# Single-voxel debugging

Craig Yanitski

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## 1 Single-voxel setup

Here we will examine the current setup of the calculations of `kosmatau3d`. These will give a basis on how the probabilistic calculation works for a single voxel, and what assumptions are present when using the single-voxel model. The observed intensity is calculated from the radiative transfer equation,

$$dI_\nu = -I_\nu \kappa_\nu ds + \epsilon_\nu ds, \tag{1}$$

we can assume $\kappa$ and $\epsilon$ (the absorption and emissivity coefficients, respectively) are constant in the voxel. Therefore they are calculated using the voxel-averaged emission:

$$\langle \epsilon_\nu(v_{obs}) \rangle_{vox} = \lim_{\Delta s \to 0} \left( \frac{\langle I_\nu \rangle_{vox} (v_{obs})}{\Delta s} \right), \tag{2}$$

$$\langle \kappa_\nu(v_{obs}) \rangle_{vox} = \lim_{\Delta s \to 0} \left( \frac{\langle \tau_\nu \rangle_{vox} (v_{obs})}{\Delta s} \right), \tag{3}$$

where $\Delta s$ is the size of the voxel, and $\langle \cdots \rangle_{vox}$ indicates a property averaged over the voxel. In order to properly understand these voxel-averaged values, it is necessary to have some insight for what is happening inside the voxel. The clumpy PDR is approximated by an ensemble of spherically-symetric KOSMA-$\tau$ 'clumps'. The number of clumps with a particular mass ($N_j$) follows the clump mass distribution:

$$\frac{\mathrm{d}N}{\mathrm{d}M} = \mathcal{A} M^{-\alpha}. \tag{4}$$

Here we adopt $\alpha = 1.84$ from Heithausen et al. (1998), and $\mathcal{A}$ is a constant. Henceforth the subscript $j$ will refer to a property specific for clumps with mass $M_j$.

There are three types of velocity one needs to consider:

- $v_{vox}$: The average radial velocity of the gas in the voxel. For testing purposes, this is set to zero. (ie. The observed intensities should follow a Gaussian centered at 0.)

- $v_{j,i}$: The internal velocities in the voxel. This is used for the radial velocity of the modeled clumps in the ensemble. This is calculated on-the-fly using $v_{j,i} \in [v_{vox} - 3\sigma_{ens,j}, v_{vox} + 3\sigma_{ens,j}]$ with step size,

$$\delta v = \min\left(\frac{\sigma_{ens}}{n_{velocity}}, \frac{\sigma_{cl}}{n_{velocity}}\right).$$

Initial testing had shown that $n_{velocity} = 3$ is sufficient. $j$ refers to a clump mass in the ensemble (which may have a different intrinsic velocity dispersion $\sigma_{cl,j}$) while $i$ refers to the internal velocity. The number of internal velocities are $\geq 6n_{velocity} + 1$.

- $v_{obs}$: The observing velocities of the emission. This is required as an argument to the voxel initialisation, and it is independent of the step size chosen for $v_{obs}$.

Now the number of clumps with a particular radial velocity $v_{j,i}$ is determined by the number of clumps of a particular mass $N_j$ and velocity distribution of the ensemble $\sigma_{ens,j}$.

$$\Delta N_{j,i} = \frac{N_j}{\sqrt{2\pi}\sigma_{ens,j}} \exp\left(-\frac{(v_{vox} - v_{j,i})^2}{2\sigma_{ens,j}^2}\right) \delta v_j, \tag{5}$$

where $\delta v_j$ is the aforementioned step size in $v_{j,i}$. The probability $p_{j,i}$ of having $k_{j,i}$ clumps in a line-of-sight observed at velocity $v_i$ is determined by Binomial distribution of the number of clumps at that velocity:

$$p_{j,i} = \binom{\Delta N_{j,i}}{k_{j,i}} p_j^{k_{j,i}} (1 - p_j)^{\Delta N_{j,i} - k_{j,i}}, \tag{6}$$

where $p_j$ is equivalent to the area-filling factor of clump $j$ ($p_j = \frac{\pi R_j^2}{\Delta s^2}$). If $p_j N_{j,i} > 5$, then a Gaussian expression is used with $\mu_{j,i} = p_j N_{j,i}$ and $\sigma_{j,i} = \sqrt{N_{j,i} p_j (1 - p_j)}$.

For having $k_{j,i}$ clumps in a line-of-sight, the intensity and optical depth ($I_{\nu,j,i}$ & $\tau_{\nu,j,i}$) can be calculated.[1] Here the subscript $\nu$ means the properties refer to a particular transition (which is what we obtain from the KOSMA-$\tau$ grid).

$$I_{\nu,j,i}(v_{obs}) = k_{j,i} I_{cl,\nu,j} \exp\left(\frac{(v_i - v_{obs})^2}{2\sigma_{cl,j}^2}\right), \tag{7}$$

$$\tau_{\nu,j,i}(v_{obs}) = k_{j,i} \tau_{cl,\nu,j} \exp\left(\frac{(v_i - v_{obs})^2}{2\sigma_{cl,j}^2}\right), \tag{8}$$

where the factor $\exp(\frac{(v_{j,i} - v_{obs})^2}{2\sigma_{cl,j}^2})$ accounts for the contribution of the clumps with radial velocity $v_{j,i}$ at observing velocity $v_{obs}$. Finally the intensity and optical depth can be averaged over the voxel using all possible combinations and their corresponding probabilities.

$$\langle I_\nu \rangle_i (v_{obs}) = \sum_k \left[\Big(\prod_j p_{j,i}(k_{j,i})\Big)\Big(\sum_j I_{\nu,j,i}(v_{obs})\Big)\right], \tag{9}$$

[1] This is incorrect as stated, but it is presented as such to agree with Andree-Labsch et al. (2015) as well as the corresponding code. For correctness, it is better to calculate $\epsilon_{\nu,j,i}$ rather than $I_{\nu,j,i}$. In the original implementation, the equation used is $\epsilon_{\nu,j,i} = \frac{I_{\nu,j,i}}{\Delta s}$.

$$\langle\tau_\nu\rangle_i(v_{obs}) = -\ln\left\{\sum_k\left[\left(\prod_j p_{j,i}(k_{j,i})\right)\exp\left(-\sum_j \tau_{\nu,j,i}(v_{obs})\right)\right]\right\}, \tag{10}$$

and finally summing over the contributions of the clumps at all velocities:

$$\langle I_\nu\rangle_{vox}(v_{obs}) = \sum_i \langle I_\nu\rangle_i(v_{obs}), \tag{11}$$

$$\langle\tau_\nu\rangle_{vox}(v_{obs}) = \sum_i \langle\tau_\nu\rangle_i(v_{obs}). \tag{12}$$

Here the sums and products ensure we consider contributions from all clump masses at all radial velocities, since there is a velocity dispersion to each clump's intensity and optical depth. Now we can finally substitute these into the radiative transfer equation to determine the intensity we expect to observe from this voxel, accounting for any background intensity $I_{bg,\nu}$:

$$I_{\mathrm{vox},\nu}(v_{obs}) = \frac{\epsilon_\nu(v_{obs})}{\kappa_\nu(v_{obs})}\left(1 - e^{-\kappa_\nu(v_{obs})\Delta s}\right) + I_{bg,\nu}e^{-\kappa_\nu(v_{obs})\Delta s}. \tag{13}$$

# 2 Calculation error

There is clearly some issue with the single voxel calculation, since there is an absorption feature that should not be present. Perhaps this was noticed initially when setting up the single-voxel model, but at the time it was dismissed due to the nonphysical model parameters (a volume filling factor $f_V > 1$). Yoko has explored more of the parameter space to compare with observations, though, and encountered this problem again. In this use-case, an over-filled voxel is used to compare to various lines-of-sight. This makes enough sense as the clumps overflow behind the voxel. I now need to revise my intensity calculations not only to correct this absorption feature, but to ensure that the previous calculations (without this error) also agree.

For a densely-filled voxel, there could exist a saturation plateau in the intensity profile $I(v_{obs})$, however the error is that there still exists some additional absorption. Due to the calculation of the voxel intensity (see §1), there are two separate modes of calculation: standard and normalised. The standard calculation of the intensity uses the clump numbers calculated using $\Delta N_{j,i}$, while the normalised calculation resizes the voxel to ensure a given number of the largest clump are included in the voxel (typically 1 for the dense clumpy ISM). There is also part of the code which resizes the voxel if it is too small to fit the largest clump. It is the combination of these two features that make debugging this error more difficult. For that reason, I will debug these calculation methods separately. What follows in this section and the next are just for voxels normalised to have 1 of the largest clump in the ensemble. The un-normalised comparison will follow in a later version of this document.

## 2.1 The correction

The issue identified thus-far is that the probabilistic description has been applied to the averaged *intensity* rather than the *emissivity*, and therefore there exists some excess absorption in the plateau region. The proposed fix for this is to modify the equation for $I_{\nu,j,i}(v_{obs})$ to calculate instead $\epsilon_{\nu,j,i}(v_{obs})$:

$$\epsilon_{\nu,j,i}(v_{obs}) = k_{j,i}\left(\frac{I_{cl,\nu,j}}{L_{vox}}\right)\left(\frac{\tau_{cl,\nu,j}}{[1-\exp(-\tau_{cl,\nu,j})]}\right)\exp\left(\frac{(v_{j,i}-v_{obs})^2}{2\sigma_{cl,j}^2}\right). \quad (14)$$

$L_{vox}$ in this equation is the line-of-sight length of the voxel. An over-filled voxel will thus have $L_{vox} = f_V \Delta s$. This leads to a voxel-averaged emissivity of,

$$\langle\epsilon_\nu\rangle_i(v_{obs}) = \sum_i \left[\Big(\prod_j p_{j,i}(k_{j,i})\Big)\Big(\sum_j \epsilon_{\nu,j,i}(v_{obs})\Big)\right]. \quad (15)$$

The corresponding modification for the optical depth in terms of opacity is,

$$\kappa_{\nu,j,i}(v_{obs}) = \frac{\tau_{\nu,j,i}(v_{obs})}{L_{vox}}, \quad (16)$$

$$\langle\kappa_\nu\rangle_i(v_{obs}) = -\ln\left\{\sum_i \left[\Big(\prod_j p_{j,i}(k_{j,i})\Big)\exp\Big(-\sum_j \kappa_{\nu,j,i}(v_{obs})\times\Delta s\Big)\right]\right\}, \quad (17)$$

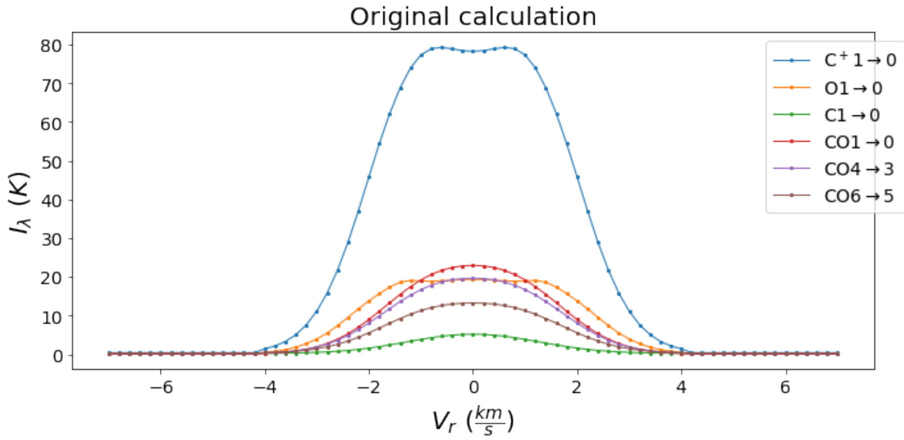
though this is essentially just the same calculation as before.

At least this is how the intended modification to the code should work. Its implementation tries to remain as faithful to this description as possible, but it was noted that there are still a couple errors. Therefore a couple of flags were added to choose the type of implementation: `test_calc` and `test_fv`. `test_calc` chooses whether or not the test calculation is used, which will definitely affect the emissivity. `test_fv` tests a form of the calculation that should have been in the code from the beginning. Since only partially- to fully-filled voxels are considered in the 3D models ($f_V \leq 1$), all of the computations depend on the extent of the voxel, $\Delta s$. This is not true in the case of an over-filled voxel ($f_V > 1$), where the excess clumps are assumed to be located just behind the voxel. In this case of an over-filled voxel, the calculations are modified to ensure it is still physically correct. (ie. The voxel essentially becomes a column, with the voxel size $\Delta s$ determining the observed area and the depth adjusted by $f_C \equiv \max(1, f_V)$.) As a crude approximation, this changes equations such as the voxel-averaged opacity to $<\kappa_\nu> = \frac{<\tau_\nu>_{vox}}{f_C \Delta s}$. This ensures all of the clumps are contained in the voxel being calculated. In the case of an over-filled voxel, the voxel calculated is actually a rectangle.

For the following tests in this section, we will use the same parameters used to identify the issue. This used one clump mass $M_{cl} = 10 M_\odot$, voxel size $\Delta s = 0.1 pc$, ensemble dispersion $\sigma_{ens} = 1 \frac{km}{s}$, ensemble mass $M_{vox} = 10^1 M_\odot$, hydrogen number density $n_H = 10^5 cm^{-3}$, and far-UV radiation $\chi = 10^4 \chi_0$. The `test_fv` flag will always be set true, since this is the required method of calculation, and for this setup we will have $f_V \approx 4$. We will just be looking at the difference between the new calculation as described and the original calculation.

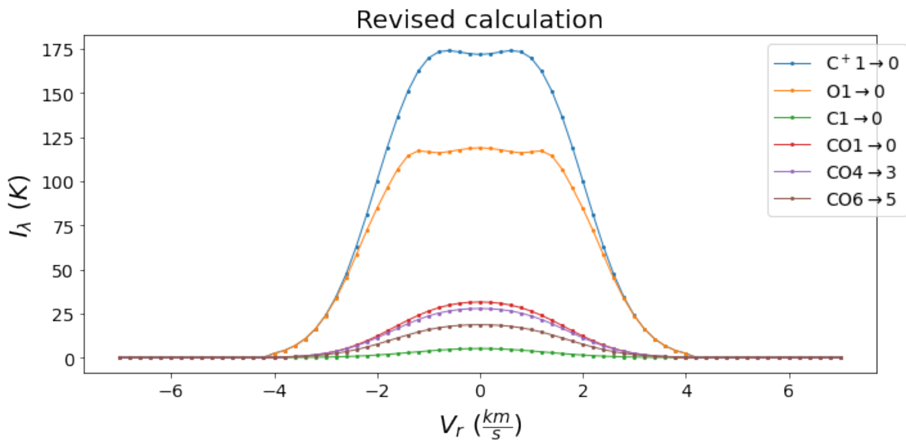
## 2.2 Original calculation

Here we will see the original form of the calculation, which tries to treat clump intensities as additive. As seen, there is a strange absorption feature for the CII $1 \rightarrow 0$ and OI 163 $\mu$m transitions.



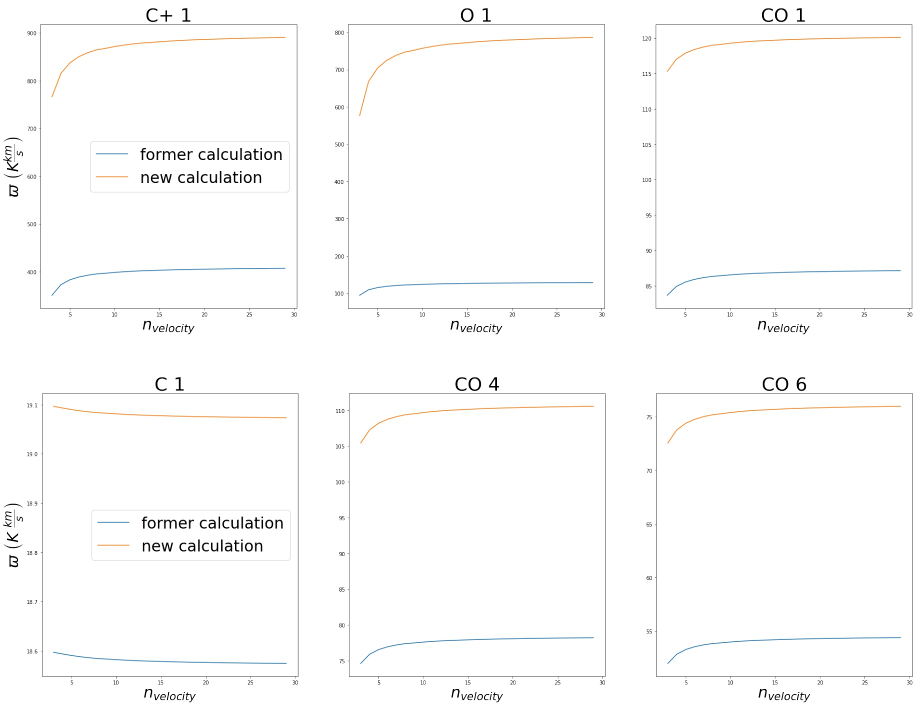

## 2.3 Revised calculation

Fixing the calculation to correctly treat the clump emissivities as additive, we see that the self-absorption features are still apparent for the CII $1 \rightarrow 0$ and OI 163 $\mu$m transitions.

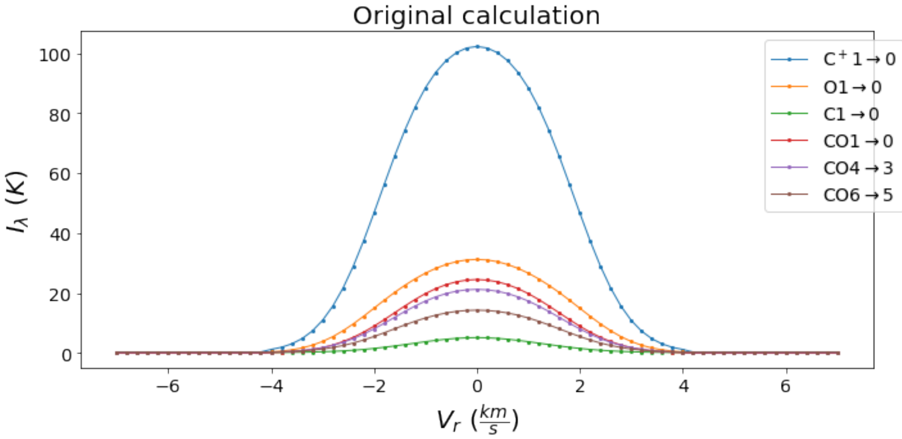


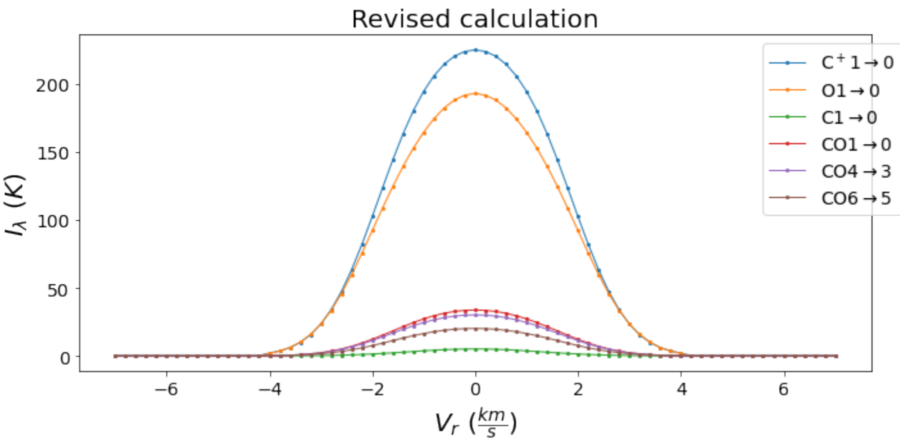
## 2.4 Convergence test

Another issue that might exist is that the internal velocity grid is too coarse. To this end, I implemented an option to change $n_{velocity}$, which affects the internal velocity grid spacing calculation ($\delta v = \frac{\sigma_{ens,j}}{n_{velocity}}$). Below I show the convergence of the integrated intensity $\varpi$ for a few transitions.




Clearly there should be a smaller step size for the internal velocity grid ($n_{velocity} = 10$ seems sufficient). What is quite alarming is the difference in the converged $\varpi$ for the new calculation and the old calculation. We can now recalculate the voxels in §2.2 and §2.3.






## 2.5 Summary/Issues

The issue appears to be in the internal velocity grid spacing $\delta v_j$. This fixes the self-absorption effect in both the original and the revised calculations. The issue is now that the new calculations give a much higher intensity for the transitions that had these self-absorption features. This is not the end of the issue, though. As noted by Markus a month ago, the intensity value used in the plots is the integrated intensity. That means the intensity profile of the single clump used in the calculation is incorrect. It could very-well be that the difference between these calculations would decrease if the code uses the correct clump emissivity/opacity. To that end, I guess I have a question for Markus: is it possible to get the maximum emissivity/opacity of the clumps in the grid (which is assumed to be the peak of a Gaussian with velocity dispersion $\sigma_{cl} \approx 0.71 \frac{km}{s}$)?