (WA) in NGC 3783
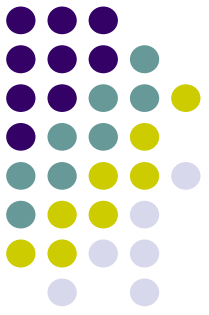

Temperature profile
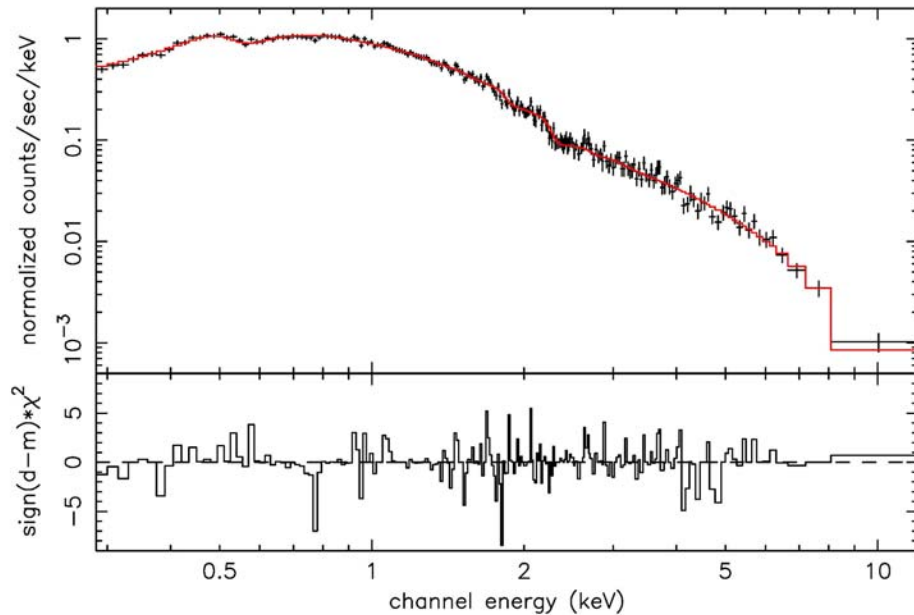1 constant pressure cloud

Oxygen ionization fracion
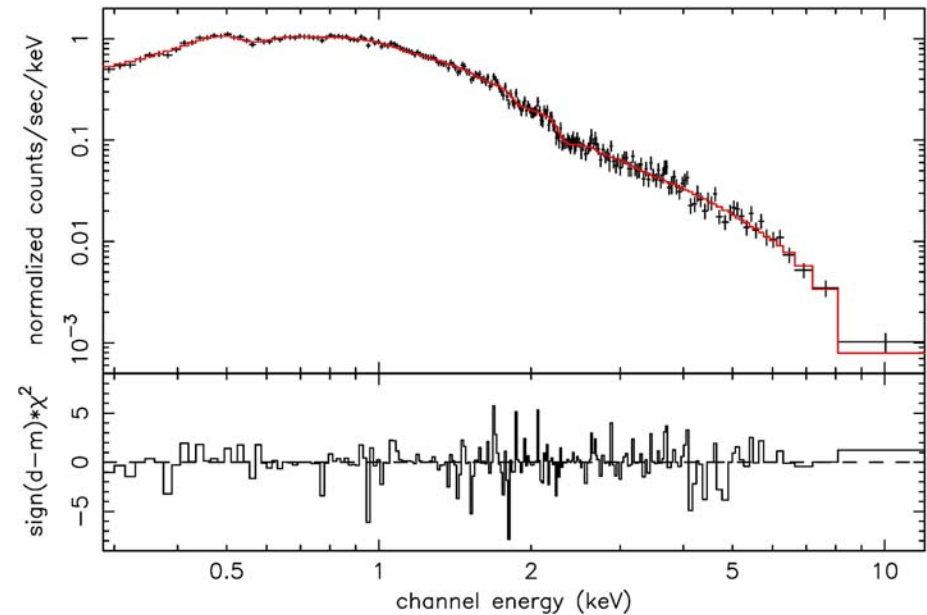Ptotx2500c4e22v150nh5

Application to *XMM-Newton* data

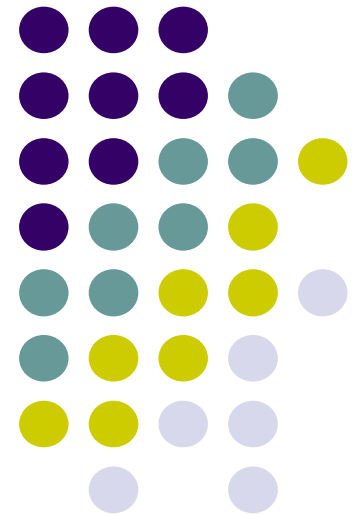## Modeling the X-ray spectra of ULXs

wabs x tbvarabs x (diskbb + po)

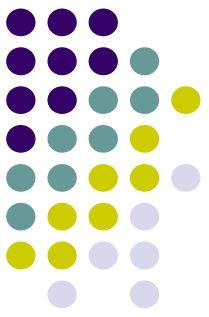χ^2 = 221.1/214 (1.04)

wabs x tbvarabs x (Temi + Tabs)

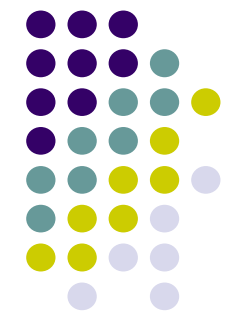χ^2 = 213.5/213 (1.00)

Additional slides

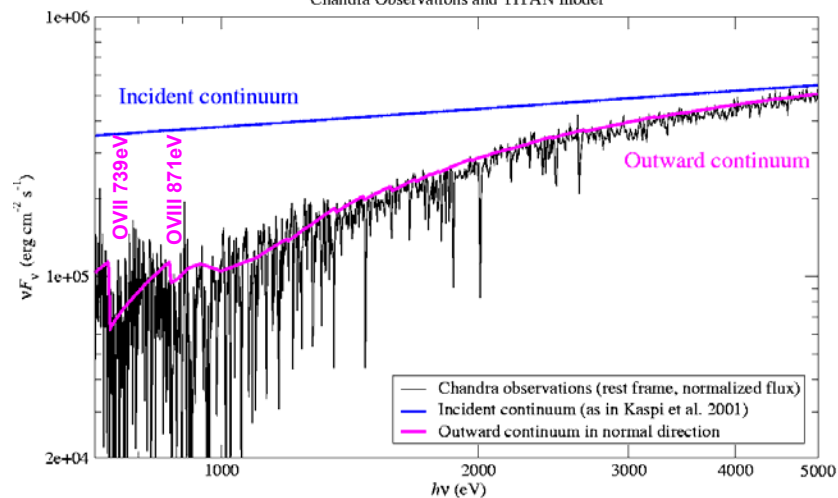# TITAN photo-ionization code

- Computes the gas structure in thermal and ionization equilibrium (locally and globally)

- 102 ions and atoms: H, He, C, N, O, Ne, Mg, Si, S, Fe

- Modes: constant density, gaseous pressure or total pressure

- Calculates multi-angle spectra (outward, reflected and transmitted)

- Accounts for Compton heating/cooling (coupled with NOAR)

- Parameters' optimal range:
  - $10^5 < n_H < 10^{14}$ cm^{-3}
  - $N_H < 10^{26}$ cm^{-2}
  - $8000 < T < 10^7$ K
  - $10 < \xi < 10^5$ erg cm s^{-1}

NGC 3783 *Chandra* modeling

NGC 3783
Chandra Observations and TITAN model

Incident continuum

OVII 739eV
OVIII 871eV

Outward continuum

Chandra observations (rest frame, normalized flux)
Incident continuum (as in Kaspi et al. 2001)
Outward continuum in normal direction

NGC 3783
Chandra observations and TITAN model

Chandra data
TITAN model (xi 2500, coldens
TITAN model (xi 2500, coldens
TITAN model (xi 2500, coldens

NGC 3783
Chandra observations and TITAN model

Si XIII
Si XIV
Si XIV
Mg XII
Si XIII
S XV

Chandra data
best TITAN model (xi=2500, coldens=3e22, total spe)
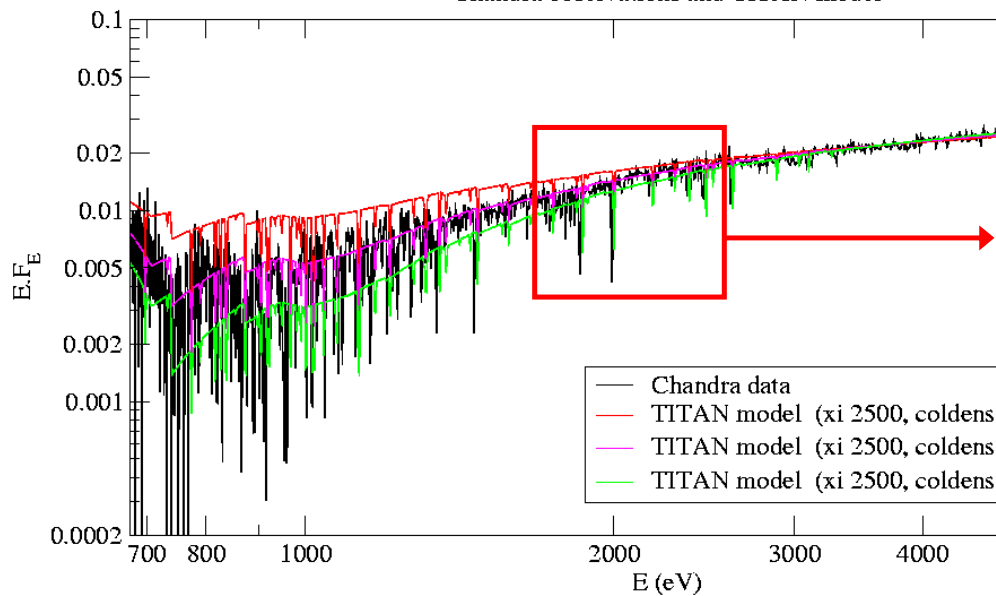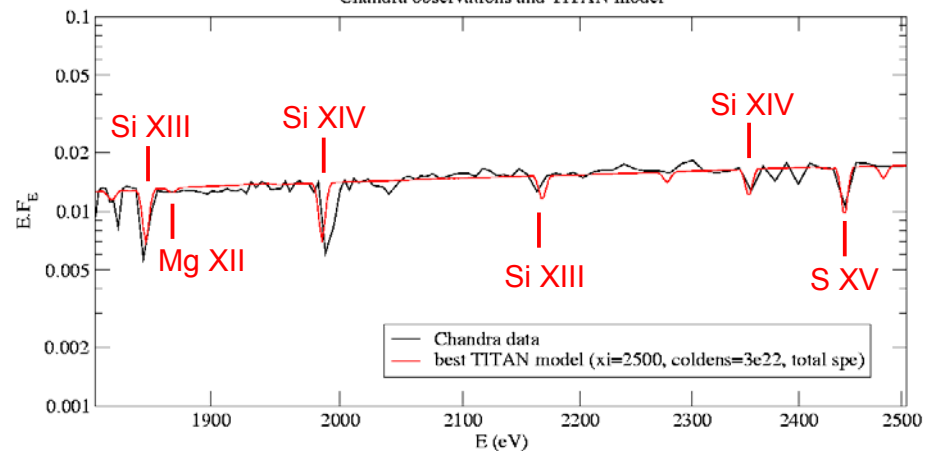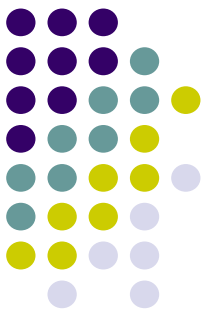
TITAN interface: Web

First web interface for launching TITAN models