Development and Implementation of a 2D-RZ Geometry Short-Characteristics Radiation Transport Method for SPECT3D

1. Introduction

SPECT3D has the capability to compute non-LTE atomic level populations for 1-D and 2-D plasmas. This includes the capability of including the effects of photoexcitation and photoionization in the multi-level atomic rate equations. Several options are available for computing photoexcitation and photoionization rates, including an escape probability model (for bound-bound transitions) and a multi-angle *long-characteristics* model. The term *long-characteristics* refers to the case when the radiative transfer equation is solved, for a given ray on the angle grid, along all volume elements seen by that ray (*i.e.*, each ray passes through the entire plasma). Computation of photoexcitation and photoionization rates in each volume element is obtained by solving the equation of radiative transfer at a number of discrete frequency and angle points, integrating over angles to get the mean intensity in each volume element, and integrating the transition cross section over frequency to get the photoexcitation and photoionization rates.

The advantage of using the multi-angle long-characteristics model is that it is accurate. However, the CPU time required can be prohibitive when using complex atomic models (due to the large number of transitions and frequency points) and/or the spatial grid has a large number of volume elements (in particular, for multi-dimensional plasma grids). Alternatively, the escape probability model is significantly faster in terms of CPU, but suffers from the fact that it: (1) is an approximation in the case of bound-bound transitions, as it neglects radiation from outside the volume element of interest and neglects the effects of overlapping transitions; and (2) is not used at all in modeling bound-free transitions.

Because of the limitations of the escape probability and multi-angle long-characteristics models, we have developed a multi-angle *short-characteristics* model that provides for considerably better accuracy than the escape probability model, and requires much less CPU time as compared to the long-characteristics model. In addition, we have implemented the short-characteristics model using a novel approach in which the number of adjacent volume elements over which the radiative transfer equation is solved is variable. This approach allows for considerable flexibility in making trade-offs between accuracy and CPU time, and allows users to assess the sensitivity of SPECT3D results to potential uncertainties in the numerical radiative transfer technique applied.

In this section we describe the new short-characteristics model implemented in SPECT3D that is used in post-processing plasma grids with 2D R-Z geometry. Results are presented for benchmark calculations performed to assess the accuracy of the numerical model. Results are also presented from timing studies involving simulations with atomic models and spatial grids of varying sophistication. *These studies show that SPECT3D calculations utilizing the short-characteristics model typically require ~ 10^1 to 10^2 less CPU time than those utilizing the long-characteristics model, while still providing a reasonable level of accuracy.*

2. Short-N Characteristics Method and 2DRZ Geometry

In the 2DRZ geometry, all physical parameters are expressed in terms of cylindrical coordinates (ρ-φ-z) and are assumed to be independent of φ. That is, azimuthal symmetry is assumed. Spatial variations of physical parameters are thus reduced to the dependence on ρ-z coordinates.

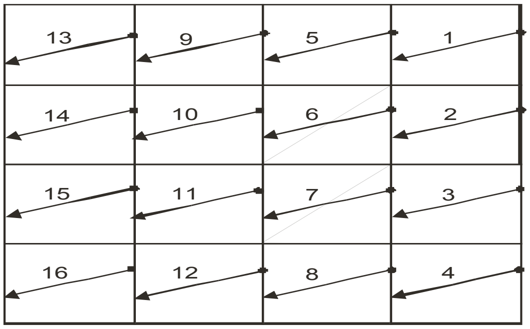
Physically, however, the plasma is in three-dimensional space, and thus the radiative transfer calculations must be done in a three-dimensional spatial grid. The corresponding three-dimensional spatial grid is a series of toriods obtained by rotating the initial 2D ρ-z spatial grid about the axis ρ = 0. A significant consequence of generating a three dimensional grid from 2DRZ geometry (for radiative transfer calculations), is that a ray that passes through the plasma, intersecting several different volume elements, will have different angles relative to each different volume element.

In applying the long characteristic method for radiative transfer, all rays passing through each volume element at each angle will be considered. As discussed above, this leads to a numerically intensive calculation. This in turn leads us to consider a short characteristic method in order to reduce the CPU-time requirements for the radiative transfer calculations.

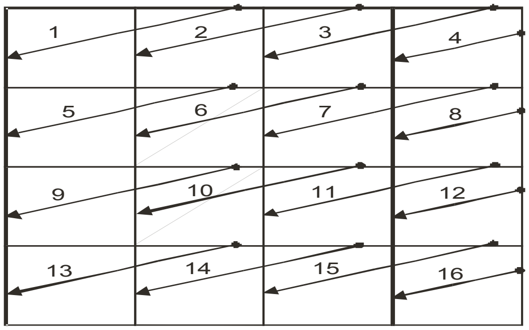
The basic idea of short characteristic methods is to reduce the radiative transfer calculations to a series of "short" spatial segments (rather than through "long" segments that extend throughout the plasma as in the long characteristic methods). Each short segment is contained within a single volume element and its beginning and ending points are at the walls of the volume element. The direction of the short segment is set by the numerical angular grid of the radiative transfer calculation. The intensity at the beginning of the segment is set by the corresponding intensities of the adjacent volume element (or by the boundary conditions of the plasma if the volume element under consideration is at the spatial boundary of the plasma). For each volume element and for each angle, the radiative transfer computations needed are done along the single volume element with the boundary conditions given by the previous volume element. This significantly reduces the amount of required radiative transfer computations, and thus the required CPU time.

During the development of this work we found that the accuracy of the short characteristic methods could be increased, while still significantly reducing the CPU time, by extending the radiative transfer calculations over "N" volume cells, where N is a small integer (rather than fixing N=1 as in the standard short characteristics method). In the current version of SPECT3D "N" is set to a default value of 3 and is modifiable by the user. We denote this approach as the "Short-N Characteristics Method". In Figure 1 we show a simplified schematic representation of the method. Below we show results obtained for different N.

In addition to the gain in CPU time efficiency, the short-N characteristic method also has the advantage of less memory requirements compared with the long characteristic method. For the calculations with the highest spatial resolution with the most detailed atomic model considered here (spatial grid of 150x80; 404 atomic energy levels for Ar), the short-N method with N=3 required ~580MB of RAM, while the same model with the long characteristic method required ~890MB of RAM.



N=1



N=2

Figure 1. Simplified schematic illustration of the Short-N characteristic method for N=1 (above) and N=2 (below). The arrows indicate the short segments through which the radiative transfer (rt) calculations will be done. The numbers above the arrows indicate the order in which rt calculations will be done.

3. Geometric Calculations

Since Spect3D post processes hydrodynamic data with arbitrary spatial grids, geometric calculations are implemented after the hydro data is read and before the actual radiative transfer computations. The geometric calculations are independent of the values of intensities and in particular of the photon energies considered. The results from these computations are stored in memory and accessed as needed during the radiative transfer calculations. Hence the geometric computations do not significantly increase the CPU-time required for post processing hydrodynamic data.

In these computations, geometric parameters for each volume element and for each angle (such as intersection positions of short segments with volume element walls, relative angles, etc.) are calculated and stored. The required interpolation parameters for intensities, as well as the corresponding dependences with respect to the short-N characteristic method are also determined and stored. The order of the different short-N segments, on which the radiative transfer computations are done, is also determined at this point to ensure that corresponding boundary conditions for each short segment will have been computed before the radiative transfer computations are done on the given segment.

4. Radiative Transfer Computations

Radiative transfer computations are performed on the short-N segments in the order previously determined by the geometric calculations. First, radiative transfer computations are done on short-N segments that have a beginning point at the boundary of the plasma, followed by computations in adjacent volume elements in inward directions. The process will continue, eventually computing on short-N segments in the outward directions until every short-N segment has been computed upon.

Mean intensities are then calculated for each volume element, and the general numerical iterative process described above proceeds until atomic level populations converge.

5. CPU-time efficiency: Short-N Characteristics vs. Long Characteristics

The gain in CPU-time-efficiency of the short-N radiative transfer method vs. the long radiative method will depend on the size of the spatial grid. For a spatial grid of n×n the respective CPU-times approximately vary with 'n' as

$$\text{Long-Characteristics (Radiative-Transfer-Time)} \sim n^3$$

$$\text{Short-N-Characteristics (Radiative-Transfer-Time)} \sim n^2$$

That is, short-N characteristics methods will be of the order of 'n' times more efficient that the long-characteristic method. The larger the spatial grid, the larger the relative efficiency of the short-N method will be.

Now, the total CPU-time for post processing a hydro data file is dominated by two sets of computations: first, the radiative transfer itself, which is the focus of the efforts described here, and second, the calculation of the opacities used in the radiative transfer. In turn, the opacity-calculation-time is proportional to the number of volume elements in the spatial grid, that is

$$\text{Opacity-Calculation-Time} \sim n^2$$

Thus, the relative gain in CPU-time efficiency with the short-N method will increase for higher spatial resolutions and will also increase for less-detailed atomic models that require less time for the opacity calculations.

As we show below, post processing a high spatial resolution hydro data file with detailed atomic models that took several weeks on a single CPU system with the long-characteristic method, can now be done within 36 hours on the same computer system with the short-N method.

6. Comparison with Analytic Results

As with the earlier long characteristic method implemented in *SPECT3D*, the short-N characteristic method has been tested against analytic results. In particular, we consider a plasma, with a uniform source function S_ν, occupying a cylindrical volume of height H and radius R, represented with a spatial grid of 10×20 ($\rho \times z$).

In Figure 2 we show the plots of the mean intensity vs. radius for optical depths, τ_R, along the radial direction of (left) τ_R=1.825 and (right) τ_R=0.165 respectively, and for the value of the short-N-parameter of N=3, superimposed with the analytic solutions. We see from Figure 2 that the differences between the numerical short-N mean intensities and the analytic mean intensities are larger towards the center of the cylinder (r=0, z=0). This is because the intensities in these regions, in all directions, are obtained through the radiative transfer calculations over many short-N segments (rather than through a single ray as in the long characteristic methods).

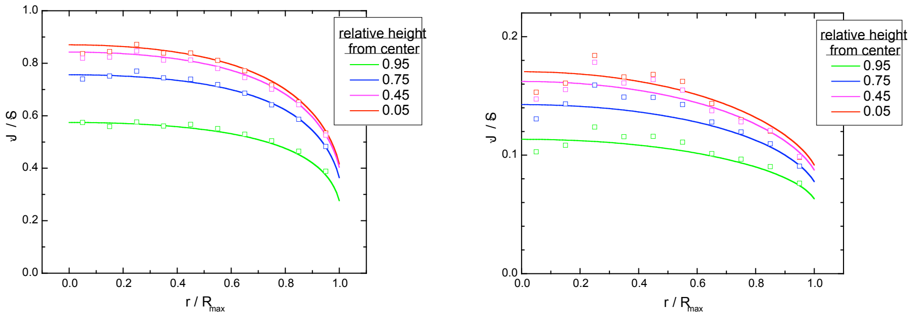


Figure 2. Spatial variation of the mean intensity for a plasma on a 2DRZ grid calculated using the short-N characteristic method (open squares) for N=3. Results are shown for several heights within the cylinder. The solid lines are the analytic solutions. (left) τ_R=1.825; (right) τ_R=0.165.

As a consistency check, in Figure 3 we show plots of the mean intensity vs. radius for optical depths along the radial direction of (left) τ_R=1.825 and (right) τ_R=0.165 respectively, but for the value of the short-N-parameter of N=20. As expected, the agreement with the analytic solution is excellent.

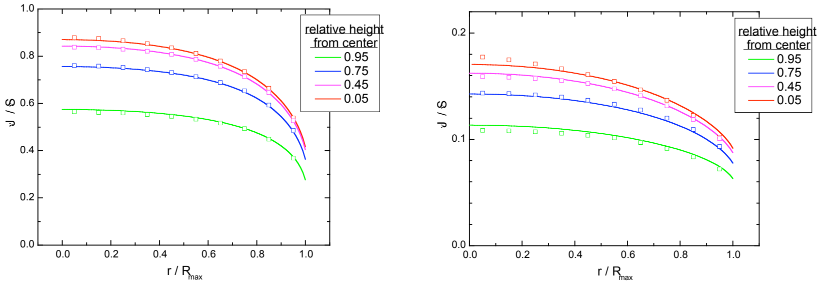


Figure 3. Spatial variation of the mean intensity for a plasma on a 2DRZ grid calculated using the short-N characteristic method (open squares) for N=20. Parameters are the same as in Figure 2.

7. Results and Discussion – Ar Doped Problem

The results shown in this section correspond to the same physical problem: A spherical plastic shell with radius 0.028 cm and thickness of 0.002 cm filled with Ar-doped deuterium (0.05% Ar). The temperature of the Ar-doped deuterium varies from 1500 eV at the

plasma center to 200 eV at the plastic shell. The density of the Ar-doped deuterium varies from 0.3 g cm^{-3} at the plasma center to 0.5 g cm^{-3} at the plastic shell.
These physical parameters correspond to an idealized model for a typical ICF (Inertial Confinement Fusion) experiment at the time of implosion stagnation.

Azimuthal symmetry is assumed and all cases are computed under 2DRZ geometry. What varies in the different cases of this section is the spatial resolution implemented and the atomic model used for Ar in the calculations.

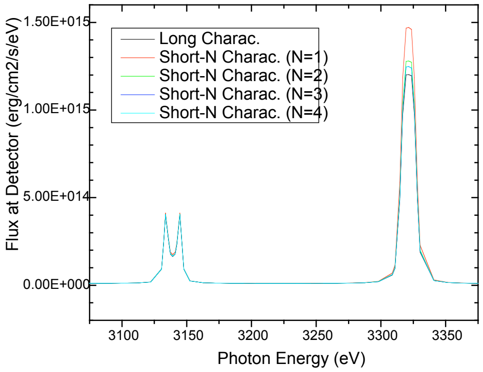


Figure 4. Spectra produced by the long characteristic method and the short-N method for different values of the N-parameter. The spatial grid of the problem is 10x10 and a simple atomic model of 11 (eleven) energy levels for Ar was used.

In Figure 4 we show plots of the spectra produced by the long characteristic method and the short-N method for different values of the N-parameter for a low spatial resolution of 10x10 and a simple atomic model for Ar of 11 (eleven) energy levels. In Figures 4 we show plots of the spectra produced by the long characteristic method and the short-N method for N=1 and N=2, for a low spatial resolution of 10x10 and a detailed atomic model for Ar of 404 energy levels. Note that the agreement with the long characteristic method tends to increase with larger N, illustrating that the accuracy of the short-N method increases with the N-parameter.

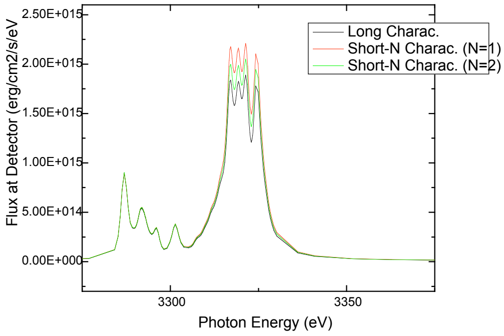


Figure 5. Spectra produced by the long characteristic method and the short-N method for N=1 and N=2. The spatial grid of the problem is 10x10 and a detailed atomic model of 404 energy levels for Ar was used.

In Tables 1 to 6, we show the comparison of CPU times between the short-N characteristic method and the long characteristic method applied to the Ar Doped problem for three spatial resolutions of 10 x 10, 50 x 50 and 150 x 80, and two atomic models for Ar with 11 and 404 energy levels. By comparing the fourth and sixth columns of the tables, we note that the relative gain in efficiency for the complete *SPECT3D* computation is less than the relative gain in efficiency of the radiative transfer calculation. This because a significant part of the *SPECT3D* computations is for opacity calculations that are performed previous to the radiative transfer calculations. The effects on the CPU-time due to the opacity calculations can be clearly seen by comparing the fourth and sixth columns of the tables. One can see that, although the relative gain in efficiency in the radiative transfer calculations is similar for all tables, the relative gain for the total SPECT3D computation is considerably higher for the simpler atomic models (odd numbered tables) since it requires significantly fewer opacity calculations.

Radiative Transfer Method	N-Param.	Total Time	Total Time Long / Total Time Short-N	Radiative Transfer Time	Radiative Transfer Time Long / Radiative Transfer Time Short-N	% diff (with respect to Long Charac.)
Long Charac.	N/A	04m 58s	1.00	04m 44s	1.00	0.00%
Short-N Charac.	1	38s	7.84	15s	18.93	21.45%
Short-N Charac.	2	46s	6.48	24s	11.83	5.83%
Short-N Charac.	3	56s	5.32	35s	8.11	3.15%
Short-N Charac.	4	67s	4.45	45s	6.31	3.09%

Table 1. Comparison of CPU times between the short-N characteristic method and the long characteristic method applied to an Ar Doped problem for a lowl resolution of 10x50 and a simple atomic model for Ar of 11 energy levels. Column 1: Radiative transfer method. Column 2: N-Parameter. Column 3: Total CPU time used for the *SPECT3D* simulation. Column 4: Ratio between the total CPU time for the long characteristic method and the total CPU time for the given radiative transfer method. Column 5: CPU time for the radiative transfer calculations. Column 6: Ratio of the CPU time for the radiative transfer calculations between the long characteristic method and the given radiative transfer method. Column 7: Percentage difference of the spectral intensity at the peak of the strongest line of the obtained spectrum with the given radiative transfer method, measured with respect to the value obtained through the long characteristic method.

Radiative Transfer Method	N-Param.	Total Time	Total Time Long / Total Time Short-N	Radiative Transfer Time	Radiative Transfer Time Long / Radiative Transfer Time Short-N	% diff (with respect to Long Charac.)
Long Charac.	N/A	01h 26m 37s	1.00	45m 12s	1.00	0.00%
Short-N Charac.	1	01h 01m 52s	1.40	02m 29s	18.20	17.52%
Short-N Charac.	2	01h 03m 07s	1.37	03m 59s	11.35	9.17%
Short-N Charac.	3	01h 04m 29s	1.34	05m 36s	8.07	6.07%
Short-N Charac.	4	01h 25m 02s	1.02	09m 21s	4.83	6.03%

Table 2. Comparison of CPU times between the short-N characteristic method and the long characteristic method applied to an Ar Doped problem for a low spatial grid resolution of 10x10 and a detailed atomic model for Ar of 404 energy levels. The columns of the table are same as Table 1.

Radiative Transfer Method	N-Param.	Total Time	Total Time Long / Total Time Short-N	Radiative Transfer Time	Radiative Transfer Time Long / Radiative Transfer Time Short-N	% diff (with respect to Long Charac.)
Long Charac.	N/A	04h 19m 33s	1.00	04h 16m 12s	1.00	0.00%
Short-N Charac.	1	10m 33s	24.60	06m 17s	48.49	39.34%
Short-N Charac.	2	12m 33s	20.68	07m 34s	33.86	19.57%
Short-N Charac.	3	15m 20s	16.92	10m 20s	24.79	10.74%
Short-N Charac.	4	17m 33s	14.79	12m 37s	20.31	6.85%
Short-N Charac.	5	23m 39s	10.97	17m 51s	14.35	4.82%

Table 3. Comparison of CPU times between the short-N characteristic method and the long characteristic method applied to an Ar Doped problem for a mid-spatial resolution of 50x50 and a simple atomic model for Ar of 11 energy levels. The columns are the same as in Table 1.

Radiative Transfer Method	N-Param.	Total Time	Total Time Long / Total Time Short-N	Radiative Transfer Time	Radiative Transfer Time Long / Radiative Transfer Time Short-N	% diff (with respect to Long Charac..)
Long Charac.	N/A	02d 00h 02m 10s	1.00	01d 15h 19m 30s	1.00	0.00%
Short-N Charac.	1	13h 24m 55s	3.58	51m 52s	45.49	19.84%
Short-N Charac.	2	15h 55m 51s	3.02	01h 28m 20s	26.71	11.52%
Short-N Charac.	3	16h 21m 19s	2.94	01h 55m 55s	20.35	6.84%
Short-N Charac.	4	16h 24m 28s	2.93	02h 20m 40s	16.77	4.26%
Short-N Charac.	5	16h 48m 00s	2.86	02h 45m 23s	14.27	2.90%

Table 4. Comparison of CPU times between the short-N characteristic method and the long characteristic method applied to an Ar Doped problem for a mid-spatial resolution of 50x50 and a detailed atomic model for Ar of 404 energy levels. The columns are the same as in Table 1.

Radiative Transfer Method	N-Param.	Total Time	Total Time Long / Total Time Short-N	Radiative Transfer Time	Radiative Transfer Time Long / Radiative Transfer Time Short-N	% diff (with respect to Long Charac.)
Long Charac.	N/A	01d 07h 30m 40s	1.00	01d 07h 16m 40s	1.0	0.00%
Short-N Charac.	1	36m 11s	52.25	23m 50s	78.74	44.05%
Short-N Charac.	2	45m 40s	41.40	33m 42s	55.69	24.84%
Short-N Charac.	3	54m 17s	34.83	42m 24s	44.26	18.77%
Short-N Charac.	4	01h 03m 30s	29.77	51m 33s	36.40	14.78%
Short-N Charac.	5	01h 11m 49s	26.33	59m 44s	31.42	11.00%
Short-N Charac.	6	01h 19m 02s	23.92	01h 07m 06s	27.97	8.45%
Short-N Charac.	7	01h 27m 21s	21.64	01h 15m 20s	24.91	6.92%

Table 5. Comparison of CPU times between the short-N characteristic method and the long characteristic method applied to an Ar Doped problem for a high spatial grid resolution of 150x80 and a simple atomic model for Ar of 11 energy levels. The columns of the table are same as Table 1

Radiative Transfer Method	N-Param.	Total Time	Total Time Long / Total Time Short-N	Radiative Transfer Time
Long Charac.	N/A	> 14d 00h 00m 00s	1.00	--
Short-N Charac.	1	01d 07h 11m 10s	> 10.77	03h 18m 53s
Short-N Charac.	2	01d 08h 36m 30s	> 10.30	04h 56m 04s
Short-N Charac.	3	01d 10h 13m 50s	> 9.82	06h 27m 09s
Short-N Charac.	4	01d 10h 40m 50s	> 9.69	07h 40m 10s
Short-N Charac.	5	01d 11h 59m 00s	> 9.34	08h 56m 13s
Short-N Charac.	6	01d 13h 33m 40s	>8.95	10h 23m 07s
Short-N Charac.	7	01d 14h 39m 40s	> 8.69	11h 36m 38s

Table 6. Comparison of CPU times between the short-N characteristic method and the long characteristic method applied to an Ar Doped problem for a high spatial grid resolution of 150x80 and a detailed atomic model for Ar of 404 energy levels. The columns of the table are same as the first five columns of Table 1

In Figure 5.6 we show plots of the spectra produced by the long characteristic method and the short-N method for different values of the N-parameter for a high spatial resolution of 150x80 and a simple atomic model for Ar of 11 (eleven) energy levels, and find conclusions similar to those of the low spatial resolution model of Figures 4 and 5.

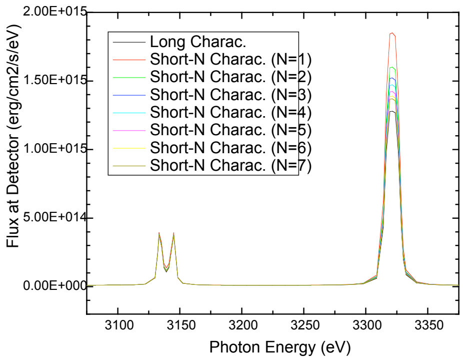


Figure 6. Spectra produced by the long characteristic method and the short-N method for different values of the N-parameter. The spatial grid of the problem is 150x80 and a simple atomic model of 11 (eleven) energy levels for Ar was used.

In Figure 7 we plot the ratio of the total CPU times for *SPECT3D* calculation using the long characteristic method and the short-N characteristic method for N=3 vs. the square root of the total number of volume elements in the spatial grid. In Figure 7, we see that significant increases in the time efficiency of the radiative transfer calculations are gained with the Short-N characteristic method with respect to the long characteristic method. We also see that the relative gain in efficiency increases with higher spatial resolution, approximately in proportion to the number of volume elements along a single dimension.

The most “realistic” computation considered here, the one with the high spatial resolution of 150x80 and a detailed atomic model of 404 energy levels for Ar, shows a gainx in CPU-time efficiency for the total *SPECT3D* computation of over a factor of ten.

This run that previously took several weeks with the long characteristic method, is now running within 36 hours with the Short-N method without loss of accuracy.

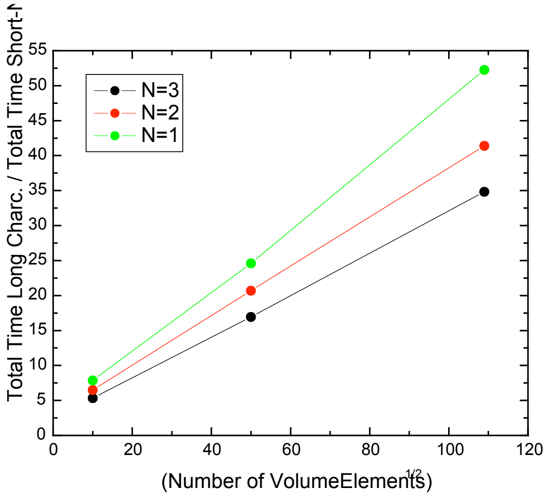


Figure 7. Ratio of the total CPU times for the post processing of *SPECT3D* between the long characteristic method and the short-N characteristic method for N = 1, 2 and 3 vs. the square root of the total number of volume elements in the spatial grid.

8. Summary and Conclusions

- We have developed a new radiative transfer method named "Short-N Characteristic", and have implemented it in the *SPECT3D* plasma simulation application for 2DRZ geometries. The method is a hybrid between the standard long characteristic methods and the standard short characteristic methods.
- The Short-N radiative transfer method has the advantage of simultaneously keeping the accuracy of the long characteristic methods and the CPU-time efficiency of the standard short characteristic methods.
- The implementation of the method has been successfully tested against analytical solutions in 2DRZ geometries.
- In one of the benchmarking tests, for a high spatial resolution of 150x80 with a detailed atomic model of 404 energy levels, a run that previously took several weeks with the long characteristic method, is now running within 36 hours with the Short-N method without loss of accuracy.
- We are currently working on implementing the Short-N characteristic method for other geometries within the *SPECT3D* plasma simulation application software.