Prof. P. Koumoutsakos, G. Tauriello
ETH Zentrum, CLT F 12, C 11
CH-8092 Zürich

Solution 4

Issued: 8.4.2013

Question 1: Conservation of Energy

There are two way to look at this problem: A more general one involves the proof that the total energy functional is a first integral for Hamiltonian systems. We are considering Hamiltonian systems of the form

$$\dot{\mathbf{p}} = -H_q(\mathbf{p}, \mathbf{q}), \qquad \dot{\mathbf{q}} = H_p(\mathbf{p}, \mathbf{q}) \tag{1}$$

where $H_q = \nabla_q H = (\partial H / \partial \mathbf{q})^T$ and $H_p = \nabla_p H = (\partial H / \partial \mathbf{p})^T$ are the column vectors of the partial derivatives. We want to show that the Hamiltonian function $H(\mathbf{p}, \mathbf{q})$ representing the total energy is a first integral of the above system.

Let $H'(\mathbf{p}, \mathbf{q}) = (\partial H / \partial \mathbf{p}, \partial H / \partial \mathbf{q})$. It follows that:

$$\frac{dH}{dt} = \frac{\partial H}{\partial \mathbf{p}} \left(\frac{\partial \mathbf{p}}{\partial t} \right)^T + \frac{\partial H}{\partial \mathbf{q}} \left(\frac{\partial \mathbf{q}}{\partial t} \right)^T = -\frac{\partial H}{\partial \mathbf{p}} \left(\frac{\partial H}{\partial \mathbf{q}} \right)^T + \frac{\partial H}{\partial \mathbf{q}} \left(\frac{\partial H}{\partial \mathbf{p}} \right)^T = 0$$

The second way is system specific for the given Hamiltonian of the N-body problem and using the chain rule for differentiation: Note that our system is:

$$\begin{cases} m_i \dot{\mathbf{v}}_i = \displaystyle\sum_{j=1; j \neq i}^{N} \mathbf{F}_{ij}(t), & (2) \\ \dot{\mathbf{x}}_i = \mathbf{v}_i(t). & (3) \end{cases}$$

The Hamiltonian for this system, representing the total energy, is given by

$$H(\mathbf{p}, \mathbf{q}) = T(\mathbf{p}) + U(\mathbf{q}) = \frac{1}{2} \sum_{i=1}^{N} \frac{1}{m_i} \mathbf{p}_i^T \mathbf{p}_i + \sum_{i=2}^{N} \sum_{j=1}^{i-1} V_{ij} \left(\|\mathbf{q}_i - \mathbf{q}_j\| \right), \tag{4}$$

where $\mathbf{q}_i = \mathbf{x}_i$ are the positions, $\mathbf{p}_i = m_i \mathbf{v}_i$ are the momenta, $T(\mathbf{p})$ is the kinetic energy and $U(\mathbf{q})$ is the potential energy.

Now:

$$\begin{aligned}
\frac{d}{dt}T(\mathbf{p}) &= \frac{d}{dt}\frac{1}{2}\sum_{i=1}^{N}\frac{1}{m_i}\mathbf{p}_i\cdot\mathbf{p}_i = \sum_{i=1}^{N} m_i\mathbf{v}_i\cdot\dot{\mathbf{v}}_i \\
\frac{d}{dt}U(\mathbf{q}) &= \frac{d}{dt}\sum_{i=2}^{N}\sum_{j=1}^{i-1}V_{ij}(||\mathbf{q}_i-\mathbf{q}_j||) = \sum_{i=2}^{N}\sum_{j=1}^{i-1}\frac{d}{dt}V_{ij}(||\mathbf{q}_i-\mathbf{q}_j||) \\
&= \sum_{i=2}^{N}\sum_{j=1}^{i-1}\frac{\partial V_{ij}}{\partial\mathbf{q}_i}\cdot\dot{\mathbf{q}}_i+\frac{\partial V_{ij}}{\partial\mathbf{q}_j}\cdot\dot{\mathbf{q}}_j = \sum_{i=2}^{N}\sum_{j=1}^{i-1}\frac{V'_{ij}}{||\mathbf{q}_i-\mathbf{q}_j||}(\mathbf{q}_i-\mathbf{q}_j)\cdot(\dot{\mathbf{q}}_i-\dot{\mathbf{q}}_j) \qquad (5) \\
&= -\sum_{i=2}^{N}\sum_{j=1}^{i-1}\mathbf{F}_{ij}\cdot\dot{\mathbf{q}}_i+\mathbf{F}_{ji}\cdot\dot{\mathbf{q}}_j = -\sum_{i=1}^{N}\sum_{j=1;j\neq i}^{N}\mathbf{F}_{ij}\cdot\dot{\mathbf{q}}_i \\
&= -\sum_{i=1}^{N}\dot{\mathbf{q}}_i\cdot\left(\sum_{j=1;j\neq i}^{N}\mathbf{F}_{ij}\right) = -\sum_{i=1}^{N}m_i\mathbf{v}_i\cdot\dot{\mathbf{v}}_i
\end{aligned}$$

We now immediately see that $\frac{d}{dt}H(\mathbf{p},\mathbf{q}) = \frac{d}{dt}T(\mathbf{p}) + \frac{d}{dt}U(\mathbf{q}) = 0$.

Question 2: Conservation of Momentum

Remember that $\mathbf{q}_i, \mathbf{p}_i \in R^3$ represent the position and momentum of the i-th particle of mass m_i, and $V_{ij}(r)$ $(i > j)$ is the interaction potential between the i-th and j-th particle. The equations of motion are:

$$\dot{\mathbf{q}}_i = \frac{1}{m_i}\mathbf{p}_i, \qquad \dot{\mathbf{p}}_i = \sum_{j=1;j\neq i}^{N}\nu_{ij}\left(\mathbf{q}_i-\mathbf{q}_j\right) \qquad (6)$$

Since we have $\nu_{ij} = \nu_{ji} = -V'_{ij}(r_{ij})/r_{ij}$ with $r_{ij} = ||\mathbf{q}_i - \mathbf{q}_j||$, we can proceed to prove the conservation of the linear and angular momentum. Linear momentum is defined as $\mathbf{P} = \sum_{i=1}^{N}\mathbf{p}_i$. It follows:

$$\frac{d}{dt}\mathbf{P} = \frac{d}{dt}\sum_{i=1}^{N}\mathbf{p}_i = \sum_{i=1}^{N}\dot{\mathbf{p}}_i = \sum_{i=1}^{N}\sum_{j=1;j\neq i}^{N}\nu_{ij}\left(\mathbf{q}_i-\mathbf{q}_j\right)$$

Noting the symmetry $\nu_{ij} = \nu_{ji}$, we can clearly see that all terms of the last double sum cancel out to zero.

Regarding angular momentum $\mathbf{L} = \sum_{i=1}^{N}\mathbf{q}_i\times\mathbf{p}_i$:

$$\begin{aligned}
\frac{d}{dt}\mathbf{L} &= \frac{d}{dt}\sum_{i=1}^{N}\mathbf{q}_i\times\mathbf{p}_i = \sum_{i=1}^{N}\left(\dot{\mathbf{q}}_i\times\mathbf{p}_i+\mathbf{q}_i\times\dot{\mathbf{p}}_i\right) \\
&= \sum_{i=1}^{N}\frac{1}{m_i}\mathbf{p}_i\times\mathbf{p}_i + \sum_{i=1}^{N}\sum_{j=1;j\neq i}^{N}\mathbf{q}_i\times\nu_{ij}\left(\mathbf{q}_i-\mathbf{q}_j\right) \\
&= -\sum_{i=1}^{N}\sum_{j=1;j\neq i}^{N}\mathbf{q}_i\times\nu_{ij}\mathbf{q}_j = 0.
\end{aligned}$$

Note that we have used that $\nu_{ij} = \nu_{ji}$ and the properties of the cross product $\mathbf{a}\times\lambda\mathbf{b} = \lambda\mathbf{a}\times\mathbf{b} = \lambda\left(\mathbf{a}\times\mathbf{b}\right)$, $\mathbf{a}\times(\mathbf{b}+\mathbf{c}) = \mathbf{a}\times\mathbf{b}+\mathbf{a}\times\mathbf{c}$, $\mathbf{a}\times\mathbf{a} = 0$ and $\mathbf{a}\times\mathbf{b} = -\mathbf{b}\times\mathbf{a}$.

Question 3: Conservation with forward Euler

The results for the forward Euler scheme are plotted and analyzed in the following question.

Question 4: Conservation with Velocity Verlet

```cpp
void Simulation::run(double time_end, double dt, const bool bEulerStepping)
{
    // Compute number of timesteps
    const size_t nsteps = (size_t)(time_end/dt);

    // Perform simulation repeating computation of accelerations and particles' status update
    for (size_t step = 0; step < nsteps; ++step)
    {
        // Dump output file every now and then (value of 50 works well for slow
        // I/O of ETH machines but can be reduced to 20 or so on faster ones)
        if (step % 50 == 0)
        {
            _dumpToFile(step, step*dt);
            _diag(step, step*dt);

            cout << "Completion: " << setprecision(2) << step*100./nsteps << "%" <<endl;
        }

        // Perform a time integration step
        if (bEulerStepping)
        {
            // using forward Euler
            _computeAccelerations();
            _updatePositions(dt);
            _updateVelocities(dt);
        }
        else
        {
            // using velocity Verlet
            if (step == 0) _computeAccelerations();

            // perform 4 steps of Velocity Verlet
            _updateVelocities(dt*0.5);
            _updatePositions(dt);
            _computeAccelerations();
            _updateVelocities(dt*0.5);
        }
    }
}
```

Listing 1: Simulation.cpp

Inspection of Fig. 1 shows that the forward Euler (FE) scheme fails to conserve the momenta, and they quickly diverge. On the other hand, Velocity Verlet (VV) seems to perform significantly better at preserving them constant over the amount of time simulated usign the same time-step as the FE scheme.

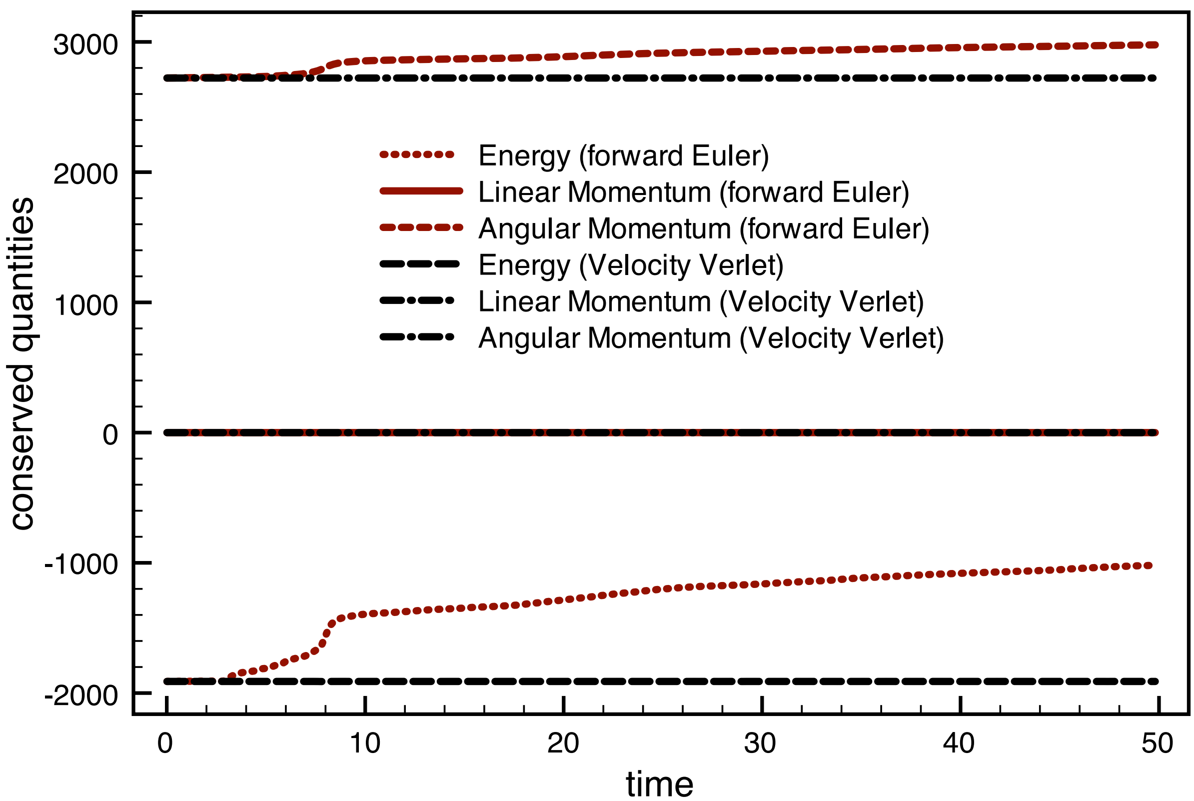

Figure 1: Momenta evolution with time by using two different integration Schemes. Forward Euler and Velocity Verlet.