A database of pressure equilibrium models with the TITAN code

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Although extremely useful in different astronomical contexts, models in pressure equilibrium are seldom applied to the highly ionized gas in the vicinity of strong X-ray sources. This is mainly due to the lack of such a computation option in the principal codes available to the community, as well as to the fact such models require very sensitive and time-consuming computations. The photoionization code TITAN, developed by our team, fulfills this gap allowing for the treatment of the ionized gas in constant gas pressure or total (gas+radiation) pressure. It gives as output the ionization, density, and temperature structures, as well as the reflected, emitted outward, and absorbed spectra. In an effort to provide the community with a ready-to-use set of constant total pressure models, TITAN is being used to compute a grid of results covering a wide range in ionization parameter, column density, and shape of the incident ionizing continuum; the computed models correspond thus to different gas conditions and can be applied to various research subjects. Such grids of models can be easily imported into XSPEC and used to fit all kinds of X-ray spectra. In addition, they can be used to simulate satellite data, an extremely useful feature in the preparation of future X-ray missions, such as Simbol-X or Con-X. The models will be stored in the Simulation Data Center at Paris Observatory and granted access through VO facilities.

TITAN – What is it?

It's a stationary, photoionization-transfer code for dense, warm, and optically thick or thin media, irradiated by an X-ray continuum

- It assumes a 1D plane-parallel geometry with a slab of gas illuminated on one side
- Includes all relevant processes: photoionization, radiative and di-electronic recombination, collisional ionization, ionization by high-energy photons, Auger processes, fluorescence, radiative and collisional excitation/de-excitation, etc.
- Computes the gas structure in ionization and thermal equilibrium
- It can work under constant density, constant gas pressure or constant total pressure
- Coupled with the NOAR code: accounts for Compton heating/cooling and may cover a large Energy range (0.1–4 10^5 eV)
- Atomic data (NIST): 102 ions and atoms of H, He, C, N, O, Ne, Mg, Si, S, Fe, amounting to ~1000 lines
- Parameters' optimal range: $10^5 < n_H < 10^{14}$ cm^{-3} $N_H < 10^{26}$ cm^{-2}; $8000 < T < 10^8$ K $10 < \xi < 10^5$ erg cm s^{-1}

It provides…

- Ionization, temperature, density structures…
- Outward, transmitted and reflected spectra, in multiple directions

TITAN – What is it for?

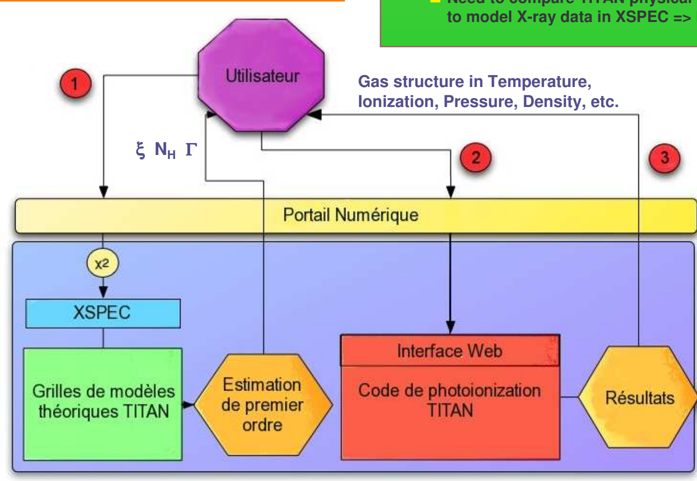
Scientific applications: e.g. the central regions of Active Galactic Nuclei (AGN), X-ray binaries, Ultra-soft Luminous X-ray sources (ULXs) …

Observational applications: interpretation of high-quality X-ray spectra from *Chandra, XMM-Newton, Suzaku,* etc. and preparation of future X-ray missions (*Con-X*, *XEUS*, *Simbol-X, …)*

The need for a database of results

TITAN modeling capabilities required by a growing astrophysical community working on X-ray spectra of AGN, ULXs, X-ray binaries…

- TITAN computes the exact transfer (ALI) for ~1000 lines and the continuum => longer computation times than other approximate methods (constant P_{tot} ~30h)
- TITAN allows for the modeling of regions in total pressure equilibrium => certain expertise needed, hand-check for convergence and possible instabilities
- Several domains of applicability: physical parameters can vary over a large range => quick, first-order estimation of the physical parameters needed prior data modelling
- Need to compare TITAN physical models with available phenomenological tools, and to model X-ray data in XSPEC => FITS table models for XSPEC



Grids benchmark

Focused on a TITAN particularity: models in total pressure equilibrium

- Started by a small number of varying parameters characterizing the ionized medium: the ionization parameter ξ, the column density N_H, and and power-law photon index Γ
- Parameters covered by the test grids:
  - Ionization parameter $1000 \leq \xi \leq 4000$ erg cm s^{-1}
  - 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 grids (45 models each) in absorption, emission (in multiple directions), and reflection (in multiple directions), for different resolutions

Interoperability with XSPEC

FITS `table models`, usable in XSPEC (a package for X-ray data reduction and analysis)

- Allows for spectra modeling, different models comparison, and data simulation
- Permits a first order estimation of the fitting parameters ξ, N_H and Γ (step 1 in figure)
- These parameters could, in a second step, be used for a full model computation (model launch though the web, via the Paris Obs. Numerical Simulations Data Center)
- On-line support to TITAN modeling will be provided to registered users

TITAN models in the Paris Observatory Numerical Simulations Data Center

Database of photoionization models, including not only the simulated spectra, but also information on the Temperature, Pressure, Ionization…

- Perspectives: extend grids to ~1000 models (thanks to LUTH cluster Titanic, IDRIS)
- Enlarge the parameter's range:
  - Ionization parameter $10 \leq \xi \leq 10^5$
  - Incident continuum (power-law) photon index: $1.2 \leq \Gamma \leq 3.6$
  - Ionized medium column density: $10^{20} \leq N_H \leq 10^{24.5}$
- Extend the energy range encompassed by the models
- Account for different resolutions (different instruments)
- On-going and future automation and documentation efforts:
  - Develop interface tools between TITAN, XSPEC, and the user
  - Databases for all pertinent information produced by the code (T, P, ions, …)
  - Workflow issues concerning coupling with the NOAR code
- Storing and computation needs: ~1 Ko/model (for R=300, range 0.3–12 keV)), computation time for a constant Ptot model ≤ 30 h