

Jordan-Magnus Methods for Cosmological Perturbation Theory

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This report investigates methods to integrate coupled systems of first-order ordinary differential equations with highly oscillatory solutions. These results inform the adaptability of community codes used to solve the Einstein-Boltzmann equations in cosmological perturbation theory. We first clarify the distinctions between Magnus expansion and multiple-scale analysis based approaches and contrast their suitability for use in cosmological perturbation theory. We then motivate the improved empirical performance demonstrated by a proposed modified Magnus expansion method known as the “Jordan-Magnus” method. Following this we generalize this approach, implementing a numerical routine that can be applied to arbitrarily sized systems and find it doesn’t outperform standard Magnus expansion methods. We also develop and implement a Chebyshev spectral collocation stepping method which offers improved accuracy and run-time for a five variable toy cosmology compared to Runge-Kutta and Magnus methods as well as offering improved flexibility through adaptive order.

Candidate Statement: Except where specific reference is made to the work of others, this work is original and has not been already submitted either wholly or in part to satisfy any degree requirement at this or any other university.

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I. INTRODUCTION

A. Background and Motivation

The Λ CDM concordance model of the Universe explains the large-scale structure and evolution of the cosmos to high precision using only six parameters[1]. In order to compare theory with data, sophisticated Boltzmann solvers have been developed to evolve the perturbation equations of the early universe from primordial times to the current epoch[2, 3]. Central to these techniques is the integration of a set of coupled oscillatory linear ordinary differential equations. Thus far, semi-analytic approximations and numerical tricks have allowed cosmologists to produce efficient codes that infer cosmological

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parameters to unprecedented accuracy specific to Λ CDM models. However, advances must be made to improve the adaptability of the codes for use on arbitrary cosmological models. The Boltzmann codes represent a popular set of these community tools in precision cosmology, including CLASS[4], CAMB[5] and PyCOSMO[6], which numerically integrate the Einstein-Boltzmann equations. These are linear first order ordinary differential equations (ODEs) describing the time evolution of linear perturbations to the interacting constituents of our universe. They display highly oscillatory solutions and so render conventional numerical approaches inefficient [7]. The current codes rely on a suite of theory-dependent tricks and approximations to improve computational efficiency. This motivates the development of more generalized theory-independent methods to solve these equations.

The Astrophysics group at Cambridge has made significant progress on techniques for solving these types of equations [8, 9]. Previous work by the group has explored efficient combinations of the standard Runge-Kutta method and Wentzel-Kramers-Brillouin approximation [10]. However, these methods have not been extended to larger coupled systems as required for cosmological models. Further work then found that Magnus expansion methods offer improved performance over linear stepping routines [8] for larger systems. Furthermore, an approach dubbed the ‘Jordan-Magnus’ method was proposed as a potentially improved, modified Magnus routine. But it has yet to be developed in a fully numerical routine that could be applied to arbitrary systems and its performance investigated. The aim of this project was originally to focus on extending the “Jordan Magnus” method proposed in [8] to arbitrary multivariate systems and examine its performance. We also decided to explore alternative approaches, contrasting the suitability of multiple scale analysis and Magnus expansion methods for Einstein-Boltzmann systems as well as developing a spectral collocation stepping method which showed promising performance on a five variable radiation dominated cosmological model.

B. Structure

Section II provides a brief background on the relevant cosmology and how equations of the form studied in this project arise in the field. The subsequent sections are structured around the three main objectives of the project and the relevant theory and results for each are combined and presented separately:

- Section III: Contrasting Magnus expansion methods and multiple-scale analysis and their suitability for use in cosmological perturbation theory.
- Section IV: Developing and testing a routine to implement a numerical Jordan-Magnus Method for coupled systems.

- Section V: Developing and analysing the performance of a spectral collocation method.

II. COSMOLOGICAL PERTURBATION THEORY

In cosmology, the Einstein-Boltzmann equations describe the evolution of the Universe on large scales. These equations are a set of differential equations that couple the dynamics of the metric to the distribution of matter and radiation in the Universe.

One important simplification is that perturbations are treated as linear around a homogeneous, isotropic background. This approach is beneficial for studying the growth of structure in the Universe. In linear perturbation theory, the matter and radiation distributions appearing in the stress-energy tensor $T_{\mu\nu}$ are described by perturbations to their density, velocity, and temperature fields. These fields can be expanded in terms of spherical harmonics and Fourier modes, which leads to a set of coupled ordinary differential equations (ODEs) for the Fourier coefficients. These perturbations in general could be scalar, vector, or tensor objects. Still, they can be shown to decompose separately in Fourier space with modes of different wave vectors evolving independently[11].

A. Photon CDM Cosmology

The dynamics of non-equilibrium perturbations are described using the Boltzmann equation:

$$\frac{df_i}{dt} = C_i [\{f_j\}], \quad (1)$$

where f_i are the distribution functions of the various particles, and C_i is a functional of the f_i and the metric describing the interactions between the components. The components include baryonic and dark matter, radiation and dark energy all interacting with the metric and via other processes. These other processes include familiar phenomena such as the Thomson scattering between electrons and photons or Coulomb scattering between protons and electrons. In perfect equilibrium $\frac{df_i}{dt} = 0$. So we consider non-equilibrium perturbations. The relevant theory deriving the dynamical equations of such systems, known as the Einstein-Boltzmann equations, can be found in textbooks including Modern Cosmology by Dodelson and Theory of Cosmological Perturbations by Mukhanov[11, 12]. They can be parameterised such that they take simple form[13]:

$$\dot{\mathbf{x}}(t) = \mathbf{A}(t)\mathbf{x}(t). \quad (2)$$

As a simple cosmological test for our numerical methods we use, for continuity, the same model parameterised in previous work for a radiation dominated universe containing only photons, cold dark matter and the

metric[8]. Here we use the Freedman-Robertson-Walker (FRW) metric which can be written using conformal time η ,

$$ds^2 = a^2(\eta)(1 + 2\Phi)d\eta^2 - (1 - 2\Psi)\delta_{ij} dx^i dx^j, \quad (3)$$

which presents the most general metric describing a

homogeneous, isotropic, expanding universe. One can restrict the analysis to scalar metric perturbations in this metric. With $a(\eta)$ being the usual cosmological scale factor, and in units where $c = 1$. There is freedom in coordinate choices representing our system, termed the gauge. A useful choice is the conformal Newtonian gauge used above where Φ and Ψ are the metric perturbations. This model simplifies to a five dimensional system of the form:

$$\begin{bmatrix} \dot{\Theta}_0 \\ \dot{\Theta}_1 \\ \dot{\delta} \\ \dot{v} \\ \dot{\Phi} \end{bmatrix} = \begin{bmatrix} -2\mathcal{H}\Omega_\gamma & -k & -\frac{1}{2}\mathcal{H}\Omega_{dm} & 0 & -\frac{k^2}{3\mathcal{H}} - \mathcal{H} \\ \frac{k}{3} & 0 & 0 & 0 & \frac{k^2}{3} \\ -6\mathcal{H}\Omega_\gamma & 0 & -\frac{3}{2}\mathcal{H}\Omega_{dm} & -ik & -\frac{k^2}{\mathcal{H}} - 3\mathcal{H} \\ 0 & 0 & 0 & -H & -ik \\ -2\mathcal{H}\Omega_\gamma & 0 & -\frac{1}{2}\mathcal{H}\Omega_{dm} & 0 & -\frac{k^2}{3\mathcal{H}} - \mathcal{H} \end{bmatrix} \begin{bmatrix} \Theta_0 \\ \Theta_1 \\ \delta \\ v \\ \Phi \end{bmatrix}, \quad (4)$$

where $\mathbf{x} = [\Theta_0, \Theta_1, \delta, v, \Phi]^T$ respectively represent perturbations to the multipole moments of the temperature field for the photon distribution; dark matter over-density field; velocity component parallel to wavevector \mathbf{k} field and metric.

III. MAGNUS METHODS VS MULTIPLE-SCALE ANALYSIS

A. Magnus Expansion

First, it is instructive to define the Magnus expansion, which follows from significant work exploring solutions to initial value problems for coupled linear ODES[14–16]. These equations can be expressed in the form of (5) where \mathbf{A} is a time-dependent $n \times n$ matrix.

$$\dot{\mathbf{x}}(t) = \mathbf{A}(t)\mathbf{x}(t) \quad (5)$$

The Magnus expansion approach expresses a solution to the system using some unknown square matrix function $\Omega(t, t_0)$. A series solution is postulated for $\Omega(t, t_0)$ and

$$\Omega_n(t) = \sum_{j=1}^{n-1} \frac{B_j}{j!} \sum_{\substack{k_1+\dots+k_j=n-1 \\ k_1, k_2, \dots, k_j \geq 1}} \int_{t_0}^t [\Omega_{k_1}(t'), [\Omega_{k_2}(t'), [\Omega_{k_3}(t'), \dots, [\Omega_{k_j}(t'), \mathbf{A}(t')]]] \dots dt'. \quad (11)$$

Note this requires n-fold nested integrals. B_j are the

the system solution expressed as,

$$\mathbf{x}(t) = \exp \left(\sum_{k=1}^{\infty} \Omega_k(t) \right) \mathbf{x}_0. \quad (6)$$

Using the relation,

$$\frac{d}{dt} (e^\Omega) e^{-\Omega} = A(t), \quad (7)$$

the time derivative of Ω can be related to the generating function of the Bernoulli numbers and the adjoint endomorphism of Ω using a Poincare-Hausdorff matrix identity:

$$\Omega' = \frac{\text{ad}_\Omega}{\exp(\text{ad}_\Omega) - 1} A. \quad (8)$$

Then it is possible to recursively solve for Ω in terms of \mathbf{A} similar to a continuous analogue of the Baker-Campbell-Hausdorff formula:

$$e^X e^Y = e^Z \quad (9)$$

$$Z = X + Y + \frac{1}{2}[X, Y] + \frac{1}{12}[X, [X, Y]] - \frac{1}{12}[Y, [X, Y]] + \dots \quad (10)$$

Thus the terms in the Magnus expansion are obtained by the equation below:

Bernoulli numbers with $B_1 = -1/2$. The first few terms

of this are:

$$\begin{aligned}\Omega_1(t) &= \int_0^t A(t_1) dt_1, \\ \Omega_2(t) &= \frac{1}{2} \int_0^t dt_1 \int_0^{t_1} dt_2 [A(t_1), A(t_2)].\end{aligned}\quad (12)$$

A sufficient condition for this series to converge for $t \in [0, T]$ is $\int_0^T \|A(s)\|_2 ds < \pi$ where $\|\cdot\|_2$ denotes a matrix norm. $\Omega_1(t)$ coincides exactly with the exponent in the case of a scalar system and the subsequent terms can be seen as the corrections needed for an exponential representation, i.e. lie group, enforced upon the system where Ω or terms in its expansion are part of the lie algebra of the lie group on the solution. It has been demonstrated from previous work that the Magnus expansion is a practically distinct approach to a higher dimensional generalisation of the WKB method[8]. We further clarify here the distinction between the more general multiple-scale analysis approach from Magnus series expansion based methods.

B. Multiple-Scale Analysis

From this point on we present new material, discussing multiple-scale analysis, not previously explored in relation to cosmological perturbation theory.

Multiple scale analysis is used when a system can be characterised by behaviour on disparate timescales. The approach classifies the techniques to construct uniformly valid approximations to the solutions of perturbation problems where solutions simultaneously depend on these different scales. Some other popular perturbation techniques including the WKB approximation, whose success motivated exploration of generalisations for coupled systems, can be considered special cases of this general approach. It involves introducing new time scale variables through which an asymptotic expansion solution can be constructed in new independent variables. These new degrees of freedom can be used to eliminate secular terms in the solution process, which then provide constraints to fix an approximate solution of the system. For example the popular WKB approximation can be derived this way for single dependent variable systems where the behaviour is well described by fast oscillation and slow modulation time scales. Here harmonic oscillation is taken to be the dominant analytic behaviour from which the system is perturbed. We elucidate this example, as derived in [17], below to motivate the more general approach that could be applied to larger systems of coupled equations,

$$y''(t) + \omega^2(\varepsilon t)y(t) = 0. \quad (13)$$

In order to use the multiple-scale approach on (13) we must transform it into a form where the system is explicitly perturbed from something we can analytically solve.

Therefore, we transform to a fixed-frequency oscillator with a small perturbation term:

$$y'' + y + \varepsilon (\text{some function of } y) = 0. \quad (14)$$

In order to achieve this we choose new time scales $\tau = \varepsilon t$ and an arbitrary $T = f(t)$. Using the chain rule to transform the derivatives of (13) we obtain:

$$\frac{d^2}{dT^2}y + \frac{f''(t)}{[f'(t)]^2} \frac{d}{dT}y + \frac{\omega^2(\varepsilon t)}{[f'(t)]^2}y = 0. \quad (15)$$

The form in (14) can be achieved if we choose

$$f'(t) = \omega(\varepsilon t),$$

so that $T = f(t) = \int^t \omega(\varepsilon x)dx = \frac{1}{\varepsilon} \int^\tau \omega(s)ds$. Now we express the solution as an asymptotic series

$$y = Y_0(T, \tau) + \varepsilon Y_1(T, \tau) + \dots,$$

where $\tau = \varepsilon t$. Substituting all these results into (14) we obtain to zeroth and first order in perturbation hierarchy, the following relations:

$$\begin{aligned}\frac{\partial^2 Y_0}{\partial t^2} + \omega^2(\tau)Y_0 &= 0 \\ \frac{\partial^2 Y_1}{\partial t^2} + \omega^2(\tau)Y_1 &= -2 \frac{\partial^2 Y_0}{\partial t \partial \tau}.\end{aligned}\quad (16)$$

As intended we can now substitute the known solution $Y_0 = A(\tau)e^{iT} + A^*(\tau)e^{-iT}$ into the second relation in equation 16. This produces the expression:

$$\begin{aligned}\frac{\partial^2 Y_1}{\partial T^2} + Y_1 &= -ie^{iT} \left[\frac{2}{\omega} \frac{dA}{d\tau} + \frac{\omega'(\tau)}{\omega^2(\tau)} A \right] \\ &\quad + ie^{-iT} \left[\frac{2}{\omega} \frac{dA^*}{d\tau} + \frac{\omega'(\tau)}{\omega^2(\tau)} A^* \right].\end{aligned}\quad (17)$$

In order to eliminate secularity and permit a bounded asymptotic solution we are forced to require that the square bracketed terms vanish. This constraint allows us to solve for $A(\tau)$, which is proportional to $1/\sqrt{\omega(\tau)}$. This fixes an approximate solution of the system which reproduces the WKB approximation:

$$Y_0 = \frac{1}{\sqrt{\omega(\tau)}} \exp \left[\pm \frac{i}{\varepsilon} \int^\tau \omega(s)ds \right]. \quad (18)$$

Similarly, in principle this procedure can be extended to arbitrary systems represented by (5) and has shown promise in fields including that of open quantum systems [18] and weakly non-linear ODE systems[19].

1. First, the characteristic timescales of the system must be identified and the equation transformed to a form where it is a perturbation in small parameter ε away from a system with a known solution.

2. Then the time variable t is promoted to an infinite collection $T = \{\tau_0, \tau_1, \tau_2, \dots\}$ of independent variables τ_n , each one a function of the perturbative parameter ε such that $\tau_n = \varepsilon^n t$, $n = 0, 1, 2, \dots$, with $0 < \varepsilon < 1$. This leads the temporal derivative to then correspond to an infinite sum provided by the chain rule,

$$\frac{d}{dt} = \sum_n \varepsilon^n \mathfrak{D}_n, \quad \mathfrak{D}_n = \frac{\partial}{\partial \tau_n}. \quad (19)$$

3. Then the existence of solutions, $x_i(t)$, in the form of asymptotic series in terms of this small parameter must be postulated, $x_i(t) = h_i(t_0, t_1, \dots)|_{t_j=\varepsilon^{j+1}}$ with $h_i = h_{i,0} + \varepsilon h_{i,1} + \varepsilon^2 h_{i,2} + \dots$. After substituting this solution and the modified differential operators into (5) a series of equations according to perturbation hierarchy can be obtained.
4. Just as in the WKB case, substituting the known solution of the zeroth order equations, a series of solvability conditions are obtained, which may require additional care and use of the Fredholm Alternative Theorem [19]. The constraints arrive from avoiding secularity and enforcing a bounded solution which fixes the form of an approximate solution.

C. Contrasting techniques

Both these techniques are perturbation methods, a class of tools used to find approximate analytic solutions to problems where exact analytic solutions cannot be found. However, by nature the multiple-scale perturbation scheme does not seem appropriate for our purposes, which seek to investigate and develop cosmology independent numerical methods. Multiple-scale analysis requires knowledge of an analytic solution that approximately describes dominant system behaviour on some characteristic fast time scale. Thus it biases any numerical method we might develop by constraining cosmological models to those displaying predictable behaviour simple enough to construct a closed-form analytic description from which the system can be perturbed.

On the other hand, while the Magnus expansion solution is also a perturbation scheme, it is instead based on the assertion of an exponential lie group representation for the solution. The first order term of this solution can be calculated simply for arbitrary systems numerically using evaluations of $\mathbf{A}(t)$, without even requiring the system to have a closed form analytic representation of $\mathbf{A}(t)$. This improves flexibility for use on arbitrarily sophisticated cosmological models. The technique is used in fields including quantum dynamics because when truncating the series, an approximate solution often shares qualitative properties with the exact solution. For example, in quantum mechanics the unitary nature of the

time evolution operator is preserved. In our case this method is motivated simply because it is an alternative formulation of a series solution to an initial value problem that doesn't require any analytic knowledge of the system's behaviour. While subsequent terms in the Magnus expansion involve complicated structures, one could posit that in a step-wise integration routine a step-size in which a manageable subset of terms remains accurate can be always be identified. Furthermore, we might expect that the exponential form of the series might favour performance on oscillatory systems over linear stepping methods, which has indeed been demonstrated in previous work [8].

IV. NUMERICAL JORDAN-MAGNUS TYPE METHOD

A. Theory

The approach termed the “Jordan-Magnus Method”, as laid out in [8] is presented below. This method endeavours to improve the first Magnus expansion term solution to (5) by applying a linear transformation, letting $\mathbf{x}_P = \mathbf{P}^{-1}\mathbf{x}$, and $\mathbf{J} = \mathbf{P}^{-1}\mathbf{A}\mathbf{P}$ for some transformation matrix $\mathbf{P}(t)$. Then

$$\dot{\mathbf{x}}_P = \mathbf{A}_P \mathbf{x}_P = \left[\mathbf{J} + \left(\dot{\mathbf{P}}^{-1} \right) \mathbf{P} \right] \mathbf{x}_P, \quad (20)$$

where $\dot{\mathbf{P}}^{-1}$ denotes the time derivative of \mathbf{P}^{-1} . Then in order to choose a \mathbf{P} such that \mathbf{A}_P is as diagonal as possible, this was identified as the transformation associated with a Jordan-Normal decomposition. Let $\mathbf{A}_P = \mathbf{\Lambda} + \mathbf{K}$ where $\mathbf{\Lambda}$ is diagonal and \mathbf{K} has zeros on the diagonal.

A solution in the form of $\mathbf{x}(t) = \mathbf{M}(t)\mathbf{x}(0)$ was sought. An approximate solution can be obtained by simply neglecting \mathbf{K} ,

$$\mathbf{M}(t) \approx \mathbf{P}(t) \exp \left(\int_0^t \mathbf{\Lambda} dt_1 \right) \mathbf{P}^{-1}(0). \quad (21)$$

This avoids a potentially costly matrix exponential. Alternatively \mathbf{K} can be included to obtain:

$$\mathbf{M}(t) \approx \mathbf{P}(t) \exp \left(\int_0^t (\mathbf{\Lambda} + \mathbf{K}) dt_1 \right) \mathbf{P}^{-1}(0), \quad (22)$$

which is identified as the first term Magnus expansion solution. However, the method as presented in [8] relies on obtaining \mathbf{P} , $\mathbf{\Lambda}$ and \mathbf{K} as functions of t because there exists no stable algorithm to compute a numerical Jordan decomposition. Calculating the analytic Jordan Normal form of \mathbf{A} is prohibitive for complicated systems and so an alternative stable numerical approach was needed.

The proposed Jordan Normal decomposition was only motivated by the fact that a general square complex matrix \mathbf{A} is not guaranteed to have diagonal form. However, all matrices can be placed in Jordan Normal form.

The Jordan normal decomposition is a way of decomposing a square matrix A into a specific form written as $A = PJP^{-1}$. Where P is an invertible matrix and J is a block diagonal matrix consisting of Jordan blocks. In general, a square complex matrix A is similar to a block diagonal matrix

$$J = \begin{bmatrix} J_1 & & \\ & \ddots & \\ & & J_p \end{bmatrix},$$

where each block J_i is a square matrix of the form

$$J_i = \begin{bmatrix} \lambda_i & 1 & & \\ & \lambda_i & \ddots & \\ & & \ddots & 1 \\ & & & \lambda_i \end{bmatrix}.$$

Here, J is the Jordan matrix and J_i is the i th Jordan block, which corresponds to an eigenvalue λ_i with 1's along the superdiagonal. The size of the Jordan block is determined by the number of linearly independent generalized eigenvectors associated with λ_k .

Therefore this is always an at least near diagonal form in which generally decomposes matrices to diagonal form. The lack of stable numerical algorithm for a Jordan-Normal decomposition forced an analytical transformation in previous work[8], prohibiting use on arbitrary systems. Here we remedy this by motivating and implementing a fully numerical version of the routine and exploring its potential.

B. Jordan-Magnus Method Analysis

First, we further motivate the use of a matrix decomposition to modify the Magnus expansion method and provide some explanation for the improved empirical performance of the Jordan-magnus routine demonstrated in [8].

In previous work the routine was only applied to two variable formulations of the simple Airy and Burst equation which are represented in the form of (5) by:

$$\mathbf{x} = \begin{bmatrix} x \\ \dot{x} \end{bmatrix} \quad \text{and} \quad \mathbf{A} = \begin{bmatrix} 0 & 1 \\ -\omega^2 & 0 \end{bmatrix}, \quad (23)$$

where $\omega^2(t) = \frac{n^2-1}{(1+t^2)^2}$ and $\omega^2(t) = t$ for Burst and Airy systems respectively. While previously the Jordan-Normal decomposition was only chosen as an alternative to diagonalisation and its improved performance not motivated we argue its potential is related to being a Jordan-Chevalley decomposition. This is where the similarity transform P such that $A = P^{-1}(D+N)P$ expresses J as a sum of semisimple, in our case we require diagonal, D and nilpotent N , meaning there exists a k with $N^k = 0$. For a Jordan-Chevalley decomposition these two components commute, so that $\exp(D+N) = \exp(D)\exp(N)$,

thereby offering stability and potentially improving runtime for exponentiation of J . In the Airy and Burst cases considered previously $N = 0$ and

$$\left(\dot{\mathbf{P}}^{-1} \right) \mathbf{P} = \begin{bmatrix} \frac{\omega'}{2\omega} & -\frac{\omega'}{2\omega} \\ -\frac{\omega'}{2\omega} & \frac{\omega'}{2\omega} \end{bmatrix}. \quad (24)$$

This seems to be a special case in which a step-size can be found where the integrated off diagonal elements introduced by (24) can be made small compared to the diagonal terms of J which are proportional to ω , as both are entirely proportional to functionals of ω . Therefore, it seems sensible in this case why neglecting off diagonal terms remained accurate as demonstrated in [8] and the routine ran faster than the standard Magnus method.

However, this is not generally true for larger arbitrary systems and so it is possible neither a Jordan-Normal nor Jordan-Chevalley decomposition would guarantee improved performance because of the $\dot{\mathbf{P}}^{-1} \mathbf{P}$ term. Nevertheless, we continued to develop a numerical routine to investigate this empirically.

C. Numerical Jordan-Magnus Routine

An at least near Jordan-Chevalley decomposition of a general unstructured matrix can be obtained using both a Schur decomposition or eigendecomposition. We found that using numerical eigendecomposition proved slow and unreliable. Convergence of the algorithm is not guaranteed for all matrices and in the case that a given matrix does not diagonalise under eigendecomposition then a similarity transformation will fail to decompose the matrix to a near diagonal form. The A_P values computed were often near singular and resulted in the exponentiation routine failing and the stepping matrix forcing the solution to vanish.

Instead we made use of the faster and generally more reliable numerical algorithm available for the real Schur transformation. The real Shur transformation can be described by $A = QTQ^{-1}$, where Q is a unitary matrix, and T is a quasi-upper triangular matrix. In quasi-triangular form, square 2-dimensional blocks describing complex-value eigenvalue pairs may extrude from the diagonal. In the case that a matrix cannot be cast into diagonal form then this still always produces a near diagonal form.

We numerically computed the Ω series expansion using the approach from [14] where A_p is Taylor expanded from the midpoint of each step,

$$\mathbf{A}_P(t) = \sum_{j=0}^{\infty} a_j (t - t_{1/2})^j \quad \text{where} \quad a_j = \left. \frac{1}{j!} \frac{d^n \mathbf{A}_P}{dt^n} \right|_{t=t_{1/2}}. \quad (25)$$

Then Ω is calculated to fourth order in timestep h via,

$$\Omega^{[4]} = \alpha_1 - \frac{1}{12} [\alpha_1, \alpha_2] + \mathcal{O}(h^5), \quad (26)$$

where $\alpha_j = h^j a_{j-1}$ and the alpha coefficients were calculated using Simpson's Newton-Cotes quadrature rules using a linear combination of three function evaluations of $A_p(t)$. This required 6 Schur decompositions and function evaluations of $A(t)$ per trial step. This method was similarly used to calculate the standard numerically evaluated Magnus expansion to fourth order. We also used the same standard adaptive step-size algorithm presented in Appendix A[7] used in previous work [8] for both RKF4(5) and Magnus type methods for consistent comparison.

D. Results

The performance of the new numerical Jordan-Magnus type method to integrate the simple two variable formulation of the Burst equation and a separate two variable system with,

$$A(t) = \begin{pmatrix} 0 & 1 \\ \frac{1}{t^2} - 4t^2 & -\frac{1}{t} \end{pmatrix}, \quad (27)$$

can be seen in Figures 2 and 3. We can see that the run-time of the JM method is much larger than either RKF4(5) or standard Magnus expansion. However, the stepsize is competitive with the standard magnus expansion and much better than RKF4(5) in regions of fast oscillation, as is especially pronounced in the central region of Figure 2 and end region of Figure 3.

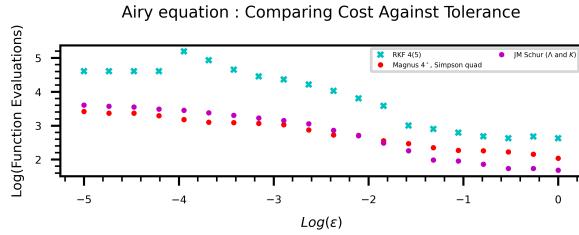


FIG. 1. Plot in \log_{10} space comparing the number of function evaluations required to integrate Airy equation from $t = 1$ to $t = 35$ against varying tolerance (ϵ) value, with all other parameters required for the adaptive step-size algorithm the same as presented in Figure 2. Each result is averaged over ten integration runs.

In order to compare whether this improvement in step-size corresponds to an increase in computational efficiency we look to the number of function evaluations required to integrate over the whole region in Figure 1. This presents a platform and code independent comparison of computational efficiency which is especially relevant when applied to systems with costly function evaluations, such as cosmologies considering a modified gravity with a complex numerical form. We see that in general the standard Magnus method is comparable with the Jordan Magnus method, becoming more competitive

at stricter tolerances. This indicates that the improved step-size in oscillatory regions does not compensate for the increased number of function evaluations required for each step and over the whole integration region.

The method failed to be reliably applied to the larger multivariate cosmological system. Here the routine on many time steps fails to exponentiate the new A_p term which often had a structure which led to overflow errors. When off-diagonal terms were omitted the method became too inaccurate to consider and so was not considered useful for general systems. This is a problem that the standard magnus method could face as well, as the ability to evaluate the costly matrix exponential deteriorates for larger system sizes, ill conditioned input matrices and matrices with significant structure. However, we found this modified method far more inhibited in practice.

V. SPECTRAL METHOD

A. Spectral Collocation on a Chebyshev Grid

Chebyshev spectral collocation methods are a class of numerical methods based on the use of Chebyshev polynomials as basis functions to approximate the solution of a differential equation. Chebyshev polynomials are a family of orthogonal polynomials defined on the interval [-1,1]. They are defined recursively with simple recurrence relations which makes them well-suited for use as basis functions in numerical methods. The formula for the n -th Chebyshev polynomial $T_n(x)$ is:

$$T_n(x) = \cos(n \cos^{-1}(x)) \quad (-1 \leq x \leq 1).$$

Or, alternatively:

$$T_n(x) = \sum_{k=0}^{\lfloor n/2 \rfloor} \frac{(-1)^k (2n-2k)!}{k!(n-k)!(n-2k)!} \left(\frac{x-1}{2}\right)^{n-2k} \text{ for } n \in \mathbb{N},$$

where $\lfloor n/2 \rfloor$ denotes the greatest integer less than or equal to $n/2$.

A spectral collocation method involves first discretizing the differential equation using a set of collocation points that are chosen based on the Chebyshev nodes. The Chebyshev nodes are the roots of the Chebyshev polynomial of degree n , where n is the number of collocation points used. Once the collocation points have been chosen, the differential equation is transformed into a system of algebraic equations using the Chebyshev polynomials as basis functions.

The system of algebraic equations is then solved to obtain the coefficients of the Chebyshev polynomial expansion of the solution. The solution can then be reconstructed by summing the Chebyshev polynomial expansion with the computed coefficients. The accuracy of the solution depends on the number of collocation points

Burst equation ($n = 60$) : Comparing Integration Methods

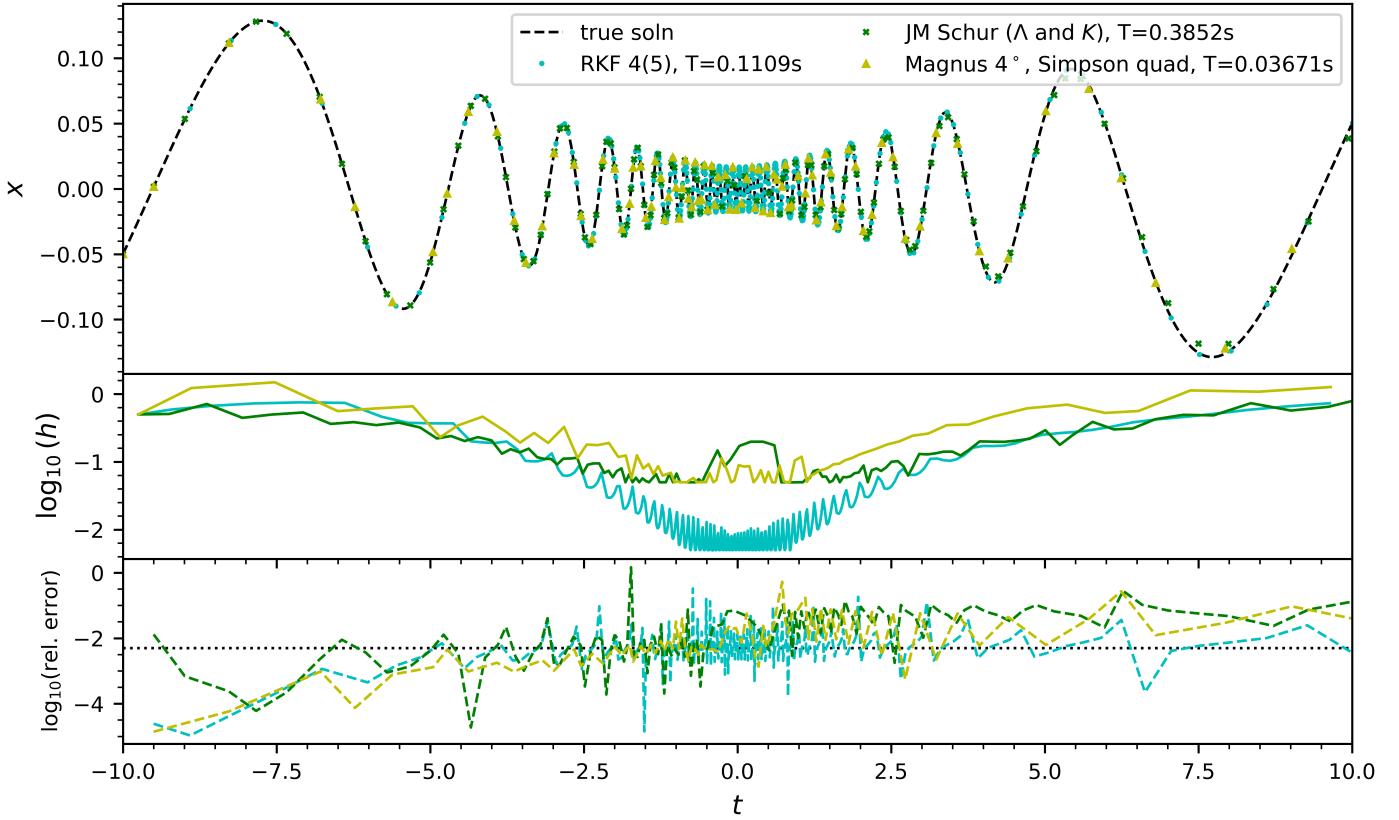


FIG. 2. Plot integrating Burst equation with Magnus and Runge-Kutta methods using adaptive step-size control. For the Magnus solutions $\epsilon = 0.005$, $a_{\text{tol}} = 0.005$, $r_{\text{tol}} = 1$. For the RKF4(5) solution, $\epsilon_{\text{RKF}} = 0.005$, $a_{\text{tol}} = 1$, $r_{\text{tol}} = 2$. Initial stepsize $h_0 = 0.5$, $h_{\text{max}} = 10$, $h_{\text{min}} = 0.01$ for Magnus methods. For RKF4(5) $h_{\text{max}} = 2.5$, $h_{\text{min}} = 0.005$. TOP: the integration results. MIDDLE: $\log_{10} |h|$ where h = stepsize. BOTTOM: $\log_{10} |\text{relative error}|$. The ϵ line shows the target error of $\epsilon = 0.005$.

used, with higher numbers of collocation points resulting in more accurate solutions.

The advantages these methods hold include offering adaptive order, such that the order of error convergence goes as $\mathcal{O}(h^p)$ in number of collocation points chosen p and stepsize h , as well as improved stability over stiff systems.

B. Numerical Method

We adapted the initial value problem collocation method found in [20] for single variable second order differential equations to generalise for use on systems of coupled first order ordinary differential equations. This method is capable of achieving an arbitrarily high order error convergence in time step in a simple manner.

On the standard interval $[-1, 1]$ the $n + 1$ Chebyshev nodes are $\tilde{\tau}_l = \cos(l\pi/n)$, $l = 0, 1, \dots, n$. The standard $(n+1) \times (n+1)$ differentiation matrix \tilde{D}_n is filled according to [21]. Rescaling to the time-step interval $[t_i, t_i + h]$

gives nodes:

$$\tau_l = t_i + \frac{h}{2}[1 + \cos(l\pi/n)], \quad l = 0, 1, \dots, n.$$

The re-scaled matrix $D_n = (2/h)\tilde{D}_n$. Using these Chebyshev nodes $\{\tau_l\}_{l=0}^n$ and differentiation matrices a general first order ODE may then be discretized over the interval $t \in [t_i, t_i + h]$ by the linear system

$$F\mathbf{u} := (D' + A')\mathbf{u} = \mathbf{0}$$

where $\mathbf{u}_j := \{u_j(\tau_l)\}_{l=0}^n$ are the node value vectors of each dependent variable x_j stacked on top of each other. The A' corresponds to $-A(t)$ from (5) transformed such that each element is replaced with a square diagonal matrix of size $n + 1$ with node evaluations on the diagonal, to allow coupling between dependent variables. Furthermore, D' now represents a block diagonal matrix with m blocks of D_n , where m is the number of dependent variables. One must also enforce initial conditions via

$$u_{j,n} = u_j(t_i), \quad (D_n \mathbf{u}_j)_n = u'_j(t_i),$$

2D eq. $x = t^{-1}\cos(t^2)$: Comparing Integration Methods

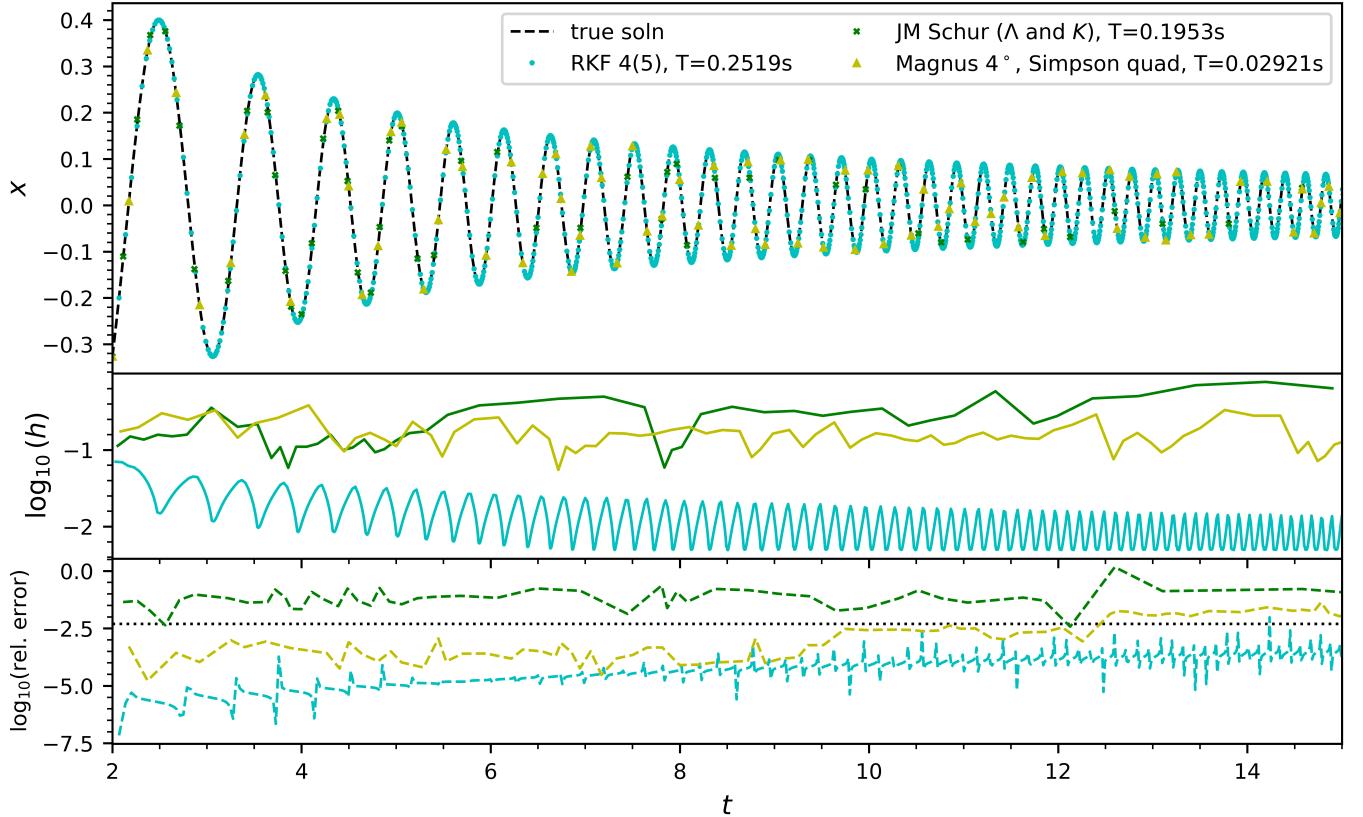


FIG. 3. Plot integrating 2 dependent variable system parameterised according to (27) with numerical Magnus and Runge-Kutta methods using adaptive stepsize control. The layout and parameters are the same as in Figure 2.

for each dependent variable. Stacking these conditions as rows gives the over determined $m \cdot (n+3) \times (m \cdot (n+1))$ linear system,

$$\begin{bmatrix} F \\ (D_{j,n})_{n,:} \\ (I_{j,n})_{n,:} \end{bmatrix} \mathbf{u} = \begin{bmatrix} 0_n \\ u'_j(t_i) \\ u_j(t_i) \end{bmatrix},$$

which is solved in the least-squares sense via singular value decomposition. This is computed with $\mathcal{O}((n+1) \cdot m)^3$ cost in number of dependent variables and collocation nodes. As part of the stepping procedure, $u_j(t)$ at the interval's upper end can be read off as the first element (since nodes π_l are ordered backwards) of the variables solution vector \mathbf{u} , and its derivative as the first element of $D_n \mathbf{u}$. These then serve as the initial conditions for the subsequent time-step.

C. Results

From Figure 4 we see that when applied to a two variable formulation of the Airy equation as in (23) the

method behaves well and as expected with the error appearing at $\mathcal{O}(h^p)$ in step-size h and number of collocation nodes p , with machine precision at the linear solve step providing a lower bound around (10^{-16}). This inhibits analysis at higher collocation points where we expect the differentiation matrices to start becoming badly conditioned anyway.

The spectral method is shown in Figure 5 to perform with superior accuracy for a range of collocation points as low as 8 at larger step-sizes when applied to the Airy system. This again exhibits the expected $\mathcal{O}(h^p)$ behaviour where the minimum error of the routine is again bounded by machine precision at the linear solve step.

We also demonstrate on a radiation dominated photon CDM Cosmology that with careful consideration of step-size and number of collocation nodes even a simple fixed step-size protocol can outperform Runge-Kutta and Magnus expansion stepping methods in Figures 6 and 7. The run time is competitive with a 4th and 6th order numerical Magnus expansion methods and significantly better than the RKF4(5) routine with similar or lower error than the other routines. This motivates use of an adaptive step-size algorithm and we propose a simple ex-

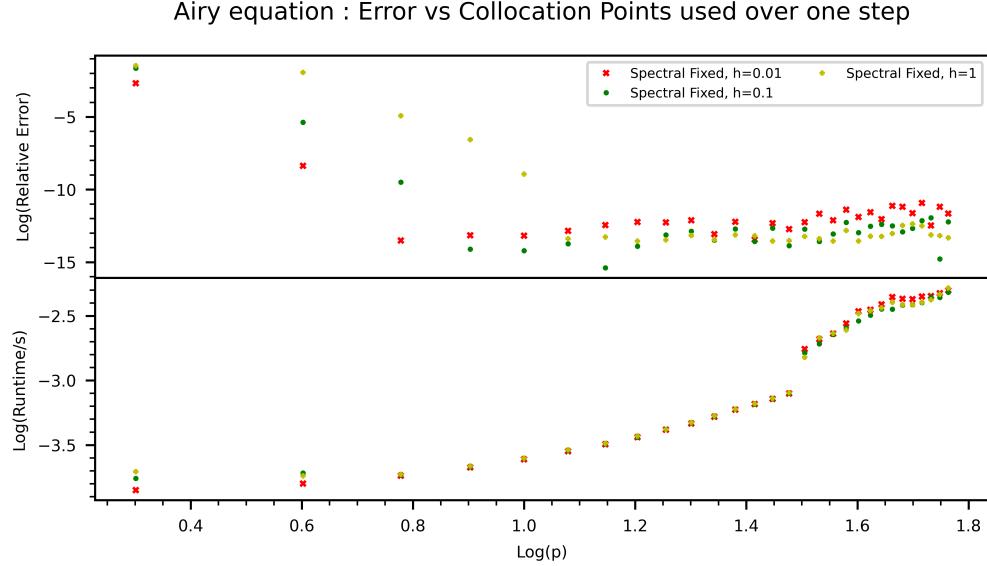


FIG. 4. Plot in \log_{10} space comparing relative error introduced over one step and run-time against number of collocation points, p , used when performed on the Airy equation, starting at $t=1$. Each value is averaged over 1000 runs.

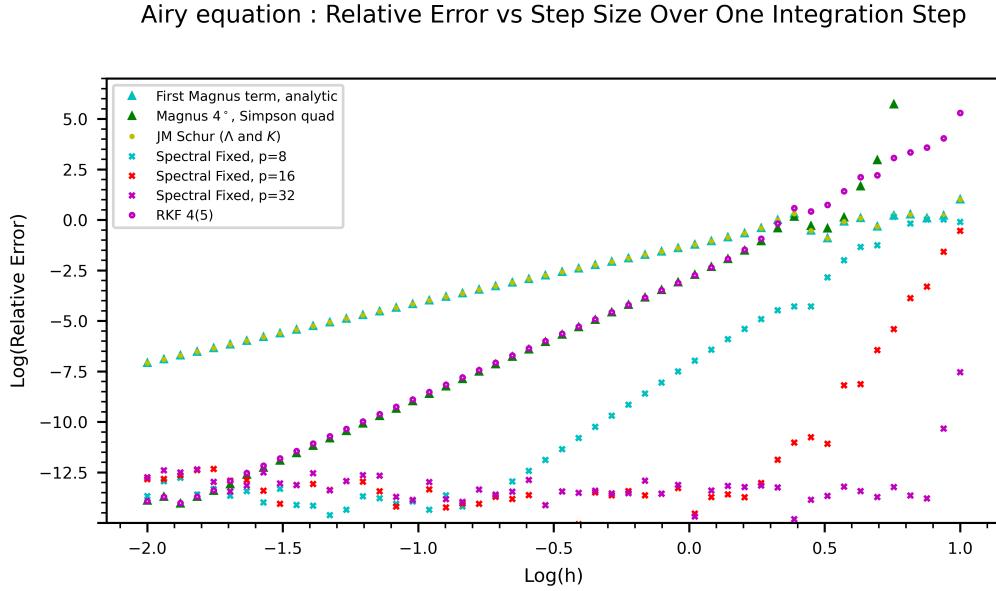


FIG. 5. Plot in \log_{10} space comparing relative error introduced over one step against step-size, h , when a stepping integration was performed on the Airy equation, starting at $t=1$. Each value is averaged over 1000 runs.

ample, presented in Appendix B, for which we have not yet found tolerances that give accurate integration. However it could serve as a basis for future work in optimising an adaptive algorithm to continue.

VI. DISCUSSION

This project focused on exploring the Jordan-Magnus method and alternative approaches to efficiently integrate coupled systems of first order ODEs whose solutions display highly oscillatory behaviour.

Our first objective was to contrast the differences between multiple-scale and Magnus expansion methods. We generalised the distinction explored previously be-

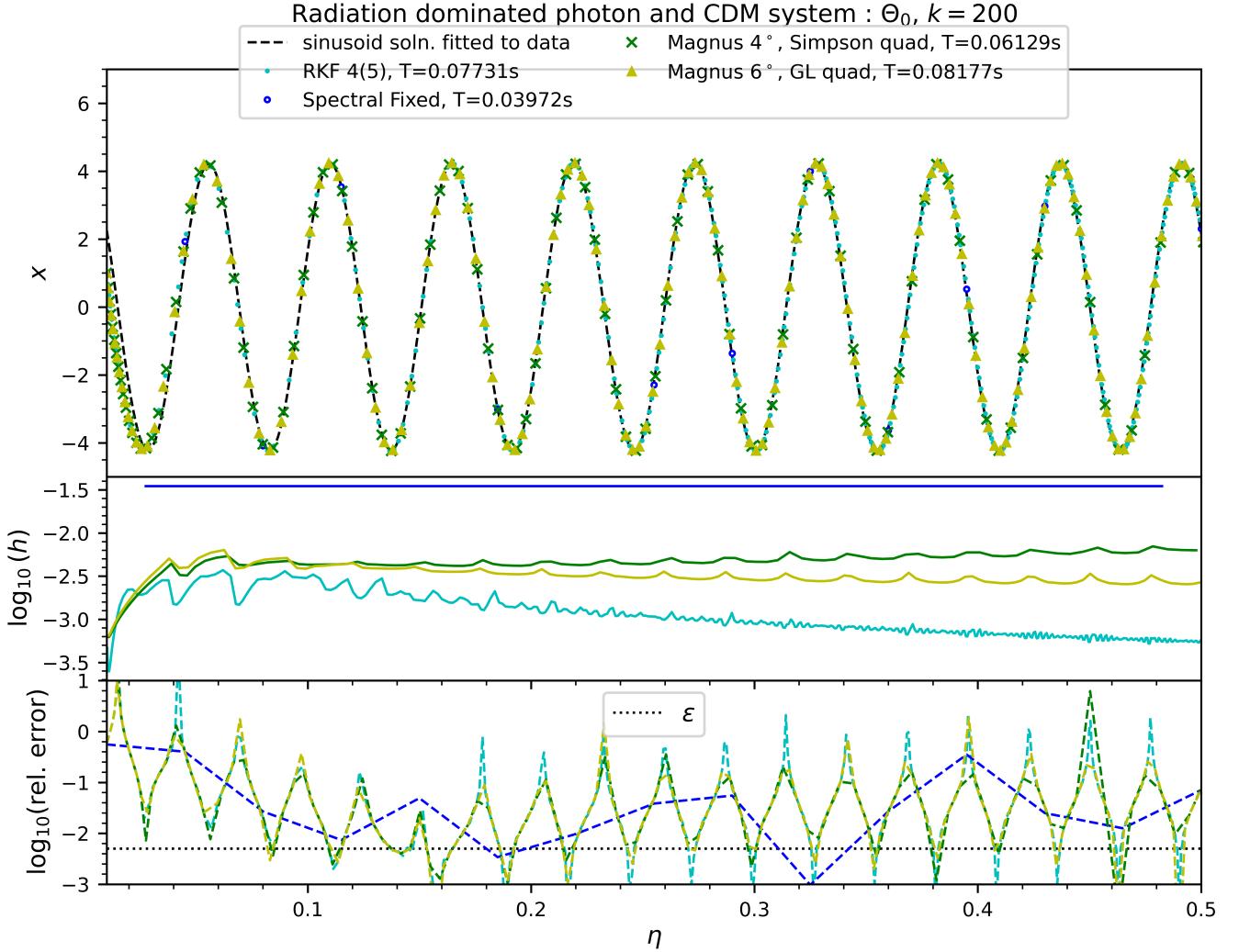


FIG. 6. Comparing numerical integration methods on the photon & CDM system. The black dashed line is the analytic solution for large $k\eta$ which is $C_0 \cos(k(\eta + C_1)/\sqrt{3})$ where C_0, C_1 are coefficients fitted to the RKF4(5) data. The initial conditions are $\eta_0 = 0.01, \mathbf{x}_0 = [1, 2, 1, 2, 1]$. The parameters are $k = 200, h_0 = 0.025, h_{\min} = 0.00025, h_{\max} = 2.5, \epsilon = 0.005$. For the Magnus methods $a_{\text{tol}} = 0.005, r_{\text{tol}} = 1$, for the RKF4(5) method $a_{\text{tol}} = 4, r_{\text{tol}} = 2$. For the spectral method $p = 8$. The layout is as in Figure 2.

tween the Magnus expansion and the WKB approximation [8]. We also discussed that while both are perturbative approaches, the multiple-scale approach too narrowly constrains practical implementation by requiring analytic knowledge of dominant solution behaviour on the fastest time scale of the system. Therefore, Magnus based approaches which do not require any prediction related to the solution nor even require a closed form representation of the system of equations offers greater flexibility to step-wise integration routines on arbitrary cosmological models.

Secondly, we aimed to generalise the Jordan-Magnus method to a fully numerical routine applicable to arbitrary coupled systems. We discussed that such routines may not theoretically promise improved performance on general systems over standard Magnus expansion meth-

ods. Furthermore, empirically our routine which relied on an alternative Schur decomposition failed to outperform fourth order numerical Magnus expansion or Runge-Kutta methods or be applied to larger systems including the five variable cosmological model considered here.

Finally, we aimed to explore the use of spectral collocation methods which have not previously been applied to the Einstein-Boltzmann equations. We implemented a Chebyshev collocation routine which was capable of outperforming both standard RKF4(5) and Magnus expansion based routines with a fixed step-size integration over a cosmological system. Like the numerical Magnus expansion based approach, this method only requires function evaluations of $\mathbf{A}(t)$ and does not require a closed form analytic representation of the system. Furthermore, while alternative methods including

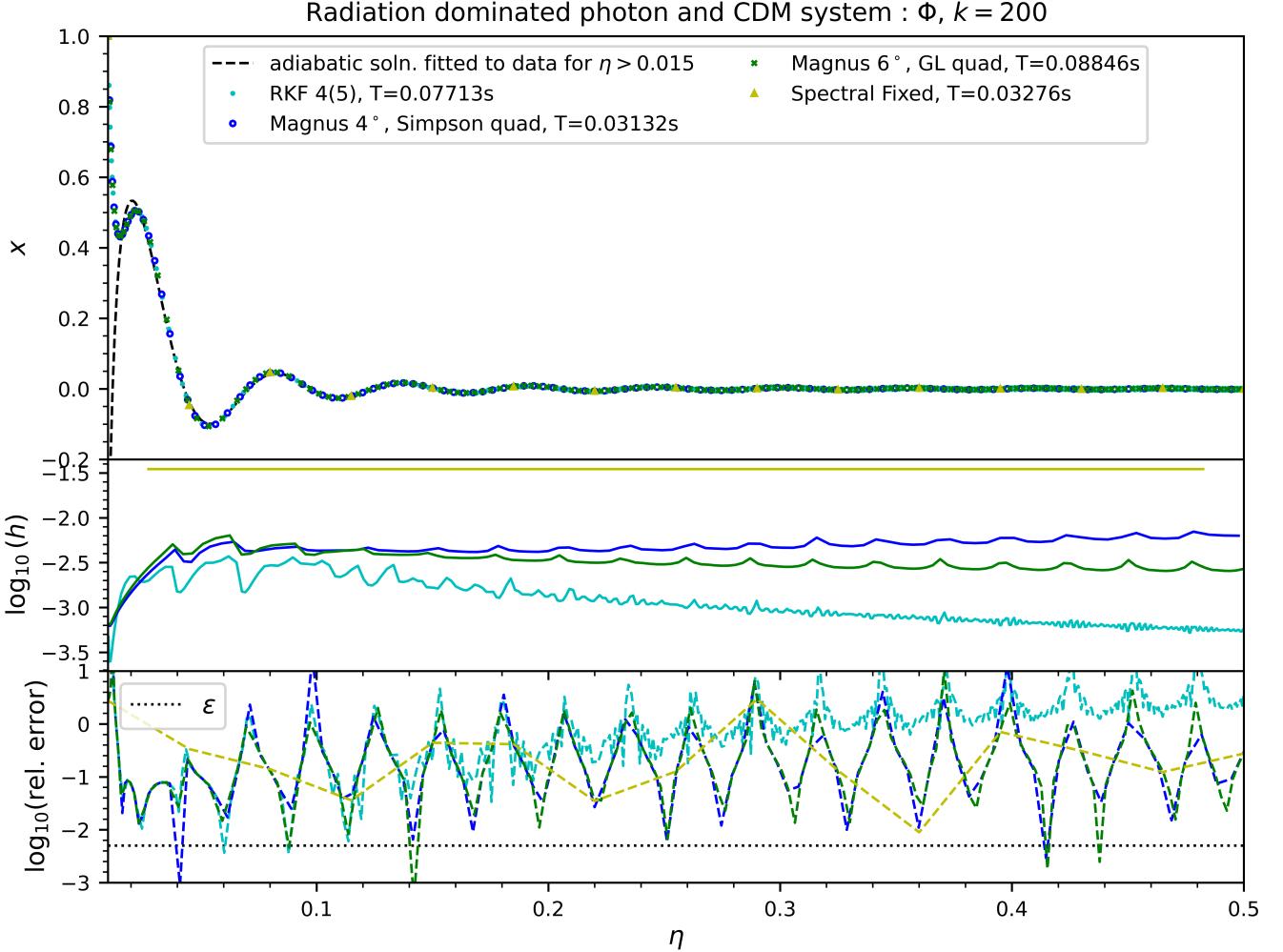


FIG. 7. Comparing numerical integration methods on the photon & CDM system, showing potential Φ . The black dashed line is the adiabatic solution fitted to the RKF4(5) data for $\eta \geq 0.05$. The initial conditions and all other parameters are as in Figure 6

Runge-Kutta methods offer flexibility only in step-size ‘h-adaptivity’, spectral methods additionally offer a tunable order of error convergence in step-size ‘p-adaptivity.’ Therefore a potential hybrid, ‘hp-adaptivity,’ that is well optimised could further improve computational efficiency in an adaptive routine. We propose a simple adaptive routine example as a basis for future work. Spectral collocation methods have not previously been used for initial value problems like this before and so optimising the hp-adaptivity control in adaptive stepping algorithms presents a promising area to explore for future research.

VII. CONCLUSION

This report has investigated Magnus expansion and spectral based methods to integrate highly oscillatory systems of coupled linear ODEs, with a focus on application to the Einstein-Boltzmann equations.

The first result in this report is to have clarified that multiple-scale analysis and Magnus expansion based methods are distinct perturbative approaches and argue that Magnus methods are more suited for use in cosmological perturbation theory and stepping integration routines.

The second result is to have generalised the method proposed in [8] for multivariate systems without requiring analytic Jordan-Normal forms. We have tested the method against simple two variable systems and found the method fails to outperform standard Magnus expansion methods.

Finally, we have developed and implemented a generalised Chebyshev spectral collocation stepping method which offers improved flexibility in terms of adaptive order of error convergence as well as step-size and outperforms RKF4(5) and Magnus expansion based methods on a five variable cosmological model. We also propose a simple adaptive step-size algorithm for this routine

which serves as a basis for future work to optimise hp-adaptivity.

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Appendix A: Adaptive Step-Size Routine for RKF4(5) and Magnus Methods

The routine is the same as that used in previous work [8] as presented in Press & Flannery (1992) [23].

To estimate an error for each step we use the standard method of estimating \mathbf{x}_{n+1} with a step of size h , and another using two steps of size $h/2$, \mathbf{x}_{n+1}^* . The error computed by $\Delta_i = |\mathbf{x}_{in+1}^* - \mathbf{x}_{in+1}|$ for each component i .

The maximum tolerable error is $\Delta_i^{\max} = \epsilon(a_{\text{tol}} + r_{\text{tol}}|\mathbf{x}_{in+1}^*|)$, where a_{tol} and r_{tol} parameterise the absolute and relative error tolerance, and ϵ is a small scale factor. The adaptive routine then follows as:

1. Calculate \mathbf{x}_{n+1}^* and \mathbf{x}_{n+1} for stepsize h .
2. Calculate Δ_i and Δ_i^{\max} and the error ratio $R = \sqrt{\frac{1}{N} \sum_i^N (\Delta_i / \Delta_i^{\max})^2}$
3. If $R \leq 1$ compute a new h as $h_{\text{new}} = hSR^{-1/(\nu+1)}$ where $S =$ safety factor ~ 0.98 , $\nu =$ order of method. Go to 5 .

4. Else if $R > 1$ compute a new h as $h_{\text{new}} = hSR^{-1/\nu}$. If $h_{\text{new}} < h_{\min}$ set $h_{\text{new}} = h_{\min}$ and go to 5 . Otherwise go to 1 .
5. If $h_{\text{new}} < 0.2h$ set $h_{\text{new}} = 0.2h$. If $h_{\text{new}} > h_{\max}$ set $h_{\text{new}} = h_{\max}$. If $h_{\text{new}} > 10h$ set $h_{\text{new}} = 10h$.
6. Use current \mathbf{x}_{n+1}^* as the estimate. Advance time. Set $h = h_{\text{new}}$. Go to next step.

Appendix B: Adaptive Step-Size Routine for Spectral Method

The routine is inspired by the adaptive step-size routine for single dependent variable systems developed in [20]. To estimate an error for each step we compute \mathbf{x}_{n+1} with p collocation points, and the same step again using $2p$ collocation points, \mathbf{x}_{n+1}^* . The error is calculated by taking the worst offender from $\Delta_i = |\mathbf{x}_{i,n+1}^* - \mathbf{x}_{i,n+1}|$. We also define the change in characteristic scale of the system, Δ_{scale} , as the sum of absolute differences between $\frac{1}{\|A(t)\|}$ at all consecutive collocation nodes within a step, where Frobenius norm $\|A(t)\|$ is used as a frequency indicator.

The maximum tolerable error is set as a free parameter to choose, Δ^{\max} , as well as an additional scale tolerance, A_{tol} . The adaptive routine then follows as:

1. Calculate \mathbf{x}_{n+1}^* and \mathbf{x}_{n+1} for stepsize h .
2. Calculate Δ_i and Δ_{scale}
3. If $\Delta_i \leq \Delta^{\max}$ and $\Delta_{\text{scale}} \leq A_{\text{tol}}$ compute a new h as $h_{\text{new}} = 2h$. If $h_{\text{new}} > h_{\max}$ set $h_{\text{new}} = h_{\max}$. Go to 5 .
4. Else if $\Delta_i > \Delta^{\max}$ and $\Delta_{\text{scale}} > A_{\text{tol}}$, compute a new h as $h_{\text{new}} = 0.5h$. If $h_{\text{new}} < h_{\min}$ set $h_{\text{new}} = h_{\min}$ and go to 5 . Otherwise go to 1 .
5. Use current \mathbf{x}_{n+1}^* as the estimate. Advance time. Set $h = h_{\text{new}}$. Go to next step.

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- [1] D. Scott, The standard model of cosmology: A skeptic's guide (2018), arXiv:1804.01318 [astro-ph.CO].
- [2] C.-P. Ma and E. Bertschinger, Cosmological perturbation theory in the synchronous and conformal newtonian gauges, *The Astrophysical Journal* **455**, 7 (1995).
- [3] U. Seljak and M. Zaldarriaga, A line-of-sight integration approach to cosmic microwave background anisotropies, *The Astrophysical Journal* **469**, 437 (1996).
- [4] J. Lesgourgues, The cosmic linear anisotropy solving system (class) i: Overview (2011).
- [5] A. Lewis, A. Challinor, and A. Lasenby, Efficient computation of cosmic microwave background anisotropies in closed friedmann-robertson-walker models, *The Astrophysical Journal* **538**, 473 (2000).
- [6] A. Refregier, L. Gamper, A. Amara, and L. Heisenberg, Pycosmo: An integrated cosmological boltzmann solver (2017).
- [7] W. Press, S. Teukolsky, W. Vetterling, and B. Flannery, *Numerical Recipes: The Art of Scientific Computing*, 3rd ed. (Cambridge University Press, 2007).
- [8] J. Bamber and W. Handley, Beyond the runge-kutta-wentzel-kramers-brillouin method, *Physical Review D* **101**, 10.1103/physrevd.101.043517 (2020).
- [9] F. J. Agocs, W. J. Handley, A. N. Lasenby, and M. P. Hobson, Efficient method for solving highly oscillatory ordinary differential equations with applications to phys-

- ical systems, Phys. Rev. Res. **2**, 013030 (2020).
- [10] W. J. Handley, A. N. Lasenby, and M. P. Hobson, The runge-kutta-wentzel-kramers-brillouin method (2016).
- [11] S. Dodelson, *Modern Cosmology* (Academic Press, Elsevier Science, 2003).
- [12] V. Mukhanov, H. Feldman, and R. Brandenberger, Theory of cosmological perturbations, Physics Reports **215**, 203 (1992).
- [13] S. Nadkarni-Ghosh and A. Refregier, The einstein–boltzmann equations revisited, Monthly Notices of the Royal Astronomical Society **471**, 2391 (2017).
- [14] S. Blanes, F. Casas, J. Oteo, and J. Ros, The magnus expansion and some of its applications, Physics Reports **470**, 151 (2009).
- [15] A. Iserles, On the numerical analysis of rapid oscillation, (2004).
- [16] W. Magnus, On the exponential solution of differential equations for a linear operator, Commun. Pure Appl. Math. **7**, 649 (1954).
- [17] W. Eckhaus, *Studies in non-linear stability theory*, Vol. 6 (Springer Science & Business Media, 2012).
- [18] D. Bernal-García, B. Rodríguez, and H. Vinck-Posada, Multiple-scale analysis of open quantum systems, Physics Letters A **383**, 1698 (2019).
- [19] P. Jakobsen, Introduction to the method of multiple scales (2016), arXiv:1312.3651 [math.AP].
- [20] F. J. Agocs and A. H. Barnett, An adaptive spectral method for oscillatory second-order linear odes with frequency-independent cost (2022), arXiv:2212.06924 [math.NA].
- [21] L. Trefethen, *Spectral Methods in MATLAB*, EngineeringPro collection (Society for Industrial and Applied Mathematics, 2000).
- [22] jarb2, jarb2/beyond_the_rkwkb_method: First release (2019).
- [23] W. H. Press, S. A. Teukolsky, W. T. Vetterling, and B. P. Flannery, *Numerical Recipes in C*, 2nd ed. (Cambridge University Press, Cambridge, USA, 1992).
- [24] J. Lees-Miller, J. Hammersley, and R. Wilson, Theoretical maximum capacity as benchmark for empty vehicle redistribution in personal rapid transit, Transportation Research Record: Journal of the Transportation Research Board , 76 (2010).