

SEI: An efficient and accurate method for calculating line profiles from spherically expanding winds

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Abstract

The SEI method for calculating line profiles in spherically symmetric expanding envelopes is introduced. Instructions are provided for the operation of the SEI codes maintained in the CCP7 program library, including a description of the required input data, performance statistics and an example calculation.

1 Method

S.E.I.= **S**obolev source function with **E**xact **I**ntegration of the transfer equation.

The SEI method has been described by Lamers, Cerrutti-Sola and Perinotto (1987). It is a method for calculating the profiles of lines formed in spherically symmetric expanding envelopes. The sourcefunction is solved in the Sobolev-approximation, and the transfer-equation is integrated exactly. This program can be used for the fitting of observed lineprofiles; *e.g.* P Cygni profiles, broad emission lines, absorption lines with extended violet absorption wings, etc. Examples of the different kind of profiles which can be obtained by this method are given in the original paper (Lamers et al, 1987). The SEI method is almost as accurate as the Comoving Frame method. The profiles can differ drastically from those calculated with the Sobolev method.

The program requires the input of the velocity law of the envelope $v(x)$, the turbulent velocity (Gaussian) in the envelope v_{turb} , the optical depth of the line as a function of velocity $\tau(v)$, the collisional term (if any) in the sourcefunction, and the underlying photospheric spectrum (contin. or abs. lines). If the predicted lines are compared with the observed profiles, these physical parameters can be derived from the linefitting. **N.B.** This program does not solve the statistical equilibrium equations in the wind. That is why the optical-depth law has to be specified.

Examples of applications of the SEI method to the study of the winds of O stars and of Planetary Nebulae can be found in Groenewegen and Lamers (1989a,b) and Perinotto et al. (1989).

There are two types of SEI programs: SEISING for the calculation of singlet lines and SEIDOU B for the calculation of doublet lines with radiative interaction. Both programs are in FORTRAN IV and run on a VAX or on an IBM-compatible PC. The following sections describe their use and their implementation in the CCP7 library.

2 Program SEIDOU B3

The first part of the program collects the input data, sets up a prespecified distance grid (**XS**) and a pre-specified grid of impact parameters for the lines of sight (**PX**) for which the transfer equation will be solved. It also calculates the turbulent profile and its integral (the error function) at prespecified wavelength points (**DELW**), expressed in terms of the normalized velocity $w = v/v_{\infty}$.

The second part of the program calculates the source function of the blue and the red components in the prespecified distance grid **XS**. The source function of the blue component (**SOUB**) is directly calculated from the escape probabilities. The source function of the red components (**SOUBR**) involves the contribution

from the blue component at radiatively coupled points, and involves an integration over angle (**XMR**). This integration is done by means of a fourth order Gaussian quadrature method over certain μ -intervals. This part of the program takes only about 10 seconds in most cases.

The third part of the program solves the transfer equation for each chosen wavelength point (**WPROF(JF)**) of the profile and each line of sight (**PX(JP)**). The integration is done by calculating the integrand at the prespecified wavelength steps (**DELW(IG)**). The program automatically takes care of the overlap of the contributions of the two components, which are separated by a normalized velocity (**SEP**). This results in a grid of intensities for each line of sight.

The fourth part of the program calculates the flux by integration of the intensities over the different lines of sight. The result is a table of wavelengths (**WPROF**), **PHOT** is the photospheric flux at that wavelength, **FUNCA** is the flux from the area of the wind in front of the star (always less than 1 for scattering lines), **FUNCB** is the flux from the region surrounding the stellar disc. The sum of **FUNCA** and **FUNCB** is the total flux at that wavelength.

3 Input to SEIDOU3 for the calculation of doublet lines

3.1 Physical Parameters

The requested input is explained below. All wavelengths and velocities are expressed in terms of the normalized velocity $w(x)$ with $x = r/R_*$, such that $w_\infty = 1$. These parameters are also described in the initial SEI paper (Lamers et al. 1987).

Velocity-law:

$$w(x) = w_0 + (1 - w_0)(1 - 1/x)^\gamma \equiv v(x)/v_\infty$$

$$w_0 = w(x = 1)$$

Optical depth law:

$$\tau(w) = T_{\text{tot}}(w_0/w_1)^{\alpha_1}(1 - (w_0/w_1)^{1/\gamma})^{\alpha_2}; \text{ for } w_0 \leq w < w_1$$

$$\tau(w) = 0; \text{ for } w_1 \leq w \leq 1$$

$$T_{\text{tot}} = \int_{w_0}^{w_1} \tau(w)$$

The choice of the parameterization of $\tau(w)$ is justified in Lamers et al. 1987. T_{tot} is related to the column density of the absorbing ions: $T = (\pi e^2/mc)f\lambda_0 N_i/v_\infty$.

Source function:

$$S_\nu(x) = \frac{\beta_c(x)I_\nu^* + \epsilon B_\nu(x)}{\beta + \epsilon}$$

β is the escape probability for line photons and β_c is the penetration probability for continuum photons. $\epsilon = C_{ul}/A_{ul}$, the ratio of collisional to radiative deexcitations, is proportional to the density and is given by:

$$\epsilon = \epsilon_0 \frac{w_0}{x^2 w(x)}$$

Planck function: a distance dependence may be introduced into the Planck function in the wind in order to simulate coronae or cold winds. This only plays a role if the collisional terms are important, *i.e.* $\epsilon > 0$ (*e.g.* WR-stars or Balmer-lines).

$$B_\nu/I_c = (B_\nu/I_c)_0 \exp(-a_T(w - w_0))$$

So T increases outwards if $a_T < 0$
decreases $a_T > 0$
constant $a_T = 0$

3.2 Variable namelist

- WO, GAMMA** : The initial velocity (w_0) and the velocity exponent (γ). These two specify the adopted velocity-law which is a ‘ β -type’ law. In this program the traditional ‘ β ’ is called ‘ γ ’ to avoid confusion with the escape probability.
- TTOTB, TTOTR** : The integrated radial optical depths (T_{tot}) of the blue and red components. In most doublets **TTOTB=2*TTOTR**.
- ALFA1, ALFA2** : Exponents describing the run of opacity (or ion density) with velocity (α_1, α_2).
- SEP** : Separation of the rest-wavelength of the two components in terms of v_∞ , **SEP** = $(\Delta\lambda/\lambda)(c/v_\infty)$.
- W1** : Extent of the optical depth $\tau(w)$. $\tau(w) = 0$ for $w > w_1$. In most cases $w_1 = 1$ for resonance lines.
- EPSOB, EPSOR** : The parameter describing the collisional term of the sourcefunctions (ϵ_0). $\epsilon_0 = 0$ for resonance lines in O stars, and positive for Wolf-Rayet stars with emission lines or for Balmer-lines in extended atmospheres.
- BICO, AT** : The Planck function in the wind, normalized to the continuum intensity (B_ν/I_c), is specified by its value $(B_\nu/I_c)_0$ at $x = 1$, and by the parameter a_T which describes the variation of temperature in the wind. This is only important if ϵ_0 is non-zero.
- WGAUS** : The “turbulent velocity” w_T in the wind, where $w_T = v_{\text{turb}}/v_\infty$.
- IGMAX** : Number of wavelength-points through the turbulent profile used for the integration of the transfer-equation. Usually 11 is good for an initial calculation and 15 is good for the final profile, unless **WGAUS** is larger than 0.3 or so. **IGMAX** must be an odd number!
- APHOTB, APHOTR** : The optical depth in the center of the photospheric profiles of the blue and red components. Set to 0 if there is no photospheric line.
- WPHOTB, WPHOTR** : The photospheric profile is assumed to be the absorption due to a Gaussian profile. **WPHOT** is the Gaussian width.
- PRSTART, PREND, PRSTEP** : These specify the wavelengths at which the flux will be calculated, expressed in units of v_∞ measured from the rest wavelength of the blue component. **PRSTART** and **PREND** are shortest and longest wavelengths, **PRSTEP** is the step-size. For instance **PRSTART=-1.3, PREND=+2.5, PRSTEP=0.2** results in 20 wavelengths (-1.3, -1.1, ... +2.3, +2.5).

3.3 Constants for numerical accuracy

These constants are set in the program, but can be changed if necessary. The user is advised to test the accuracy and its dependence on these parameters.

- XMAX** : Maximum distance from the star for solving transfer equation:
XMAX=1000.
- NXS** : Number of depth steps for the calculation of the source-functions. The resulting depth steps (**XS**) are spaced logarithmically:
NXS=30 or **50**.
- NPIN** : The number of lines of sight in front of the disc is **4*NPIN**:
NPIN=2.
- NPOUT** : The number of lines of sight next to the stellar disc is **4*NPOUT**:
NPOUT=6 or **8** is okay.

4 Input to SEISING3 for the calculation of single lines

The program SEISING3 can be used for the calculation of single lines. It is faster than SEIDOU3 and requires less input data. The input parameters are **WO, GAMMA, TTOT, ALFA1, ALFA2, W1, EPSO, BICO, AT, WGAUS, IGMAX, APHOT, WPHOT, PRSTART, PREND, PRSTEP**. Of course SEIDOU3 may be used for calculating profiles for singlet lines simply by setting the optical depths of the red component to zero, *i.e.* **TTOTR=0, APHOTR=0**.

5 Example

Examples of input and output data are provided for both programs in order to verify their implementation. The same dataset is used in each case, except that the red component is excluded from the SEISING3 calculation.

5.1 Input parameters

Parameter	SEIDOU3	SEISING3
W0	0.01	0.01
GAMMA	1.	1.
TTOTB	2.	2.
TTOTR	1.	
SEP	0.5	
ALFA1	1.	1.
ALFA2	1.	1.
W1	1.	1.
EPSOB	0.	0.
EPSOR	0.	
BICO	1.	1.
AT	0.	0.
WGAUS	0.1	0.1
IGMAX	15	15
APHOTB	2.	2.
WPHOTB	0.3	0.3
APHOTR	1.	
WPHOTR	0.3	
PRSTART	-1.8	-1.8
PREND	+1.8	+1.8
PRSTEP	0.1	0.1

Figure 1: Photospheric (broken line) and nett (solid line) line profiles calculated for a star with a spherically symmetric expanding envelope using the SEI method. Cases are shown for singlet (SEISING3) and doublet (SEIDOU3) lines calculated using the input data given in §4.1.

5.2 Output

The output of the program is written into a file named SEIDOUT3.DAT for SEIDOU3 (or SEISOUT3.DAT for SEISING3). Part of the output will appear on the screen during execution.

5.3 CPU-time

The source function at 50 gridpoints takes about 5 seconds on a microVAX 3500. The time for the solution of the transfer equation is approximately

$$T(\text{sec CPU}) = 0.013 * [\text{IGMAX} * \text{NPROF} * (\text{NPIN} + \text{NPOUT})]$$

So a typical doublet profile of $\text{NPROF}=37$ (37 wavelength-points), $\text{IGMAX}=15$ and $\text{NPIN}=2$ and $\text{NPOUT}=6$ will take about 32 seconds. A singlet profile (using SEISING3) takes about 20 seconds.

6 CCP7 implementation

The FORTRAN source for programs SEISING3 and SEIDOUNB3 is stored online, along with example input and output data, further documentation and other utility programs in the CCP7 program library. Details of access to the library have been given in this Newsletter (Jefferly, 1990). The SEI programs may be found in subdirectory

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UK.AC.ST-AND.STAR::CCP7DISK:[CCP7.SEI]
```

and its subdirectories. A VMS BACKUP saveset containing the programs and associated material may be found in

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UK.AC.ST-AND.STAR::CCP7DISK:[CCP7.SAVESETS]SEI.BCK
```

and may be obtained by file transfer over JANET. The distributed version of SEISING3 differs slightly from that received from Henny Lamers in that much of the input and output has been modified for consistency with SEIDOUNB3. The calculated line profiles have not been altered.

6.1 SEITODIPSO

For users obtaining the SEI programs from the CCP7 library and familiar with the STARLINK program DIPSO (Howarth & Murray 1991), a utility program called SEITODIPSO is available to convert the output (either from file SEIDOUT3.DAT or from SEISOUT3.DAT) into a format suitable for input to DIPSO.

The program requires a few inputs: the user must select whether an SEIDOUNB3 or SEISING3 calculation is to be formatted, and must decide whether to preserve the normalized wavelength units, or to transform the profile wavelengths to Angstroms. In the latter case, action depends on the type of calculation. For a doublet, the user must supply the wavelengths (\AA) of both components of the doublet. v_∞ is recovered automatically from the parameter **SEP** ($= (\Delta\lambda/\lambda)(c/v_\infty)$) used in the SEIDOUNB3 calculation. For a singlet, the user must supply both the wavelength (\AA) of the line and the required v_∞ (km/s).

The photospheric and envelope profiles are written to files SEIPHOT.SP0 and SEIWIND.SP0 respectively, with data used in their computation transferred to their two line headers. These may be read into DIPSO with the command **SPORD**. Fig. 1 was prepared solely using SEISING3, SEIDOUNB3, SEITODIPSO and DIPSO.

References

- Groenewegen, M.A.T. & Lamers, H.J.G.L.M., 1989. *Astron. Astrophys. Suppl.* **79**, 359.
'The winds of O-stars. I: an analysis of the UV line profiles with the SEI method'
- Groenewegen, M.A.T., Lamers, H.J.G.L.M. & Pauldrach, A.W.A., 1989. *Astron. Astrophys.* **221**, 78.
'The winds of O-stars. II: the terminal velocities of stellar winds of O-type stars'
- Howarth, I.D. & Murray, J., 1991. *Starlink User Note* 50.13
'DIPSO: A friendly spectrum analysis program'
- Jeffery, C.S., 1990. *CCP7 Newsletter* No. 14, p.43.
'CCP7GUEST — Accessing the CCP7 library: A User Guide'
- Lamers, H.J.G.L.M., Cerrutti-Sola, M. & Perinotto, M., 1987. *Astrophys. J.* **314**, 726.
'The "SEI" method for accurate and efficient calculations of the profiles in spherically symmetric stellar winds'
- Perinotto, M., Cerutti-Sola, M. & Lamers, H.J.G.L.M., 1989. *Astrophys. J.* **337**, 382.
'Winds from Central Stars of Planetary Nebulae'

Problems?

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