Numerical methods for the evolution of primordial perturbations

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Introduction

Bayesian analysis of the cosmic microwave background (CMB) allows us to constrain cosmological parameters and infer the physics of the early universe. The forward modelling phase of Bayesian inference involves calculation of the likelihood function ($\mathcal{L}$) of the model parameters. To get to $\mathcal{L}$, one needs to numerically solve linear, **ordinary differential equations with oscillatory solutions** *efficiently*. Currently these kind of calculations are the bottleneck of the inference process, as traditional numerical methods struggle to trace oscillatory solutions with high enough precision and acceptable speed. The **Runge–Kutta–Wentzel–Kramers–Brillouin method (RKWKB)**, proposed by Handley et al. [2016], combines known approaches to speed up such calculations by stepping over several wavelengths at a time. Here we present an implementation of RKWKB used to calculate primordial power spectra of primordial curvature perturbations, but the method is in general applicable to any system which requires rapid solution of linear differential equations, e.g. perturbative analyses.

Cosmology of primordial perturbations

- The Mukhanov–Sasaki equation governs the time-evolution of quantum mechanical fluctuations (seeds of late-time cosmic structure) in the early universe.
- Baumann [2009] derive it as:

$$\ddot{\mathcal{R}}_k + \left(\frac{H}{2} + \frac{\dot{z}}{z}\right)\dot{\mathcal{R}}_k + \left(\frac{k}{a}\right)^2 \mathcal{R}_k = 0$$

- H is the Hubble parameter, a the scale factor, $z = \frac{a\dot{\phi}}{H}$, and k is the characteristic wavenumber of the perturbation $\mathcal{R}_k$.
- This is just an oscillator with damping term γ and time-dependent frequency ω, which changes slowly in some region.
- The time-dependence of ω and γ are determined by

$$\dot{H} + H^2 = \frac{1}{3}\left[\dot{\phi}^2 - V(\phi)\right], \quad H^2 = \frac{1}{3}\left[\frac{1}{2}\dot{\phi}^2 + V(\phi)\right], \quad 0 = \ddot{\phi} + 3H\dot{\phi} + \frac{dV}{d\phi}.$$

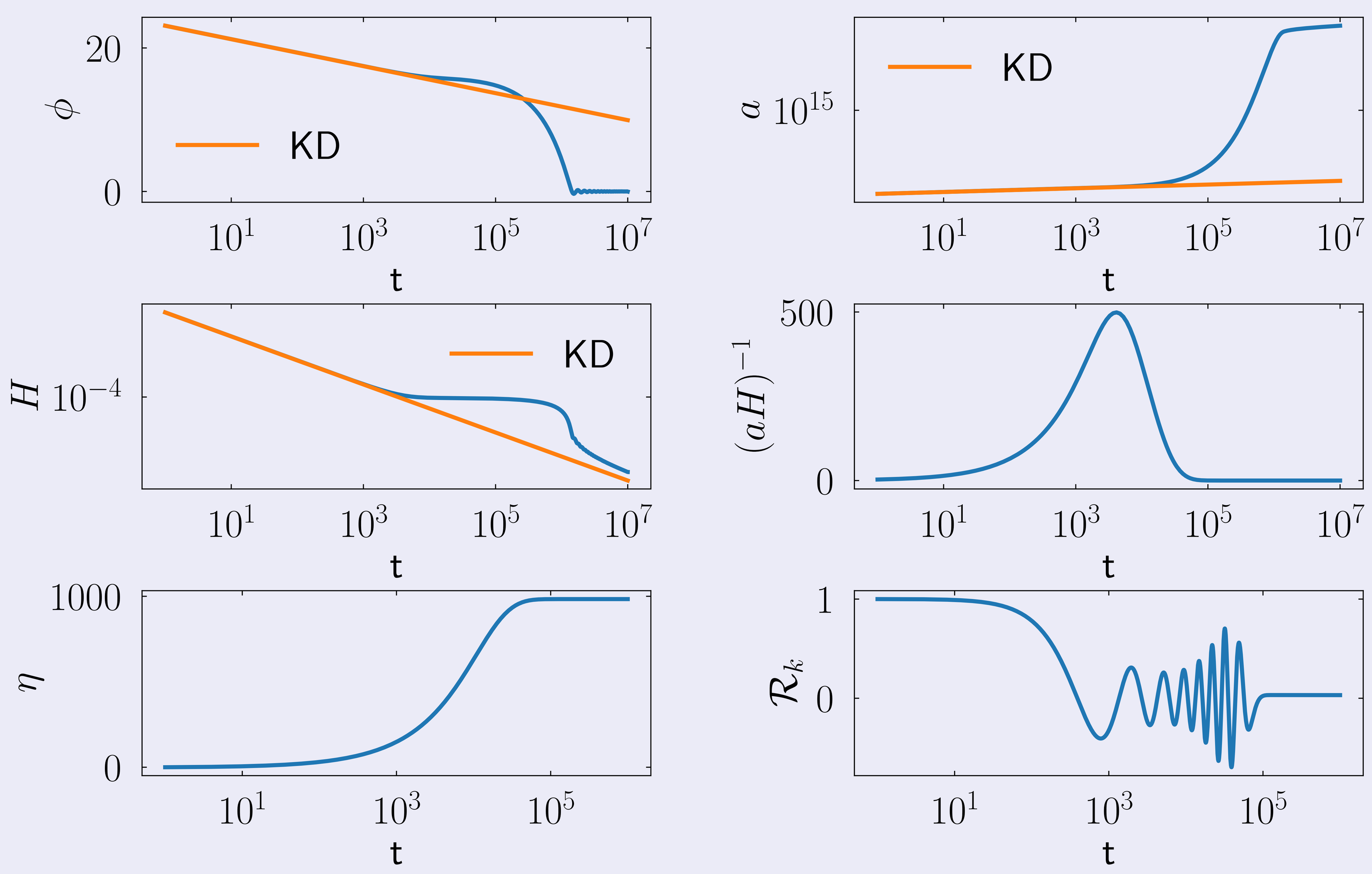


Figure: Evolution of the cosmological background and of a typical perturbation mode (bottom right panel) in our inflationary model. 'KD' refers to the type of initial conditions set.

RKWKB

- In general, RKWKB solves equations of the form:

$$\ddot{x} + 2\gamma(\boldsymbol{y})\dot{x} + \omega^2(\boldsymbol{y})x = 0,$$
$$\boldsymbol{F}(\boldsymbol{y}) = \dot{\boldsymbol{y}}.$$

- **RK** stepping procedures solve differential equations by stepping along a solution, extrapolating the solution via a Taylor series at each step.
- **WKB** methods provide good analytic approximations to oscillatory solutions.
- **RKWKB** combines these two by using WKB approximations to extrapolate the solution at each step of an adaptive RK stepping method.
- **Adapting the stepsize** based on estimates of the local error allows RKWKB to take large strides in regions where the frequency changes slowly.
- RKWKB **dynamically switches** between using a WKB approximation or a Runge–Kutta–Fehlberg 4(5) solution to predict the next step.

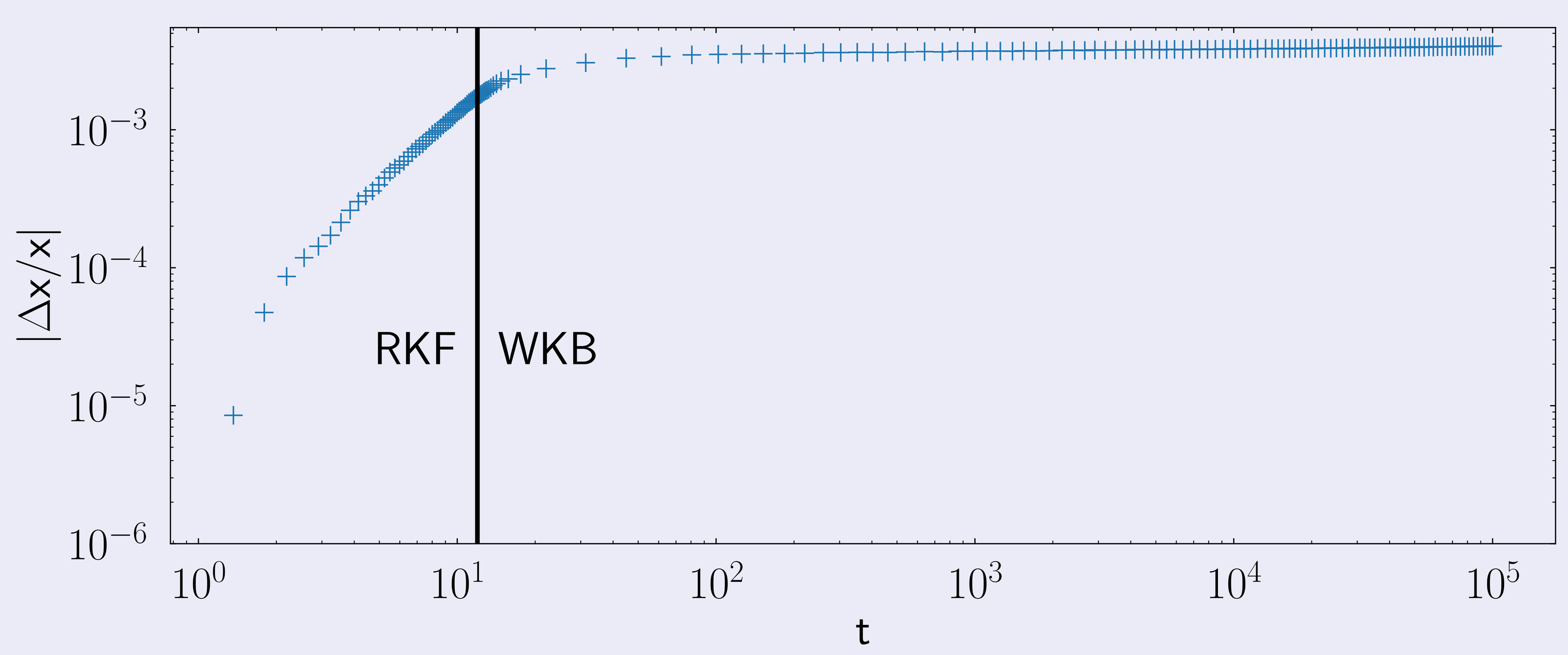


Figure: Relative error in RKWKB's solution to the Airy equation ($\omega \sim t^{1/2}, \gamma = 0$). The first few steps are taken with the RKF45 method, then the algorithm switches to taking WKB steps as the frequency changes more slowly at later times. The error stays bounded but the stepsize increases polynomially.

RKWKB in action

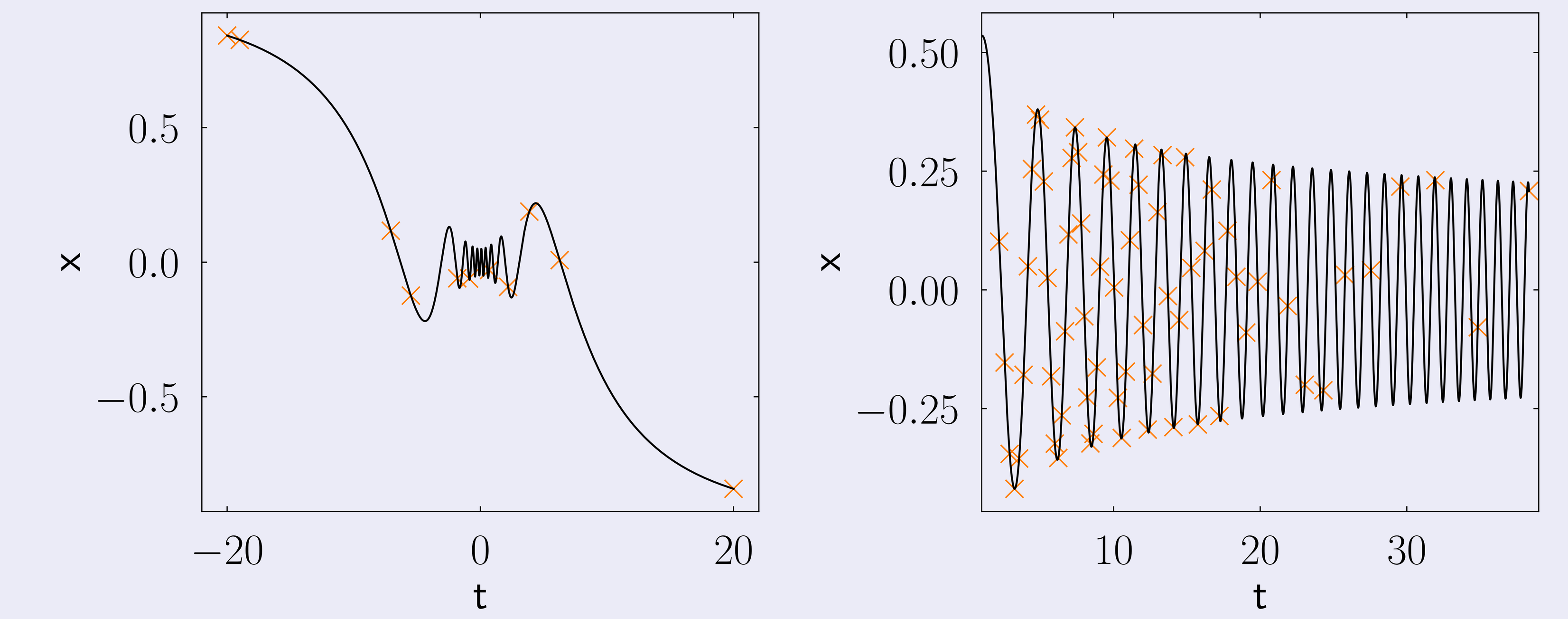
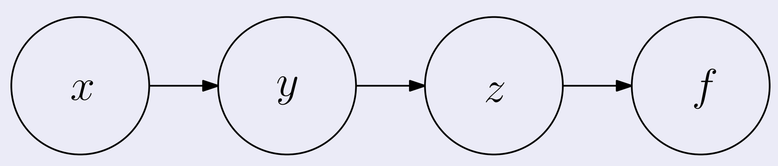


Figure: RKWKB's steps (orange crosses) while solving the 'burst' equation (left) and the Airy equation (right).

Automatic Differentiation (AD)

- RKWKB requires at least up to the second time derivatives of the frequency and damping term of the equation being solved.
- These need to be computed on-the-fly, with high precision and speed.
- **AD** operates near machine precision by applying the chain rule and storing intermediate results.
- Independently of the number of variables a function takes, AD takes a few times longer than the function itself to be evaluated.
- Symbolic differentiation can differentiate expressions, but AD can differentiate algorithms.



$$\frac{\partial f}{\partial x} = \frac{\partial f}{\partial z} \cdot \frac{\partial z}{\partial x}$$
$$\frac{\partial z}{\partial x} = \frac{\partial z}{\partial y} \cdot \frac{\partial y}{\partial x}$$
$$\frac{\partial y}{\partial x} = \frac{\partial y}{\partial x} \cdot \frac{\partial x}{\partial x}$$

Figure: Reverse-mode AD of the function $f(z(y(x)))$.

Results

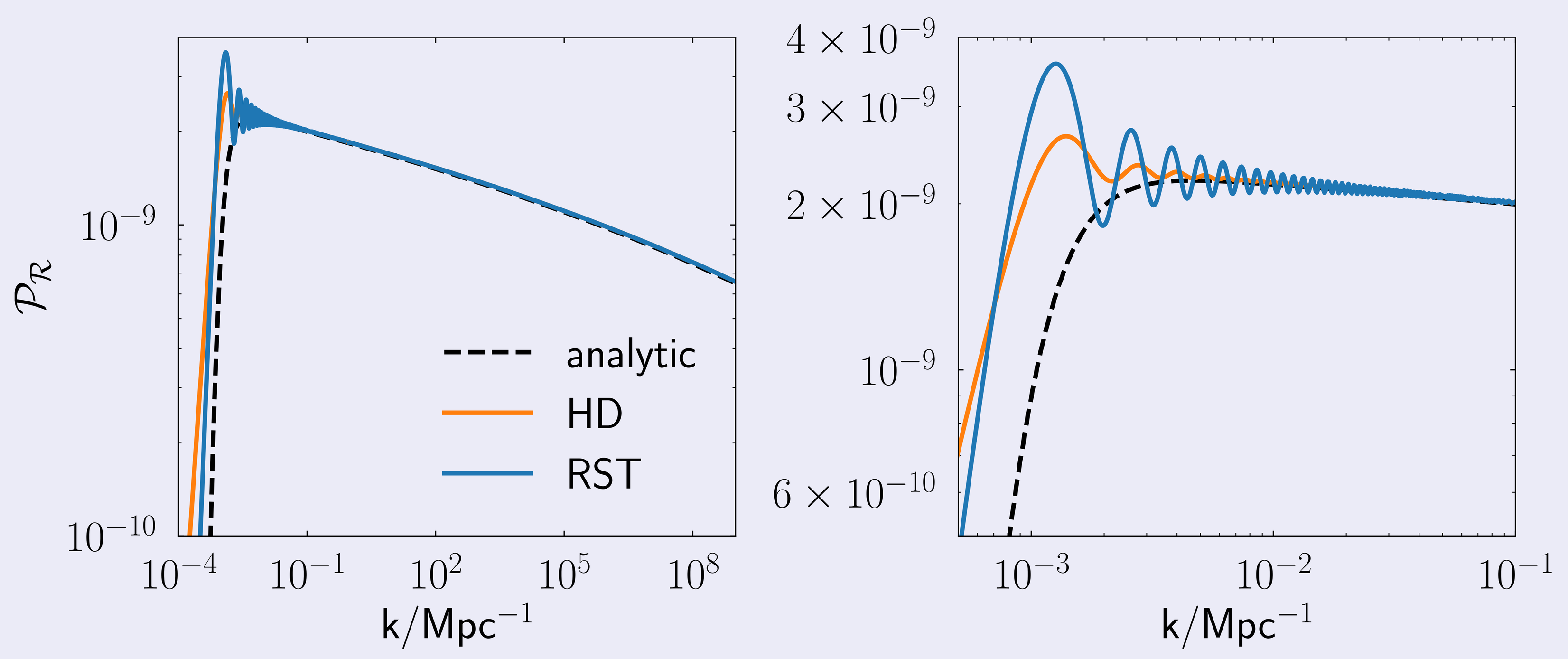


Figure: Primordial power spectra generated with RKWKB. 'HD' and 'RST' refer to different initial conditions - alternative initial conditions are easily explored with RKWKB. No other method can solve the Mukhanov–Sasaki at large values of k such as this.

Further work and applications

- Equations with oscillatory solutions are abound in physics. RKWKB can speed up the computation of their solutions.
- RKWKB (once fully optimised) could speed up the training of a neural network-based proxy for fast likelihood computation.
- RKWKB could possibly be generalised to solve coupled oscillators of the form $\ddot{\boldsymbol{x}} = A(\boldsymbol{y})\boldsymbol{x}$, where A is a matrix.

References

D. Baumann. TASI Lectures on Inflation. *ArXiv e-prints*, July 2009.

W. J. Handley, A. N. Lasenby, and M. P. Hobson. The Runge-Kutta-Wentzel-Kramers-Brillouin Method. *ArXiv e-prints*, December 2016.