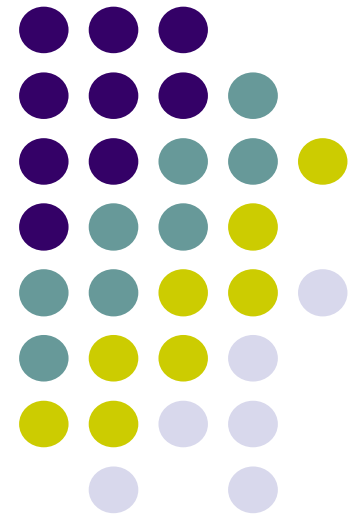


Development of theoretical databases with TITAN

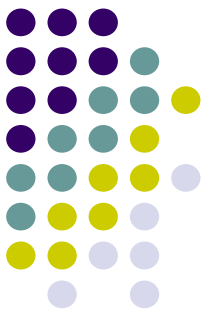


Anabela C. Gonçalves

LUTh, Observatoire de Paris



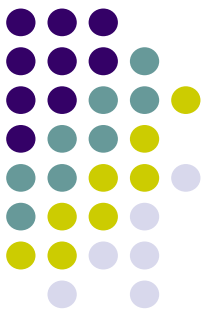
Paris Observatory Numerical Gate



Its mission...

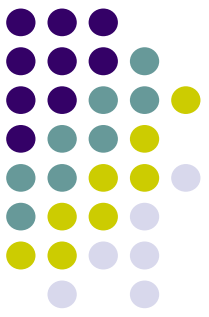
- To list, to promote, and to optimize the use of **numerical tools and codes (modeling and simulation)** developed at Paris Observatory
- By providing an easy access to the codes and related information
- By offering a “computation structure” for running the codes: provides both memory/hard disk space 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

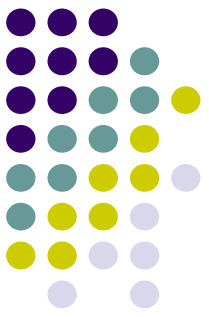
- Three grids' projects are presently contemplated:
 - Database of diluted clouds' models: **PDR code** (MIS team, LUTh)
Project phase: stand by
 - Database of collapsing clouds' models: **Ramses/MHD codes**
(PI: P. Hennebelle, LERMA)
Project phase: computation, validation, documentation
 - Database 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

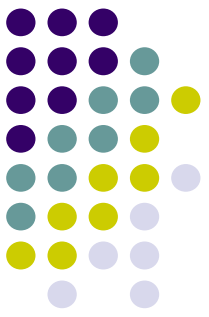
- Provides: ionization, temperature, and density structures for media in constant density, constant gas pressure, or **constant total pressure**
- Also: outward, transmitted and reflected **spectra** in multiple directions
- **Scientific applications:** theoretical modeling of Active Galactic Nuclei (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

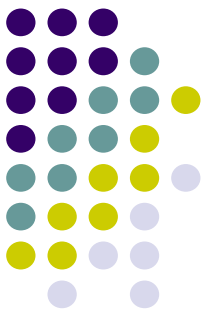
- TITAN models compute the exact transfer for ~ 1000 lines and the continuum => **longer computation times** (~ 30 h for constant P_{tot})
- TITAN allows for the modeling of regions in total pressure equilibrium, solves the thermal instabilities => **complex models, hand-check** for convergence, choice 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

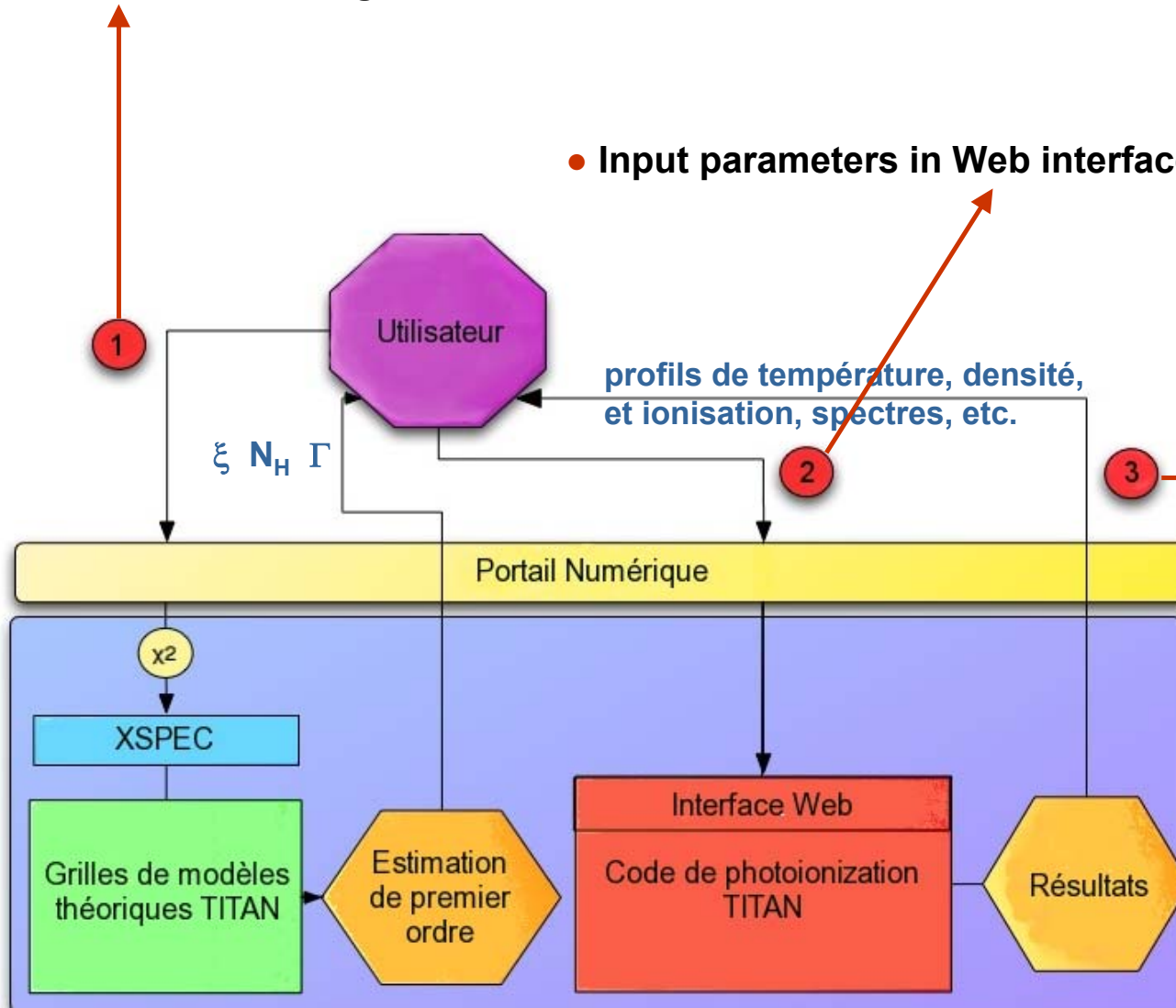
- Started by a small number of varying parameters characterizing the ionized medium: ξ , N_{H} , and Γ
- Parameters covered by the first test grids:
 - Ionization parameter $1000 \leq \xi \leq 4000 \text{ erg cm s}^{-1}$
 - Incident continuum (a power-law) photon index: $2.1 \leq \Gamma \leq 3.3$
 - Ionised medium column density: $10^{22} \leq N_{\text{H}} \leq 10^{23} \text{ cm}^{-2}$
- Computed multiple sets of grids, for different resolutions
 - Absorption grid
 - Emission grids in multiple directions ($\sim 7' - 37.5^\circ$, $37.5 - 60^\circ$, $60 - 83.5^\circ$)
 - Reflection grids in multiple directions (same angles)



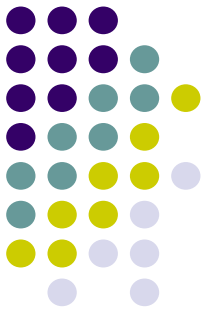
TITAN interface: XSPEC, Web

- Confrontation of grids of results with the data: first order estimation

- Input parameters in Web interface => full model computation



- 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

```
anabela@bob75-2-82-67-146-115.fbx.proxad.net: /home/anabela/OPM/titan-noar - Terminal - Konsole
Session  Édition  Affichage  Signets  Configuration  Aide
XSPEC>model atable{Tabs.fits}
Model: TITAN_ab<1>
Input parameter value, delta, min, bot, top, and max values for ...
      1.4      0.3      1.4      1.4      2.3      2.3
1:TITAN_ab:alpha>1.8
      1000      1.5E+03      1E+03      1E+03      4E+03      4E+03
2:TITAN_ab:xi>2200
      1E+22      4.5E+22      1E+22      1E+22      1E+23      1E+23
3:TITAN_ab:NH>3e22
      0      -0.001      0      0      5      5
4:TITAN_ab:Redshift>0
      1      0.01      0      0      1E+24      1E+24
5:TITAN_ab:norm>1e-3
-----
Model: TITAN_ab<1>
Model Fit Model Component Parameter Unit Value
par par comp
  1  1  1  TITAN_ab alpha 1.80000 +/- 0.00000
  2  2  1  TITAN_ab xi 2200.00 +/- 0.00000
  3  3  1  TITAN_ab NH 3.000000E+22 +/- 0.00000
  4  4  1  TITAN_ab Redshift 0.00000 frozen
  5  5  1  TITAN_ab norm 1.000000E-03 +/- 0.00000

Files being used for table models:
Model comp File
  1 Tabs.fits
-----
```

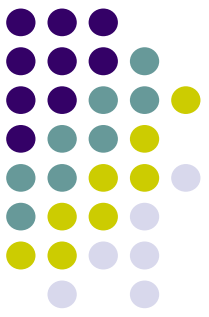
File Edit Tools Help

1 2 3

Select
 All
Invert

1	1.400000E+00	1.000000E+03	1.000000E+22
2	1.400000E+00	1.000000E+03	5.500000E+22
3	1.400000E+00	1.000000E+03	1.000000E+23
4	1.400000E+00	2.500000E+03	1.000000E+22
5	1.400000E+00	2.500000E+03	5.500000E+22
6	1.400000E+00	2.500000E+03	1.000000E+23
7	1.400000E+00	4.000000E+03	1.000000E+22
8	1.400000E+00	4.000000E+03	5.500000E+22
9	1.400000E+00	4.000000E+03	1.000000E+23
10	1.700000E+00	1.000000E+03	1.000000E+22
11	1.700000E+00	1.000000E+03	5.500000E+22
12	1.700000E+00	1.000000E+03	1.000000E+23
13	1.700000E+00	2.500000E+03	1.000000E+22
14	1.700000E+00	2.500000E+03	5.500000E+22
15	1.700000E+00	2.500000E+03	1.000000E+23
16	1.700000E+00	4.000000E+03	1.000000E+22
17	1.700000E+00	4.000000E+03	5.500000E+22
18	1.700000E+00	4.000000E+03	1.000000E+23
19	2.000000E+00	1.000000E+03	1.000000E+22
20	2.000000E+00	1.000000E+03	5.500000E+22
21	2.000000E+00	1.000000E+03	1.000000E+23
22	2.000000E+00	2.500000E+03	1.000000E+22
23	2.000000E+00	2.500000E+03	5.500000E+22
24	2.000000E+00	2.500000E+03	1.000000E+23
25	2.000000E+00	4.000000E+03	1.000000E+22

Go to: Edit cell:



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)

The Meudon PDR code

Cloud parameters | Grains parameters | Transfer

Model name:

Chemistry file:

Size (Av):

Density [cm⁻³]:

Radiation field (left):

Radiation field (right):

External source

Spectral type:

User defined source:

Distance [pc]:

Thermal balance

Temperature [K]:

Equation of state: Symmetrical profile

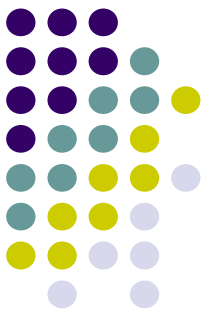
Specific density profile:

Pressure [cm⁻³ K]:

Cosmic rays ionization rate:

Turbulent velocity [km/s]:

Number of iterations:



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: $10^{20} \leq N_{\text{H}} \leq 10^{24.5}$
 - Storage needs ~1 Ko/model (R=300), computation time ≤ 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, ...)

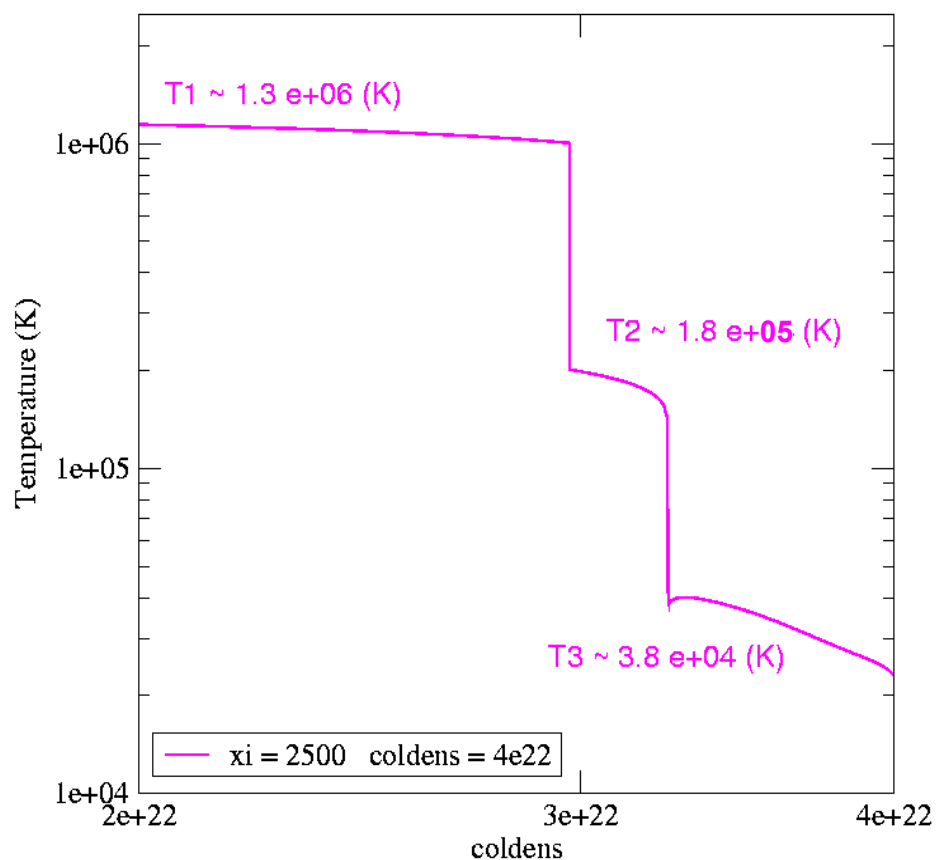


Application to *Chandra* data

Modeling the Warm Absorber (WA) in NGC 3783

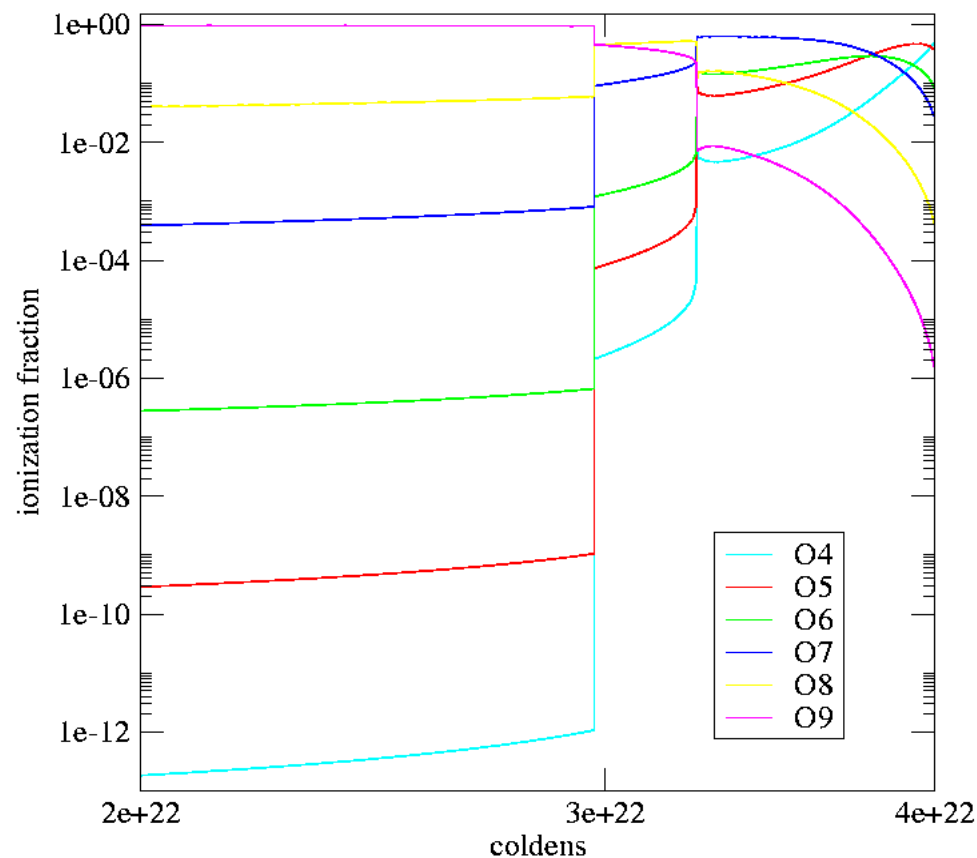
Temperature profile

1 constant pressure cloud

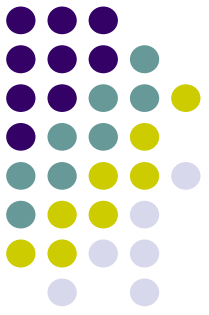


Oxygen ionization fraction

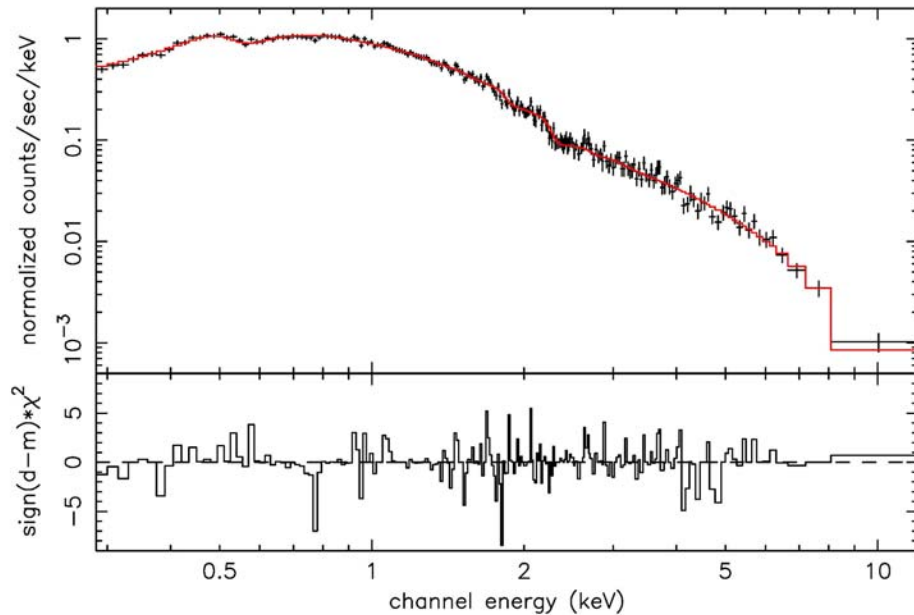
Ptotx2500c4e22v150nh5



Application to *XMM-Newton* data

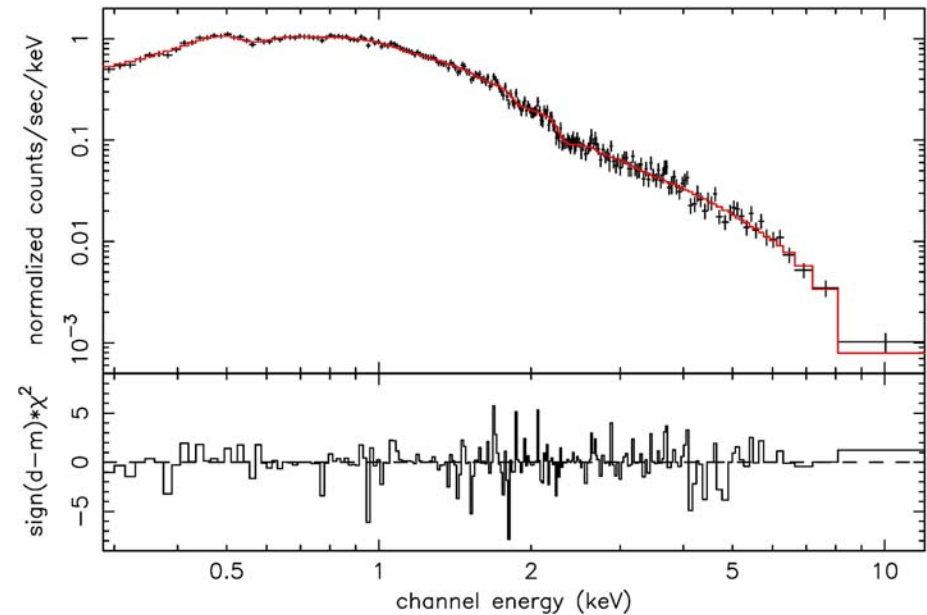


Modeling the X-ray spectra of ULXs



wabs x tbvarabs x (diskbb + po)

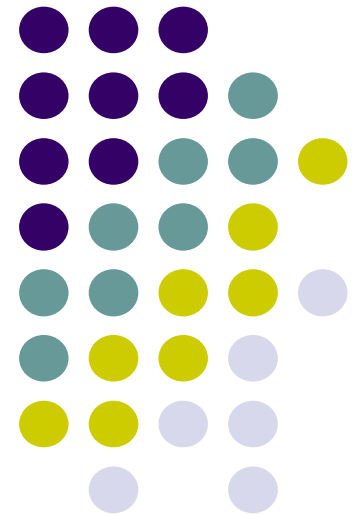
$$\chi^2 = 221.1/214 (1.04)$$



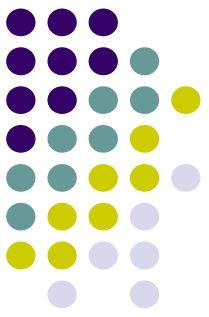
wabs x tbvarabs x (Temi + Tabs)

$$\chi^2 = 213.5/213 (1.00)$$

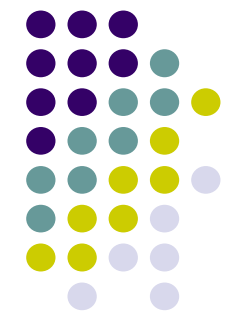
Additional slides



TITAN photo-ionization code

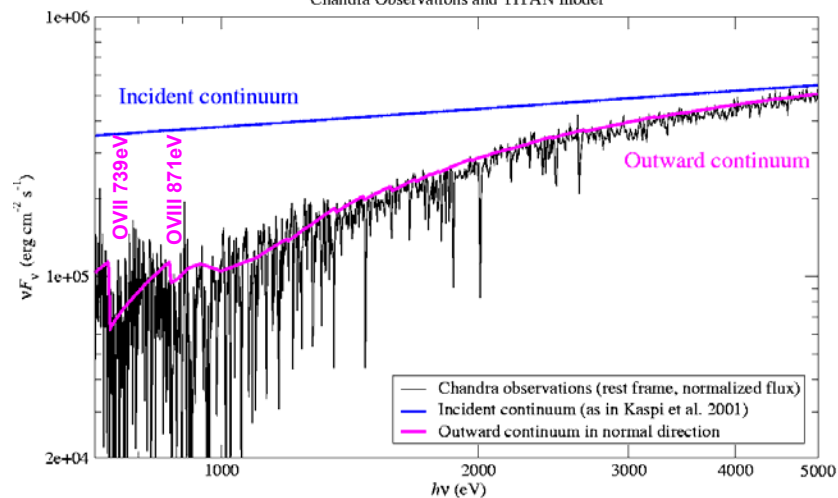


- Computes the gas structure in thermal and ionization equilibrium (locally and globally)
- 102 ions and atoms: H, He, C, N, O, Ne, Mg, Si, S, Fe
- Modes: constant density, gaseous pressure or total pressure
- Calculates multi-angle spectra (outward, reflected and transmitted)
- Accounts for Compton heating/cooling (coupled with NOAR)
- Parameters' optimal range:
 - $10^5 < n_{\text{H}} < 10^{14} \text{ cm}^{-3}$
 - $N_{\text{H}} < 10^{26} \text{ cm}^{-2}$
 - $8000 < T < 10^7 \text{ K}$
 - $10 < \xi < 10^5 \text{ erg cm s}^{-1}$

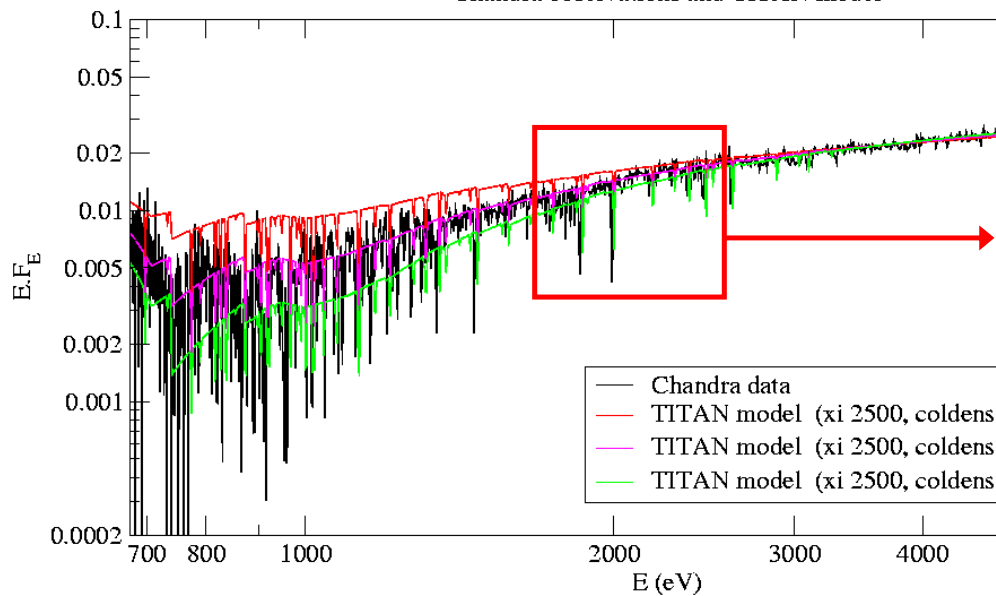


NGC 3783 *Chandra* modeling

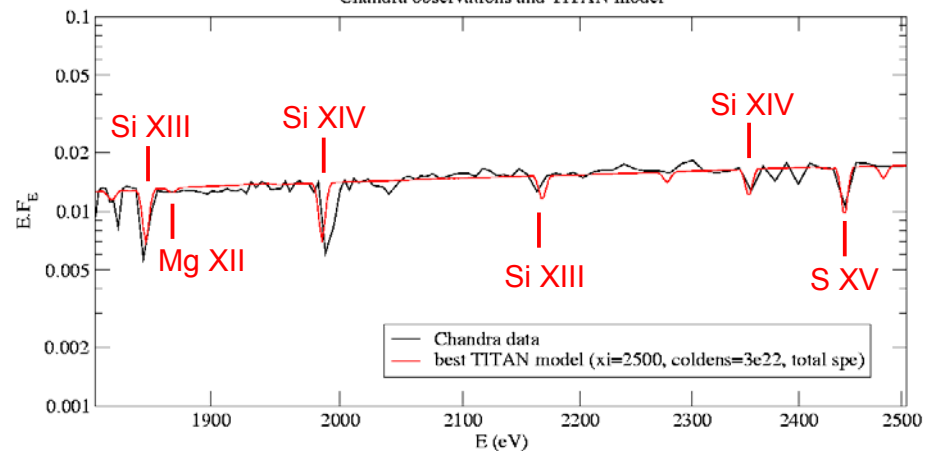
NGC 3783
Chandra Observations and TITAN model

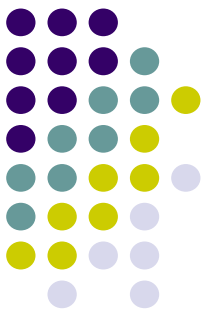


NGC 3783
Chandra observations and TITAN model




NGC 3783
Chandra observations and TITAN model





TITAN interface: Web

First web interface for launching TITAN models

 **Portail de simulations numériques**

TITAN : Modélisation des milieux photoionisés

Ensembles de paramètres

Enregistrer l'ensemble de paramètres sous le nom:

Type de paramètres d'entrée [parfile]: * ?

Upload an input parameter file: aucun fichier sélectionné ?

Session name [titre]: * ?

Type of atomic data [fichatomic]: * ?

Upload an atomic data file: aucun fichier sélectionné ?

hydrostatic equilibrium [idens]: * ?

Surface hydrogen density (units cm) [nhinit]: * ?

Initial temperature (units K) [tinit]: * ?

Total column density (units cm⁻²) [coldens]: * ?

Turbulent velocity (units km/s) [vturb]: * ?

Index for a power-law density [dendex]: * ?