The PHOENIX Model Atmosphere Package

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PHOENIX version 16

- integrated /1D and /3D versions
- same micro-physics from 1D to 3D
- new EOS (ACES)
- dust formation/destruction $\rightarrow$ DRIFT (Helling & Woitke)
- massively parallel:
  - multi-stage domain decomposition
  - MPI
  - weak & strong scaling verified to 4k+ processes

Applications

PHOENIX v16 is being used to model

- “all” types of normal stars
- nova and supernova atmospheres
- very low mass stars, brown dwarfs & Exoplanet atmospheres
- irradiated planets/stars
- terrestrial planets
- disks (proto-planetary, AGN)

Model Construction

- Basic Physical Model
  - spherical shell
  - static (stars) or expanding (novae, winds, SNe)
  - hydrostatic or hydrodynamical equilibrium
  - central source provides energy

Model Construction

- Constraint equations:
  - energy conservation
    $\rightarrow$ temperature structure
  - momentum conservation
    $\rightarrow$ pressure & velocity structure

Model Construction

- "Auxiliary" equations:
  - Radiative transfer equation
  - solved via (non-local) operator splitting
  - full characteristics based method

Model Construction

- Radiative transfer equation
  - 1 or 3D
  - time independence
  - problem: scattering (dust, lines)

$$\frac{\partial}{\partial t} I(\nu, \vec{x}, \hat{\vec{n}}) + \hat{\vec{n}} \cdot \nabla I(\nu, \vec{x}, \hat{\vec{n}}) = \chi(\nu, \vec{x}) \left(S(\nu, \vec{x}) - I(\nu, \vec{x}, \hat{\vec{n}}) \right)$$

- solve for large optical depths & strong scattering
- allow for irradiation, velocity fields

3DRT Framework

- Cartesian (spherical, cylindrical) coordinates
- voxel grid ("cells")
  - physical data constant within a voxel
  - solve RT inside the voxels
- grid coordinates, e.g., $[-n_x, +n_x]$
- $\rightarrow$ voxel coordinates from $(-n_x, -n_y, -n_z)$ to $(+n_x, +n_y, +n_z)$

Data size

- small grid:
- $n_x = n_y = n_z = 32$
- $\rightarrow (2 * 32 + 1)^3 = 274\,625$ voxels
- compare to typically 64 to 128 grid points in 1D!
- large grid:
- $n_x = n_y = n_z = 128$
- $\rightarrow (2 * 128 + 1)^3 = 16\,974\,593$ voxels
- $\rightarrow$ one scalar physical variable (e.g., T) $\rightarrow 129$ MB

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3DRT Framework

- solution through operator splitting

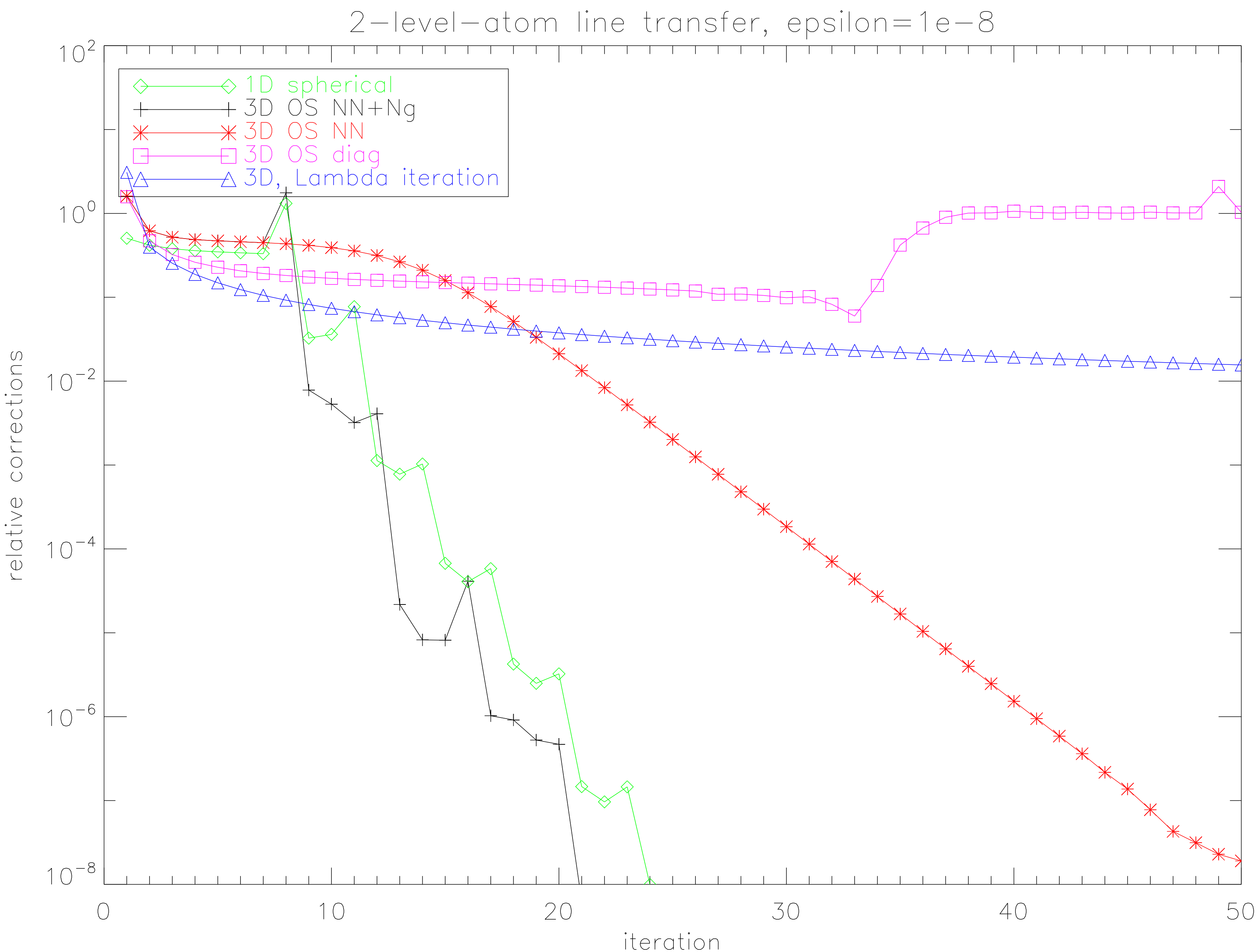
$$[1 - \Lambda^*(1-\epsilon)]\,\bar{J}_{\rm new} = \bar{J}_{\rm fs} - \Lambda^*(1-\epsilon)\bar{J}_{\rm old},$$

  where $\bar{J}_{\rm fs} = \Lambda S_{\rm old}$.
- need method to perform FS
- need method to construct Λ^*

Computation of Λ^*

- tri-diagonal operator in the 1D case
- $\rightarrow$ nearest neighbor Λ^* in 3D
- 1D: considers interaction of point with two direct neighbors
- 3D: interaction of a voxel with the $3^3 - 1 = 26$ surrounding voxels
- (or 6 neighbors in strictly face-centered view)
- 3D: storage requirements large but worth it!

convergence: $\epsilon_l = 10^{-8}$



Model Construction

- "Auxiliary" equations:
  - equation of state $\rightarrow (T, P_{\rm gas}, \rho)$ relation
    - high temperatures:
      (hot stars, Supernovae, novae)
      $\rightarrow$ need to include many ions
    - low temperatures:
      (Brown dwarfs, Jupiter-like planets, cool novae)
      $\rightarrow$ need to include 100's of molecules & dust species
  - ACES EOS (Travis Barman), valid above 100 K

Molecules

Selected molecules considered in the EOS

NH	C_2	CN	CO	MgH	CaH	SiH	TiO	H_2O	H_2
N_2	NO	CO_2	O_2	ZrO	VO	MgS	SiO	AlH	HCl
HF	HS	TiH	AlO	BO	CrO	LaO	MgO	ScO	YO
SiF	NaCl	CaOH	HCN	C_2H_2	CH_4	CH_2	C_2H	HCO	NH_2
LiOH	C_2O	AlOF	NaOH	MgOH	AlO_2	Al_2O	AlOH	SiH_2	SiO_2
H_2S	OCS	KOH	TiO_2	TiOCl	VO_2	FeF_2	YO_2	ZrO_2	BaOH
LaO_2	C_2H_4	C_3	SiC_2	CH_3	C_3H	NH_3	C_2N_2	C_2N	CaF_2
AlOCl	Si_2C	CS_2	$CaCl_2$	AlF	CaF	Si_2	SiS	CS	AlCl
KCl	CaCl	TiS	TiCl	SiN	AlS	AL_2	FeO	SiC	TiF_2
FeH	LiCl	NS	NaH	SO	S_2	$AlBO_2$	AlClF	$AlCl_2$	AlF_2
$AlOF_2$	AlO_2H	Al_2O_2	$BeBO_2$	OBF	HBO	HBO_2	HBS	BH_2	BO_2H_2
BH_3	H_3BO_3	KBO_2	$LiBO_2$	$NaBO_2$	BO_2	$BaCl_2$	BaF_2	BaO_2H_2	BaClF
$BeCl_2$	BeF_2	BeOH	BeH_2	BeH_2O_2	Be_2O	Be_3O_3	ClCN	CHCl	CHF
CHP	CH_3Cl	KCN	NaCN	BeC_2	C_2HCl	C_2HF	$(NaCN)_2$	C_4	C_5
CaO_2H_2	MgClF	SiH_3Cl	$FeCl_2$	K_2Cl_2	$MgCl_2$	Na_2Cl_2	$TiOCl_2$	$SrCl_2$	$TiCl_2$
$ZrCl_2$	$TiCl_3$	$ZrCl_3$	$ZrCl_4$	CrO_2	SiH_3F	OTiF	SiH_2F_2	MgF_2	SrF_2
ZrF_2	TiF_3	ZrF_4	FeO_2H_2	SrOH	$(KOH)_2$	$(LiOH)_2$	MgO_2H_2	$(NaOH)_2$	SrO_2H_2
PH_2	PH_3	SiH_4	Si_2N	PO_2	SO_2	P_4	Si_3	NO_2	NO_3
C_3N	C_2H_3	C_4H	HC_3N	C_4H_2	CH_3CN	HC_5N	C_6H	C_4H_4	C_6H_2
HC_7N	C_4H_4S	C_4H_4O	C_4H_6	C_6H_4	HC_9N	C_5H_5N	C_6H_5O	C_6H_6	C_6H_6O
$HC_{11}N$	OH^-	CH^-	C_2^-	OH	CH	CN^-	SiH^-	H_2^-	HS^-
CS^-	FeO^-	BO^-	$AlCl_2{}^-$	$AlF_2{}^-$	$AlOF_2{}^-$	$AlOH^-$	$CO_2{}^-$	NO^+	$H_2{}^+$
TiO^+	ZrO^+	$AlOH^+$	$BaOH^+$	HCO^+	$CaOH^+$	$SrOH^+$	H_3O^+	H_3^+	

Liquids & Solids

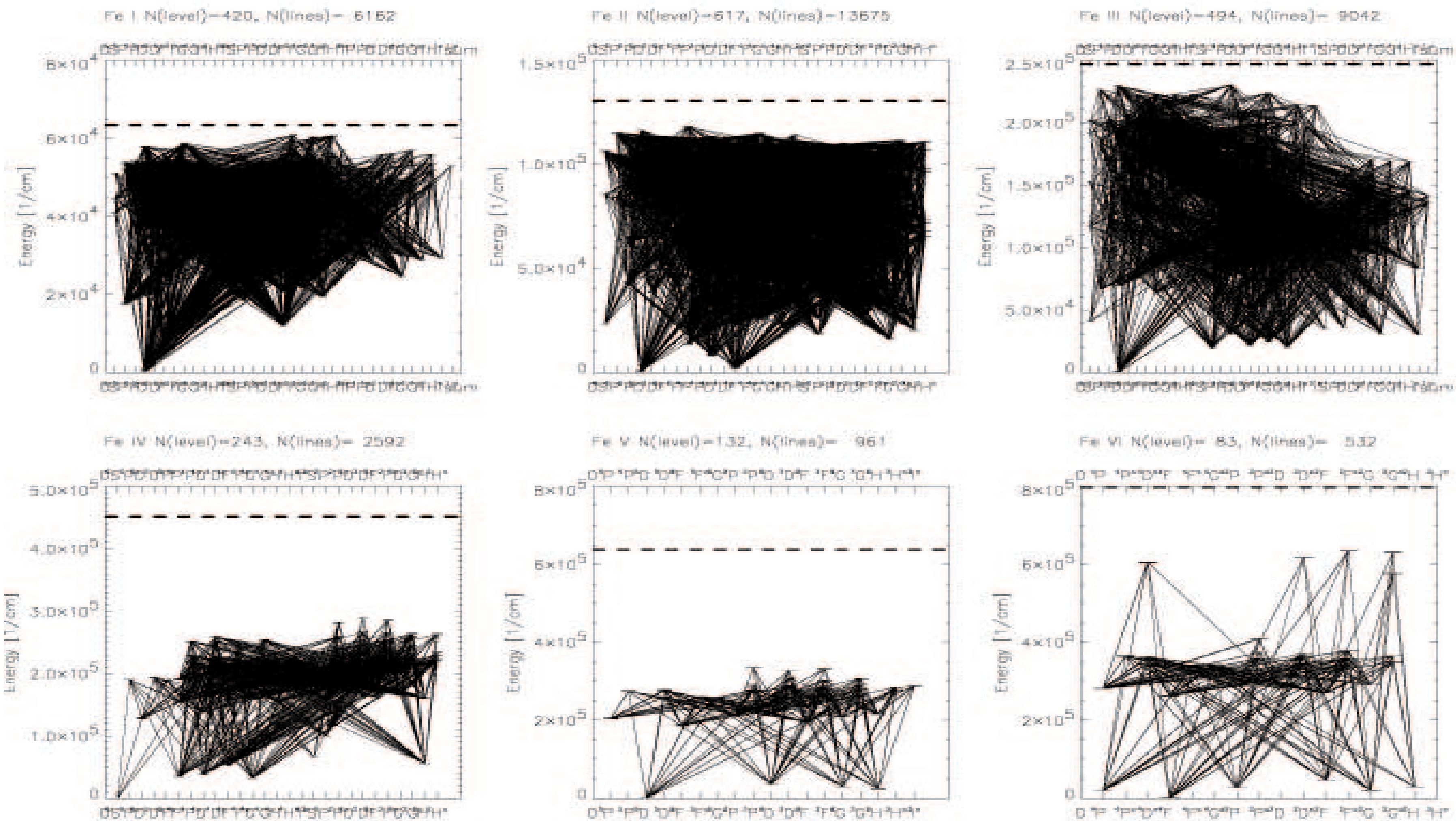
Selected liquid/dust species considered in the EOS

Al/l	B/l	Ba/l	Be/l	Ca/l	Cr/l	Cu/l	Fe/l	K/l
Li/l	Mg/l	Mn/l	Na/l	Nb/l	Ni/l	P/l	S/l	Si/l
Sr/l	Ti/l	V/l	Zn/l	Zr/l	BeO/l	ClK/l	NbO/l	OSr/l
ClNa/l	VO/l	B_2Ti/l	$BaCl_2$/l	$CaCl_2$/l	Cl_2Fe/l	Cl_2Sr/l	O_2Si/l	Li_2O/l
Mg_2Si/l	Cu_2O/l	Cl_3Fe/l	Cr_2O_3/l	NiS_2/l	$BLiO_2$/l	Cl_2S_2/l	Ni_3S_2/l	Al_2O_3/l
O_3V_2/l	Cl_5Nb/l	Nb_2O_5/l	$B_4K_2O_7$	$B_4Na_2O_7$	Li_2O_3Si	$B_4Li_2O_7$	$Mg_3O_8P_2$	$Al_3F_{14}N$
B_5H_9/l	$H_{10}O_8S$	$B_8K_2O_{13}$	$B_{10}H_{14}$	Al	B	Ba	Be	C
Ca	Co	Cr	Cu	Fe	Li	Mg	Mn	Na
Nb	Ni	P	S	Si	Sr	Ti	V	Zn
Zr	MgO	FeS	CaO	CaS	MgS	TiN	AlN	NiS
MnS	TiO	VO	CuO	FeO	TiC	SiC	ZrC	H_2O
TiO_2	ZrO_2	SiO_2	FeS_2	NiS_2	Mg_3N_2	Ni_3S_2	Ti_2O_3	Ti_3O_5
Ti_4O_7	V_2O_3	Al_2O_3	Al_2O_3	Al_2O_3	Al_2O_3	Al_2S_3	Cr_2O_3	$CaTiO_3$
$MgTiO_3$	$MgSiO_3$	$CaSiO_3$	$MnSiO_3$	Na_2SiO_3	K_2SiO_3	Fe_2SiO_4	Ca_2SiO_4	Mg_2SiO_4
$ZrSiO_4$	Fe_2O_3	Fe_3O_4	$MgAl_2O_4$	$MgTi_2O_5$	Al_2SiO_5	$CaMgSi_2$	Ca_2MgSi	Ca_2Al_2S
$CaAl_2Si$	$KAlSi_3O$	$NaAlSi_3$	Al_6Si_2O	MgC_2	Cr_3C_2	Mg_2C_3	Al_4C_3	Cr_7C_3
$Cr_{23}C_6$								

Model Construction

- statistical equilibrium equations
  $\longrightarrow$ relate the population of each energy level to non-local radiation field and to collisional processes
- radiative transfer & statistical equilibrium equations are *intricately coupled*
  $\longrightarrow$ must be solved together
  $\longrightarrow$ statistical equations are inherently *non-local* $\Rightarrow$

Fe NLTE model atoms



Model Construction

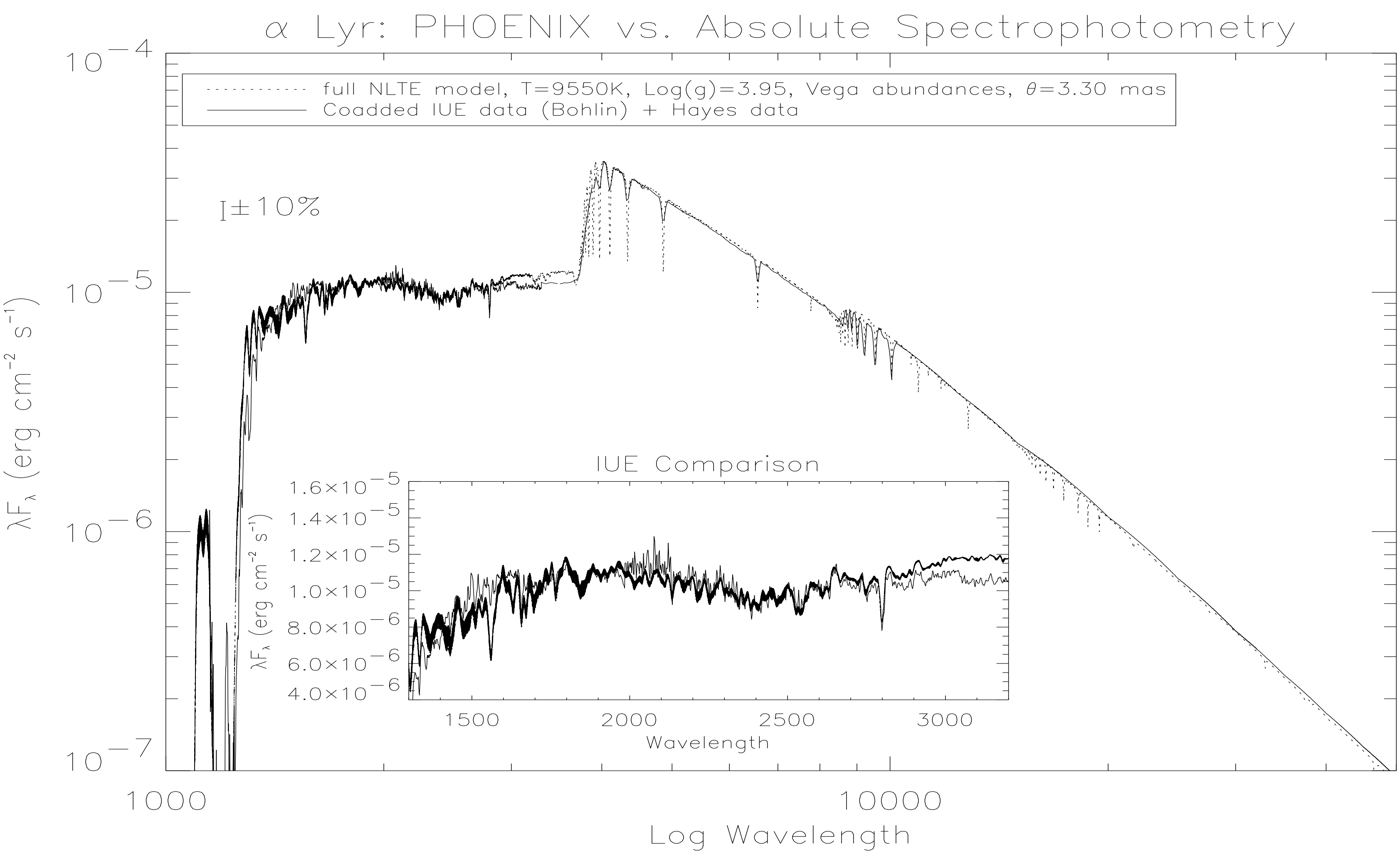
- atomic line blanketing: $\approx 5 - 30 \times 10^6$ lines dynamically selected from a list of 83×10^6 lines
- molecular line blanketing: $\approx 15 - 600 \times 10^6$ lines dynamically selected from a list of 1.2×10^9 lines
- direct opacity sampling of line blanketing
- depth dependent line profiles
  $\rightarrow$ no ODF or opacity sampling tables (NLTE!).
- special profiles for important lines

Computational Problem

- 1D (serial) CPU time: 1–6 CPU days
- 3D (serial) CPU time: 10 CPU *years*
- Solution: parallel computing
  - dramatically reduces wallclock time per model
  - allows efficient use of existing large supercomputer facilities
  - 1D: 8-16 CPUs for a few hours
  - 3D: 4096 CPUs for one day

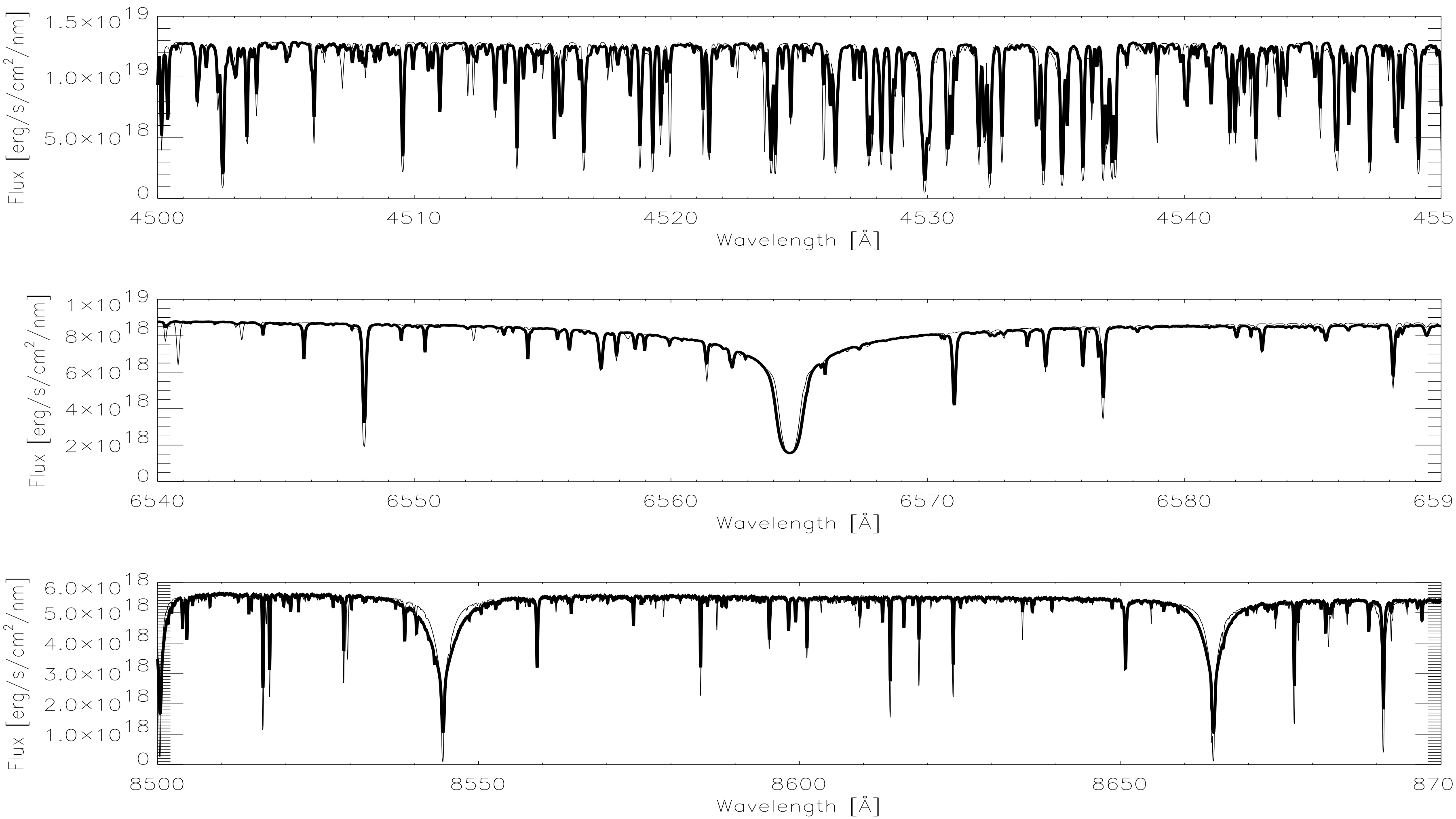
Results: A stars

- models work well for A0V's ...



Results: solar type stars

- models work well for G2V's . . .



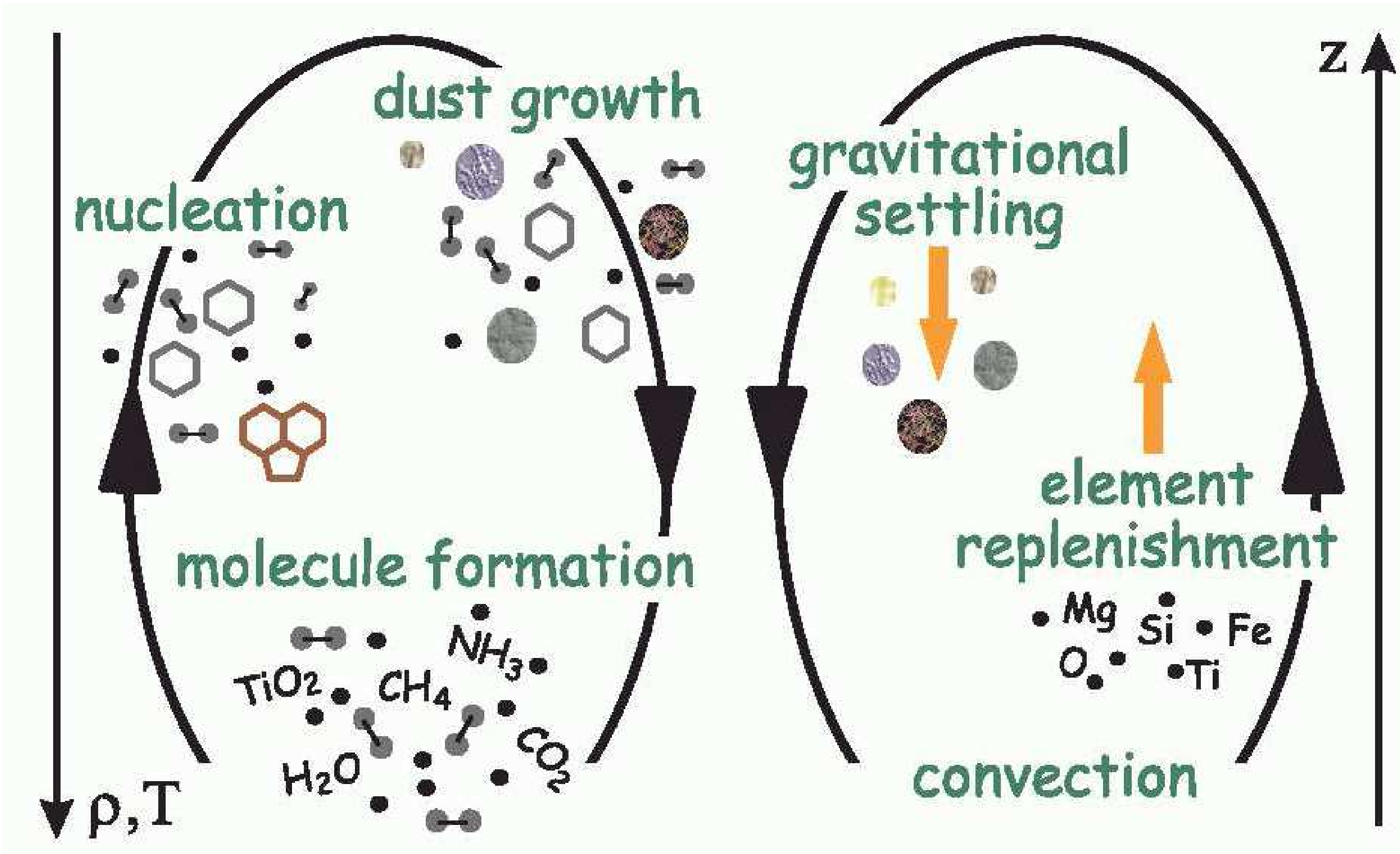
Dust formation/destruction

- directly couple DRIFT (Helling & Woitke) dust model to PHOENIX model atmospheres
  - PHOENIX $\rightarrow$ provides atmosphere structure $(T, P_g, \ldots)$
  - DRIFT $\rightarrow$ compute dust formation/destruction (cloud deck)
  - $\rightarrow$ feedback to PHOENIX
  - $\rightarrow$ new atmosphere structure
  - iterate to convergence

DRIFT dust mode

- Helling & Woitke
- stationary solution
- nucleation rates for $(TiO_2)_N$ seeds
- 7 most important solids used (TiO_2, Al_2O_3, Fe, SiO_2, MgO, $MgSiO_3$, Mg_2SiO_2)
- mixing by convection + overshooting
- grain size distribution via moments

DRIFT dust mode

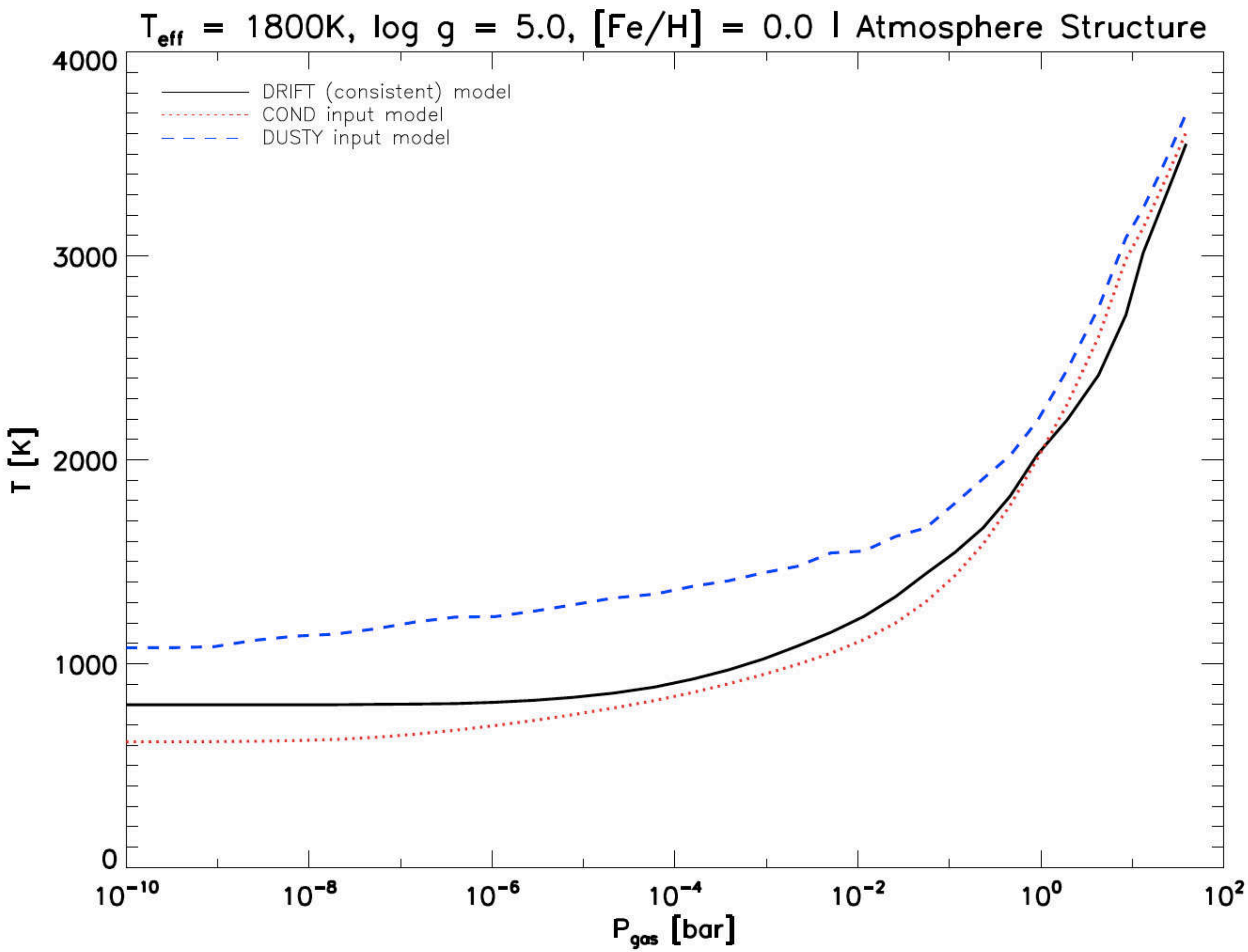


- Helling et al (2001)

DRIFT-PHOENIX models

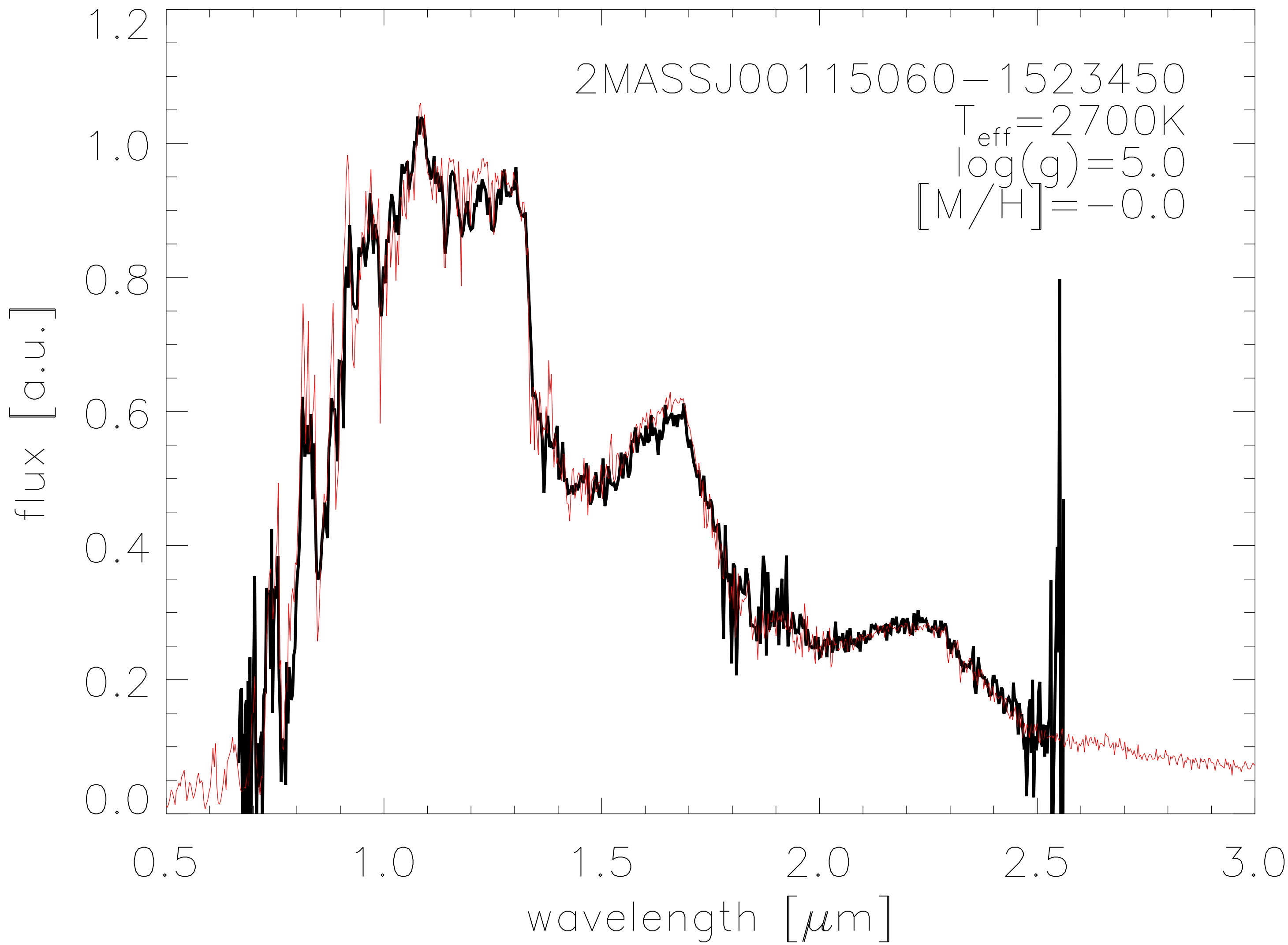
- location of convection zone crucial for dust formation!
- considering feedback dust formation vs. atmosphere structure crucial
- cloud deck depends on model parameters

atmosphere structure feedback



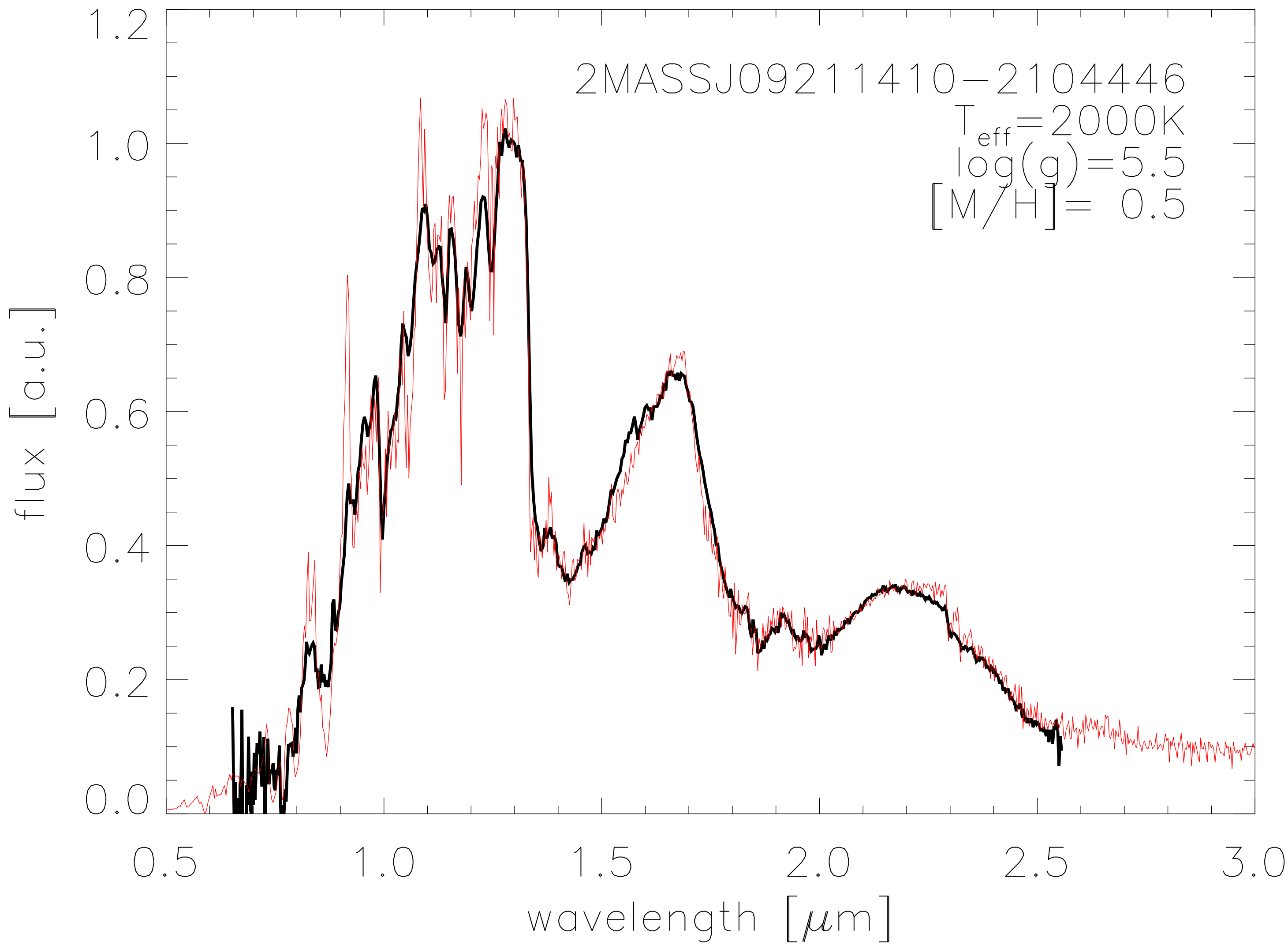
- Dissertation M. Dehn (2007)

Application: good fits



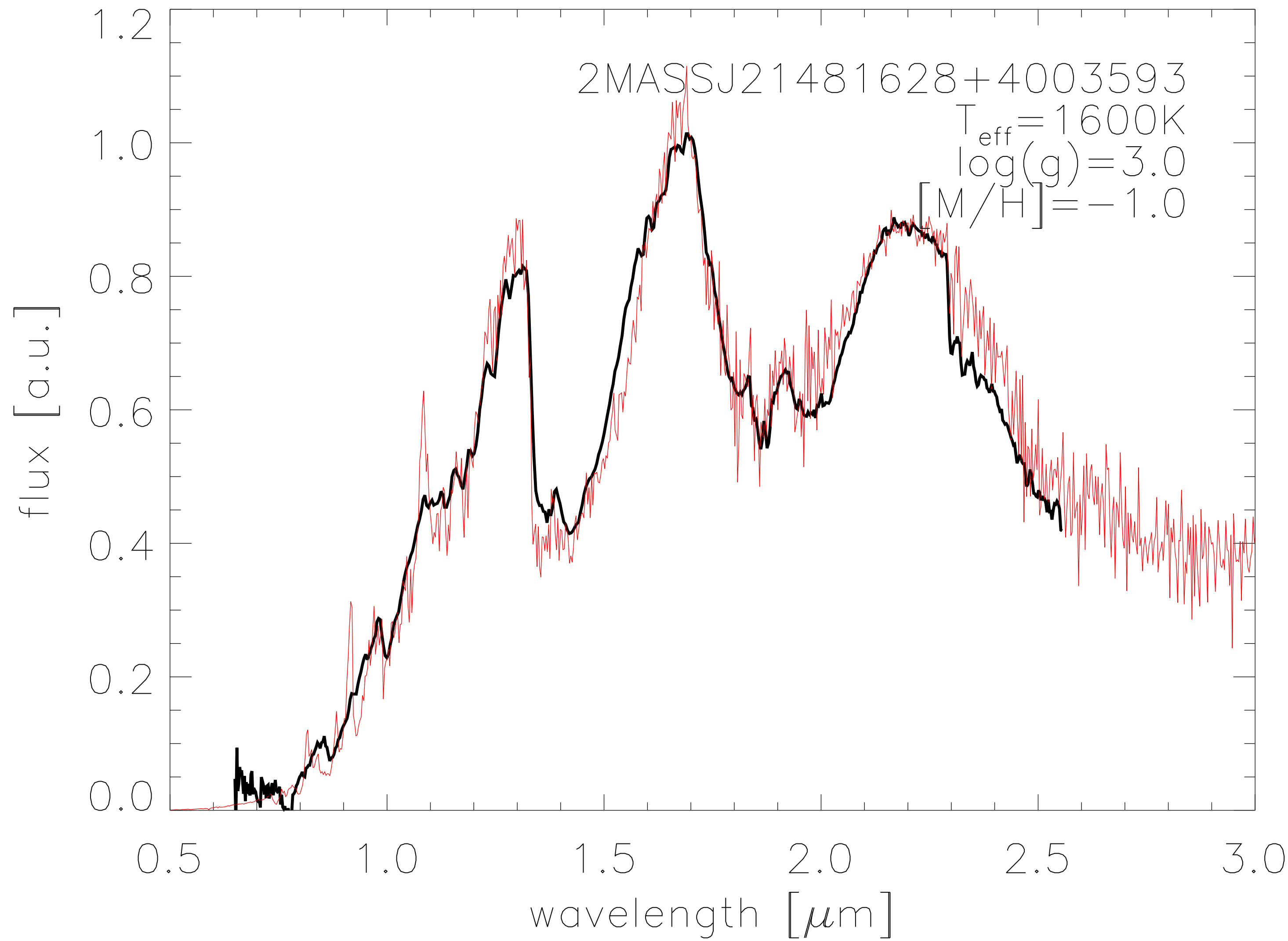
Witte et al (2011)

Application: good fits



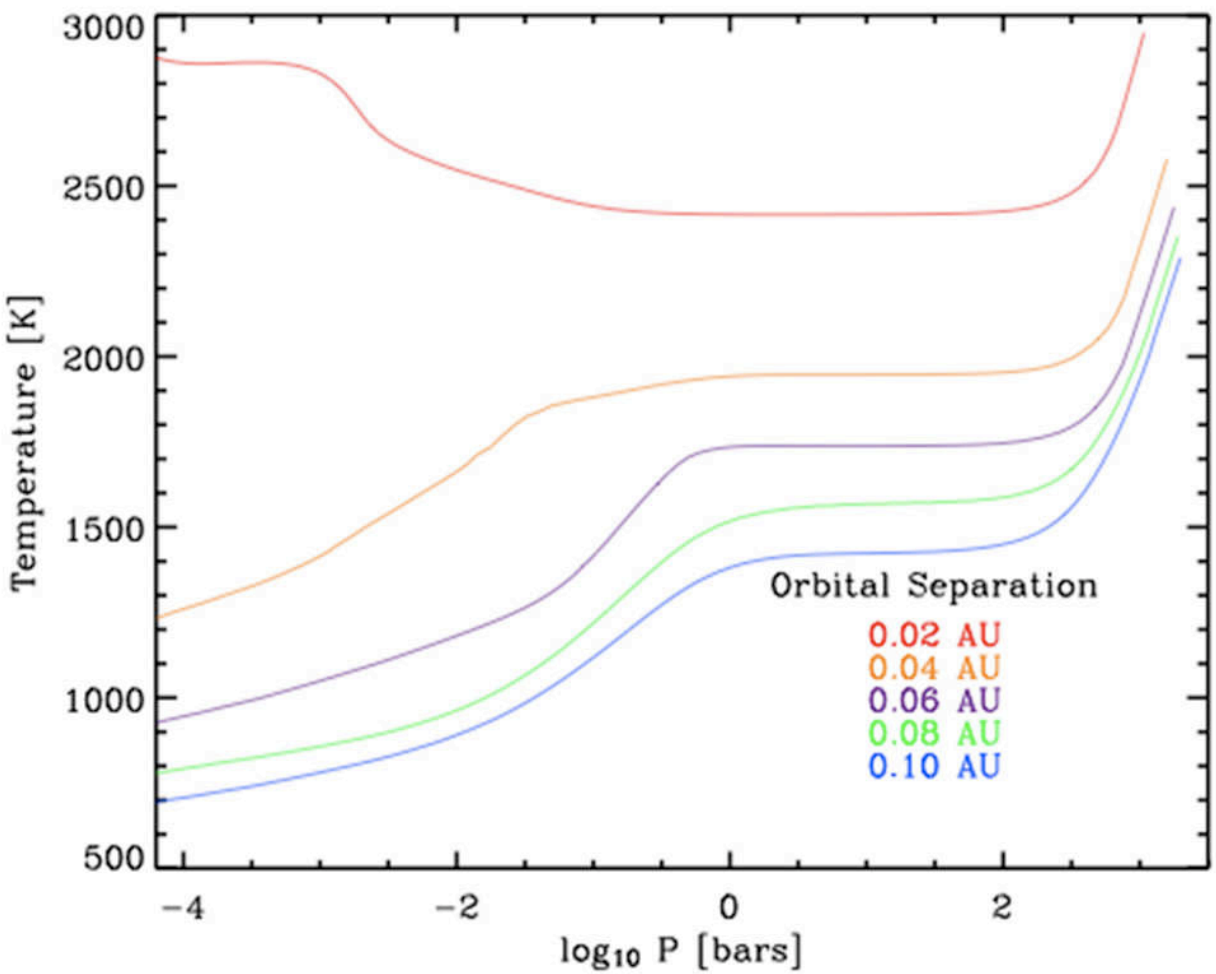
Witte et al (2011)

Application: good fits



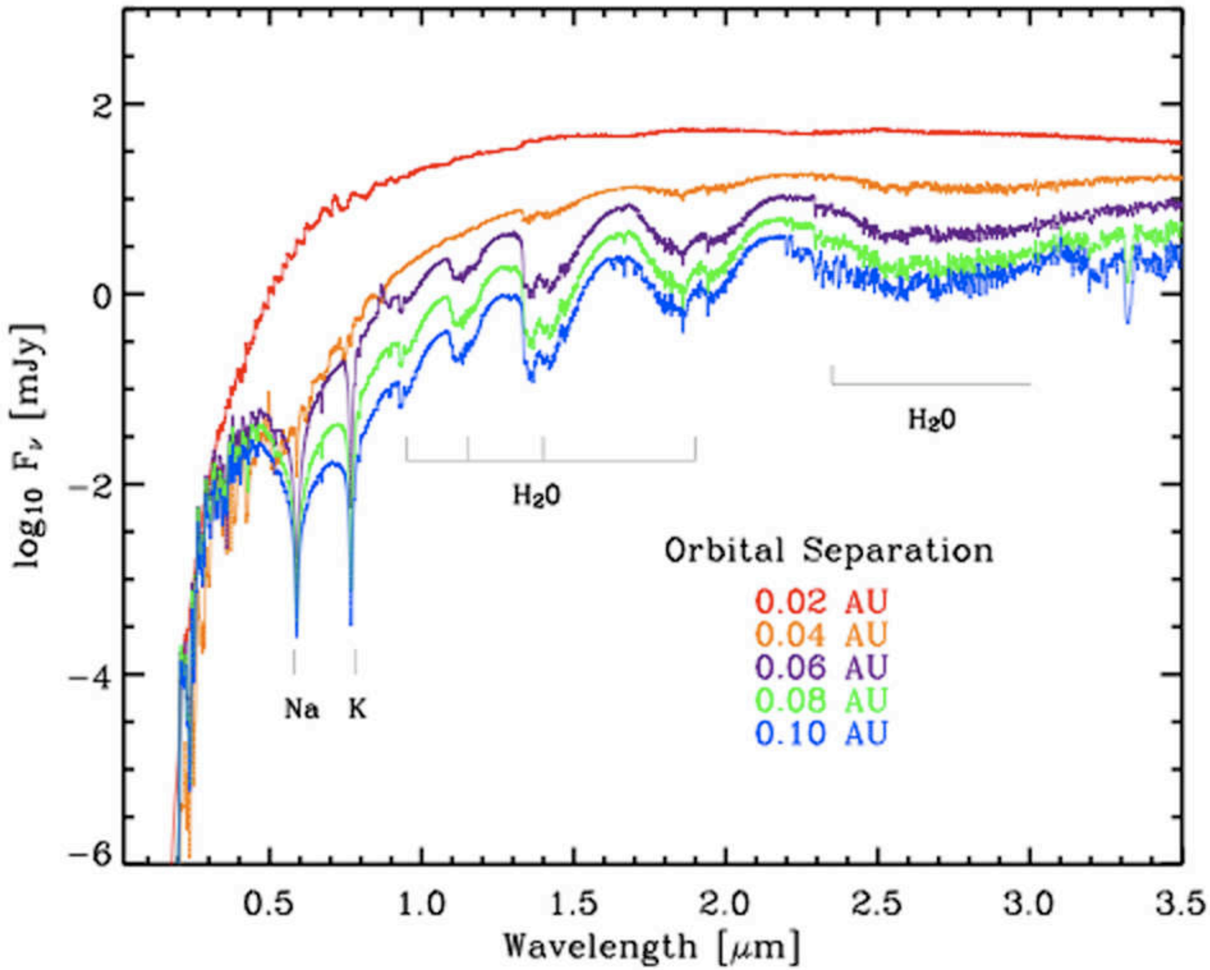
Witte et al (2011)

Irradiation



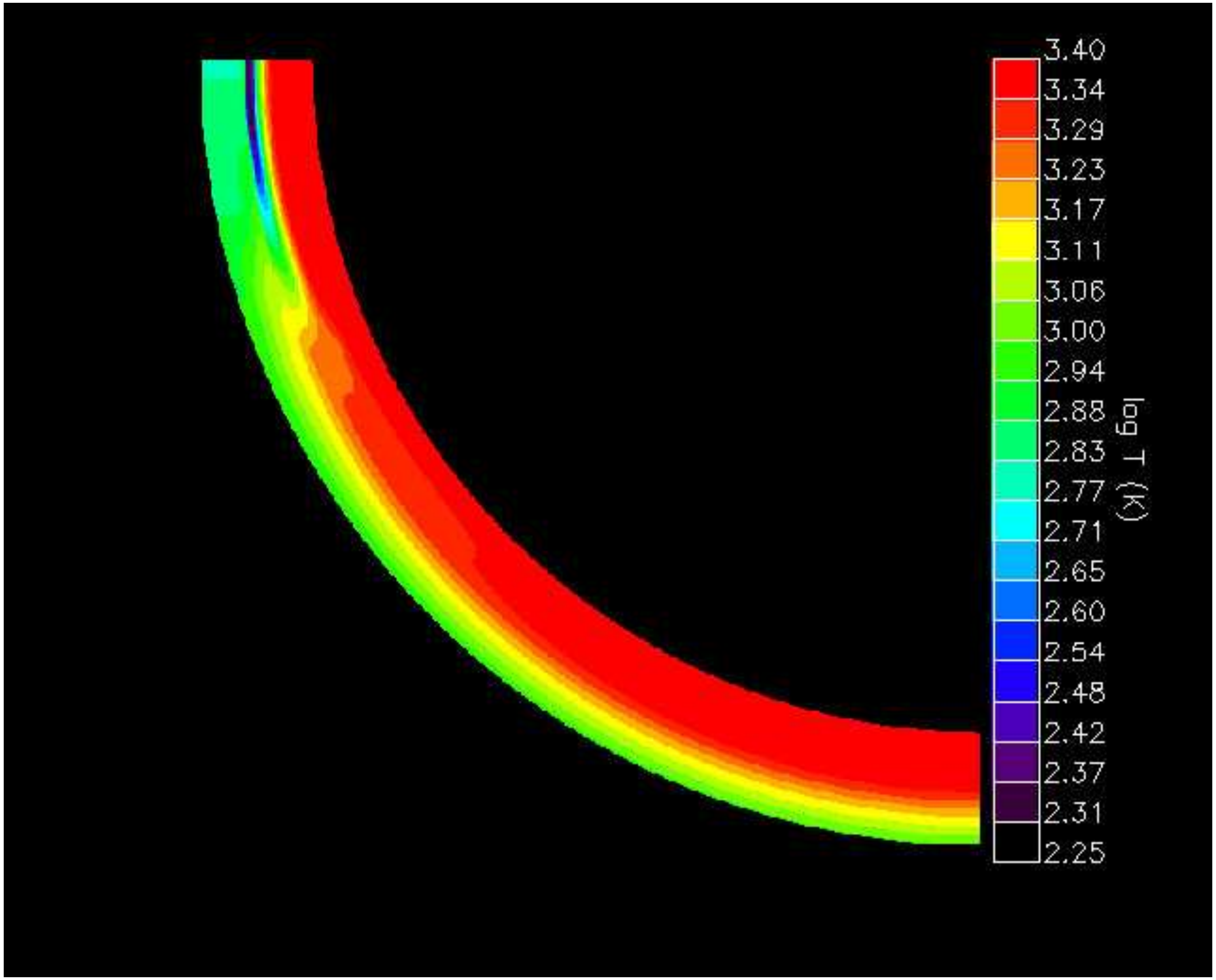
- temperature structure for different separations

Irradiation



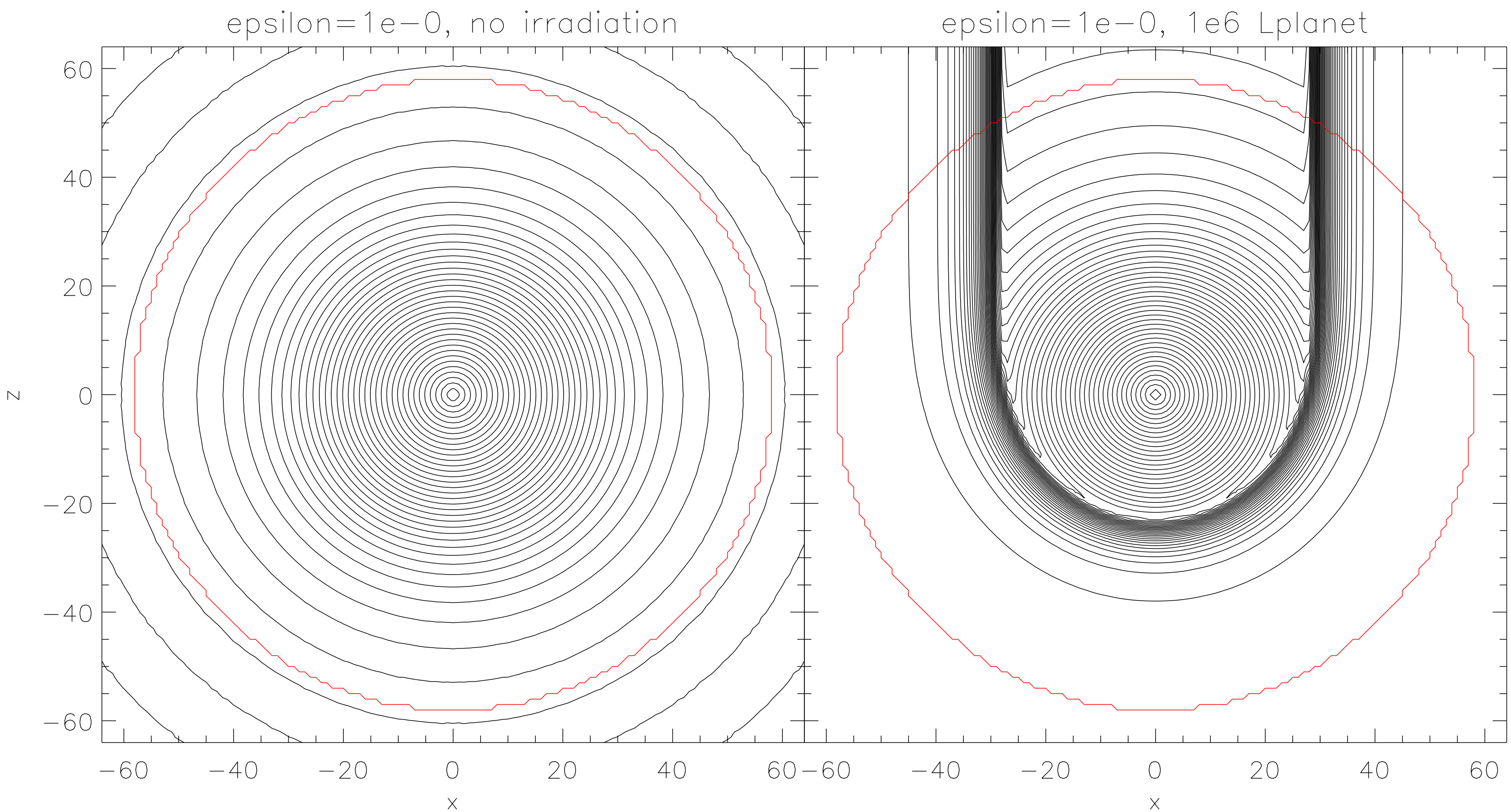
- EGP spectra for different separations

Results: 2D structure

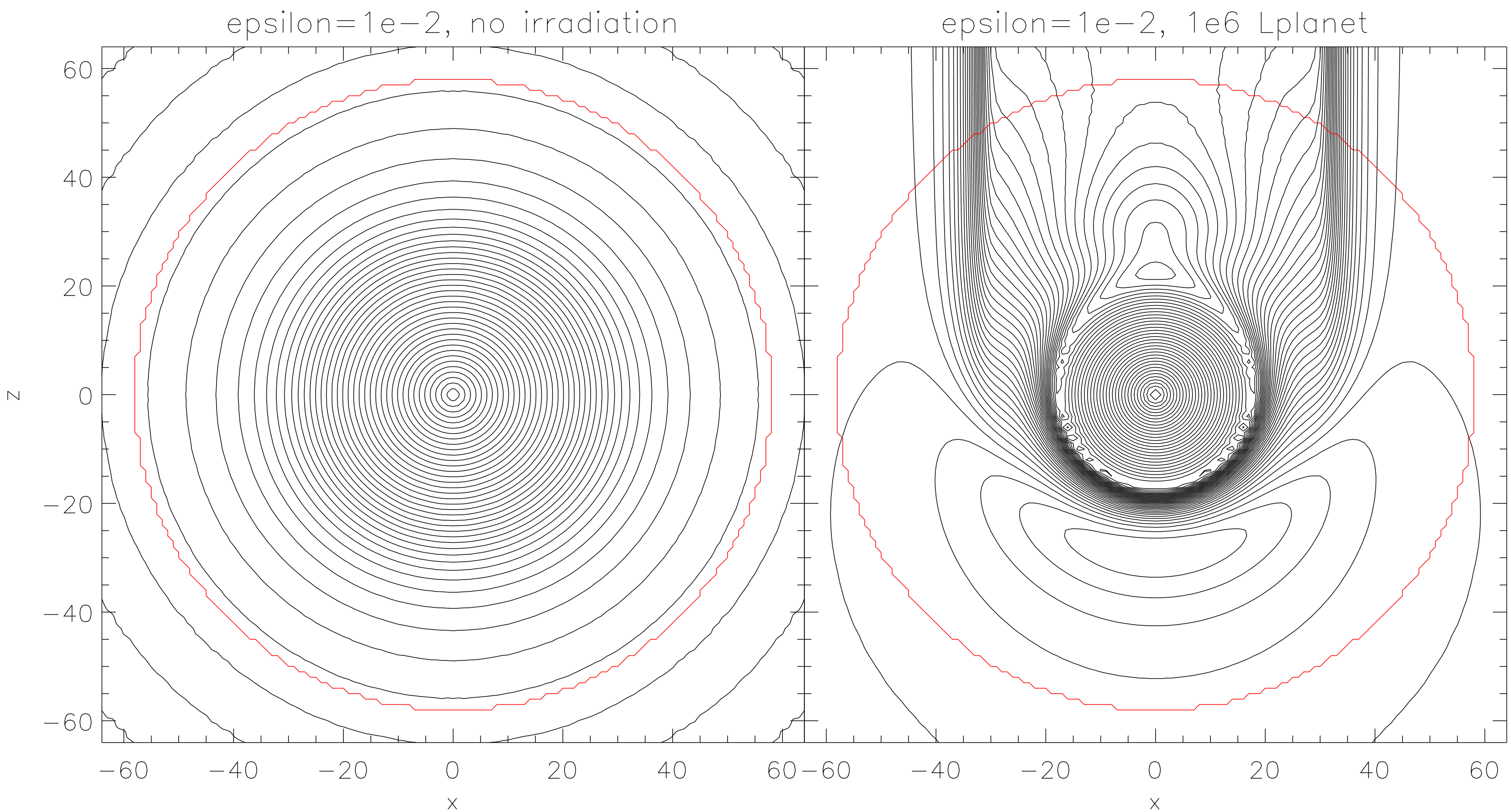


roll the movie!

Results: 3DRT w/ irradiation



Results: 3D w/ irradiation



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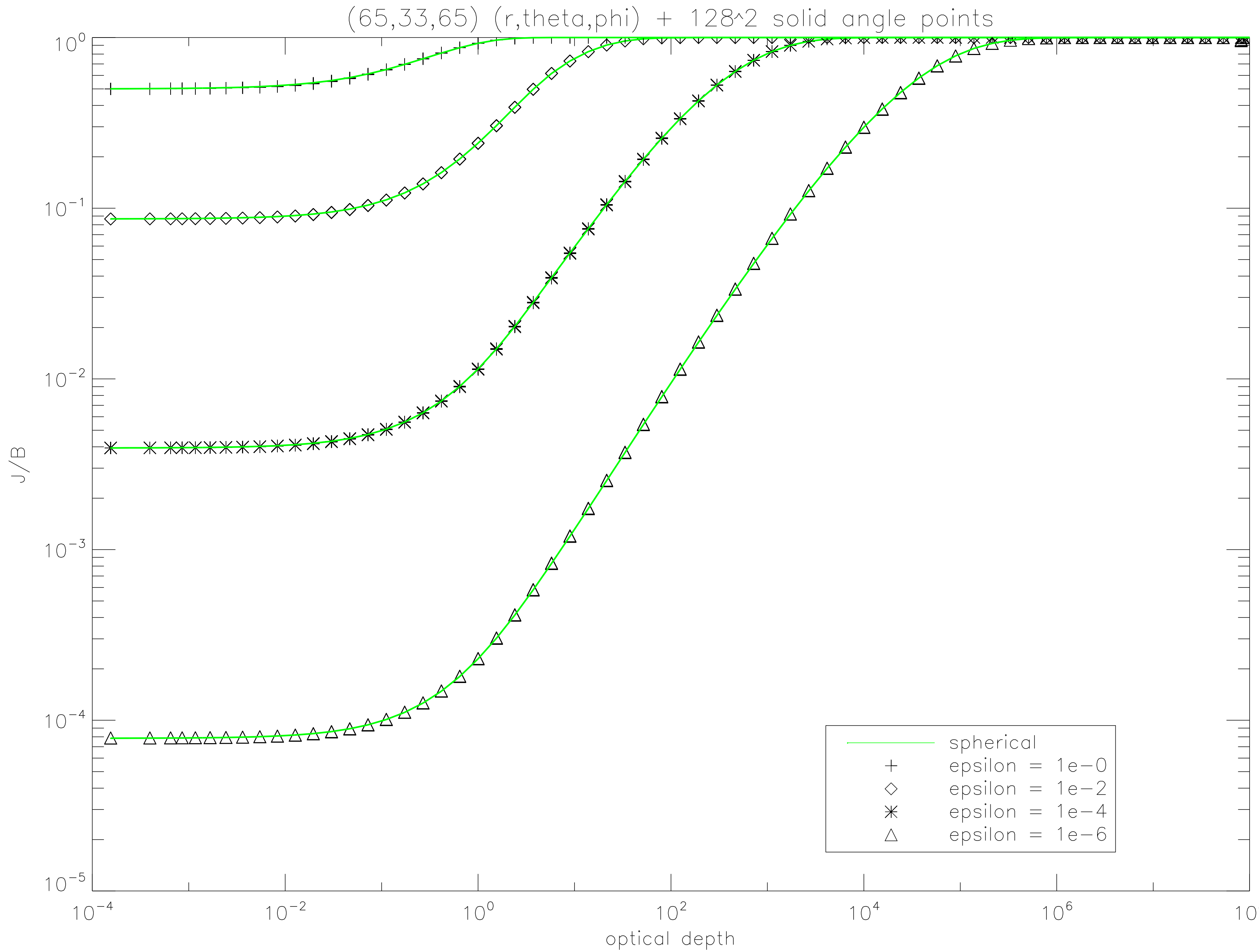
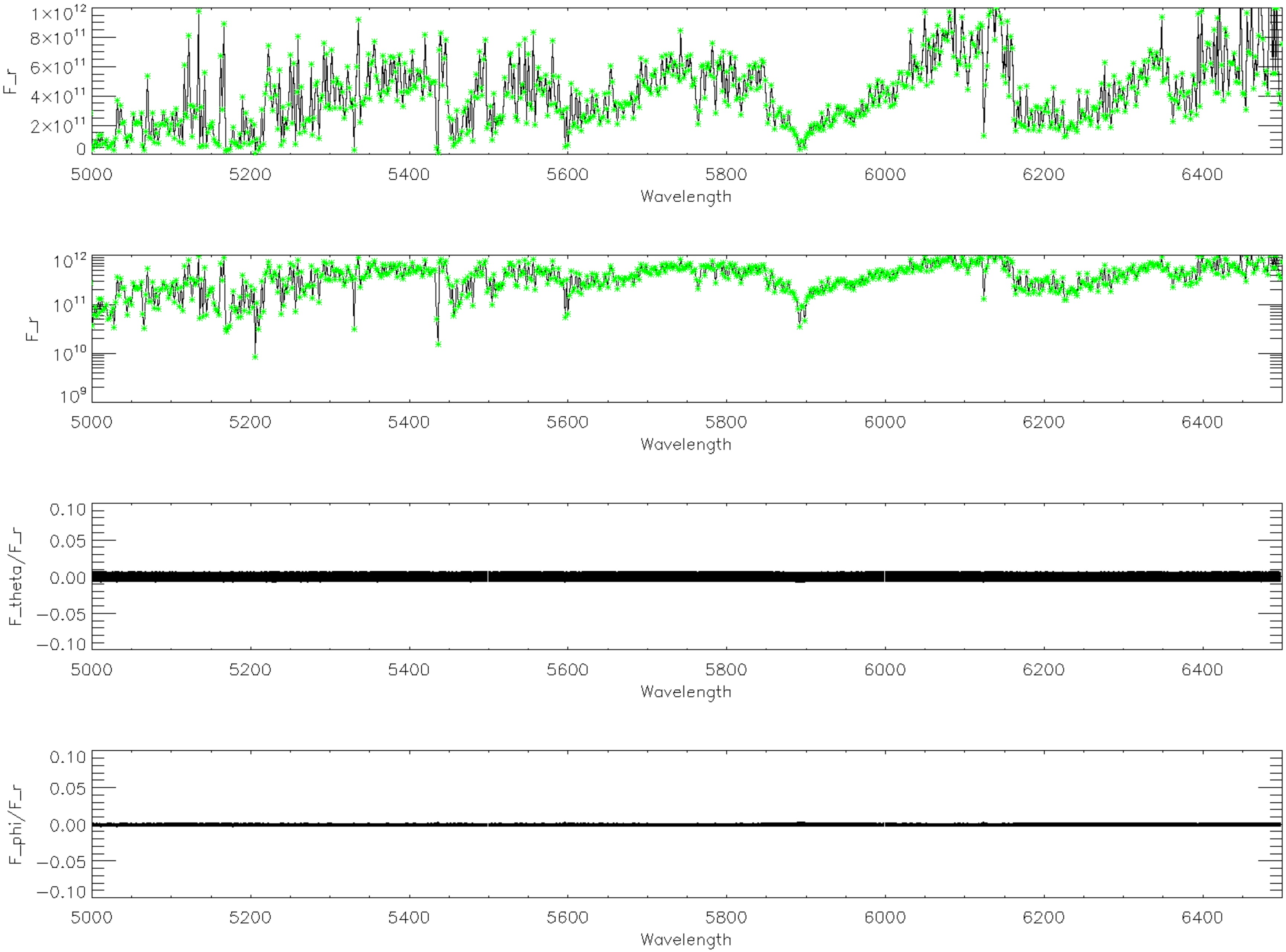
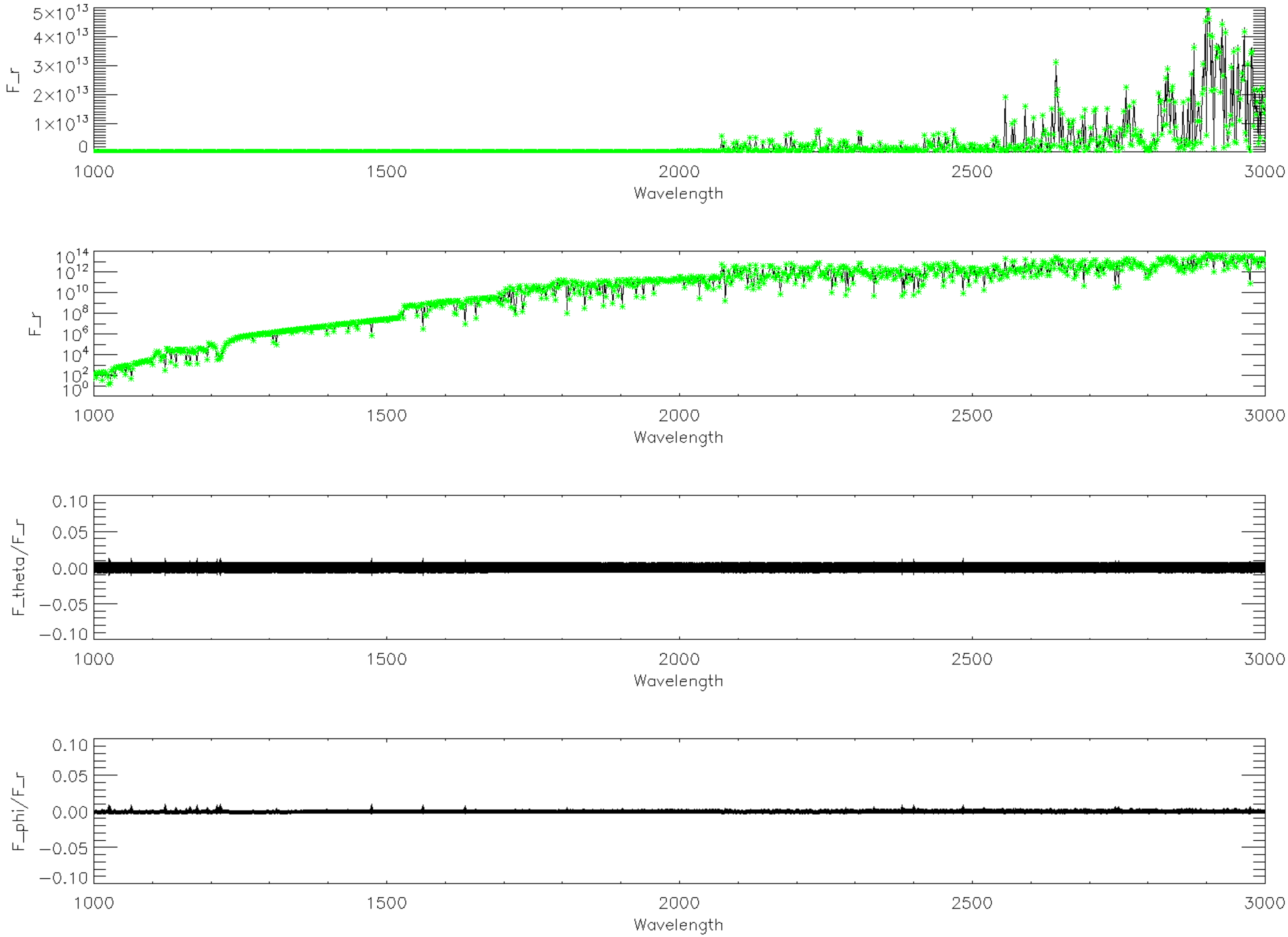
spherical 3D coordinates



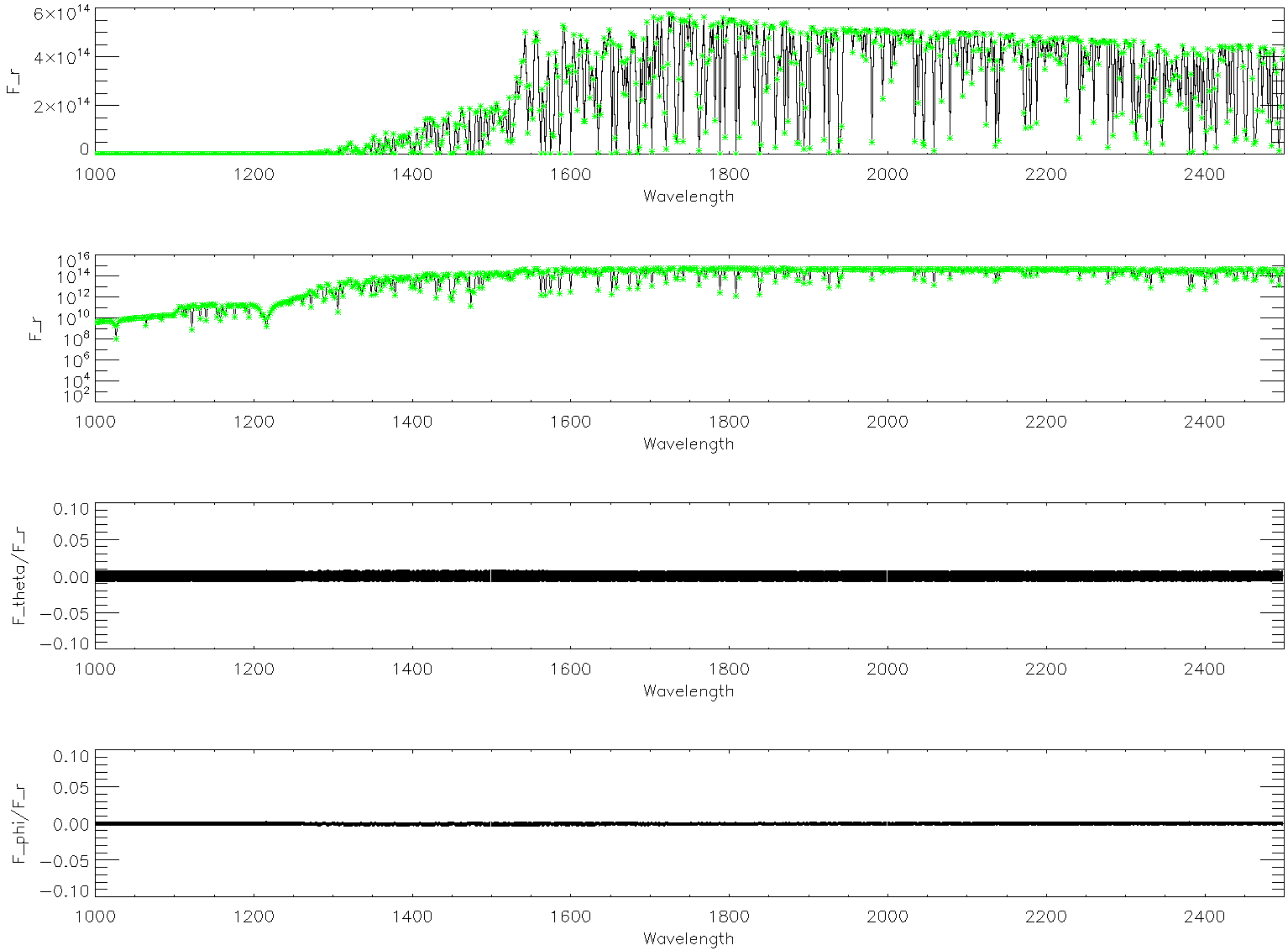
PHOENIX 1D vs 3D: 3000K



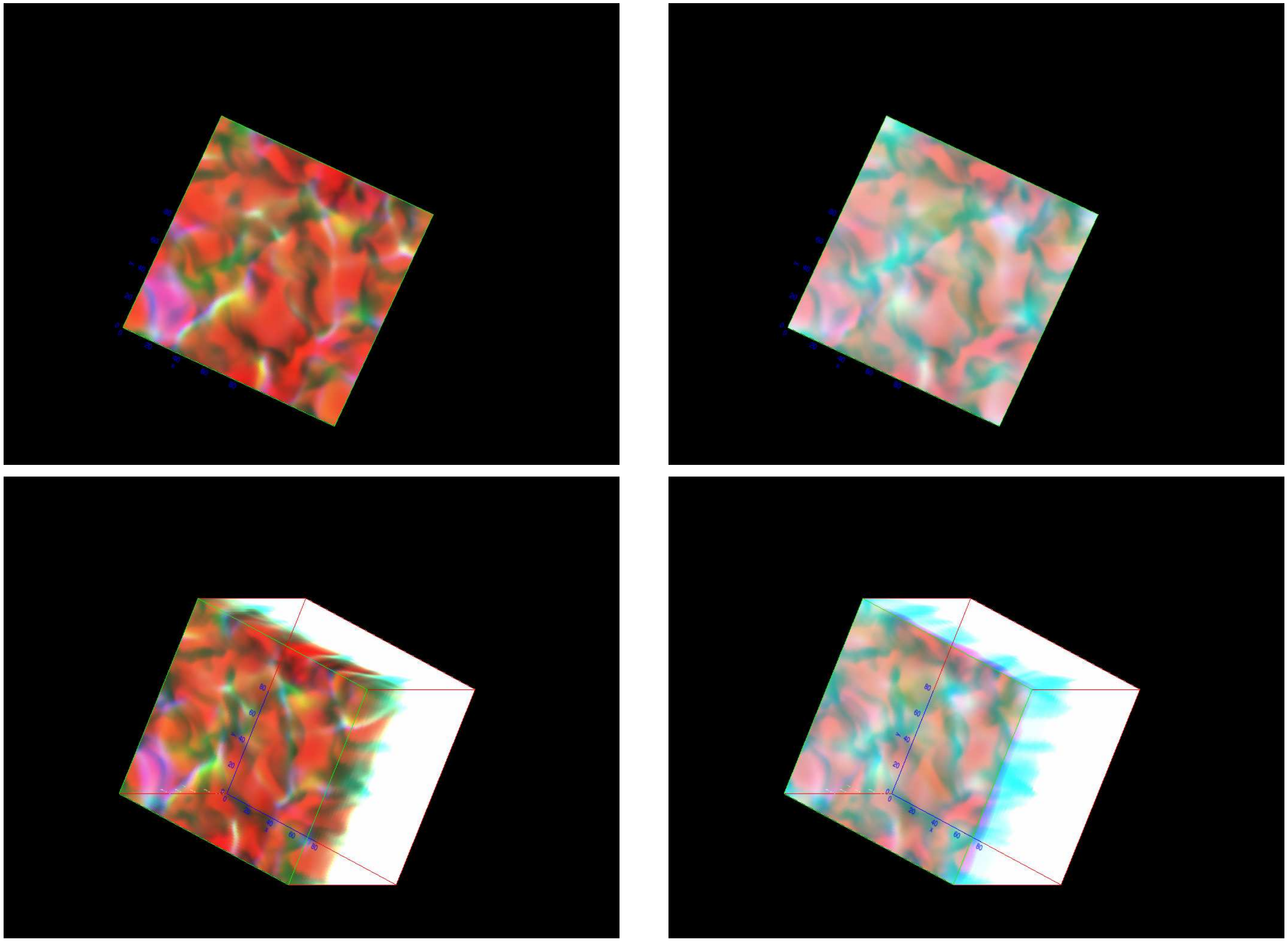
PHOENIX 1D vs 3D: 5700K



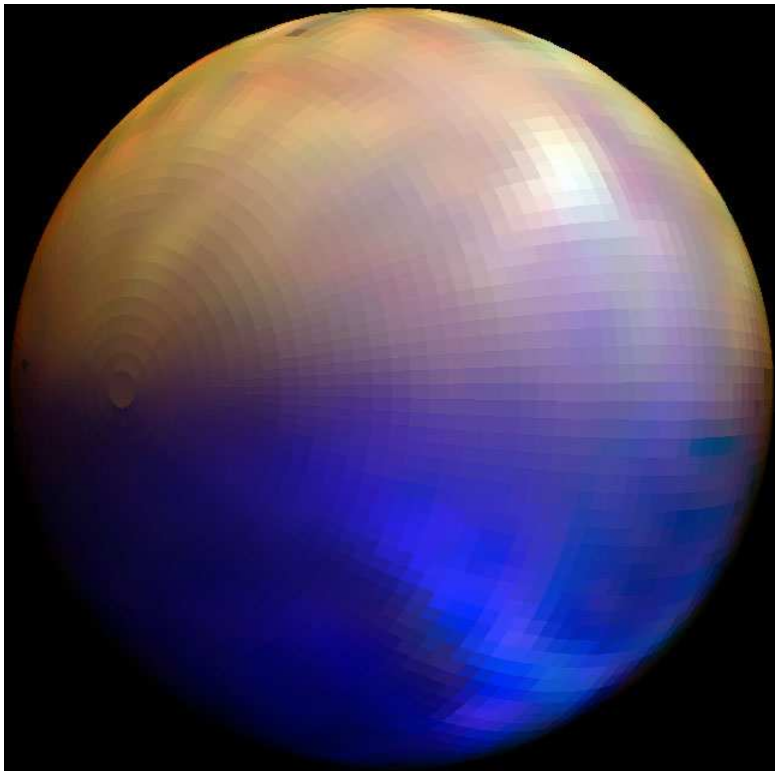
PHOENIX 1D vs 3D: 9000K

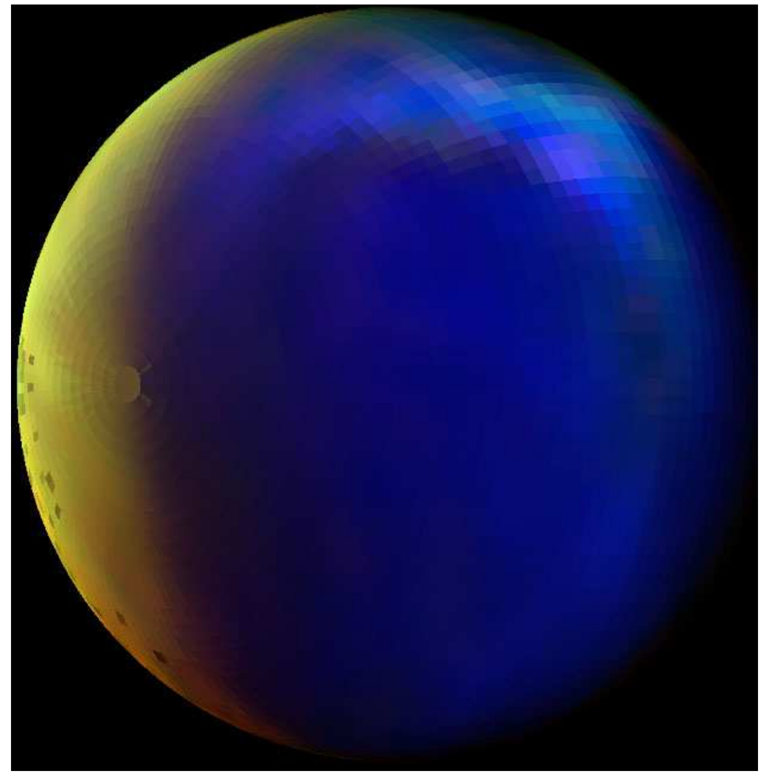


3D visualization: hydro model, line



3D visualization: GCM planet





Conclusions: The Future

- better/more detailed line profiles
- optical properties of dust particles
  $\rightarrow$ materials physics!
- detailed models of dust formation
  $\rightarrow$ composition/sizes/shapes
- non-equilibrium effects $\rightarrow$ NLTE+NLCE
- multi-D RT calculations $\rightarrow$ irradiation