# 4D Grid-fitting of UV-optical Spectra of Massive Stars. I. Numerical Technique and its Associated Uncertainties Postprint

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**Date:** 2025-09-28T12:14:27+00:00

## Abstract

The best way to check the validity of our theories (models) is by direct comparison with the experiment (observations). However, this process suffers from numerical inaccuracies, which are not frequently studied and often remain mostly unknown. In this study, we focus on addressing the numerical inaccuracies intrinsic to the process of comparing theory and observations. To achieve this goal, we built four-dimensional (4D) spectral grids for Wolf-Rayet stars (WC and WN spectral classes) and blue supergiants characterized by low metallicity similar to that of the Small Magellanic Cloud. In contrast to lighter (three-dimensional) grids, which rely on a priori assumptions about certain stellar parameters (e.g., wind velocity) and thus have limited applicability, our 4D grids vary four independent parameters, enabling more flexible and broadly applicable spectral fitting. Utilizing these 4D grids, we developed and validated a fitting approach facilitating direct fits to observed spectra. Through rigorous testing on designated "test" models, we demonstrated that the numerical precision of derived essential stellar parameters, including effective temperature, mass-loss rate, luminosity, and wind velocity, is better than 0.05 dex. Furthermore, we explored the influence of unaccounted factors, including variations in the metal abundances, wind acceleration laws, and clumping, on the precision of the derived parameters. The results indicate that the first two factors have the strongest influence on the numerical accuracy of the derived stellar parameters. Variations in abundances predominantly influenced the mass-loss rate for weak-wind scenarios, while effective temperature and luminosity remained robust. We found that the wind acceleration law influences the numerical uncertainty of the derived wind parameters mostly for models with weak winds. Interestingly, different degrees of clumping demonstrated good precision for spectra with strong winds, contrasting with a decrease in the precision for weak-wind cases. We found also that the accuracy of our approach depends on spectral range and the inclusion of ultraviolet spectral range improves the precision of derived parameters, especially for an object with weak winds.

## Full Text

## Preamble

Research in Astronomy and Astrophysics, 25:075012 (21pp), 2025 July https://doi.org/10.1088/1674-4527/addbc6 CSTR: 32081.14.RAA.addbc6

### 4D Grid-fitting of UV-optical Spectra of Massive Stars. I. Numerical Technique and its Associated Uncertainties

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Received 2025 March 3; revised 2025 April 28; accepted 2025 May 19; published 2025 June 16

## Abstract

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**Key words:** stars: Wolf-Rayet -stars: winds, outflows -methods: numerical -stars: massive

## 1. Introduction

The extreme temperatures and luminosities of massive stars provide a large amount of ionizing photons, leading to extreme non-local thermal equilibrium (non-LTE) conditions in their expanding atmospheres. Additionally, the mass-loss rate and velocity structure of the wind contribute to altering the density profile of massive star atmospheres. This makes the spectral analysis of massive stars a complex problem achievable only after development of sophisticated model atmosphere codes.

By utilizing stellar atmosphere modeling, it becomes feasible to derive essential physical properties of massive stars. These include fundamental parameters such as effective temperature (T*), luminosity (L), mass-loss rate (M), and terminal wind velocity (v∞). These parameters play crucial roles as inputs in various models related to stellar structure and evolution, necessitating accurate knowledge of their values.

Typically, the interpretation of spectra from massive stars strongly relies on model atmospheres, and a precise spectroscopic analysis should incorporate a multi-wavelength comparison between observations and models. Currently, there is no established standard approach for deriving stellar parameters using complete spectral information, and different studies often produce significantly different results. In general, such discrepancies may be attributed to disparities in atomic data, model atmosphere codes, numerical methods, and/or analysis techniques. Nonetheless, adopting a consistent approach that incorporates full spectral information has the potential to produce more comparable results and enhance our understanding of massive star evolution.

Over the past decades, significant progress in computer hardware and astronomical software has allowed for the inclusion of iron line blanketing and microclumping in models (Hillier & Lanz 2001; Gräfener et al. 2002), leading to more realistic stellar spectra. The realism of these spectra can be revealed solely through direct comparison of theory with observed data. Given the complexity of stellar atmosphere models, we must have a tool (e.g., numerical technique) to carry out such comparison. Three primary sources of inaccuracy arise during this comparison: (a) inaccuracies inherent in the theory; (b) inaccuracies introduced by the experiment (observations); (c) inaccuracies of the numerical technique for comparing theory and observations.

For the latter, the terms numerical uncertainty, numerical precision, and numerical accuracy will be used throughout the text. Evaluating the overall accuracy of the model lies beyond the scope of our research. In this study, our emphasis is placed on addressing the numerical inaccuracies resulting from the process of comparing theory and observations (item (c) above). This task is fundamentally significant because it serves as a bridge connecting theory with observations. If our method of comparing theory and observations bears significant uncertainties, it could obscure the interpretation of the physical parameters we derive, regardless of how accurate our theory and observations are.

To achieve this goal (evaluation of uncertainties of the numerical technique for comparing theory and observations), we need a "work field." We have calculated four-dimensional (4D) grids of stellar atmosphere models for massive stars, aiming to develop and assess a rigorous method for deriving stellar parameters through direct fitting of observed spectra. The four "axes" of these grids are effective temperature (T*), luminosity (L), mass-loss rate (M), and terminal wind velocity (v∞). Although it is well known, we recall that such a choice of basic parameters is due to the fact that the spectrum of a massive star is determined by the ionization structure of its wind. At a given point in the stellar wind, the latter basically depends on the ratio of ionizing photons to gas number density. The stellar luminosity and temperature (controlling the shape of the underlying continuum) are responsible for the available ionizing photons, while the mass-loss rate and wind velocity set the gas number density, which determines the shape of line profiles in the spectrum.

Spectral grid-modeling may adopt "lighter" grids (e.g., three-dimensional (3D) grids) provided we have a priori information on some basic stellar parameters. It is our understanding that this is possible only for the terminal wind velocity of a massive star, and in such a case all model spectra in the 3D grid will have the same stellar wind value. However, such a 3D grid will have limited applications: it is suitable only for analysis of the specific object at hand or for spectra of massive stars with stellar wind velocities not very different from the value adopted in the corresponding 3D spectral grid. An illustrative application of a 3D grid and its use for determining fundamental physical parameters is found in Zhekov et al. (2020).

We note that "lighter" spectral grids have been actively used in the last two-three decades, with the Potsdam Wolf-Rayet Models being probably the best example of using stellar atmosphere models for deriving stellar parameters of an appreciable number of massive stars in a consistent manner (Hamann et al. 2019; Sander et al. 2019 and references therein). However, these are two-dimensional (2D) grids and their use relies on analysis of continuum-normalized spectra. On the one hand, this makes the comparison between theory and observations more efficient in terms of technical (computer) resources. On the other hand, it adopts some approximate relations (scaling laws) for the stellar parameters, meaning it is done at the expense of not using all available information about physical conditions in the spectral-formation regions (stellar winds). Thus, our choice for a "work field" in this study is to make use of 4D grids of spectral models of massive stars.

This paper is organized as follows: In Section 2, we describe the employed model of stellar atmospheres and outline the approach developed for directly fitting stellar spectra. In Section 3, we evaluate the expected accuracy of derived stellar parameters by fitting "test" spectra of models with randomly chosen stellar parameter values. In Section 4, we discuss possible implications of our results. We present our conclusions in Section 5.

## 2.1. The Model of Stellar Atmosphere

For the purposes of our investigation, we use the non-LTE radiative transfer code CMFGEN (Hillier & Miller 1998; Hillier & Lanz 2001). This software is a comprehensive atmosphere code that incorporates full line-blanketing, specifically engineered to address the challenges posed by solving the statistical equilibrium and radiative transfer equations in spherical geometry.

In CMFGEN, the determination of stellar effective temperature follows the Stefan–Boltzmann law with a reference radius specified at a particular value for Rosseland optical depth. For OB stellar models, we have opted for a reference optical depth of 2/3, whereas for WN and WC stars, given their strong winds, we have chosen a reference optical depth of 20. This choice ensures that the stellar radii do not extend into the wind region. The formula for computing effective temperature is as follows:

$$T_* = \left( \frac{L}{4\pi\sigma R_*^2} \right)^{1/4}$$

Here, L denotes the stellar luminosity, $\sigma$ is the Stefan–Boltzmann constant, and R* is the specified radius for the reference Rosseland opacity.

From observations, we know that the winds of massive stars exhibit non-uniform characteristics, characterized by the presence of inhomogeneities or "clumps." These clumps have a notable impact on the appearance of stellar spectra, making it imperative to model non-uniform stellar atmospheres. CMFGEN provides a mechanism to account for optically thin clumping, often referred to as microclumping. This approach is grounded in the concept that the stellar wind is composed of clumps characterized by heightened density and dimensions smaller than the mean free path of photons. These clumps possess an increased density, expressed as a clumping factor denoted as D, in comparison to the average wind density (see Hamann & Koesterke 1998 for detailed description). The models are calculated with the assumption that the clumps are created by a volume filling factor represented by the reciprocal of D, designated as f, assuming that the regions between clumps contain minimal matter. This factor follows the relationship f = 1/D.

In our models, f∞ = 0.1, described by the following clumping law introduced in Martins et al. (2009):

$$f(r) = f_\infty + (1 - f_\infty)\exp\left(-\frac{v(r)}{v_{\mathrm{cl}}}\right)$$

Here, r is the distance from the star, v(r) is the wind velocity, and vcl is the velocity value from which clumping is taken into account. We have chosen the clumping to start at vcl = 30 km $\mathrm{s}^{-1}$.

It is important to note that CMFGEN does not solve the wind momentum equation. Consequently, the structure of the wind velocity must be predefined. In our models, we describe the wind velocity structure using a standard $\beta$-type velocity law with a specific exponent set to $\beta = 1$. This velocity law is connected to the hydrostatic section of the wind, situated just below the sonic point, where the wind velocity attains the local speed of sound. We note that the turbulent gas velocity (vturb) contributes to the "micro-structure" of the wind, and a specific value must be adopted.

Selecting uniform values for the volume filling factor, velocity-law exponent, and turbulent velocity is done with the intention of reducing the number of independent parameters within the models. Adopting uniform parameter values of $\beta$, f∞, and vturb can be regarded as conventional in the field of spectral modeling for massive Wolf-Rayet stars (e.g., Hamann et al. 2019; Sander et al. 2019 and references therein). It is important to acknowledge that there may be valid reasons to explore alternative values for these parameters in specific situations, particularly when seeking closer alignment with actual physical conditions and observational data.

## 2.2. Description of WN, WC and BSG Grids

The spectral characteristics of a massive star are intricately tied to the ionization structure of its stellar wind. Broadly speaking, the ionization state within a specific region of the stellar wind depends on the equilibrium between the quantity of ionizing photons and the gas density in that region. Although the primary sources of ionizing photons are generally the stellar luminosity and temperature, the density structure of the wind is predominantly determined by the mass-loss rate and wind velocity. Consequently, these four parameters (L, T*, M, and v∞) serve as the fundamental physical parameters defining the features of stellar spectra. Therefore, we have chosen these parameters as the primary inputs for our model grids.

Considering all of this and the needs of our future studies, we have calculated model grids for nitrogen-rich (WN) and carbon-rich (WC) Wolf-Rayet stars, as well as blue supergiants (BSGs) characterized by low metallicity similar to the Small Magellanic Cloud (SMC). Throughout the text, we will denote them as the WC grid, WN grid, and SMC grid. Each CMFGEN model in our grids incorporates the elements H, He, C, N, O, Ne, Mg, Al, Si, P, S, Ar, Ca, and Fe.

The chosen parameter ranges for varying L, M, v∞, and T* are appropriate for these objects (see, e.g., Hamann et al. 2019; Sander et al. 2019, and references therein) and the corresponding selected values are given in Table 1 . For the WN and WC grids, the adopted abundances are from van der Hucht et al. (1986). For the SMC grid, the adopted He abundance is 25% by mass, while the other elements have metallicity of [Fe/H] = $-0.95$ dex (Choudhury et al. 2018).

For the turbulent velocity, a value of vturb = 20 km $s^{-1}$ throughout the wind is used for the Wolf-Rayet grids, while a value of vturb = 10 km $s^{-1}$ is used for the SMC grid.

While we are actively working to expand the BSG grids to higher metallicities and the WR grids to a broader parameter space, it is important to emphasize that building grids is not the main focus of this study. Instead, these grids are provisional and even temporary, as key assumptions—such as metallicity, clumping, velocity law, etc.—remain uncertain.

## 2.3. 4D Grid Modeling—A New Approach to Direct Nonlinear Fitting of Stellar Spectra

The objective of this study is to develop a numerical methodology for grid-fitting stellar spectra of massive stars and estimate its corresponding numerical uncertainties. To accomplish this, it is crucial to compare theoretical and fitted spectra with established stellar parameters. However, in reality this is not possible, and associated uncertainties from numerical fitting techniques often remain ambiguous. Only through clear understanding of these numerical uncertainties can we gauge the reliability of any parameters derived from comparison of theoretical spectra with real observations.

As demonstrated by Zhekov et al. (2020), our choice is to carry out direct fitting of an observed spectrum with a theoretical spectrum "extracted" from a grid of theoretical spectra (Section 2.2). In that study, we used 3D spectral grids, while we deal here with the technically more complex (but physically more sophisticated) case of 4D grids. Thus, our fitting procedure has two parts: (a) how we calculate a model spectrum using a 4D spectral grid; (b) how we estimate the "similarity (correspondence)" between observed and theoretical spectra. It is important to emphasize that for fitting procedures of this nature, whether working with absolutely calibrated observed spectra or observed magnitudes (i.e., using spectral energy distribution), a crucial requirement is having knowledge of the distance to the studied object.

It is important to mention that our fitting procedure operates in log-log space. In other words, each applied interpolation works with the logarithm of the dependent function (specifically, the spectrum, which represents spectral density) and the logarithm of the independent variable. This choice ensures that all approximations result in physically meaningful positive values for the function (i.e., spectral density).

**Calculating a model spectrum.** In our model grids, we provide precise spectra exclusively at the grid nodes. Nevertheless, to generate spectra for parameter values that fall between these nodes, we must utilize an approximation method. We tried various approximations and found that the most reliable—that is, the most stable and with acceptable accuracy—is linear interpolation in log-log space. Since we deal with 4D grids, by analogy with the 2D case for which the standard procedure is bilinear interpolation, we perform quadrilinear interpolation. So, to calculate a spectrum for a set of stellar parameters (T*, M, log L, v∞) in a specific 4D "cube," we perform linear interpolation consecutively from 1D through 2D and 3D up to 4D, that is, along all the "axes" of the 4D "cube." Figure 1 [Figure 1: see original paper] presents a schematic diagram of the quadrilinear interpolation. We recall that bilinear interpolation is of higher order (higher accuracy) than linear approximation (e.g., see Section 3.6 in Press et al. 1992), thus the adopted quadrilinear interpolation is of higher order than bilinear interpolation.

An important detail is the choice of the independent variable for the interpolation process. Understandably, the basic case is to choose the logarithm of actual physical parameters as independent variables for the quadrilinear interpolation along each dimension of the 4D grid. Let us denote this the "basic approximation" or B-approximation. On the other hand, since line emission is a very important feature in the spectra of massive stars of early types, we consider two other cases of the independent variable: the emission measure scale and the transformed radius. Those two are somehow indicative of the stellar wind emission. We denote these cases EM-approximation and RT-approximation, respectively.

We note that the emission processes that take place in formation of the stellar wind emission are two-particle collisions. So, it is natural to expect that line and continuum emission of various ionic species are proportional to the emission measure scale:

$$\mathrm{EM} \propto \int n_e n_i \, dV$$

where n is the gas number density and V is the corresponding volume for a specific ion, and each line-emission volume is proportional to the third power of the reference radius (R*, see Equation (1)), because the latter sets the scale of the emission region in the stellar wind of a massive star.

The term transformed radius (Rt) was introduced by Schmutz et al. (1989) and has been used in modeling observed spectra of massive stars (see Hamann et al. 2019; Sander et al. 2019 and references therein). In terms of stellar parameters, it reads:

$$R_t = R_* \left(\frac{v_\infty}{M}\right)^{2/3}$$

where again we made use of Equation (1).

As seen from Equations (3) and (4), both interpolation variables depend on all the basic stellar parameters considered in this study. Therefore, when performing grid interpolation, we can use any of these variables only for one of the "axes" of our 4D grid that is directly responsible for the stellar wind emission (i.e., M and v∞). So, for the EM-approximation and RT-approximation we use the corresponding interpolation variable on one of these two axes and adopt linear interpolation on the other three axes (as in the B-approximation). As a result, our fitting procedure has five approximation cases to calculate a model spectrum based on a 4D grid of stellar atmosphere model spectra: one B-approximation, two EM-approximations, and two RT-approximations.

**Match between observed and theoretical spectra.** A standard way in spectral fitting is to adopt some likelihood estimator (LE) to check how well a theoretical spectrum matches an observed one. As a rule, the minimum value of this LE defines a set of fitting parameters reproducing the observed spectrum "best." We explored spectral fitting with different LEs ( $^2$-minimization among others) and achieved best results with estimators based on absolute deviations between observed and theoretical spectra:

$$z_i = \mathrm{Sp}_{\mathrm{obs}}(\lambda_i) - \mathrm{Sp}_{\mathrm{mod}}(\lambda_i)$$

Since we fit an observed spectrum, the model spectrum is subject to interstellar extinction (reddening), meaning we fit for five parameters: four stellar parameters (T*, M, log L, v∞) and E(B−V).

Our fitting procedure adopts the following robust LEs:

$$\mathrm{LE}_1 = \sum_i |z_i|$$

$$\mathrm{LE}_2 = \sum_i \ln\left(1 + \frac{z_i^2}{2\sigma^2}\right)$$

$$\mathrm{LE}_3 = \sum_i \frac{|z_i|}{1 + |z_i|/\sigma}$$

$$\mathrm{LE}_4 = \sum_i \tanh\left(\frac{|z_i|}{\sigma}\right)$$

$LE_1$ is the sum of absolute deviations between observed and model spectra. $LE_2$ is defined by analogy with the Cauchy distribution (e.g., see Section 15.7 in Press et al. 1992). $LE_3$ and $LE_4$ are experimental estimators that have the property of decreasing the weight of deviant points in the fit while searching for the minimum of an LE-function. We note that the $LE_2$-, $LE_3$-, and $LE_4$-function behavior is similar to that of the standard $LE_1$-function for small values of z , but $LE_2$-, $LE_3$-, and $LE_4$-functions are more robust for deviant points. Such points might result from observational uncertainties as well as from uncertainties in numerical approximations.

On the technical side, we adopted the downhill simplex method to search for the minimum of the LE-function, as its algorithm is exemplified in the amoeba procedure (see Section 10.4 in Press et al. 1992). In summary, our 4D-grid fitting process consists of the following steps. First, an individual fit obtains the "best" set of model parameters by making use of the five approximations previously described: one B-approximation, two EM-approximations, and two RT-approximations. Specifically, it picks the result from that approximation which provides the smallest minimum of the LE-function at hand. Second, we carry out a spectral fit for each of the four LE-functions defined above (see Equation (5)). As a result, we derive four "best" sets of stellar parameters that define a model spectrum matching the observed one, and the mean of these four "best" sets constitutes the solution from our fitting process.

## 3. Test Results

The accuracy of derived stellar parameters from 4D-grid fitting of observed spectra relies on the quality of the observed spectra and the fitting approach used. An illustration of how 4D-grid fitting can estimate stellar parameters from fitting an observed spectrum is provided in Appendix A. However, before estimating a reliable range of derived stellar parameters, it is imperative to investigate and establish the level of uncertainties arising from applying the fitting procedure.

For each spectral approximation, we performed tests to compare results from the amoeba procedure and those from a gradient method to search for the minimum of a function (e.g., the Davidson-Fletcher-Powell algorithm, see Section 10.7 in Press et al. 1992), and the derived "best"sets of parameters were identical. So, we adopted the downhill simplex method in this study because it does not require calculations of derivatives, thus introducing less numerical noise (uncertainties).

In order to investigate this, we carried out tests for each of the 4D grids of model spectra (WC, WN, and SMC grids). Specifically, for each grid we calculated over 20 synthetic spectra using the CMFGEN code. These were used as "perfect" observed spectra in the ultraviolet (UV)-optical domain. For each "perfect" observed spectrum, we used a set of stellar parameters randomly chosen within the boundaries of the corresponding 4D grid. Each "perfect" observed spectrum was subject to interstellar reddening, the value of which was randomly chosen as well. In addition, some fiducial value for the distance (e.g., 2000 pc) was associated with each object. We then fitted these test spectra to derive the corresponding stellar parameters. Differences between input and derived values provide estimates of expected accuracy from using our fitting procedure. We also performed additional tests by adding Gaussian noise to the "perfect" observed spectra ( "noisy" observed spectra), which could be considered a more realistic representation of observed spectra.

We note that stars with strong winds, such as those represented by WN and WC grids, typically exhibit UV-optical spectra richer in line emission than those from the SMC grid, which correspond to objects with weaker winds. As a result, we would expect that stellar wind parameters for objects with strong winds would be derived with better accuracy by our 4D-grid fitting procedure.

**Objects with strong winds.** Results from tests for the "perfect" observed spectra of WC and WN stars are shown in Figures 2 [Figure 2: see original paper] and 3 [Figure 3: see original paper], respectively. Detailed results from these tests, along with those for "noisy" observed spectra, are presented in Table 2 . It is evident that all absolute deviations of derived stellar parameters from their respective input values are well within the limits of (smaller than) 0.05 dex. Moreover, the mean absolute deviation for the WC and WN samples is significantly below 0.05 dex. However, we opt for a more conservative approach by assuming that numerical uncertainty is determined by the maximum deviation observed in the tests (shown in the "max" column of Table 2). Interestingly, this uncertainty limit (0.05 dex) also holds for the case of "noisy" test spectra (Table 2).

**Objects with weak winds.** Figure 4 [Figure 4: see original paper] ( "perfect" observed spectra) and Table 2 ( "perfect" and "noisy" observed spectra) present results from tests for SMC objects. As in the case of objects with strong winds, the mean absolute deviation of derived stellar parameters is appreciably less than the accuracy limit of 0.05 dex. However, we see that occasionally larger deviations occur (in 1% of cases). In general, we may conclude that in both cases (strong and weak winds), numerical uncertainty of derived stellar parameters is not worse than 0.05 dex. But it is interesting to check whether the spectral range of observed spectra may have some effect on parameter accuracy as well.

**Spectral range.** Results from tests for "perfect" observed spectra of WC, WN, and SMC objects in the optical (3150–11000 Å) are given in Table 3 . We see again that numerical accuracy of derived parameters is not worse than 0.05 dex for objects with strong winds (WC and WN spectra). However, the quality of derived parameters slightly deteriorates for objects with weak winds (SMC spectra): the fraction of cases with parameter accuracy greater than 0.05 dex increases from 1% to 8%. Thus, it is reasonable to conclude that the larger the spectral range and the better the quality of observed spectra of massive stars, the better constrained are the derived stellar parameters from 4D-grid fitting.

## 4. Discussion

It is essential to acknowledge that our fitting technique works within the framework of stellar atmosphere models, relying on certain assumptions about key properties such as chemical composition, wind velocity profile ($\beta$-law), and volume filling factor (clumping). However, this limitation applies to any study based on stellar atmosphere models. What if actual stellar properties do not correspond to those adopted in this study? It is indeed reasonable to expect some variation within a specific spectral class. Factors such as abundances, wind acceleration law, and clumping might display a degree of variability around assumed "typical" values, though generally within certain expected limits. Thus, we will next address this issue in some detail.

We aim to explore the effect of conducting 4D-grid fitting on observed spectra of objects whose abundances, wind acceleration laws, and clumping deviate from the values adopted in our 4D grids. We will also briefly address the case of 4D grid-fitting of "composite" spectra of massive stars (e.g., massive binaries).

### 4.1. Abundances

For each of the 4D grids considered in our study (WC, WN, and SMC), we defined an additional abundance set labeled "Add." (Table 4 ). The additional WC set is based on WC abundances for galactic metallicity as defined in Sander et al. (2012), and the additional WN set represents the WN abundance set for galactic metallicity as defined in Hamann & Gräfener (2004) with helium mass fraction of 0.78. The additional SMC abundance set exhibits metal abundances that have approximately doubled (see Table 4 for details).

For each 4D grid, we prepared "perfect" observed spectra having the same stellar parameters as described in Section 3, but their abundances were those from the "Add."set for WC, WN, and SMC objects. We used our 4D-grid fitting procedure and the corresponding results are shown in Figures B1, B2, and B3 respectively.

In general, changes in abundances affect the derived parameters, with the most important change being in derived mass-loss rate values. In the case of strong winds (i.e., in the WN and WC grids), alterations in abundances also result in corresponding changes in log L. This is understood as the density profile, specific to a given chemical element in the stellar wind, undergoing changes solely due to variations in mass-loss rate, and the ionization structure must adapt to align with the observed spectrum. Consequently, the ionization agent (luminosity) is affected. In the case of weak winds (i.e., SMC grid), there are practically no changes in derived values of effective temperature and luminosity (T* and log L). This is because stellar wind emission is not the dominant part of the spectrum; therefore, its changes do not lead to changes in other stellar parameters.

## 4.2. Wind Acceleration Law

We recall that the 4D grids in this study were built adopting a wind acceleration law with $\beta = 1$. For each 4D grid, we prepared two additional sets of “perfect” observed spectra having the same stellar parameters as described in Section 3 and values of $\beta = 0.5$ and $\beta = 2$. This means we explore the impact on derived parameters if a massive star has a faster accelerating ($\beta = 0.5$) or slower accelerating ($\beta = 2$) wind compared to that adopted in our 4D grids ($\beta = 1$). Results from fits of these spectra with our 4D-grid fitting procedure are shown in Figures B4, B5, and B6.

It is evident that there are appreciable systematic changes in derived stellar parameters, and in general their accuracy worsens. For strong winds, it could be assumed to be not worse than 0.1 dex for all stellar parameters. However, for weak winds, the stellar wind parameters may have larger deviations (up to 0.2 dex) while effective temperature and luminosity are recovered very well.

We think the reason for such systematic changes is that different $\beta$-laws result in considerable changes to the velocity and density profiles of the stellar-wind plasma. Therefore, there are large changes in the ionization structure of the emission region of various ionic species as well. In addition, the 4D-fitting procedure tries to handle this within the available 4D grid. For example, if the ionization structure “moves in” closer to the star, it chooses smaller stellar wind velocities, and the opposite is valid if the ionic structure “moves out” further from the star. Next, it adjusts the amount of line emission by choosing the value of the mass-loss rate. In turn, different values of the latter may cause some changes in derived luminosity values. Moreover, effective temperature also plays a role since its value influences ionization structure by defining the “typical” energy of ionizing photons. In other words, the complex behavior of derived stellar parameters follows from the strong nonlinearity of emission formation from massive stars of early spectral types.

Considering the significant impact of wind acceleration on determined stellar parameters, we believe that the $\beta$-law could serve as a promising candidate for expanding the grid-fitting procedure by adding another “dimension”in the future. It is worth recalling that the $\beta$-law is an approximation to the velocity profile in winds of massive stars. A more realistic velocity profile can be modeled only if radiative hydrodynamics models are adopted. However, given their complexity and need for computer resources, using such models to confront theory and observations by direct fitting of observed spectra of numerous specific objects does not seem feasible. Thus, we feel confident that expanding our fitting procedure by adding the $\beta$-law “dimension” is a reasonable step to take.

## 4.3. Clumping

It is generally assumed that massive stars with different mass-loss rates that scale with their corresponding volume filling factors ($f\infty^2$) have very similar spectra, provided other stellar parameters are kept fixed. Our 4D fitting procedure relies on approximations of the model spectrum, leading to introduction of numerical noise. To check the effect of the latter on this scaling law, we prepared an additional set of "perfect" observed spectra having the same stellar parameters as described in Section 3 and a value of f∞ = 0.25, but the mass-loss rates were scaled according to the scaling law: log M_{new} = log M_{old} + 0.2. This means that stellar parameters derived from applying our 4D-grid fitting procedure should remain the same as before. Results from fits of these spectra are shown in Figures B7, B8, and B9.

We see that for strong winds, although there are some small systematic changes in derived parameters, the clumping scaling law seems to work acceptably: the derived stellar parameters are still within numerical accuracy of 0.05 dex as before (f∞ = 0.1). In contrast, when it comes to weak winds, the alteration in mass-loss rate values is not insignificantly small. We attribute this behavior to the imperfect nature of the clumping scaling law, where minor residuals are compounded with uncertainties arising from numerical approximations to model spectra adopted in our 4D-grid fitting procedure.

Note that stellar atmosphere models of massive stars typically assume a constant filling factor. However, a physically more realistic approach would involve clumping that varies with distance from the star. Such variability becomes feasible when analyzing individual objects across diverse spectral domains like UV, optical, and radio. An illustration of such approach can be found in Zhekov et al. (2020) (see also appendix A in that source).

Another fundamental assumption in these stellar atmosphere models is that the interclump medium has negligible contribution to the stellar spectrum; in other words, the intercloud space is "void of matter." However, it seems improbable that such "empty" space exists in winds of massive stars. It is more likely that winds of massive stars consist of a two-component flow: a massive component composed of clumps and a low-density component that fills the interclump space. Evidence supporting this two-component picture also arises from analysis of X-ray emission from colliding-wind binaries, which are binary systems consisting of two massive stars (see discussion in Section 4.3 of Zhekov et al. 2020). We thus believe that addressing possible emission from the low-density wind component (interclump matter) is needed, and we plan to try carrying out even simple estimates in a future study.

## 4.4. 4D Grid-fitting of "Composite" Spectra

A "composite" spectrum may arise, for example, from a binary system in which both components are massive stars. If the studied object is a wide binary (orbital period of hundreds of days or years), then wind-absorption effects for either massive-star spectrum by its binary companion might be neglected. So, the total ( "composite" ) spectrum would be a sum of two spectra subject to common reddening (interstellar absorption). An interesting (and simple) case to consider is when the stellar components in a massive binary are of quite different spectral class (type). In such a case, we can adopt 4D grid-fitting (using two different grids) because the spectral vectors are independent (none of the component spectra could mimic the other one). Again, it is interesting to evaluate the level of uncertainties of derived stellar parameters when adopting 4D grid-fitting to a “composite” spectrum.

To address this, we made use of test spectra of WC and WN stars ( “perfect observed spectra” ) as described in Section 3. We constructed more than 20 “composite” WC+WN spectra by combining individual WC and WN model spectra and applying common reddening to the resulting summed spectrum. These spectra were fitted with our 4D-grid procedure, where at each step of the fitting process a spectrum is calculated from each of the grids (WC and WN) and the total model spectrum is the sum of both spectra.

Results from 4D grid-fitting to the “composite” WC+WN test spectra are given in Table 5 . As in tests of fitting spectra of single massive stars, we explored different spectral ranges: UV-optical (1150–11000 Å) and optical (3150–11000 Å). Interestingly, numerical accuracy of derived parameters is not worse than 0.05 dex in the case of UV-optical spectra, and in just one case (for one stellar parameter, i.e., in less than 1%) it exceeds that boundary. These results are quite encouraging for using 4D grid-fitting of observed “composite” spectra of massive stars (e.g., wide massive binaries). We note that this procedure can be easily “upgraded” for more complex cases, e.g., “composite” spectra with three spectral components. Results from applying 4D grid-fitting in such a case are given in Zhekov & Petrov (2025).

## 5. Conclusions

We have developed a novel technique that enables direct fitting of observed spectra. To validate this technique, we calculated 4D grids of model spectra for early spectral-class massive stars, specifically Wolf-Rayet stars (WC and WN spectral classes) and BSGs with low metallicity similar to those of the SMC. These model grids served as a testing ground for developing and testing our technique, as well as for estimating expected numerical uncertainties. We demonstrated that this approach achieves numerical precision not exceeding 0.05 dex when estimating essential stellar parameters—effective temperature, mass-loss rate, luminosity, and terminal wind velocity. This was confirmed through rigorous testing on designated “test” models. Even when Gaussian noise was added to synthetic spectra, the mean absolute deviation consistently remained well below 0.05 dex for objects exhibiting both weak and strong stellar winds.

It is essential to note that actual accuracy of derived physical parameters depends not only on the fitting approach but also on how well simplifying assumptions in the models and underlying theory reflect real conditions in stellar winds. However, without such numerical uncertainty estimates, even the most sophisticated methods would be unreliable for deriving and interpreting stellar parameters for physical analysis. Our results are encouraging and provide strong support for our goal of deriving fundamental stellar parameters from spectral analysis with the highest attainable accuracy.

It is essential to note that accuracy of derived parameters depends on the spectral range, and inclusion of UV spectral range contributes to improved parameter derivations, particularly for objects with weak winds. This underscores the importance of selecting appropriate spectral range for comprehensive and accurate stellar parameter determination.

We explored the influence of unaccounted factors such as variations in metal abundances, wind acceleration law, and degree of clumping on precision of derived parameters. Notably, we found that variations in abundances predominantly affected derived mass-loss rate values, particularly evident in weak-wind scenarios represented by our SMC grid. Interestingly, for weak winds, derived values of effective temperature and luminosity remained largely unaffected by abundance changes.

Furthermore, our tests revealed significant influence of wind acceleration law on accuracy of determined stellar parameters, with noticeable decrease in precision, particularly up to 0.2 dex for objects with weak winds. In contrast, application of different degrees of clumping demonstrated good parameter precision (less than 0.05 dex) for objects with strong winds, but resulted in decreased precision up to 0.2 dex for objects with weak winds. This dichotomy underscores the interplay between degree of clumping and strength of stellar wind, emphasizing the need for careful consideration of these factors in pursuit of precise stellar parameter determinations. Consequently, our clumping scaling law is effective for objects characterized by strong winds, whereas its application to objects with weak winds results in significant decline in precision, up to 0.2 dex.

These results affirm that real accuracy of stellar parameters derived from any fitting technique using theoretical models will strongly depend on systematic errors arising from simplifying assumptions inherent in the theoretical models. Specifically, a critical inference from our investigation is that precise information about the wind velocity law is required to ensure reliable determination of stellar parameters. Consequently, we plan to expand the parameter space by including models with diverse values of $\beta$. This is necessary to enhance accuracy of stellar wind parameter determinations.

On the technical side, we see at least two ways to achieve better accuracy in derived stellar parameters: (a) build "denser" model grids; (b) improve numerical approximation of model spectra. In practical terms, denser model grids with smaller parameter steps can enhance accuracy of derived stellar parameters within the 4D grid fitting framework. However, this approach demands significant computational resources and time due to the complexity of the grid-building process, which is not easily automated. The need for numerical approximation arises because stellar atmosphere codes cannot produce detailed spectra of all chemical elements "instantaneously." While it would be ideal to avoid numerical approximations, it is currently not feasible. In this respect, accuracy of derived stellar parameters improves if we manage to find a "better" numerical approximation than those used in Section 2.3 of this study.

Finally, we note that when analyzing observed spectra of massive stars there might be two major issues as illustrated by numerical experiments in this study. First, the wind of a real object may have a velocity profile different from that adopted in our 4D grids ($\beta$-law with $\beta = 1$). Second, its chemical composition may deviate from the abundance set used to calculate these grids. Moreover, the "combined" effect of both issues is hard to foresee. While the first issue could be handled by adding a new "dimension" to the grids (whether "globally" or "locally," as discussed above), we do not think it is feasible to adopt the same approach for handling chemical composition from fitting observed spectra of massive stars. The reason is that it is not possible to define a "global" parameter that could describe the variety of changes in the spectrum due to different chemical elements. Alternatively, adding more "dimensions"to the grids even only for the most abundant elements is hardly the way to go. Therefore, this "combined" effect needs to be addressed in detail, and the corresponding solution will likely adopt some iteration procedure that must be carefully tested —a complex task that we plan to consider in a follow-up study.

## Acknowledgments

This research is based on observations made with the International Ultraviolet Explorer (IUE), obtained from the MAST data archive at the Space Telescope Science Institute, which is operated by the Association of Universities for Research in Astronomy, Inc., under NASA contract NAS 5-26555. This research has made use of NASA's Astrophysics Data System and the SIMBAD astronomical database, operated by CDS at Strasbourg, France. We thank the anonymous referee for valuable comments and suggestions, which helped improve this manuscript.

## Data Availability

The calculated 4D grids (792 WC spectra, 432 WN spectra, and 600 SMC spectra) as well as their future updates (if any) will be available from this link: https://drive.google.com/drive/u/1/folders/16gLnF2Z3abES8CPUOxI2dKBw8j58MW6_. The model spectra are in the range 1000–11000 Å with sampling of 1 Å.

## Appendix A: 4D-grid Fitting of the UV-optical Spectrum of WR 23

The accuracy of derived stellar parameters of a studied object generally depends on the quality of its observed spectra. We recall that the 4D fitting procedure works with spectra in absolute flux units. Therefore, photometric absolute uncertainties associated with the observed spectrum will impact derived stellar parameters. Additionally, spectral resolution (and sampling) should not be very  "crude," because that will result in inaccurate emission line profiles which in turn would deteriorate quality of derived stellar wind velocity.

The distance to the studied object, along with its associated uncertainties, is another physical quantity important for obtaining reliable stellar parameters. Specifically, it plays a key role in estimating stellar luminosity, which subsequently affects derived values of both mass-loss rate and stellar temperature. This relationship arises because the continuum is primarily determined by stellar luminosity. Thus, changing the distance, which leads to changes in luminosity, causes changes in ionization structure of the stellar wind. To maintain consistency with the observed spectrum, adjustments are necessary. This involves "back-adjusting" the ionization structure by modifying mass-loss rate and stellar temperature, with the latter being particularly significant as it determines the quantity of photoionizing photons emitted.

The focus of this study is not to derive stellar parameters of massive stars; however, in this appendix we provide an example of how the 4D grid-fitting procedure can be applied to real observations. Therefore, WR 23 was selected as a demonstration case. WR 23 is categorized as a Wolf-Rayet star of the WC (carbon-rich) subtype (e.g., the Galactic Wolf-Rayet Catalogue; Rosslowe & Crowther 2015) at a Gaia distance of 2.3 ± 0.1 kpc (Crowther et al. 2023). The optical spectrum of WR 23 was taken from the STELIB spectroscopic library, which has an intermediate spectral resolution of  3 Å, sampling of 1 Å, and overall absolute photometric uncertainty of 3% (Le Borgne et al. 2003).

We expanded the spectral range by making use of the UV spectrum of WR 23 from the International Ultraviolet Explorer (IUE): the data are taken from the Mikulski Archive for Space Telescopes (MAST). The IUE spectrum has sampling of 1.68 Å at wavelengths $\lambda < 1979$ Å and 2.67 Å at wavelengths $\lambda >$ 1979 Å.

Our fitting procedure of observed spectra consists of the following steps. First, we prepare the 4D grid of model spectra for the corresponding spectral binning (sampling) of the observed spectrum at hand. Then, we derive stellar parameters using the approach described in Section 2.3 for the nominal distance of 2.3 kpc to WR 23. We also derive stellar parameters for cases of upper (2.4 kpc) and lower (2.2 kpc) limits to the distance. Finally, we repeat these fits for the three distance values, performing 4D fitting twice for each case to account for absolute photometric uncertainties: i.e., considering the flux to be 3% higher or lower than nominal flux. In all fits, we adopt the Galactic extinction curve of Fitzpatrick (1999) with RV = 3.1.

Derived stellar parameters and their associated uncertainties are given in Figures A1 [FIGURE:A1], A2 [FIGURE:A2], and Table A1 [TABLE:A1]. Note that the highest contribution to uncertainties of derived parameters is due to errors in distance to WR 23. Because luminosity scales as the square of distance, the highest impact is on derived stellar luminosity, and uncertainties on absolute flux then accumulate, adding extra uncertainty. But in general, uncertainties from distance and absolute flux are somehow "redistributed" between derived values of luminosity, mass-loss rate, and stellar temperature. It is worth noting that wind velocity remains unaffected by this redistribution, likely because wind velocity is mostly "confined" by emission-line profiles.

If any stellar parameters we are fitting for are already constrained from other studies, we can incorporate that prior information by keeping the parameter fixed at its known value and then proceed to fit remaining parameters. Nevertheless, among the four fundamental stellar parameters, only terminal wind velocity can be constrained reliably from observations.

Interestingly, the derived terminal velocity from 4D grid-fitting, using no a priori information about its value, is in good correspondence with the value of 2280 km $s^{-1}$ from classical analysis of IUE spectra of massive stars by Prinja et al. (1990) and of 2342 km $s^{-1}$ by Niedzielski & Skorzynski (2002). This is valid both for fits to the entire spectrum (UV-optical) of WR 23 and only to its optical spectrum (Table A1).

In general, results of fitting UV-optical and only optical spectrum of WR 23 are in acceptable correspondence with each other (see also Section 3). We attribute this to the presence of many strong emission lines that help constrain physical parameters of the studied massive stars better. Nevertheless, it is our understanding that the former (results from fitting the entire spectrum) should be considered more reliable. Finally, we note that reddening curves with $RV \neq 3.1$ can be used in our 4D-grid fits, but this can be adopted only if corresponding information is available from other studies.

## Appendix B: Tests with Different Abundances, Wind Acceleration Law and Volume Filling Factor

In the figures below, we provide results from 4D-grid modeling (fitting) of test spectra ( "perfect" observed spectra) for objects considered in this work (WC, WN, and SMC). These tests are aimed at checking corresponding effects if chemical composition (Figures B1 [FIGURE:B1], B2 [FIGURE:B2], and B3 [FIGURE:B3]), stellar wind acceleration (Figures B4 [FIGURE:B4], B5 [FIGURE:B5], and B6 [FIGURE:B6]), and clumping (Figures B7 [FIGURE:B7], B8 [FIGURE:B8], and B9 [FIGURE:B9]) in observed objects differ from those used to build our 4D spectral grids of model spectra.

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