DFTL analysis

Notations

In this section, we describe the notations used for the rest of the paper. The Position of the ith particle at the nth instant is denoted by $\mathbf{x}_i^n$. The Velocity of the ith particle at the nth instant is denoted by $\mathbf{v}_i^n$. The Time Step size is denoted by Δt. The Separation between all the particles is assumed to be constant and is denoted as d. The External Forces are denoted by $\mathbf{f}$ (Assumed to be constant). The Damping Constant included in the DFTL paper is denoted by $s_{damping}$. The Position calculated of the ith particle at the nth instant by the Position Based Dynamics (PBD) is denoted by $\mathbf{p}_i^n$. Also, we assume all the variables to be continuous and differentiable

[RN: No need to capitalize "position", "velocity", etc.]

[VR: Oh okay. It would be very cumbersome to remove them now, so if we make any other draft then I will take care of it]

Equations of motion

The equations of motion of an inextensible chain of n particles are

$$
\begin{aligned}
m_i \frac{d^2\mathbf{x}_i}{dt^2} &= \mathbf{f}_i + \lambda_{i+1}\nabla_{\mathbf{x}_i} c_{i+1} + \lambda_i \nabla_{\mathbf{x}_i} c_i && \forall i = 1, \dots, n, \\
c_i &= 0 && \forall i = 1, \dots, n.
\end{aligned}
$$

The DFTL method exactly satisfies $c_i = 0$ for all i at every time step. Therefore, we only need to prove that it also satisfies the equation for $d^2\mathbf{x}_i/dt^2$ in the limit, i.e. that there exist constraint forces θ_i such that

$$
\begin{aligned}
\frac{\mathbf{x}_i^n - \mathbf{x}_i^{n-1}}{\Delta t} &= \mathbf{v}_i^n + O(\Delta t), && \text{(V.E)} \\
m_i \frac{\mathbf{v}_i^n - \mathbf{v}_i^{n-1}}{\Delta t} &= \mathbf{f}_i^n + \theta_{i+1}^n \nabla_{\mathbf{x}_i^n} c_{i+1}^n + \theta_i^n \nabla_{\mathbf{x}_i^n} c_i^n + O(\Delta t) && \text{(A.E)}
\end{aligned}
$$

Proof

The equations given in the DFTL paper can be rewritten as follows

$$\mathbf{p}_i^n = \mathbf{x}_i^{n-1} + \Delta t \mathbf{v}_i^{n-1} + \Delta t^2 \mathbf{f}_i^n, \tag{1}$$

$$\mathbf{x}_i^n = \mathbf{x}_{i-1}^n + d\frac{\mathbf{p}_i^n - \mathbf{x}_{i-1}^n}{\|\mathbf{p}_i^n - \mathbf{x}_{i-1}^n\|}, \tag{2}$$

$$\mathbf{v}_i^n = \frac{\mathbf{x}_i^n - \mathbf{x}_i^{n-1}}{\Delta t} - s_{damping}\frac{\Delta \mathbf{x}_{i+1}}{\Delta t} \tag{3}$$

where $\Delta \mathbf{x}_{i+1} = \mathbf{x}_{i+1}^n - \mathbf{p}_{i+1}^n$.

[RN: Instead of manual line breaks and resetting \parindent you can simply `\usepackage{parskip}` in your document preamble.]

[VR: Thanks for this. Wasn't aware about it.]

Now from the experimentations that were concluded by us, we know that the equation (3) has the improper correction term which leads to impractical velocities. Now to get rid of this, we can re-construct this method in an other format which will have the same state of motion as the original DFTL method. Thus this new set of equations will be:

$$\mathbf{p}_i^n = \mathbf{x}_i^{n-1} + \Delta t \mathbf{v}_i^{n-1} + \Delta t^2 \mathbf{f}_i^n - s_{damping}\Delta \mathbf{x}_{i+1}, \tag{4}$$

$$\mathbf{x}_i^n = \mathbf{x}_{i-1}^n + d\frac{\mathbf{p}_i^n - \mathbf{x}_{i-1}^n}{\|\mathbf{p}_i^n - \mathbf{x}_{i-1}^n\|}, \tag{5}$$

$$\mathbf{v}_i^n = \frac{\mathbf{x}_i^n - \mathbf{x}_i^{n-1}}{\Delta t} \tag{6}$$

where $\Delta \mathbf{x}_{i+1} = \mathbf{x}_{i+1}^{n-1} - \mathbf{p}_{i+1}^{n-1}$.

[RN: You obtain these equations simply by defining the new $\mathbf{v}_i^n$ to be the old $\mathbf{v}_i^n$ plus $s_{damping}\frac{\Delta \mathbf{x}_{i+1}}{\Delta t}$, right?]

[VR: The modification for $\mathbf{v}_i^n$ as you stated is correct but I would rather say that these new equations are obtained by transferring the $s_{damping}$ term while getting the $\mathbf{p}_i^n$.]

Here, if we go through these equations then we can deduce that the positions $\mathbf{x}_i^n$ for all the particles i and all the times n will be the same for both the methods. Now the above set of equations implies that we will have two different set of constraints for all the particles. One will be the upstream constraints (between particles i and i+1) and the other will be the downstream constraints (between particles i and i-1). Now the equations (4) to (6) can be inferred in the following manner:

- While trying to obtain the positions for the physical system at first time step, the above constraint solver module will get the predicted positions by ignoring the constraints and using the initial system information. Done in equation (4)

- Now after this, the solver will resolve all the conflicting downstream constraints and report a corrected system. This is done by equation (5). Now, the solver will also store the information of the change in position of any particle i in Δx_i

- Then the system will update the velocities for all the particles for this time step update.

- Now for getting the system state in the next time step while obtaining the predicted positions for the particle i, the solver will also include the saved position change for the particle (i+1). This is done in the equation (4). And thus this entire sequence of calculations will keep getting repeated

- Thus for obtaining the system information at time (n+1), the equation (4) will be using the upstream constraints, which got ignored at time n, in order to get the predicted positions at time (n+1). And then in equation (5), the downstream constraints for the system are solved using the Follow-the-leader method at time (n+1). Thus, here we account for both the upstream and downstream constraints for all the particles thus achieving a balanced mass distribution.

We will now prove correctness of the solver module for the modified system of DFTL equations. Now, we can also write the projection from $\mathbf{p}_i$ to $\mathbf{x}_i$ in terms of the constraint gradients. From this, We have the ith constraint as

$$c_i^n = \|\mathbf{x}_i^n - \mathbf{x}_{i-1}^n\| - d, \tag{7}$$

$$\nabla_{\mathbf{x}_i^n} c_i^n = \frac{\mathbf{x}_i^n - \mathbf{x}_{i-1}^n}{\|\mathbf{x}_i^n - \mathbf{x}_{i-1}^n\|}, \tag{8}$$

$$\nabla_{\mathbf{x}_{i-1}^n} c_i^n = -\frac{\mathbf{x}_i^n - \mathbf{x}_{i-1}^n}{\|\mathbf{x}_i^n - \mathbf{x}_{i-1}^n\|}, \tag{9}$$

So, Using the above equations, we can transform our equations as

$$\begin{aligned}
\mathbf{x}_i^n &= \mathbf{x}_{i-1}^n + d\frac{\mathbf{p}_i^n - \mathbf{x}_{i-1}^n}{\|\mathbf{p}_i^n - \mathbf{x}_{i-1}^n\|} && (10)\\
&= \mathbf{p}_i^n + \underbrace{(d - \|\mathbf{p}_i^n - \mathbf{x}_{i-1}^n\|)}_{\lambda_i^n} \underbrace{\frac{\mathbf{p}_i^n - \mathbf{x}_{i-1}^n}{\|\mathbf{p}_i^n - \mathbf{x}_{i-1}^n\|}}_{\nabla_{\mathbf{x}_i^n} c_i^n} && (11)\\
&= \mathbf{p}_i^n + \lambda_i^n \nabla_{\mathbf{x}_i^n} c_i^n && (12)
\end{aligned}$$

[RN: Instead of λ_i^n let us call it δ_i^n or something, to distinguish it from the λ in (A.E.). After all, they are not the same — to get the equations to match we will need the $\lambda = \delta/\Delta t^2$, right?]
[VR: Updated that variable in the (A.E) equation rather. So that is now *theta* as you can see in equation (21)]

Now, we can also write from the equation (5) that

$$\frac{\mathbf{p}_i^n - \mathbf{x}_{i-1}^n}{\|\mathbf{p}_i^n - \mathbf{x}_{i-1}^n\|} = \frac{\mathbf{x}_i^n - \mathbf{x}_{i-1}^n}{\|\mathbf{x}_i^n - \mathbf{x}_{i-1}^n\|} \tag{13}$$

From the equation of $\nabla_{\mathbf{x}_i^n} c_i^n$ in the equation (8), and using it along with the previous equation in equation (5) gives

$$\mathbf{x}_i^n - \mathbf{x}_{i-1}^n = d\nabla_{\mathbf{x}_i^n} c_i^n \tag{14}$$

Also, using the definition of $\Delta\mathbf{x_{i+1}}$ and the equation (12), we get

$$\frac{\Delta\mathbf{x_{i+1}}}{\Delta t} = \frac{\lambda_{i+1}^{n-1}\nabla_{\mathbf{x}_{i+1}^{n-1}} c_{i+1}^{n-1}}{\Delta t} \tag{15}$$

Now, we can see that the equation (6) will be consistent with the Velocity Convergence Equation $(V.E)$. Thus, we need to obtain an equation assuming the form of $(A.E)$ from our equations.

Making the use of equation (4) and equation (15), we obtain:

$$\mathbf{p}_i^n - \mathbf{x}_i^{n-1} - \Delta t\mathbf{v}_i^{n-1} - \Delta t^2\mathbf{f}_i^n = -s_{damping}\lambda_{i+1}^{n-1}\nabla_{\mathbf{x}_{i+1}^{n-1}} c_{i+1}^{n-1} \tag{16}$$

Using equation (12) and the above equation, we can eliminate the term of $\mathbf{p}_i^n$ and obtain:

$$(\mathbf{x}_i^n - \lambda_i^n\nabla_{\mathbf{x}_i^n} c_i^n) - \mathbf{x}_i^{n-1} - \Delta t\mathbf{v}_i^{n-1} - \Delta t^2\mathbf{f}_i^n = -s_{damping}\lambda_{i+1}^{n-1}\nabla_{\mathbf{x}_{i+1}^{n-1}} c_{i+1}^{n-1} \tag{17}$$

The above equation can be restructured to give the below equation:

$$(\mathbf{x}_i^n - \mathbf{x}_i^{n-1}) - \Delta t\mathbf{v}_i^{n-1} = \Delta t^2\mathbf{f}_i^n - s_{damping}\lambda_{i+1}^{n-1}\nabla_{\mathbf{x}_{i+1}^{n-1}} c_{i+1}^{n-1} + \lambda_i^n\nabla_{\mathbf{x}_i^n} c_i^n \tag{18}$$

Making the use of equation (6) and dividing both the L.H.S and R.H.S by Δt^2, we obtain:

$$\frac{\mathbf{v}_i^n - \mathbf{v}_i^{n-1}}{\Delta t} = \mathbf{f}_i^n + \left(\left(\frac{\lambda_i^n}{\Delta t^2}\right)\nabla_{\mathbf{x}_i^n} c_i^n\right) - s_{damping}\left(\left(\frac{\lambda_{i+1}^{n-1}}{\Delta t^2}\right)\nabla_{\mathbf{x}_{i+1}^{n-1}} c_{i+1}^{n-1}\right) \tag{19}$$

For our analysis, where $\Delta t \to 0$, we can approximate the gradient at $(n-1)^{th}$ time to be the gradient at n^{th} time step. Though it should be more meaningful to try to infer that:

$$\left(\left(\frac{\lambda_{i+1}^n}{\Delta t^2}\right)\nabla_{\mathbf{x}_{i+1}^n} c_{i+1}^n\right) = \left(\left(\frac{\lambda_{i+1}^{n-1}}{\Delta t^2}\right)\nabla_{\mathbf{x}_{i+1}^{n-1}} c_{i+1}^{n-1}\right) + O(\Delta t) \tag{20}$$

The question is *How to do so?* Also, $\nabla_{\mathbf{x}_i^n} c_i^n = -\nabla_{\mathbf{x}_{i-1}^n} c_i^n$ (From the equations (8) and (9)).
[RN: In principle these quantities $(\lambda_{i+1}/\Delta t^2)\nabla_{\mathbf{x}_{i+1}} c_{i+1}$ should be approximating the constraint force on particle $i+1$. So the difference between their values at times t and $t+\Delta t$ can be $O(\Delta t)$ only if the constraint forces are continuous over time. This follows from smoothness and nondegeneracy of the constraint functions (in the continuous case, denoting $\mathbf{J}$ to be the Jacobian of the constraint function vector $\mathbf{c} = [c_1, c_2, \dots]^T$,

$$
\begin{aligned}
& \mathbf{c} = 0 \\
\implies & \mathbf{Jv} = 0 \\
\implies & \mathbf{Ja} + (\tfrac{\mathrm{d}}{\mathrm{d}t}\mathbf{J})\mathbf{v} = 0
\end{aligned}
$$

which along with $\mathbf{Ma} = \mathbf{f} + \mathbf{J}^T\boldsymbol{\lambda}$ allows you to show that $\boldsymbol{\lambda}$ is continuous as long as $\mathbf{J}$ is full rank and $\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{J}$ is continuous.) However it still remains to show that the discrete λs approximate the constraint forces to within $O(\Delta t)$. Maybe one can show this using the third equation above, i.e. that the λs computed with DFTL satisfy

$$\mathbf{JM}^{-1}(\mathbf{f} + \mathbf{J}^T\boldsymbol{\lambda}) + (\tfrac{\mathrm{d}}{\mathrm{d}t}\mathbf{J})\mathbf{v} = O(\Delta t).$$

Not sure if this is above your pay grade.]
[VR: Yeah this looks complicated to me. These different variables involved expand to pretty complicated terms and it nowhere seems like on expanding those variables and performing some algebraic simplifications, the above equation would directly get reduced to a term of $O(\Delta t)$.]
[VR: Also I had a doubt. If you look at the equation (19), then it can be said that for the particle (i), apart from having a constraint force corresponding to $(\lambda_{i+1}/\Delta t^2)\nabla_{\mathbf{x}_{i+1}} c_{i+1}$, there would also be a constraint force corresponding to $(\lambda_i/\Delta t^2)\nabla_{\mathbf{x}_i} c_i$. Thus there are two terms of constraint forces involved, one for the upstream constraint and other for the downstream constraint. So how would $\mathbf{Ma} = \mathbf{f} + \mathbf{J}^T\boldsymbol{\lambda}$ hold, with λ as $(\lambda_i/\Delta t^2)$ for the particle (i)?]

If we could prove that λ_i^n follows an order of Δt^2 then we can replace the fractions $\left(\frac{\lambda_i^n}{\Delta t^2}\right)$ by some other constants θ_i^n. *How to do so?*
[VR: Can you let me know about this too?]

By applying the above mentioned ideas, the equation (19) would get converted to:

$$\frac{\mathbf{v}_i^n - \mathbf{v}_i^{n-1}}{\Delta t} = \mathbf{f}_i^n + \left((\theta_i^n)\,\nabla_{\mathbf{x}_i^n} c_i^n\right) + s_{damping}\left(\left(\theta_{i+1}^n\right)\nabla_{\mathbf{x}_i^n} c_{i+1}^n\right) + O(\Delta t) \quad (21)$$

Thus, here we can see that when the value of $s_{damping}$ is 1, then the above equation gets reduced to the equation $(A.E)$. Thus, we can see that for this method, the velocity convergence equation $(V.E)$ is satisfied for all the values of $s_{damping}$, while the acceleration convergence equation $(A.E)$ is satisfied when $s_{damping}$ is 1.

Thus our method will converge to a physically accurate solution in the limits of $\Delta t \to 0$, when we use the value of $s_{damping}$ as 1.