

Numerical Approximations of Particle Motion within a Torus and on a Plane

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1 Introduction

The motion of a particle along a surface can be modeled using a combination of physics, differential equations, and numerical analysis. Considering three primary forces (gravity, friction, and the normal force), a system of six differential equations can be derived from the implicit equation of a surface. In particular, a torus and a plane were considered.

To visualize the motion, determining exact solutions for a system of six differential equations is generally unrealistic and computationally expensive. However, numerical methods can be implemented instead. In this report, two methods were considered: a 2-step BDF method and a 2-step Adams-Bashforth method. Respectively, the methods are implicit and explicit, and both are of order 2. Convergence of each methods when applied to a plane was numerically determined in MATLAB by observing the error between one of the two methods and a pair of high order Runge-Kutta methods, the latter of which serves as a decent alternative to the exact solution.

Although differential equations were also derived for the torus, the analysis performed with the example for a plane was not repeated with a torus. The basic framework for analyzing the errors of a method when applied to a torus exists in this report nonetheless.

2 Theory

Denote the position of a particle in \mathbb{R}^3 by $\vec{x} = [x \ y \ z]^T$. Let $\dot{\vec{x}} = \vec{v}$ (velocity) and $\ddot{\vec{x}} = \vec{a}$ (acceleration). For a particle moving along a surface defined by $f(x, y, z) = 0$, there are three primary forces at play:

Force Due to Gravity: $m\vec{g}$,

Normal Force: $\frac{\vec{\nabla} f}{\|\vec{\nabla} f\|}N$, and

Force Due to Friction: $-\mu\frac{\vec{v}}{\|\vec{v}\|}N$,

where m is the particle mass, μ is the friction coefficient, and N is some constant. By Newton's Law, the sum of forces that act on the particle is the product of the mass and acceleration of the particle. Then

$$\begin{aligned} m\vec{a} &= m\vec{g} - \mu\frac{\vec{v}}{\|\vec{v}\|}N + \frac{\vec{\nabla} f}{\|\vec{\nabla} f\|}N \\ \Rightarrow \vec{a} &= \vec{g} - \frac{\mu}{m} \cdot \frac{\vec{v}}{\|\vec{v}\|}N + \frac{1}{m} \cdot \frac{\vec{\nabla} f}{\|\vec{\nabla} f\|}N \end{aligned} \quad (1)$$

Note that twice differentiating the surface equation $f(x, y, z) = 0$ gives

$\mathbf{H}\vec{v} \cdot \vec{v} + \vec{\nabla} f \cdot \vec{a} = 0$, where \mathbf{H} is the Hessian matrix corresponding to the implicit surface

equation $f(x, y, z) = 0$. Then Equation (1) implies

$$\begin{aligned}
& \mathbf{H}\vec{v} \cdot \vec{v} + \vec{\nabla}f \cdot \left(\vec{g} - \frac{\mu}{m} \cdot \frac{\vec{v}}{\|\vec{v}\|}N + \frac{1}{m} \cdot \frac{\vec{\nabla}f}{\|\vec{\nabla}f\|}N \right) = 0 \\
\Rightarrow & \mathbf{H}\vec{v} \cdot \vec{v} + \vec{\nabla}f \cdot \vec{g} - \frac{\mu}{m} \cdot \frac{\vec{\nabla}f \cdot \vec{v}}{\|\vec{v}\|}N + \frac{1}{m} \cdot \frac{\vec{\nabla}f \cdot \vec{\nabla}f}{\|\vec{\nabla}f\|}N = 0 \\
\Rightarrow & m\mathbf{H}\vec{v} \cdot \vec{v} + \vec{\nabla}f \cdot m\vec{g} - \frac{d}{dt}f(x, y, z) \frac{N}{\|\vec{v}\|} + \frac{\|\vec{\nabla}f\|^2}{\|\vec{\nabla}f\|}N = 0 \\
\Rightarrow & -\frac{d}{dt}0 \frac{N}{\|\vec{v}\|} + \|\vec{\nabla}f\|N = -m\mathbf{H}\vec{v} \cdot \vec{v} - \vec{\nabla}f \cdot m\vec{g} \\
\Rightarrow & N = \frac{-m\mathbf{H}\vec{v} \cdot \vec{v} - \vec{\nabla}f \cdot m\vec{g}}{\|\vec{\nabla}f\|}. \tag{2}
\end{aligned}$$

3 Torus

The surface equation f defined for a torus centered at the origin is

$$f(x, y, z) = (\sqrt{x^2 + y^2} - R)^2 + z^2 - r^2 = 0, \tag{3}$$

for some positive constants $R, r \in \mathbb{R}$. From Equation (3), we can compute the gradient and Hessian matrix of f via partial differentiation. For ease of further computations, let

$$\begin{aligned}
\vec{\omega} &= [x \ y \ z \ x' \ y' \ z']^T \\
&= [\omega_1 \ \omega_2 \ \omega_3 \ \omega_4 \ \omega_5 \ \omega_6]^T \\
\alpha &= \omega_4^2 + \omega_5^2 + \omega_6^2, \\
\beta &= \omega_1\omega_5 - \omega_2\omega_4, \text{ and} \\
\lambda &= \omega_1^2 + \omega_2^2.
\end{aligned}$$

Then the gradient and Hessian matrix of f respectively are

$$\begin{aligned}
\vec{\nabla}f &= \left[-2\frac{(\sqrt{\lambda} - R)\omega_1}{\sqrt{\lambda}} \quad -2\frac{(\sqrt{\lambda} - R)\omega_2}{\sqrt{\lambda}} \quad -2\omega_3 \right]^T, \text{ and} \\
\mathbf{H} &= \begin{bmatrix} -2 + \frac{2R\omega_2^2}{\sqrt{\lambda^3}} & -\frac{2R\omega_1\omega_2}{\sqrt{\lambda^3}} & 0 \\ -\frac{2R\omega_1\omega_2}{\sqrt{\lambda^3}} & -2 + \frac{2R\omega_1^2}{\sqrt{\lambda^3}} & 0 \\ 0 & 0 & -2 \end{bmatrix}.
\end{aligned}$$

Now, we can compute the scalar N associated with the normal force and the force due to friction. Note that the norm used in Equation (2) is the Euclidean norm. Then we have

$$\begin{aligned}
N &= \frac{-m\mathbf{H}\vec{v} \cdot \vec{v} - \vec{\nabla}f \cdot m\vec{g}}{\|\vec{\nabla}f\|} \\
&= \frac{-m \left[-2 \left(\alpha - \frac{R\beta^2}{\sqrt{\lambda^3}} \right) \right] - (-2m(-g)\omega_3)}{2r} \\
&= \frac{m}{r} \cdot \left(\alpha - \frac{R\beta^2}{\sqrt{\lambda^3}} - g\omega_3 \right). \tag{4}
\end{aligned}$$

With careful computations, it follows from Equation (4) that

$$\dot{\vec{\omega}} = \begin{bmatrix} \omega'_1 \\ \omega'_2 \\ \omega'_3 \\ \omega'_4 \\ \omega'_5 \\ \omega'_6 \end{bmatrix} = \begin{bmatrix} \omega_4 \\ \omega_5 \\ \omega_6 \\ \frac{1}{(r\lambda)^2\sqrt{\alpha}} \left(\sqrt{\lambda^3} \cdot (g\omega_3 - \alpha) + R\beta^2 \right) \left(\omega_1\sqrt{\alpha} \cdot (\sqrt{\lambda} - R) + \mu r\omega_4\sqrt{\lambda} \right) \\ \frac{1}{(r\lambda)^2\sqrt{\alpha}} \left(\sqrt{\lambda^3} \cdot (g\omega_3 - \alpha) + R\beta^2 \right) \left(\omega_2\sqrt{\alpha} \cdot (\sqrt{\lambda} - R) + \mu r\omega_5\sqrt{\lambda} \right) \\ -g + \frac{1}{r^2\sqrt{\alpha}\lambda^3} \cdot \left(\sqrt{\lambda^3} \cdot (g\omega_3 - \alpha) + R\beta^2 \right) \left(\omega_3\sqrt{\alpha} + \mu\omega_6r \right) \end{bmatrix}.$$

4 Plane

The surface equation f defined for a plane in \mathbb{R}^3 is

$$f(x, y, z) = ax + by + cz + d = 0, \quad (5)$$

for some constants $a, b, c, d \in \mathbb{R}$. From Equation (5), we can compute the gradient and Hessian matrix of f by taking partial derivatives. Then the gradient and Hessian matrix of f respectively are

$$\vec{\nabla} f = [a \quad b \quad c]^T, \text{ and}$$

$$\mathbf{H} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}.$$

Now, we can compute the scalar N associated with the normal force and the force due to friction. Note that the norm used in Equation (2) is the Euclidean norm. Let

$$\vec{\sigma} = [x \quad y \quad z \quad x' \quad y' \quad z']^T$$

$$= [\sigma_1 \quad \sigma_2 \quad \sigma_3 \quad \sigma_4 \quad \sigma_5 \quad \sigma_6]^T.$$

Then we have

$$N = \frac{-m\mathbf{H}\vec{v} \cdot \vec{v} - \vec{\nabla} f \cdot m\vec{g}}{\|\vec{\nabla} f\|}$$

$$= \frac{-m(0) - m(c)(-g)}{\sqrt{a^2 + b^2 + c^2}}$$

$$= \frac{mcg}{\sqrt{a^2 + b^2 + c^2}}. \quad (6)$$

With careful computations, it follows from Equation (6) that

$$\dot{\vec{\sigma}} = \begin{bmatrix} \sigma'_1 \\ \sigma'_2 \\ \sigma'_3 \\ \sigma'_4 \\ \sigma'_5 \\ \sigma'_6 \end{bmatrix} = \begin{bmatrix} \sigma_4 \\ \sigma_5 \\ \sigma_6 \\ \frac{cg}{a^2 + b^2 + c^2} \left(a - \mu\sigma_4 \sqrt{\frac{a^2 + b^2 + c^2}{\sigma_4^2 + \sigma_5^2 + \sigma_6^2}} \right) \\ \frac{cg}{a^2 + b^2 + c^2} \left(b - \mu\sigma_5 \sqrt{\frac{a^2 + b^2 + c^2}{\sigma_4^2 + \sigma_5^2 + \sigma_6^2}} \right) \\ g \left(\frac{c}{a^2 + b^2 + c^2} \left(c - \mu\sigma_6 \sqrt{\frac{a^2 + b^2 + c^2}{\sigma_4^2 + \sigma_5^2 + \sigma_6^2}} \right) - 1 \right) \end{bmatrix}. \quad (7)$$

5 Numerical Methods

Consider the Initial Value Problem (IVP):

$$\begin{cases} y'(t) &= f(t, y(t)), \\ y(t_0) &= y_0. \end{cases}$$

To determine A-stability for an s -step multistep method defined by

$$\sum_{m=0}^s a_m y_{n+m} = h \sum_{m=0}^s b_m f(t_{n+m}, y_{n+m}),$$

for some $a_m, b_m \in \mathbb{R}, m = 0, 1, \dots, s$, and where $n = 0, 1, \dots, N$ for some $N \in \mathbb{N}$, consider the IVP

$$\begin{cases} y'(t) &= \lambda y(t), \\ y(t_0) &= y_0, \end{cases}$$

for some $\lambda \in \mathbb{C}$ where $\operatorname{Re}(\lambda) < 0$. Let $z = h\lambda$, then let

$$\eta(\omega, z) = \sum_{m=0}^s (a_m - zb_m)\omega^m.$$

By a lemma, a multistep method is A-stable iff $b_s > 0$ and the roots of $\eta(\omega, z)$ at $z = it$, (i.e. $\omega_i(it)$), are in the closed complex unit disk. If $\eta(\omega, it)$ is of the form $\alpha\omega^2 + \beta\omega + \gamma$ for some $\alpha, \beta, \gamma \in \mathbb{C}$, then by another lemma, the roots $\omega_i(it)$ are in the closed complex unit disk if and only if

- (1) $|\alpha| \geq |\gamma|$,
- (2) $||\alpha|^2 - |\gamma|^2| \geq |\alpha\bar{\beta} - \beta\bar{\gamma}|$, and
- (3) if $\alpha = \gamma$, then $|\beta| \leq 2|\alpha|$.

In addition, for multistep methods, we can verify a method is of order p if

$$\sum_{m=0}^s a_m \omega^m - \left(\sum_{m=0}^s b_m \omega^m \right) \ln \omega = O(|\omega - 1|^{p+1})$$

as $\omega \rightarrow 1$.

5.1 2-step 2-order Backward Differentiation Formulae (BDF)

A 2-step BDF is given by

$$y_{n+2} - \frac{4}{3}y_{n+1} + \frac{1}{3}y_n = \frac{2}{3}hf(t_{n+2}, y_{n+2}),$$

where $n = 0, 1, \dots, N$ for some N . All BDFs are constructed such that they have an order equal to the number of steps. In fact, by a theorem, we know that any BDF of order between 1 and 6, inclusive, converges. To determine if the method is A-stable, we derive

$$\eta(\omega, it) = \left(1 - \frac{2}{3}it\right)\omega^2 - \frac{4}{3}\omega + \frac{1}{3}.$$

Clearly, $\eta(\omega, it)$ is of the form $\alpha\omega^2 + \beta\omega + \gamma$ where $\alpha = 1 - \frac{2}{3}it$, $\beta = -\frac{4}{3}$, and $\gamma = \frac{1}{3}$. We now claim that the roots satisfy $|\omega_i(it)| < 1$.

Proof.

$$\begin{aligned}
|\alpha| \geq |\gamma| &\iff \left| 1 - \frac{2}{3}it \right| \geq \left| \frac{1}{3} \right| \\
&\iff \left| 1 - \frac{2}{3}it \right|^2 \geq \left| \frac{1}{3} \right|^2 \\
&\iff 1 + \frac{4}{9}t^2 \geq \frac{1}{9} \\
&\iff \frac{4}{9}t^2 + \frac{8}{9} \geq 0 \\
&\iff t^2 + 2 \geq 0 \\
||\alpha|^2 - |\gamma|^2| \geq |\alpha\bar{\beta} - \beta\bar{\gamma}| &\iff \left| \left| 1 - \frac{2}{3}it \right|^2 - \left| \frac{1}{3} \right|^2 \right| \geq \left| \left(1 - \frac{2}{3}it \right) \left(-\frac{4}{3} \right) - \left(-\frac{4}{3} \right) \left(\frac{1}{3} \right) \right| \\
&\iff \left| 1 + \frac{4}{9}t^2 - \frac{1}{9} \right| \geq \left| -\frac{4}{3} + \frac{8}{9}it + \frac{4}{9} \right| \\
&\iff \left| \frac{4}{9}t^2 + \frac{8}{9} \right|^2 \geq \left| \frac{8}{9}it - \frac{8}{9} \right|^2 \\
&\iff \left| \frac{1}{2}t^2 + 1 \right|^2 \geq |it - 1|^2 \\
&\iff \frac{1}{4}t^4 + t^2 + 1 \geq t^2 + 1 \\
&\iff \frac{1}{4}t^4 \geq 0 \\
&\iff t^4 \geq 0
\end{aligned}$$

The third condition is not applicable since $\alpha \neq \gamma$. □

Then since $b_2 > 0$ and the roots of $\eta(\omega, it)$ satisfy $|\omega_i(it)| < 1$, the 2-step 2-order BDF is A-Stable.

5.2 2-step Adams-Bashforth Method

A 2-step A-B method is given by

$$y_{n+2} - y_{n+1} = h \left(\frac{3}{2}f(t_{n+1}, y_{n+1}) - \frac{1}{2}f(t_n, y_n) \right),$$

where $n = 0, 1, \dots, N$ for some N . We now claim that this method has order 2.

Proof. Let $\omega = x + 1$. Then

$$\begin{aligned}
&\sum_{m=0}^2 a_m(x+1)^m - \left(\sum_{m=0}^2 b_m(x+1)^m \right) \ln(x+1) \\
&= (x+1)^2 - (x+1) - \left(\frac{3}{2}(x+1) - \frac{1}{2} \right) \left(x - \frac{1}{2}x^2 + O(x^3) \right) \\
&= x^2 + 2x + 1 - x - 1 - \left(\frac{3}{2}x + 1 \right) \left(x - \frac{1}{2}x^2 + O(x^3) \right) \\
&= x^2 + x - \left(\frac{3}{2}x^2 - \frac{3}{4}x^3 + O(x^4) + x - \frac{1}{2}x^2 + O(x^3) \right) \\
&= x^2 + x - (x^2 + x + O(x^3)) \\
&= O(x^3) \\
&= O(x^{2+1})
\end{aligned}$$

Thus the order of the 2-step A-B method is 2. □

Since $b_2 = 0$, we automatically know that the method is not A-stable, but we can still determine a linear stability region. For this method we have

$$\eta(\omega, z) = \omega^2 - \left(-1 - \frac{3}{2}z \right) \omega + \frac{1}{2}z.$$

Solving for ω , we get

$$\omega = \frac{1}{2} + \frac{3}{4}z \pm \sqrt{\frac{1 + z + \frac{9}{4}z^2}{4}}.$$

Then the linear stability domain (LSD) is the set of all $z \in \mathbb{C}$ such that $|\omega| \leq 1$. Figure 1 below illustrates the LSD in the complex plane.

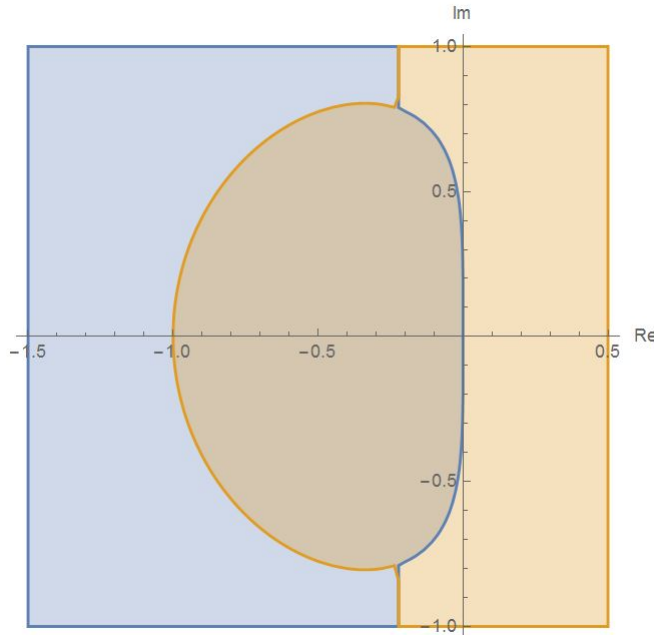


Figure 1: The LSD for a 2-step A-B method, as the intersection of both shaded regions.

6 Implementation of Numerical Methods on a Plane

The IVP associated with a plane has initial conditions. For the purposes of this project, suppose that a particle is moving freely along a plane with initial position (x_0, y_0, z_0) and initial velocity (x'_0, y'_0, z'_0) , the latter of which is tangential to the plane. Furthermore, we cannot simply pick any initial position or velocity and satisfy the conditions. Assuming the plane spans all of \mathbb{R}^3 , if we choose any x_0 and y_0 for an initial position, we can calculate a value for z_0 for which the initial position is on the plane such that

$$z_0 = \frac{-ax_0 - by_0 - d}{c}.$$

To ensure that we have a initial velocity tangent to the plane, we determine a spanning set of \mathbb{R}^3 that uniquely defines the plane. To do this, we need the normal vector \vec{n} of the plane. In this case, \vec{n} is the gradient $[a \ b \ c]^T$. We seek to compute two vectors \vec{v}_1, \vec{v}_2 perpendicular to the normal vector, An easy choice for \vec{v}_1 would be to choose $[b \ -a \ 0]$. For \vec{v}_2 we can choose $\vec{n} \times \vec{v}_1 = [-ac \ -bc \ a^2 + b^2]^T$. Then for any $\alpha, \beta \in \mathbb{R}$, any vector \vec{v} for the plane defined by $ax + by + cz + d = 0$ can be written as

$$\vec{v} = \alpha \vec{v}_1 + \beta \vec{v}_2 = \alpha \begin{bmatrix} -b \\ a \\ 0 \end{bmatrix} + \beta \begin{bmatrix} -ac \\ -bc \\ a^2 + b^2 \end{bmatrix} = \begin{bmatrix} -\alpha b - \beta ac \\ \alpha a - \beta bc \\ \beta(a^2 + b^2) \end{bmatrix}.$$

In other words, we can pick any real values for α and β that determine an initial velocity (x'_0, y'_0, z'_0) that is tangent to the plane.

6.1 Example

Suppose we have the following parameters and initial conditions:

$\mu = 0.1$	$g = 9.8\text{m/s}^2$	Simulation Time = 10s	
$a = 5$	$b = 2$	$c = 3$	$d = 4$
$x_0 = 5\text{m}$	$y_0 = -2\text{m}$	$\alpha = 100$	$\beta = -1$

Then $z_0 \approx -8.33\text{m}$ and $(x'_0, y'_0, z'_0) = (185\text{m/s}, -506\text{m/s}, 29\text{m/s})$. To implement these methods on the system of 6 differential equations described in Equation (7), MATLAB was used. For each method, an "exact" solution (computed by a pair of high-order Runge-Kutta methods) was used. Each subsequent step size, starting from 0.4 and ending at 0.0125, is half of the previous step size. The errors, calculated as the infinity norm of the difference of the method and the "exact" solution, were computed for the x , y , and z components of the position. Table 1 below gives both the errors e_i at step size h and the ratios $\frac{e_i}{e_{i+1}}$.

Method	e_i	h	Error		
			x	y	z
BDF	e_1	0.4	1.60×10^{-3}	1.02×10^{-3}	3.34×10^{-3}
	e_2	0.2	5.81×10^{-4}	3.10×10^{-4}	1.18×10^{-3}
	e_3	0.1	1.31×10^{-4}	6.88×10^{-5}	2.63×10^{-4}
	e_4	0.05	2.68×10^{-5}	1.73×10^{-5}	5.61×10^{-5}
	e_5	0.025	7.06×10^{-6}	3.86×10^{-6}	1.43×10^{-5}
	e_6	0.0125	1.75×10^{-6}	8.89×10^{-7}	3.56×10^{-6}
A-B	e_1	0.4	2.16×10^{-3}	9.57×10^{-4}	4.24×10^{-3}
	e_2	0.2	5.52×10^{-4}	2.44×10^{-4}	1.08×10^{-3}
	e_3	0.1	1.39×10^{-4}	6.18×10^{-5}	2.73×10^{-4}
	e_4	0.05	3.50×10^{-5}	1.55×10^{-5}	6.87×10^{-5}
	e_5	0.025	8.77×10^{-6}	3.89×10^{-6}	1.72×10^{-5}
	e_6	0.0125	2.20×10^{-6}	9.75×10^{-7}	4.31×10^{-6}

Method	e_i/e_{i+1}	Error Ratio		
		x	y	z
BDF	e_1/e_2	2.750	3.293	2.843
	e_2/e_3	4.423	4.503	4.464
	e_3/e_4	4.905	3.983	4.699
	e_4/e_5	3.793	4.477	3.908
	e_5/e_6	4.039	4.339	4.034
A-B	e_1/e_2	3.920	3.913	3.919
	e_2/e_3	3.960	3.957	3.960
	e_3/e_4	3.980	3.979	3.980
	e_4/e_5	3.990	3.989	3.990
	e_5/e_6	3.995	3.995	3.995

Table 1: Errors and error ratios for each method at various step sizes.

For each method, the order is 2. Since we reduce each successive step size by a factor of 2, we want to observe from the data above in Table 1 that $\lim_{i \rightarrow \infty} \frac{e_i}{e_{i+1}} = 2^2 = 4$ in an effort to numerically show that the methods converge. For the 2-step A-B method, this is clear. If we did not know that the method converges we can now observe numerically that the error ratios converge to $2^2 = 4$. For the 2-step BDF method, the error ratios clearly appear to revolve around 4, slowly getting closer to 4. However, they do not converge as nicely as the error ratios for the A-B method. This may potentially be due to technical limitations of MATLAB or the fact that a pair of high-order R-K methods was used in place of an exact solution. Nonetheless, the ratios appear to get closer to 4, although somewhat erratically. Thus, given the initial parameters specified earlier applied to a plane, the 2-step BDF and 2-step A-B methods appear to converge.

7 Conclusion

Basic knowledge of physics states that the sum of acting forces on a particle is equal to the product of mass and acceleration of the particle. Considering force due to gravity, force due to friction, and the normal force, a system of six differential equations can be derived for a surface. Using the implicit surface equations for a torus and a plane, the systems of differential equations were derived.

To visualize the motion of a particle across a plane, two numerical methods were implemented: a 2-step BDF method and a 2-step Adams-Bashforth method. These methods are implicit and explicit, respectively, and both methods are of order 2. From theory, we know that both methods must converge. Therefore, as a confirmation that either method is implemented correctly on a system of differential equations, we can look at the ratios of the errors for different size sizes. Since each consecutive step size was reduced by a factor of 2, the ratios should be expected to converge to 4.

When testing method accuracy numerically, initial conditions and parameters must not be arbitrary. Thus, an example of a plane with specified parameters was used to observe the convergence of the both methods. If different parameters and initial conditions were chosen, then the resulting methods would be expected to converge as well, although the rate at which the methods converge may vary.

The basic framework for applying the methods to a torus was also included in this report, so a similar approach to the example of a plane can be taken.

8 References

Alwanou, G., Baramidze, G., Housman, J., Kavouklis, C., Sulakova, J., Zager, M. (n.d.).
Problem 6: Frictional Sliding on Surface of Variable Curvature.