# MiMeS: Misalignment Mechanism Solver

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#### Abstract

We introduce a C++ header-only library that solves the Axion equation of motion, MiMeS. MiMeS makes no assumptions regarding the cosmology and the thermal mass of the axion, which allows the user to consider various cosmological scenarios and axion-like models. MiMeS also includes a convenient python interface, which allows the user to use it without writing any code in C++, with minimum overhead.

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# 1 Introduction

The axion is a hypothetical particle that was originally introduced in order to solve the strong CPproblem of the standard model (SM) [1, 2, 3]. Furthermore, the axion is assumed to acquire a non-zero vacuum expectation value (VEV), which results in the spontaneous breaking of a global symmetry, called Peccei-Quinn (PQ). That is the axion is a pseudo-Nambu-Goldstone boson. Moreover, it also appears to be a valid dark matter (DM) candidate [4, 5, 6], as it is electrically neutral and long-lived. The axion starts, at very early time, with a VEV close to the PQ breaking scale (usually much higher than 100GeV), but due to the expansion of the Universe it eventually ends oscillating around zero. This oscillation results in an apparent constant number of axion particles (or constant energy of the axion field) today, which can account for the observed [7] DM relic abundance. Apart form the axion, there are other hypothetical particles (for early examples of such particles see [8, 9]; and [10] for a review), called axion-like particles (ALPs), which are not related to the strong CP-problem. That is, these ALPs, interact with the SM in a different way than the axion. However, they can still account for the DM of the Universe. From the point of view of their DM abundance, both axions and ALPs, follow the same dynamics (similar EOM). The only difference between the two is their mass. The mass of the axion is dictated by QCD, while it is model-dependent for other ALPs. Therefore, the cosmological evolution of both axions and ALP is often discussed together (see, for example ref. [11]).

In this article, introduce a header-only C++ library, MiMeS, <sup>1</sup> that solves the axion (or ALP) EOM, where both the mass and the underlying cosmological evolution are treated as user inputs. Therefore, MiMeS can be used to compute the relic abundance of axions or ALPs, in a wide variety of cases. Moreover, one can use MiMeS in python scripts, without having to write any C++ code.

<sup>&</sup>lt;sup>1</sup>MiMeS is distributed under the MIT license. A copy of this license should be available in the MiMeS root directory. If you have not received one, you can find it at github.com/dkaramit/MiMeS/blob/master/LICENSE.

This paper is organized as follows: In section 2, we introduce the EOM and show how it can be solved approximately. Also, we introduce the notation that MiMeS follows, we derive the "adiabatic invariant" of the system, and discuss how it is used. In the next section, we introduce MiMeS, by showing how it can be downloaded, compiled, an ran for the first time. Also, we explain in detail all the parameters that MiMeS as a user input at run-time. In section 4, we discuss the few assumption that MiMeS makes, its default compile-time options and user input, and how the user can change them. Moreover, we provide a complete example in both C++ and python.

# 2 Physics background

Although there are several works in the literature (such as [12, 11]) that can provide a insight on the cosmological evolution of axions, in this section we define, derive, and discuss various quantities we need, in order to understand how MiMeS works in detail.

**The EOM** The axion field is usually expressed in terms of the so-called axion angle,  $\theta$ , as  $A = \theta f_a$ , with  $f_a$  the scale at which the PQ symmetry breaks. <sup>2</sup> The axion angle follows the EOM

$$\left(\frac{d^2}{dt^2} + 3H(t) \frac{d}{dt}\right)\theta(t) + \tilde{m}_a^2(t) \sin\theta(t) = 0, \qquad (2.1)$$

with H(t) the Hubble parameter (determined by the cosmology), and  $\tilde{m}_a(t)$  the time (temperature) dependent mass of the axion. MiMeS expects the mass to be of the form

$$\tilde{m}_a^2(T) = \frac{\chi(T)}{f_a^2} \,,$$
 (2.2)

and  $\chi$  a function of the temperature. For the QCD axion, this has been calculated using lattice simulations in [13]. <sup>3</sup>

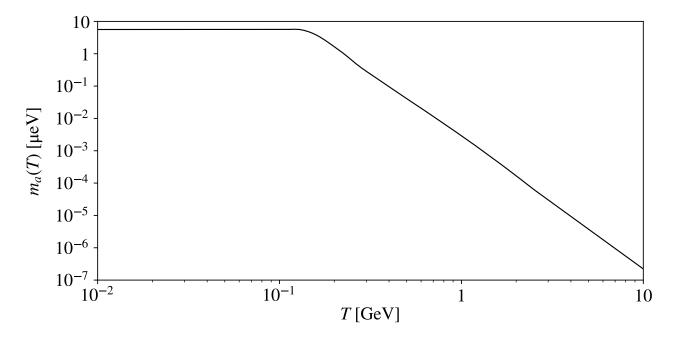


Figure 1: The mass of the axion as a function of the temperature for  $f_a = 10^{12}$  GeV, using the data provided in ref. [13].

<sup>&</sup>lt;sup>2</sup>If in a model under study, there is no  $f_a$ , this parameter is still expected by MiMeS, but the user can set  $f_a = 1$ .

<sup>&</sup>lt;sup>3</sup>The data provided by ref. [13] are used by MiMeS out-of-the-box. However, the user is free to change them.

**Initial conditions** Assuming that the PQ symmetry breaks before inflation, the initial conditions (i.e. at some t=0, after inflation) for the EOM is random. However, we note that  $\tilde{m}_a \to 0$  (see Fig. (1)) – i.e.  $\tilde{m}_a \ll H$  – at very early times. Therefore, after inflation, the EOM is simply

$$\left(\frac{d^2}{dt^2} + 3H(t) \frac{d}{dt}\right)\theta(t) = 0, \qquad (2.3)$$

which is solved by  $\theta = \theta_{\rm ini} + C \int_0^t dt' \left(\frac{a(t'=0)}{a(t')}\right)^3$ , with  $\theta_{\rm ini}$  a constant and a the scale factor of the Universe. That is, as the Universe expands, and as long as  $\tilde{m}_a \ll H$ ,  $\theta \to \theta_{\rm ini}$ . Since we would like to calculate the relic abundance of axions, we can integrate eq. (2.1) from a time after inflation (call it  $t = t_{\rm ini}$ ) such that  $\dot{\theta}|_{t=t_{\rm ini}} = 0$  and  $\theta|_{t=t_{\rm ini}} = \theta_{\rm ini}$ . This is the most common case (there are exceptions to this; e.g. [14]), and it is what MiMeS uses.

# 2.1 The WKB approximation

In order to solve analytically eq. (2.1), we assume  $\theta \ll 1$ , which results in the linearised EOM

$$\left(\frac{d^2}{dt^2} + 3H(t) \frac{d}{dt} + \tilde{m}_a^2(t)\right)\theta(t) = 0.$$
 (2.4)

Using a trial solution  $\theta_{\rm trial} = \exp\left[i\int dt \left(\psi(t) + 3/2 \ i \ H(t)\right)\right]$ , and defining  $\Omega^2 = \tilde{m}_a^2 - \frac{9}{4}H^2 - \frac{3}{2}\dot{H}$  we can transform the eq. (2.4) to

$$\psi^2 = \Omega^2 + i \dot{\psi} \,, \tag{2.5}$$

which has a formal solution  $\psi = \pm \sqrt{\Omega^2 + i\dot{\psi}}$ . In the WKB approximation, we assume a slow time-dependence; that is  $\dot{\psi} \ll \Omega^2$  and  $\dot{\Omega} \ll \Omega^2$ . Then we can approximate  $\psi$  as

$$\psi \approx \pm \Omega + \frac{i}{2} \frac{d \log \Omega}{dt} \,, \tag{2.6}$$

which results in the general solution of eq. (2.4)

$$\theta \approx \frac{1}{\sqrt{\Omega}} \exp\left(-\frac{3}{2} \int dt \ H\right) \left[ A \cos\left(\int dt \ \Omega\right) + B \sin\left(\int dt \ \Omega\right) \right] \ .$$
 (2.7)

Applying, then, the initial conditions  $\dot{\theta}|_{t=t_{\rm ini}}=0$  and  $\theta|_{t=t_{\rm ini}}\approx\theta_{\rm ini}$ , we arrive at

$$\theta(t) \approx \theta_{\rm ini} \sqrt{\frac{\Omega_{\rm ini}}{\Omega(t)}} \left(\frac{a}{a_{\rm ini}}\right)^{-3/2} \cos\left(\int_{t_{\rm ini}}^{t} dt' \ \Omega(t')\right) .$$
 (2.8)

In order to further simplify this approximate result, we note that  $\theta$  deviates from  $\theta_{\rm ini}$  close to  $t=t_{\rm osc}$  – corresponding to  $T=T_{\rm osc}$ , the so-called "oscillation temperature" –  $\tilde{m}_a|_{t=t_{\rm osc}}=3H|_{t=t_{\rm osc}}$ , which is defined as the point at which the axion begins to oscillate. This observation allows us to set  $t_{\rm ini}=t_{\rm osc}$ . Moreover, at  $t>t_{\rm osc}$ , we approximate  $\Omega\approx\tilde{m}_a$ , as  $H^2$  and  $\dot{H}$  become much smaller than  $\tilde{m}_a{}^2$  quickly after  $t=t_{\rm osc}$ . Finally, the axion angle takes the form

$$\theta(t) \approx \theta_{\rm osc} \left(\frac{3}{4}\right)^{1/4} \sqrt{\frac{\tilde{m}_a|_{t=t_{\rm osc}}}{\tilde{m}_a(t)}} \left(\frac{a}{a_{\rm osc}}\right)^{-3/2} \cos\left(\int_{t_{\rm osc}}^t dt' \ \tilde{m}_a(t')\right) , \qquad (2.9)$$

where  $\theta_{\rm osc} = \theta|_{t=t_{\rm osc}}$ . This equation is further simplified if we assume that  $\theta_{\rm osc} \approx \theta_{\rm ini}$ , i.e.

$$\theta(t) \approx \theta_{\rm ini} \left(\frac{3}{4}\right)^{1/4} \sqrt{\frac{\tilde{m}_a|_{t=t_{\rm osc}}}{\tilde{m}_a(t)}} \left(\frac{a}{a_{\rm osc}}\right)^{-3/2} \cos\left(\int_{t_{\rm osc}}^t dt' \ \tilde{m}_a(t')\right) . \tag{2.10}$$

It is worth mentioning that the accuracy of this approximation depends, in general, on  $T_{\rm osc}$ ; it determines the difference between  $\theta_{\rm ini}$  and  $\theta_{\rm osc}$ , the deviation of  $\dot{\theta}|_{t=t_{\rm osc}}$  from 0, and whether  $\dot{\Omega} \ll \Omega^2$ .

**Axion energy density** In the small angle approximation, the energy density of the axion is

$$\rho_a = \frac{1}{2} f_a^2 \left[ \dot{\theta}^2 + \tilde{m}_a^2 \theta^2 \right] . \tag{2.11}$$

For the relic abundance of axions, we need to calculate their energy density at very late times. That is,  $\dot{\tilde{m}}_a = 0$ ,  $\tilde{m}_a \gg H$  and  $\dot{H} \ll H^2$ . After some algebra, we obtain the approximate form of the energy density as a function of the scale factor (a)

$$\rho_a \approx \frac{m_a}{2} f_a^2 \theta_{\rm ini}^2 \tilde{m}_a(a_{\rm osc}) \left(\frac{a_{\rm osc}}{a}\right)^3 , \qquad (2.12)$$

which shows that the energy density of axions at late times scales as the energy density of matter; *i.e.* the number of axion particles is conserved. If there is a period of entropy injection to the plasma for  $T < T_{\text{osc}}$ , the axion energy density gets diluted, since

$$a^3 s = \gamma \ a_{\rm osc}^{3} s_{\rm osc} \Rightarrow \left(\frac{a_{\rm osc}}{a}\right)^3 = \gamma^{-1} \frac{s}{s_{\rm osc}},$$
 (2.13)

with  $\gamma$  the amount of entropy injection to the plasma between  $t_{\text{osc}}$  and t. Therefore, the present (at  $T = T_0$ ) energy density of the axion, becomes

$$\rho_{a,0} = \gamma^{-1} \frac{s_0}{s_{\text{osc}}} \frac{1}{2} f_a^2 m_a \tilde{m}_{a,\text{osc}} \theta_{\text{ini}}^2, \qquad (2.14)$$

with  $m_a$  the mass of the axion at  $T=T_0$ . Notice that the explicit dependence on  $f_a$  cancels, since  $\tilde{m}_a \sim 1/f_a$ . That is,  $f_a$  only affects the energy density of the axions through its impact on  $T_{\rm osc}$ .

### 2.2 Notation

The EOM (2.1) depends on time, which is not very useful variable in cosmology. Therefore, we introduce

$$u = \log \frac{a}{a_{\text{ini}}} \,, \tag{2.15}$$

which results in

$$\frac{dF}{dt} = H\frac{dF}{du}$$

$$\frac{d^2F}{dt^2} = H^2 \left(\frac{d^2F}{du^2} + \frac{1}{2}\frac{d\log H^2}{du}\frac{dF}{du}\right).$$
(2.16)

The EOM in terms of u, then, becomes

$$\frac{d^2\theta}{du^2} + \left[\frac{1}{2}\frac{d\log H^2}{du} + 3\right]\frac{d\theta}{du} + \left(\frac{\tilde{m}_a}{H}\right)^2 \sin\theta = 0.$$
 (2.17)

Notice that in a radiation dominated Universe

$$\frac{d\log H^2}{du} = -\left(\frac{d\log g_{\text{eff}}}{d\log T} + 4\right)\delta_h^{-1},\,$$

with  $\delta_h = 1 + \frac{1}{3} \frac{d \log h_{\text{eff}}}{d \log T}$ . In a general cosmological setting, if the expansion rate is dominated by an energy density that scales as  $\rho \sim a^{-c}$ ,  $\frac{d \log H^2}{du} = -c$ . We notice that close to rapid particle annihilations and decays, the evolution of the energy densities change, and  $\frac{d \log H^2}{du}$  can only be computed numerically.

Moreover, it is worth mentioning that the EOM 2.17 with the initial condition  $\theta(u=0) = \theta_{\text{ini}}$  and  $d\theta/du(u=0) = 0$  can be written as a system of first order ordinary differential equations

$$\frac{d\zeta}{du} + \left[\frac{1}{2}\frac{d\log H^2}{du} + 3\right]\zeta + \left(\frac{\tilde{m}_a}{H}\right)^2 \sin\theta = 0.$$

$$\frac{d\theta}{du} - \zeta = 0.$$
(2.18)

This form of the EOM is what MiMeS uses, as it is suitable for integration via Runge-Kutta methods – which are briefly discussed in Appendix A.

## 2.3 Adiabatic invariant and the anharmonic factor

The small angle approximation does not allow us to solve the EOM 2.1 analytically. Moreover, even for  $\theta \ll 1$ , the WKB approximation fails to capture the dynamics before the adiabatic conditions are met, and result in an inaccurate axion relic abundance. Therefore, a numerical integration should be preferred. Furthermore, in order to reduce the computation time, the numerical integration needs to stop as soon as the axion begins to evolve adiabatically. After this point, we can correlate its energy density at later times, using an "adiabatic invariant", which can be defined for oscillatory systems with varying period.

**Definition of the adiabatic invariant** Given a system with Hamiltonian  $\mathcal{H}(\theta, p; t)$ , the equations of motion are

$$\dot{p} = -\frac{\partial \mathcal{H}}{\partial \theta} , \ \dot{\theta} = \frac{\partial \mathcal{H}}{\partial p} .$$
 (2.19)

Moreover, we note that

$$d\mathcal{H} = \dot{\theta} dp - \dot{p} d\theta + \frac{\partial \mathcal{H}}{\partial t} dt . \tag{2.20}$$

If this system exhibits closed orbits (e.g. if it oscillates), we define

$$J \equiv C \oint p \ d\theta \ , \tag{2.21}$$

where the integral is over a closed path (e.g. a period, T), and C indicates that J can always be rescaled with a constant. This quantity is the adiabatic invariant of the system, if the Hamiltonian varies slowly during a cycle. That is,

$$\frac{dJ}{dt} = C \oint \left( \dot{p} \ d\theta + p \ d\dot{\theta} \right) = C \int_{t}^{t+T} \frac{\partial \mathcal{H}}{\partial t'} \ dt' \approx T \left. \frac{\partial \mathcal{H}(t')}{\partial t'} \right|_{t'=t} \approx 0 \ .$$

**Application to the axion** The Hamiltonian that results in the EOM of eq. (2.1) is

$$\mathcal{H} = \frac{1}{2} \frac{p^2}{f_a^2 \ a^3} + V(\theta) \ a^3 \ , \tag{2.22}$$

with

$$p = f_a^2 \ a^3 \ \dot{\theta} \tag{2.23}$$

$$V(\theta) = \tilde{m}_a^2 f_a^2 (1 - \cos \theta) . \tag{2.24}$$

Notice that the Hamiltonian varies slowly if  $\tilde{m}_a(T)/\tilde{m}_a \ll \tilde{m}_a$  and  $H \ll \tilde{m}_a$ , which are the adiabatic conditions. When these conditions are met, the adiabatic invariant for this system becomes

$$J = \frac{\oint p \ d\theta}{\pi f_a^2} = \frac{1}{\pi f_a^2} \oint \sqrt{2 \left(\mathcal{H}(\theta) - V(\theta) \ a^3\right) \ f_a^2 a^3} \ d\theta = \frac{2}{\pi f_a^2} \int_{-\theta_{\text{peak}}}^{\theta_{\text{peak}}} \sqrt{2 \left(\mathcal{H}(\theta_{\text{peak}}) - V(\theta) \ a^3\right) \ f_a^2 a^3} \ d\theta \ , \tag{2.25}$$

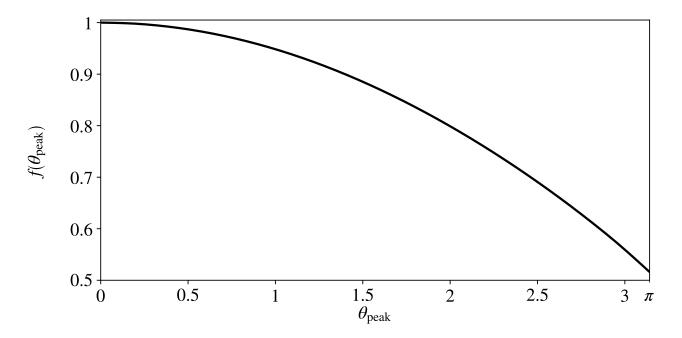


Figure 2: The anharmonic factor for  $0 \le \theta_{\text{peak}} < \pi$ .

where we note that  $\theta_{\text{peak}}$  denotes the maximum of  $\theta$  – the peak of the oscillation, which corresponds to p = 0. That is,  $\mathcal{H}(\theta_{\text{peak}}) = V(\theta_{\text{peak}})$   $a^3$ . Therefore, the adiabatic invariant, takes the form

$$J = \frac{2\sqrt{2}}{\pi f_a} \int_{-\theta_{\text{peak}}}^{\theta_{\text{peak}}} \sqrt{V(\theta_{\text{peak}}) - V(\theta)} a^3 d\theta = \frac{2\sqrt{2}}{\pi} \tilde{m}_a a^3 \int_{-\theta_{\text{peak}}}^{\theta_{\text{peak}}} \sqrt{\cos \theta - \cos \theta_{\text{peak}}} d\theta , \quad (2.26)$$

where, for the last equality, we have used the adiabatic conditions, i.e. negligible change of  $\tilde{m}_a$  and a during one period. Usually, the adiabatic invariant is written as [15, 16]

$$J = a^3 \tilde{m}_a \theta_{\text{peak}}^2 f(\theta_{\text{peak}}) , \qquad (2.27)$$

where

$$f(\theta_{\text{peak}}) = \frac{2\sqrt{2}}{\pi\theta_{\text{peak}}^2} \int_{-\theta_{\text{peak}}}^{\theta_{\text{peak}}} d\theta \sqrt{\cos\theta - \cos\theta_{\text{peak}}} , \qquad (2.28)$$

is called the anharmonic factor, with  $0.5 \lesssim f(\theta_{\text{peak}}) \leq 1$  (see Fig. (2)).

The role of the adiabatic invariant in the axion relic energy density The adiabatic invariant allows us to calculate the maximum value of the angle  $\theta$  at late times from its corresponding value at some point just after the adiabatic conditions where fulfilled.

In order to do this, we can numerically integrate eq. (2.1), and identify the maxima of  $\theta$ . <sup>4</sup> Once the adiabatic conditions are fulfilled, we can stop the integration at a peak,  $\theta_{\text{peak},*}$  – which corresponds to  $T = T_*$  and  $a = a_*$ . Then, the value of the maximum angle today ( $\theta_{\text{peak},0} \ll 1$ ) is related to  $\theta_{\text{peak},*}$  via

$$\theta_{\text{peak},0}^{2} = \left(\frac{a_{*}}{a_{0}}\right)^{3} \frac{\tilde{m}_{a,*}}{m_{a}} f(\theta_{\text{peak},*}) \theta_{\text{peak},*}^{2} = \gamma^{-1} \frac{s_{0}}{s_{*}} \frac{\tilde{m}_{a,*}}{m_{a}} f(\theta_{\text{peak},*}) \theta_{\text{peak},*}^{2}.$$
 (2.29)

Plugging this into eq. (2.11) (with  $\dot{\theta} = 0$ , i.e. at today's peak), we arrive at the energy density today

$$\rho_{a,0} = \gamma^{-1} \frac{s_0}{s_*} m_a \tilde{m}_{a,*} \frac{1}{2} f_a^2 \theta_{\text{peak},*}^2 f(\theta_{\text{peak},*}), \qquad (2.30)$$

<sup>&</sup>lt;sup>4</sup>MiMeS identifies the maxima in real time, so it stops as soon as the system becomes adiabatic.

where  $\gamma$  is the entropy injection coefficient between  $T_*$  and  $T_0$ , defined from

$$a^{3}(T_{0}) \ s(T_{0}) = \gamma \ a^{3}(T_{*}) \ s(T_{*})$$
 (2.31)

Notice that eq. (2.30) is similar to the corresponding WKB result (2.14) at  $t_{\rm osc} \to t_*$ , multiplied by the anharmonic factor  $f(\theta_{\rm peak,*})$ . So, the numerical integration is needed in order to correctly identify  $T_*$  and  $\theta_{\rm peak,*}$ , which are greatly affected by the underlying cosmology (especially in cases where entropy injection is active close to  $T_{\rm osc}$ ) and whether  $\theta_{\rm ini} \gtrsim 1$  [16, 17].

# 3 MiMeS usage

The latest stable version of MiMeS is available in https://github.com/dkaramit/MiMeS/tree/stable, which can also be obtained by running: <sup>5</sup>

```
git clone -b stable https://github.com/dkaramit/MiMeS.git
```

It is important to note that MiMeS relies NaBBODES [18] and SimpleSplines [19]. These are two libraries developed independently, and in order to get MiMeS with the latest version of these libraries, one needs to run following commands

```
git clone https://github.com/dkaramit/MiMeS.git
```

- cd MiMeS
- 3 git submodule init
- 4 git submodule update --remote

This downloads the master branch of MiMeS; and NaBBODES [18] and SimpleSplines [19] as submodules. This guaranties that MiMeS uses the most updated version of these libraries, although it may not be stable.

Once everything is downloaded successfully, we can go inside the MiMeS directory, and run "bash configure.sh" and "make". The bash script configure.sh, just writes some paths to some files, formats the data files provided in an acceptable format (in section 4.2 the format is explained), and makes some directories. The makefile is responsible for compiling some examples and checks, as well as the shared libraries that needed for the python interface. If everything runs successfully, there should be two new directories exec and lib. Inside exec, there are several executables that ready to run, in order to ensure that the code runs (e.g. no segmentation fault occurs). For example, exec/AxionSolve\_check.run, should print the values of the parameters  $\theta_{\rm ini}$  and  $f_a$ , the oscillation temperature and the corresponding value of  $\theta$ , the evolution of the axion (e.g. temperature,  $\theta$ ,  $\rho_a$ , etc.), and the values of various quantities on the peaks of the oscillation. In the directory lib, there are several shared libraries for the python interface.

Although there are various options available at compile-time, we first discuss how MiMeS can be used, in order for the role of these options to be clear.

#### 3.1 First steps

There are several examples in C++ (MiMeS/UserSpace/Cpp) and python (MiMeS/UserSpace/Python), as well as jupyter notebooks (MiMeS/UserSpace/JupyterNotebooks), that show in detail how MiMeS can be used. Here, we discuss the various functions one may use as it will provide some insight for the following discussions.

#### 3.1.1 Using MiMeS in C++

The class that is responsible for the solution of the EOM is mimes::Axion<LD, Solver, Method>, located in MiMeS/src/Axion. However, in order to use it, we have to define the mass of the axion as a function of the temperature and  $f_a$ . The axion mass is defined as an instance of the mimes::AxionMass<LD>, which is defined in the header file MiMeS/src/AxionMass/AxionMass.hpp. We should note that LD

<sup>&</sup>lt;sup>5</sup>Instructions on how git can be installed can be found in https://github.com/git-guides/install-git.

is the numerical type we use  $(e.g. \ long \ double)$ . The other template arguments are related to the differential equation solver, and their role will be explained in later sections.

Therefore, at the top of the main .cpp file, we need to include

```
#include "src/AxionMass/AxionMass.hpp"
#include "src/Axion/AxionSolve.hpp"
```

Notice that if the this .cpp file is not in the root directory of MiMeS, we need to compile it using the flag -Ipath-to-root, "path-to-root" the relative path to the root directory of MiMeS; e.g. if the .cpp is in the MiMeS/UserSpace/Cpp/Axion directory, this flag should be -I../../.

The mass of the axion can be defined in two ways; either via a data file or as a user defined function.

**Axion mass form data file** In many cases, axion mass cannot be written in a closed form. In these cases, the user may provide a data file. Then, the axion mass can be defined via this file as

```
mimes::AxionMass<LD> axionMass(chi_PATH, minT, maxT);
```

The template parameter LD can be a numeric type (e.g. double or long double). The argument chi\_PATH is a (relative or absolute) path to a file with two columns; T (in GeV) and  $\chi$  (in GeV<sup>4</sup>), with increasing T. In this case, the axion mass is interpolated between the temperatures minT and maxT. These two parameters are just suggestions, and the actual interpolation limits, TMin and TMax, are chosen as the closest temperatures in the data file. That is, in general, TMin  $\geq$  minT and TMax  $\leq$  maxT. Beyond these limits, the mass is assumed to constant by default. However, one can change this by using

```
axionMass.set_ma2_MAX(ma2_MAX);
axionMass.set_ma2_MIN(ma2_MIN);
```

with ma2\_MAX and ma2\_MIN the axion mass squared as functions (or any other callable objects) with signatures LD ma2\_MAX(LD T, LD fa) and LD ma2\_MIN(LD T, LD fa). These functions are called for  $T \geq TMax$  and  $T \leq TMin$ , respectively. Usually, in order to ensure continuity of the axion mass, one needs to know TMin, TMax,  $\chi(TMin)$ , and  $\chi(TMax)$ ; which can be found by calling axionMass.getTMin(), axionMass.getChiMin(), and axionMass.getChiMax(), respectively.

**Axion mass function** In some cases, the dependence of the axion mass on the temperature is known. If this is the case, the user can define the axion mass via

```
mimes::AxionMass<LD> axionMass(ma2);
```

with ma2 the axion mass squared as a callable object with signature LD ma2(LD T, LD fa).

**The EOM solver** Once the axion mass is defined, we can declare a variable that will be used to solve the EOM, as

```
mimes::Axion<LD,Solver,Method> ax(theta_i, fa, umax, TSTOP, ratio_ini,

N_convergence_max, convergence_lim, inputFile, &axionMass, initial_step_size,

minimum_step_size, maximum_step_size, absolute_tolerance, relative_tolerance,

beta, fac_max, fac_min, maximum_No_steps);
```

Here, LD should be the numeric type to be used; it is recommended to use long double, but other choices are also available as we discuss later. Moreover Solver and Method depend on the type of Runge-Kutta (RK) the user chooses. The available choices are shown in table 4. A discussion on RK methods is given in Appendix A.

The various parameters are as follows:

- 1. theta\_i: initial angle.
- 2. fa: the PQ scale.

- 3. umax : if u > umax the integration stops (remember that  $u = \log(a/a_i)$ ). Typically, this should be a large number ( $\sim 1000$ ), in order to avoid stopping the integration before the axion begins to evolve adiabatically.
- 4. TSTOP: if the temperature drops below this, integration stops. In most cases this should be around  $10^{-4}$  GeV, in order to be sure that any entropy injection has stopped before integration stops (since BBN bounds [20, 21] should not be violated).
- 5. ratio\_ini: integration starts when  $3H/\tilde{m}_a \approx \text{ratio_ini}$  (the exact point depends on the file "inputFile", which we will see later).
- 6. N\_convergence\_max and convergence\_lim: integration stops when the relative difference between two consecutive peaks is less than convergence\_lim for N\_convergence\_max consecutive peaks.
- 7. inputFile: relative (or absolute) path to a file that describes the cosmology. the columns should be:  $u \ T \ [\text{GeV}] \ \log H$ , sorted so that u increases. <sup>6</sup> It is important to remember that MiMeS assumes that the entropy injection has stopped before the lowest temperature of given in inputFile. Since MiMeS is unable to guess the cosmology beyond what is given in this file, the user has to make sure that there are data between the initial temperature (which corresponds to ratio\_ini, and TSTOP).
- 8. axionMass: an instance of the mimes::AxionMass<LD> class, passed by pointer.
- 9. initial\_stepsize (optional): initial step the solver takes.
- 10. maximum\_stepsize (optional): This limits the step-size to an upper limit.
- 11. minimum\_stepsize (optional): This limits the step-size to a lower limit.
- 12. absolute\_tolerance (optional): absolute tolerance of the RK solver
- 13. relative\_tolerance (optional): relative tolerance of the RK solver. Generally, both absolute and relative tolerances should be 10<sup>-8</sup>. In some cases, however, one may need more accurate result (e.g. if f\_a is extremely high, the oscillations happen violently, and the system destabilizes). Whatever the case, if the tolerances are below 10<sup>-8</sup>, long doubles have be used. MiMeS by default uses long double variables, in order to change it see the options available in section 4.2.
- 14. beta (optional): controls how agreesive the adaptation is. Generally, it should be around but less than 1.
- 15. fac\_max, fac\_min (optional): the stepsize does not increase more than fac\_max, and less than fac\_min. This ensures a better stability. Ideally, fac\_max= ∞ and fac\_min= 0, but in reality one must tweak them in order to avoid instabilities.
- 16. maximum\_No\_steps (optional): maximum steps the solver can take Quits if this number is reached even if integration is not finished.

In order to understand the role of the optional parameters, some basic techniques of Runge-Kutta methods are discussed in Appendix A.

The EOM (2.17), then can be solved using

# ax.solveAxion();

Once the EOM is solved, we can access  $T_{\rm osc}$ ,  $\theta_{\rm osc}$ , and  $\Omega h^2$  via ax.T\_osc, ax.theta\_osc, and ax.relic. The entire evolution (the points the integrator took) of the axion angle is stored in ax.points, which is a two-dimensional std::vector<LD>, with the columns corresponding to a, T [GeV],  $\theta$ ,  $d\theta/du$ ,  $\rho_a$ .

<sup>&</sup>lt;sup>6</sup>One can run "bash MiMeS/src/FormatFile.sh inputFile" in order to sort it and remove any unwanted duplicates. See Appendix F for details of MiMeS/src/FormatFile.sh.

Moreover, the peaks of he oscillation are stored in another two-dimensional std::vector<LD>, with the columns corresponding to a, T [GeV],  $\theta_{\rm peak}$ ,  $d\theta/du=0$ ,  $\rho_a$ , J. We should note that the peaks are identified using linear interpolation between integration points, in order to ensure that  $d\theta/du=0$ . That is, the values stored in ax.peaks do not exist in ax.points. Finally, the local errors (see Appendix A) of the integration points of  $\theta$  and  $\zeta$  are stored in ax.dtheta and ax.dzeta.

Changing axion mass definition The axion mass definition can change at any time by changing the data file (or ma2\_MIN and ma2\_MAX) or using using

```
ax.set_ma2(ma2);
```

with ma2 a callable object with signature LD ma2(LD T, LD fa).

However, since integration starts at a temperature determined by ratio\_ini, if the mass changes (including the definitions beyond the interpolation limits), we have to remake the interpolation of the underlying cosmology described by the parameter inputFile. Thus, if we change the definition of the mass, we need to call

```
ax.restart();
```

This function remakes the interpolations, clears all vector, and sets all variables to 0.

Changing initial condition The final member function is mimes::Axion::setTheta\_i, which allows the user to set a different  $\theta_{\text{ini}}$  without generating another instance. <sup>7</sup> This function is used as

```
ax.setTeta_i(new_theta_ini);
```

where new\_theta\_ini is the new value of  $\theta_{\rm ini}$ . Running this function resets all variables to 0 (except T\_osc and a\_osc, since they should not change), and clears all std::vector<LD> variables, which allows the user to simply run "ax.solveAxion();" as if ax was a freshly defined instance.

# 3.1.2 Using MiMeS in python

The modules for the python interface are located in MiMeS/src/interfacePy. Although the usage of the AxionMass and Axion classes is similar to the C++ case, it is worth showing explicitly how the python interface works. One should keep in mind that the various template arguments discussed in the C++ case have to be chosen at compile-time. That is, for the python interface, one needs to choose the numeric type, and RK method to be used when the shared libraries are compiled. This is done by assigning the relevant variable in MiMeS/Definitions.mk before running "make". The various options are discussed in section 4.1, and outlined in table 5.

The two relevant classes are defined in the modules interfacePy.AxionMass and interfacePy.Axion, and can be loaded in a python script as

```
from sys import path as sysPath
from os import path as osPath
sysPath.append(osPath.join(osPath.dirname(__file__), 'path_to_src'))
from interfacePy.AxionMass import AxionMass
from interfacePy.Axion import Axion
```

It is important that 'path\_to\_src' provides the relative path to the MiMeS/src directory. For example, if the script is located in MiMeS/UserSpace/Python, 'path\_to\_src' should be '../../src'.

**Axion mass definition via a data file** As before, we first need to define the axion mass. Similarly to the previous case, in order to define the axion mass via a file, we use

```
AxionMass axionMass(chi_PATH, minT, maxT)
```

<sup>&</sup>lt;sup>7</sup>Since the interpolations of the data of inputFile are made inside the constructor of the mimes::Axion<LD,Solver,Method>class, mimes::Axion<LD,Solver,Method>::setTheta\_i is a faster choice if ones needs to solve the EOM for a different initial condition.

Here, the constructor requires the same parameters as in C++. Moreover, the axion mass beyond the interpolation limits can be changed via

```
axionMass.set_ma2_MAX(ma2_MAX)
axionMass.set_ma2_MIN(ma2_MIN)
```

Although the naming is the same as in the C++ case, there is an important difference. Namely, ma2\_MAX and ma2\_MIN have to be functions (that take T and  $f_a$  as arguments and return  $\tilde{m}_a{}^2$ ), and cannot be any other callable object. The reason is that MiMeS uses the ctypes module, which only works with objects compatible with C. Moreover, the values of TMin, TMax,  $\chi(\text{TMin})$ , and  $\chi(\text{TMax})$  can be obtained by axionMass.getTMin(), axionMass.getTMax(), axionMass.getChiMax(), respectively.

### Axion mass definition via a function Again this can be done as

```
AxionMass axionMass(ma2)
```

with ma2 the axion mass squared, which should be a function (not any callable object) of T and  $f_a$ .

Importand note Once an AxionMass is no longer required, to call the destructor. In this case, we can run

```
del axionMass
```

The reason is that MiMeS constructs a pointer for every instance of the class, which needs to be deleted manually.

#### The EOM solver We can define an Axion instance as follows

```
ax=Axion(theta_i, fa, umax, TSTOP, ratio_ini, N_convergence_max, convergence_lim,
inputFile, axionMass, initial_step_size, minimum_step_size, maximum_step_size,
absolute_tolerance, relative_tolerance, beta, fac_max, fac_min, maximum_No_steps)
```

Here the input parameters are the same as in the C++ case (the usage of the class can be found by running ?Axion after loading the module). The only slight difference compared to the C++ case is that the axionMass instance is not passed as a pointer; it is done internally using ctypes.

Using the defined variable (ax in this example), we can simply run

```
ax.solveAxion()
```

in order to solve the EOM of the axion. In contrast to the C++ implementation, this only gives us access to  $T_{\rm osc}$ ,  $\theta_{\rm osc}$ , and  $\Omega h^2$ ; the corresponding variables are ax.T\_osc, ax.theta\_osc, and ax.relic. In order to get the evolution of the axion field, we need to run

```
ax.getPoints()
```

This will make numpy arrays that contain the scale factor (ax.a), temperature (ax.T),  $\theta$  (ax.theta), its derivative with respect to u (ax.zeta), and the energy density of the axion (ax.rho\_axion).

Moreover, in order to get the various quantities on the peaks of the oscillation, we can run

```
ax.getPeaks()
```

This makes numpy arrays that contain the scale factor (ax.a\_peak), temperature (ax.T\_peak),  $\theta$  (ax.theta\_peak), its derivative with respect to u (ax.zeta\_peak, which should be equal to 0), the energy density of the axion (ax.rho\_axion\_peak), and the values of the adiabatic invariant on the peaks (ax.adiabatic\_invariant).

Moreover, we can run the following

```
ax.getErrors()
```

in order to store the local errors (see Appendix A) of  $\theta$  and  $\zeta$  in ax.dtheta and ax.dzeta, respectively.

Changing axion mass definition We can change the axion mass by changing the file, ma2\_MIN and ma2\_MAX, or using

```
ax.set_ma2(ma2)
```

with ma2 a function that takes T and  $f_a$ , and returns the  $\tilde{m}_a^2$ . As in the C++ case, if the definition of the mass of the axion changes (including the definitions beyond the interpolation limits), we have to call

```
ax.restart()
```

in order to remake the interpolation of cosmological quantities and reset the various variables.

Changing the initial condition The initial condition  $\theta_{\text{ini}}$  can be changed using

```
ax.setTeta_i(new_theta_ini)
```

which is faster than running the constructor again, since all the interpolations are reused. However, running this function, erases all the arrays, and resets all variables to 0 (except T\_osc and a\_osc, as they should not change).

Importand note The Axion class constructs a pointer to an instance of the underlying mimes::Axion class, which has to be manually deleted. Therefore, once ax is used it must be deleted, *i.e.* we need to run

```
del ax
```

We should note that this must run even if we assign another instance to the same variable ax, otherwise we risk running out of memory.

# 4 Assumptions and user input

MiMeS only makes a few, fairly general, assumptions. First of all, it is assumed that the axion energy density is always subdominant compared to radiation or any other component of the Universe, and that decays and annihilations of particles have a negligible effect on the axion energy density. Moreover, the initial condition is always assumed to be  $\theta_{t=t_{\rm ini}} = \theta_{\rm ini}$  and  $\dot{\theta}|_{t=t_{\rm ini}} = 0$ . Furthermore, it is also assumed that  $3H/\tilde{m}_a$  increases monotonically at high temperatures. Also, it is assumed that the entropy of the plasma is resumes its conserved status at a temperature higher than the minimum temperature of inputFile (which is required by the constructor of the mimes::Axion<LD,Solver,Method> class). Finally, MiMeS does not try to predict anything regarding the cosmology. Therefore, the temperatures in inputFile must cover the entire region of integration; i.e. the maximum temperature has to be larger than the one required to reach ratio\_ini, while the minimum one should be lower than TSTOP.

# 4.1 Options at Compile-time

The user has a number of options regarding different aspects for the code. If MiMeS is used without using the available makefiles, then they must use the correct values for the various template arguments, explained in Appendix B. The various choices we for the shared libraries used by the python interface are given in MiMeS/Definitions.mk while the corresponding options for the C++ examples are in the Definitions.mk files in the directories inside the subdirectories of MiMeS/UserSpace/Cpp. The options correspond to different variables, which are

- 1. rootDir: the relative path of root directory of MiMeS.
- 2. LONG: this should be either long or omitted. If omitted, the type of the numeric values is double (double precision). On the other hand, if LONG=long, the type is long double. Generally, using double should be enough. For the sake of numerical stability, however, it is advised to always use LONG=long, as it a safer option. The reason is that the axion angle redshifts, and can become very

small, which introduces "rounding errors". Moreover, if the parameters absolute\_tolerance or absolute\_tolerance are chosen to be below  $\sim 10^{-8}$ , then double precision numbers may not be enough, and LONG=long is preferable. This choice comes at the cost of speed; double precision operations are usually preformed much faster. It is important to note that LONG defines a macro with the same name (in the C++ examples), which then defines the macro (again in the C++ examples) as #define LD LONG double. The macro LD, then is used as the corresponding template argument in the various classes. We point out again that if one chooses not to use the makefile files, the template arguments need to be known at compile-time. So the user has to define them in the code.

- 3. LONGpy: the same as LONG, but for the python interface. One should keep in mind that this cannot be changed inside python scripts. It just instructs ctypes what numeric type to use. Since the preferred way to compiled the shared libraries is via running "make" in the root directory of MiMeS, this variable needs to be defined inside MiMeS/Definitions.mk. By default, this variable is set to long, since this is the most stable choice in general.
- 4. SOLVER: MiMeS uses the ordinary differential equation (ODE) integrators of ref. [18]. Currently, there are two available choices; Rosenbrock and RKF. The former is a general embedded Rosenbrock implementation and it is used if SOLVER=1, while the latter is a general explicit embedded Runge-Kutta implementation and can be chosen by using SOLVER=2 (a brief description of how these algorithms are implemented can be found in Appendix A). By default MiMeS uses is SOLVER=1, because the axion EOM tends to oscillate rapidly. However, in some cases, a high order explicit method may also work. Note that this variable defines a macro that is then used as the second template argument of the mimes::Axion<LD,Solver,Method> class. The preferred way to do it in the shared libraries is via the MiMeS/Definitions.mk file, however, the user if free to compile everything in a different way. In this case, the various Definitions.mk files, are not being used, and the user must define the relevant arguments in the code where MiMeS is used.
- 5. METHOD: Depending on the type of solver is chosen, there are some available methods. 8
  - For SOLVER=1, the available methods are METHOD=RODASPR2 and METHOD=ROS34PW2. The RODASPR2 choice is a fourth order Rosenbrock-Wanner method (more information can be found in ref. [22]). The ROS34PW2 choice corresponds to a third order Rosenbrock-Wanner method [23].
  - For SOLVER=2, the only reliable method available in NaBBODES is the Dormand-Prince [24] chosen if METHOD=DormandPrince, which is an explicit Runge-Kutta method of seventh order.

This variable defines a macro (with the same name) that is passed as the third template parameter of mimes::Axion<LD,Solver,Method> (i.e.METHOD<LD> in the place of Method). If the compilation is not done via the makefile files, the user must define the relevant template arguments in the code.

- 6. CC: the C++ compiler that one chooses to use. The default option is CC=g++, which is the GNU C++ compiler, and is available for all systems. Another option is to use the clang compiler, which is chosen by CC=clang -lstdc++. MiMeS is mostly tested using g++, but clang also seems to work (and the resulting executables are sometimes faster), but the user has to make sure that their version of the compiler of choice supports the C++ 17 standard, otherwise MiMeS probably will not work.
- 7. OPT: Optimization level of the compiler. By default, this is OPT=03, which produces executables that are marginally faster than OPT=01 and OPT=02, but significantly faster than OPT=00. There

<sup>&</sup>lt;sup>8</sup>It is worth mentioning that NaBBODES is built in order to be a template for all possible Rosenbrock and explicit Runge-Kutta embedded methods, and one can provide their own Butcher tableau if they want to use another method, as shown in Appendix A.

is another choice, OPT=Ofast, but it can cause various numerical instabilities, and is generally considered dangerous – although we have not observed any problems when running MiMeS.

It is important to note, once again, that the variables that correspond to template arguments must be known at compile time. Thus, if the compilation is done without the help of the various makefile files, the template arguments must be given, otherwise compilation will fail. <sup>9</sup> For example, the choice LONG=long, SOLVER=1, and METHOD=RODASPR2 will be used to compile the shared libraries (and C++ example in MiMeS/UserSpace/Cpp/Axion) with mimes::Axion<long double,1,RODASPR2<long double>>. In order to fully understand the template arguments, the signatures of all classes and functions are given in Appendix B.

### 4.2 User input

# 4.2.1 Compile-time input

Files MiMeS requires files that provide data for the relativistic degrees of freedom (RDOF) of the plasma, and the anharmonic factor. Although MiMeS is shipped with the standard model RDOF found in [25], and a few points for  $f(\theta_{\text{peak}})$  introduced in eq. (2.28), the user is free change them via the corresponding variables in Paths.mk (in the root directory of MiMeS). Moreover, there is a set of data for the QCD axion mass as calculated in ref.[13]. The variables pointing to these data files are cosmoDat, axMDat, and anFDat, for the RDOF, axion mass, and the anharmonic factor; respectively.

The format of the files has to be the following:

- The RDOF data must be given in three columns; T (in GeV),  $h_{\text{eff}}$ , and  $g_{\text{eff}}$ .
- The axion mass data must be given in two columns; T (in GeV),  $\chi$  (in GeV<sup>4</sup>). Here,  $\chi$  is defined as in eq. (2.2). The user can provide a function instead of data for the axion mass, by leaving the axMDat variable empty.
- The data for the anharmonic factor must be give in two columns  $\theta_{\text{peak}}$   $f(\theta_{\text{peak}})$ ; with increasing  $\theta_{\text{peak}}$ .

The paths to these files should be given at compile time. That is, once Paths.mk changes, "bash configure.sh" and then "make" must be ran. The user can change the content of the data files (without changing their paths), in order to use them without compiling MiMeS again. However, the user has to make sure that all the files are sorted so that the values of first column increase (with no duplicates or empty lines). In order to ensure this, it is advised to run "bash FormatFile.sh path-to-file" (in Appendix F there are some details on MiMeS/src/FormatFile.sh), in order to format the file (that should exist in "path-to-file") so that it complies with the requirements of MiMeS.

These paths are stored as strings in MiMeS/src/misc\_dir/path.hpp at compile-time (they are defined as constexpr), and can be accessed once this header file is included. The corresponding variables are cosmo\_PATH, chi\_PATH, and anharmonic\_PATH, for the path to data file of the plasma quantities,  $\chi(T)$ , and  $f(\theta_{\text{peak}})$ ; respectively. Although, the axion mass data file may be omitted – since the axion mass is defined by the user, the variable chi\_PATH is still useful if the axion mass is defined via a data file, as it is automatically converted to an absolute path. <sup>10</sup>

#### 4.2.2 Run-time input

The run-time user input is described in sec. 3. The user has to provide at least the parameters that describe the axion evolution,  $\theta_{\text{ini}}$  and  $f_a$ .

Moreover, the maximum allowed value of u and the minimum value of T, allow the user to decide when the integration has to stop even if the axion has not reached its adiabatic evolution. Ideally,

<sup>&</sup>lt;sup>9</sup>In C++ the template arguments are part of the definition of a class; if the template arguments are not known, the class is not even constructed.

<sup>&</sup>lt;sup>10</sup>Absolute paths have the advantage to be accessible from everywhere else in the system. Thus, executables that seek the corresponding files can be called and copied easily.

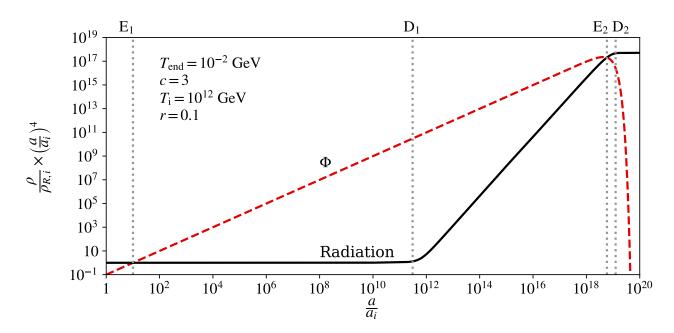


Figure 3: The energy densities of the plasma and a hypothetical decaying fluid. The parameters of the cosmological scenario  $T_{\rm END}=10^{-2}$  GeV, c=3,  $T_{\rm ini}=10^{12}$  GeV, and r=0.1; the parameters follow the definitions in ref. [27].

 $\mathtt{umax} = \infty$  and  $\mathtt{TSTOP} = 0$ , but  $\mathtt{MiMeS}$  is designed to be as general as possible and there may be cases where one needs to stop the integration abruptly. <sup>11</sup>

Furthermore, ratio\_ini allows the user to choose a desired point at which the interpolation of the data in inputFile begins. This can save valuable computation time as well as memory, as only the necessary data are stored and searched. Generally, for ratio\_ini> 10<sup>3</sup>, the relic abundance becomes independent from ratio\_ini, but one has to choose it carefully, in order to find a balance between accuracy and computation time.

Finally, the convergence conditions -i.e. N\_convergence\_max and convergence\_lim - allow the user to decide when the adiabatic evolution of the axion begins. Generally, the relic abundance does not have a strong dependence on these parameters as long as N\_convergence\_max> 3 and convergence\_lim< $10^{-1}$  (i.e. the adiabatic invariant does not vary more that 10% for three consecutive peaks of the oscillation). However, we should note that greedy choices (e.g. N\_convergence\_max= 100 and convergence\_lim=  $10^{-5}$ ) are dangerous, as  $\theta$  tends to oscillate rapidly and destabilize the differential equation solver. Therefore, these parameters should be chosen carefully, in order to ensure that integration stops when axion has reached its adiabatic evolution, without destabilising the EOM.

## 4.3 Complete Examples

Although one can modify the examples provided in MiMeS/UserSpace, in this section we show a complete example in both C++ and python. The underlying cosmology is assumed to be an EMD scenario. <sup>12</sup>. and the evolution of the energy densities of the plasma and a fluid  $\Phi$  is shown in Fig. (3). The various regime changes are indicated as  $T_{\rm E_{1,2}}$  – corresponding to the first and second time where  $\rho_{\Phi} = \rho_{\rm R}$ , and  $T_{\rm D_{1,2}}$  – which correspond to the start and end of entropy injection (for more precise definition see [27]). Regarding the axion, this cosmological scenario alters its evolution, since both the Hubble parameter and the entropy of the plasma change significantly. This results in a shift in the oscillation temperature, and the dilution of the axion energy density.

Moreover, we will use the QCD axion mass of ref. [13]. For the axion mass beyond the minimum

<sup>&</sup>lt;sup>11</sup>These two variables are not optional, because the user must be aware of them, in order to choose them according to their needs.

<sup>&</sup>lt;sup>12</sup>In terms of the parametrisation introduced in ref. [26, 27], the early matter dominated case is defined via  $T_{\rm end} = 10^{-2}$  GeV, c = 3,  $T_{\rm ini} = 10^{12}$  GeV, and r = 0.1.

and maximum temperatures,  $T_{\min, \max}$ , in the corresponding data file, we will take

$$\tilde{m}_{a} = \begin{cases} \frac{\chi(T_{\min})}{f_{a}^{2}} & \text{for } T < T_{\min} \\ \frac{\chi(T_{\max})}{f_{a}^{2}} \left(\frac{T}{T_{\max}}\right)^{-8.16} & \text{for } T > T_{\max} \end{cases}$$

$$(4.1)$$

# 4.3.1 complete example in C++

In order to write a C++ program that uses MiMeS in order to solve the EOM 2.19, we must include the header files src/AxionMass/AxionMss.hpp and src/Axion/AxionSolve.hpp. In the example at hand, the main function should contain the definition of the axion mass

```
// use chi_PATH to interpolate the axion mass.
     mimes::AxionMass<LD> axionMass(chi_PATH,0,mimes::Cosmo<LD>::mP);
2
3
     /* This is the axion mass squared beyond the interpolation limits
4
     for the current data. If you don't specify them, the axion mass
5
     is taken to be constant beyond these limits */
     /*set ma2 for T>TMax*/
8
     long double TMax=axionMass.getTMax();
9
     long double chiMax=axionMass.getChiMax();
10
     axionMass.set_ma2_MAX(
11
        [&chiMax,&TMax](long double T, long double fa){
12
           return chiMax/fa/fa*std::pow(T/TMax,-8.16);
13
14
     );
15
16
     /*set ma2 for T<TMin*/
17
     long double TMin=axionMass.getTMin();
18
     long double chiMin=axionMass.getChiMin();
19
     axionMass.set_ma2_MIN(
20
        [&chiMin,&TMin](long double T, long double fa){
21
           return chiMin/fa/fa;
22
23
     );
```

It should be noted that, since we have used chi\_PATH, we need to include the path.hpp header file from MiMeS/src/misc\_dir. Moreover, we note that we have used as parameter mimes::Cosmo<LD>::mP, which is the Planck mass, as a static member of the Cosmo class (described in Appendix B), in order to interpolate the mass up to  $T = m_P$ , i.e. the entire possible mass range.

Following, the axion EOM can be solve as

This program should solve the axion EOM. However, one needs to print anything that they need. For example, the relic abundance is printed by adding std::cout<<ax.relic<<"\n"; after ax.solveAxion();. It should be noted that, in order to make sure that the code is compiled successfully, one should add at the top of the file any other header they need. In particular, in this case, we need to add #include<iostream>, in order to be able to use std::cout.

Parameter choice It should be noted that the string that is assigned to the variable inputFile, is the path of file that exists in MiMeS/UserSpace/InputExamples. Also, rootDir is a constant static (char[]) variable that is defined in MiMeS/src/path.hpp, and it is automatically generated when bash configure.sh is executed. Moreover, the other parameters used in the constructor are:

```
\bullet beta= 0.9
• theta_i = 0.1
                             • convergence_lim= 10^{-2}
• fa = 10^{16} \text{ GeV}
                              • initial_stepsize= 10^{-1}
                                                                • fac_max = 1.2
• umax =500
                              • maximum_stepsize= 10^{-1}
                                                                • fac_min= 0.8
• TSTOP= 10^{-4} \text{ GeV}
                                                                • maximum_No_steps= 10^7
                              • minimum_stepsize= 10^{-8}
• ratio ini= 10^3
                              • absolute_tolerance= 10^{-11}
• N_convergence_max= 15
                             • relative_tolerance= 10^{-11}
```

Template arguments Furthermore, The first template parameter is long double, which means that all the numeric types (apart from integers like maximum\_No\_steps) have "long double" precision. which is useful when considering low tolerances as in this example. The second and third template parameters are responsible for the Runge-Kutta method we use. That is, n this case, the second template parameter – 1 – means that we use a Rosenbrock method, with the method being RODASPR2. Notice that the method also needs a template parameter that is used to declare all member variables of the RODASPR2 class as long double.

Compilation Before we compile, we have to make sure that we have already executed bash configure.sh. Assuming that we name the file that contains the code axionExample.cpp, and it is located in MiMeS/UserSpace, an executable can be produced as

```
g++ -03 -std=c++17 -lm -I../ -o axion axionExample.cpp

or

clang -lstdc++ -03 -std=c++17 -lm -I../ -o axion axionExample.cpp
```

Both of these commands should create an executable that solves the axion EOM. That is, assuming we have a terminal open in MiMeS/UserSpace, we can run ./axion, and get the results we chose. It should be noted that all paths that MiMeS uses by default are written as absolute paths when we run bash ./configure.sh. Therefore, if the inputFile variable is also an absolute path, the executable can be copied and used in any other directory of the same system. However, it should be preferred that executables are kept under the MiMeS directory, in order to be able to compile them with different data file paths if needed.

The entire code This example consists of only a few lines of code, which, including the change in the axion mass beyond the interpolation limit, is

```
#include<iostream>
     //include everything you need from MiMeS
     #include"src/Axion/AxionSolve.hpp"
3
     #include"src/AxionMass/AxionMass.hpp"
4
     #include"src/Cosmo/Cosmo.hpp"
5
     #include"src/misc_dir/path.hpp"
6
7
     int main(){
8
        // use chi_PATH to interpolate the axion mass.
9
        mimes::AxionMass<LD> axionMass(chi_PATH,0,mimes::Cosmo<LD>::mP);
10
11
        /*set \tilde{m}_a^2 for T \geq T_{\max}*/
12
        long double TMax=axionMass.getTMax();
13
        long double chiMax=axionMass.getChiMax();
14
        axionMass.set_ma2_MAX(
15
           [&chiMax,&TMax](long double T, long double fa){
16
```

```
return chiMax/fa/fa*std::pow(T/TMax,-8.16);
17
           }
18
        );
19
20
        /*set \tilde{m}_a^2 for T \leq T_{\min}*/
21
        long double TMin=axionMass.getTMin();
22
        long double chiMin=axionMass.getChiMin();
        axionMass.set_ma2_MIN(
24
           [&chiMin,&TMin](long double T, long double fa){
25
              return chiMin/fa/fa;
26
        );
28
29
30
        std::string inputFile = std::string(rootDir)+
31
           std::string("/UserSpace/InputExamples/MatterInput.dat");
32
33
        mimes::Axion<long double, 1, RODASPR2<long double> >
        ax(0.1, 1e16, 500, 1e-4, 1e3, 15, 1e-2, inputFile, &axionMass,
35
        1e-1, 1e-8, 1e-1, 1e-11, 1e-11, 0.9, 1.2, 0.8, int(1e7));
36
37
        ax.solveAxion();
38
        std::cout<<ax.relic<<"\n";</pre>
40
41
42
        return 0;
     }
43
```

We should point out that another example is given in MiMeS/UserSpace/Cpp/Axion, where all parameters are taken as command-line inputs, the various compilation-time options can be given MiMeS/UserSpace/Cpp/Axion/Definitions.mk, and then compiled using make. Therefore, the user can just modify this code in order to meet their needs. That is, using this example, one only needs to add their preferred definition of ma2\_MAX and ma2\_MIN — or change the axionMass variable (in MiMeS/src/static.hpp) using a function as mentioned in section 4.2.1 without writing the entire program themselves.

**Alternative axion mass definition** For this particular example, we could have used the approximate definition of the axion mass

$$\tilde{m}_a^2 \approx m_a^2 \times \left\{ \left( \frac{T_{\rm QCD}}{T} \right)^{8.16} & \text{for } T \ge T_{\rm QCD} \\ 1 & \text{for } T \le T_{\rm QCD} \end{cases} \right.$$

$$(4.2)$$

where  $T_{\rm QCD}\approx 150~{\rm MeV}$  and  $m_a=\frac{3.2\times 10^{-5}~{\rm GeV^4}}{f_a{}^2}$ . This can be done by substituting the axionMass definition (lines 9-28) with

```
auto ma2 = [](long double T,long double fa){
    long double TQCD=150*1e-3;
    long double ma20=3.1575e-05/fa/fa;
    if(T<=TQCD){return ma20;}
    else{return ma20*std::pow((TQCD/T),8.16);}
};
mimes::AxionMass<LD> axionMass(ma2);
```

# 4.3.2 complete example in python

In order to be able use the AxionMass and Axion classes in python, we need to import the corresponding modules from MiMeS/src/interfacePy. That is, assuming that the script from which we intend to im-

port MiMeS/src/interfacePy/Axion/Axion.py and MiMeS/src/interfacePy/Axion/AxionMass.py is in MiMeS/UserSpace, we can import the classs by writing the following

```
#add the relative path for MiMeS/src
from sys import path as sysPath
from os import path as osPath
sysPath.append(osPath.join(osPath.dirname(__file__), '../src'))

from interfacePy.AxionMass import AxionMass #import the AxionMass class
from interfacePy.Axion import Axion #import the Axion class
from interfacePy.Cosmo import mP #import the Planck mass
```

Once everything we need is imported, we can simply follow the steps outlined in section 3.1.2. For the example at hand, we can create an instance of the AxionMass class as

```
# AxionMass instance
     axionMass = AxionMass(r'../src/data/chi.dat',0,mP)
2
3
     # This is the axion mass squared beyond the interpolation limits for the current data.
4
     # If you don't specify them, the axion mass is taken to be constant beyond these limits
5
     TMax=axionMass.getTMax()
6
     chiMax=axionMass.getChiMax()
7
     TMin=axionMass.getTMin()
8
9
     chiMin=axionMass.getChiMin()
10
     axionMass.set_ma2_MAX( lambda T,fa: chiMax/fa/fa*pow(T/TMax,-8.16) )
11
     axionMass.set_ma2_MIN( lambda T,fa: chiMin/fa/fa )
12
```

Then we can simply create an instance of the Axion class as

```
#in python it is more convenient to use relative paths
inputFile = "./InputExamples/MatterInput.dat"

ax = Axion(0.1, 1e16, 500, 1e-4, 1e3, 15, 1e-2, inputFile, axionMass,
1e-1, 1e-8, 1e-1, 1e-11, 0.9, 1.2, 0.8, int(1e7))
```

Again, the parameters for the constructor are the same as in the C++ example. The axion EOM, then, is solved using

```
ax.solveAxion()
```

In contrast to the C++ usage of this function, this only stores the  $\theta_{\rm ini}$ ,  $f_a$ ,  $\theta_{\rm osc}$ ,  $T_{\rm osc}$ , and  $\Omega h^2$  in the variables ax.theta\_i, ax.fa, ax.theta\_osc, ax.T\_osc, and ax.relic; respectively. Therefore, we can print the relic abundance by calling print(ax.relic). In order to get the integration points (i.e. the evolution of the angle and the other quantities), the quantities at the peaks, and the local integration errors, we need to call

```
#this gives you all the points of integration
ax.getPoints()

#this gives you the peaks of the oscillation
ax.getPeaks()

#this gives you local integration errors
ax.getErrors()
```

The documentation of any python function can be read directly inside the script using? as a prefix. For example, in order to see what the functionality and usage of the getPeaks function, we can call "?ax.getPeaks", and its documentation will be printed.

As already mentioned, it is important to always delete any instance of the AxionMass and Axion classes once they are not needed. In this case this is done by calling

```
del ax del axionMass
```

Compilation of the shared library As described in section 4.2.1, we may need to change the default data file paths, or the various compilation options. This is done through the variables in MiMeS/Definitions.mk and MiMeS/Paths.mk described in section 4.1.

Once we have chosen everything according to our needs, the library can be created by opening a terminal inside the root directory of MiMeS and running

```
bash configure.sh
make lib/Axion_py.so
```

The entire code As in the C++ example, this example consists of only a few lines of code. The script we described here is

```
#add the relative path for MiMeS/src
     from sys import path as sysPath
     from os import path as osPath
3
     sysPath.append(osPath.join(osPath.dirname(__file__), '../src'))
4
     from interfacePy. AxionMass import AxionMass #import the AxionMass class
     from interfacePy. Axion import Axion #import the Axion class
     from interfacePy.Cosmo import mP #import the Planck mass
8
9
     # AxionMass instance
10
     axionMass = AxionMass(r'../src/data/chi.dat',0,mP)
11
12
     # define \tilde{m}_a{}^2 for T \leq T_{\min}
13
     TMin=axionMass.getTMin()
14
     chiMin=axionMass.getChiMin()
15
     axionMass.set_ma2_MIN( lambda T,fa: chiMin/fa/fa )
16
17
     # define \tilde{m}_a{}^2 for T \geq T_{\rm max}
18
     TMax=axionMass.getTMax()
19
     chiMax=axionMass.getChiMax()
20
     axionMass.set_ma2_MAX( lambda T,fa: chiMax/fa/fa*pow(TMax/T),8.16) )
21
22
     #in python it is more convenient to use relative paths
23
     inputFile = inputFile="./InputExamples/MatterInput.dat"
24
25
     ax = Axion(0.1, 1e16, 500, 1e-4, 1e3, 15, 1e-2, inputFile, axionMass,
26
     1e-1, 1e-8, 1e-1, 1e-11, 1e-11, 0.9, 1.2, 0.8, int(1e7))
27
28
     ax.solveAxion()
29
30
     print(ax.relic)
31
32
     #once we are done we should run the destructor
33
     del ax
34
     del axionMass
35
```

One can find a complete example, including the option to create several plots, in the script MiMeS/UserSpace/Python/Axion.py. Also, the same example can be used interactively, in jupyter notebook environment, that can be found in MiMeS/UserSpace/JupyterNotebooks/Axion.ipynb. One can read the comments, and change all different parameters, in order to examine how the results are affected.

Alternative axion mass definition In order to use the approximate axion mass as defined in eq. (4.2), we could replace the definition of the axionMass variable (lines 10-21) with

```
1  def ma2(T,fa):
2    TQCD=150*1e-3
3    ma20=3.1575e-05/fa/fa
4    if T<=TQCD:
5        return ma20;
6    return ma20*(TQCD/T)**8.16
7    axionMass = AxionMass(ma2)</pre>
```

#### 4.3.3 Results

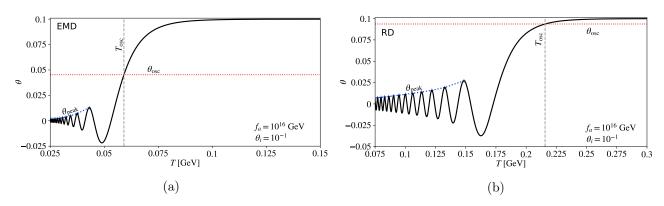


Figure 4: The evolution of the axion angle,  $\theta$ , with the temperature in early matter dominated (a) and radiation dominated (b) cases. For the EMD case, the  $\theta_{\rm ini}$  is chosen so that  $\Omega h^2 = 0.12$ .

In Fig. (4a) we show the evolution of  $\theta$  for temperatures  $T \in [0.025, 0.15]$  GeV, where the vertical line indicates  $T_{\rm osc}$ , while the horizontal one the corresponding value of  $\theta$ ,  $\theta_{\rm osc}$ . Also, the blue curve connects the peaks of the oscillation. For comparison, in Fig. (4b) we also show the evolution of the angle in a radiation dominated Universe with constant entropy (i.e. standard cosmological scenario). From these figures, we can see that the effect of an early matter domination reduces the amplitude of oscillation – due to the injection of entropy – as well the oscillation temperature – due to the increase of the Hubble parameter. Furthermore, the angle at  $T = T_{\rm osc}$  in the EMD scenario is much smaller that the corresponding value in the standard cosmological case, since the entropy injection causes the scale factor to be larger compared to the scale factor at the same temperature. Moreover, in Fig. (5), we show the relative local error of integration as well as a histogram of the number of integration steps for 0.025 GeV < T < 0.15 GeV. The local relative errors, defined in Appendix A, are shown

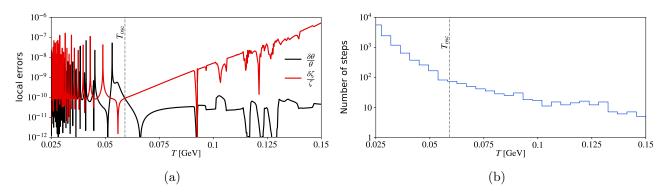


Figure 5: (a) Local relative errors of  $\theta$  and  $\zeta$  for the temperature range  $0.025 \text{GeV} \leq T \leq 0.15 \text{GeV}$ . (b) Histogram of number of points in the same temperature range.

in Fig. (5a). The black and red lines correspond to  $\delta\theta/\theta$  and  $\delta\zeta/\zeta$ , respectively. This figure indicates that the local errors are relatively well behaved for  $T > T_{\rm osc}$ , and they only start to oscillate violently

once the oscillations start. However, the adaptation of the integration step seems to work, as the errors are kept below  $\sim 10^{-7}$  (the relative error of zeta is large because  $\zeta \approx 0$  before the  $T_{\rm osc}$ ). In order to examine how the step-size is adapted to the difficulty of the problem, we also show a histogram which show how many integration steps are taken for fixed temperature intervals. <sup>13</sup> In this figure, we see that the number of integration steps increases rapidly for temperatures below the oscillation temperature. This is expected, since integration becomes more difficult as the frequency of the oscillation increases  $-\tilde{m}_a/H$  increases rapidly for  $T < T_{\rm osc}$ . That is, the local integration error tends to increase. Thus, in order to reduce the local error, the embedded RK method we employ, reduces the step-size. This means that for  $T \lesssim T_{\rm osc}$  the number of integration steps increase drastically. This is the general picture of how adaptation happens. However, one has to experiment with all the available parameters, in order to solve the axion EOM as accurately and fast as possible.

# 5 Acknowledgements

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# 6 Summary

We have introduced MiMeS; a header-only library written C++ that is used to compute the axion (or ALP) relic abundance, by solving the corresponding EOM, in a user defined underlying cosmology. MiMeS makes only a few assumptions, which allows the user to explore a wide range ALP and cosmological scenarios.

In this manuscript, we have provided a detailed explanation on how to use MiMeS, by showing examples in both C++ and python (paragraphs (3.1) and (4.3)). We have described the user input that is expected, and the various options available (sections (3) and (4)). Moreover, in the Appendix, we provide a detailed review of all the internal components that comprise MiMeS. We briefly discuss the Runge-Kutta methods that MiMeS uses, and show how the user can implement their own. We explain the functionality of all the classes, modules, and utilities. Also, we provide a detailed input and option guide.

In the future, MiMeS will be extended in several ways. First, we should implement new functionality that will allow the user to automatically compare against various experimental data (although, there is already an available module [28] that can be used for this goal). This is going to be helpful, as the user will only need to use one program (or script) to compute what is needed. We also aim to supplement MiMeS with the option to produce ALPs via interactions of the plasma (e.g. freeze-out/in), which may be useful in certain cases. Moreover, a later version of MiMeS may allow the user to define different initial condition for  $\zeta$  as well, since there are cases where this is needed (e.g. [14]). Finally, MiMeS will continue to improve by correcting mistakes, or implementing suggestions by the community.

# Appendix

# A Basics of embedded Runge-Kutta Mehtods

Runge-Kutta (RK) methods are employed in order to solve an ordinary differential equation (ODE), or a system of ODEs of first order. <sup>14</sup> Although there are some very insightful sources in the literature (e.g. [29, 30, 31]) we give a brief overview of them in order to help the user to make appropriate decisions when using MiMeS.

 $<sup>^{13}</sup>$  More precisely, the histogram is made by dividing the the temperature range 0.025 GeV  $\lesssim T \lesssim 0.15$  GeV to 30 bins of equal size.

<sup>&</sup>lt;sup>14</sup>Boundary value problems, and higher order differential equations are expressed as first order ODEs, and then solved. Similarly to eq. (2.19).

The general form of a system of first order of ODEs is

$$\frac{d\vec{y}}{dt} = \vec{f}(\vec{y}, t) , \qquad (A.1)$$

with given initial condition  $\vec{y}(0)$ . Also, the components of  $\vec{y}$  denote the unknown functions. Note that we can always shift t to start at 0, which simplifies the notation. In order to solve the the system of eq. (A.1), an RK method uses an iteration of the form

$$\vec{y}_{n+1} = \vec{y}_n + h \sum_{i=1}^s b_i \ \vec{k}_i \ , \tag{A.2}$$

with n denoting the iteration number, h the "step-size" that is used to progress t;  $t_{n+1} = t_n + h$ . Moreover, s,  $b_i$  and  $\vec{k}_i$  define the corresponding RK method. For example, the classic Euler method is an RK method with s = 1, b = 1, and  $\vec{k}_1 = \vec{f}(y_n, t_n)$ . Methods with  $\vec{k}$  that depends on previous step  $(i.e. \ \vec{k} = \vec{k} \ [y_n, t_n])$ , are called explicit, while the ones that try to also predict next step  $(i.e. \ \vec{k} = \vec{k} \ [y_n, t_n; y_{n+1}, t_{n+1}])$  are called implicit. <sup>15</sup>

# A.1 Embedded RK methods

A large category of RK methods are the so-called embedded RK methods. These methods make two estimates for the same step simultaneously – without evaluating  $\vec{k}$  many times within the same iteration. Therefore, together with the iteration of eq. (A.2), a second estimate is given by

$$\vec{y}_{n+1}^* = \vec{y}_n + h \sum_{i=1}^s b_i^* \vec{k}_i , \qquad (A.3)$$

with  $b_i^*$  is an extra parameter that characterise the "embedded" method of different order (typically, one order higher that the estimate A.2). The local (for the step  $t_{n+1}$ ) error divided by the scale of the solution, then, estimated as

$$\Delta \equiv \sqrt{\frac{1}{N} \sum_{d=1}^{N} \left( \frac{y_{n+1,d} - y_{n+1,d}^*}{\Lambda_d} \right)^2} , \qquad (A.4)$$

where n the iteration number, N the number of ODEs, d the component of  $\vec{y}$ , and  $\Lambda_d$  defined as

$$\Lambda_d = \text{Atol} + \max\left(|y_{n+1,d}|, |y_{n+1,d}^*|\right) \text{ Rtol}, \qquad (A.5)$$

with Atol and Rtol the absolute and relative tolerances that characterise the desirable accuracy we want to achieve; user defined values, typically Atol=Rtol $\ll$  1. With these definitions, the desirable error is reached when  $\Delta \lesssim 1$ .

**Step-control** The definition A.4, allows us to adjust the step-size h in such way that  $\Delta \approx 1$ . That is, we take trial steps, and h is adapted until  $\Delta \approx 1$ . A simple adaptive strategy adjusts step-size, using

$$h \to \beta \ h \max \left[ f_{\min}, \min \left( \Delta^{-\frac{1}{p+1}}, f_{\max} \right) \right] ,$$
 (A.6)

with p the order of the RK method (p+1 is the order of the embedded one),  $\beta$  a bias factor of the adaptive strategy (typically  $\beta$  is close but below 1), used to adjust the tendency of h to be somewhat smaller than what the step-control predicts. Also,  $f_{min}$  and  $f_{max}$  are the minimum and maximum allowed factors, respectively, that can multiply  $\beta$  h, used in order to avoid large fluctuations that can destabilise the process. All these parameters are chosen by the user, in order to make the step-control process as aggressive or safe as needed.

MiMeS	Runge-Kutta
absolute_tolerance	Atol
relative_tolerance	Rtol
b	β
fac_min	$f_{ m min}$
fac_max	$f_{ m max}$

Table 1: Correspondence between the user MiMeS user input and the RK parameters described in the text.

Correspondence between MiMeS parameters and RK ones The various parameters that MiMeS are described in section 4.2. The correspondence between them and the RK parameters is given in table 1.

# A.2 Explicit embedded RK methods

Explicit methods use only the information of the previous step in order to compute  $\vec{k}_i$  from

$$\vec{k}_i = \vec{f} \left( \vec{y}_n + h \left( \sum_{j=1}^{i-1} a_{ij} \vec{k}_j \right), t_n + c_i h \right), \quad \forall i = 1, 2, \dots, s ,$$
 (A.7)

with  $a_{ij}$ ,  $c_i$ , together with  $b_i$  and  $b_i^*$ , consist the so-called Butcher tableau of the corresponding method. For explicit methods this is usually presented as

It should be noted that  $c_i = \sum_{j=1}^{s} a_{ij}$ .

#### A.3 Rosenbrock methods

Explicit RK methods, encounter instabilities when a system is "stiff"  $^{16}$ ; e.g. when it oscillates rapidly, or has different elements at different scales. These problems are somewhat resolved by trying to predict the next step inside  $\vec{k}$ ; i.e. in implicit methods. However, then one has to solve a non-linear set of equations in order to compute  $\vec{y}_{n+1}$ , which is generally a slow process, as the Newton method (or some variation) needs to be applied. However, there exist another way, a compromise between explicit and implicit methods. Linearly implicit RK methods, usually called Rosenbrock methods – with popular improvements as Rosenbrock-Wanner methods, introduce parameters in the diagonal of the Butcher tableau A.8 and linearise the system of non-linear equations (for details, see [30]). In these methods,  $\vec{k}$  is determined by

$$\left(\hat{I} - \gamma h \hat{J}\right) \cdot \vec{k}_i = h \vec{f} \left(\vec{y}_n + \sum_{j=1}^{i-1} a_{ij} \vec{k}_j, t_n + c_i h\right) + h^2 \left(\gamma + \sum_{j=1}^{i-1} \gamma_{ij}\right) \frac{\partial \vec{f}}{\partial t} + h \hat{J} \cdot \sum_{j=1}^{i-1} \gamma_{ij} \vec{k}_j, \qquad (A.9)$$

<sup>&</sup>lt;sup>15</sup>Generally, by substituting implicit methods  $y_{n+1}$  as in eq. (A.2), we end up with a system of equations that need to be solved in order to compute  $\vec{k}$ .

<sup>&</sup>lt;sup>16</sup>A definition of stiffness can be found in [30, 29].

which is written in such a way that everything is evaluated at  $t = t_n$ . In eq. (A.9),  $\hat{J} = \frac{\partial f}{\partial \vec{y}}$  the Jacobian of the system of ODEs,  $\hat{I}$  the unit matrix with dimension equal to the number of ODEs. Moreover,  $\gamma$  and  $\gamma_{ij}$  are parameters that characterise the method (along with  $a_{ij}$ ,  $c_i$ ,  $b_i$ , and  $b_i^*$ ).

Implementing a new Butcher tableau in NaBBODES As already mentioned, MiMeS uses NaBBODES, which supports the implementation of new Butcher tableaux. This is done by adding a new class (or struct) inside the header file METHOD.hpp that can be found in MiMeS/src/NaBBODES/RKF for the explicit RK and MiMeS/src/NaBBODES/Rosenbrock for the Rosenbrock embedded methods. All the new parameters must be public, constexpr static variables, of a type that is the template parameter of the method. For example, the Heun-Euler method can be implemented by adding the following code in MiMeS/src/NaBBODES/RKF/METHOD.hpp

```
/*---Implementation of the Heun-Euler method----*/
     /*----It shouldn't be used for MiMeS, since it is likely to fail----*/
2
3
     //LD is the numeric type (\ie double, or long double).
4
     template<class LD>
5
     //use struct because its variables are public by default.
6
     struct HeunEuler{
        static constexpr unsigned int s=2; // HeunEuler is a 2-stage RK
        static constexpr unsigned int p=1; // first order, with embedded p+1=2
9
10
        //these are aliases for the arrays
11
        using arr=std::array<LD,s>;
        using arr2=std::array<std::array<LD,s>,s>;
13
14
        static constexpr arr b=\{0.5,0.5\}; // this is b_i
15
        static constexpr arr bstar=\{0.5,0.5\}; // this is b_i^*
16
        static constexpr arr c={0,1}; // remember that c_i = \sum_i a_{ij}
17
18
        // this is a_{ij}
19
        static constexpr arr2 a={
20
21
           arr{0,0},
           arr{1,0}
22
        };
23
     };
24
```

In order to implement the ROS3w [23] method, one can add the following code in the header file MiMeS/src/NaBBODES/Rosenbrock/METHOD.hpp

```
/*----Implementation of the ROS3w method----*/
     /*----It shouldn't be used, since it is likely to fail to produce a result-----*/
2
3
4
     //LD is the numeric type (i.e. double, or long double).
5
     template<class LD>
6
     struct ROS3w{
7
        static constexpr unsigned int s=3; // 3-stage
8
        static constexpr unsigned int p=2; // second order (embedded order is p+1)
9
10
11
        //aliases for the arrays
        using arr=std::array<LD,s>;
12
        using arr2=std::array<std::array<LD,s>,s>;
13
14
        static constexpr arr b=\{0.25, 0.25, 0.5\}; // this is b_i
15
        // this is b_i^*
16
        static constexpr arr bstar={ 0.746704703274,0.1144064078371,0.13888888888888};
17
```

```
18
         static constexpr arr c={0,2/3.,4/3.}; // remember that c_i = \sum_{i=1}^{n} a_{ij}
19
         static constexpr LD gamma=0.4358665215084; // this is \gamma
20
21
         // this is a_{ij}
22
         static constexpr arr2 a={
23
            arr{0,0,0},
24
            arr{2/3.,0,0},
25
            arr{2/3.,2/3.,0}
26
         };
27
28
         // this is \gamma_{ij}
29
         static constexpr arr2 g={
30
            arr{0,0,0},
31
            arr{0.3635068368900,0,0},
32
            arr{-0.8996866791992,-0.1537997822626,0}
33
         };
34
      };
35
```

How to compile MiMeS in order to use the newly implemented method Once a new Butcher tableau is implemented, the mimes::Axion class can use it. This class, just needs the name of method assigned to the corresponding template argument; Method. A convenient way to do this, is to define a macro using the -D flag of the compiler, and use macro as the corresponding template parameter of the mimes::Axion class. Alternatively, if one uses the makefile files, a method can be chosen by adding it in the corresponding Definitions.mk file; e.g. as METHOD=ROS3w for the ROW3 method. <sup>17</sup>

# B C++ classes

MiMeS is designed as an object-oriented header-only library. That is, all the basic components of the library are defined as classes inside header files. All the classes relevant to the use of MiMeS are under the namespace mimes.

### B.1 Cosmo class

The mimes::Cosmo<LD> class is responsible for interpolation of the various quantities of the plasma. Its header file is MiMeS.src/Cosmo/Cosmo.hpp, and needs to be included in order to use this class. The template parameter LD is the numeric type that will be used, e.g. double. The constructor of this class is

```
template<class LD>
mimes::Cosmo<LD>(std::string cosmo_PATH, LD minT=0, LD maxT=mimes::Cosmo<LD>::mP)
```

The argument  $cosmo_PATH$  is the path of the data file that contains T (in GeV),  $h_{eff}$ ,  $g_{eff}$ , with increasing T. The parameters minT and maxT are minimum and maximum interpolation temperatures. These temperatures are just limits, and the action interpolation is done between the closest temperatures in the data file. Moreover, beyond the interpolation temperatures, both  $h_{eff}$  and  $g_{eff}$  are assumed to be constants.

Interpolation of the RDOF, allows us to define various quantities related to the plasma; e.g. the entropy density is defined as  $s = \frac{2\pi^2}{45} h_{\rm eff} T^3$ . These quantities are given as the member functions:

- template<class LD> LD mimes::Cosmo<LD>::heff(LD T):  $h_{\rm eff}$  as a function of T.
- template<class LD> LD mimes::Cosmo<LD>::geff(LD T):  $g_{eff}$  as a function of T.

<sup>&</sup>lt;sup>17</sup>One needs to make sure to use the correct Solver template argument (or SOLVER variable in the Definitions.mk files), otherwise compilation will fail.

- template<class LD> LD mimes::Cosmo<LD>::dheffdT(LD T):  $dh_{\rm eff}/dT$  as a function of T.
- template<class LD> LD mimes::Cosmo<LD>::dgeffdT(LD T):  $dg_{\rm eff}/dT$  as a function of T.
- template<class LD> LD mimes::Cosmo<LD>::dh(LD T):  $\delta_h=1+\frac{1}{3}\frac{d\log h_{\rm eff}}{d\log T}$  as a function of T.
- template<class LD> LD mimes::Cosmo<LD>::s(LD T): The entropy density of the plasma as a function of T.
- template<class LD> LD mimes::Cosmo<LD>::rhoR(LD T): The energy density of the plasma as a function of T.
- template<class LD> LD mimes::Cosmo<LD>::Hubble(LD T): The Hubble parameter assuming radiation dominated expansion as a function of T.

Moreover, there are several cosmological quantities are given as members variables:

- template<class LD> constexpr static LD mimes::Cosmo<LD>::T0: CMB temperature today [32] in GeV.
- template<class LD> constexpr static LD mimes::Cosmo<LD>::h\_hub: Dimensionless Hubble constant [32].
- template<class LD> constexpr static LD mimes::Cosmo<LD>::rho\_crit: Critical density [32] in GeV<sup>3</sup>.
- template<class LD> constexpr static LD mimes::Cosmo<LD>::relicDM\_obs: Central value of the measured DM relic abundance [7].
- template<class LD> constexpr static LD mimes::Cosmo<LD>::mP: Planck mass [32] in GeV.

#### B.2 AnharmonicFactor class

The class mimes::AnharmonicFactor<LD> is responsible interpolating the anharmonic factor as defined in eq. (2.28). The corresponding header file is MiMeS/src/AnharmonicFactor/AnharmonicFactor.hpp.

The constructor of this class is

```
template < class LD>
mimes::AnharmonicFactor < LD>(std::string anharmonic_PATH)
```

Again, the template argument LD is a numeric type, and the anharmonic\_PATH string is the path of the data file with data for  $\theta_{\text{peak}}$  (which should be in increasing order) and  $f(\theta_{\text{peak}})$ .

The member function that MiMeS uses is the overloaded call operator

```
template<class LD> LD mimes::AnharmonicFactor<LD>::operator()(LD theta_peak)
```

This function returns the value of the anharmonic factor at  $\theta_{\text{peak}}$  =theta\_peak. Although, there is no need to call this function beyond the interpolation limits (as long as the data file contains  $0 \le \theta_{\text{peak}} \le \pi$ ), it is important to note that the anharmonic factor is taken to be constant beyond these limits.

#### B.3 AxionMass class

The mimes::AxionMass<LD> class is responsible for the definition of the axion mass. The header file of this class is MiMeS/src/AxionMass/AxionMass.hpp. Its usage and member functions are described in the examples given in sections (3.1) and (4.3). However, it would be helpful to outline them here.

The class has two constructors. The first one is

```
template<class LD>
mimes::AxionMass<LD>(std::string chi_PATH, LD minT=0, LD maxT=mimes::Cosmo::mP)
```

The first argument, chi\_PATH, is the path to a data file that contains two columns; T (in GeV) and  $\chi$  (in GeV<sup>4</sup>), with increasing T. The arguments minT and maxT are the interpolation limits. These limits are used in order to stop the interpolation in the closest temperatures that exist in the data file. That is the actual interpolation limits are  $T_{\min} \ge \min$ T and  $T_{\max} \le \max$ T. Beyond these limits, by default, the axion mass is assumed to be constant. However, this can be changed by using the member functions

```
void set_ma2_MIN(std::function<LD(LD,LD)> ma2_MIN)
void set_ma2_MAX(std::function<LD(LD,LD)> ma2_MAX)
```

Here, ma2\_MIN and ma2\_MAX are functors that define the axion mass squared beyond the interpolation limits. In order to ensure that the axion mass is continuous, usually we need  $T_{\min}$ ,  $T_{\max}$ ,  $\chi(T_{\min})$ , and  $\chi(T_{\max})$ . These values can be obtained using the member functions

- template<class LD> LD mimes::AxionMass<LD>::getTMin(): This function returns the minimum interpolation temperature,  $T_{\min}$ .
- template<class LD> LD mimes::AxionMass<LD>::getTMax(): This function returns the maximum interpolation temperature,  $T_{\text{max}}$ .
- ullet template<class LD> LD mimes::AxionMass<LD>::getChiMin(): This function returns  $\chi(T_{\min})$ .
- template<class LD> LD mimes::AxionMass<LD>::getChiMax(): This function returns  $\chi(T_{\text{max}})$ .

An alternative way to define the axion mass is via the constructor

```
template<class LD>
mimes::AxionMass<LD>(std::function<LD(LD,LD)> ma2)
```

Here, the only argument is the axion mass squared,  $\tilde{m}_a$ , defined as a callable object. Once an instance of the class is defined, we can get  $\tilde{m}_a^2$  using the member function

```
template<class LD> LD mimes::AxionMass<LD>::ma2(LD T, LD fa)
```

We should note that ma2 is a public std::function<LD(LD,LD)> member variable. Therefore, it can be assigned using the assignment operator. However, in order to change its definition, we can also use the following member function:

```
template<class LD> void mimes::AxionMass<LD>::set_ma2(std::function<LD(LD,LD)> ma2)
```

#### B.4 AxionEOM class

The mimes::AxionEOM<LD> class is not useful for the user. However, it is responsible for the interpolation of the underlying cosmology, and the definition of the axion EOM 2.19, which is passed to the ODE solver of NaBBODES.

The constructor of the class is

```
template<class LD>
mimes::AxionEOM<LD>(LD fa, LD ratio_ini, std::string inputFile, AxionMass<LD> *axionMass)
```

The role of the arguments are discussed in section (3.1.1) and (4.2.2) as well as in table 2. One the instance is created, the interpolations are constructed by calling the member function

```
template<class LD> void mimes::AxionEOM<LD>::makeInt()
```

Then, the temperature as a function of  $u = \log a/a_{\rm ini}$ , is given via the member function

```
template<class LD> LD mimes::AxionEOM<LD>::Temperature(LD u)
```

Another useful member function is

```
template<class LD> LD mimes::AxionEOM<LD>::logH2(LD u)
```

This function returns  $\log H^2$  as a function of u. Moreover, its derivative,  $\frac{d \log H^2}{du}$ , is computed using

```
template<class LD> LD mimes::AxionEOM<LD>::dlogH2du(LD u)
```

It should be noted that the highest interpolation temperature is determined by ratio\_ini while the lower interpolation temperature is the one given in the data file inputFile. Beyond these limits, all functions are assumed to be constant. Therefore, one should be careful, and choose an appropriate ratio\_ini, and provide a lower temperature at which any entropy injection has stopped and the axion has reached its adiabatic evolution.

Finally, the actual EOM is given an overloaded call operator

```
template<class LD>
void mimes::AxionMass<LD>::operator()(std::array<LD,2> &lhs, std::array<LD,2> &y, LD u)
```

Here, the inputs are  $u = \log a/a_{\text{ini}}$ ,  $y[0] = \theta$ , and  $y[1] = \zeta$ ; which are used to calculate the components of the EOM, with  $lhs[0] = \frac{d\theta}{du}$  and  $lhs[1] = \frac{d\zeta}{du}$ .

### B.5 Axion class

The mimes::Axion<LD,Solver,Method> class is the class that combines all the others, and actually solves the axion EOM 2.19. Its header file is MiMeS/src/Axion/AxionSolve.hpp, and its constructor is

```
template<class LD, const int Solver, class Method>
mimes::Axion< LD, Solver, Method<LD>>(LD theta_i, LD fa, LD umax, LD TSTOP,
LD ratio_ini, unsigned int N_convergence_max, LD convergence_lim,
std::string inputFile, AxionMass<LD> *axionMass, LD initial_step_size=1e-2,
LD minimum_step_size=1e-8, LD maximum_step_size=1e-2, LD absolute_tolerance=1e-8,
LD relative_tolerance=1e-8, LD beta=0.9, LD fac_max=1.2, LD fac_min=0.8,
unsigned int maximum_No_steps=10000000)
```

The various arguments are discussed in section (3.1.1) and (4.2.2); and outlined in table 2. The member function responsible for solving the EOM is

```
template < class LD, const int Solver, class Method>
void mimes::Axion < LD, Solver, Method < LD >::solveAxion()
```

Once this function finishes, the results are stored in several member variables.

The quantities  $a/a_{\rm ini}$ , T,  $\theta$ ,  $\zeta$ ,  $\rho_a$ , at the integration steps are stored in

```
template<class LD, const int Solver, class Method>
std::vector< std::vector<LD> > mimes::Axion< LD, Solver, Method<LD> >::points
```

The quantities  $a/a_{\rm ini}$ , T,  $\theta$ ,  $\zeta$ ,  $\rho_a$ , J, at the peaks of the oscillation are stored in

```
template < class LD, const int Solver, class Method>
std::vector < std::vector < LD> > mimes::Axion < LD, Solver, Method < LD> >::peaks
```

Note that these points are computed using linear interpolation between two integration points with a change in the sign of  $\zeta$ .

The local integration errors for  $\theta$  and  $\zeta$  are stored in

```
template<class LD, const int Solver, class Method>
std::vector<LD> mimes::Axion< LD, Solver, Method<LD>>::dtheta

template<class LD, const int Solver, class Method>
std::vector<LD> mimes::Axion< LD, Solver, Method<LD>>::dzeta
```

Moreover, the oscillation temperature,  $T_{\rm osc}$ , and the corresponding values of  $a/a_{\rm ini}$  and  $\theta$  are given in

```
template < class LD, const int Solver, class Method>
LD mimes::Axion < LD, Solver, Method < LD > :: T_osc

template < class LD, const int Solver, class Method>
LD mimes::Axion < LD, Solver, Method < LD > :: a_osc
```

```
template<class LD, const int Solver, class Method>
  LD mimes::Axion< LD, Solver, Method<LD>>::theta_osc
```

Also, the entropy injection between the last peak  $(T = T_{\text{peak}})$  and today  $(T = T_0)$ ,  $\gamma$  (defined as in eq. (2.31)), is given in

```
template<class LD, const int Solver, class Method>
LD mimes::Axion< LD, Solver, Method<LD>>::gamma
```

The relic abundance is stored in the following member variable

```
template < class LD, const int Solver, class Method>
D mimes::Axion < LD, Solver, Method < LD >::relic
```

We can set another initial condition,  $\theta_{\rm ini}$ , using

```
template<class LD, const int Solver, class Method>
void mimes::Axion< LD, Solver, Method<LD> >::setTheta_i(LD theta_i)
```

We should note that running this function all variables are cleared. So we lose all information about the last time axionSolve() ran.

In case the mass of the axion is changed, we also need to remake the interpolation (i.e. run mimes::AxionEOM::makeInt()). This is done using

```
template < class LD, const int Solver, class Method>
void mimes:: Axion < LD, Solver, Method < LD > >:: restart()
```

Again, this function clears all member variables. So it should be used with caution.

Finally, there is static mimes::Cosmo<LD> member variable

```
template<class LD, const int Solver, class Method>
static mimes::Cosmo<LD> mimes::Axion< LD, Solver, Method<LD>>::plasma
```

This variable can be used without an instance of the mimes::Axion<LD,Solver,Method> class.

# C python interface

The various python modules, classes, and functions are designed to work exactly in the same way as the ones in C++. All the modules are located in src/interfacePY, so it is helpful to add the MiMeS/src path to the system path at the top of every script that uses MiMeS. This is done by adding

```
from sys import path as sysPath
sysPath.append('path_to_src')
```

The available models are Cosmo, AxionMass, and Axion, each defines a class with the same name.

# C.1 Cosmo class

The Cosmo module defines the Cosmo class, which contains information about the plasma. The relevant shared library (lib/libCosmo.so) is obtained by compiling MiMeS/src/Cosmo/Cosmo.cpp using make lib/libCosmo.so.

The class can be imported by running

```
from interfacePy.Cosmo import Cosmo
```

Its constructor is

```
Cosmo(cosmo_PATH, minT=0, maxT=mP)
```

The argument  $cosmo\_PATH$  is the path (a string) of a data file that contains T (in GeV),  $h_{eff}$ ,  $g_{eff}$ , with accenting T. The second and third arguments, minT and maxT, are minimum and maximum interpolation temperatures, with the interpolation being between the closest temperatures in the data file. Moreover, beyond these limits, both  $h_{eff}$  and  $g_{eff}$  are assumed to be constants. It is important to note that the class creates a void pointer that gets recasted to mimes::Cosmo<LD> in order to call the various member functions. This means that once an instance of Cosmo is no longer needed, it must be deleted, in order to free the memory that it occupies. An instance, say cosmo, is deleted using

del cosmo

The member functions of this class are:

- Cosmo.heff(T):  $h_{\text{eff}}$  as a function of T.
- Cosmo.geff(T):  $g_{\text{eff}}$  as a function of T.
- Cosmo.dheffdT(T):  $dh_{\rm eff}/dT$  as a function of T.
- Cosmo.dgeffdT(T):  $dg_{\rm eff}/dT$  as a function of T.
- Cosmo.dh(T):  $\delta_h = 1 + \frac{1}{3} \frac{d \log h_{\rm eff}}{d \log T}$  as a function of T.
- Cosmo.s(T): The entropy density of the plasma as a function of T.
- Cosmo.rhoR(T): The energy density of the plasma as a function of T.
- Cosmo. Hubble (T): The Hubble parameter assuming radiation dominated expansion as a function of T.

The several cosmological quantities are given as members variables:

- Cosmo. TO: CMB temperature today [32] in GeV.
- Cosmo.h\_hub: Dimensionless Hubble constant [32].
- Cosmo.rho\_crit: Critical density [32] in GeV<sup>3</sup>.
- Cosmo.relicDM\_obs: Central value of the measured DM relic abundance [7].
- Cosmo.mP: Planck mass [32] in GeV.

Note that these values can be directly imported from the module, without declaring an instance of the class, as

```
from interfacePy.Cosmo import TO, h_hub, rho_crit, relicDM_obs, mP
```

# C.2 AxionMass class

The AxionMass class is defined in the module with the same name that can be found in the directory MiMeS/src/interfacePy/AxionMass. This class is responsible for the definition of the axion mass. This module loads the corresponding shared library from MiMeS/lib/libma.so, which is created by compiling MiMeS/src/AxionMass/AxionMass.cpp using "make lib/libma.so". Its usage is described in the examples given in sections (3.1) and (4.3). Moreover, this class is used in the same way as mimes::AxionMass<LD>. However, we should append in this section the definition of its member functions in python.

The class is imported using

```
from interfacePy.AxionMass import AxionMass
```

The constructor is

AxionMass(\*args)

and can be used in two different ways.

First, one can pass three arguments, i.e.

```
AxionMass(chi_PAT, minT, maxT)
```

The first argument is the path to a data file that contains two columns; T (in GeV) and chi (in GeV<sup>4</sup>), with increasing T. The arguments minT and maxT are the interpolation limits. These limits are used in order to stop the interpolation in the closest temperatures in chi\_PATH. That is the actual interpolation limits are  $T_{\min} \ge \min$ T and  $T_{\max} \le \max$ T. Beyond these limits, by default, the axion mass is assumed to be constant. However, this can be changed by using the member functions

```
AxionMass.set_ma2_MIN(ma2_MIN)
AxionMass.set_ma2_MAX(ma2_MAX)
```

Here, ma2\_MIN(T,fa) and ma2\_MAX(T,fa), are functions (not any callable object), should take as arguments T and fa, and return the axion mass squared beyond the interpolation limits. In order to ensure that the axion mass is continuous, usually we need  $T_{\min}$ ,  $T_{\max}$ ,  $\chi(T_{\min})$ , and  $\chi(T_{\max})$ . These values can be obtained using the member functions

- AxionMass.getTMin(): This function returns the minimum interpolation temperature,  $T_{\min}$ .
- AxionMass.getTMax(): This function returns the maximum interpolation temperature,  $T_{\text{max}}$ .
- AxionMass.getChiMin(): This function returns  $\chi(T_{\min})$ .
- AxionMass.getChiMax(): This function returns  $\chi(T_{\rm max})$ .

An alternative way to define the axion mass is via the constructor

```
AxionMass(ma2)
```

Here, ma2(T,fa) is a function (not any callable object) that takes T (in GeV) and  $f_a$ , and returns  $m_a^2(T)$  (in GeV). As in the other python classes, once the instances of this class are no longer needed, they must be deleted using the destructor, del.

The member function that returns  $\tilde{m}_a^2$  is

```
AxionMassma2(T,fa)
```

We should note that another ma2 can be changed using the following member function:

```
AxionMass.set_ma2(ma2)
```

Again, ma2(T,fa) is a function (not any callable object) that takes T (in GeV) and  $f_a$ , and returns  $m_a^2(T)$  (in GeV).

#### C.3 Axion class

The class Axion, solves the axion EOM 2.19. This class is defined in MiMeS/interfacePy/Axion/Axion.py, and imports the corresponding shared library. This library is compiled by running make lib/Axion\_py.so, and its source file is MiMeS/src/Axion/Axion-py.cpp. As in the previous classes, its usage is similar to the C++ version.

Its constructor is

```
Axion(theta_i, fa, umax, TSTOP,
ratio_ini, unsigned int N_convergence_max, convergence_lim,
inputFile, axionMass, initial_step_size=1e-2,
minimum_step_size=1e-8, maximum_step_size=1e-2, absolute_tolerance=1e-8,
relative_tolerance=1e-8, beta=0.9, fac_max=1.2, fac_min=0.8,
unsigned int maximum_No_steps=10000000)
```

Again, the various arguments are discussed in section (3.1.1) and (4.2.2); and can also be found in table 2. Notice one important difference between this and the C++ verison of this class; the instance of AxionMass, axionMass, is passed by value (there are no pointers in python). However, internally, the constructor converts this instance to a pointer, which is then passed to the underlying C function responsible for creating the relevant instance.

The member function responsible for solving the EOM is

#### Axion.solveAxion()

Once this function is finished, the following member funcions are available

- Axion.T\_osc: the oscillation temperature,  $T_{\rm osc}$ , in GeV.
- Axion.a\_osc:  $\frac{a}{a_{\rm ini}}$  at the oscillation temperature.
- Axion.theta\_osc:  $\theta_{\rm osc},~i.e.~\theta$  at  $T_{\rm osc}.$
- Axion.gamma: the entropy injection between the last peak  $(T = T_{\text{peak}})$  and today  $(T = T_0)$ ,  $\gamma$  (defined as in eq. (2.31)).
- Axion.relic The relic abundance of the axion.

The evolution of  $a/a_{\rm ini}$ , T,  $\theta$ ,  $\zeta$ ,  $\rho_a$  at the integration steps, is not automatically accessible to user, but they can be made so using

### Axion.getPoints()

Then, the following member variables are filled

- Axion.a: The scale factor over its initial value,  $\frac{a}{a_{\rm ini}}$ .
- Axion.T: The temperature in GeV.
- Axion.theta: The axion angle,  $\theta$ .
- Axion.zeta: The derivative of  $\theta$ ,  $\zeta \equiv \frac{d\theta}{d\log(a/a_{\rm ini})}$ .
- Axion.rho\_axion: The axion energy density in GeV<sup>4</sup>.

Moreover, the function

### Axion.getPeaks()

fills the (numpy) arrays Axion.a\_peak, Axion.T\_peak, Axion.theta\_peak, Axion.zeta\_peak, Axion.rho\_axion\_peak, and Axion.adiabatic\_invariant with the quantities  $a/a_{\rm ini}$ , T,  $\theta$ ,  $\zeta$ ,  $\rho_a$ , J, at the peaks of the oscillation. These points are computed using linear interpolation between two integration points with a change in the sign of  $\zeta$ .

The local integration errors for  $\theta$  and  $\zeta$  are stored in Axion.dtheta and Axion.dzeta, after the following function is run

#### Axion.getErrors()

Another initial condition,  $\theta_{\rm ini}$ , can be used without declaring a new instance using

### Axion.setTheta\_i(theta\_i)

We should note that running this function all variables are cleared.

As in the previous python classes, once an instance of the Axion class is no longer needed, it needs to be deleted, by calling the destructor, del.

Important difference between the C++ version Since the axion mass is passed by value in the constructor, a change of the AxionMass instance has no effect on the Axion instance that uses it. Therefore, if the definition of the axion mass changes, one has to declare a new instance of the Axion class. The new instance can be named using the name of the previous one, if the latter is deleted by running its destructor.

# D WKB module

The WKB module can be used to calculate the axion relic abundance using the WKB approximation discussed in section 2. The module can be imported using

```
from interfacePy import WKB
```

It contains the definition of a function that returns the relic abundance using the WKB approximation, which is

```
WKB.relic(Tosc, theta_osc ,ma2, gamma=1,
cosmo=Cosmo(_PATH_+r'/src/data/eos2020.dat',0,Cosmo.mP))
```

Here, Tosc is the oscillation temperate, ma2(T,fa) is  $m_a^2(T)$  as a function that takes T and  $f_a$  as arguments, cosmo an instance of the Cosmo class, and gamma the entropy injection (as defined in eq. (2.13)).

Moreover, there is a function that helps to determine  $T_{\rm osc}$  and  $\gamma$ , which is

```
WKB.getPoints(fa, ma2, inputFile, cosmo=Cosmo(_PATH_+r'/src/data/eos2020.dat',0,Cosmo.mP))
```

The arguments fa, inputFile,  $f_a$ , and cosmo the path to a file that describes the cosmology (described in table 2),  $f_a$  (in GeV), an instance of the Cosmo class, respectively. This function returns  $\gamma$  (the entropy injection between Tosc and today) and  $T_{\rm osc}$ .

# E The ScanScript module

The python interface of MiMeS has two simple classes that help to scan over  $\theta_{\text{ini}}$  and  $f_a$ , in parallel. These two classes can be imported from the module ScanScript.

Tis module is based on the bash script MiMeS/src/util/parallel\_scan.sh, which automatically performs scans in parallel. This script is used as

```
bash src/util/parallel_scan.sh executable cpus inputFile
```

Here, executable is the path to an executable, cpus the number of instances of the executable to launch simultaneously, and inputFile a file that contains the arguments the executable expects. This file should contain arguments for the executable in each line. This script, then, separates all in arguments in the inputFile in batches of size cpus, and runs one batch at a time.

#### E.1 The Scan class

The Scan class writes a time-coded file (so it would be unique) with columns that correspond to  $\theta_{\rm ini}$ ,  $f_a$  (GeV),  $\theta_{\rm osc}$ ,  $T_{\rm osc}$  (in GeV), and  $\Omega h^2$ , for every combination of  $\theta_{\rm ini}$  and  $f_a$  that are passed as input. This class is imported using

```
from interfacePy.ScanScript import Scan
```

```
Its constructor is
```

```
ScanScript.Scan(cpus,table_fa,table_theta_i,umax,TSTOP,ratio_ini,

N_convergence_max,convergence_lim,inputFile,

PathToCppExecutable, break_after=5*60,break_time=5,break_command='',

initial_step_size=1e-2, minimum_step_size=1e-8, maximum_step_size=1e-2,

absolute_tolerance=1e-8, relative_tolerance=1e-8,

beta=0.9, fac_max=1.2, fac_min=0.8, maximum_No_steps=int(1e7))
```

Some arguments are the same as in the Axion class, and their definition can be found in table 2. The other arguments are

- cpus: number of points to run simultaneously (number of cpus available).
- table\_fa: table of  $f_a$  to scan.
- table\_theta\_i: table of  $\theta_{\rm ini}$  to scan
- PathToCppExecutable: path to an executable that takes theta\_i, fa, umax, TSTOP, ratio\_ini, N\_convergence\_max, convergence\_lim, and inputFile; and prints theta\_i, fa, theta\_osc, T\_osc, and relic.
- break\_after, break\_time: take a break after break\_after seconds for break\_time seconds.
- break\_command (optional): before it takes a break, run this system command (this may be a script to send the results via e-mail, or back them up).

The scan runs using the method

```
Scan.run()
```

For every value of  $f_a$ , this method calls another one Scan.run\_batch(), which in turn calls the bash script MiMeS/src/util/parallel\_scan.sh with arguments PathToCppExecutable, cpus, and a file that contains all the inputs for PathToCppExecutable for all values in table\_theta.

As the scan runs, it prints the number of batches that have been evaluated, the mean time it takes to evaluate one batch, and an estimate of the remaining time. It should be noted that if the scan exits before it finishes, the next run will continue from the point at which it was stopped even if the inputs have changed. In order to start from the beginning, the user must delete the file count.\_mimes\_.

#### E.2 The ScanObs class

The ScanObs class scans for different values of  $f_a$  (given as a table) and finds the value of  $\theta_{\rm ini}$  closer to the observed DM relic abundance. The result file is a time-coded file with columns correspond that to  $\theta_{\rm ini}$ ,  $f_a$  (in GeV),  $\theta_{\rm osc}$ ,  $T_{\rm osc}$  (in GeV), and  $\Omega h^2$ . It is imported using

from interfacePy.ScanScript import ScanObs

Its constructor is

```
ScanScript.ScanObs(cpus,table_fa,len_theta,umax,TSTOP,ratio_ini,
N_convergence_max,convergence_lim,inputFile,axionMass,
PathToCppExecutable, relic_obs,relic_err_up,relic_err_low,
cosmo=Cosmo(_PATH_+r'/src/data/eos2020.dat',0,Cosmo.mP),
break_after=5*60,break_time=5,break_command='',
initial_step_size=1e-2, minimum_step_size=1e-8, maximum_step_size=1e-2,
absolute_tolerance=1e-8, relative_tolerance=1e-8,
beta=0.9, fac_max=1.2, fac_min=0.8, maximum_No_steps=int(1e7)
```

Here, len\_theta is the number of different values of  $\theta$  to be used in the search of a value closer to the central value of the observed DM relic abunance. The arguments relic\_obs, relic\_err\_up, relic\_err\_low are the central value of  $\Omega h^2$ , and its upper and lower error; respectively. All the other arguments have already been defined previously.

The scan runs using the method

```
ScanObs.run()
```

For every value of  $f_a$ , this method first calculates the relic abundance for  $\theta_{\rm ini} \ll 1$ , and finds the value of  $\theta_{\rm ini}$  that would result in  $\Omega h^2 = {\tt relic\_obs}$ ;  $\theta_{\rm ini}^{\rm (approx)}$ . This is easy to do, since for  $\theta_{\rm ini} \ll 1$ , the EOM becomes independent of  $\theta_{\rm ini}$ .

Then, it creates an array, table\_theta, of size len\_theta that contains values of  $\theta_{\rm ini}$  between  $Min(0.85 \ \theta_{\rm ini}^{\rm (approx)}, 1)$  and  $Max(1.2 \ \theta_{\rm ini}^{\rm (approx)}, \pi)$ . Then it calls ScanObs.run\_batch(), which works as Scan.run\_batch().

Similarly to the Scan class, if the scan exits before it finishes, the next run will continue from the point at which it was stopped. In order to start from the beginning, delete the file count.\_mimes\_.

### E.3 FT class

The FT class, defined in FT module that can be found in src/interfacePy/FT, is used to format the ticks when plotting using matplotlib [33]. The class can be imported using

The various arguments are

- \_M\_xticks,\_M\_yticks: A list for the major ticks in the x and y axes, respectively.
- \_M\_xticks,\_M\_yticks: A list for the major ticks in the x and y axes, respectively, for which no number is printed.
- \_m\_xticks,\_m\_yticks: A list for the minor ticks in the x and y axes, respectively.
- xmin, xmax (ymin, ymax): Minimum and maximum of the x (y) axes, respectively.
- xscale, yscale: The scale of the x and y axes, respectively. The available values are "linear", "log", and "symlog".

Instances of FT should be defined after subplots have been defined, because the code seems clearer. Once this is done, we can format the ticks of a subplot, sub, using

```
FT.format_ticks(plt,sub)
```

It is important to not that plt is the matplotlib.pyplot module that is usually imported as

```
import matplotlib.pyplot as plt
```

# Example of FT

Consider as an example the plot of  $f(x) = e^{-\frac{1}{2}x^2}$  for  $-5 \le x \le 5$ . In order to do this, we need to run

```
import numpy as np#you usually need numpy
2
     #---these are for plots---#
3
     import matplotlib.pyplot as plt
     #load the FT module
6
     from sys import path as sysPath
     sysPath.append('../../src')
     from interfacePy.FT import FT
9
10
     fig=plt.figure(figsize=(9,4))
11
     fig.subplots_adjust(bottom=0.15, left=0.15, top = 0.95, right=0.9, wspace=0.0, hspace=0.0)
12
     sub = fig.add_subplot(1,1,1)
13
14
     x=np.linspace(-5,5,500)
15
     sub.plot(x,np.exp(-1/2. * x**2))
16
```

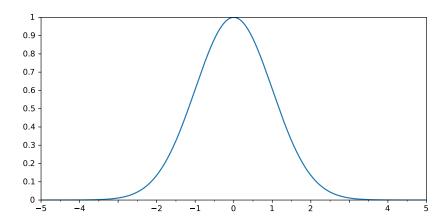


Figure 6: Example plot obtained by using the FT class.

Now we can format the ticks using FT. For the shake of this example, for the x-axis, we choose as major ticks all integrs except 3 and -3, and minor ticks the halves of each major tick. Also, for the y-axis, we choose to only show major ticks for every 0.1 in the interval of interest. Finally, we set the plot limits as  $x \in [-5, 5]$  ad  $y \in [0, 1]$ , using linear scale for both. This can be done as

```
#set major ticks
     _M_xticks=[i for i in range(-5,6)]
2
     _{M_{yticks}=[i/10. \text{ for i in range}(0,11)]}
3
     #set major ticks that will not have a label
5
     _M_xticks_exception=[-3,3]
6
     _M_yticks_exception=[]
     _{m_xticks=[i+j/2. for i in range(-5,6) for j in [0,1]]}
9
     _m_yticks=[]
10
     ft=FT(_M_xticks, _M_yticks, _M_xticks_exception, _M_yticks_exception, _m_xticks, _m_yticks,
11
        xmin=-5, xmax=5, ymin=0, ymax=1, xscale='linear', yscale='linear')
12
13
     ft.format_ticks(plt,sub)
14
```

The resulting plot is shown in Fig. (6).

# F Utilities

There are various utilities, that can be found MiMeS/src/util, which can be used to make the use of MiMeS easier. In this section we will show how they work, and when they should be used.

## F.1 FormatFile.sh

This is a bash script that formats a data file so that it is compatible with the interpolation assumptions. It takes a path to a file as an arguments, and it returns the same file, sorted (in ascenting order) with respect to the first column, removes duplicate and empty lines, and it removes the last "new line" (i.e.  $\n$ ). The script is called as

```
bash MiMeS/src/util/FormatFile.sh path_to_dat_file
```

Here path\_to\_dat\_file is a path to the data file we would like to replace with the formatted one. Notice that FormatFile.sh must be ran in order to ensure that the cosmological input needed by the mimes::Axion<LD,SOLVER,METHOD<LD>> class, is acceptable.

Moreover, note that FormatFile.sh is ran every time configure.sh is called, in order to format the data files for the RDOFs,  $\chi(T)$ , and the anharmonic factor, in order to ensure that they comply with what MiMeS expects.

#### F.2 timeit.sh

This script takes two arguments. The first should be a path to an executable, the second a file that contains arguments to passed to the executable. The script, then, runs the executable, and prints in stderr the time it took (is seconds) to run it. It is important to note that each argument of the executable should be in a different line of the file. <sup>18</sup>

The script is called as

```
bash MiMeS/src/util/timeit.sh path_to_executable path_to_dat_file
```

This script is useflul for running the example code in MiMeS/UserSpace/Cpp/Axion/Axion.cpp, which is compiled by calling "make examples" in the root directory of MiMeS. The executable that results from the compilation of this source, Axion.run, expects the same arguments as the constructor of the mimes::Axion<LD,SOLVER,METHOD<LD>> class (see section B). This means that we can write a file (call it INPUT) that contains all these arguments in each line, and simply run

```
bash MiMeS/src/util/timeit.sh MiMeS/UserSpace/Cpp/Axion/Axion.run INPUT
```

The files KinationInputs, MatterInputs, and RDInputs; in MiMeS/UserSpace/Cpp/Axion, show these files should look like in different cases.

#### F.3 Timer C++ class

The class mimes::util::Timer, defined in MiMeS/src/util/timeit.hpp, can be used in order to time processes in C++. An instance of this class prints its life-time – *i.e.* time from the moment it was created until it went out of scope – in stderr. Instances of this class are intended to be used inside a scope in order to count te time it took to run a block of code. For example the time it takes to compute  $\sum_{i=0}^{10^4} i$  can be determined as

```
#include "src/util/timeit.hpp"
2
     int main(){
3
4
        auto sum = 0;
5
           Timer _timer_;
6
            for(auto i=0; i<=10000; ++i){ ++sum;}</pre>
        }
8
9
        return 0;
10
     }
11
```

### F.4 linspace function

The function linspace, defined in MiMeS/src/util/linspace.hpp, is used to generate linearly spaced numbers between some boundary. This function is overloaded; there are two functions with the same name and different signature. The first one is

```
/*linspace where the list is pushed in a vector that is pass by reference*/
template<class LD>
void mimes::util::linspace(LD min, LD max, unsigned int length, std::vector<LD> &X)
```

Here, X is cleared, and gets filled with lenght linearly spaced numbers min and max.

The overloaded version of this function is

foo

 $<sup>^{18} \</sup>mbox{For example}$  , if we have an executable that takes two arguments, let's assume the first is 3 and the second is "foo", the file should read:

```
/*linspace where the list returned as a vector*/
template<class LD>
std::vector<LD> mimes::util::linspace(LD min, LD max, unsigned int length)
```

This function does not get a reference to a std::vector<LD>, instead it return one.

# F.5 logspace function

The function logspace, defined in MiMeS/src/util/logspace.hpp, is used to generate  $log_{10}$  spaced points between a given boundary. The signatures of this function are

```
/*logspace where the list is pushed in a vector that is pass by reference*/
template<class LD>
void mimes::util::logspace(LD min, LD max, unsigned int length, std::vector<LD> &X)

/*logspace where the list returned as a vector*/
template<class LD>
std::vector<LD> mimes::util::logspace(LD min, LD max, unsigned int length)
```

Both of these functions work as linspace.

# F.6 map function

The function map, defined in MiMeS/src/util/map.hpp, applys a function of an std::vector, and fills anther std::vector with the result. The signatures of this function are

```
/*The list is pushed in a vector that is pass by reference*/
template<class LD>
void map(const std::vector<LD> &X, std::function<LD(LD)> func, std::vector<LD> &Y)

/*The list returned as a vector*/
template<class LD>
std::vector<LD> map(const std::vector<LD> &X, std::function<LD(LD)> func)
```

Both of these functions evaluate func (a callable object) for every element of X. If another std::vector is given, then it is cleared and filled with the results, otherwise the function returns a std::vector with the values of func(X).

# G Quick guide to the user input

We present tables (2), (3), and (4), with the various available run-time inputs, required files, and template arguments. In table 5 we show the available compile-time options, that can be used when compiling using the various makefile files.

	User run-time input.
theta_i	Initial angle.
fa	The PQ scale.
umax	Once $u = \log a/a_i > \text{umax}$ , the integration stops. Typical value: $\sim 500$ .
TSTOP	Once $T < \texttt{TSTOP}$ , integration stops. Typical value: $10^{-4}$ GeV.
ratio_ini	Integration starts at $u$ with $3H/\tilde{m}_a \approx \text{ratio\_ini}$ . Typical value: $\sim 10^3$ .
N_convergence_max convergence_lim	Integration stops when the relative difference between two consecutive peaks is less than convergence_lim for N_convergence_max consecutive peaks.
inputFile	Relative (or absolute) path to a file that describes the cosmology. The columns should be: $u T [\text{GeV}] \log H$ , with acceding $u$ . Entropy injection should have stopped before the lowest temperature of given in inputFile.
axionMass	Instance of mimes::AxionMass <ld> class. In C++ this instance is passed as a pointer to the constructor of the mimes::Axion<ld,solver,method> class, while in python it is simply passed as a variable.</ld,solver,method></ld>
initial_stepsize	Initial step-size of the solver. Default value: $10^{-2}$ .
minimum_stepsize	Lower limit of the step-size. Default value: $10^{-8}$ .
maximum_stepsize	Upper limit of the step-size. Default value: $10^{-2}$ .
absolute_tolerance	Absolute tolerance of the RK solver (see also table 1). Default value: $10^{-8}$ .
relative_tolerance	Relative tolerance of the RK solver (see also table 1). Default value: $10^{-8}$ .
beta	Aggressiveness of the adaptation strategy (see also table 1). Default value: 0.9.
fac_max, fac_min	The step-size does not change more than fac_max and less than fac_min within a trial step (see also table 1). Default values: 1.2 and 0.8, respectively.
maximum_No_steps	If integration needs more than maximum_No_steps integration stops.  Default value: 10 <sup>7</sup> .

Table 2: Table of run-time user input.

# Required data files, with corresponding variables in MiMeS/Paths.mk.

cosmoDat	Relative path to data file with $T$ (in GeV), $h_{\rm eff}$ , $g_{\rm eff}$ . If the path
	changes one must run bash configure.sh and make.
axMDat	Relative path to data file with $T$ (in GeV), $\chi$ (defined from eq. (2.2)). If the path changes one must run bash configure.sh and make. This variable can be omitted, since the user can define an AxionMass instance using any path.
anFDat	Relative path to data file with $\theta_{\text{peak}}$ , $f(\theta_{\text{peak}})$ . If the path changes one must run bash configure.sh and make.

Table 3: Paths to the required data files.

# References

[1] R. D. Peccei and H. R. Quinn, CP Conservation in the Presence of Instantons, Phys. Rev. Lett. 38 (1977) 1440–1443.

# Template arguments. LD This template argument appears in all classes of MiMeS. The preferred choice should be either long double. However, in many cases double can be used. The user should be careful, as the later can lead to a inaccurate result; especially for low tolerances, and small values of $\theta$ . Solver This is the second template argument of the mimes::Axion<LD,Solver,Method> class. The available choices are Solver=1 for Rosenbrock method, and Solver=2 for explicit RK method. The third template argument of the mimes::Axion<LD,Solver,Method> Method class. Its value depends on the choice of Solver; For Solver=1, Method can be either RODASPR2<LD> (fourth order) or ROS34PW2<LD> (third order). For Solver=2, Method can only be DormandPrince<LD> (seventh order). Notice that the definitions of the various method classes, also need a template argument, LD, that must be the same as thi first template argument of the mimes::Axion<LD,Solver,Method> class. If one defines their own Butcher table (see Appendix A), then they would have to follow their definitions and assumptions.

Table 4: Template arguments of the various MiMeS classes.

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- [15] D. H. Lyth, Axions and inflation: Sitting in the vacuum, Phys. Rev. D 45 (1992) 3394–3404.

rootDir	The relative path of root directory of MiMeS. Relevant only when compiling using make. Available in all Definitions.mk.
LONG	long for long double or empty for double. This is defines a macro in the source files of the various C++ examples. Available in Definitions.mk inside the various subdirectories of MiMeS/UserSpace/Cpp.
LONGpy	long or empty. Same as LONG, applies in the python modules. Available in MiMeS/Definitions.mk.
SOLVER	In order to use a Rosenbrock method SOLVER=1. For explicit RK method, SOLVER=2. This defines a macro that is passes as the second template argument of mimes::Axion <ld,solver,method>. The corresponding variable in MiMeS/Definitions.mk applies to the python modules. The variable in MiMeS/UserSpace/Cpp/Axion/Definitions.mk applies to the example in the same directory.</ld,solver,method>
METHOD	Depending of the solver, this macro should name one of its available methods. For SOLVER=1, METHOD=RODASPR2 (fourth order) or ROS34PW2 (third order). For SOLVER=2, METHOD=DormandPrince (seventh order). There is a macro (METHOD) used by the shared library MiMeS/lib/Axion_py.so. The corresponding variable in MiMeS/Definitions.mk applies to the python modules. The variable in MiMeS/UserSpace/Cpp/Axion/Definitions.mk applies to the examples in the that directory.
	Compiler options
CC	The preferred C++ compiler (g++ by default). Corresponding variable in all Definitions.mk files.
OPT	Optimization level of the compiler. Available options OPT=01, 02, 03 (be default). By Corresponding variable in all Definitions.mk files.

Table 5: User compile-time input. These are available in the various Definitions.mk files, which are used when compiling using make.

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