

SolPOC: a Python Package for Modelling the Optical Coating Used in Solar Thermal Energy Systems

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Abstract. Solar collectors of all types (thermal or photovoltaic, with or without concentration) require one or more surface treatments during their solar radiation conversion. These treatments are made up of thin layers of materials stacked that constitute mirrors, glass panes, thermal absorbers, or cover the junctions of PV cells. To allow all stakeholders in the solar community to easily model the optical behavior of their thin layer stacks we propose our in-house code. SolPOC (Solar Performances Optimization Code) is a Python Package specifically designed to provide a better understanding of coatings, thin film deposition of materials for solar energy applications and especially for Solar Thermal Energy Systems. The package includes a stable and fast method to calculate the spectral reflectivity, transmissivity, and absorptivity of a stack of thin films over the full solar spectrum and maximize the solar performance of the stack by optimizing its characteristics. SolPOC comes with several optimization methods, a script using multiprocessing pool tools, and a comprehensive database of refractive indices of real materials. The code has already produced major scientific advances in research on coatings for solar thermal systems. It is simple to use for non-coder users, automatically saves important results and is freely available on GitHub with a complete documentation and tutorials.

Keywords: Thin Layers, Modelling, Solar Energy, Optics

1. Introduction

Harvesting solar energy for heat production using Concentrated Solar Thermal (CST), for electricity production using Concentrated Solar Power (CSP) or for a variety of systems (Solar Thermal Systems, building and photovoltaic), all require materials with optically efficient surface properties, which can be provided by thin layer stacks. We can cite as examples the nanometric thin layer of silver or aluminum for a solar mirror, or the thin stack used for ensuring antireflective properties [1], [2]. In the case of solar thermal receivers for CSP, they should be highly absorptive in the solar range (0.28 – 4 μm) to harvest as much solar radiation as possible, but also have low emissivity in the infrared range (1 – 50 μm) to reduce radiative thermal losses [3], [4]. This effect, called “spectral selectivity” can easily be achieved using multilayered coating architectures [5]. All these coatings that need to be optically designed and optimized in terms of layer thicknesses and compositions, to guarantee their high optical performance.

In conclusion, harvesting solar energy requires materials with high quality surface properties, which can be provided by thin layer stacks.

Working on the development of solar energy coatings we have developed our own in-house code to solve Maxwell's equations in multilayered thin film structures. This allows us to easily model the optical properties (reflectance, transmittance and absorptance) of any thin film coating. This code is used for studying, modeling and optimizing a wide variety of optical surfaces treatments, using the following features:

1. Calculate the optical properties of a large number of stacked thin layers in the solar spectral domain.
2. Compile optical data from a large variety of materials, including custom materials that can easily be added by the users.
3. Optimize the characteristics of these stacks to accommodate a wide range of thin layer combinations and functionalities, thus proposing efficient designs of multilayer stacks.

Given the number of challenges involved, we now seek to share our code with the solar research community as a ready-to-use and free software that fills the gap of existing solutions. The whole project, named SolPOC (Solar Performance Optimization Code) is now free and available as a Python package through the PyPI repository with source code hosted on GitHub [6], [7]. Furthermore, we have provided comprehensive documentation, example scripts and tutorials (using Jupyter Notebooks) all located on the GitHub platform. SolPOC has been designed to serve as a readily accessible solution in the field of coatings for solar energy, keeping in mind the fundamental principles of Open Science. The software is distributed under a GPL-3.0 license.

2. Overview of SolPOC

The Solar Performance Optimization Code (SolPOC) package is tailored for investigating coatings, thin film deposition, and materials utilized in solar energy applications, including solar thermal, concentrated solar thermal, Concentrated Solar Power (CSP), photovoltaics (PV), low-e windows, buildings, and others. It provides user-friendly and comprehensive tools designed for the thermal solar community. SolPOC quickly and easily computes the reflectivity, transmissivity, and absorptivity over a full solar spectrum of a stack of thin films and is accessible for non-coder users.

2.1 General overview of SolPOC Python Package

SolPOC is a free, tunable, versatile, and fast code designed for research in the field of solar energy coatings. The code operates within the Python 3 programming environment. Our approach aligns with an open-source and reproducibility policy. The code is freely available on GitHub or can be installed directly using the "`pip install solpoc`" command from any Python terminal. Examples and Ready-to-use scripts are also provided and can be easily used, using the "`!solpoc-init`" command. The GitHub page includes a comprehensive user guide, several Jupyter Notebook tutorials, and numerous examples. The target goal of SolPOC is to assist researchers in the solar community by easily simulating and managing multilayer thin films, enabling them to test, evaluate and optimize new thin layer architectures for solar energy.

2.2 Optical properties of multilayer thin films

We have implemented in SolPOC a very fast and stable calculation of optical properties of thin layer stacks using the Abélès formalism method [8]. This crucial step allows us to calculate the reflectivity, transmissivity and absorptivity of one or several thin layers stacks (up to 150 layers) using the complex refractive index of each materials used. The selected Abélès formalism

method (which is different from Transfer Matrix Method, known as TMM) provides the best compromise between time and stability compared to TMM according to the literature [9].

To meet the specific needs of the solar community, the calculation of optical properties is done across a wide solar domain extending to infrared, typically from 280 nm to 2500 nm with a 5 nm step and extending up to 30 μm . Regarding the large size of the spectral domain and the need of accuracy (SolarPACES reflectance Guideline strongly recommend a 5 nm step) we have vectorized the core code structure around NumPy package [10]. It allows us to maximize computational efficiency, which strongly reduces the calculation time per CPU [11]. In-house benchmarking shows us a calculation time using SolPOC are shorter than those other codes, such as TMM Fast, Solcore or PyMoosh [12], [13], [14].

2.3 Materials for solar thin layers stack

The raw data used for calculating optical properties are the refractive indices ($N = n + ik$) of each used material used. SolPOC offers an extensive database containing optical properties for 130 types of materials, particularly those relevant to solar thermal energy systems. The database includes metals, dielectrics, conductive oxides, and some semiconductors. All these materials have been carefully selected by the authors through a critical review of scientific literature and technical catalogs [15], [16]. We propose a preselected dataset, with refractive indices measured on thin films rather than bulk materials, using experimental measurements rather than modeling, and studies with numerous measurement points to minimize reliance on interpolation and extrapolation by the code. Most selected data cover a broad solar spectral range (280 – 2500 nm) and often extend into the mid-infrared range to reduce errors in calculating solar properties or radiative losses [17], [18]. The complete database is accessible directly through the package, allowing users to quickly test coating architectures without requiring a download. Advanced users can follow the user guide and incorporate their own refractive index data by simply adding text files to a local folder.

Additionally, the code incorporates an Effective Medium Approximations (EMA) method, allowing the possibility to use composite layers in the thin film architectures. These composite layers can include, for example, porous layers (such as a mixture of air and dielectric, like porous SiO_2 used in antireflective coating) or cermets (combinations of metal inclusions within a dielectric matrix, used in Spectrally Selective Thermal Absorber (SSTA)). The Bruggeman theory is implemented into SolPOC. This theory is frequently used in the solar community and has already been discussed in the literature and in our previous papers [2], [19].

2.4 Optimize the thin layers stack

The major aim of the Solar Performance Optimization Code (SolPOC) is to design highly effective thin layer stacks for solar thermal energy systems. In most cases, an optimized multilayer stack is achieved through a careful selection of materials, but more importantly, through precise determination of the optimum thickness of each thin layer and the volume fractions in the case of composite material. SolPOC can optimize the entire thin layer stack to achieve high solar efficiency (e.g., highest solar reflectance or heliothermal efficiency for SSTA), including different layer compositions in the case of composite layers (porous or cermet). Many objective functions (quantitative estimation of the solar performance of a given multilayer stack) are already implemented and described in the code documentation. Additional inputs, as ASTM G173-03 AM1.5 reference solar spectra or common solar cell spectral response are already also available [20], [21]

SolPOC offers various evolutionary algorithms such in-house Genetic Algorithm (GA) method, Differential Evolution (DE), Particles Swarm Optimization (PSO), and the One plus One ((1+1)-ES) algorithm. It also includes a simulated annealing method for comparison (a non-gradient-based optimization method) [22], [23]. Each optimization algorithm has its own pros and cons, but we recommend using PSO or Differential Evolution (DE). Bennet et al. have

shown in their work that the gradient free method DE can reach high quality results, even superior to Needle performance, a classical optimization often used in the multilayer community [24], [25]. At the end, SolPOC package provides a multiprocessing pool tools script that is "ready to use" for non-coder users. This enables each optimization to be run multiple times in parallel, which increases the robustness and reliability of the results. The shape of the solar spectrum (if used) introduces numerous local minima in the optimization process. For complex thin layer stacks (up to four layers) we recommend running the optimization process multiple times. This is straightforward when using SolPOC.

SolPOC has already driven significant scientific progress in solar thermal coatings research and is currently being used in the SelHySol research project for developing spectrally selective surfaces for compact hybrid PV/CST solar receivers [26].

3. Results

Fig 1 provides an overview of SolPOC application [8]. After describing the stack (number of layers and materials used) the user selects one objective function integrated into the package (such as maximized solar reflectance, for instance) or creates their own. Additionally, solar spectra or other parameters like human eye sensitivity or PV cell spectral efficiency are directly incorporated and can be easily changed. Subsequently, the software optimizes the stack using one of the six available global optimization methods, which can include optimizing thin layer thicknesses, compositions (for cermet or porous materials), or even the ideal value of refractive index. This procedure is iterated multiple times, facilitated by parallelizable code, which enables the determination of an optimized stack and ensures confidence in the optimization outcomes. Finally, the code automatically saves different figures or data to help the users in result interpretation.

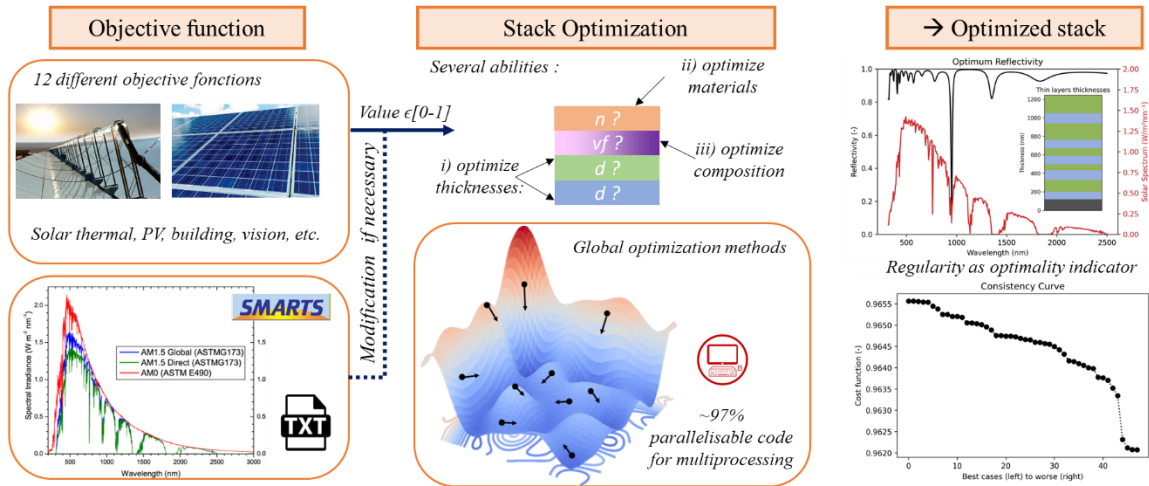


Figure 1. SolPOC offers a wide range of objective functions suitable for solar energy and other. After choosing global optimization method, the code quickly optimizes the stack [8].

3.1 Example: Spectrally Selective Thermal Absorber

To illustrate one potential use of SolPOC, we propose a coating optimization for a Spectrally Selective Thermal Absorber used for CSP applications. This well-known case within the CSP community involves maximizing heliothermal efficiency. It is defined as the solar energy absorbed minus radiative thermal losses divided by the total available solar energy, all calculated under a given concentration ratio and the thermal absorber's temperature. Equations can easily be found in SolPOC documentation or in literature [6], [19]. To ensure the spectrally selective effect, which guarantees good heliothermal efficiency, we propose using two different materials: tungsten (W) and aluminum oxide (Al_2O_3) to create a three-layer stack (W/W-

$\text{Al}_2\text{O}_3/\text{Al}_2\text{O}_3$) deposited on an iron substrate (Fe), all present in SolPOC materials database. In this example, maximizing the heliothermal efficiency of the thin layer stack involves finding the ideal thickness of each thin layer and the optimal composition for the cermet (named the volume fraction, the volumic percentage of W in $\text{W-Al}_2\text{O}_3$) for a total of four parameters. Thus, the use of an optimization code like SolPOC is necessary.

Once the SolPOC package is properly installed, the user can open the ready-to-use optimization script (optimization_multiprocess.py). The script's usage is detailed in the user guide and in the Jupyter Notebooks. The GitHub repository also contains a pre-configured file, and the associated results presented here (tutorial_selective_coating.py). This optimization script is straightforward to use: all the necessary variables are grouped and described, effectively creating a sort of GUI. We made this choice to ensure the script is easy to use for non-coders while allowing advanced users to easily adapt and modify the code for their specific needs. Note that all specific functions related to the solar energy system, such as modeling the optical properties of the stack over a full solar spectrum, evaluating heliothermal efficiency, or specially tuned evolutionary optimizations, are provided by SolPOC.

The left plot (**Figure 2**) shows the spectral reflectivity of the optimized stack, which exhibits a typical spectrally selective effect, indicating that the optimization has been well-executed. SolPOC automatically adapts the figure related to reflectivity according to the specific case (in this instance, evaluating heliothermal efficiency). The stack's reflectivity (in black) is presented alongside the ASTM G173-03 DC solar spectrum (in red) and a blackbody curve (in orange), calculated based on the thermal absorber temperature (here, 300°C). Note that the blackbody curve is illustrative; its shape is normalized to match the maximum of the solar spectrum (in red). The reflectivity is minimized in the solar domain (solar absorptance: 94.22%) and maximized in the infrared domain (thermal emissivity at 300°C : 8.62%). The total heliothermal efficiency (under a concentration factor of 80) is maximized at 93.25%. The figure on the right provides a global overview of the optimized stack, with each layer's thickness accurately scaled. Each material is represented with a thematic color according to its refractive index. Other files and figures provided by SolPOC allow the user to easily identify the optimum thickness of each thin layer, which are as follows: 165 nm of W, 103 nm of $\text{W-Al}_2\text{O}_3$ with 26.5% volumetric fraction, and 76 nm of Al_2O_3 .

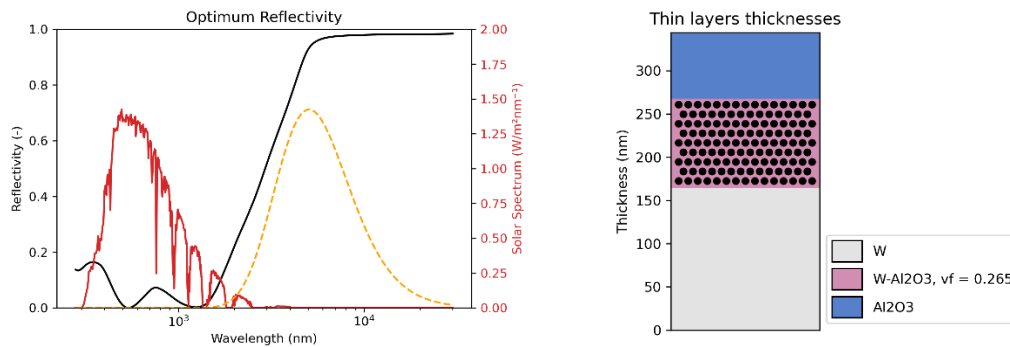


Figure 2. At left, the optimum reflectivity curve, with a solar AM 1.5 DC solar spectra and a black body ($T = 300^\circ\text{C}$). A right: a global overview of the $\text{W/W-Al}_2\text{O}_3/\text{Al}_2\text{O}_3$ stack

When using SolPOC as planned, each optimization can be repeated several times, with low impact on calculation thanks to a multiprocessing implementation. Even non-coder users get to profit from each core of their CPU, even on modern calculation station (SolPOC is frequently used unto a 48 cores server). As example, the estimate parallelizable portion of the code reaching 97.07% according to Amdahl's law [27]. In these cases, repeat the optimization 8 times take a total of 93 s, under a classical laptop. Using the proposed evolutionary optimization method (Specific version of Differential Evolution [25]), each run found the same optimum value (here 93.25% was found systematic), meaning the same thin layers thickness in all the optimized stack.

By choosing to make SolPOC freely available to anyone we hope to help the solar community easily study, model and optimize their thin layer stacks for solar thermal energy systems and other.

Data availability statement

All the code of the package, written in Python, is freely available on a GitHub repository. The GitHub repository also includes various tutorials, a user guide with different documentation and several Jupyter notebooks. SolPOC is an evolving and collaborative project that we are continuously working on. Please keep in mind that the announced version and the associated DOI are currently up to date but may change quickly.

Name: SolPOC

Code repository on GitHub : <https://github.com/SolPOCandCo/SolPOC>

Code repository on PyPi: <https://pypi.org/project/solpoc/>

Licence: GNU General Public License v3.0

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Author contributions

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Thalita Drumond: Software, Validation, Writing - original draft

Amine Mahammou: Resource, Validation

Denis Langevin: Formal analysis, Validation, Writing – original draft

Antoine Moreau: Formal analysis, Validation, Writing – review & editing.

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Competing interests

The authors declare that they have no competing interests.

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References

- [1] A. Grosjean, A. Soum-Glaude, and L. Thomas, "Replacing silver by aluminum in solar mirrors by improving solar reflectance with dielectric top layers," *Sustainable Materials and Technologies*, vol. 29, p. e00307, Sep. 2021, doi: [10.1016/J.SUSMAT.2021.E00307](https://doi.org/10.1016/J.SUSMAT.2021.E00307).
- [2] A. Grosjean, A. Soum-Glaude, P. Neveu, and L. Thomas, "Comprehensive simulation and optimization of porous SiO₂ antireflective coating to improve glass solar transmittance for solar energy applications," *Solar Energy Materials and Solar Cells*, vol. 182, pp. 166–177, Aug. 2018, doi: [10.1016/J.SOLMAT.2018.03.040](https://doi.org/10.1016/J.SOLMAT.2018.03.040).
- [3] C. Atkinson, C. L. Sansom, H. J. Almond, and C. P. Shaw, "Coatings for concentrating solar systems – A review," *Renewable and Sustainable Energy Reviews*, vol. 45, pp. 113–122, 2015, doi: <https://doi.org/10.1016/j.rser.2015.01.015>.
- [4] Flamant Gilles, "Matériaux pour le solaire à concentration," in *Le solaire à concentration*, ISTE., 2021.
- [5] A. Soum-Glaude, I. Bousquet, L. Thomas, and G. Flamant, "Optical modeling of multi-layered coatings based on SiC(N)H materials for their potential use as high-temperature solar selective absorbers," *Solar Energy Materials and Solar Cells*, vol. 117, pp. 315–323, 2013, doi: [10.1016/j.solmat.2013.06.030](https://doi.org/10.1016/j.solmat.2013.06.030).
- [6] Antoine Grosjean and Thalita Drumond, "SolPOC." Accessed: Apr. 22, 2024. [Online]. Available: <https://github.com/SolPOCandCo/SolPOC>
- [7] "Python Package Index - PyPI," 2023, Python Software Foundation. Accessed: Nov. 28, 2023. [Online]. Available: <https://pypi.org/>
- [8] Antoine Grosjean et al., "Solar Performance Optimization Code for the optical response of multilayer stacks in Python: SolPOC," *SciPost*, Accessed: Apr. 22, 2024. [Online]. Available: https://scipost.org/submissions/scipost_202403_00005v1/
- [9] D. Langevin, P. Bennet, A. Khairah-Walieh, P. Wiecha, O. Teytaud, and A. Moreau, "PyMoosh : a comprehensive numerical toolkit for computing the optical properties of multilayered structures," Sep. 2023, [Online]. Available: <http://arxiv.org/abs/2309.00654>
- [10] F.-G. Aranzazu et al., "Parameters and Method to Evaluate the Reflectance Properties of Reflector Materials for Concentrating Solar Power Technology Under Laboratory Conditions, Official Reflectance Guideline Version 3.1," 2020.
- [11] A. Luce, A. Mahdavi, F. Marquardt, and H. Wankerl, "TMM-Fast, a transfer matrix computation package for multilayer thin-film optimization: tutorial," *Journal of the Optical Society of America A*, vol. 39, no. 6, p. 1007, Jun. 2022, doi: [10.1364/josaa.450928](https://doi.org/10.1364/josaa.450928).
- [12] Alexander Luce, "TMM Fast." Accessed: Sep. 13, 2023. [Online]. Available: https://github.com/MLResearchAtOSRAM/tmm_fast
- [13] Moreau Antoine, Bennet Pauline, Langevin Denis, and Wiecha Peter, "PyMoosh." Accessed: Sep. 12, 2023. [Online]. Available: <https://github.com/AnMoreau/PyMoosh>
- [14] D. Alonso-Álvarez, T. Wilson, P. Pearce, M. Führer, D. Farrell, and N. Ekins-Daukes, "Solcore: a multi-scale, Python-based library for modelling solar cells and semiconductor materials," *J Comput Electron*, vol. 17, no. 3, pp. 1099–1123, 2018, doi: [10.1007/s10825-018-1171-3](https://doi.org/10.1007/s10825-018-1171-3).
- [15] M. N. Polyanskiy, "Refractive index database." Accessed: Sep. 11, 2023. [Online]. Available: <https://refractiveindex.info>
- [16] "Schott Optical Glass Datasheets," 2023. Accessed: Sep. 11, 2023. [Online]. Available: obtained from <http://www.schott.com>
- [17] A. Soum-Glaude, I. Bousquet, M. Bichotte, S. Quoizola, L. Thomas, and G. Flamant, "Optical Characterization and Modeling of Coatings Intended as High Temperature Solar Selective Absorbers," *Energy Procedia*, vol. 49, pp. 530–537, Jan. 2014, doi: [10.1016/J.EGYPRO.2014.03.057](https://doi.org/10.1016/J.EGYPRO.2014.03.057).
- [18] Aránzazu Fernández-García et al., "Guidelines Parameters and Methode to Evaluate the Reflectance Properties OF Materials for Concentrating Solar Power Technology Under Laboratory Conditions," *Official Reflectance Guideline Version 3.1 April 2020*, 2020.
- [19] A. Grosjean, A. Soum-Glaude, and L. Thomas, "Influence of operating conditions on the optical optimization of solar selective absorber coatings," *Solar Energy Materials and Solar Cells*, vol. 230, p. 111280, Sep. 2021, doi: [10.1016/J.SOLMAT.2021.111280](https://doi.org/10.1016/J.SOLMAT.2021.111280).

- [20] D. R. Myers, K. Emery, and C. Gueymard, "Proposed reference spectral irradiance standards to improve concentrating photovoltaic system design and performance evaluation," in Conference Record of the Twenty-Ninth IEEE Photovoltaic Specialists Conference, 2002., 2002, pp. 923–926. doi: [10.1109/PVSC.2002.1190731](https://doi.org/10.1109/PVSC.2002.1190731).
- [21] S. Winter and D. Friedrich, "Effects of the New Standard IEC 60904-3:2008 on the Calibration Results of Common Solar Cell Types," 2009, doi: [10.4229/24thEUPVSEC2009-4AV.3.67](https://doi.org/10.4229/24thEUPVSEC2009-4AV.3.67).
- [22] J. Kennedy and R. Eberhart, "Particle Swarm Optimization," page 1942--1948. Proceedings of the IEEE International Conference on Neural Networks, Ed., 1995. doi: <http://dx.doi.org/10.1109/ICNN.1995.488968>.
- [23] R. Storn and K. Price, "Differential Evolution – A Simple and Efficient Heuristic for global Optimization over Continuous Spaces," Journal of Global Optimization, vol. 11, no. 4, pp. 341–359, 1997, doi: [10.1023/A:1008202821328](https://doi.org/10.1023/A:1008202821328).
- [24] M. A. Barry et al., "Evolutionary algorithms converge towards evolved biological photonic structures," Sci Rep, vol. 10, no. 1, Dec. 2020, doi: [10.1038/s41598-020-68719-3](https://doi.org/10.1038/s41598-020-68719-3).
- [25] P. Bennet, "Optimisation numérique des structures photoniques," 2022. [Online]. Available: <http://www.theses.fr/2022UCFAC052/document>
- [26] A. Mahammou et al., "Spectrally Selective Mirror Coatings for Hybrid PV/CSP Receivers," in 29th SolarPACES Conference, October 10 – October 13, 2023, Sydney, Australia, Sydney Australia.
- [27] D. P. Rodgers, "Improvements in Multiprocessor Sgstem Design," 1985.