

MATH 728B, WATER MOLECULE, HOMEWORK III

Review of Notation. Consider a system of N particles with masses M_a and positions R_a , $a = 1, \dots, N$, relative to the inertial frame $(\hat{\mathbf{e}}_1, \hat{\mathbf{e}}_2, \hat{\mathbf{e}}_3)$. The position of the *center of mass* is given by $\bar{R} = M_{tot}^{-1} \sum_{a=1}^N M_a R_a$, where $M_{tot} = \sum_{a=1}^N M_a$ is the total mass. The *total linear momentum* $\Pi_{tot} = \sum_{a=1}^N M_a \dot{R}_a$ can be written as $M_{tot} \dot{\bar{R}}$. Newton's Laws dictate that this momentum must evolve according to the equation $\dot{\Pi}_{tot} = F_{tot}$, where F_{tot} is the vector sum of all the (external and internal) forces acting on the system. If $F_{tot} = 0$ then $\Pi_{tot} = M_{tot} \dot{\bar{R}}$ is independent of time, and hence $\bar{R}(t) = \bar{R}(0) + t\Pi_{tot}/M_{tot}$. The *total angular momentum* $\Lambda_{tot} = \sum_{a=1}^N R_a \times M_a \dot{R}_a$ can be written as $\Lambda_{tot} = \bar{R} \times \Pi_{tot} + \sum_{a=1}^N (R_a - \bar{R}) \times M_a (\dot{R}_a - \dot{\bar{R}})$. Another consequence of Newton's Laws is that $\dot{\Lambda}_{tot} = \sum_{a=1}^N R_a \times F_a$, where F_a is the total force (external and internal) exerted on particle a . The quantity $\sum_{a=1}^N R_a \times F_a$ is called the *total torque*. If this is also zero then Λ_{tot} is independent of time. Since $\bar{R} \times \Pi_{tot}$ is independent of time it follows that $\Lambda = \sum_{a=1}^N (R_a - \bar{R}) \times M_a (\dot{R}_a - \dot{\bar{R}})$ is independent of time. This quantity is called the *total angular momentum relative to the center of mass*. The *total kinetic energy* is defined as $T_{tot} = \frac{1}{2} \sum_{a=1}^N M_a \|\dot{R}_a\|^2$, and can be written as $T_{tot} = \frac{1}{2} M_{tot} \|\dot{\bar{R}}\|^2 + \frac{1}{2} \sum_{a=1}^N M_a \|\dot{R}_a - \dot{\bar{R}}\|^2$. Define the *moment of inertia tensor* \mathbb{I} to be $\mathbb{I} = \sum_{a=1}^N M_a [\|R_a - \bar{R}\|^2 \mathbf{1} - (R_a - \bar{R})(R_a - \bar{R})^T]$. Define the *spatial angular velocity* Ω such that $\Lambda = \mathbb{I}\Omega$. Then $\frac{1}{2} \sum_{a=1}^N M_a \|\dot{R}_a - \dot{\bar{R}}\|^2 = \frac{1}{2} \Omega \cdot \Lambda + \frac{1}{2} \sum_{a=1}^N M_a \|\dot{R}_a - \dot{\bar{R}} - \Omega \times (R_a - \bar{R})\|^2 = T_{rot} + T_{int}$. Even though Λ is independent of time and $\Lambda = \mathbb{I}\Omega$, we generally have that both \mathbb{I} and Ω depend on time. However we can simplify this time dependence as much as possible by defining a *body pose* whose origin is the center of mass \bar{R} and whose coordinate axes are given by $A = (\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3)$, where these axes are attached to the body in some manner. There are body versions of many spatial quantities: $R_a - \bar{R} = Ar_a$, $\Lambda = A\lambda$, $\Omega = A\omega$, and $\mathbb{I}A = \mathbb{A}i$. If there is no internal vibration, i.e. for a rigid body, i is independent of time. In general i fluctuates slightly as a result of vibrations for semirigid bodies, but may change drastically for systems which consist of coupled semirigid subunits (like proteins). But at least it is independent of the overall rotational motion of the body frame (unlike \mathbb{I}). The *angular velocity of the body frame* $\tilde{\omega}$ is defined by the rule $\dot{A} = A[\tilde{\omega} \times]$. The *apparent angular momentum in the body frame* \mathbf{j} is defined to be $\mathbf{j} = \sum_{a=1}^N r_a \times M_a \dot{r}_a$. An extremely important relation is that $\lambda = i\tilde{\omega} + \mathbf{j}$. These quantities allow us to write $T_{rot} = \frac{1}{2} \omega \cdot \lambda = \frac{1}{2} \tilde{\omega} \cdot i\tilde{\omega} + \frac{1}{2} (i^{-1}\mathbf{j}) \cdot \mathbf{j} + \tilde{\omega} \cdot \mathbf{j}$ and $T_{int} = \frac{1}{2} \sum_{a=1}^N M_a \|\dot{r}_a\|^2 - \frac{1}{2} (i^{-1}\mathbf{j}) \cdot \mathbf{j}$. The matrix A containing the body frame can be coordinatized by a vector $\mathbf{v} \in \mathbb{R}^3$, whose direction gives the axis of rotation and whose length $\theta = \|\mathbf{v}\|$ is the angle of rotation in the positive sense (via the right hand rule). We have $A(\mathbf{v}) = \mathbf{1} \cos(\theta) + \mathbf{v}\mathbf{v}^T \frac{1-\cos(\theta)}{\theta^2} + [\mathbf{v} \times] \frac{\sin(\theta)}{\theta}$. From this we derive the formula $\tilde{\omega} = S(\mathbf{v})\dot{\mathbf{v}}$, where $S(\mathbf{v}) = \mathbf{1} \frac{\sin(\theta)}{\theta} + \mathbf{v}\mathbf{v}^T \frac{1}{\theta^2} (1 - \frac{\sin(\theta)}{\theta}) + [\mathbf{v} \times] \frac{1-\cos(\theta)}{\theta^2}$, and $S(\mathbf{v})^{-1} = \mathbf{1} \frac{\theta \sin(\theta)}{2(1-\cos(\theta))} + \mathbf{v}\mathbf{v}^T \frac{1}{\theta^2} (1 - \frac{\theta \sin(\theta)}{2(1-\cos(\theta))}) + [\mathbf{v} \times] \frac{1}{2}$. For large biomolecular systems we usually assume $\dot{\bar{R}} = 0$ and $\Lambda = 0$, so that $T_{tot} = T_{int}$.

The Kinetic Energy. The vectors r_a , and the moment of inertia tensor

$$\mathbf{i} = \sum_{a=1}^N M_a [\|r_a\|^2 \mathbf{1} - r_a r_a^T],$$

can be expressed as functions of the internal coordinates $\mathbf{q} = \langle q^1, \dots, q^{3N-6} \rangle$. The time derivatives $\dot{r}_a = \sum_{j=1}^{3N-6} \frac{\partial r_a}{\partial q^j} \dot{q}^j$ are functions of \mathbf{q} and their time derivatives $\dot{\mathbf{q}} = \langle \dot{q}^1, \dots, \dot{q}^{3N-6} \rangle$ since $\frac{\partial r_a}{\partial q^j}$ is a function of \mathbf{q} for each j . Thus the total kinetic energy can be expressed in terms of the variables $\bar{R}, \dot{\bar{R}}, \mathbf{v}, \dot{\mathbf{v}}, \mathbf{q}$ and $\dot{\mathbf{q}}$. We have

$$T_{tot} = \frac{1}{2} M_{tot} \|\dot{\bar{R}}\|^2 + \frac{1}{2} [S(\mathbf{v})\dot{\mathbf{v}}] \cdot \mathbf{i} S(\mathbf{v})\dot{\mathbf{v}} + [S(\mathbf{v})\dot{\mathbf{v}}] \cdot \mathbf{j} + \frac{1}{2} \sum_{a=1}^N M_a \|\dot{r}_a\|^2.$$

The apparent angular momentum can be expressed in terms of $\dot{\mathbf{q}}$: $\mathbf{j} = \sum_{a=1}^N r_a \times M_a \dot{r}_a = \sum_{j=1}^{3N-6} (\sum_{a=1}^N r_a \times M_a \frac{\partial r_a}{\partial q^j}) \dot{q}^j$. The vectors $\mathbf{A}_j(\mathbf{q}) = \mathbf{i}^{-1} (\sum_{a=1}^N r_a \times M_a \frac{\partial r_a}{\partial q^j})$, $j = 1, \dots, 3N-6$, comprise what is called the *mechanical connection 1-form*. It is convenient to define a $3 \times (3N-6)$ matrix $\mathbf{A}(\mathbf{q})$ whose j th column vector is $\mathbf{A}_j(\mathbf{q})$. Thus $\mathbf{j} = \sum_{j=1}^{3N-6} \mathbf{i} \mathbf{A}_j(\mathbf{q}) \dot{q}^j = \mathbf{i} \mathbf{A}(\mathbf{q}) \dot{\mathbf{q}}$.

The internal kinetic energy $T_{int} = \frac{1}{2} \sum_{a=1}^N M_a \|\dot{r}_a\|^2 - \frac{1}{2} (\mathbf{i}^{-1} \mathbf{j}) \cdot \mathbf{j}$ is a function only of \mathbf{q} and $\dot{\mathbf{q}}$. In fact there is a $(3N-6) \times (3N-6)$ symmetric matrix $\tau(\mathbf{q})$ such that $T_{int} = \frac{1}{2} \dot{\mathbf{q}}^T \tau(\mathbf{q}) \dot{\mathbf{q}}$. Explicitly we have

$$\tau(\mathbf{q})_{jl} = \sum_{a=1}^N M_a \frac{\partial r_a}{\partial q^j} \cdot \frac{\partial r_a}{\partial q^l} - \mathbf{A}_j(\mathbf{q}) \cdot \mathbf{i} \mathbf{A}_l(\mathbf{q}).$$

The symmetric matrix $\tau(\mathbf{q})_{jl}$ is called the *Riemannian metric on shape space*.

The total kinetic energy now becomes

$$T_{tot} = \frac{1}{2} M_{tot} \|\dot{\bar{R}}\|^2 + \frac{1}{2} [S(\mathbf{v})\dot{\mathbf{v}}] \cdot \mathbf{i} S(\mathbf{v})\dot{\mathbf{v}} + [S(\mathbf{v})\dot{\mathbf{v}}] \cdot \mathbf{i} \mathbf{A}(\mathbf{q}) \dot{\mathbf{q}} + \dot{\mathbf{q}}^T [\tau(\mathbf{q}) + \mathbf{A}(\mathbf{q})^T \mathbf{i} \mathbf{A}(\mathbf{q})] \dot{\mathbf{q}}.$$

The momentum conjugate to q^j is $p_j = \frac{\partial T_{tot}}{\partial \dot{q}^j} = \lambda \cdot \mathbf{A}_j(\mathbf{q}) + [\tau(\mathbf{q}) \dot{\mathbf{q}}]_j$, where $\lambda = \mathbf{i} \dot{\omega} + \mathbf{j} = \mathbf{i} [S(\mathbf{v})\dot{\mathbf{v}} + \mathbf{A}(\mathbf{q}) \dot{\mathbf{q}}]$. Let $\mathbf{p} = \langle p_1, \dots, p_{3N-6} \rangle$. Therefore $\mathbf{p} = \mathbf{A}(\mathbf{q})^T \lambda + \tau(\mathbf{q}) \dot{\mathbf{q}}$. The momentum conjugate to the i th component of \mathbf{v} is $\pi_i = \frac{\partial T_{tot}}{\partial \dot{v}_i} = [S(\mathbf{v})]_i \cdot \lambda$. Thus $\boldsymbol{\pi} = \langle \pi_1, \pi_2, \pi_3 \rangle = S(\mathbf{v})^T \lambda$. We can use these quantities to eliminate $\dot{\mathbf{q}}$ and $\dot{\mathbf{v}}$:

$$\begin{aligned} \dot{\mathbf{q}} &= \tau(\mathbf{q})^{-1} [\mathbf{p} - \mathbf{A}(\mathbf{q})^T S(\mathbf{v})^{-T} \boldsymbol{\pi}], \\ \dot{\mathbf{v}} &= S(\mathbf{v})^{-1} \{ [\mathbf{i}^{-1} + \mathbf{A}(\mathbf{q}) \tau(\mathbf{q})^{-1} \mathbf{A}(\mathbf{q})^T] S(\mathbf{v})^{-T} \boldsymbol{\pi} - \mathbf{A}(\mathbf{q}) \tau(\mathbf{q})^{-1} \mathbf{p} \}. \end{aligned}$$

The total kinetic energy can be expressed in terms of these variables.

$$\begin{aligned} T_{tot} &= \frac{1}{2M_{tot}} \|\boldsymbol{\Pi}_{tot}\|^2 + \frac{1}{2} [\mathbf{i}(\mathbf{q})^{-1} S(\mathbf{v})^{-T} \boldsymbol{\pi}] \cdot S(\mathbf{v})^{-T} \boldsymbol{\pi} \\ &\quad + \frac{1}{2} [\mathbf{p} - \mathbf{A}(\mathbf{q})^T S(\mathbf{v})^{-T} \boldsymbol{\pi}] \cdot \tau(\mathbf{q})^{-1} [\mathbf{p} - \mathbf{A}(\mathbf{q})^T S(\mathbf{v})^{-T} \boldsymbol{\pi}]. \end{aligned}$$

This expression leads directly to Hamiltonian equations of motion for a rotating and vibrating system, where the Hamiltonian is $h = T_{tot} + V(\mathbf{q})$. An advantage of this form of the equations of motion is that the vector \mathbf{v} is found along with the other quantities. One disadvantage is that the effect of conservation of angular momentum is hidden. This is reflected in the fact that the Hamiltonian depends on \mathbf{v} only through the quantity $\lambda = S(\mathbf{v})^{-T}\boldsymbol{\pi}$. It is possible to write equations of motion only involving the variables $\lambda, \mathbf{q}, \mathbf{p}$. The Hamiltonian is

$$\begin{aligned}\tilde{h}(\lambda, \mathbf{q}, \mathbf{p}) &= \frac{1}{2M_{tot}}\|\Pi_{tot}\|^2 + \frac{1}{2}[\mathbf{i}(\mathbf{q})^{-1}\lambda] \cdot \lambda \\ &\quad + \frac{1}{2}[\mathbf{p} - \mathbf{A}(\mathbf{q})^T\lambda] \cdot \tau(\mathbf{q})^{-1}[\mathbf{p} - \mathbf{A}(\mathbf{q})^T\lambda] + V(\mathbf{q}).\end{aligned}$$

It follows that Π_{tot} and Λ are conserved. The first term is the energy of translational motion, the second is the energy of rotational motion, and the last is the residual kinetic energy. The Hamiltonian (Poisson) equation of motion for λ is the familiar $\dot{\lambda} = \lambda \times \tilde{\omega}$:

$$\dot{\lambda} = \lambda \times \{[\mathbf{i}(\mathbf{q})^{-1} + \mathbf{A}(\mathbf{q})\tau(\mathbf{q})^{-1}\mathbf{A}(\mathbf{q})^T]\lambda - \mathbf{A}(\mathbf{q})\tau(\mathbf{q})^{-1}\mathbf{p}\}.$$

The quantity $\|\lambda\|^2$ is conserved, so one can coordinatize this sphere (say using stereographic coordinates u and v) and eliminate the radial degree of freedom. Numerical integration of the resulting minimal (symplectic!) system in the variables $u, v, \mathbf{q}, \mathbf{p}$ would automatically conserve numerically both linear and angular momentum, whereas using the above (Poisson but not symplectic) equation for λ will not necessarily conserve $\|\lambda\|^2$ numerically. But it is not always worthwhile to go to such lengths to accomplish such exact momentum conservation. The Hamiltonian equation for \mathbf{q} is

$$\dot{\mathbf{q}} = \tau(\mathbf{q})^{-1}[\mathbf{p} - \mathbf{A}(\mathbf{q})^T\lambda].$$

The Hamiltonian equation for \mathbf{p} is ($l = 1, \dots, 3N - 6$)

$$\begin{aligned}\dot{p}_l &= -\frac{1}{2}\lambda \cdot \frac{\partial[\mathbf{i}(\mathbf{q})^{-1}]}{\partial q^l}\lambda - \frac{1}{2}[\mathbf{p} - \mathbf{A}(\mathbf{q})^T\lambda] \cdot \frac{\partial[\tau(\mathbf{q})^{-1}]}{\partial q^l}[\mathbf{p} - \mathbf{A}(\mathbf{q})^T\lambda] \\ &\quad + \frac{\partial[\mathbf{A}(\mathbf{q})^T]}{\partial q^l}\lambda \cdot \tau(\mathbf{q})^{-1}[\mathbf{p} - \mathbf{A}(\mathbf{q})^T\lambda] - \frac{\partial V(\mathbf{q})}{\partial q^l}\end{aligned}$$

The first term on the right is usually associated with *centripetal forces*. The third term on the right is associated with *Coriolis forces*. These two terms vanish when $\lambda = 0$.

If these equations are solved for $\lambda, \mathbf{q}, \mathbf{p}$ as functions of t then \mathbf{v} can be found by solving

$$\dot{\mathbf{v}} = S(\mathbf{v})^{-1}\{[\mathbf{i}(\mathbf{q})^{-1} + \mathbf{A}(\mathbf{q})\tau(\mathbf{q})^{-1}\mathbf{A}(\mathbf{q})^T]\lambda - \mathbf{A}(\mathbf{q})\tau(\mathbf{q})^{-1}\mathbf{p}\}.$$

Then the positions of the particles can be found from the equations $R_a = \bar{R} + A(\mathbf{v})r_a(\mathbf{q})$.

Another question concerns initial conditions. Suppose we want to choose initial conditions so that the system has linear momentum Π_{tot} and angular momentum Λ_{tot} . We may choose $\bar{R}(0), \mathbf{v}(0), \mathbf{q}(0), \mathbf{p}(0)$ arbitrarily. These choices correspond to choosing the initial positions to be $R_a(0) = \bar{R}(0) + A(\mathbf{v}(0))r_a(\mathbf{q}(0))$. Then we define $\lambda(0) = A(\mathbf{v}(0))^T\Lambda_{tot}$.

The initial total energy is $\tilde{h}(\lambda(0), \mathbf{q}(0), \mathbf{p}(0))$, and it needs to be in a physically reasonable range. To determine the corresponding choice of initial velocities use the formulae

$$\begin{aligned}\dot{\mathbf{q}}(0) &= \tau(\mathbf{q}(0))^{-1}[\mathbf{p}(0) - \mathbf{A}(\mathbf{q}(0))^T \lambda(0)], \\ \tilde{\omega}(0) &= \mathbf{i}(\mathbf{q}(0))^{-1} \lambda(0) - \mathbf{A}(\mathbf{q}(0)) \dot{\mathbf{q}}(0),\end{aligned}$$

$$\dot{R}_a(0) = \frac{\Pi_{tot}}{M_{tot}} + A(\mathbf{v}(0)) \left\{ \tilde{\omega}(0) \times r_a(\mathbf{q}(0)) + \sum_{j=1}^{3N-6} \frac{\partial r_a}{\partial q^j}(\mathbf{q}(0)) \dot{q}^j(0) \right\}.$$

Specifics for a Water molecule. For a water molecule we have hydrogen atoms at R_1, R_2 and an oxygen atom at R_3 , and internal coordinates l_1, l_2, α . The body frame has its z axis pointing from the oxygen to the first hydrogen, and its x axis perpendicular to this in the half plane containing the second hydrogen. We compute that

$$r_1 = \begin{pmatrix} -\frac{M_2 l_2 \sin \alpha}{M_{tot}} \\ 0 \\ \frac{(M_2 + M_3) l_1 - M_2 l_2 \cos \alpha}{M_{tot}} \end{pmatrix}, r_2 = \begin{pmatrix} \frac{(M_1 + M_3) l_2 \sin \alpha}{M_{tot}} \\ 0 \\ -\frac{M_1 l_1 + (M_1 + M_3) l_2 \cos \alpha}{M_{tot}} \end{pmatrix}, r_3 = \begin{pmatrix} -\frac{M_2 l_2 \sin \alpha}{M_{tot}} \\ 0 \\ -\frac{M_1 l_1 + M_2 l_2 \cos \alpha}{M_{tot}} \end{pmatrix}$$

The moment of inertia tensor is $\mathbf{i} = \frac{1}{M_{tot}} \begin{pmatrix} a & 0 & b \\ 0 & c & 0 \\ b & 0 & d \end{pmatrix}$ where

$$\begin{aligned}a &= M_2(M_1 + M_3)l_2^2 \cos^2 \alpha - 2M_1M_2l_1l_2 \cos \alpha + M_1(M_2 + M_3)l_1^2, \\ b &= -M_2l_2 \sin \alpha[(M_1 + M_3)l_2 \cos \alpha - M_1l_1], \\ c &= M_1(M_2 + M_3)l_1^2 - 2M_1M_2l_1l_2 \cos \alpha + M_2(M_1 + M_3)l_2^2, \\ d &= (M_1 + M_3)M_2l_2^2 \sin^2 \alpha.\end{aligned}$$

Its inverse is

$$\mathbf{i}^{-1} = \begin{pmatrix} \frac{M_1 + M_3}{M_1 M_3 l_1^2} & 0 & -\frac{[(M_1 + M_3)l_2 \cos \alpha - M_1 l_1]}{M_1 M_3 l_1^2 l_2 \sin \alpha} \\ 0 & \frac{M_{tot}}{c} & 0 \\ -\frac{[(M_1 + M_3)l_2 \cos \alpha - M_1 l_1]}{M_1 M_3 l_1^2 l_2 \sin \alpha} & 0 & \frac{c}{M_1 M_1 M_3 l_1^2 l_2^2 \sin^2 \alpha} - \frac{M_1 + M_3}{M_1 M_3 l_1^2} \end{pmatrix}.$$

Also the apparent angular momentum $\mathbf{j} = \sum_{a=1}^3 r_a \times M_a \dot{r}_a$ in the body frame is

$$\mathbf{j} = \begin{pmatrix} 0 \\ -\frac{M_2}{M_{tot}} [M_1 \sin \alpha (l_1 \dot{l}_2 - l_2 \dot{l}_1) + (M_1 l_1 l_2 \cos \alpha - (M_1 + M_3) l_2^2) \dot{\alpha}] \\ 0 \end{pmatrix}.$$

In class we derived a complicated expression for τ , but as one can see we only need τ^{-1} :

$$\tau(\mathbf{q})^{-1} = \begin{pmatrix} \frac{1}{M_3} + \frac{1}{M_1} & \frac{\cos \alpha}{M_3} & -\frac{\sin \alpha}{M_3 l_2} \\ \frac{\cos \alpha}{M_3} & \frac{1}{M_3} + \frac{1}{M_2} & -\frac{\sin \alpha}{M_3 l_1} \\ -\frac{\sin \alpha}{M_3 l_2} & -\frac{\sin \alpha}{M_3 l_1} & \frac{c}{M_1 M_2 M_3 l_1^2 l_2^2} \end{pmatrix}.$$

For the water molecule a simple potential energy is

$$V(l_1, l_2, \alpha) = k_1(l_1 - l_1^0)^2 + k_2(l_2 - l_2^0)^2 + k_\alpha(\alpha - \alpha_0)^2.$$

For the parameter values see Water Molecule, Homework I.

Final Computation Project, Due Friday, Dec. 14. Use Maple to find the matrix $\mathbf{A}(\mathbf{q})$ for the water molecule. Use Maple to explicitly derive the 9 differential equations of motion for the variables $\lambda, \mathbf{q}, \mathbf{p}$. Also explicitly find the 3 differential equations for \mathbf{v} given $\lambda, \mathbf{q}, \mathbf{p}$ as functions of t (see the discussion above).

Assume $\Pi_{tot} = 0$, and $\bar{R} = 0$ for all time. Write a Matlab function that computes $\tilde{h}(\lambda, \mathbf{q}, \mathbf{p})$. Assume $\mathbf{v}(0) = \mathbf{0}$, so that $\lambda(0) = \Lambda_{tot}$. By trial and error find a choice of $\lambda(0), \mathbf{q}(0), \mathbf{p}(0)$ so that $E = \tilde{h}(\lambda(0), \mathbf{q}(0), \mathbf{p}(0))$ is between $1 \cdot 10^{-3}$ and $2 \cdot 10^{-3} \cdot \text{amu} \cdot \text{angstrom}^2 \cdot \text{fs}^{-2}$. Compute the corresponding initial positions and velocities of all the atoms.

Write a Matlab function which accepts $\mathbf{v}, \lambda, \mathbf{q}, \mathbf{p}$ as arguments and computes the right-hand-sides of the 12 differential equations for these quantities that you found above using Maple. Solve your system of ordinary differential equations on Matlab using ode45 with the choice of initial conditions you found by trial and error. Recover from the numerical solution of this system the actual positions of the atoms as functions of time.

Use NAMD to solve for the motion of a water molecule with the initial positions and velocities you found above. Compare the final positions and velocities to those that you computed using Matlab (after solving the system). For how many fs do they basically agree? Use VMD to watch the movie of your rotating and vibrating water molecule.

Turn in copies of your Matlab functions, and a written account of your results.