I. INTRODUCTION

Primordial Black Holes (PBHs) were first considered in [1, 2]. They could have been formed in the very early Universe due to the gravitational collapse of cosmological perturbations in the radiation epoch. Within this hypothesis PBHs can be generated as a consequence of high non-linear peaks in the primordial distribution of density perturbations. While at Cosmic Microwave Background Radiation (CMB) scales the amplitudes of the curvature perturbations are too small to generate a significant amount of PBHs, there is currently no hard bound on their amplitudes at smaller scales, leaving open the possibility of having a large fraction of the Dark Matter (DM) in the form of PBHs.

Recently, several studies have addressed the problem of estimating PBH abundances from the power spectrum and including the effect of non-Gaussianities [3–9]. In [8] it was proved using peak theory that abundances of PBHs generated by the inflationary power spectrum depend strongly on the shape of the peak. The abundance turned out to be exponentially sensitive to the threshold $\delta_c$ of PBH formation. Analytical estimation obtained so far [10, 11] are too poor to be used in this respect and therefore numerical techniques are needed (although see [12]).

Numerical simulations of PBH formation started some time ago with [13, 14], where $\delta_c$ was computed and a universal scaling law (depending only on the fluid type) for the mass of the BH. The scaling relation was similar to the one obtained from the gravitational collapse of a scalar field [15, 16].

Later in [17–21] numerical simulations were performed reproducing the scaling behavior up to very small values near the threshold. The value of the scaling exponent matched with the one quoted in the literate got from a perturbative treatment [22, 23], and from numerical collapse simulations [24].

Motivated by the recent perspectives on primordial black hole and the implications in cosmology, we have addressed this problem, focusing to obtain an efficient numerical method to compute the threshold $\delta_c$ and estimate the mass $M_{\text{BH}}$. In this paper, for first time, we simulate the gravitational collapse of curvature perturbations leading the formation of PBHs using Misner-Sharp equations with the implementation of pseudo-spectral method technique, which has been already used in general relativity with a great success [29, 30]. We have been able to compute the threshold $\delta_c$ with an accuracy of $O(10^{-5})$ for different perturbations, the results match with the ones quoted in the literature. Moreover, to avoid the breaking of the simulation due to the formation of the singularity, instead to implement null coordinates, we have used an excision technique. The mass is then found by the use of an analytical approximation of the mass accretion asymptotic behavior. We present for first time, the values of the black hole mass for the higher allowed values in the case of a Gaussian curvature perturbation. Here we also show a deviation from the scaling law of up to $O(15\%)$ in the higher end of PBH masses. Our publicly accessible code can be found in https://sites.google.com/fqa.ub.edu/albertescriva/home.
II. MISNER-SHARP EQUATIONS

The Misner-Sharp equations \cite{26} describes the motion of a spherically symmetric relativistic fluid. The starting point is to consider an ideal fluid with energy momentum tensor \( T^{\mu\nu} = (p + \rho)u^\mu u^\nu + pg^{\mu\nu} \) with the following line element:

\[
ds^2 = -A(r,t)\,dt^2 + B(r,t)\,dr^2 + R(r,t)^2\,d\Omega^2, \tag{1}
\]

where \( d\Omega^2 = d\theta^2 + \sin^2(\theta)d\phi^2 \) is the line element of a 2-sphere and \( R(r,t) \) is the areal radius. The components of the four velocity \( u^\mu \) (which are equal to the unit normal vector orthogonal to the hyperspace at cosmic time \( t \) \( u^\mu = n^\mu \)), are given by \( u^t = 1/A \) and \( u^r = 0 \) for \( i = r, \theta, \phi \). From now on, we will use units \( G = \mu = 1 \).

In the Einstein field equations appear the following quantities:

\[
\frac{1}{A(r,t)} \frac{\partial R(r,t)}{\partial t} = D_t R \equiv U(r,t), \tag{2}
\]

\[
\frac{1}{B(r,t)} \frac{\partial R(r,t)}{\partial r} = D_r R \equiv \Gamma(r,t), \tag{3}
\]

where \( D_t \) and \( D_r \) are the proper time and distances derivatives. \( U \) is the radial component of the four-velocity associated to an Eulerian frame. It measures the radial velocity of the fluid with respect to the centre of coordinates. From the Einstein equations one finds that the generalized Lorentz factor \( \Gamma \) is:

\[
\Gamma = \sqrt{1 + U^2 - \frac{2M}{R}}, \tag{4}
\]

where \( M(r,t) \) is the Misner-Sharp mass, defined as

\[
M(r,t) \equiv \int_0^R 4\pi R^2 \rho R' \,dr = \int_0^r \rho \Gamma d^3V. \tag{5}
\]

This mass includes contributions from the kinetic energy and gravitational potential energies. Finally, the Misner-Sharp equations governing the evolution of a spherically symmetric collapse in non-linear full general relativity are:

\[
D_t U = -\left[ \frac{\Gamma}{(\rho + p)} D_r p + \frac{M}{R^2} + 4\pi R p \right], \tag{6}
\]

\[
D_t R = U, \tag{7}
\]

\[
D_r p = -\frac{(\rho + p)}{R^2} D_r (UR^2), \tag{8}
\]

\[
D_r M = -4\pi R^2 U p, \tag{9}
\]

\[
D_r A = -\frac{A}{\rho + p} D_r p. \tag{10}
\]

To close the system we need to give the equation of state of the fluid, which in our context is \( p = \omega \rho \). The boundary conditions in order to solve the system are \( R(r = 0, t) = 0 \), which leads \( U(r = 0, t) = 0 \) and \( M(r = 0, t) = 0 \). Then, by spherical symmetry we have \( D_r p(r = 0, t) = 0 \). At \( r \to \infty \) we want to match with the Friedmann-Robertson-Walker (FRW) background, but in a numerical simulation we have to handle with a finite grid. Then, to math the outer point of the grid with the FRW solution and to avoid reflections from pressure waves, we have used the condition \( D_r p(r = r_f, t) = 0 \) (where \( r_f \) if the outer point of the grid). Eq. (6) is called the Hamiltonian constraint, we will use it later on for numerical checks. Eq. (10) can be solved analytically imposing \( A(r_f, t) = 1 \) to match with the FRW spacetime \cite{31}. This gives:

\[
A(r,t) = \left( \frac{\rho_o(t)}{\rho(r,t)} \right)^{\frac{\omega}{1 + \omega}}, \tag{11}
\]

where \( \rho_o(t) = \rho_0(t_0/t)^2 \) is the energy density of the FRW background and \( \rho_0 = 3H_0^2/8\pi \). Using the definitions of Eq. (12), we can rewrite Misner-Sharp equations in a more convenient way to perform the numerical simulations:

\[
\dot{U} = -A \left[ \frac{\omega}{1 + \omega} \frac{\rho'}{R^2} + \frac{M}{R^2} + 4\pi R \omega \rho \right], \tag{12}
\]

\[
\dot{R} = AU, \tag{13}
\]

\[
\dot{\rho} = -A \rho (1 + \omega) \left( \frac{U}{R} + \frac{U'}{R'} \right), \tag{14}
\]

\[
\dot{M} = -4\pi A \omega \rho UR^2, \tag{15}
\]

where \( (\cdot) \) and \( (\cdot)' \) represents the time and radial derivative respectively. At superhorizon scales the metric Eq. (16) can be approximated, at leading order in gradient expansion, by the following metric \cite{18}:

\[
ds^2 = -dt^2 + a^2(t) \left[ \frac{dr^2}{1 - K(r)^2} + r^2 d\Omega^2 \right]. \tag{16}
\]

The cosmological perturbation will be encoded in the initial curvature \( K(r) \). At leading order in gradient expansion, the product \( K(r)^2 \) is proportional to the compaction function \( C(r) = \frac{2[M(r,t) - M_h(r,t)]}{R(r,t)} \), which represents a measure of the mass excess inside a given volume. More specifically,

\[
C(r,t) = \frac{2[M(r,t) - M_h(r,t)]}{R(r,t)}. \tag{17}
\]

We now define the location of the maxim of \( C(r) \) as \( r_m \), which is also the typical length scale of the initial perturbation \cite{31}. By defining \( \epsilon(t) = R_H(t)/a(t)r_m \), one can solve Misner-Sharp equations at leading order in \( \epsilon \ll 1 \). \( R_H(t) = 1/H(t) \) is the cosmological horizon and \( r_m \) is the length scale of the perturbation. This approach is the so-called long wavelength approximation \cite{32} (or gradient expansion). We have:
\[ A(r, t) = 1 + e^2(t) \tilde{A}(r), \]
\[ R(r, t) = a(t)r(1 + e^2(t) \tilde{R}(r)), \]
\[ U(r, t) = H(t)R(r, t)(1 + e^2(t) \tilde{U}(r)), \]
\[ \rho(r, t) = \rho_b(t)(1 + e^2(t) \tilde{\rho}(r)), \]
\[ M(r, t) = \frac{4\pi}{3} \rho_b(t)R(r, t)^3(1 + e^2(t) \tilde{M}(r)), \]

where for \( \epsilon \to 0 \) we recover the (FRW) solution. The perturbations of the tilde variables in the linear regime were computed in [33], which we summarize here:

\[
\tilde{\rho}(r) = \frac{3(1 + \omega)}{5 + 3\omega} \left[ K(r) + \frac{r}{3} K'(r) \right] r_m^2,
\]
\[
\tilde{U}(r) = -\frac{1}{5 + 3\omega} K(r) r_m^2,
\]
\[
\tilde{A}(r) = -\frac{\omega}{1 + \omega} \tilde{\rho}(r),
\]
\[
\tilde{M}(r) = -3(1 + \omega) \tilde{U}(r),
\]
\[
\tilde{R}(r) = -\frac{\omega}{(1 + 3\omega)(1 + \omega)} \tilde{\rho}(r) + \frac{1}{1 + 3\omega} \tilde{U}(r).
\]

The background evolution equations are: \( H(t) = H_0(t_0/t) \), \( a(t) = a_0(t/t_0)^{\alpha} \) and \( R_H(t) = R_H(t_0)(t/t_0) \) where \( a_0 = a(t_0) \), \( H_0 = H(t_0) = \alpha/t_0 \) and \( R_H(t_0) = 1/H_0 \). Moreover we define \( \alpha = 2/3(1 + \omega) \).

The amplitude of a cosmological perturbation can be measured by the mass excess within a spherical region:

\[
\delta(r, t) = \frac{1}{V} \int_0^R 4\pi R^2 \frac{\rho - \bar{\rho}}{\bar{\rho}} R' dr,
\]

where \( V = 4\pi R^3/3 \) and at leading order in \( \epsilon \) gives:

\[
\delta(r, t) = \left( \frac{1}{aH r_m} \right)^2 \tilde{\delta}(r),
\]

where \( \tilde{\delta}(r) = f(w)K(r)r_m^2 \) and \( f(\omega) = 3(1 + \omega)/(5 + 3\omega) \). In the long wavelength approximation, \( C(r, t) \approx C(r) = f(\omega)K(r)r^2 = r^2 \delta(r)/r_m^2 \) [33], which yields \( C(r_m) = \delta(r_m) = \tilde{\delta}_m \). Because of the above definitions the value of \( r_m \) is given by the solution of:

\[
K(r_m) + \frac{r_m}{2} K'(r_m) = 0.
\]

After the initial conditions are given the compaction function starts to evolve non-linearly and becomes time dependent. The first apparent horizon is then formed whenever the peak of the compaction function is about one (for a more formal discussion see [34]). We define the threshold for primordial black hole formation as \( \delta_e \) such that a PBH is formed whenever \( \delta(r_m) \geq \delta_e \).\(^1\)

\[\text{III. PSEUDO-SPECTRAL TECHNIQUE}\]

Instead of using a Lagrangian hydrodynamic technique, we have implemented the Pseudo-spectral Chebyshev collocation method to compute the spatial derivatives part of the Eqs. [13]. The time evolution is instead solved with fourth-order explicit Runge-Kutta method. In the following we explain the use of the pseudo-spectral technique, see also [35] and [36].

Consider a function \( f(x) \) and fit with \( N_{\text{cheb}} \) Chebyshev polynomials (although could be any kind of orthonormal function). More specifically we can define the approximated function:

\[
f_{N_{\text{cheb}}}(x) = \sum_{k=0}^{N_{\text{cheb}}} c_k T_k(x),
\]

where \( T_k(x) \) are the Chebyshev polynomial of order \( k \). The coefficients \( c_k, k = 0, 1, \ldots, N_{\text{cheb}} \) are then obtained by solving \( f_{N_{\text{cheb}}}(x_k) = f(x_k) \) where \( x_k = \cos(k\pi/N_{\text{cheb}}) \).

Those points are called Chebyshev collocation points and correspond to \( T'_k(x_k) = 0 \). The solution is

\[
f_{N_{\text{cheb}}}(x) = \sum_{k=0}^{N_{\text{cheb}}} L_k(x)f(x_k),
\]

\[
L_k(x) = \frac{(-1)^{k+1}(1 - x^2)T_{N_{\text{cheb}}}(x)}{\tilde{c}_k N_{\text{cheb}}(x - x_k)},
\]

where \( \tilde{c}_k = 2 \) if \( k = 0, N \) and \( \tilde{c}_k = 1 \) in other cases. The functions \( L_k \) are called Lagrange interpolation polynomials. With this we can easily obtain the \( p \) derivative to be:

\[
f^{(p)}_{N_{\text{cheb}}}(x_i) = \sum_{k=0}^{N_{\text{cheb}}} L_k^{(p)}(x_i)f_{N_{\text{cheb}}}(x_k).
\]

Defining the Chebyshev differentiation matrix \( D^{(p)} = \{L_k^{(p)}(x_i)\} \) we have:

\[
D_{i,j}^{(1)} = \frac{\tilde{c}_i}{\tilde{c}_j} \left( \frac{1}{x_i - x_j} \right)^{i+j} (i \neq j), i, j = 1, \ldots, N_{\text{cheb}} - 1,
\]

\[
D_{i,i}^{(1)} = \frac{-x_i}{2(1 - x_i^2)}, i = 1, \ldots, N_{\text{cheb}} - 1,
\]

\[
D_{0,0}^{(1)} = -D_{N_{\text{cheb}}, N_{\text{cheb}}}^{(1)} = \frac{2N_{\text{cheb}}^2 + 1}{6}.
\]

We use the following identity to compute the diagonal terms of the matrix \( D \) quoted before:

\[
D_{i,i}^{(1)} = N_{\text{cheb}}^{N_{\text{cheb}} - 1} \sum_{j=0,j \neq i}^{N_{\text{cheb}}} D_{i,j}^{(1)},
\]

which gives a substantial improvement regarding the round-off errors in the numerical computations (see [36] for details).

\(^1\) Here we use a slightly different notation for \( \delta_m \) from the paper of [33] to avoid confusion due to the use of the linear extrapolation.
The crucial advantage of spectral methods in comparison with finite differences is that the error decays exponentially in \( N_{\text{cheb}} \). With finite-difference instead, error decays like \( 1/N^v \), where \( N \) is again the sample of points and \( v \) is a positive number. Moreover a crucial differences with respect to finite differences is that at a given point is computed globally taking into account the value of the all the other points, in comparison with finite differences where the derivative at a given point only takes into account the neighbours.

In our particular case, the domain of the radial coordinate is given by \( \Omega = [r_{\text{min}}, r_{\text{max}}] \) where \( r_{\text{min}} = 0 \) and \( r_{\text{max}} = N_H R_H(t_0) \). \( N_H \) is the number of initial cosmological horizon, which in general is taken to be \( N_H \approx 90 \) as it is done in the literature \[17\]. Since our domain is not \([-1, 1]\) (which is the domain for the Chebyshev polynomials), we need to shift the domain:

\[
\tilde{x}_k = \frac{r_{\text{max}} + r_{\text{min}}}{2} + \frac{r_{\text{max}} - r_{\text{min}}}{2} x_k.
\]

\( \tilde{x}_k \) are the new Chebyshev points rescaled to our domain \( \Omega \). In the same way, the Chebyshev matrix can be rescaled in a straightforward way using the chain rule:

\[
\tilde{D} = 2 \frac{r_{\text{max}} - r_{\text{min}}}{2} D.
\]

To implement a Dirichlet boundary condition at given \( x_k \), such that \( f(x = x_k) = u_{D,bc} \), it is only needed to fulfil \( f N_{\text{cheb}}(x = x_k) = u_{D,bc} \). Instead, in case of Newmann condition such that \( f^{(1)}(x = x_k) = u_{N,bc} \), then \( (D \cdot f N_{\text{cheb}})(x = x_k) = u_{N,bc} \). The stability of the method depends on the value of \( N_{\text{cheb}} \) and \( dt \) used. An increment of the spatial resolution will require an enough small time step \( dt \) to avoid instabilities during the evolution.

\[\text{IV. NUMERICAL PROCEDURE}\]

In all our numerical simulations we are setting \( t_0 = 1 \) and \( a_0 = 1 \), which yields \( H_0 = 1/2 \) and \( R_B(t_0) = 2 \). For the length scale of the perturbation, we have taken \( r_m = 10 R_B(t_0) \) as done in the literature \[18\]. This ensures that the long wavelength approximation is fulfilled. To find \( \delta_c \) we have implemented a bisection method which scans different regimes of \( \delta \) until finding the range in which the collapse will happen. The threshold \( \delta_c \) is defined as the mid point of this range.

It’s useful to know that \( \delta_c \) is bounded from above by \( \delta_c = f(\omega) \). This can be directly inferred by noticing that \( \Gamma^2 = 1 - K(r)r^2 \). The numerical procedure that we have established is described as follows:

- Set up the number of Chebyshev points \( N_{\text{cheb}} \) and create the grid of points \( x_k \). This yields the Chebyshev differentiation matrix \( D \).
- Introduce the initial time step \( dt_0 \) and the length scale value \( r_m \).
- Choose a lower and an upper bound in \( \delta \) to perform the domain of the bisection method. In our case, we have chosen \( \delta_{\text{max}} = 2/3 \) and \( \delta_{\text{min}} = 2/5 \) \[12\] (although this can be changed to establish a domain closer to \( \delta_c \) to reduce the computational time).
- Given a curvature profile \( K(r) \), such that \( K(r) = AK(r) \) with \( K(0) = 1 \), compute the tide perturbations in the other hydrodynamical magnitudes following Eqs.\[19\] \[18\], except by the curvature amplitude \( A \) that multiplies all this perturbations.
- Once the bisection method starts and a value of \( \delta_m \) is taken, the corresponding value of \( A \) is computed to set up the profile \( K(r) \).
- Use the four-order Runge-Kutta equations to integrate the equations at each time-step \( dt \), imposing as well boundary conditions at each internal time step.
- Compute at each iteration time the value of the peak of the compaction function \( C_{\text{peak}} \). Once it approaches \( C_{\text{peak}} \approx 1 \) an apparent horizon is formed. This corresponds to a given value of \( \delta_{c,yes} \). Next step is search for a lower value of \( \delta_c \) via bisection method modifying the bound such that \( \delta_c \in [\delta_{\text{min}}, \delta_{c,yes}] \) and we go to the next iteration in the bisection. Otherwise, if \( C_{\text{peak}} \approx C_{\text{min}} \) (in our simulations we take in general \( C_{\text{min}} \approx 0.3 \), this is related to the fact that \( \delta_{\text{min}} = 2/5 \) then the perturbation disperse (it is not going to form a black hole) getting a value \( \delta_{c,no} \) and we go to the next iteration in the bisection, modifying the bound such that \( \delta_c \in [\delta_{c,no}, \delta_{\text{max}}] \) and we go to the next iteration in the bisection.

- With the previous result, the bisection method is iterated until the difference between \( \delta_{c,yes} \) and \( \delta_{c,no} \) becomes less than the resolution that we set to compute the value of \( \delta_c, \delta_c \approx \delta_{c,yes} - \delta_{c,no} \lesssim \delta(\delta_c) \). Where we infer that \( \delta_c = (\delta_{c,yes} + \delta_{c,no})/2 \pm \delta(\delta_c) \). If during the bisection \( \delta - \delta_c \) goes beyond the resolution of the method, then the trial \( \delta \) is shifted according to \( \delta(\delta_c) \).

For the Runge-Kutta we have used the conformal time \( dt = dt_0(t/t_0)^\alpha \) as it improves significantly the running time. To test our code, we use the 2-norm of the Hamiltonian constraint equation Eq.\[33\] in all the simulations, which is expected to remain constant from the beginning if Einstein equations are correctly solved during the simulations. Specifically:

\[
\mathcal{H} = D_r M - 4\pi \Gamma \rho R^2, \quad (33)
\]

\[
\| \mathcal{H} \|_2 \equiv \frac{1}{N_{\text{cheb}}} \sqrt{\sum_k |\mathcal{H}_k|^2}. \quad (34)
\]

The resolution that we have been able to obtain is \( \delta_{c,yes} - \delta_{c,no} > 10^{-5} \).
V. TESTING THE CODE

In this section and in the rest of the paper we will test our code in a radiation dominated universe, because of its interest in PBH formation. In other words, we will fix $\omega = 1/3$ and therefore $f(\omega) = 2/3$.

A. FRW solution

Here we check that our code reproduces the FRW solution. To do that, we have computed the relative error of the different variables $\rho, U, M, R$ ( $A$ and $\Gamma$ depends on the previous ones) with respect to the FRW analytical solution. We define $\delta X_i = X(x_i) - X_b(x_i)$, where $X$ are the variables that we solve in the Misner-Sharp equations. To test our code against the FRW solution we compute the variance,

$$\|\delta X\|^2 = \frac{1}{N_{\text{cheb}}} \sum_k |\delta X_k|^2 \quad (35)$$

In Fig. 1, we see the evolution of $\|H\|_2$ in terms of different spatial resolutions. The time step for all cases has taken to be $dt_0 = 10^{-3}$.

In Fig. 2 and Fig. 3 we see $\|\delta X\|_2$ for the different hydrodynamical variables and we see a good convergence to the analytical solution. In particular, it is clear that incrementing the number of Chebyshev points the convergence to the analytical solution gets better and better. Already for $N = 6$ we have at least an $O(10^{-10})$ accuracy.

Obviously for a curvature profile that is not homogeneous the number of Chebyshev points points would need to be increased because the pressure gradients are not vanishing.

B. Curvature profiles

In this section we are going to test our code against the results obtained in [33] for centrally peaked profile, the ones relevant for cosmology [3, 5]. In other words we shall consider the following profiles for initial curvature...
perturbations:
\[ K(r) = A e^{-\frac{1}{2}(r/r_m)^2 q}, \]  
(36)
where \( q \) parametrizes the slope of the profiles.

For \( q = 1 \) we recover the Gaussian curvature profile. Here we get \( \delta_c \approx 0.49774 \pm 2 \cdot 10^{-5} \), which matches the one quoted in the literature \( (\delta_c \approx 0.5 \ [33]) \). This value was obtained by using \( dt_0 = 10^{-3} \) and \( N_{\text{cheb}} = 400 \). We have checked that this result is stable under the increment of \( N_{\text{cheb}} \) and/or the reduction of \( dt_0 \).

In addition, to check the correctness of the numerical procedure of the bisection at each iteration, we have computed \( \|H\|_2 \), which can be found in Fig. 4. We see that the constraint is violated at late times for \( \delta - \delta_c \approx O(10^{-5}) \). This sets the maximal resolution we can achieve.

Finally, in Fig. 5, we have tested our code against the different profiles parameterized by \( q \) in the range \( q \in [0.5, 14.6] \). Our results match with very good accuracy the ones of [33].

\[ \delta_c \approx 0.49774 \pm 2 \cdot 10^{-5}, \]

In Fig. 7 (the sub-critical case) \( C_{\text{peak}} \) decreases continuously as the perturbation is diluted away due to the dominance of pressure gradients.

In Fig. 8 (the critical case) \( C_{\text{peak}} \) first decreases and then bounces to re-increase again.

- From the figures 6, 7 and 8 we see that \( \Gamma \) is not constant during the evolution. This implies, as it should, that the long-wave approximation breaks down during the evolution.

- In Fig. 8 (super-critical case) we see that \( U/\Gamma \) decreases quickly in time. Instead, in Fig. 7 (sub-critical case) only a small negative value \( U/\Gamma \) is reached for early times, and after that no negative values can be found, which means that the perturbation is dispersing avoiding the collapse. The most remarkable behavior is found in the critical case Fig. 8. Here the fluid splits into two parts, one going inwards (negative \( U \)) and one outwards (positive \( U \)) generating an under-dense region. This under-dense region re-attract the fluid with a net effect of a rarefaction and compression process which gets faster and faster. This is the reason why the code is not able to follow the evolution up to the final time BH formation. As we shall see we will nevertheless be able to infer the final mass.

\[ \delta_c \]  

Let us finally remark something about the long wavelength approximation. As can be seen in Fig. 9 the threshold \( \delta_c \) has some small dependence in terms of \( \epsilon \). It is obvious that the difference between the asymptotic critical value and the one numerically found grows with \( \epsilon \).

\[ \delta_c \]  

In Fig. 6 (the super-critical case) \( C_{\text{peak}} \) grows during the evolution. From the same figure it is also evident the formation of two apparent horizons, as discussed in [33]. The outer horizon moves outwards and the inner moves faster than the outer inwards. Once the inner horizon approaches the center of coordinates the simulation breaks due to the appearance of the singularity.

\[ \delta_c \]  

In Figs. 6, 7 and 8 we see the evolution of the variables \( \rho, \Gamma, U \) and \( C \) for the Gaussian profile \( q = 1 \) in the, respectively, supercritical \( \delta \gg \delta_c \), subcritical \( \delta \ll \delta_c \) and critical \( \delta \approx \delta_c \) cases.

- In Fig. 6 (the super-critical case) we see that the \( C_{\text{peak}} \) grows during the evolution. From the same figure it is also evident the formation of two apparent horizons, as discussed in [33]. The outer horizon moves outwards and the inner moves faster than the outer inwards. Once the inner horizon approaches the center of coordinates the simulation breaks due to the appearance of the singularity.

\[ C_{\text{peak}} \]  

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In Fig. 9 (the sub-critical case) \( C_{\text{peak}} \) decreases continuously as the perturbation is diluted away due to the dominance of pressure gradients.

In Fig. 8 (the critical case) \( C_{\text{peak}} \) first decreases and then bounces to re-increase again.

- From the figures 6, 7 and 8 we see that \( \Gamma \) is not constant during the evolution. This implies, as it should, that the long-wave approximation breaks down during the evolution.

- In Fig. 8 (the super-critical case) we see that \( U/\Gamma \) decreases quickly in time. Instead, in Fig. 7 (sub-critical case) only a small negative value \( U/\Gamma \) is reached for early times, and after that no negative values can be found, which means that the perturbation is dispersing avoiding the collapse. The most remarkable behavior is found in the critical case Fig. 8. Here the fluid splits into two parts, one going inwards (negative \( U \)) and one outwards (positive \( U \)) generating an under-dense region. This under-dense region re-attract the fluid with a net effect of a rarefaction and compression process which gets faster and faster. This is the reason why the code is not able to follow the evolution up to the final time BH formation. As we shall see we will nevertheless be able to infer the final mass.

\[ \delta_c \]  

Let us finally remark something about the long wavelength approximation. As can be seen in Fig. 9 the threshold \( \delta_c \) has some small dependence in terms of \( \epsilon \). It is obvious that the difference between the asymptotic critical value and the one numerically found grows with \( \epsilon \).

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FIG. 4. Left Panel: Hamiltonian constraint for the iterations of the bisection procedure in the case of the Gaussian curvature profile whose are leading to the formation of a black hole. Right panel: Hamiltonian constraint for the iterations of the bisection procedure in the case of the Gaussian curvature profile whose perturbations are going to disperse and not form a black hole. In both cases $dt_0 = 10^{-3}$, $N_{\text{cheb}} = 400$.

FIG. 6. Dynamical evolution of the different magnitudes at a given time $t$ for a supercritical perturbation in case of $q = 1$ and $\delta = 0.51$. We have taken $dt_0 = 10^{-3}$ and $N_{\text{cheb}} = 800$ in the simulation.

D. Power-spectrum profile

In this section, we aim to provide a test of the stability of our code for profiles that differ from the ones studied before [36]. The main difference are under- and over-density oscillations away from the peak of the curvature. The profiles used here are sub-classes of the mean profiles obtained with the procedure outlined in [3] by broken power spectrums of the form...
FIG. 7. Dynamical evolution of the different magnitudes at a given time $t$ for a subcritical perturbation in case of $q = 1$ and $\delta = 0.49$. We have taken $dt_0 = 10^{-3}$ and $N_{\text{cheb}} = 800$ in the simulation.

$$P(k) = \begin{cases} 
0 & k < k_p \\
P_0 \left( \frac{k}{k_p} \right)^{-n} & k \geq k_p,
\end{cases} \quad (37)$$

which are relevant for cosmological applications \[5\]. In particular, we shall only consider the convergent cases of $n \geq 0$. In Eq. (37), $k_p$ is the wave length of the peak. After a straightforward computation, one finds that the mean curvature is

$$\bar{K}(r) = \frac{3n}{2(k_p r)^3} \left[ -k_p r \left( E_{3+n}(-ik_p r) + E_{3+n}(i k_p r) \right) + i \left( E_{4+n}(ik_p r) - E_{4+n}(-ik_p r) \right) \right], \quad (38)$$

where

$$E_n(x) = \int_1^\infty e^{-xt} \frac{t^n}{n!} dt. \quad (39)$$

From a given value of $r_m$ and $n$, we get the correspondent value of $k_p$ solving numerically Eq. (22). An important difference from these profile with respect to the ones studied before is that here we needed to consider a larger number of $N_{\text{cheb}}$ in order to capture the oscillations of the curvature. Finally, in Fig. 11 are shown the thresholds obtained for different values of $n$.

FIG. 11. Values of $\delta_c$ for different values of $n$ for the curvature profile of Eq. (38). Simulations done with $N_{\text{cheb}} \approx 700$ and $dt_0 = 10^{-3}$.

VI. MASS SPECTRUM

It is known that for $\bar{\delta}(r_m)$ close to the critical value $\delta_c$ the mass of the black hole follows the following scaling law \[14, 20, 21\]

$$M_{BH} = M_H \bar{K}(\delta - \delta_c)^\gamma, \quad (40)$$
FIG. 8. Dynamical evolution of the different magnitudes at a given time $t$ for a perturbation with $\delta \approx \delta_c$ in case of $q = 1$ and $\delta = 0.49775$. We have taken $dt_0 = 10^{-3}$ and $N_{\text{cheb}} = 800$ in the simulation.

FIG. 10. Curvature profile $\bar{K}(r)$ in terms of $n$ using Eq.(38).

where $\gamma \approx 0.36$ in radiation. In Eq.(40) the constant $K$ is a correction factor due to the choice of the reference mass $M_H \equiv 1/2H(t_m)$, where the Hubble scale has been calculated at the time $r_m H(t_m)\alpha(t_m) = 1$.

To test our code, in this section we will numerically obtain the constant $K_c$ for a Gaussian profile, and find the scaling law for large deviations from the critical value. Previous numerical computation were only performed in the region up to $\delta - \delta_c \approx 10^{-2}$. We will show in the following, for the first time, the mass range for large values of $\delta(r_m)$ up to the maximal value $2/3$.

The way we will find the mass spectrum is by the implementation of the excision technique [38, 39] which avoids the region of large curvatures in the Misner-Sharp evolution where the code would break.

The key idea of excision is that nothing inside the event horizon can affect the physics outside. The excisions follow the motion of the apparent horizon. The implementation of this technique is straightforward using spectral method, in contrast with finite differences [30], since the derivative at the excision boundary (that we have to define when we cut part of the computational domain) is computed without taking into account points that lies inside the inner boundary (in finite differences it is necessary to interpolate).

Unfortunately, the excision technique cannot be used until the formation of the black hole. This is due to the fact that the velocity of the outer horizon is too small and the initial resolution is not enough to follow the change in apparent horizon. Of course this can be solved with an implementation of adaptive mesh refinement (AMR). We will however follow here another (semi-analytical) direction.

It has been shown in [40–42] that, at the final stage of the BH formation, the mass accretion follows the law

$$
\frac{dM}{dt} = 4\pi FR^2_{BH}\rho(t) .
$$

(41)
$F$ is the accretion rate constant and it is usually numerically found to be of order $O(1)$. This approximation was already employed in the context of PBH formation from domain walls in [33].

By the condition of apparent horizon $R_{BH} = 2M_{BH}$, the previous equation is solved as:

$$M_{BH}(t) = \frac{1}{M_{a}^2 + \frac{3}{2}F \left( \frac{1}{t} - \frac{1}{t_{a}} \right)} , \quad (42)$$

where $M_{a}$ is the initial mass when the asymptotic approximation is used at the time $t_{a}$.

We will find $F$ by fitting the numerical evolution of the mass via the excision method. Once found it, the PBH mass will be inferred as the asymptotic mass at $t \to \infty$, i.e.

$$M_{BH}(t \to \infty) = \left( \frac{1}{M_{a}} - \frac{3F}{2t_{a}} \right)^{-1} . \quad (43)$$

The exact procedure we have used is the following:

- Find the location of the outer apparent horizon $(2M(r,t)/R(r,t) = 1)$ using a cubic spline interpolation (we have checked that the difference in $M(r,t)$ taking a quadratic spline interpolation are $O(0.01\%)$).

- Define an excision boundary close to the location of the apparent horizon.

- No boundary conditions are imposed in the inner excision surface and the derivative at that point is evaluated as in the usual case.

- Let evolve the code with the initial conditions in the excision region.

- Repeat for the next time step until reaching the interpolation function regime.

For the computation of the excision we have taken at least $N_{\text{cheb}} = 1000$, to increase the resolution and be able to make the excision sequentially.

In order to check when the approximation of Eq. (42) is valid, we have computed the ratio of the increment of the black hole mass respect the Hubble scale $\Psi = M/HM$, which is expected to be $\Psi < 1$ when the evolution satisfy this regime. We have made a non-linear fit in the Eq. (42) to get the parameters $t_{a}$, $M_{a}$ and $F$ to estimate the mass of the black hole. The range of numerical values that we use to make the fit are those which fulfill $\Psi \lesssim 0.1$, which works well for our purposes. We have checked that the Hamiltonian constraint is fulfill until late time, when the simulation breaks, Fig. (13). Nevertheless, we have tested that the evolution of the mass is not affected by the violation of the constraint. The results can be found in Fig. (13). Interestingly, we see a crossing for different evolution of $\Psi$ at a given time $t^*$.

The values of $F$ that we get goes from $F \in [3.5, 3.75]$ increasing the value of $\delta$. This is consistent with the one reported in [33] where a value of $F \approx 3.8$ was got for large black holes. We have check always that the fit performed is accurate, getting a variance of $\sigma_{\text{max}} \approx 10^{-5}$. The standard deviation $s_{d}$ of the parameters are $s_{d}(t_{a}) \approx 10^{-9}$, $s_{d}(M_{a}) \approx 10^{-5}$ and $s_{d}(F) \approx 10^{-5}$.

We have used the values of $M_{BH}$ in the range of $\delta \in [0.505, 0.51]$ to estimate the value of $\mathcal{K}$ from the scaling law, taking into account that $\delta_{c} = 0.49774$ and $\gamma = 0.357$.

The values of $\mathcal{K}$ in this domain of $\delta$ are $\mathcal{K} \in [5.87, 5.96]$, making an average we get $\mathcal{K} = 5.91$. This values differs in 1.9% from the value quoted in the literature with $\mathcal{K} = 6.03$. The values of $M_{BH}$ in terms of $\delta$ can be found in Fig. (14).

Finally, for first time we present the values of $M_{BH}$ for large values of $\delta$ until $\delta \approx 2/3$. We observe that the scaling law deviates at the higher end of in the $\delta$ range
up to $O(15\%)$, as can be seen in the subplot of Fig. 14.

![Fig. 14](image_url)

FIG. 14. Values of $M_{BH}/M_H$ in terms of $\delta - \delta_c$. The solid red line corresponds to the scaling law behavior with $\gamma = 0.357$, $\delta_c = 0.49774$ for $K = 6$, and the blue solid line with the numerical value for $K = 5.91$. Dark points are the values got from the fitting of Eq.(43). The subplots represents the deviation $d$ respect the numerical values and the ones coming from the scaling law. The orange vertical line is the value $\delta = 2/3$.

VII. CONCLUSIONS

We have performed numerical simulations of PBHs formations using Pseudo-spectral methods instead of the extensively used Lagrangian hydrodynamic formalism based on [25, 28]. We have been able to obtain the threshold $\delta_c$ of different curvature profiles with an accuracy of $O(10^{-5})$, which match with the ones quoted in the literature [33].

In our simulations we have used an excision technique to remove the singularity from the computational domain. To get the mass of the black hole, we have employed a semi-analytical formalism given by Eq.(42), which leads a deviation of $O(2\%)$ in the determination of the black hole mass with respect to the values quoted in the literature, in the scaling law regime. Moreover, for first time we were able to give the values of the black hole mass for large initial amplitudes, finding a deviation of $O(15\%)$ at the largest value $\delta = 2/3$ with respect to Eq(40).

Our code is an independent test of the correctness of the thresholds found earlier in the literature. Our method could be the way to solve a multidimensional collapse because the standard implementation of the hydrodynamical methods seems to fail [28]. However we leave it for future research.

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