Prospects, challenges and evolution of AGN modeling in the Astro-H Era
Rikkyo University, Tokyo, October 21-22, 2015

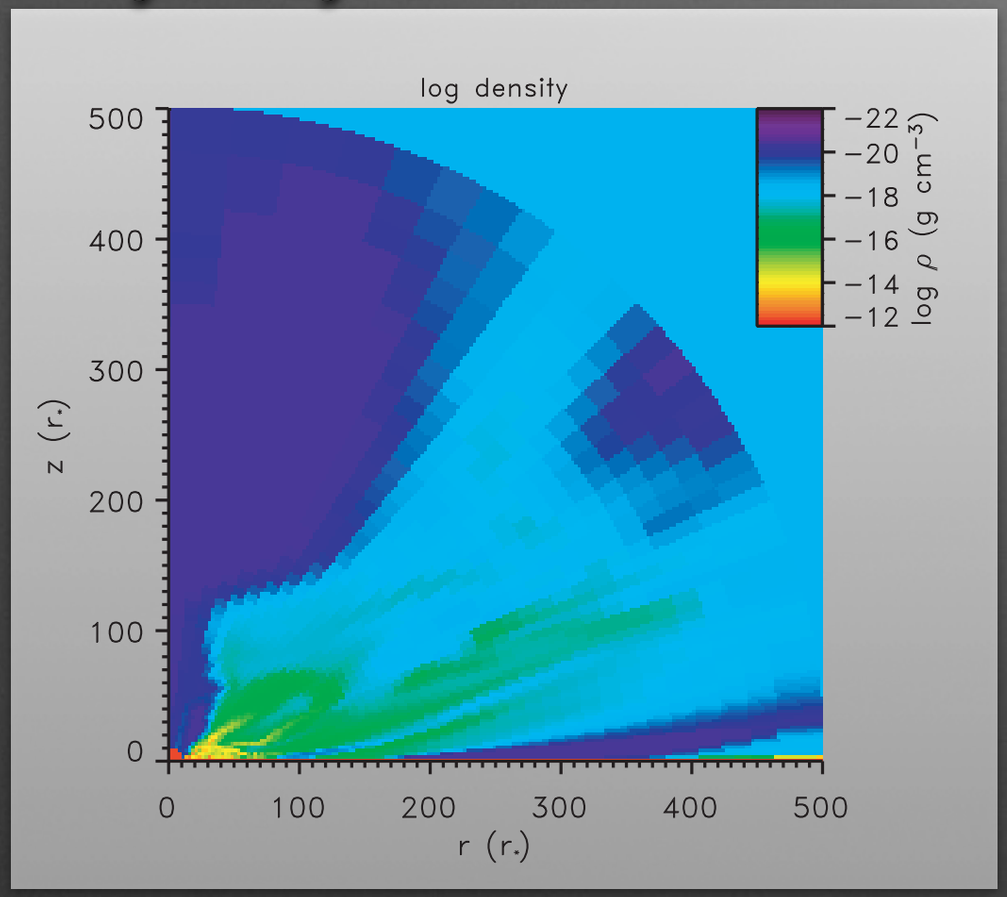
Monte Carlo Approach to Radiation Modeling of AGN

Hirokazu Odaka
ISAS/JAXA

Linking between Theory and Observation

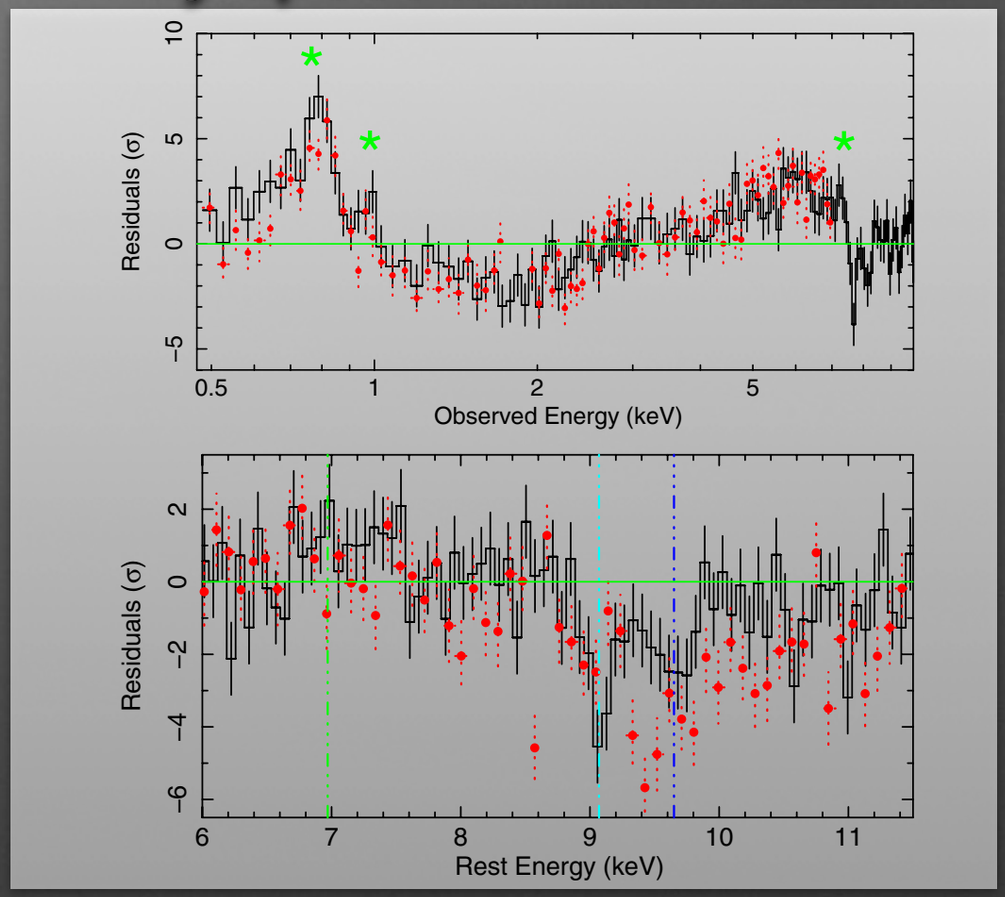
AGN outflow seen from theory and observation

Hydrodynamic simulation



Proga & Kallman 2004

X-ray spectrum with Suzaku



Reeves et al. 2009

No direct link between them!

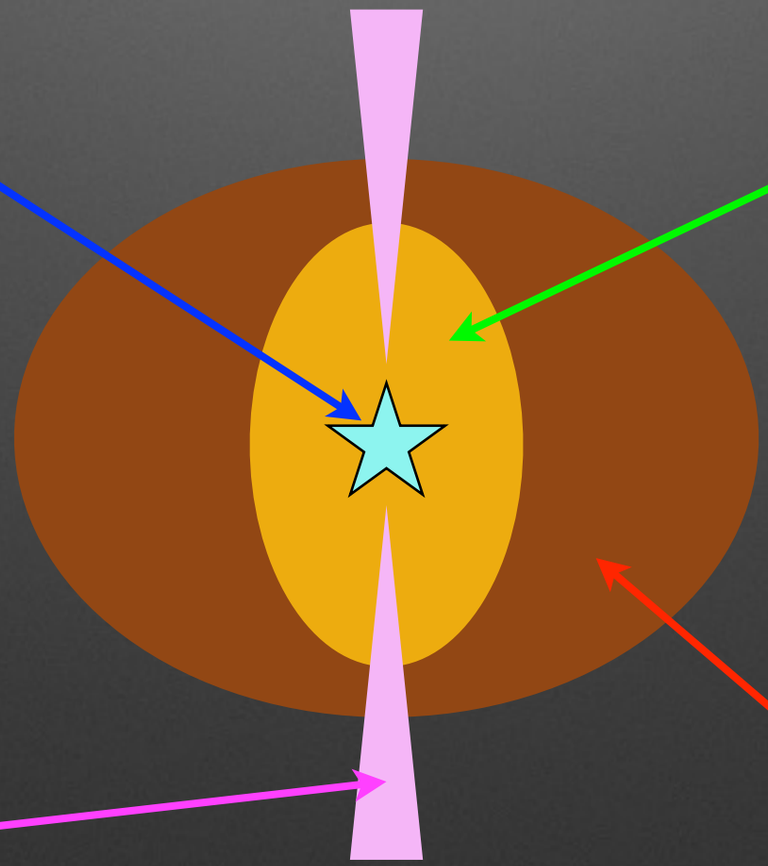
We can not directly observe the local properties (density, temperature, etc.).
To link theory to observational information, we need radiation modeling.

Structure of Accreting System

- For radiation modeling, we start with a basic picture of an accreting system.
- This structure is common both to stellar mass systems and AGN.

Central Engine
- accretion flow onto a black hole or neutron star
- emitting strong radiation

Release of gravitational energy



Photoionized Plasma
- ionized by strong radiation
- reprocessing into lines and continuum

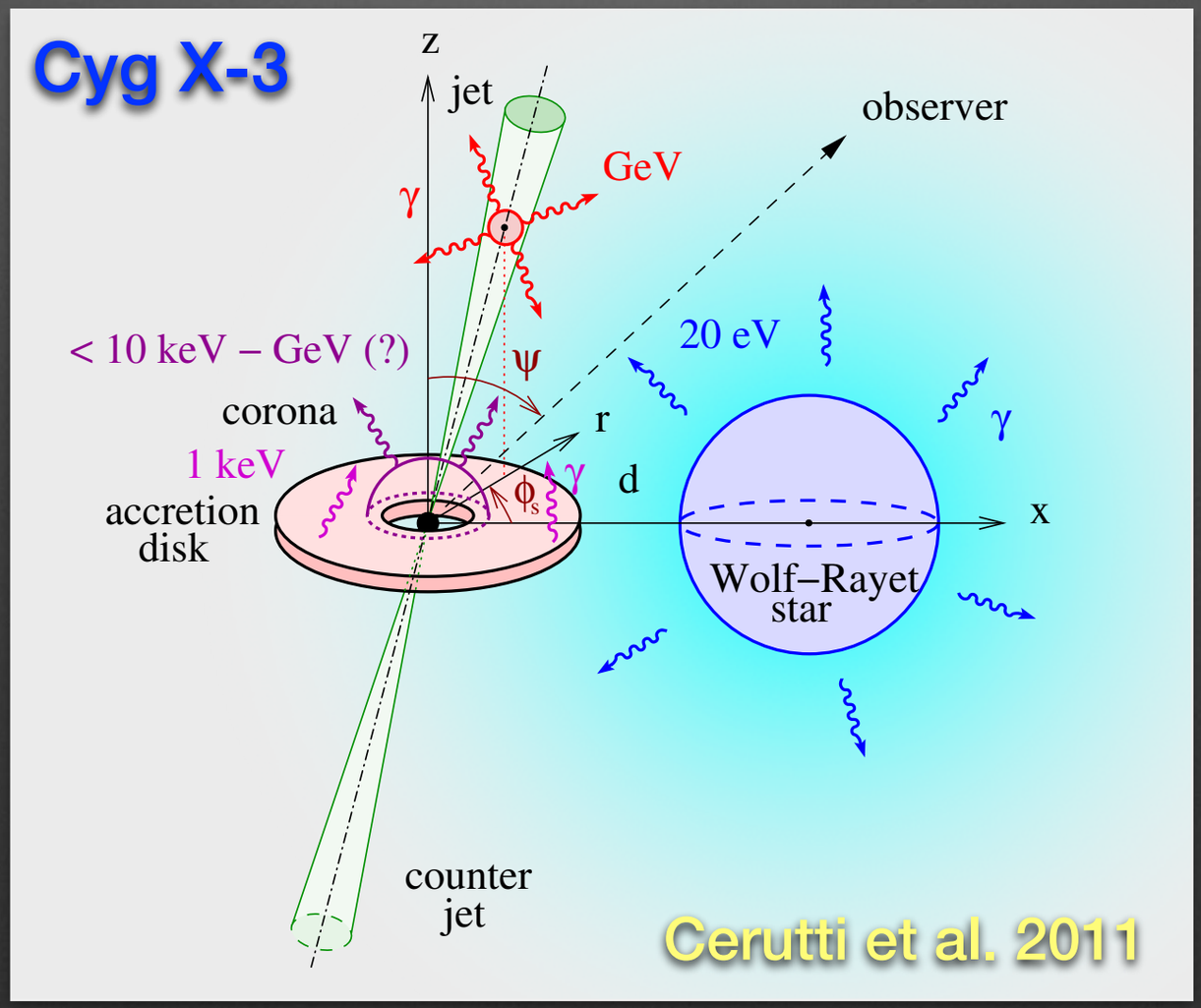
- surroundings provide matter for accretion.
- some part is outflowing.

Relativistic Jet
Energy release via mechanical power

Cold Matter
- reflecting X-rays

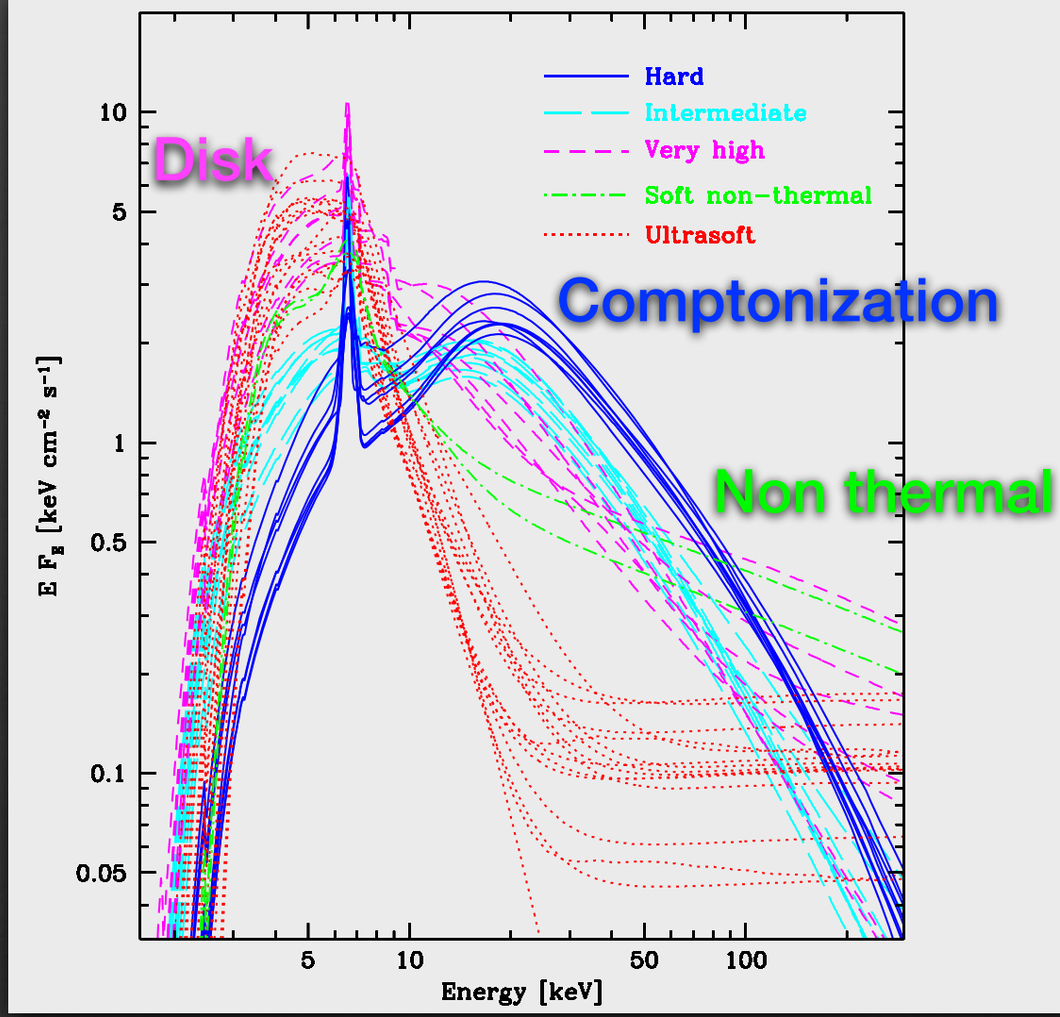
Analogy to Stellar Mass Systems

- Stellar mass systems are useful for a benchmark of AGN modeling.
- X-ray binaries (black holes or neutron stars)
- Accreting white dwarfs are also helpful since they have comparable disk temperature.



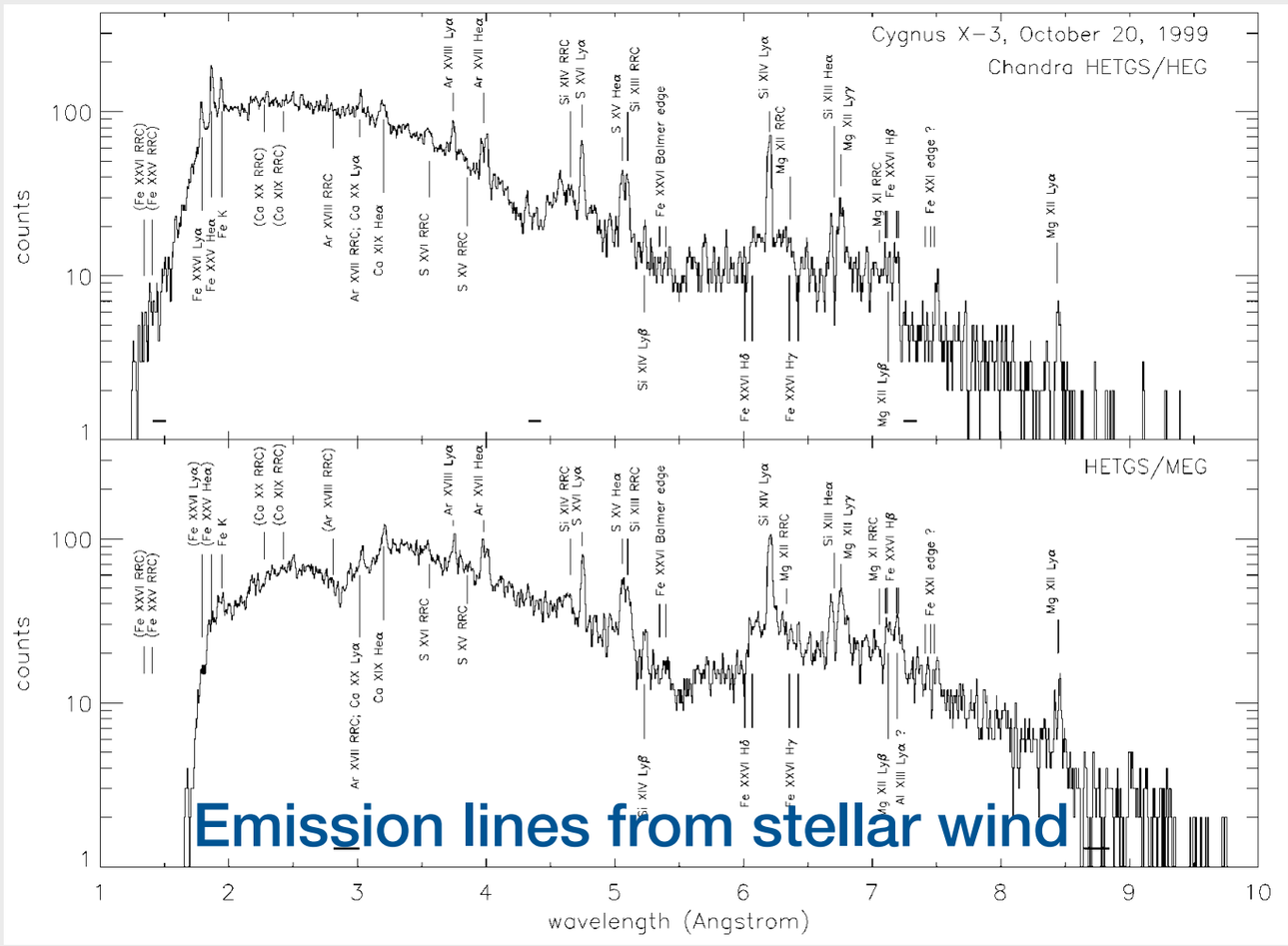
X-ray View of an Accreting Object

Cyg X-3 in a wide band (RXTE)



Hjalmarsdotter et al. 2009

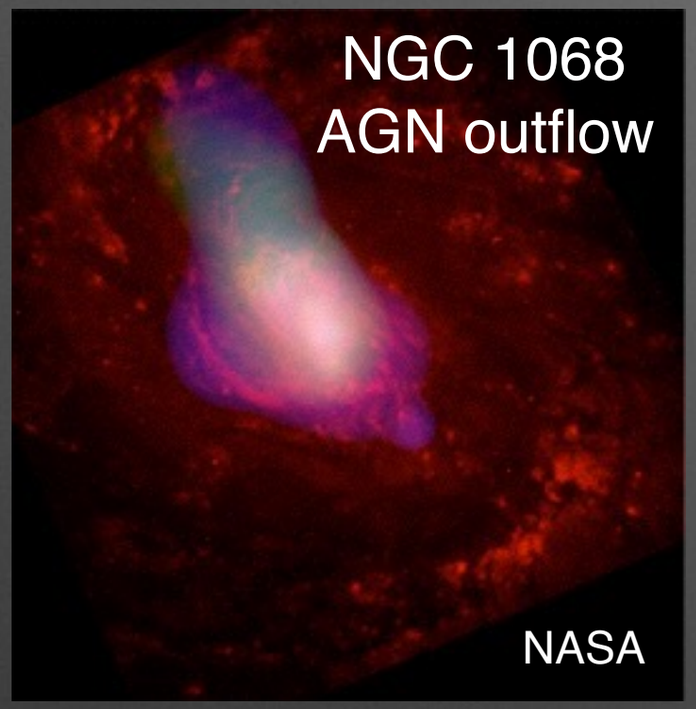
Cyg X-3 in high resolution (Chandra-HETG)



Paerels et al. 2000

X-ray features emerging from Comptonization, disk black body, disk reflection, photoionized stellar wind, etc. tell us physical conditions of the system. We need a model to interpret this spectrum.

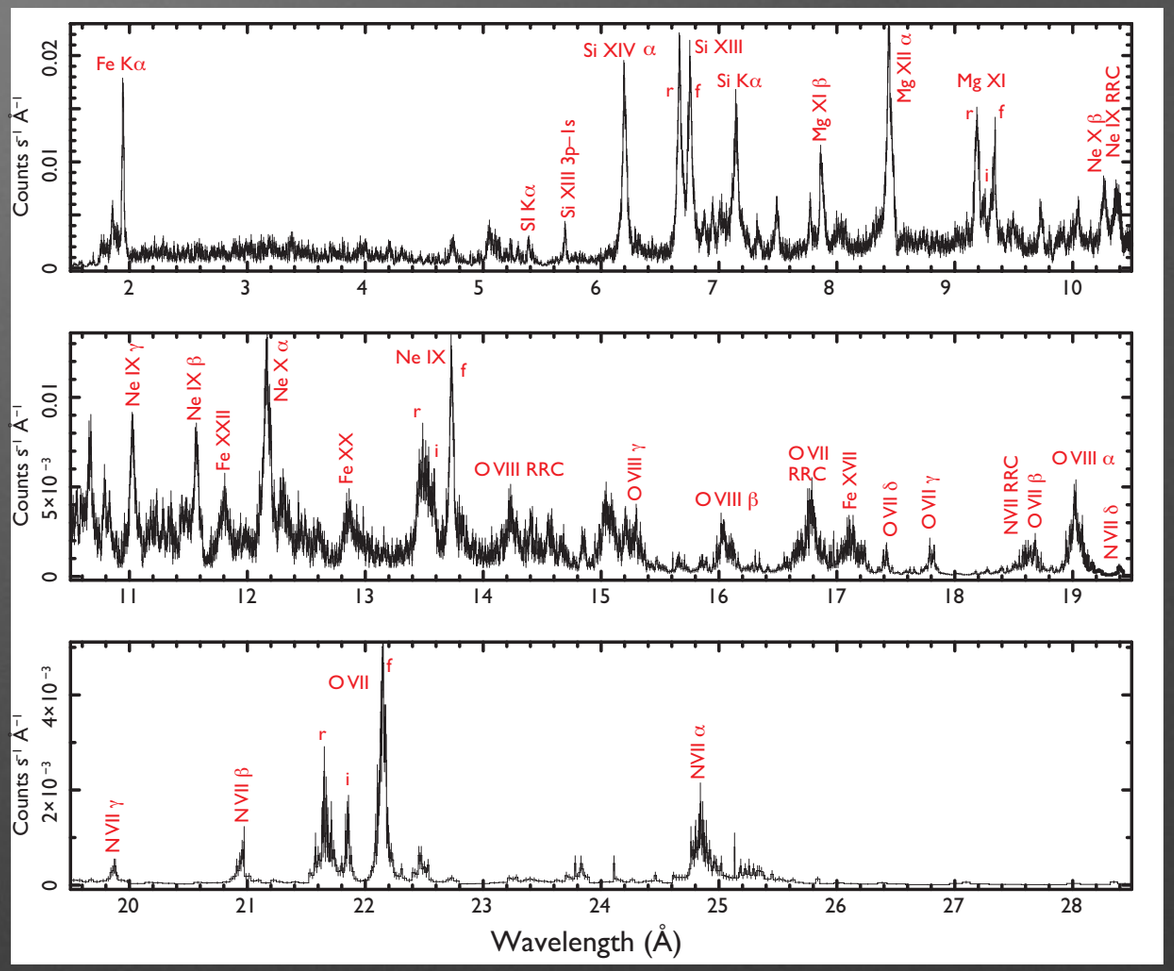
X-ray View of an Accreting Object



Chandra

←Image

Spectrum→



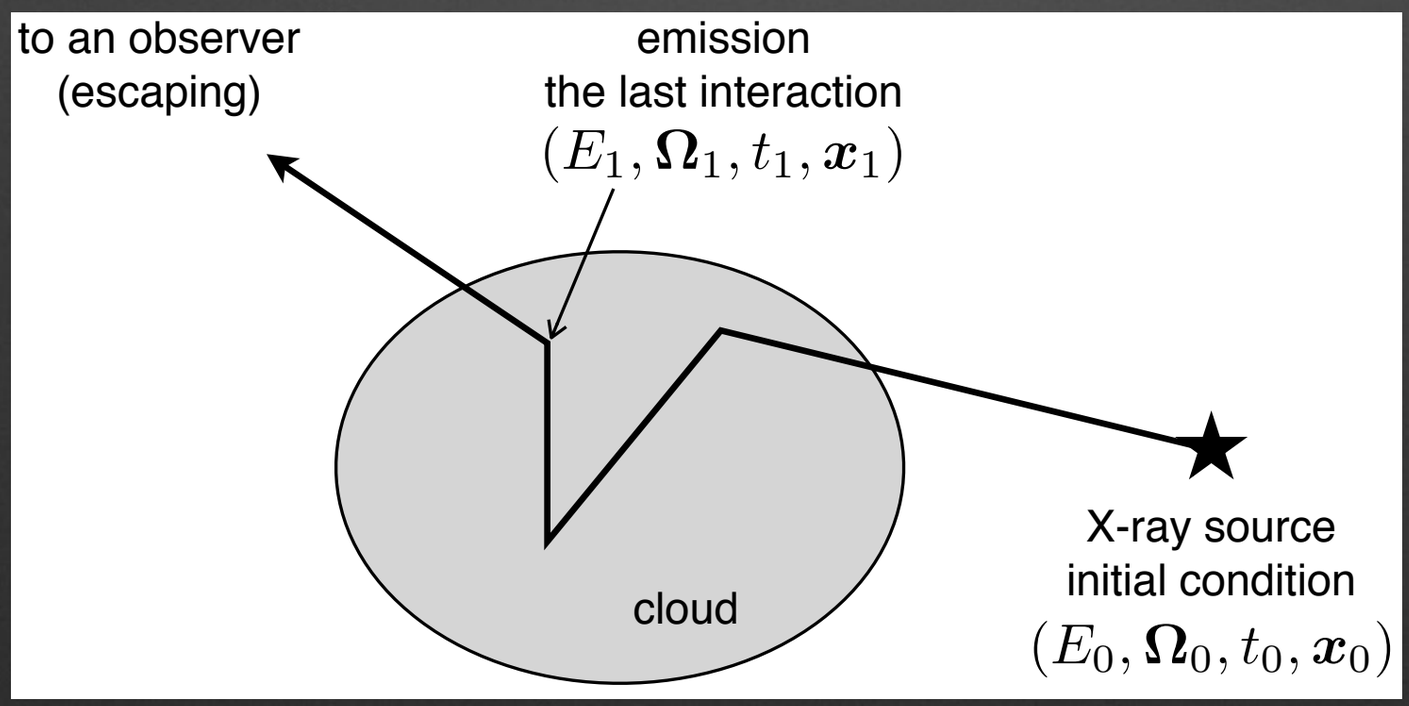
Evans+ (2009)

Monte Carlo Approach to Radiative Transfer

Recent improvement in observational instruments allows us to obtain high-quality data. Precise comparison between the data and theoretical models requires careful treatment of X-ray generation in a plasma and radiative transfer.

Monte Carlo is the simplest and the most reliable way to treat radiative transfer accurately.

The simulation tracks photons by calculating their propagation and interactions based on Monte Carlo method in a realistic geometry.



Odaka et al. 2011

MONACO

We have developed a new multi-purpose calculation framework of X-ray radiation based on Monte Carlo Simulations for observational study.

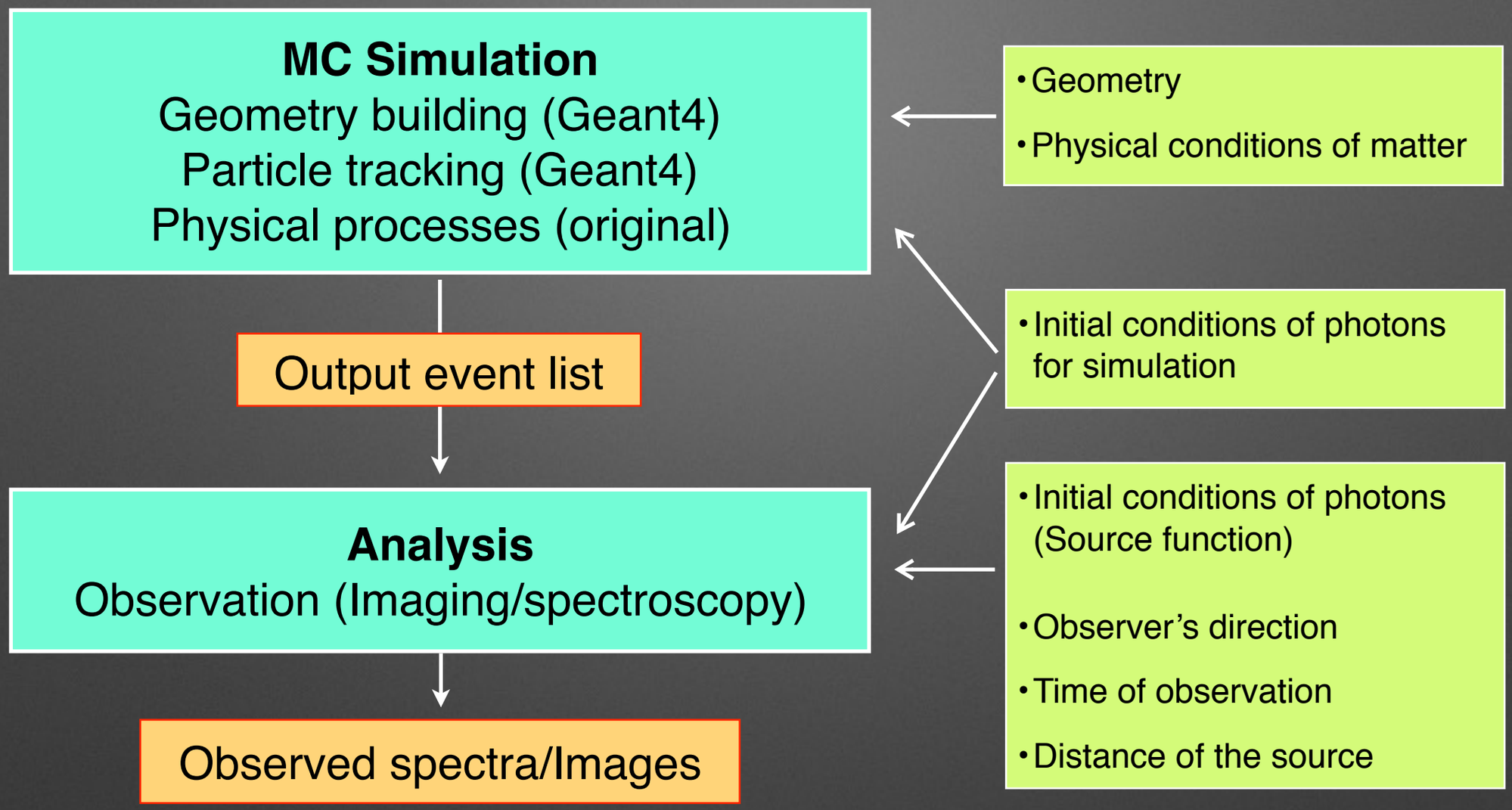
MONACO:

Monte Carlo simulation for

Astrophysics and **Co**smology

Alphonse Mucha (1897)

The MONACO Framework



- Building geometry and tracking particles: Geant4 toolkit library
  ←sophisticated treatment of complicated geometry (e.g. radiation detector simulation)
- Physical processes:
  original implementation
  ←need to treat plasma, detailed atomic processes of atoms, molecules and ions
  ←need to treat gas motion that makes Doppler effects (shifts and broadening)

Physical Processes

Several physical processes important in accretion-powered sources are implemented.

Cold matter	Photoelectric absorption followed by fluorescence and scattering by electrons bound to neutral atoms or molecules are responsible for generating spectral features of X-ray reflection - X-ray reflection nebulae (Odaka et al. 2011) - AGN molecular tori (Furui et al. in prep.)
Photoionized plasma	Gas is ionized by strong X-ray radiations in the vicinity of accreting objects. Photoionization and photoexcitation of various ion species result in emission lines and absorption lines - Stellar winds in X-ray binaries (Watanabe et al. 2006) - AGN outflows (Hagino et al. 2015, Hagino et al. submitted) - Super soft X-ray sources (bright WDs) (Wada et al. in prep.)
Comptonization	This process plays an important role in cooling a hot accretion flow through X-ray radiation - Accretion flows onto NS (Odaka et al. 2014) - Accretion flows onto BH (Odaka et al. in prep.)

Photoionization

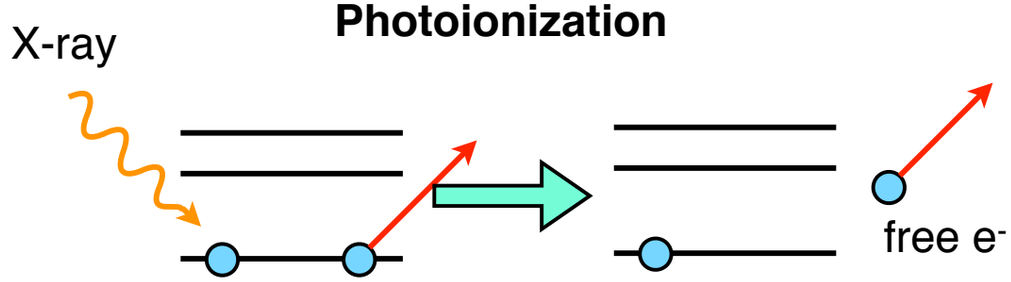
See also Astro-H White Paper “New spectral features” (arXiv:1412.1172v1)

- Stellar winds illuminated by neutron stars or black holes are best studied X-ray photoionized plasma. e.g. Vela X-1, Cyg X-3
- Watanabe et al. (2006) determined structure of the stellar wind of Vela X-1 including the wind mass-loss rate based on Chandra-HETG specta and detailed Monte Carlo modeling at different orbital phases.
- Before MC simulations, we need to calculate ionization structure (ion fractions and electron temperatures), which is determined by
  - balance between ionization and recombination, and
  - balance between heating and cooling.
- We are using *XSTAR* (Kallman) for this calculation.

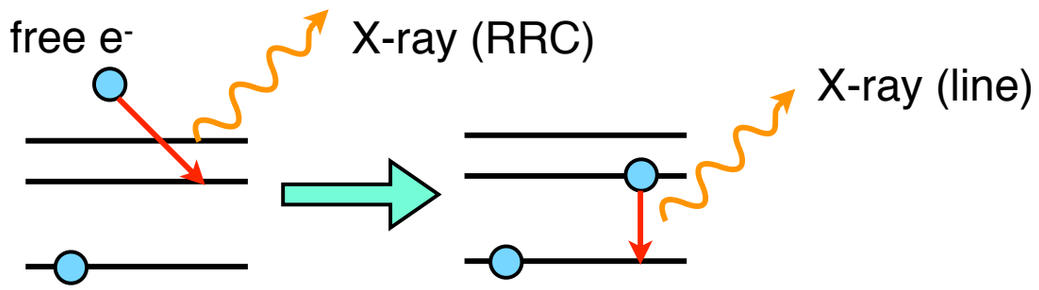
Processes in Photoionized Plasma

Two-electron ion

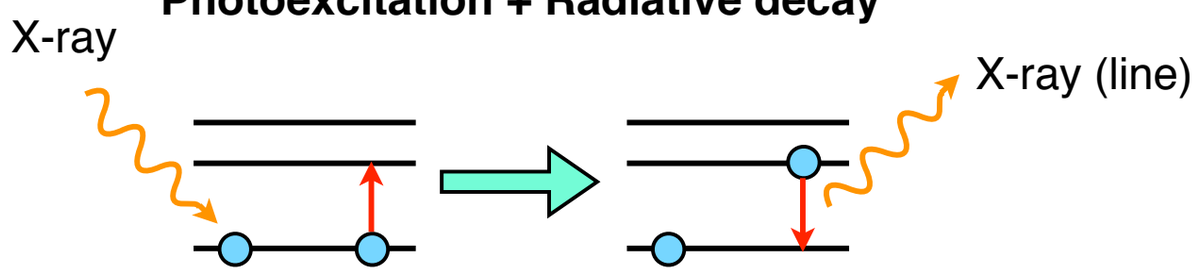
Photoionization



Radiative recombination + Radiative decay

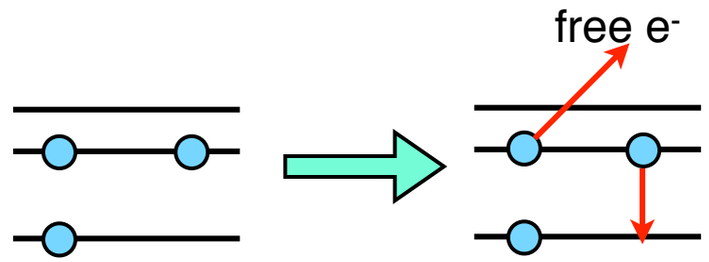


Photoexcitation + Radiative decay

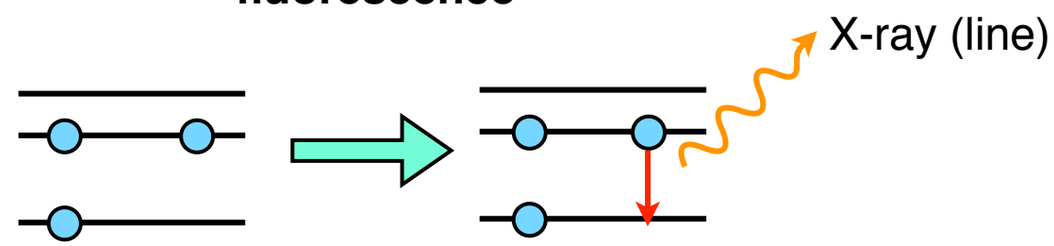


Three-electron ion in an excited state

autoionization



fluorescence



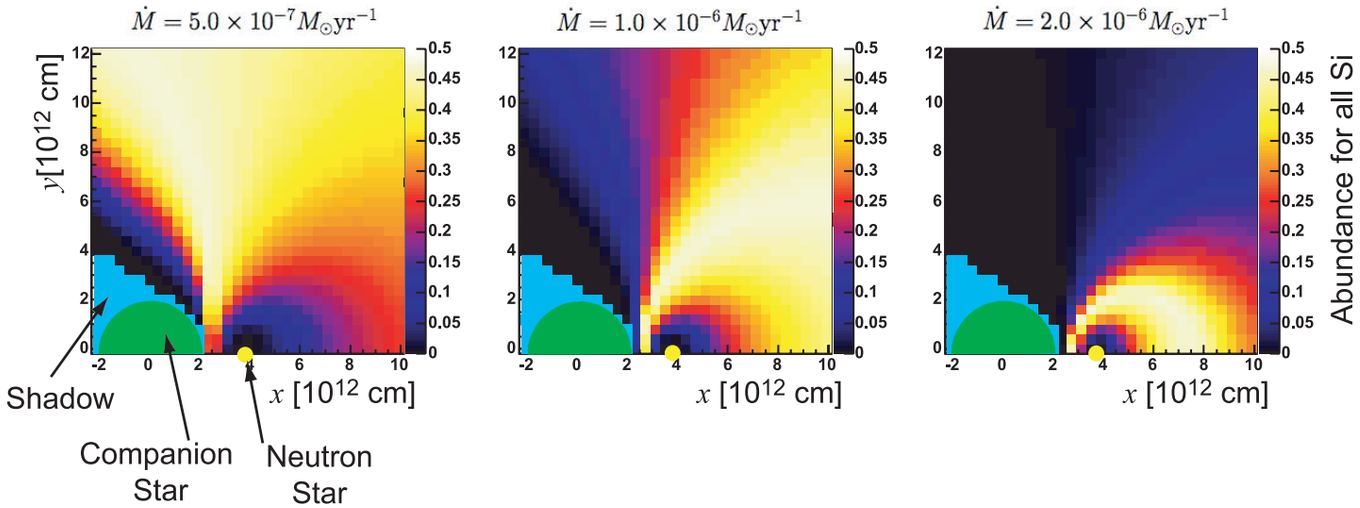
Resonance-Auger destruction:
a photon at a resonance line energy will be absorbed via resonance excitation and autoionization.

Stellar Wind in Vela X-1

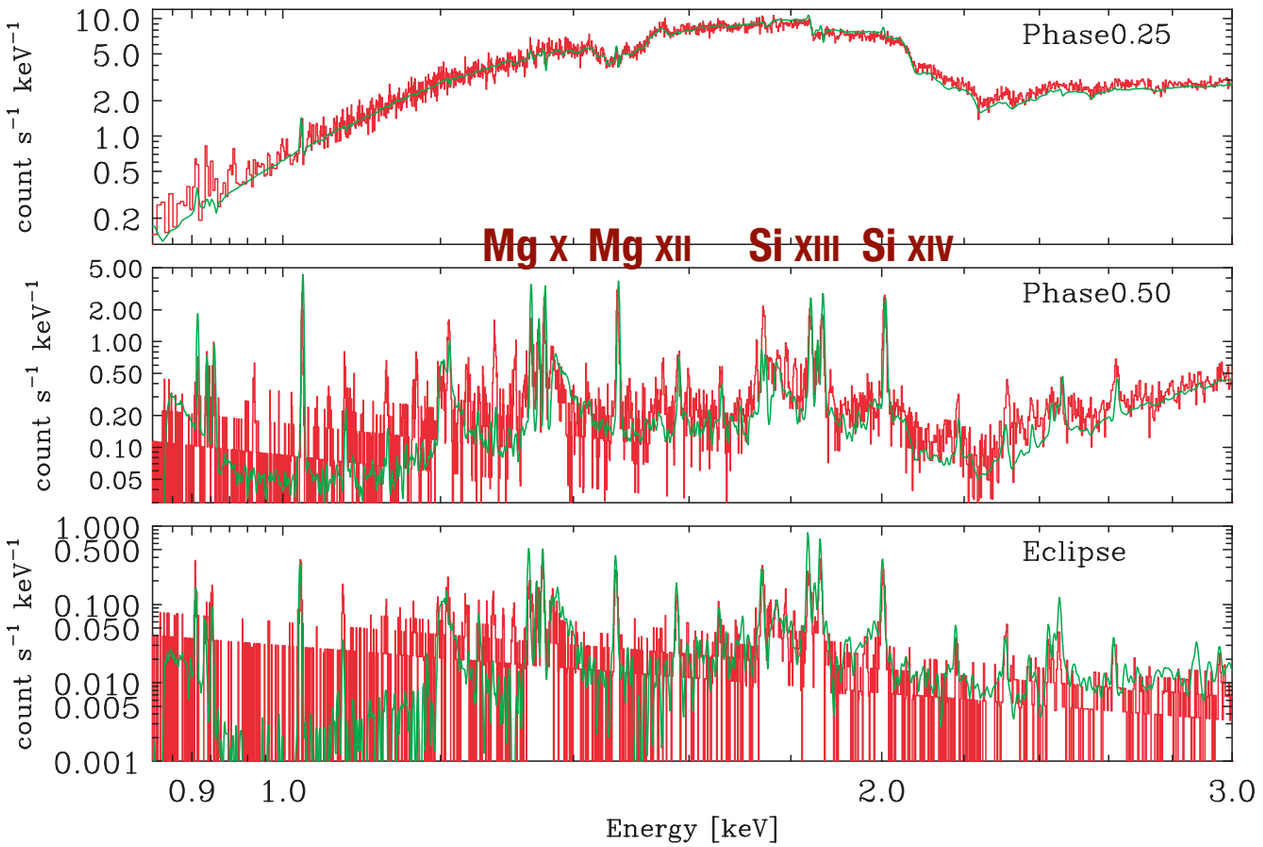
XSTAR

Ion fraction of Si XIV

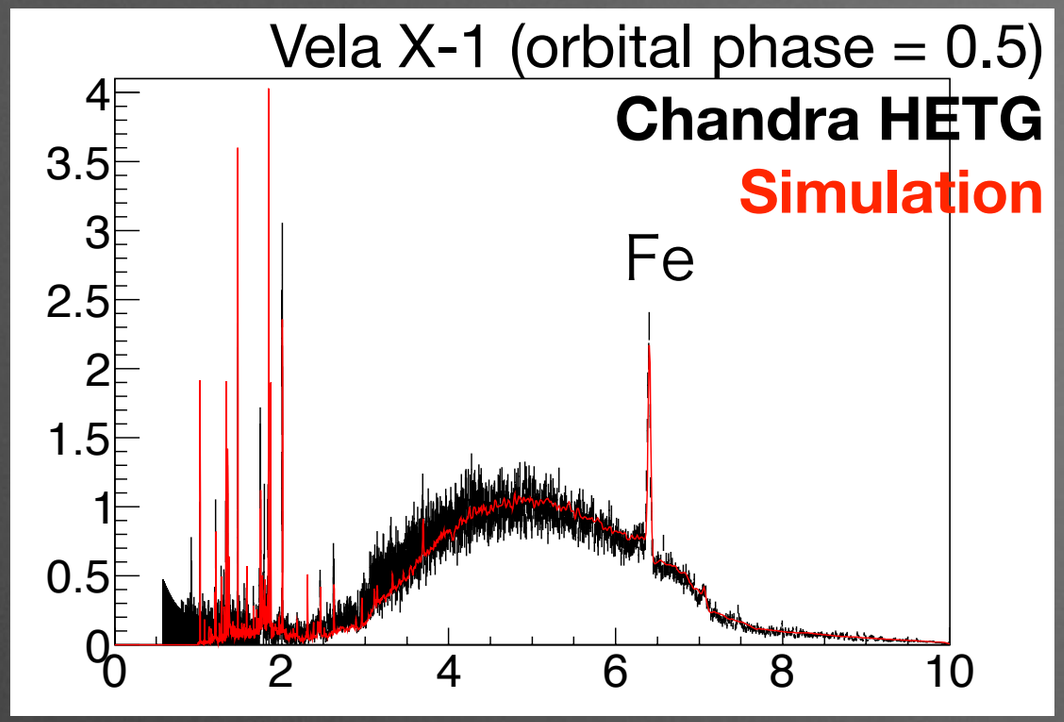
Watanabe et al. 2006

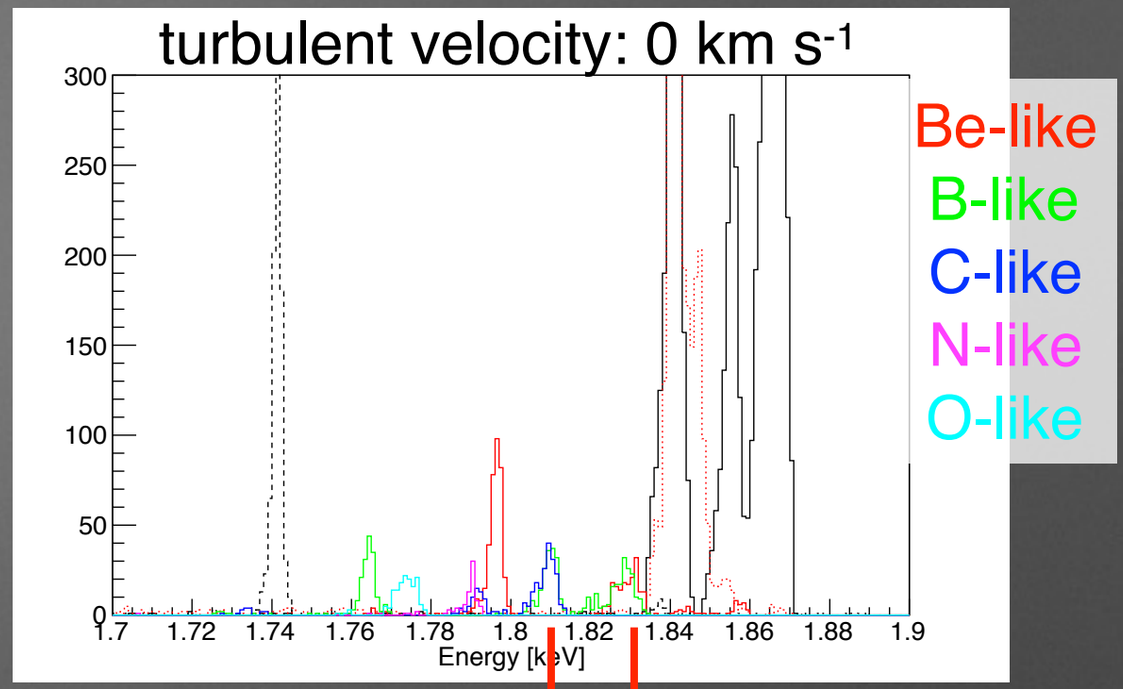


MC simulation

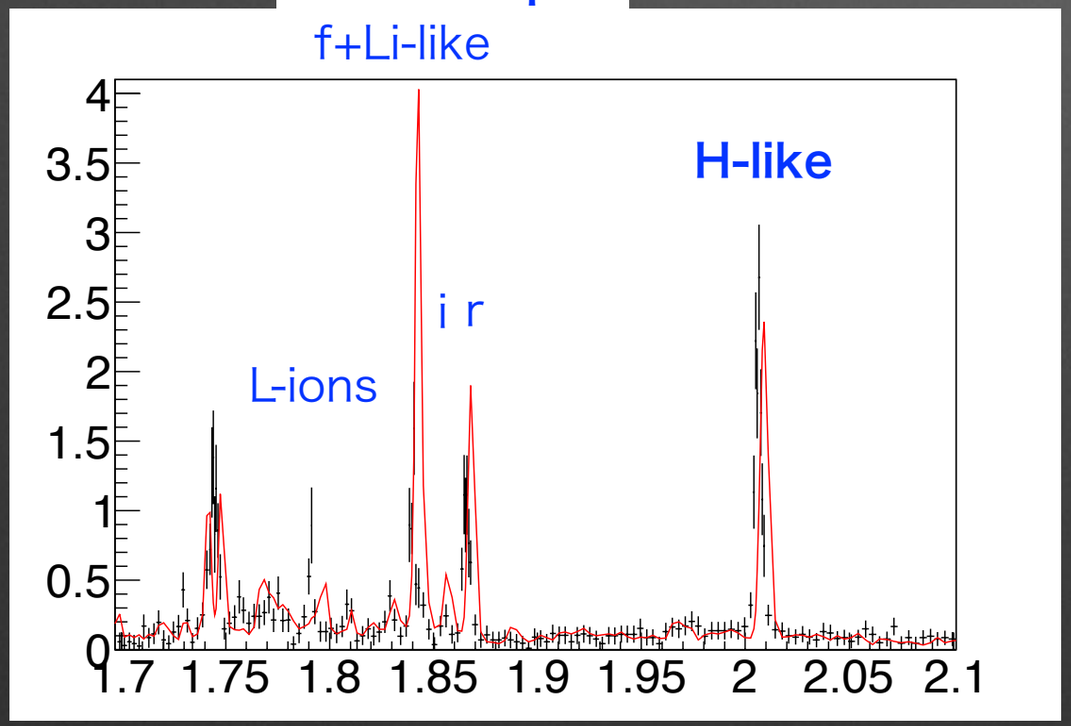


Odaka PhD thesis

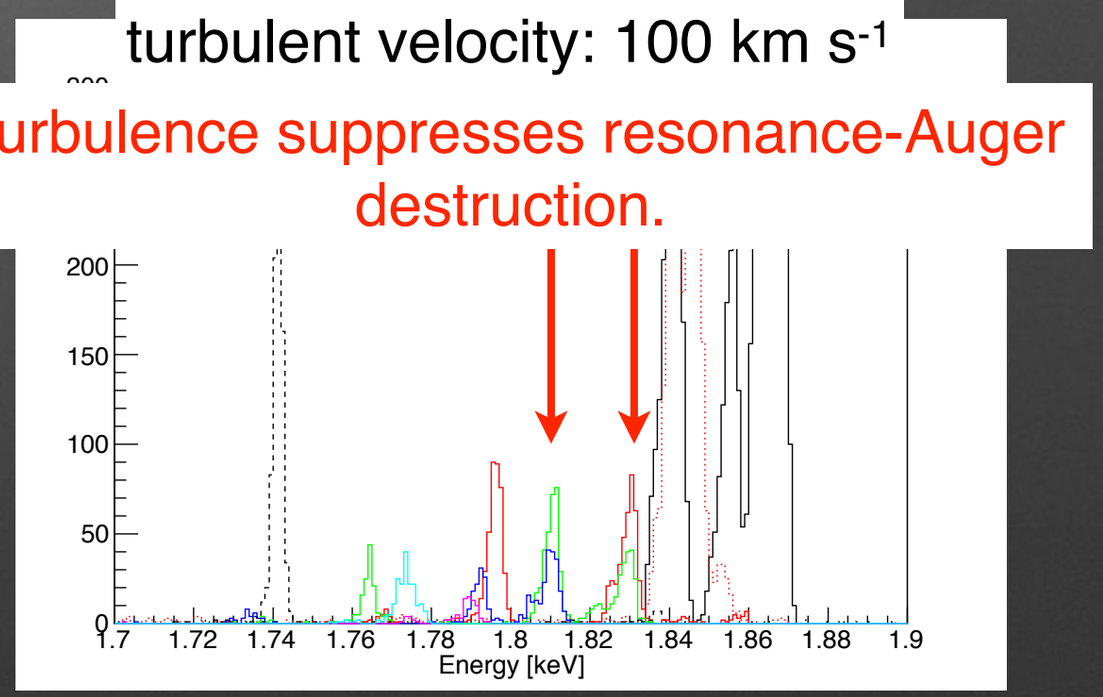




He-like triplet



First attempt to reproduce Si-K complex of Vela X-1 spectrum obtained by Chandra. Model parameters are not optimized yet.

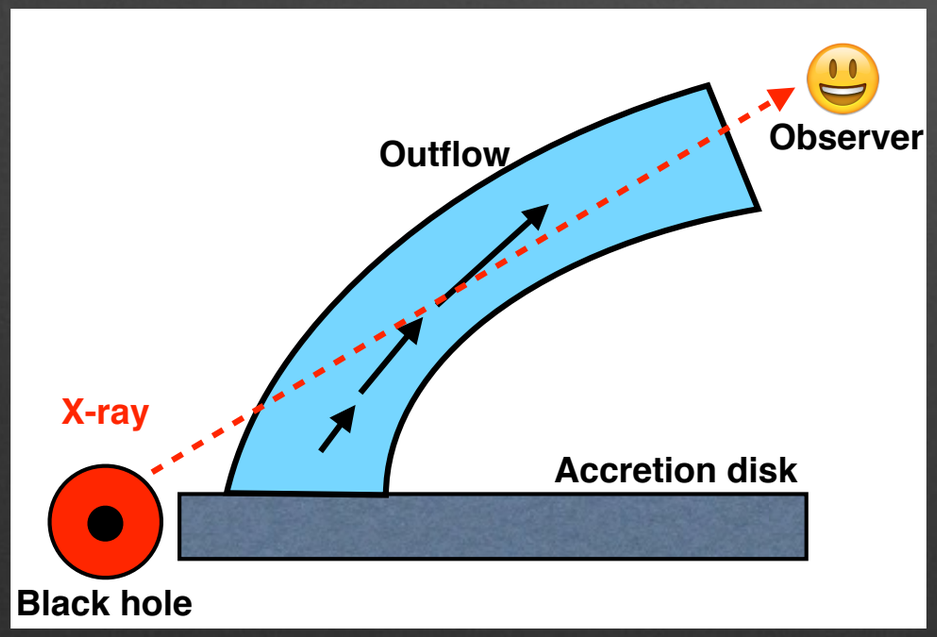


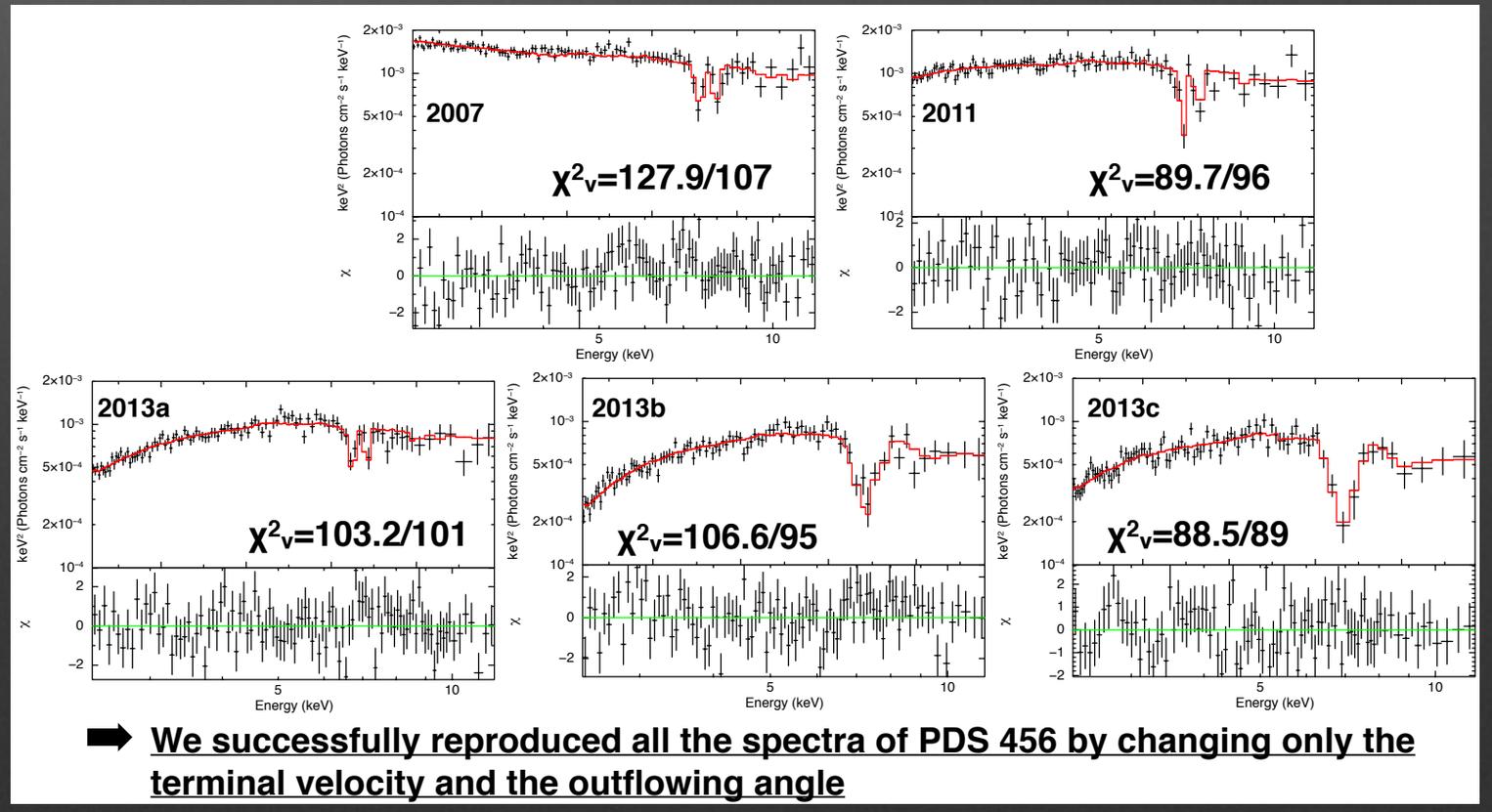
Monte Carlo simulation is a powerful tool to simulate effects of turbulence on a line spectrum.

AGN Ultra Fast Outflow

Listen to Hagino's talk!

- Some luminous quasars display deep blue-shifted absorption lines of hydrogen/helium-like ions of iron.
- Mildly relativistic (0.3c) wind arising from an accretion disk of AGN.
- The outflow is highly ionized by the luminous X-rays from the AGN central engine.



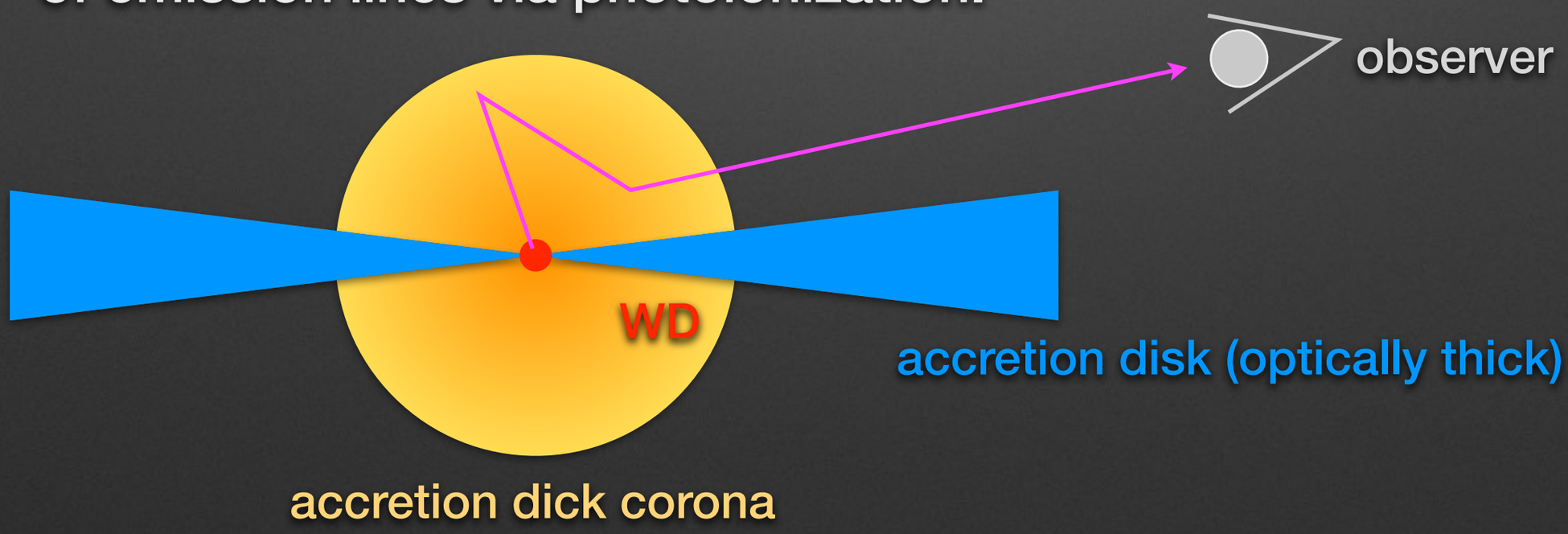


➡ **We successfully reproduced all the spectra of PDS 456 by changing only the terminal velocity and the outflowing angle**

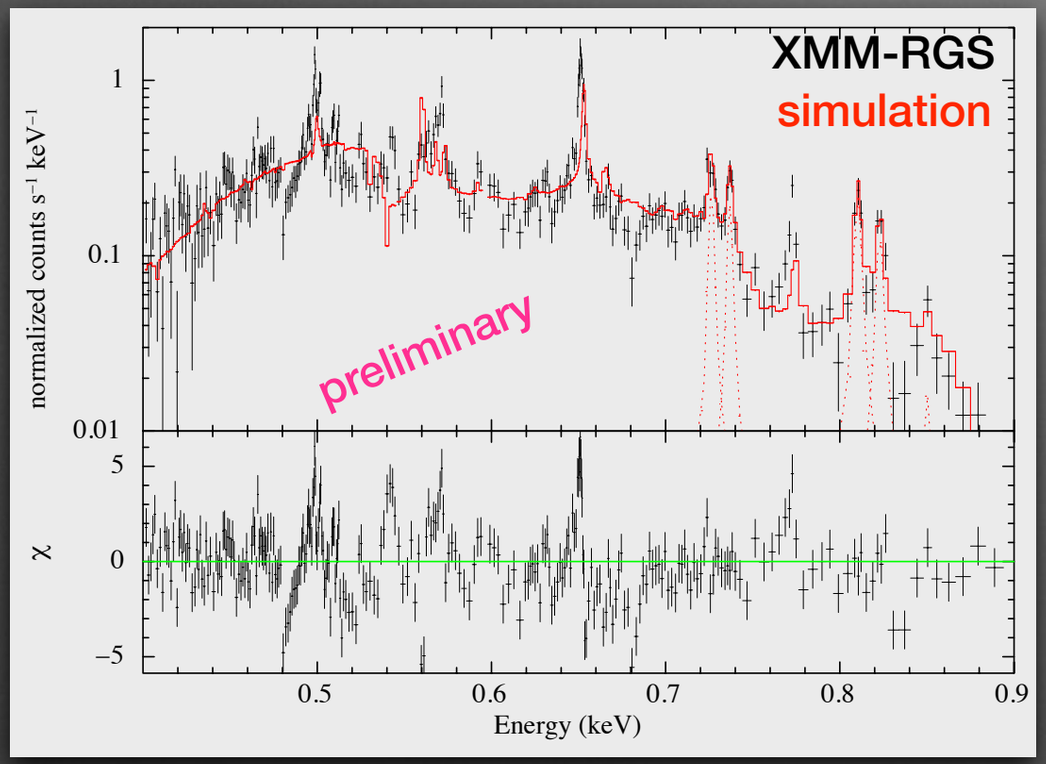
Hagino et al. 2015

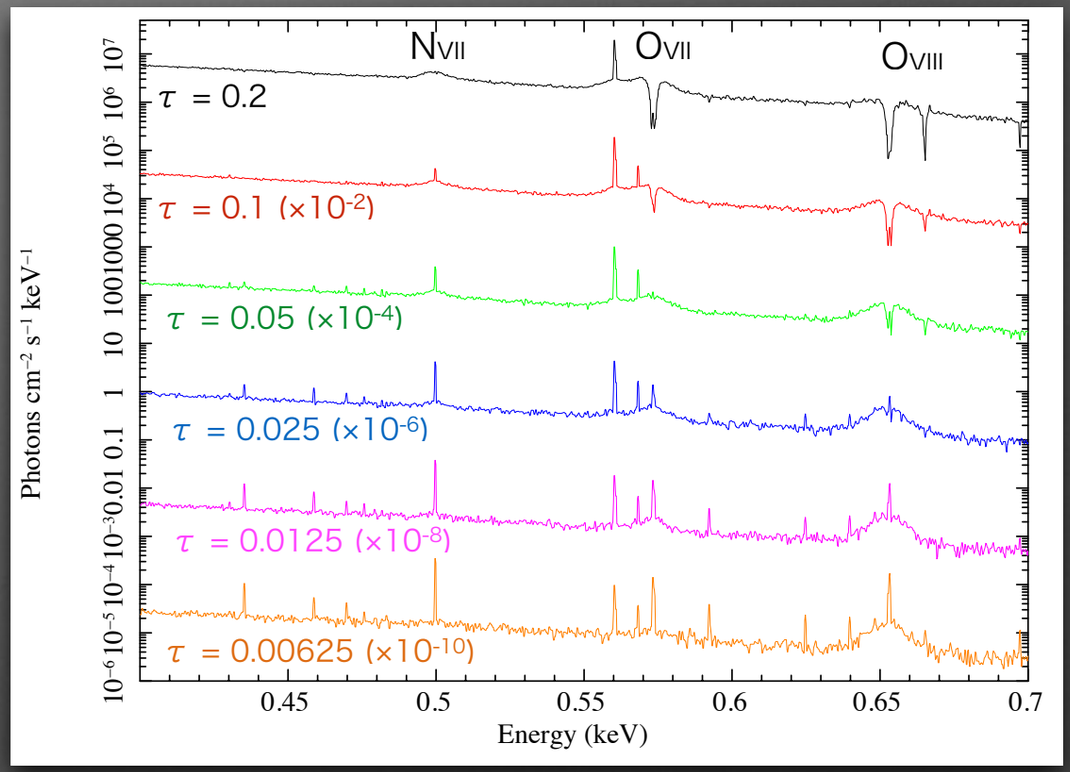
Super Soft X-ray Sources (SSS)

- Extremely bright in soft X-rays (below 0.8 keV)
- Thermonuclear burning continuously occurs on a white dwarf surface, radiating at close to the Eddington luminosity ~ 10^{38} erg s^{-1}.
- Very high accretion rate ~ 10^{-7} $M_\odot$ yr^{-1}.
- Possible progenitors of type Ia supernovae.
- There exists an accretion disk corona (ADC) which displays plenty of emission lines via photoionization.



Accretion Disk Corona in SSS



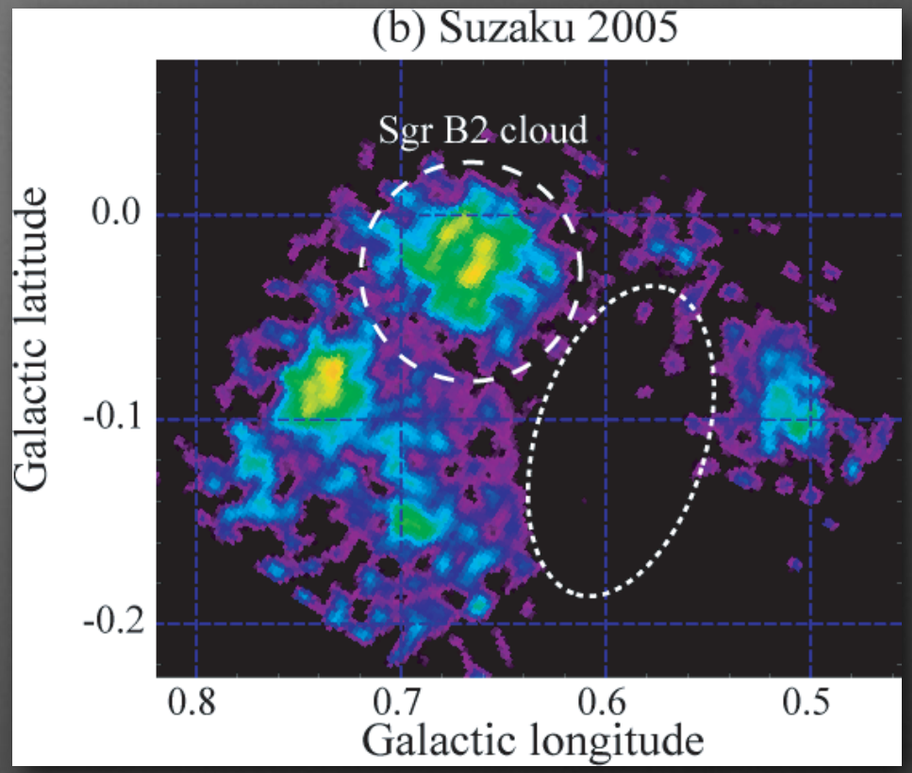


- We attempt to reproduce the high-resolution X-ray spectrum of CAL 87 (SSS in LMC) in the context of accurate photoionization modeling.
- Line red shifts imply that the corona is outflowing.
- Absence of features by resonance scattering suggests that optical depth is even thinner than reported by previous studies.

Wada et al. in prep.

Giant Molecular Cloud in the Galactic Center

- Giant molecular cloud Sgr B2 has been reflecting a past outburst of SMBH Sgr A*, displaying strong Fe fluorescence at 6.4 keV.
  It shows strong time variability over a few year scale.



- Such objects are good probes of molecular clouds themselves and the black hole activity.

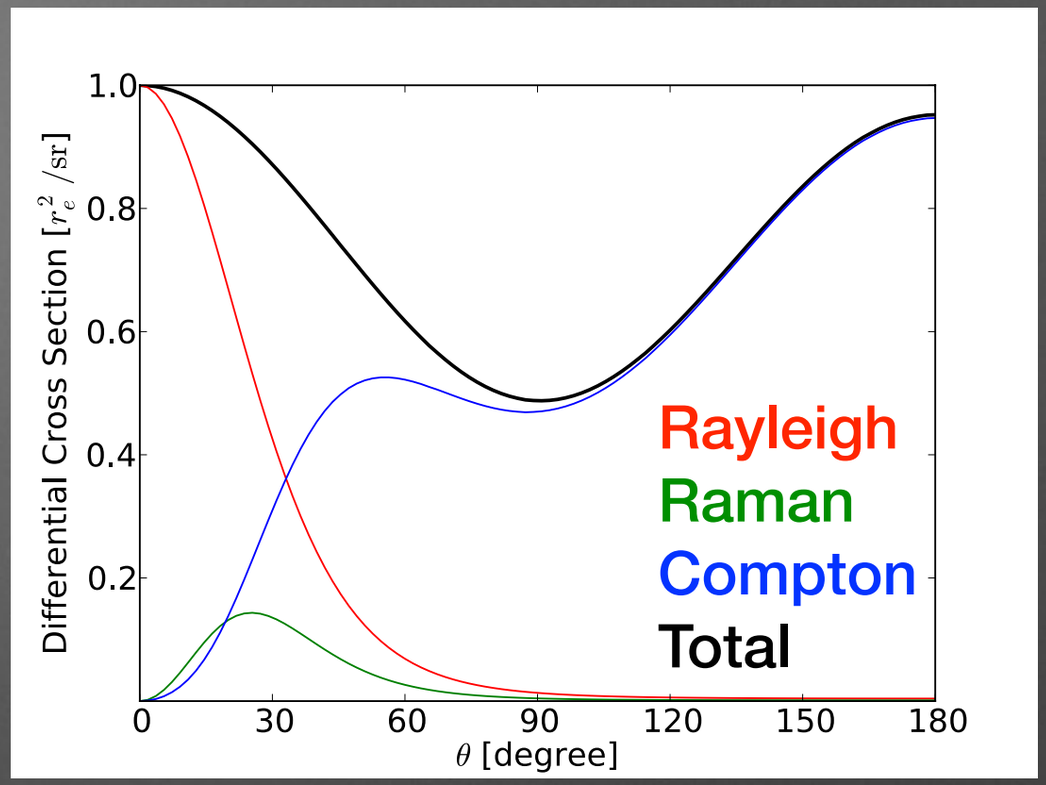
- We have to consider multiple scatterings and structure of the cloud. → Monte Carlo simulation

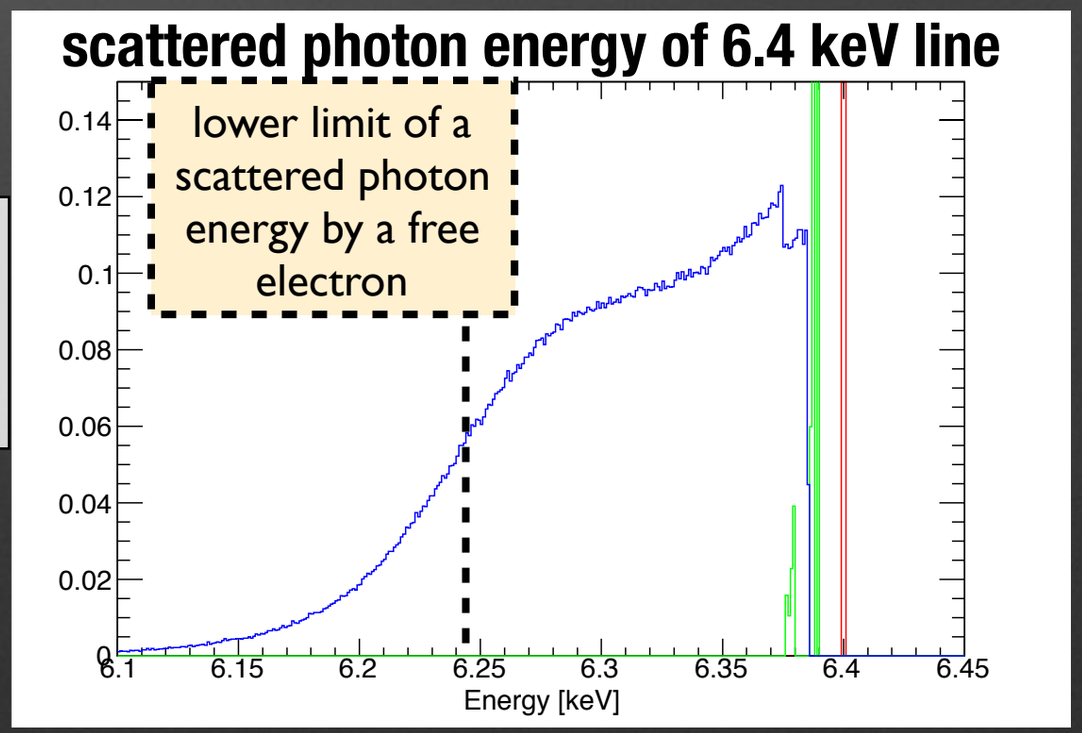
Physical Processes in Cold Matter

- Photoelectric absorption
  EPDL97 is used for cross section data.
  (Same as G4 Low Energy EM)

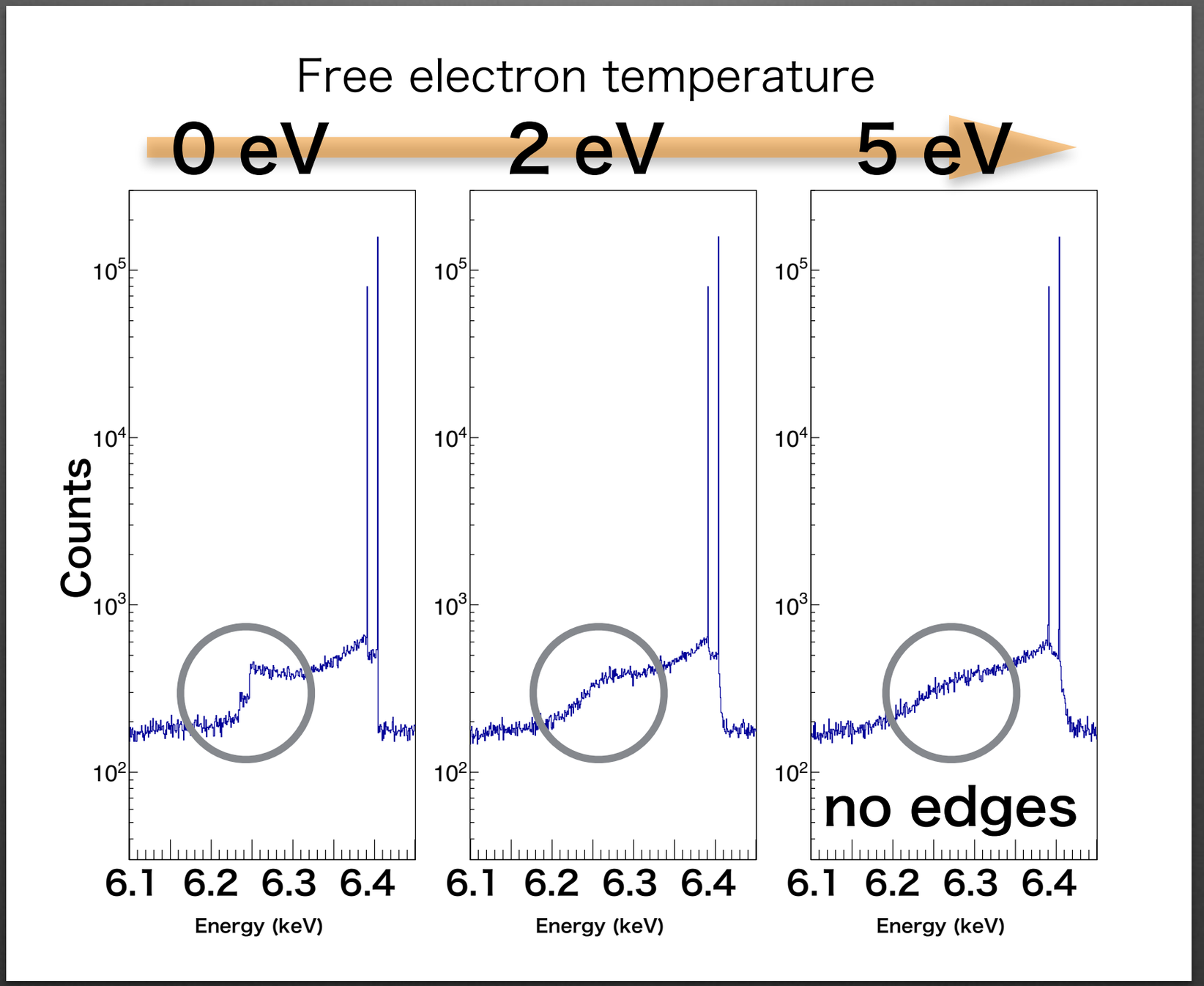
- Scattering by a bound electron
  different from the free electron case
  This process can be divided into three channels according to the final state of the target electron.
  (Sunyaev & Churazov 1996)

$$\gamma + \mathrm{X}_i \rightarrow \begin{cases} \gamma_1 + \mathrm{X}_i & \text{(ground state—Rayleigh scattering)} \\ \gamma_1 + \mathrm{X}_i^* & \text{(excited state—Raman scattering)} \\ \gamma_1 + \mathrm{X}_{i-1} + \mathrm{e}^- & \text{(free state—Compton scattering)} \end{cases}$$



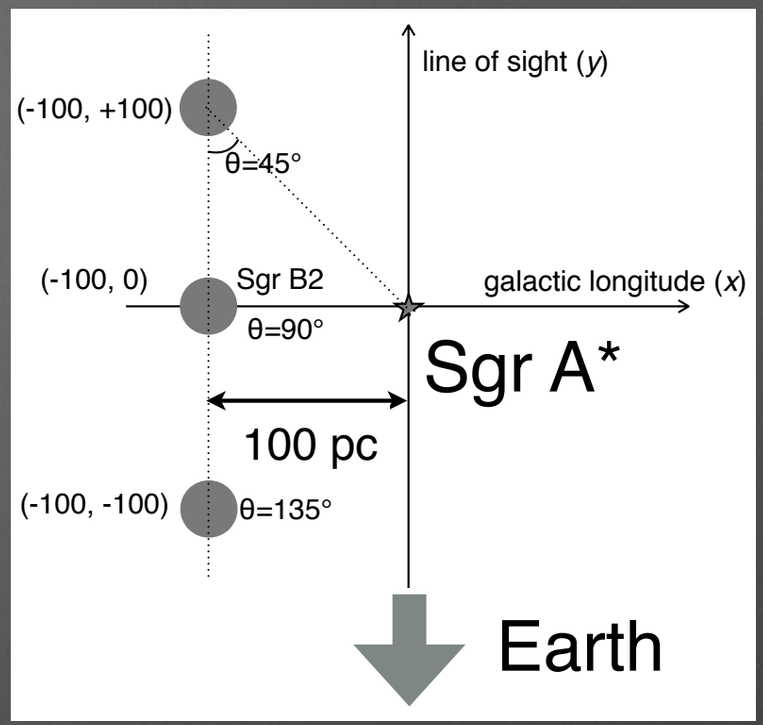


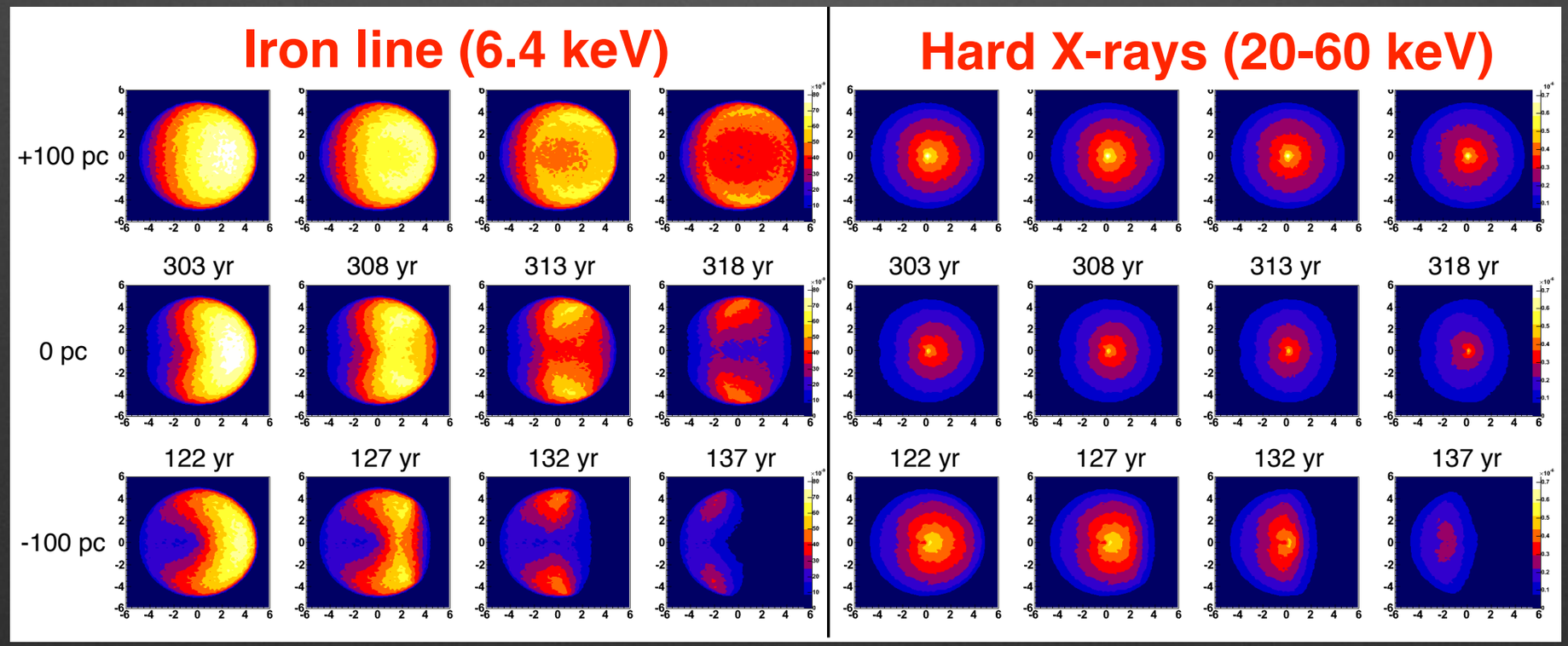
Compton Shoulder by Free Electrons



Simulation Results of the Molecular Cloud

- Giant molecular cloud Sgr B2 has been reflecting a past outburst of SMBH Sgr A*, displaying Fe fluorescence line at 6.4 keV.
- It shows strong time variability over a few year scale.
- Such objects are good probes of molecular clouds themselves and the black hole activity.

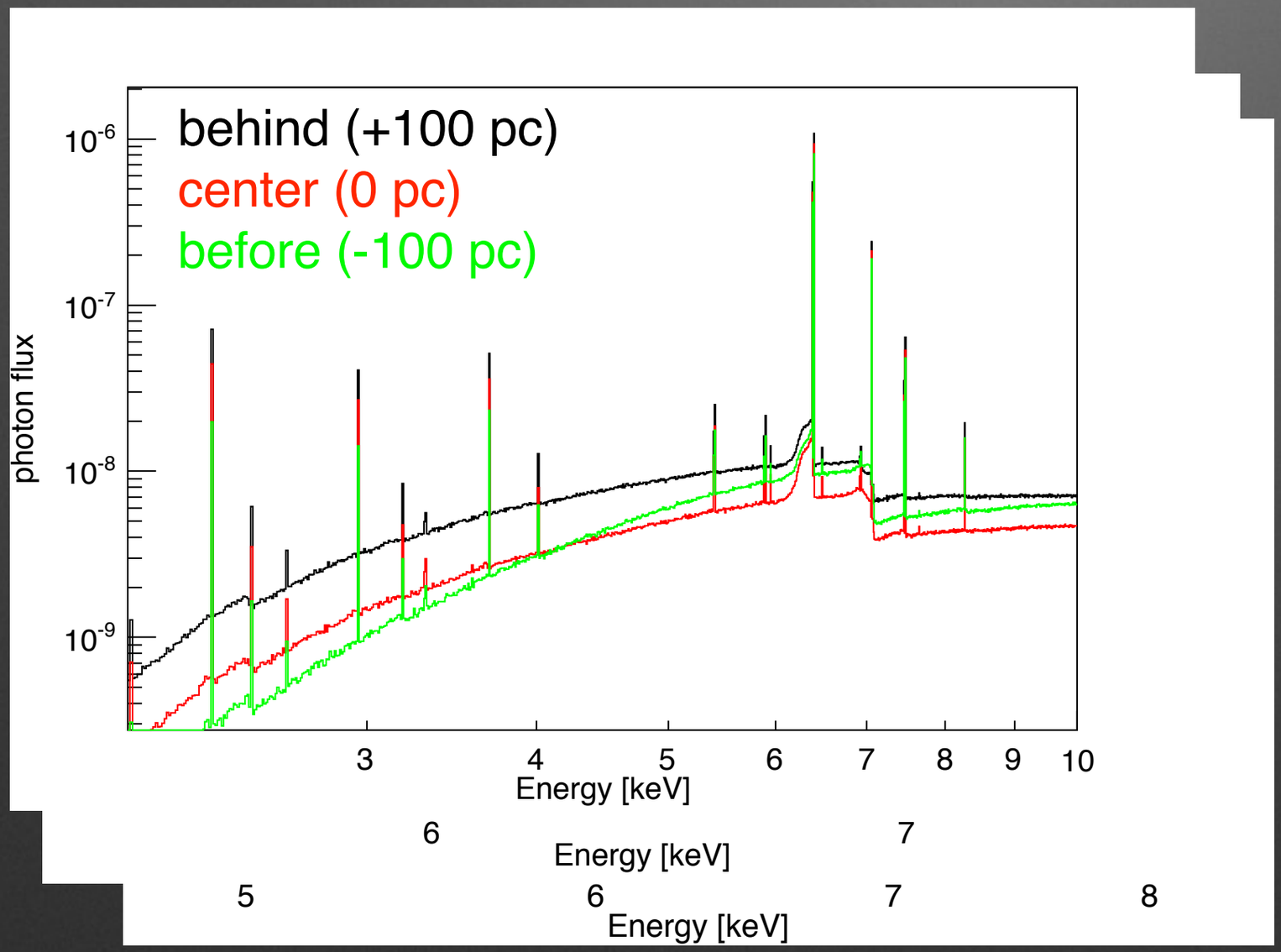


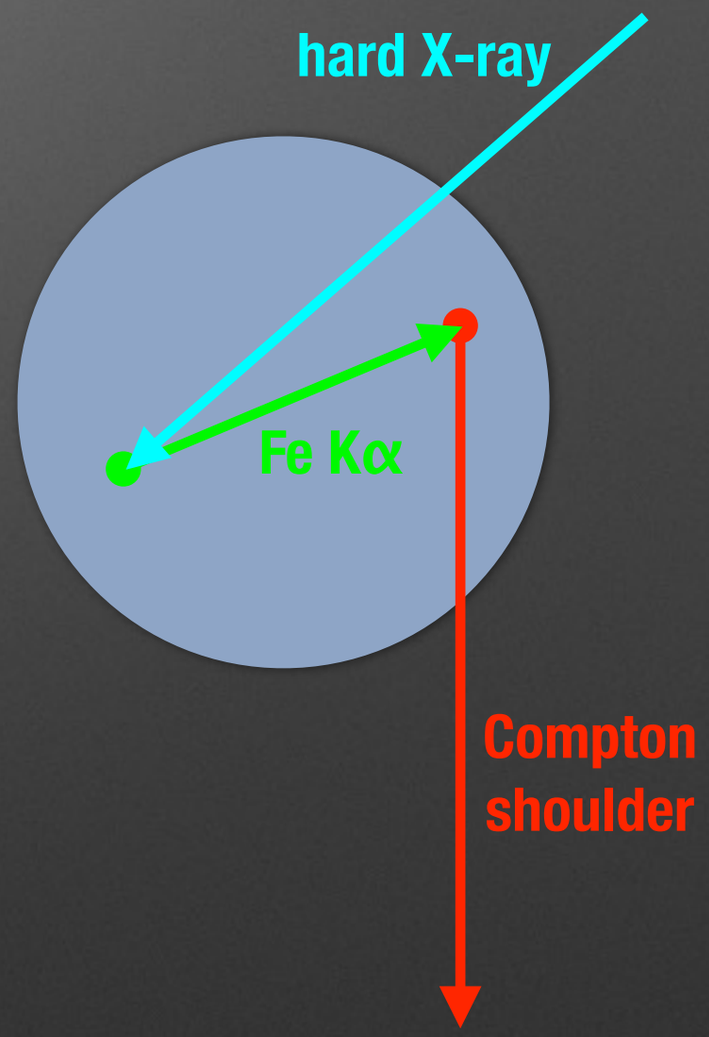


Odaka et al. 2011

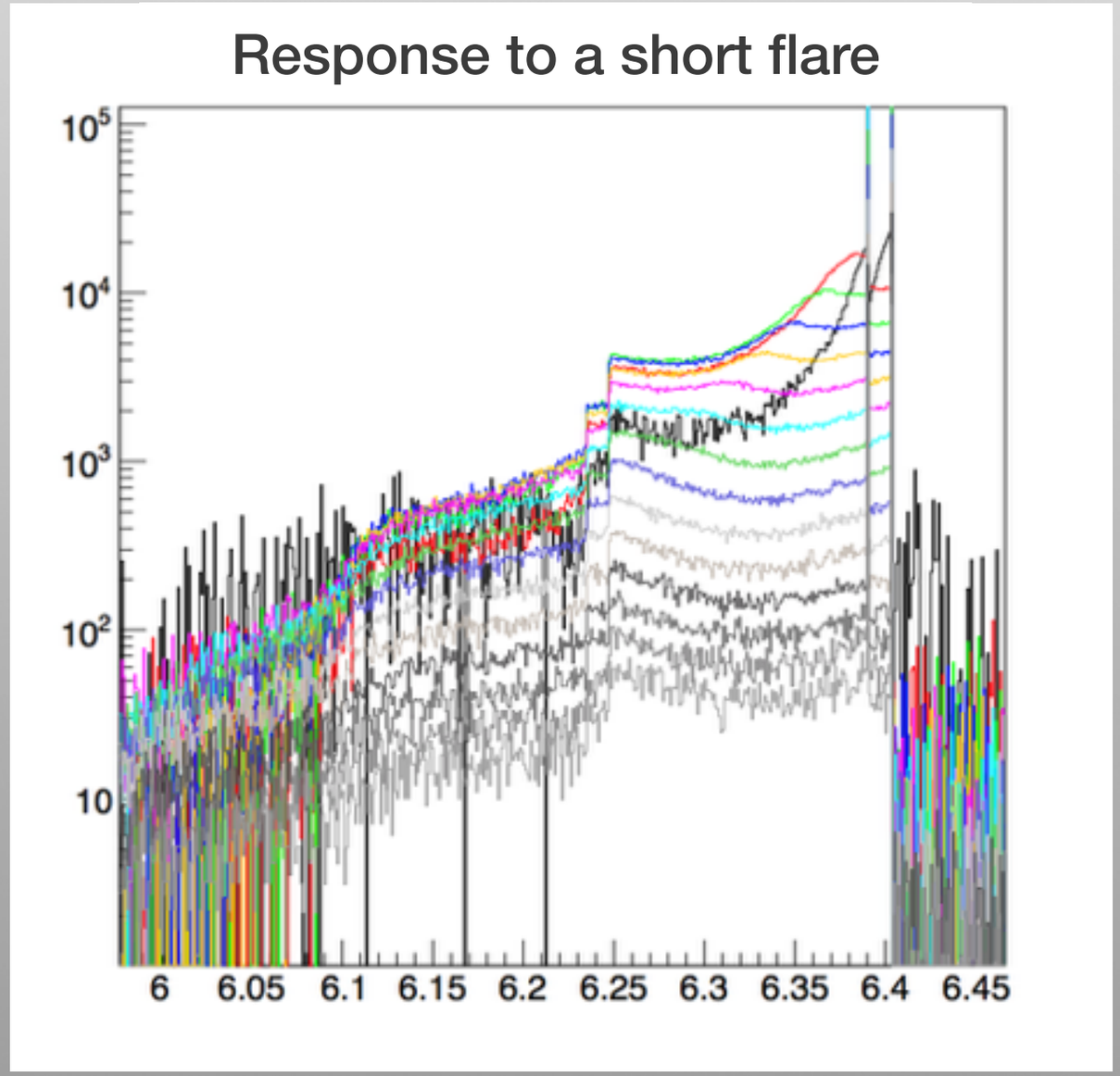
Compton Shoulders

Compton shoulder, which is produced by Compton down-scattering of strong fluorescence lines (e.g. Fe Kα), has a potential diagnostic power.

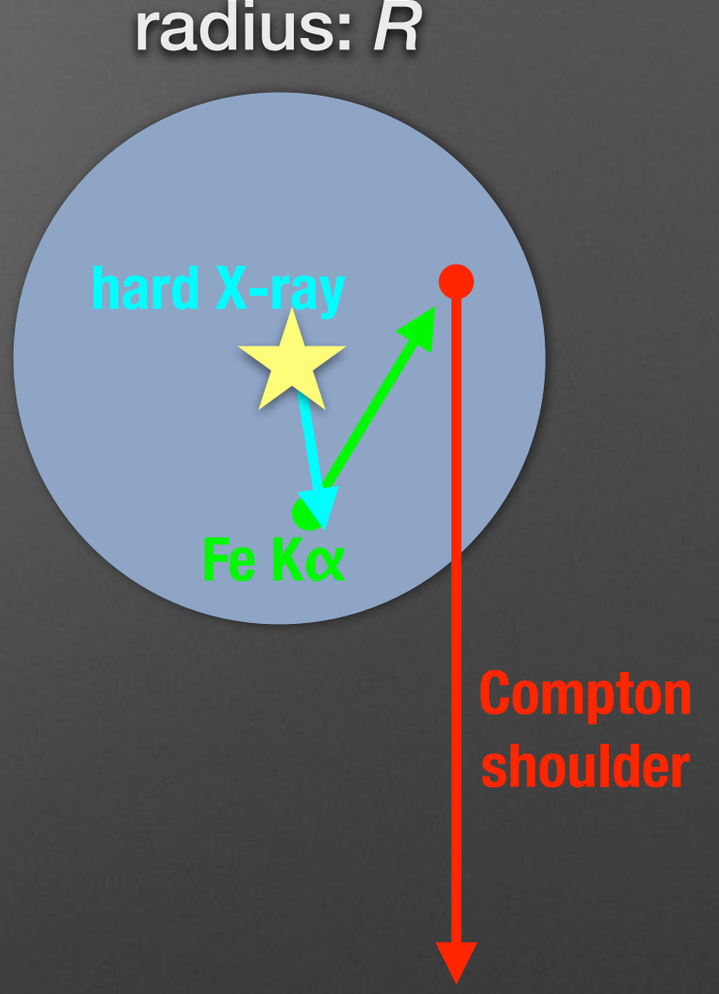




Time Evolution of Compton Shoulder



Time [R/c]
(0.0-0.1) R/c
(0.2-0.3) R/c
(0.4-0.5) R/c
(0.6-0.7) R/c
(0.8-0.9) R/c
(1.0-1.2) R/c
(1.2-1.4) R/c
...



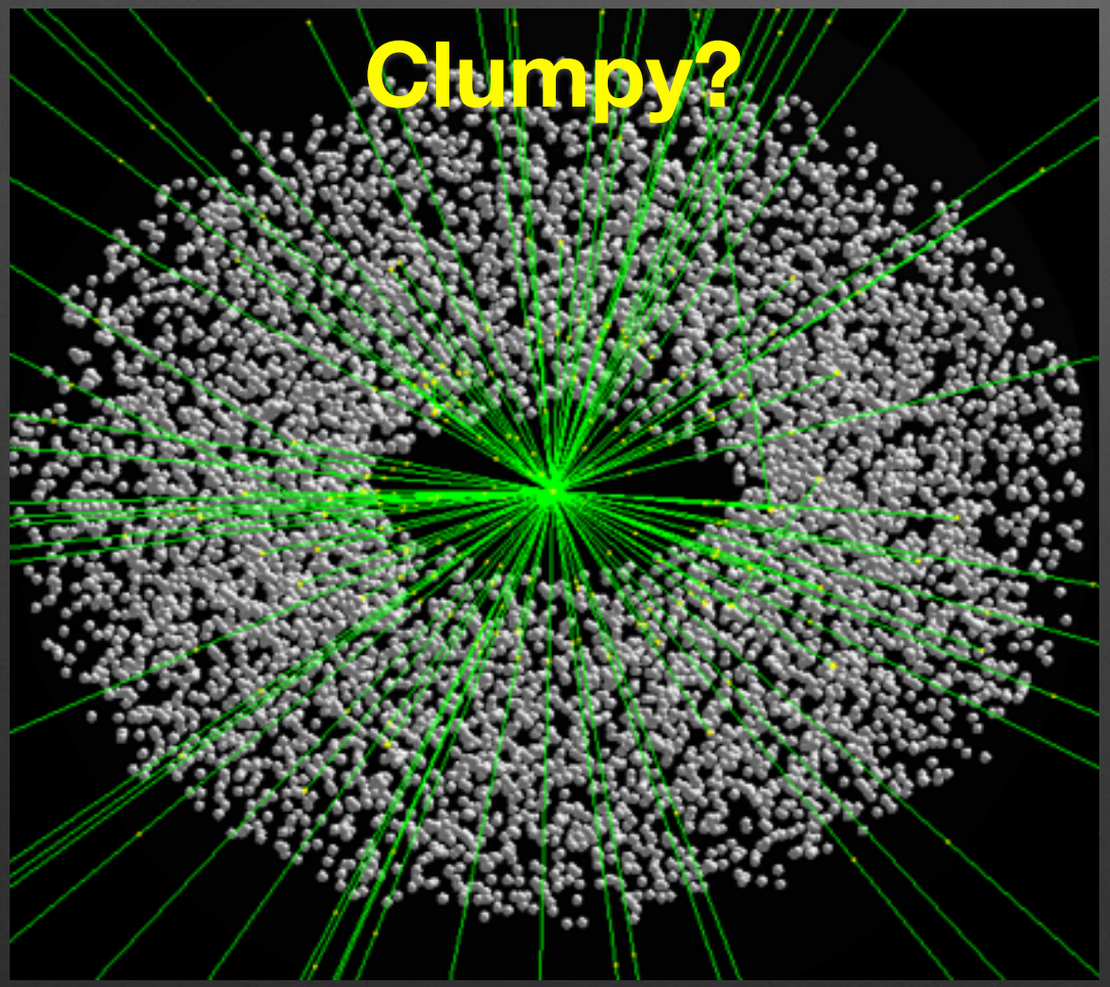
- The shoulder profile can be a probe of the temporal and spatial properties of the illuminating flare and reflecting cloud.

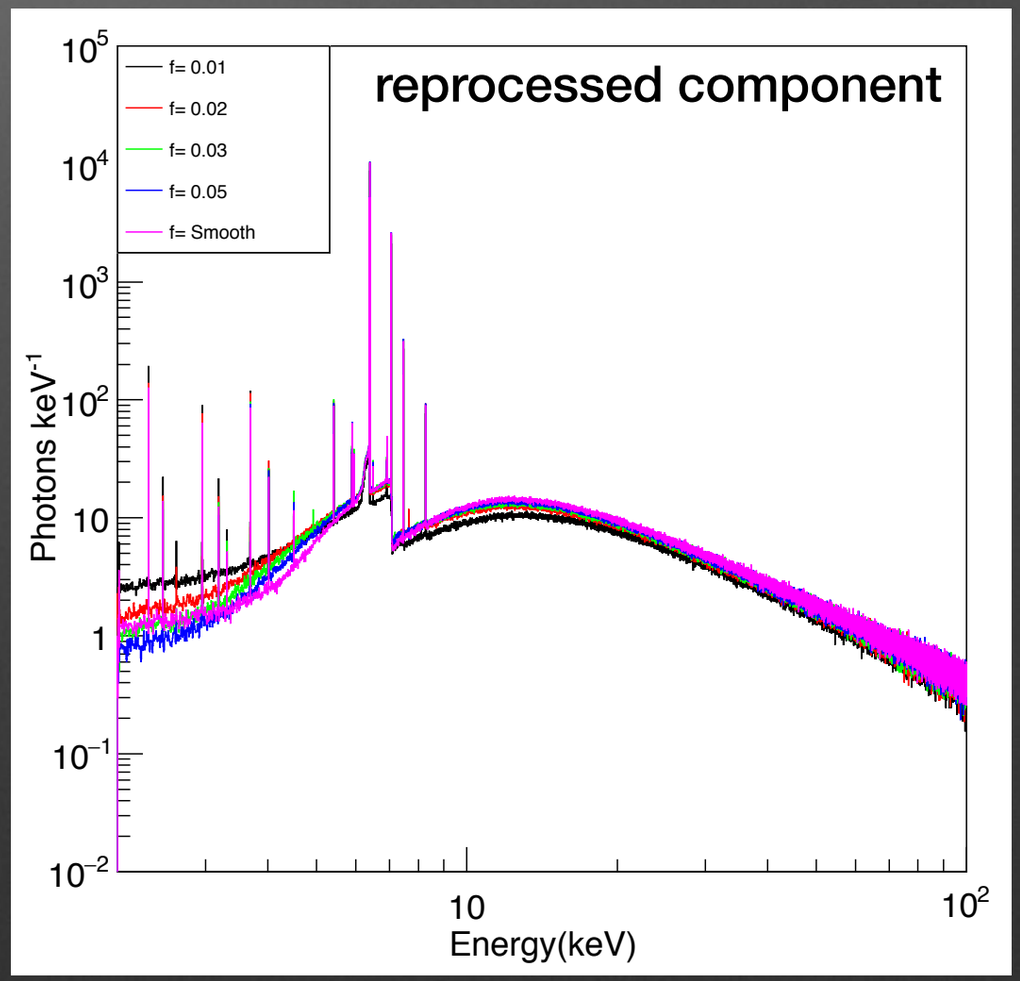
Odaka, Yoneda et al. in prep.

AGN Dusty Torus

Listen to Tanimoto's talk!

- An obscuring dusty molecular torus is believed to exist around an AGN.
- While most X-ray studies have assumed smooth torus models, infrared observations suggest that the torus has a clumpy structure.
- We build a new spectral model to extract torus parameters from X-ray observations.





Furui et al. in prep.

Comptonization

Optically thick	Analytical/numerical methods are efficient.
Not optically thick Complicated geometry High energy band	The process is essentially discrete. →Monte Carlo approach is suitable.

Using Lorentz transformation

Lab frame	Bulk motion's frame	Target electron's frame
• determine the next interaction point • see the bulk motion	• select the target electron • see the thermal motion	• calculate scattering by a rest electron

$$p^{\mu} \rightarrow p'^{\mu} \rightarrow p''^{\mu}$$

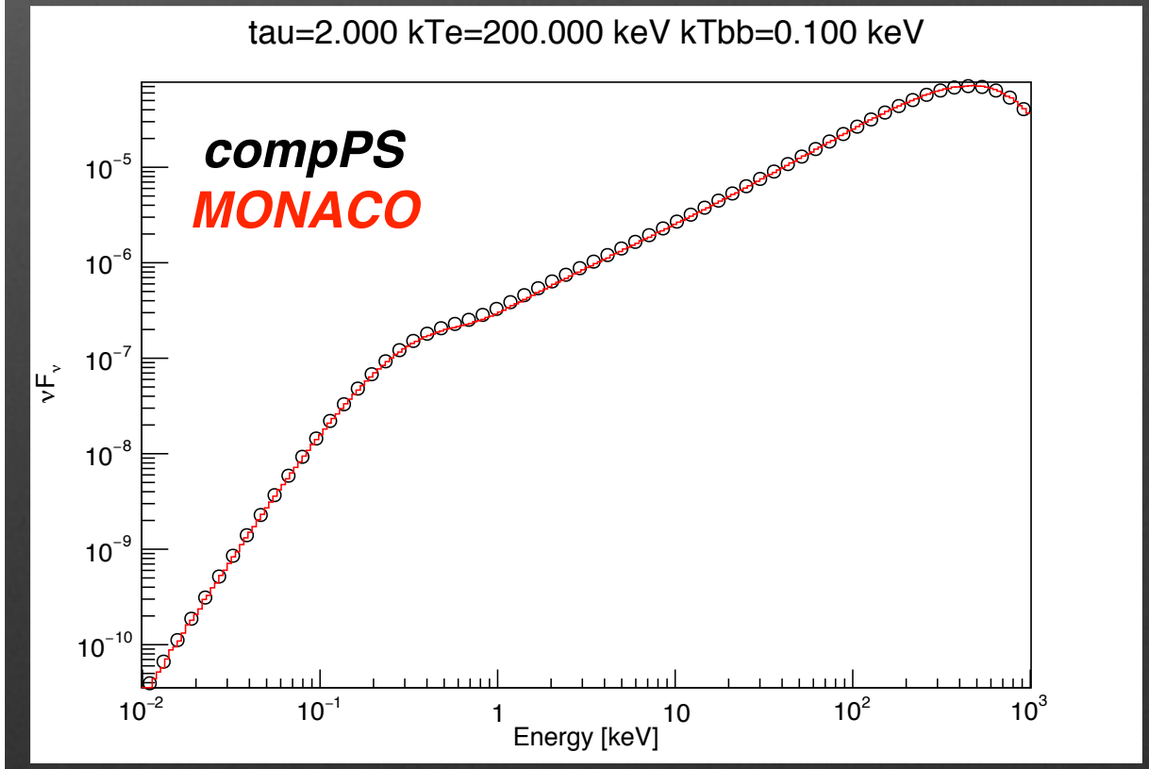
Lorentz transformation

Lorentz transformation

$$p_1^{\mu} \leftarrow p_1'^{\mu} \leftarrow p_1''^{\mu}$$

Magnetic field effects can be included.

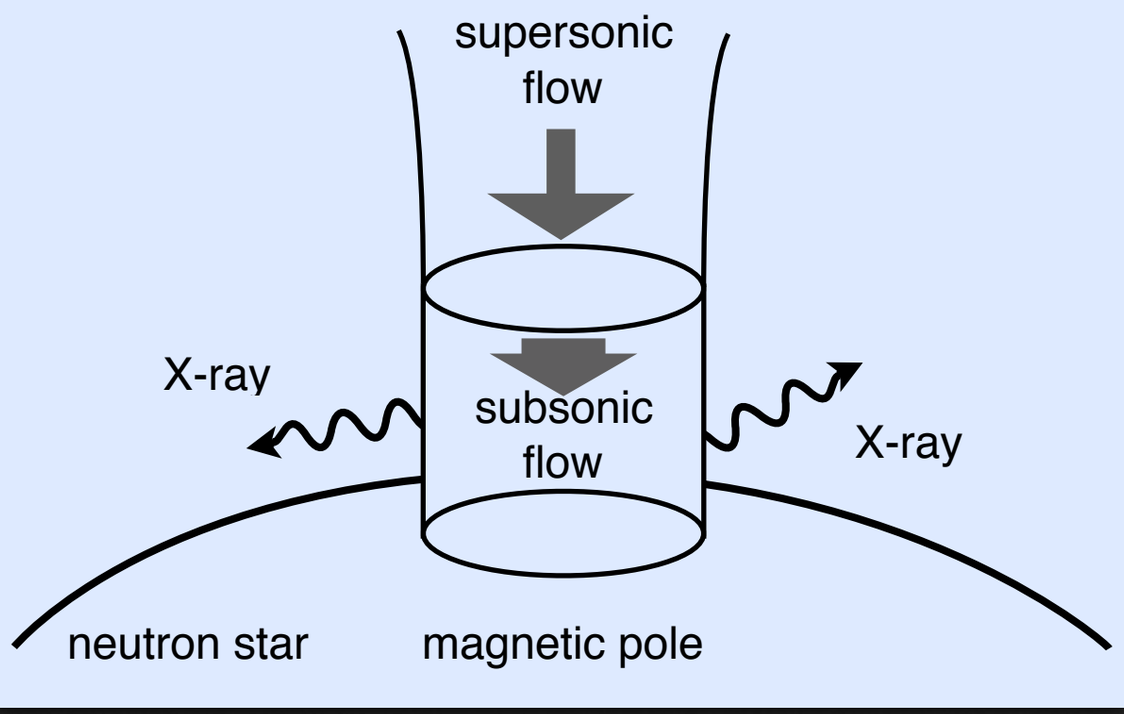
Comparison with ***compPS*** (Poutanen & Svenson, 1996)

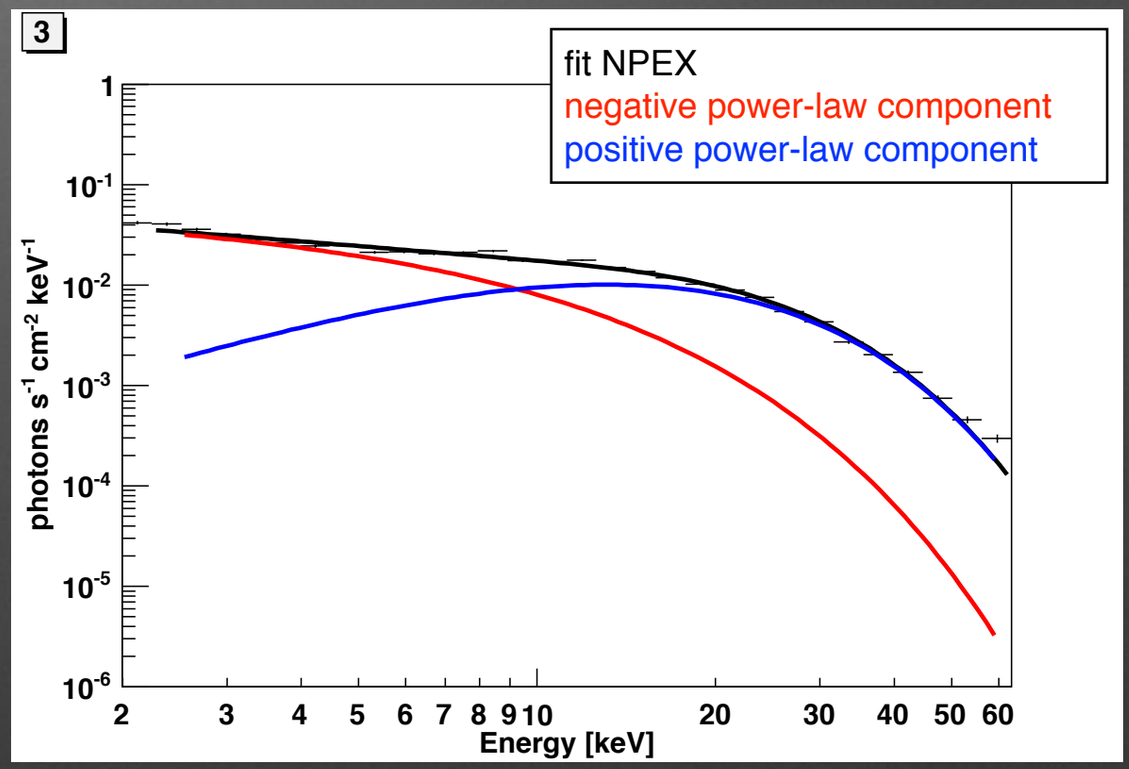


Accretion Flow onto Neutron Stars

Optically thick	Analytical/numerical methods are efficient.
Not optically thick Complicated geometry High energy band	The process is essentially discrete. →Monte Carlo approach is suitable.

Accretion column on NS
(Becker & Wolff 2007)





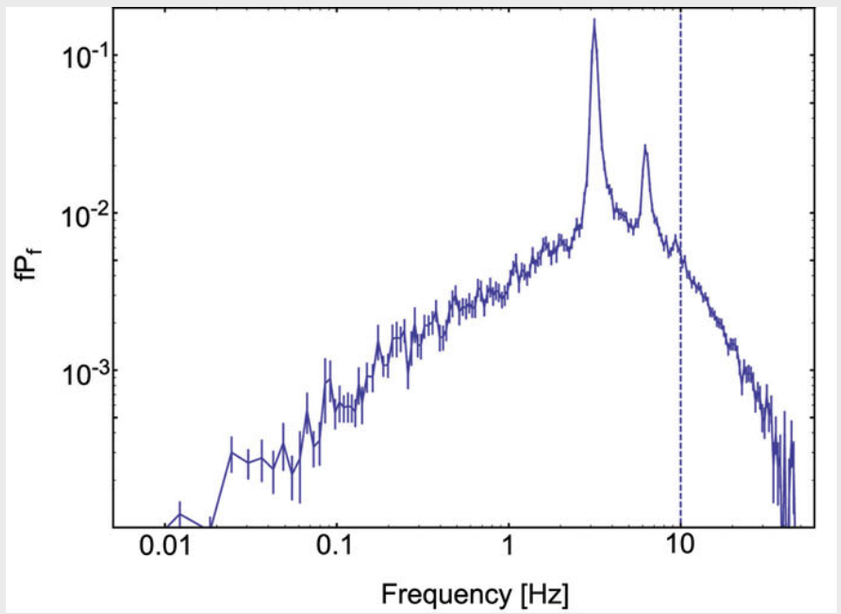
Odaka et al. 2013, 2014

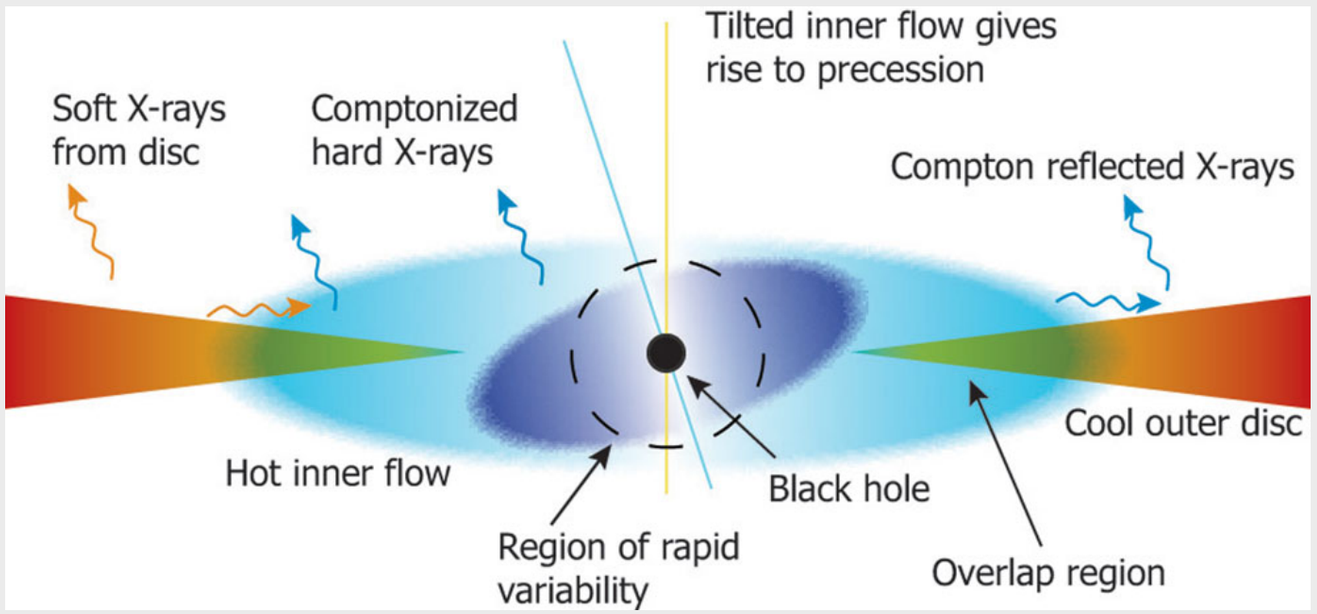
We found a set of self-consistent solutions that agree with the observations of accreting NS Vela X-1 and have reasonable model parameters.
column radius = 200 m, kTe = 6 keV, B field=2×10^{12} G

Accretion Flow onto Black Holes

- The scattering process would be much simpler than the NS case. No need to consider the strong B-field and the bulk motion.
- However, the properties of the accretion flow are highly uncertain.
- We investigate Comptonized radiation of microquasar XTE J1550–564 on its rise to outburst in 1998.
- The source showed strong low frequency QPO, which can be explained in the context of a precessing inner hot flow.

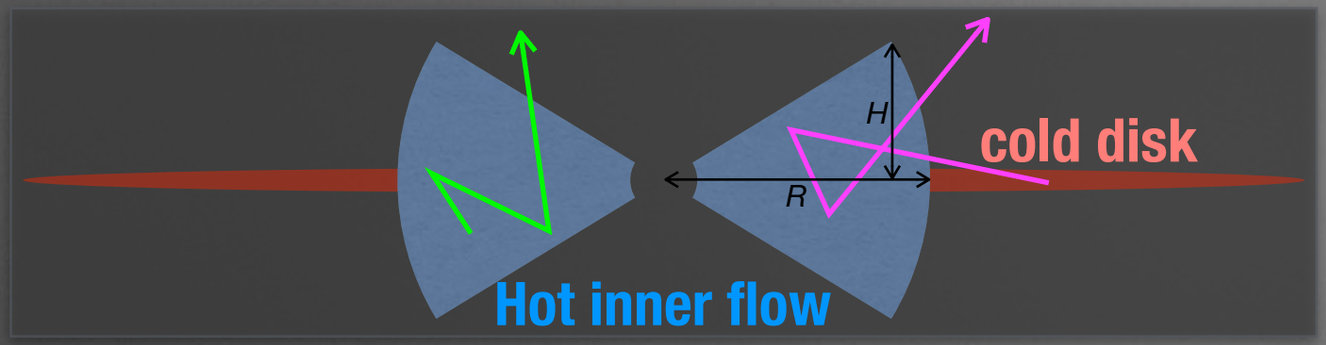
QPOs in power spectral density



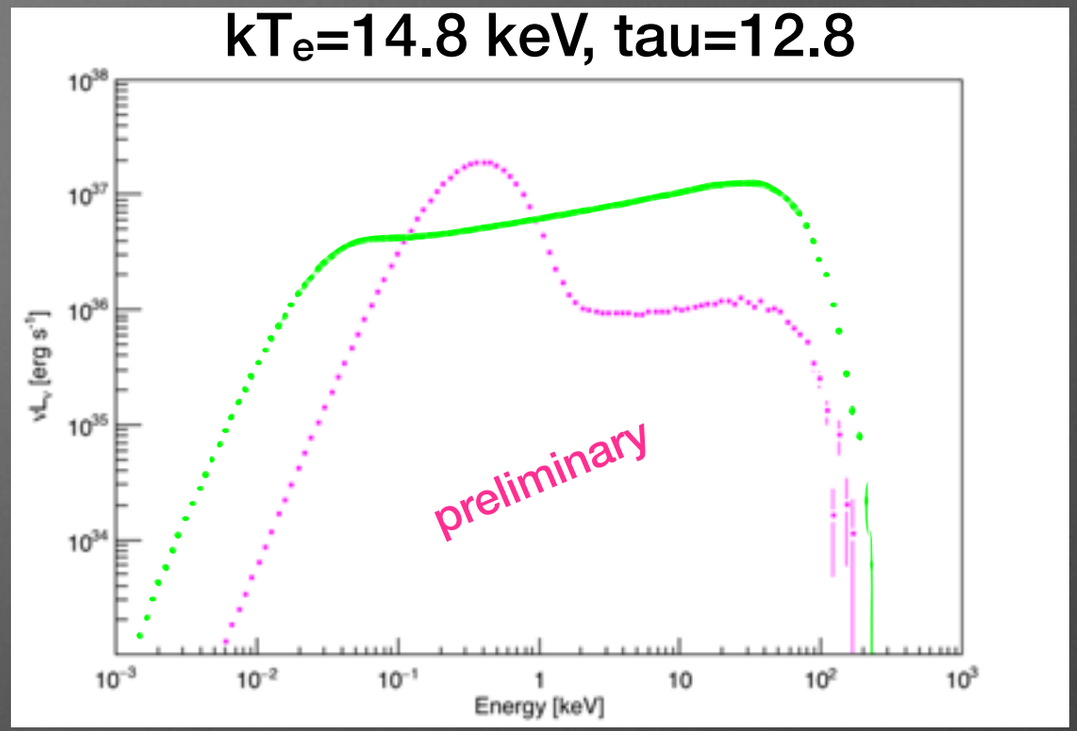


Axelsson et al. 2013

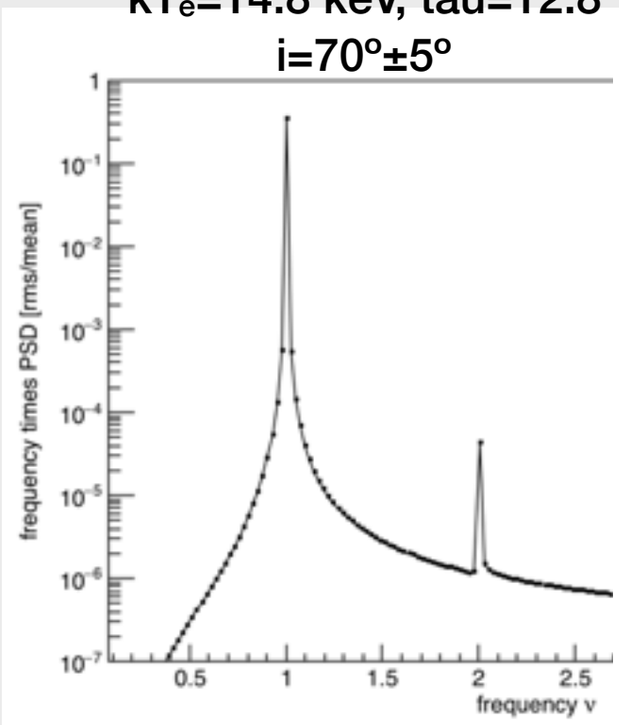
Comptonization Model



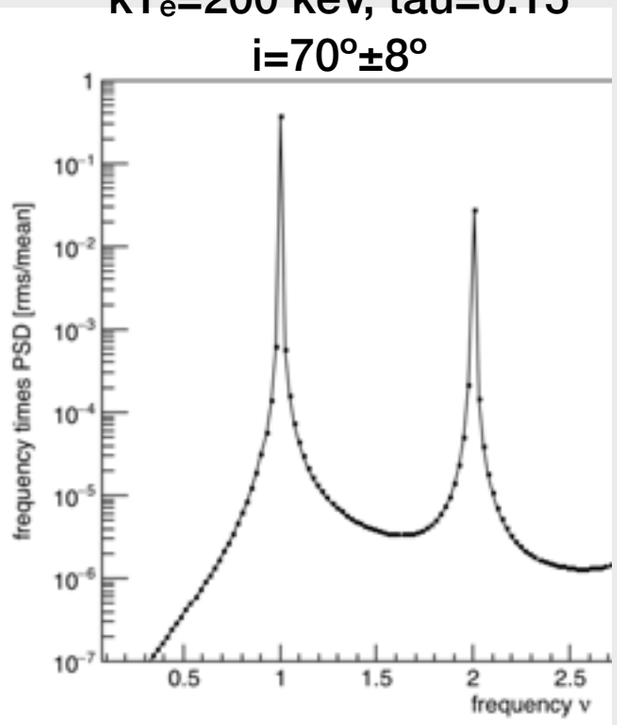
We assume cyclo-synchrotron (CS) origin of the seed photons as well as disk black body. CS can have a significant role in cooling the hot inner flow (e.g. Di Matteo et al. 1997).



the flow geometry
kT_e=14.8 keV, tau=12.8
i=70°±5°



slab geometry
kT_e=200 keV, tau=0.15
i=70°±8°



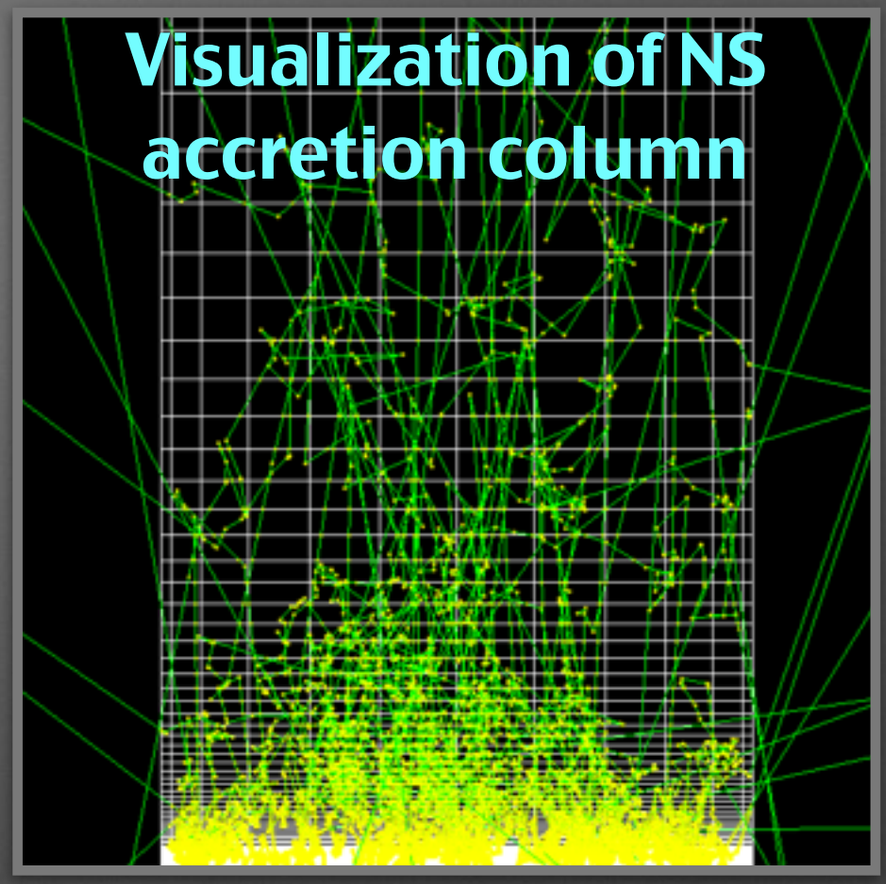
- Assuming the vertical precession of the flow (i=70°±5°), we successfully reproduced the observed level of QPO. But the first harmonic was significantly weaker than observed.
- This may implies that the flow has inhomogeneous structure with higher kTe or nonthermal electrons.

Odaka et al. in prep.

Conclusions

We have developed a general-purpose X-ray spectrum synthesizer MONACO based on Monte Caro simulation.

This MC framework will enable us to interpret high S/N data obtained by modern/future X-ray observatories including ASTRO-H.



<u>Collaborators of the MONACO project</u>
Framework: Shin Watanabe, Tadayuki Takahashi
Reflection from molecular clouds: Felix Aharonian, Dmitry Khangulyan
Compton shoulders: Hiroki Yoneda, Andrew Fabian
AGN torus: Shunya Furui, Yasushi Fukazawa, Toshihiro Kawaguchi, Masanori Ohno, Atsushi Tanimoto, Yoshihiro Ueda
Photoionized stellar winds: Shin Watanabe, Masao Sako
AGN outflows: Kouichi Hagino, Chris Done, Poshak Ghandi
Super soft X-ray sources: Kazuya Wada, Ken Ebisawa, Masahiro Tsujimoto
Accretion onto NS: Dmitry Khangulyan, Yasuyuki Tanaka, Kazuo Makishima
Accretion onto BH: Chris Done
Polarization: Paolo Coppi

Future Plans

- Full simulations of photoionized plasma.
  - to calculate ionization structure by using Monte Carlo results.
- Multi-wavelength, nonthermal processes
- General relativity