SIMULATION OF DEFORMABLE BIOLOGICAL STRUCTURES WITH A TETHERED PARTICLE SYSTEM MODEL

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ABSTRACT

A new model is proposed for the simulation of deformable biological structures such as proteins, membranes, tissues, and organs. The idea involves the use of discrete-event simulation to track the motion of large numbers of colliding particles. If two approaching particles reach an inner limiting distance, they collide, rebound outwards, and may become "tethered". When two separating tethered particles reach an outer limiting distance, then provided they remain tethered, they retract inwards. By constraining the distances between pairs of particles in this manner, a variety of deformable structures may be represented. A model of a presynaptic terminal of a nerve cell is presented as an example.

We expect the proposed tethered particle system to offer a considerably simpler alternative to existing deformable structure modeling techniques such as the finite element method (FEM). Many have noted that impulse-based simulations similar to ours are hopelessly inefficient at resolving simultaneous or nearly-simultaneous collisions of three or more particles. We therefore introduce a condition whereby multiple small colliding particles may act, temporarily, as a single body. With this approximation we hope to rectify the inefficiency of impulse-based methods without sacrificing simplicity or validity.

INTRODUCTION

The simulation of deformable structures is used for a wide range of applications in the biomedical field, including the study of physiology, the analysis of joint replacements, and the planning of surgeries [1]. The finite element method (FEM), described in [2], is likely the most popular method for such applications. The possibility of obtaining a new method, one that may be simpler or more computationally efficient, merits the investigation of alternatives.

One relatively simple alternative to the FEM is impulse-based simulation [3]. We regard an impulse as an instantaneous change in the momentum of an object. It is counterintuitive to model deformable structures with impulses, as the deformation of an object is a continuous process that may require a significant length of time. That said, if one represents a deformable structure as a network of a large number of particles, then numerous collisions and impulses between those particles may produce the effect of a gradual deformation of the overall structure. In order to construct stable networks of particles, it is necessary to include not only collisions that redirect two approaching particles away from one another, but also collisions that steer separating particles back towards one another.

This paper introduces the tethered particle system (TPS), a particle collision model in which certain pairs of particles are “tethered” to one another and may not separate beyond some fixed distance. The TPS allows one to apply relatively simple impulse-based dynamic simulation techniques to models of deformable objects. Early results suggest that the TPS holds potential at least for the simulation of microscopic biological structures such as proteins and membranes, and possibly for larger tissues and even organs.

Presented in the paper are the key formulas for collision detection and collision response in a TPS, an approximation that addresses the inefficiency of resolving large numbers of nearly-simultaneous collisions, and a model of deformable biological structures in presynaptic terminals of nerve cells.

COLLISION DETECTION

Unlike FEM-based simulations in which time is advanced at regular intervals, the TPS uses a discrete-event approach in which time is advanced to the moment when the next collision occurs. Collision detection is the task of identifying the next collision.

Suppose that particle *A* is centered at the position $\vec{u_A}$ and has the velocity $\vec{v_A}$, and particle *B* is at $\vec{u_B}$ with velocity $\vec{v_B}$. At time Δt in the future, the distance Δu between the two particles is then as follows.

$$\Delta u = \sqrt{\sum\left(\left(\left(\vec{u_B}+\vec{v_B}\cdot\Delta t\right)-\left(\vec{u_A}+\vec{v_A}\cdot\Delta t\right)\right)^2\right)} \quad (1)$$

We use the notational convention that vector multiplication is performed element by element. We also use the summation symbol as an operator that adds all vector elements, as demonstrated below.

$$[2,3,4]^2 = [2,3,4]\cdot[2,3,4] = [4,9,16]$$
$$\sum\left([2,3,4]^2\right) = \sum[4,9,16] = 29$$

Solving (1) for Δt, we obtain the following.

$$\Delta t = \frac{-b \pm \sqrt{b^2 - 4\cdot a\cdot c}}{2\cdot a} \qquad (2)$$

Where:
$$a = \sum\left(\left(\vec{v_B} - \vec{v_A}\right)^2\right)$$
$$b = 2\cdot\sum\left(\left(\vec{u_B} - \vec{u_A}\right)\cdot\left(\vec{v_B} - \vec{v_A}\right)\right)$$
$$c = \sum\left(\left(\vec{u_B} - \vec{u_A}\right)^2\right) - \Delta u^2$$

To find the time at which the next collision occurs between two specific particles, we first evaluate (2) with Δu set to the distance at which the two particles must collide. If dealing with non-penetrating spherical particles, Δu would be the sum of their radii. After evaluating (2), our collision time is the smaller finite, real, and non-negative result. With more than two particles, we must find the smallest Δt for any particle pair. Performing a simulation, we would advance time by this minimum Δt, then resolve the collision by calculating the new velocities of the colliding particles, then repeat the process.

One generally thinks of a collision as a situation in which two approaching particles rebound off one another. We refer to this type of collision as a "blocking collision". In a TPS simulation, a blocking collision occurs if two approaching particles reach an inner limiting distance $\Delta u_{blocking}$. At that point the two particles may become "tethered". A "tethering collision" occurs when two separating tethered particles reach an outer limiting distance $\Delta u_{tethering}$. At that point the connection between the particles may break, in which case the particles continue to separate. Should the particles remain tethered, however, they reflect inwards. The distance between two tethered particles is thus constrained; ignoring computational errors, the distance is at least $\Delta u_{blocking}$ and at most $\Delta u_{tethering}$.

The distances $\Delta u_{blocking}$ and $\Delta u_{tethering}$ replace Δu in (2), yielding future times for both blocking and tethering collisions.

COLLISION RESPONSE

Given the positions $\vec{u_A}$ and $\vec{u_B}$, and the velocities $\vec{v_A}$ and $\vec{v_B}$, of two particles at the time when they collide, collision response is the calculation of the new particle velocities $\vec{v_A}'$ and $\vec{v_B}'$. We now also need the masses of the particles, m_A and m_B. Derived from the law of conservation of momentum, (3) yields the new velocities given the impulse $\Delta\vec{p}$.

$$\left[\vec{v_A}', \vec{v_B}'\right] = \left[\vec{v_A} + \frac{\Delta\vec{p}}{m_A},\ \vec{v_B} - \frac{\Delta\vec{p}}{m_B}\right] \qquad (3)$$

In order to determine the impulse, it is useful to obtain the following: $\hat{u}$, a unit vector along the axis between the particles; $\vec{v_{AB}}$, the relative particle velocity; $\vec{v_{\hat{u}}}$, the relative velocity projected onto $\hat{u}$; and $\vec{v_{\hat{w}}}$ the relative velocity projected onto the plane perpendicular to $\hat{u}$.

$$\hat{u} = \frac{\left(\vec{u_B} - \vec{u_A}\right)}{\sqrt{\sum\left(\left(\vec{u_B} - \vec{u_A}\right)^2\right)}}$$
$$\vec{v_{AB}} = \vec{v_B} - \vec{v_A}$$
$$\vec{v_{\hat{u}}} = \sum\left(\vec{v_{AB}}\cdot\hat{u}\right)$$
$$\vec{v_{\hat{w}}} = \vec{v_{AB}} - \vec{v_{\hat{u}}}$$

In most cases the impulse can be calculated by the well known equation in (4), where $c_{resitute}$ is the "coefficient of restitution" that expresses the ratio of the new projected relative speed to the magnitude of the old $\vec{v_{\hat{u}}}$. The maximum value of this coefficient is 1, in which case no energy is lost in the collision, and the minimum value is 0, in which case the energy loss is maximized.

$$\Delta\vec{p} = \left(1 + c_{restitute}\right)\cdot\left(\frac{1}{m_A} + \frac{1}{m_B}\right)^{-1}\cdot\vec{v_{\hat{u}}} \qquad (4)$$

The TPS requires a distinction between the "rebounding" of two approaching particles, the "retraction" of two separating but tethered particles, and the "revolution" of two tethered particles. Each case has its own coefficient that determines the energy lost. In the case of two rebounding particles, the traditional type of collision, we obtain the impulse by substituting $c_{rebound}$ into (4). In the case of two

retracting tethered particles, we evaluate (4) with $c_{retract}$ instead. The remainder of this section will focus on revolution.

If two tethered particles are at their tethering distance and their relative velocity is perpendicular to $\hat{u}$, then the use of (4) will lead to an infinite succession of infinitesimal retraction impulses. To prevent this, we check whether a retraction impulse is sufficient to draw the two particles together at an angle of at least $\theta_{revolve}$ from perpendicular.

$$\sqrt{\sum\left(\left(c_{retract}\cdot\vec{v}_{\hat{u}}\right)^2\right)} > \tan\left(\theta_{revolve}\right)\cdot\sqrt{\sum\left(\vec{v}_{\hat{w}}^{\,2}\right)}$$

If the condition above is satisfied, then a retraction impulse is sufficient and we use (4). Otherwise, we abandon (4) and calculate an impulse that will draw the tethered particles together at an angle of $\theta_{revolve}$. We refer to this as "revolution" because, if left alone, the particles will circle one another in a series of these collisions.

To calculate the revolution impulse, we first obtain the relative direction $\hat{u}_{revolve}$ corresponding to the angle $\theta_{revolve}$.

$$\hat{u}_{revolve} = \frac{\vec{v}_{revolve}}{\sqrt{\sum\left(\vec{v}_{revolve}^{\,2}\right)}}$$

Where: $\vec{v}_{revolve} = \vec{v}_{\hat{w}} - \tan\left(\theta_{revolve}\right)\cdot\sqrt{\sum\left(\vec{v}_{\hat{w}}^{\,2}\right)}\cdot\hat{u}$

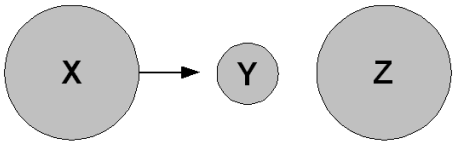
Given the previously-calculated relative velocity $\vec{v}_{AB}$, the revolution impulse given by (5) results in a new relative velocity $\vec{v}_{AB}'$ with direction $\hat{u}_{revolve}$. The magnitude of the new relative velocity is chosen based on the coefficient $c_{revolve}$. This coefficient expresses the ratio of the new relative speed to the old one; not after a single collision, but rather after one entire revolution of the two particles. Suppose $\theta_{revolve}$ is 45 degrees and $c_{revolve}=0.5$. Because it will take four collisions to achieve a full revolution, the relative speed will drop by a factor of $0.5^{1/4}$, or approximately 0.84, on each collision.

$$\Delta\vec{p} = \left(\frac{1}{m_A}+\frac{1}{m_B}\right)^{-1}\cdot\left(\vec{v}_{AB}-\vec{v}_{AB}'\right) \qquad (5)$$

Where: $\vec{v}_{AB}' = c_{revolve}^{\frac{\theta_{revolve}}{\pi}}\cdot\sqrt{\sum\left(\vec{v}_{AB}^{\,2}\right)}\cdot\hat{u}_{revolve}$

NEARLY-SIMULTANEOUS COLLISIONS

The following simple scenario reveals a problem with the model presented thus far. Particle *X* is about to collide with stationary particle *Y*, which will then collide with stationary particle *Z*.



First we assume $c_{rebound}=1$. If all particles have equal mass, particle *X* will transfer all of its momentum to *Y*, which will in turn transfer all of its momentum to *Z*. There will be only two collisions. If the mass of particle *Y* is much less than that of the other two, however, *X* will lose only a fraction of its momentum when it first collides with *Y*. In this case many nearly-simultaneous collisions will occur, with *Y* bouncing back and forth between the two larger particles. In a simulation where the mass of *Y* was a thousandth that of the other two, 70 collisions occurred in total.

The processing of these 70 collisions is a large computational effort for such a simple scenario, but when the simulation described above was repeated with $c_{rebound}<0.9$, the momentum transferred on each collision converged to zero and the simulation stalled. This well known problem with simultaneous and nearly-simultaneous collisions is described in [4], along with a constraint-based solution that requires the minimization of a linear function constrained by a system of linear inequalities. We stick to impulse-based modeling, and propose a much simpler approximation for the TPS.

Our approximation groups colliding particles for a duration of at least $\Delta t_{restitute}$, which is an arbitrary value. During this time, the grouped particles move together with the velocity $\Delta\vec{v}_{load}$, and interact as a single body with a mass equivalent to the sum of the masses of each grouped particle.

$$\vec{v}_{load} = \left(1+\frac{m_B}{m_A}\right)^{-1}\cdot\vec{v}_A + \left(1+\frac{m_A}{m_B}\right)^{-1}\cdot\vec{v}_B \qquad (6)$$

For a collision between two particles *A* and *B*, we record an impulse $\Delta\vec{p}_{AB}$ to apply via (3) after the time $\Delta t_{restitute}$ elapses. This impulse is calculated from the impulse $\Delta\vec{p}$, as given by (4) or (5), but we subtract the momentum that we effectively introduced by changing the velocities to $\Delta\vec{v}_{load}$.

$$\Delta \vec{p}_{AB} = \Delta \vec{p} - \left(\frac{1}{m_A} + \frac{1}{m_B} \right)^{-1} \cdot \vec{v}_{AB} \quad (7)$$

Returning to the scenario, suppose that particles *X* and *Y* collide at time t_{XY}. We temporarily give both particles the velocity of (6), and record the impulse $\Delta \vec{p}_{XY}$ from (7) to apply after the time reaches $t_{XY} + \Delta t_{restitute}$. But suppose that the second collision occurs at t_{YZ} before $t_{XY} + \Delta t_{restitute}$. We then evaluate (6) and (7) for particles *Y* and *Z*. Because *Y* is grouped with *X*, we use the combined mass of *X* and *Y* for the mass of *Y*. From (6) we get the new temporary velocity of all three particles, while (7) gives us $\Delta \vec{p}_{YZ}$. We now wait until time reaches $t_{YZ} + \Delta t_{restitute}$, then apply $\Delta \vec{p}_{YZ}$ between particles *Y* and *Z* using (3), still treating *X* and *Y* as a single body. Finally, without advancing time, we apply $\Delta \vec{p}_{XY}$ between particles *X* and *Y*.

By temporarily combining the masses of grouped particles, which increases the magnitude of collision impulses, our approximation dramatically reduces the number of collisions in a TPS simulation. Even if this approximation is found to introduce inaccuracy on an individual-particle level, it may not invalidate the modeled behavior of a system that includes a large number of particles. The approximation obeys conservation of momentum, and it should be noted that only a very small value of $\Delta t_{restitute}$ is needed to address the problem of nearly-simultaneous collisions.

DEFORMABLE BIOLOGICAL STRUCTURES

Using the Python programming language, we implemented discrete event simulation code to investigate TPS models of various types of deformable biological structures. Figure 1 shows a model of a presynaptic terminal, a part of a nerve cell. The deformable structures in this case are clusters of sacs called “vesicles” tethered to proteins called synapsins. These clusters formed during simulation from initially-isolated vesicle particles and synapsin particle pairs, and reacted realistically to impacts within a rigid spherical cell membrane.

The TPS can be applied to various types of deformable structures. We intend to model long proteins by chaining tethered particles together, and have begun representing deformable membranes as planar networks of particles tethered to their nearest neighbors. A TPS membrane can model microscopic structures, like nerve cell membranes, or macroscopic tissues, like the walls of veins and arteries.

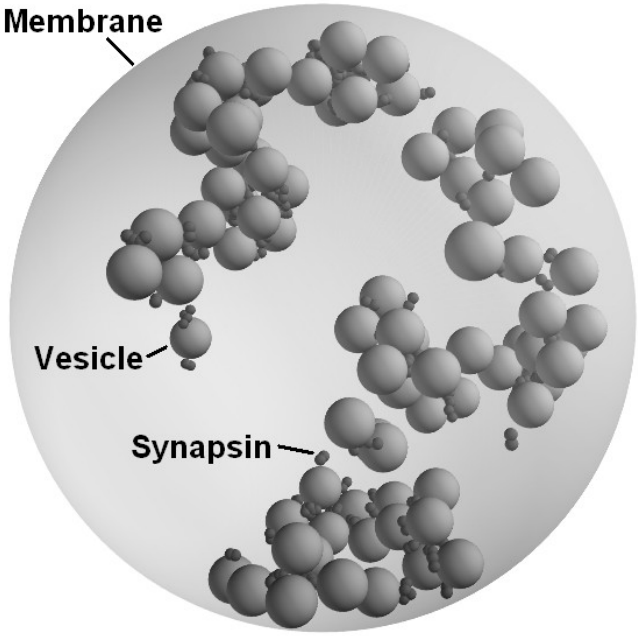


Figure 1: A simulation snapshot of a TPS model of a presynaptic terminal of a nerve cell. The membrane is modeled as a single large particle of infinite mass. It contains smaller particles representing vesicles, which are tethered to pairs of still smaller synapsin particles.

CONCLUSION

A new model, the tethered particle system, has been proposed and demonstrated for the simulation of deformable structures. The key formulas needed to implement the model have been presented. Simulation results to date suggest that the TPS has the potential to represent microscopic biological structures like those found in the modeled presynaptic terminal, and further research may demonstrate its utility for larger tissues and even organs. The TPS could be enhanced with friction, the rotation of particles, the representation of gravity as a sequence of impulses, and the inclusion of fluid dynamics using freely-moving particles or a superimposed differential equation model.

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