Report on the outcomes of a Short-Term Scientific Mission[1]

Action number: CA21126

Grantee name: Lucio Crivellari

Details of the STSM

Title: ***Novel algorithms to compute the structure of the outer layers of AGB stars***

Start and end date: 24/05/2023 to 09/06/2023

Description of the work carried out during the STSM

Description of the activities carried out during the STSM. Any deviations from the initial working plan shall also be described in this section.

Complex molecules, including nC species (carbonaceous molecules), are mostly synthesized in AGB stars and are the main candidates to drive mass loss in their outermost layers. Investigation of the formation of the above molecules will cast light on the physical processes at the origin of the formation of complex molecules and dust grains, the main purpose of the research project CA21126. The numerical computation of the outer structure of AGB stars is an essential tool for further developments of the project. In order to model both the physics and the chemistry of the cool expanding layers of AGB stars our group, at the INAF-Osservatorio Astronomico d'Abruzzo and Instituto de Astrofísica de Canarias, developed initially the VULCAN code (see Cristallo *et al.,* 2021, hereinafter Paper I). It is a Lagrangian 1D hydrodynamic code which adopts, however, the same assumptions and simplifications introduced by Bowen (1988). In particular the treatment of radiative transfer (RT) is quite rough and the determination of the radiative equilibrium temperature, essential to determine the internal energy change driven by periodic outward-moving shocks, is calculated by using the Eddington approximation for a grey plane parallel atmosphere. In order to get rid of these shortcomings we introduced an operative approach to computing the outer layers of AGB stars based on the iterative sequential procedure introduced by E. Simonneau and L. Crivellari (see Crivellari *et al*., 2021, hereinafter Paper II). It includes the solution of the monochromatic RT in spherical geometry as described in Gros *et al*. (1997).

1 This report is submitted by the grantee to the Action MC for approval and for claiming payment of the awarded grant. The Grant Awarding Coordinator coordinates the evaluation of this report on behalf of the Action MC and instructs the GH for payment of the Grant.

References

Bowen, G.H. 1988, *Ap. J.*, **329**, 299.

Cristallo, S., Piersanti, L., Gobrecht, D., Crivellari, L. and Nanni, A. 2012, *Universe*, **7(4)**, 80,

Paper I.

Crivellari, L.,Cristallo, S. and Piersanti, L. 2012, *Universe*, **7(9)**, 340, Paper II.

Gros, M., Crivellari, L. and Simonneau, E. 1997, *Ap. J.*, **489**, 331.

Last year we we wrote a code that yields a self-consistent solution of the equations that shape the structure of a stellar atmosphere. The relevant results have been already presented in Paper II. The backbone of the code is the iterative sequential procedure introduced by E. Simonneau and L. Crivellari (see *The stellar atmosphere physical system. II. An operative sequential algorithm to solve the stellar atmosphere problem*, L. Crivellari, 2019, *Serb. Astron. J*., **198**, 1), which requires an educated guess of the distribution of the temperature with geometrical depth in order to compute the intial structure of the outer layers of the stellar atmosphere, the bootstrap of the iterative procedure whose output shall be a final structure that fullils the constraint of energy conservation. The first days of the stay (since May 25th through June 1st) were devoted to achieve such a physically consistent initial structure.

In the successive step (June 2nd to June 4th) we revised the bolometric radiative transfer equation for the radiation field integrated over the whole frequency range, which is at the core of the temperature correction that will yield the temperature that warrants the radiative equilibrium and successively worked out the numerical criteria to achieve the convergence to the physically correct solution.

Eventually (June 5^{h} through June 8th) we converted the original code into the TEIDE subroutine, that was successfully implemented into the VULCAN code, described in Paper I. The encouraging results so far achieved pave the way to the further full development of the VULCAN code. The last day was devoted to a throughout discussion of the physical soundness of the numerical algorithms employed and their future improvement. There was no time for approaching the parallelization of the code, one of the goals indicated in the Working Plan of the APPLICATION FORM.

Description of the STSM main achievements and planned follow-up activities

Description and assessment of whether the STSM achieved its planned goals and expected outcomes, including specific contribution to Action objective and deliverables, or publications resulting from the STSM. Agreed plans for future follow-up collaborations shall also be described in this section.

The preliminary results obtained by running the up-to-dated version of VULCAN turned out satisfactory. We are looking forward to the next mission, whose goal will be the ultimate version of the VULCAN code, to be delivered for use within the objectives of the Action. The presentation of the numerical methods employed and the discussion of the results will be the subject of a major paper.

However the robustness of the code shall be verified when the formation of shocks produced by a periodical piston mechanism is duly taken into account. The propagation of shocks induces large variations of the physical conditions of the outer circumstellar layers, which could result in numerical instabilities brought about by an inadequate choice of the radial mesh on which the structure of the stellar atmosphere is computed. As discussed at the end of the stay, physical improvements shall be introduced in a near future, among them the inclusion of radiation pressure into the equation of

hydrostatic equilibrium and a proper parametrization of the dissipation of non-radiative energy in the overall energy balance equation.