Derivatives and interface to the retrieval

M. Höpfner

Abstract: The simultaneous determination of the atmospheric spectrum and it's derivatives with respect to various atmospheric and instrumental parameters is the basis for the use of KOPRA in retrieval processors. In this part the basic principles implemented for the calculation of derivatives with respect to atmospheric quantities are described. The derivatives with respect to instrumental parameters are summarized.

1 Introduction

Besides the calculation of the atmospheric spectrum convolved with the instrumental line shape and the field-of-view of the interferometer KOPRA is dedicated to the determination of the derivatives of the spectrum with respect to various retrieval parameters (which are just called 'parameters' in the following). The parameters can roughly be subdivided in two parts: the atmospheric ones and the ones describing the instrumental performance. Atmospheric parameters are:

- temperature
- pressure
- volume mixing ratio
- non-LTE/LTE population ratio
- temperature gradient
- volume mixing ratio gradient
- atmospheric continuum

Instrumental parameters are:

- line-of-sight
- offset
- scale
- wavenumber shift
- ils-parameters

This subdivision reflects the internal procedure for the calculation of derivatives: the atmospheric derivatives need to be considered during the ray-tracing and mass calculation, during the absorption-coefficient determination and during the radiative transfer. Instrumental derivatives are determined after the monochromatic spectrum is known: during the ils-convolution and fov-calculation and the offset/scale addition/multiplication. Derivatives with respect to pressure are not supported by KOPRA in a fast way but calculated numerically. In the following we will first describe the principles for the calculation of atmospheric derivatives and then for instrumental ones. At the end the interface to retrieval approaches via various possible parameterizations of the retrieval quantities is presented.

2 Calculation of derivatives wrt atmospheric parameters

2.1 The formulas

In order to explain the implemented method for the calculation of derivatives wrt atmospheric parameters we start with the formula for the radiative transfer:

$$S = B(T_{back}) \prod_{i=1}^{N} \tau_i + \sum_{i=1}^{N} \tilde{J}_i (1 - \tau_i) \prod_{k=i+1}^{N} \tau_k \qquad (1)$$

i is the index for the layers with layer 1 the farthest and layer N the nearest with respect to the observer. $\tilde{J}_i$ is the source function for layer i and τ_i the single layer transmission:

$$\tau_i = exp\left[-\delta_i\right] \tag{2}$$

δ_i is the optical depth for layer i:

$$\delta_i = \delta_{e,Aerosol,i} + \sum_{g=1}^{G} \left[\sigma_{a,ig} + \sum_{b=1}^{B_g} \alpha_{igb} \sigma_{a,igb} \right] u_{ig} \tag{3}$$

$\delta_{e,Aerosol,i}$ is the optical depth of aerosol extinction, $\sigma_{a,ig}$ the absorption coefficient for all LTE bands of gas g, $\sigma_{a,igb}$ the LTE absorption coefficient for NLTE band b of gas g, α_{igb} the ratio of NLTE to LTE absorption coefficient for NLTE band b of gas g, u_{ig} the column density for gas g in layer i, $B_g$the number of NLTE bands for gas g, and G the number of gases.
In the most simple case:

$$\tilde{J}_i = B(T_{Air,i}), \tag{4}$$

i.e. the Planck function for the Curtis-Godson temperature of air for layer i.
For NLTE and more exact calculations:

$$\tilde{J}_i = \frac{\hat{J}_i}{\delta_i} = \frac{B(T_{Air,i})\delta_{a,Aerosol,i} + \sum_{g=1}^{G} \left[B(T_{ig})\sigma_{a,ig} + \sum_{b=1}^{B_g} J_{igb}\alpha_{igb}\sigma_{a,igb} \right] u_{ig}}{\delta_i} \tag{5}$$

$\delta_{a,Aerosol,i}$ is the optical depth of aerosol absorption, $B(T_{ig})$ the Planck function for the Curtis-Godson temperature of gas g for layer i, and J_{igb} the NLTE source function for NLTE band b of gas g and layer i.
The aim is the calculation of the derivatives of the spectrum S with respect to the atmospheric retrieval parameters q_m of some quantity. This can be written as:

$$\frac{dS}{dq_m} = \sum_{i=1}^{N} \left(\frac{dS}{d\tilde{J}_i} \frac{d\tilde{J}_i}{dq_m} + \frac{dS}{d\tau_i} \frac{d\tau_i}{dq_m} \right). \tag{6}$$

Parallel to the radiative transfer calculation the derivative of the radiance with respect to the layer transmission is determined by

$$\begin{aligned} \frac{dS}{d\tau_i}\tau_i &= B(T_{back}) \prod_{k=1}^{N} \tau_k + \sum_{j=1}^{i-1} \tilde{J}_j (1-\tau_j) \prod_{k=j+1}^{N} \tau_k - \tilde{J}_i \prod_{k=i}^{N} \tau_k \\ &= \prod_{k=i}^{N} \tau_k \left[B(T_{back}) \prod_{k=1}^{i-1} \tau_k + \sum_{j=1}^{i-1} \tilde{J}_j (1-\tau_j) \prod_{k=j+1}^{i-1} \tau_k - \tilde{J}_i \right] \\ &= \prod_{k=i}^{N} \tau_k \left[S_{i-1} - \tilde{J}_i \right] \end{aligned} \tag{7}$$

The last term (1st row) is the derivative of the emission of layer i attenuated by all layers between i and the observer and the first two terms (1st row) are the derivative of the attenuation for the radiation of each layer up to layer i. Note that the sum (1st row) is the sum over the contribution functions for layer 1 to layer i-1. The formula in the 3rd row is essential for the implementation in the radiative transfer

code: the derivative of the spectrum wrt transmission of layer i can be calculated successively when the radiance leaving layer i-1 (S_{i-1}) and the source function of the actual layer is known.
The derivative of the spectrum wrt the source function of layer i is just:

$$\frac{dS}{d\tilde{J}_i} = (1-\tau_i) \prod_{k=i+1}^{N} \tau_k \tag{8}$$

At this point we have to distinguish between the various kinds of atmospheric parameters wrt which we want to calculate the derivatives.

2.1.1 Derivatives wrt volume mixing ratio and volume mixing ratio gradient parameters

We neglect the dependence of the source function and the absorption coefficients on volume mixing ratio (through Curtis-Godson temperature and pressure) and need only to determine the derivative of the layer transmission:

$$\begin{aligned} \frac{d\tau_i}{dq_{vmr,mg}} &= -\tau_i \frac{d\delta_i}{dq_{vmr,mg}} = -\tau_i \frac{d\delta_i}{du_{ig}} \frac{du_{ig}}{dq_{vmr,mg}} \\ &= -\tau_i \left[\sigma_{a,ig} + \sum_{b=1}^{B_g} \alpha_{igb} \sigma_{a,igb} \right] \frac{du_{ig}}{dq_{vmr,mg}} \end{aligned} \tag{9}$$

$q_{vmr,mg}$ is the m^{th} (vmr or vmr-gradient) parameter for gas g.
Hence, during the calculation of the path variables the derivatives of the partial columns u_{ig} of gas g for each layer i with respect to the vmr (or vmr gradient) parameters must be determined.

2.1.2 Derivatives wrt aerosol absorption coefficient parameters

a) for cases in which $\tilde{J}_i = B(T_{Air,i})$, the source term is not dependent on aerosol absorption and therefore:

$$\begin{aligned} \frac{d\tau_i}{dq_{Aerosol,m}} &= -\tau_i \frac{d\delta_i}{dq_{Aerosol,m}} \\ &= -\tau_i \frac{d\delta_i}{d\delta_{e,Aerosol,i}} \frac{d\delta_{e,Aerosol,i}}{dq_{Aerosol,m}} = -\tau_i \frac{d\delta_{a,Aerosol,i}}{dq_{Aerosol,m}} \end{aligned} \tag{10}$$

b) for cases in which the source term $\tilde{J}_i$ is dependent on aerosol absorption additionally to a) we have to determine:

$$\frac{d\tilde{J}_i}{dq_{Aerosol,m}} = \frac{\delta_i B(T_{Air,i}) - \hat{J}_i}{\delta_i^2} \frac{d\delta_{a,Aerosol,i}}{dq_{Aerosol,m}} \tag{11}$$

$q_{Aerosol,m}$ is the m^{th} (aerosol absorption) parameter (the microwindow dependence is skipped in this context).
Hence, during the calculation of the path variables the derivatives of the aerosol absorption optical depths $\delta_{a,Aerosol,i}$ for each layer i with respect to the aerosol absorption parameters must be determined.

2.1.3 Derivatives wrt temperature (and temperature gradient) parameters

The derivative of the layer transmission wrt temperature parameters is:

$$\frac{d\tau_i}{dq_{T,m}} = -\tau_i \frac{d\delta_i}{dq_{T,m}} = -\tau_i \frac{d\delta_i}{dT_{Air,i}} \frac{dT_{Air,i}}{dq_{T,m}} \tag{12}$$

with:

$$\begin{aligned} \frac{d\delta_i}{dT_{Air,i}} &= \frac{d}{dT_{Air,i}} \sum_{g=1}^{G} \left[\sigma_{a,ig} + \sum_{b=1}^{B_g} \alpha_{igb}\sigma_{a,igb} \right] u_{ig} \\ &= \sum_{g=1}^{G} \left[\frac{d\sigma_{a,ig}}{dT_{ig}} + \sum_{b=1}^{B_g} \left(\frac{d\alpha_{igb}}{dT_{ig}}\sigma_{a,igb} + \frac{d\sigma_{a,igb}}{dT_{ig}}\alpha_{igb} \right) \right] u_{ig} \\ &+ \sum_{g=1}^{G} \left[\sigma_{a,ig} + \sum_{b=1}^{B_g} \alpha_{igb}\sigma_{a,igb} \right] \frac{du_{ig}}{dT_{ig}} \end{aligned} \tag{13}$$

$q_{T,m}$ is the m$^{\text{th}}$ temperature (or temperature gradient) parameter.
During the calculation of the path variables the derivatives of the Curtis-Godson temperatures for air wrt the temperature parameters must be determined.
The derivatives of the absorption coefficients wrt temperature is calculated in parallel to the absorption coefficients themselves. The absorption coefficients are the product of line-intensity and line-profile:

$$\sigma_{a,ig} = \sum_{n=1}^{N_g} A_{ign}\Phi_{ign} \tag{14}$$

A_{ign} is the line intensity for line n, gas g, N_g the number of lines for gas g, and layer i and Φ_{ign} the line profile. Since the most important temperature dependence in this formula stems from the line intensity we calculate only that derivative (also because the derivative calculation of the line profile function wrt T would be too time consuming). Therefore,

$$\frac{d\sigma_{a,ig}}{dT_{ig}} = \sum_{n=1}^{N_g} \frac{dA_{ign}}{dT_{ig}}\Phi_{ign} \tag{15}$$

Two cases have to be distinguished for determination of the source function derivatives wrt temperature:
a) for cases in which $\tilde{J}_i = B\left(T_{Air,i}\right)$:

$$\frac{d\tilde{J}_i}{dq_{T,m}} = \frac{dB\left(T_{Air,i}\right)}{dT_{Air,i}} \frac{dT_{Air,i}}{dq_{T,m}} \tag{16}$$

b) for cases in which the source term $\tilde{J}_i$ is calculated for NLTE:

$$\frac{d\tilde{J}_i}{dq_{T,m}} = \frac{\delta_i \frac{d\hat{J}_i}{dT_{Air,i}} + \hat{J}_i \frac{d\delta_i}{dT_{Air,i}}}{\delta_i^2} \frac{dT_{Air,i}}{dq_{T,m}} \tag{17}$$

with:

$$\begin{aligned}\frac{d\hat{J}_i}{dT_{Air,i}} &= \frac{d}{dT_{Air,i}} B\left(T_{Air,i}\right)\delta_{a,Aerosol,i} + \sum_{g=1}^{G}\left[B\left(T_{ig}\right)\sigma_{a,ig} + \sum_{b=1}^{B_g} J_{igb}\alpha_{igb}\sigma_{a,igb}\right] u_{ig} \\ &= \frac{dB\left(T_{Air,i}\right)}{dT_{Air,i}}\delta_{a,Aerosol,i} + \sum_{g=1}^{G}\left[B\left(T_{ig}\right)\sigma_{a,ig} + \sum_{b=1}^{B_g} J_{igb}\alpha_{igb}\sigma_{a,igb}\right]\frac{du_{ig}}{dT_{ig}} \quad (18) \\ &+ \sum_{g=1}^{G}\left[\begin{array}{l}\frac{dB(T_{ig})}{dT_{ig}}\sigma_{a,ig} + B\left(T_{ig}\right)\frac{d\sigma_{a,ig}}{dT_{ig}} + \\ \sum_{b=1}^{B_g}\frac{dJ_{igb}}{dT_{ig}}\alpha_{igb}\sigma_{a,igb} + J_{igb}\left(\frac{d\alpha_{igb}}{dT_{ig}}\sigma_{a,igb} + \frac{\sigma_{a,igb}}{dT_{ig}}\alpha_{igb}\right)\end{array}\right] u_{ig}\end{aligned}$$

2.1.4 Derivatives wrt pressure parameters

The derivative of the spectrum with respect to pressure parameters is:

$$\frac{dS}{dq_{p,m}} = \sum_i\left[\frac{dS}{dp_{Air,i}}\frac{dp_{Air,i}}{dq_{p,m}} + \sum_g \frac{dS}{du_{ig}}\frac{du_{ig}}{dq_{p,m}}\right]. \quad (19)$$

The first term of this equation reads:

$$\frac{dS}{dp_{Air,i}} = -\tau_i\frac{dS}{d\tau_i}\frac{d\delta_i}{dp_{Air,i}} \quad (20)$$

with:

$$\frac{d\delta_i}{dp_{Air,i}} \approx \sum_{g=1}^{G}\left[\frac{d\sigma_{a,ig}}{dp_{ig}} + \sum_b \alpha igb\frac{d\sigma_{a,ig}}{dp_{ig}}\right] u_{ig} \quad (21)$$

The derivatives of the cross-sections $\sigma_{a,ig}$ with respect to pressure are determined during the calculation of the cross-sections. This is done numerically by recalculating the cross-sections for each path with slightly changed pressures.
The second term in 19, i.e. the dependence of partial columns on pressure parameters is determined during the calculation of integrated path values during raytracing. Mind that the partial columns do not depend linearly on the pressure due to refraction, especially at low tangent altitudes.

2.1.5 Derivatives wrt non-LTE/LTE population ratio parameters

For the determination of derivatives wrt non-LTE/LTE population ratios r we must calculate $\frac{d\tilde{J}_i}{dq_{r,m}}$ and $\frac{d\tau_i}{dq_{r,m}}$:

$$\frac{d\tau_i}{dq_{r,m}} = -\tau_i\frac{d\delta_i}{dr_{ign}}\frac{dr_{ign}}{dq_{r,m}} \quad (22)$$

with the derivative of the optical depth wrt non-LTE/LTE population ratio of a distinct state n of gas g:

$$\frac{d\delta_i}{dr_{ign}} = u_{ig}\sum_{b=1}^{B_g}\frac{d\alpha_{igb}}{dr_{ign}}\sigma_{a,igb} \quad (23)$$

The source function derivative wrt vibrational temperature is:

$$\frac{d\tilde{J}_i}{dq_{r,m}} = \frac{\delta_i \frac{d\hat{J}_i}{dT_{Vib,i}} + \hat{J}_i \frac{d\delta_i}{dr_{ign}}}{\delta_i^2} \frac{dr_{ign}}{dq_{r,m}} \tag{24}$$

with:

$$\frac{d\hat{J}_i}{dr_{ign}} = u_{ig} \sum_{b=1}^{B_g} \left(\frac{dJ_{igb}}{dr_{ign}} \alpha_{igb} + J_{igb} \frac{d\alpha_{igb}}{dr_{ign}} \right) \sigma_{a,igb} \tag{25}$$

2.2 The implementation in the radiative transfer module

In this section it is described how the formulas above are implemented in the module radtra_m. We use the variable names of the code and whenever possible a reference to the variable names in section 2.1 is made. The basic steps are:
a) go from the layer far from the observer to the layer near the observer and calculate the radiative transfer and some derivative auxiliary variables.
b) go back layer for layer from the observer to the end of the atmosphere and multiply the auxiliary variables by the transmission between the actual layer and the observer in order to get the radiance derivatives wrt each layer
c) add together the derivatives wrt each layer weighted by the influence of the retrieval parameter in each layer (post-derivation)

And now in detail:
a)
Begin with layer far from observer
For actual layer i calculate: tau = τ_i, src = $\tilde{J}_i$, opt = δ_i , srcn = $\hat{J}_i$, dopt_dcol = dopt_dcol = $\frac{d\delta_i}{du_{ig}}$, dsrc_daerabsopt = $\frac{d\tilde{J}_i}{d\delta_{a,Aerosol,i}}$, dsrc_dTvib = $\frac{d\tilde{J}_i}{dT_{Vib,i}}$, dopt_dTvib = $\frac{d\delta_i}{dT_{Vib,i}}$.
The derivatives wrt kinetic temperature are stored in the 'imaginary' parts of the variable src and opt: derivT(src) = $\frac{d\tilde{J}_i}{dT_{Air,i}}$, derivT(opt) = $\frac{d\delta_i}{dT_{Air,i}}$.
Store tau in variable tausave$_i$ for each layer
Calculate: derirad = tau*(rad-src) = $\tau_i \left[S_{i-1} - \tilde{J}_i \right]$ (see 7)
Calculate actual radiance at end of layer i: rad = derirad + src = $\tau_i \left[S_{i-1} - \tilde{J}_i \right] + \tilde{J}_i$
Calculate derivative auxiliary variables:
derivmr$_i$ = derirad * dopt_dcol
deriaer$_i$ = (1-tau) * dsrc_daerabsopt-derirad
deripla$_i$ = (1-tau) * derivT(src) - derirad * derivT(opt)
derisrc$_i$ = (1-tau) * dsrc_dTvib - derirad * dopt_dTvib

b)
go back layer for layer from the observer to the end of the atmosphere and multiply the auxiliary variables by the transmission between the actual layer and the observer in order to get the radiance derivatives wrt each layer.

Go back from i=N to i=1:
tautot = tausavei * tautot
derivmr$_{i+1}$ = derivmr$_{i+1}$ * tautot
deriaer$_{i+1}$ = deriaer$_{i+1}$ * tautot
deripla$_{i+1}$ = deripla$_{i+1}$ * tautot

$\text{derisrc}_{i+1} = \text{derisrc}_{i+1}$ * tautot

c)
add together the derivatives wrt each layer weighted by the influence of the retrieval parameter in each layer (post-derivation).

This is performed in subroutines:

derivmr: derivmr_calc@radtra_m, derivmrgrad_calc@radtra_m
deriaer: deriaer_calc@radtra_m
deripla: deriT_calc@radtra_m, deriTgrad_calc@radtra_m
derisrc: deriTvib_calc@radtra_m

2.3 Derivatives of path values wrt parameters during ray-tracing

To be able to perform the 'post-derivation', i.e. the step from the derivatives of the spectrum wrt the integrated path variables (partial columns, Curtis-Godson means) to the derivatives wrt the retrieval parameters the following quantities have to be known:

$\frac{du_{ig}}{dq_{vmr,mg}}$ derivative of partial column amount of gas g and layer i with respect to the m^{th} vmr parameter of gas g
Variable: geo()%par()%lay()%speci()%dcol()

$\frac{du_{ig}}{dq_{vmrgradient,mg}}$ derivative of partial column amount of gas g and layer i with respect to the m^{th} vmr-gradient parameter of gas g
Variable: geo()%par()%lay()%speci()%dcolgrad()

$\frac{d\delta_{a,Aerosol,i}}{dq_{Aerosol,m}}$ derivative of aerosol absorption optical depth of layer i with respect to the m^{th} aerosol absorption coefficient parameter
Variable: geo()%par()%lay()%dabsopt()

$\frac{dT_{Air,i}}{dq_{T,m}}$ derivative of Curtis-Godson-temperature of air for layer i with respect to the m^{th} T-parameter
Variable: geo()%par()%lay()%dT()

$\frac{dT_{Air,i}}{dq_{Tgradient,m}}$ derivative of Curtis-Godson-temperature of air for layer i with respect to the m^{th} T-gradient-parameter
Variable: geo()%par()%lay()%dTgrad()

$\frac{dr_{ign}}{dq_{r,m}}$ derivative of non-LTE/LTE population ratio for layer i with respect to the m^{th} non-LTE/LTE population ratio parameter
Variable: geo()%par()%lay()%speci()%iso()%state()
%dTvib_cg_dT()

$\frac{dp_{Air,i}}{dq_{p,m}}$ derivative of Curtis-Godson-pressure of air for layer i with respect to the m^{th} pressure-parameter
Variable: geo()%par()%lay()%dp()

$\frac{du_{i,g}}{dq_{p,m}}$ derivative of partial column amount of gas g and layer i with respect to the m^{th} pressure-parameter
Variable: geo()%par()%lay()%dcol()

Nearly all of these quantities are computed in integrate@ray_m where also the partial column amounts and Curtis-Godson values themselves are determined for each layer.

The procedure is simply numerical:

- change the parameter q using some increment
- recalculate the partial column, Curtis-Godson value, ...
- calculate the numeric derivative using the previously determined partial column, Curtis-Godson value for the undisturbed case

Especially in limb-observations for the derivatives of the layer pressure and column amounts with respect to the pressure parameter it is not possible to do the same procedure as just described layer by layer. Because of the dependence of refraction on pressure it is rather necessary to recalculate the whole limb path with a slightly changed pressure parameter (this has to be done for each parameter). The derivatives are then determined numerically.

3 Calculation of derivatives wrt instrumental parameters

(This is also described in more detail in Part XII: 'FOV and AILS')

- line-of-sight
  Derivatives wrt the nadir angle are determined numerically in the subroutines fovils1@ilsfov_m and envfovils@ilsfov_m: additionally to the field-of-view weighted spectrum around the nominal nadir angle another one is calculated around the nominal nadir angle plus an increment. From these two the fov derivative spectrum is determined.

- offset
  The offset derivative (which is obviously =1) is set in off_deri@offsca_m.

- scale
  The scale derivative (which is obviously equal to the spectrum itself) is set in sca_deri@offsca_m.

- wavenumber shift
  The derivative of the spectrum wrt wavenumber shift is calculated numerically in derive@ilsfov_m: the derivative in the fine-grid spectrum S is:

$$\frac{dS_k}{d\nu} = \frac{S_{k+1} - S_{k-1}}{2\Delta\nu_f}$$

  $\Delta\nu_f$ is the wavenumber fine grid distance. After that the wavenumber shift derivative on the fine grid is convolved with the ails-function.

- ils-parameters
  In the case of circular aperture the ils parameters wrt which the derivatives are determined are linear apodization and phase. These derivatives are calculated numerically in the routines ilsapo@ilsfov_m and fovils1@ilsfov_m. For this purpose the ils is recomputed with slightly modified linear apodization or phase parameters to get the derivative of the ils wrt these parameters. This ils-derivative is then convolved with the fine-grid spectrum. The same procedure is implemented for the ils parameters defined by ESA.

4 Principles of derivative and retrieval parameter handling

One main feature of KOPRA is the flexible handling of abstract retrieval parameters in order to support different retrieval strategies. Therefore, in the core of KOPRA input profile data are strictly separated from parameters used for the description of atmospheric profiles.
Derivatives are only computed with respect to parameters. I.e. if derivatives of the spectrum wrt some atmospheric quantity (e.g. the temperature) should be calculated, the profile of this quantity must be parameterized (e.g. determination of temperature parameters). On the other hand, a profile can be parameterized without derivatives being calculated (i.e. the parameters are only used for the forward calculation of the spectrum). This procedure implies that at some point in the program a transformation from the atmospheric profile to the parameter space and somewhere else a back-transformation from the parameters to the value of the atmospheric quantity is made.
The transformation into the parameter space (i.e. the initialization of the parameter vectors) is done outside the core of the forward model (in the module `inipar_m`) following the reading of input files. Here, the input profiles are transformed into parameters using some formula which has to be explicitly implemented in `inipar_m`. The parameter values are stored in the variable `para%` while the input profiles have already been read into `inprof%`.
The back-transformation is calculated during the ray-tracing and path integration (module `ray_m`) where the explicit value of the quantity at some point in the atmosphere is needed. This task is done by the `give`-functions of module `give_m`. These routines return the value of any atmospheric quantity at any position in the atmosphere. Hence, they not only perform the back-transformation from the parameters but also the interpolation of the input profiles and the distinction between parameters (using variable `para%`) and input profiles (using variable `inprof%`). Obviously, changing the transformation formulas in `inipar_m` requires also a modification of the back-transformation in `give_m` and vice versa.

5 Retrieval interface

5.1 Input from the retrieval-code

- *Which derivative should be calculated?* In $ 10 of the main KOPRA input file it has to be defined which derivatives of the spectrum should be calculated by KOPRA.

- *Atmospheric retrieval parameters:* as explained above, the atmospheric profile parameters with respect to which derivatives are determined are handled differently from the rest of the profiles. The retrieval profile parameters are stored in the variable `para%`[1] and are initialized in module `inipar_m`. In the basic version of KOPRA the profile parameters are set identical to the values at the levels given in the main KOPRA input file under $11.5 and the interpolation rule is linear in altitude and only for pressure linear in ln(altitude). For different parameterizations the user has to adjust the module `inipar_m` for initialization and the module `give_m` for the transformation from the parameter space into profile-altitude, -latitude, -longitude space (the interpolation rules).

[1] For details about the variables see Part XIX: 'Module, subroutine and variable listing and description'

The interface to the retrieval is performed through the variable `para%` by use of the module `inpdat_m`.

- *Instrumental retrieval parameters:* for initialization of the instrumental retrieval parameters the values given in the main KOPRA input file are used and for these parameters the derivatives are determined. I.e. no re-parameterization like for the atmospheric retrieval parameters is made. The interface to the retrieval is performed through variable `inst%` by use of the module `inpdat_m`.
- *Information on necessary allocations and recalculations:* for some variables during each iteration the retrieval code has to tell the forward model which ones have to be allocated and which ones should be recalculated. The recalculation concerns the leveling of the atmosphere, the determination of additional geometries for the simulation of the field-of-view, and the calculation of absorption coefficients. The relating control parameters are `sw%new_modelgeo`, `sw%new_modelgrid`, `sw%new_absco`.

5.2 Output to the retrieval-code

- *Spectra and derivatives:* all spectra and their derivatives with respect to the retrieval parameters are available through variable `outdat%` by use of module `outdat_m`.

5.3 Example for use of KOPRA in a retrieval environment

The call of KOPRA inside a retrieval program and the setting of the variables for allocation and recalculation is given in the example below.

```
! read main KOPRA input-file
  call input('input/kopra.inp')

! read retrieval input-file (belongs to the retrieval code)
  call input_invers('input/koprainv.inp')

! initialize the atmospheric retrieval parameters (module inipar_m)
  call ini_para

! for KOPRA run in the first iteration
  sw%firstrun=.true.

! variables geo%, sim%, modprof%, Sails%, deri%, mw% are not allocated
  sw%alloc_geo = 0
  sw%alloc_sim = 0
  sw%alloc_modprof = 0
  sw%alloc_Sails = 0
  sw%alloc_outdat = 0
  sw%alloc_deri = 0
  sw%alloc_mw = 0

! additional geometries for fov will be added
  sw%new_modelgeo = .true.

! the atmospheric layering will be done
```

```
  sw%new_modelgrid = .true.

! the absorption coefficients will be calculated
  sw%new_absco = .true.

! call KOPRA - first iteration
  call kopra_forwrd

! call the inversion algorithm - first iteration
  call kopra_invers

! for KOPRA run in the next iterations
  sw%firstrun=.false.

! loop on maxiter iterations
  do i = 2, maxiter

   ! additional geometries for fov will not be determined new
     sw%new_modelgeo = .false.

   ! the atmospheric layering will not be done new
     sw%new_modelgrid = .false.

   ! the absorption coefficients will be calculated new for each iteration
     sw%new_absco = .true.

   ! deallocation of various variables if necessary
     if ( sw%alloc_geo/=0 .and.&
          (sw%firstrun.or.sw%new_absco)  ) then
        call deallocate_geo(0)
        sw%alloc_geo = 0
     end if
     if ( sw%alloc_Sails /= 0 ) then
        call deallocate_Sails(0)
        sw%alloc_Sails = 0
     end if
     if (sw%alloc_deri/=0 .and. sw%firstrun ) then
        call deallocate_deri(0)
        sw%alloc_deri = 0
     end if
     if (sw%alloc_mw/=0 .and. sw%firstrun ) then
        call deallocate_mw(0)
        sw%alloc_mw = 0
     end if

   ! call KOPRA - next iterations
     call kopra_forwrd

   ! call the inversion algorithm - next iterations
     call kopra_invers
  end do
```