New Algorithm for Mixmaster Dynamics

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Abstract

We present a new numerical algorithm for evolving the Mixmaster spacetimes. By using symplectic integration techniques to take advantage of the exact Taub solution for the scattering between asymptotic Kasner regimes, we evolve these spacetimes with higher accuracy using much larger time steps than previously possible. The longer Mixmaster evolution thus allowed enables detailed comparison with the Belinskii, Khalatnikov, Lifshitz (BKL) approximate Mixmaster dynamics. In particular, we show that errors between the BKL prediction and the measured parameters early in the simulation can be eliminated by relaxing the BKL assumptions to yield an improved map. The improved map has different predictions for vacuum Bianchi Type IX and magnetic Bianchi Type VI$_0$ Mixmaster models which are clearly matched in the simulation.

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Mixmaster dynamics (MD), discovered independently by Belinskii, Khalatnikov, and Lifshitz (BKL) \cite{1} and Misner \cite{2}, describes a system in which pure gravity exhibits chaos (or at least a strong sensitivity to initial conditions). Although first discovered in vacuum spatially homogeneous cosmologies of Bianchi Type IX, MD also occurs in vacuum cosmologies of Bianchi Type VIII \cite{3} and magnetic Bianchi Type VI$_0$ \cite{4}. (Other possible arenas for MD are given by Jantzen \cite{5}.)

It is clear that the most general homogeneous cosmology exhibits MD and has been conjectured that the same is true in the inhomogeneous case \cite{1}. Much recent work \cite{6} has focused on the question of whether or not MD is chaotic in any invariant sense since computed Lyapunov exponents can be either zero or positive depending on the choice of time variable \cite{7,8,9}. The issue has recently been resolved in favor of chaos by Cornish and Levin \cite{10} who have provided a prescription to define the discrete outcomes required to exhibit the fractal basins of attraction characteristic of chaos. A parallel issue remains, however. BKL (as revised by Chernoff and Barrow \cite{11} and extended by Berger \cite{12}) derived an approximate MD as a sequence of Kasner models with a map from one Kasner epoch to the next. So far, the properties of the map have always been consistent with those of the full solution to Einstein’s equations obtained numerically \cite{7,8,12}. However, one would wish to have more precise criteria for the BKL map’s validity and perhaps to measure departures from it. In addition, one must untangle the loss of information due to the chaotic nature of the dynamics from the accumulation of errors due to finite numerical precision.

Here, we describe a new numerical algorithm for MD which represents improvement by at least two orders of magnitude over standard ODE solvers in the speed with which a Mixmaster model may be evolved toward the singularity (without any loss of accuracy). We take advantage of the fact that MD as a sequence of Kasners is equivalent to MD as a sequence of bounces (transitions between Kasners) and that evolution from one Kasner to the next is the exactly solvable Taub cosmology \cite{13}. We apply this new method to the (diagonal) Bianchi IX and magnetic Bianchi VI$_0$ examples of MD in order to compare an improved BKL map to the numerical results and to display clearly the role of numerical precision in this comparison.
The models we shall use to illustrate our method are described by the metric

\[ ds^2 = -e^{2(\alpha+\zeta+\gamma)} \, dt^2 + e^{2\alpha} (\sigma_1)^2 + e^{2\zeta} (\sigma_2)^2 + e^{2\gamma} (\sigma_3)^2 . \]  

(1)

Here \( \alpha, \zeta \) and \( \gamma \) are functions of \( t \), and \( \sigma_1, \sigma_2 \) and \( \sigma_3 \) are time independent, orthogonal forms, invariant under the group of spatial symmetries. The dynamics of these spacetimes is therefore just the determination of the logarithmic scale factors (LSFs) \( \alpha, \zeta \) and \( \gamma \) as functions of \( t \). The Einstein equations for the models may be obtained by variation of the Hamiltonian \( H = H_k + H_p \) (and the constraint \( H = 0 \)) where

\[ 2H_k = 3 \left( p_\alpha^2 + p_\zeta^2 + p_\gamma^2 \right) - 6 \left( p_\alpha p_\zeta + p_\alpha p_\gamma + p_\zeta p_\gamma \right) . \]  

(2)

The potential term \( H_p \) is a function of the LSFs and depends on the type of homogeneous cosmology being treated. For vacuum Bianchi type IX or magnetic Bianchi Type VI\(_0\), we have

\[ H_p = c^2 e^{2b\alpha} + e^{4\zeta} + e^{4\gamma} - 2 \left( a e^{2(\alpha+\zeta)} + a e^{2(\alpha+\gamma)} + d e^{2(\zeta+\gamma)} \right) . \]  

(3)

Here \( a = 1, \, b = 2, \, c = 1 \) and \( d = 1 \) for vacuum Bianchi Type IX, while \( a = 0, \, b = 1, \, c = \sqrt{\xi} \) and \( d = -1 \) for magnetic Bianchi Type VI\(_0\), and \( \xi \) is a constant that depends on the strength of the magnetic field. Note that the magnetic field in Type VI\(_0\) provides the potential wall that is furnished by curvature in Type IX. When the logarithmic scale factors are large and negative, the potential term \( H_p \) is negligible so that the dynamical system is then essentially a free particle: \( \alpha, \zeta \) and \( \gamma \) are linear functions of \( t \). This is a Kasner epoch. The bounces between epochs occur in those periods when the potential is not negligible. Since the potential consists of terms that are exponentials of the LSFs, each of the bounces occurs in a brief time period (in terms of \( t \)).

To evolve the Mixmaster spacetimes numerically we use the method of symplectic integration \[14,15\]. This method begins with a dynamical system with Hamiltonian \( H = H_1 + H_2 \) where the equations obtained by variation of \( H_1 \) and \( H_2 \) are separately exactly solvable. For a Hamiltonian \( H \) let \( U(H, \Delta t) \) be the operator that evolves the system for a time \( \Delta t \).
Consider the operator
\[ U_2(H, \Delta t) \equiv U(H_1, \Delta t/2) U(H_2, \Delta t) U(H_1, \Delta t/2) \quad . \quad (4) \]
then to second order in \( \Delta t \) the operator \( U_2(H, \Delta t) \) agrees with \( U(H, \Delta t) \). Using the operator \( U_2(H, \Delta t) \) one can, by iteration, construct evolution operators that agree with \( U(H, \Delta t) \) to any desired order. Explicitly the \( 2n+2 \) order approximation to \( U(H, \Delta t) \) is
\[ U_{2n+2}(H, \Delta t) \equiv U_{2n}(H, s_n \Delta t) U_{2n}(H, (1 - 2s_n) \Delta t) U_{2n}(H, s_n \Delta t) \quad (5) \]
where \( s_n = 1/(2 - 2^{1/(2n+1)}) \). Note that though evolution using \( U_{2n} \) is formally \( 2n \) order accurate, the error may be much smaller than one would expect. Recall that if \( H_2 = 0 \) then \( U_2 \) (and therefore \( U_{2n} \)) is exactly equal to \( U \). Similarly if the evolution takes place in a region of phase space where \( H_2 \) is extremely small then \( U_{2n} \) is an extremely good approximation to \( U \), a much better approximation than, e.g. \( 2n \) order Runge-Kutta. Thus in such regions of phase space one can take very large time steps without introducing large inaccuracy.

To apply the symplectic integration method to the homogeneous cosmologies it is necessary to divide their Hamiltonian into two pieces, each of which is exactly solvable. It turns out that \( H_k \) and \( H_p \) are each exactly solvable since \( H_k \) is a free particle Hamiltonian that yields the Kasner solution while \( H_p \) contains no momenta and thus yields trivial equations of motion. However, splitting the Hamiltonian in this way still necessitates the use of extremely small time steps at the bounces. To take full advantage of the symplectic method we would like to split the Hamiltonian in such a way that \( H_2 \) is very small in the region of phase space in which the evolution is taking place. Note that the largest contribution to the potential term is always of the form \( c^2 e^{2b\tilde{\alpha}} \) where \( b \) and \( c \) are the constants defined in (3) for \( \tilde{\alpha} \) corresponding to a magnetic wall and \( c = 1, b = 2 \) for \( \tilde{\alpha} \) corresponding to a curvature wall. Call the other two LSFs \( \tilde{\zeta} \) and \( \tilde{\gamma} \). Denote by \( \tilde{p}_{\tilde{\alpha}}, \tilde{p}_{\tilde{\zeta}} \) and \( \tilde{p}_{\tilde{\gamma}} \) the momenta corresponding to \( \tilde{\alpha}, \tilde{\zeta} \) and \( \tilde{\gamma} \) respectively. We split the Hamiltonian into \( H_1 = H_k + c^2 e^{2b\tilde{\alpha}} \) and \( H_2 = H_p - c^2 e^{2b\tilde{\alpha}} \). But \( H_1 \) is the Hamiltonian for the exactly solvable Taub model while \( H_2 \) still contains no momenta. At each time step, the code identifies the largest LSF and implements the appropriate split.
In our notation, the Taub solution is the following: Since $H_1$ is independent of $\tilde{\zeta}$ and $\tilde{\gamma}$ it follows that $\tilde{p}_\zeta$ and $\tilde{p}_\gamma$ are constants. The remaining variables evolve as follows: Define $q, k$ and $r$ by $q \equiv -\dot{\tilde{\alpha}}(t)$,
\begin{equation}
k \equiv \left[ q^2 + 6 c^2 e^{2b\tilde{\alpha}(t)} \right]^{1/2},
\end{equation}
\begin{equation}
r \equiv \ln \left( \cosh kb\Delta t + \frac{q}{k} \sinh kb\Delta t \right).
\end{equation}
Then we have
\begin{equation}
\tilde{\alpha}(t + \Delta t) = \tilde{\alpha}(t) - \frac{r}{b},
\end{equation}
\begin{equation}
\tilde{p}_\alpha(t + \Delta t) = \tilde{p}_\alpha(t) - \frac{2c^2}{k} e^{2b\tilde{\alpha}(t) - r} \sinh kb\Delta t,
\end{equation}
\begin{equation}
\tilde{\zeta}(t + \Delta t) = \tilde{\zeta}(t) + \frac{r}{b} - 6\tilde{p}_\gamma \Delta t,
\end{equation}
\begin{equation}
\tilde{\gamma}(t + \Delta t) = \tilde{\gamma}(t) + \frac{r}{b} - 6\tilde{p}_\zeta \Delta t.
\end{equation}
Note that these formulas give exact solutions of the dynamics of $H_1$. There is no approximation and no assumption that $\Delta t$ is “small.” The dynamics of $H_2$ are trivial. Since $H_2$ is independent of $\tilde{p}_\alpha$, $\tilde{p}_\zeta$ and $\tilde{p}_\gamma$ it follows that $\tilde{\alpha}$, $\tilde{\zeta}$ and $\tilde{\gamma}$ are constants. The evolution of $\tilde{p}_\alpha$ is then given by
\begin{equation}
\tilde{p}_\alpha(t + \Delta t) = \tilde{p}_\alpha(t) - \frac{\partial H_2}{\partial \tilde{\alpha}} \Delta t
\end{equation}
and correspondingly for the other momenta.

Our computer code implements the sixth order symplectic integration algorithm with this split of the Hamiltonian. The time step is increased if evolution with $\Delta t$ and $\Delta t/2$ yields the same solution to a desired accuracy. For comparison we also evolved the same Mixmaster spacetimes with a fourth order, adaptive stepsize Runge-Kutta code and a sixth order symplectic algorithm with $H = H_k + H_p$. A comparison of the results of the three codes for type IX is shown in Fig. 1 for the region around a typical bounce. Note that the symplectic integration code achieves accurate evolution in approximately one hundred times fewer steps than the Runge-Kutta code. The key here is that any adaptive step size algorithm in any ODE solver can accurately reproduce the Kasner solution. However, in standard methods, $\Delta t$ must be drastically decreased when a potential term becomes non-negligible.
If care is not taken, a too large time step will cause overshoot of the potential wall leading to numerical disaster. In the new algorithm, the largest term in (3) is identified and the appropriate Taub solution used to effortlessly propagate the trajectory through the bounce. There is no need to decrease the time step. One can easily reach $|Ω| = \frac{1}{3}|α + ζ + γ| \approx 10^{35}$ in only 50,000 time steps corresponding to more than 150 epochs. Previous simulations have reported results for fewer than 30 epochs with $|Ω| < 10^8$ while requiring significantly more computer time [8]. If the constraint is not enforced at all, none of the algorithms discussed here can evolve more than about 15 epochs with the initial data used here. To maintain accuracy, it is necessary to enforce the Hamiltonian constraint at least every few time steps depending on the precision required. Recently, Gundlach and Pullin [16] have argued that the constraints must be enforced in generic numerical relativity codes. Our new algorithm allows simulations to be run for a sufficiently large number of epochs that the need to enforce the constraint here is also seen.

Each Kasner epoch can be specified by the values of four parameters: $(u, v, p_Ω, κ)$. As shown by several authors [14,11] these parameters can be defined throughout the evolution of a Mixmaster spacetime, though they are (approximately) constant only within a Kasner epoch. Following reference [17] we define $p_Ω \equiv p_α + p_ζ + p_γ$, and the Kasner indices $p_1 = -\dot{α}/(3p_Ω)$, $p_2 = -\dot{ζ}/(3p_Ω)$ and $p_3 = -\dot{γ}/(3p_Ω)$. Now reorder the $p_i$ so that $p_1 \leq p_2 \leq p_3$. Let $\bar{α}$, $\bar{ζ}$ and $\bar{γ}$ be respectively the LSFs corresponding to $p_1$, $p_2$ and $p_3$. Define $u$, $v$ and $κ$ by

\begin{align*}
u \equiv & \frac{p_2}{p_3} \left( \frac{p_1 \bar{γ} - p_3 \bar{α}}{p_1 \bar{ζ} - p_2 \bar{α}} \right) + 1 , & (14)
κ \equiv & p_3 \left( \frac{\bar{ζ}}{p_2} - \frac{\bar{α}}{p_1} \right) . & (15)
\end{align*}

BKL made the following approximation to MD: (i) between bounces the spacetime is exactly Kasner, (ii) the bounce occurs instantaneously and (iii) at a bounce one of the LSFs vanishes. This approximation yields a rule (the BKL map) that gives the values of the parameters
in the $n+1$st epoch in terms of their values in the $n$th epoch. It is well-known that these assumptions are less valid early in the simulation and improve as the singularity is approached. For $p_{q}$, the BKL rule is

$$p_{q,n+1} = p_{q,n} \left( \frac{u_{n}^{2} - u_{n} + 1}{u_{n}^{2} + u_{n} + 1} \right).$$

(16)

For the other parameters, the BKL map depends on whether $u_{n}$ is greater than 2. For $u_{n} \geq 2$, the BKL map is $u_{n+1} = u_{n} - 1$, $v_{n+1} = v_{n} + 1$ and $\kappa_{n+1} = \kappa_{n}$. For $u_{n} \leq 2$ (referred to as an era change), the rule is $u_{n+1} = 1/(u_{n} - 1)$, $v_{n+1} = 1 + (1/v_{n})$ and $\kappa_{n+1} = v_{n}\kappa_{n}/(u_{n} - 1)$.

However, the known exact dynamics of $H_{1}$ provides a better approximation to MD than does this BKL approximate dynamics—i.e. the sequence of bounces is a better description than the sequence of Kasners. It therefore yields a better map of the parameters $(u, v, p_{q}, \kappa)$ from one epoch to the next. This “improved BKL map” actually agrees with the BKL map for $u$ and $p_{q}$ but adds corrections to $v$ and $\kappa$. Let the quantity $w$ be given by

$$w = \frac{2}{b} \ln \left( \frac{u^{2} + 1}{u p_{q}} \right)$$

(17)

where $b$ and $c$ are defined as in (3) for the vacuum Type IX and magnetic VI0 cases. Within any era the improved BKL map for $v$ and $\kappa$ is

$$v_{n+1} = v_{n} + 1 + \frac{u_{n} + 1 - v_{n}}{1 + (\kappa_{n}/w_{n})},$$

(18)

$$\kappa_{n+1} = \kappa_{n} + w_{n},$$

(19)

while for an era change the improved BKL map gives

$$v_{n+1} = 1 + \frac{1 + (w_{n}/\kappa_{n})}{v_{n} + (u_{n} + 1)(w_{n}/\kappa_{n})},$$

(20)

$$\kappa_{n+1} = v_{n}\kappa_{n} + (u_{n} + 1)w_{n}/u_{n} - 1.$$ 

(21)

Note that in the limit of vanishing $w_{n}/\kappa_{n}$ the improved BKL map agrees with the BKL map. As the singularity is approached, $|\kappa_{n}| \to \infty$ so that the BKL terms overwhelm the corrections. In Fig. 2, 20 epochs of a typical magnetic Bianchi VI0 trajectory are displayed in
the anisotropy plane. The axes are $\mathbf{18} \beta_\pm /|\Omega|$ where $\beta_+ = \frac{1}{6}(\zeta + \gamma - 2\alpha)$, $\beta_- = \frac{1}{2\sqrt{3}}(\zeta + \gamma)$ so that the exponential potential terms have fixed locations. We have chosen the vertical wall to be due to the magnetic field ($\xi e^{2\alpha}$) with the other two walls ($e^{4\xi}$, $e^{4\gamma}$) due to curvature. The epoch numbers are identical to those in Fig. 3 which shows the fractional difference between measured and predicted (on the basis of the previous measured value) values of $v$ for the BKL and improved maps for bounces off magnetic (VI) and curvature (IX) walls. It is clearly seen that extremely accurate agreement is obtained alternately for the magnetic and curvature improved maps as the trajectory correspondingly bounces off the respective walls. A new era with bounces between two curvature walls is also seen in epochs 12-14. Fig. 4 shows a later stage in the evolution when all three maps converge as expected. The results for the parameter $\kappa$ are identical.

Finally, we consider tracking an initial value of $u$ through almost 200 epochs with the Hamiltonian constraint enforced at every time step. The sequence is begun at a point where, during an era, the ODE solution follows the BKL map for $u$ to the desired precision. Unlike the predictions previously described, loss of information and numerical error are allowed to accumulate. *Mathematica* [19] is used to obtain the sequence of BKL $u$-values to 60 significant figures (SFs) while our ODE solver is run in quadruple precision (32 SFs). Integer parts for $u$ in the latter different from those predicted by the former arise in our simulation at epoch 161, precisely where a 32 SF *Mathematica* sequence completely loses precision due to era changes. In fact, examination of the $u$ sequence shows that epoch 161 begins the 32nd era, as expected. (Similarly, the double precision simulation deviates at epoch 47, the start of the 16th era.) Given initial data specified to $N$ SFs, the numerical simulation follows the true Mixmaster trajectory through $\approx N$ eras, until the initial information is lost. However, as can be deduced from Fig. 4, the numerical solution remains close to some true Mixmaster trajectory for any sequence of $N$ eras in the simulation. We emphasize here that these effects are not visible early in the simulation. Our new algorithm allows easy study of Mixmaster models for more than one hundred epochs to permit careful examination of issues relating to the validity of the (improved) BKL approximation.
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FIGURES

FIG. 1. Comparison of algorithms for MD. A typical Mixmaster bounce is shown in the anisotropy plane. Crosses indicates every 10th point on a 4th order Runge-Kutta evaluation of the trajectory, while circles indicate every 10th point for a 6th order standard symplectic evaluation. The filled squares indicate every point using the new algorithm. The inset shows the details closest to the bounce.

FIG. 2. The first 20 epochs of a typical magnetic Bianchi VI0 trajectory in the rescaled anisotropy plane where the potential is shown as a fixed equilateral triangle. Some epoch numbers are shown. The vertical potential wall is produced by the magnetic field while the others are due to curvature.

FIG. 3. Fractional difference between measured and predicted values of \( v \) vs. epoch number using the BKL prediction (crosses), the curvature wall prediction (squares), and the magnetic wall prediction (circles). Triangles mark the first epoch of an era.

FIG. 4. Convergence of the BKL and improved maps as the evolution shown in Figures 2 and 3 is continued toward the singularity. The symbols are the same as those in Fig. 3.
