APPENDIX A

Deformation and Force Simulation

The Euler-Lagrange equation of a 3D deformable body discretized using the FEM is:

$$\mathbf{M}\ddot{\mathbf{u}} + \mathbf{C}\dot{\mathbf{u}} + \mathbf{K}\mathbf{u} = \mathbf{f}, \tag{A.1}$$

where $\mathbf{u}$ is the displacement vector; $\mathbf{M}$, $\mathbf{C}$ and $\mathbf{K}$ are the *mass*, *damping* and *stiffness* matrices and $\mathbf{f}$ is the external force. Under the linear elasticity assumption, there matrices are all constant (independent w.r.t. the displacement). Based on Equation (A.1) a generalized eigen problem is defined as:

$$\mathbf{K\Phi} = \mathbf{M\Phi\Lambda}, \tag{A.2}$$

where $\mathbf{\Lambda}$ is a diagonal matrix and its diagonal elements are the corresponding eigenvalues. Solving the above equation gives us the *modal displacement matrix*, $\mathbf{\Phi}$, with the size $3n \times m$ where m is the number of modes which normally is a much smaller number than n. With $\mathbf{\Phi}$, the spatial displacement $\mathbf{u}$ can be expressed with a set of reduced coordinates as:

$$\mathbf{u} = \mathbf{\Phi q}, \tag{A.3}$$

where $\mathbf{q}$ is called the *spectral displacement*. If we substitute Equation (A.3) into Equation (A.1) and pre-multiply $\mathbf{\Phi}^{\mathrm{T}}$ at both sides of the equation, we will have a reduced or spectral version of Euler-Lagrange equation with size m:

$$\mathbf{M}_{\mathrm{q}}\ddot{\mathbf{q}} + \mathbf{C}_{\mathrm{q}}\dot{\mathbf{q}} + \mathbf{K}_{\mathrm{q}}\mathbf{q} = \mathbf{\Phi}^{\mathrm{T}}\mathbf{f}, \tag{A.4}$$

where $\mathbf{M}_{\mathrm{q}} = \mathbf{\Phi}^{\mathrm{T}}\mathbf{M\Phi}$, $\mathbf{C}_{\mathrm{q}} = \mathbf{\Phi}^{\mathrm{T}}\mathbf{C\Phi}$ and $\mathbf{K}_{\mathrm{q}} = \mathbf{\Phi}^{\mathrm{T}}\mathbf{K\Phi}$ all become diagonal matrices. However, Equation (A.4) is only able to handle small deformation because the linear strain tensor is used, otherwise the stiffness matrix will not be constant. In order to incorporate large rotational deformation, the Modal Warping technique [13] is used such that the rotation at each node is estimated and tracked by a $3n \times 1$ rotation vector $\mathbf{w}$ which is computed as the *curl* of the displacement field:

$$\mathbf{w} = \tfrac{1}{2}\nabla \times \mathbf{u} = \tfrac{1}{2}\nabla \times \mathbf{\Phi q} = \mathbf{\Psi q}, \tag{A.5}$$

where $\mathbf{\Psi}$ is a pre-computed *modal rotation matrix*. Each 3×1 component in $\mathbf{w}$ represents the axis-angle-form of rotation at a node on the finite element mesh. Based on it, we can get the rotation matrix $\mathbf{R}$. The readers can refer to [13] for the detailed derivation. The idea behind Modal Warping is embedding a local coordinate frame at each finite element node. The deformation at the node is computed with the estimated rotation removed. Thus, Modal Warping can be considered as a co-rotational form of linear modal analysis. Based on matrix $\mathbf{R}$, Equation (A.3) is then modified as $\mathbf{u} = \mathbf{R\Phi q}$, and Equation (A.4) is changed to:

$$\mathbf{M}_{\mathrm{q}}\ddot{\mathbf{q}} + \mathbf{C}_{\mathrm{q}}\dot{\mathbf{q}} + \mathbf{K}_{\mathrm{q}}\mathbf{q} = \mathbf{\Phi}^{\mathrm{T}}(\mathbf{R}^{\mathbf{T}}\mathbf{f}). \tag{A.6}$$

Equation (A.6) contains a set of decoupled ordinary differential equations (ODEs). In order to solve it, we use *average acceleration method* to linearize the ODE [44], which yields a linear system to be solved at each *time-step*:

$$\mathbf{A}\ddot{\mathbf{q}} = \mathbf{b}, \tag{A.7}$$

where $\mathbf{A} = \mathbf{M}_{\mathrm{q}} + \gamma h\mathbf{C}_{\mathrm{q}} + \beta h^2\mathbf{K}_{\mathrm{q}}$ and $\mathbf{b} = \mathbf{f}_{\mathrm{q}}{}^{t+1} - \mathbf{C}_{\mathrm{q}}\tilde{\dot{\mathbf{q}}}^{t+1} - \mathbf{K}_{\mathrm{q}}\tilde{\mathbf{q}}^{t+1}$. $\tilde{\mathbf{q}}^{t+1}$ and $\tilde{\dot{\mathbf{q}}}^{t+1}$ are displacement and velocity predictors defined as:

$$\tilde{\mathbf{q}}^{t+1} = \mathbf{q}^{t} + h\dot{\mathbf{q}}^{\mathrm{t}} + \frac{h^2}{2}(1-2\beta)\ddot{\mathbf{q}}^{t}, \tag{A.8}$$

$$\tilde{\dot{\mathbf{q}}}^{t+1} = \dot{\mathbf{q}}^{t} + (1-\gamma)h\ddot{\mathbf{q}}^{\mathrm{t}}. \tag{A.9}$$

Scalar h represents the size of the time-step, while scalars β and γ are two constants where $\beta = 1/4$ and $\gamma = 1/2$. Note the superscripts t and $t+1$ indicate the current and the next time-step. Then the unknown displacements and velocities can be expressed as:

$$\mathbf{q}^{t+1} = \tilde{\mathbf{q}}^{t+1} + \beta h^2\ddot{\mathbf{q}}^{t+1}, \tag{A.10}$$

$$\dot{\mathbf{q}}^{t+1} = \tilde{\dot{\mathbf{q}}}^{t+1} + \gamma h\ddot{\mathbf{q}}^{t+1}. \tag{A.11}$$

Substituting Equations (A.8) and (A.9) into Equations (A.10) and (A.11) yields:

$$\mathbf{q}^{\mathrm{t+1}} = \mathbf{q}^{\mathrm{t}} + h\dot{\mathbf{q}}^{\mathrm{t}} + \frac{h^2}{2}\left(\frac{1}{2}(\ddot{\mathbf{q}}^{\mathrm{t}} + \ddot{\mathbf{q}}^{\mathrm{t+1}})\right), \tag{A.12}$$

$$\dot{\mathbf{q}}^{\mathrm{t+1}} = \dot{\mathbf{q}}^{\mathrm{t}} + h(\tfrac{1}{2}(\ddot{\mathbf{q}}^{\mathrm{t}} + \ddot{\mathbf{q}}^{\mathrm{t+1}})), \tag{A.13}$$

which are Equations (6) and (7) in Section 5.3.

The users' manipulation and interaction is realized with *Lagrange Multiplier Method*. When position constraints are applied, an elementary matrix $\mathbf{E}$ is used to pick out the constraint nodes and the linear position constraint can be formulated as $\mathbf{Jq} = \mathbf{c}$, where $\mathbf{J} = \mathbf{ER\Phi}$ is the constraint matrix. $\mathbf{c}$ is a vector representing the desired displacements of constrained nodes. The constrained version of the time-integration equation is written as :

$$\begin{pmatrix} \mathbf{A} & (\beta h^2\mathbf{J})^{\mathrm{T}} \\ \beta h^2\mathbf{J} & \mathbf{0} \end{pmatrix}\begin{pmatrix} \ddot{\mathbf{q}} \\ \boldsymbol{\lambda} \end{pmatrix} = \begin{pmatrix} \mathbf{b} \\ \mathbf{c} - \mathbf{J}\tilde{\mathbf{q}} \end{pmatrix}, \tag{A.14}$$

where $\boldsymbol{\lambda}$ is the vector of the unknown *Lagrange Multipliers*. Let $\tilde{\mathbf{J}} = \beta h^2\mathbf{J}$ and $\tilde{\mathbf{c}} = \mathbf{c} - \mathbf{J}\tilde{\mathbf{q}}$, Equation (A.14) can then be expressed as:

$$\begin{pmatrix} \mathbf{A} & \tilde{\mathbf{J}}^{\mathrm{T}} \\ \tilde{\mathbf{J}} & \mathbf{0} \end{pmatrix}\begin{pmatrix} \ddot{\mathbf{q}} \\ \boldsymbol{\lambda} \end{pmatrix} = \begin{pmatrix} \mathbf{b} \\ \tilde{\mathbf{c}} \end{pmatrix}. \tag{A.15}$$

Solving Equation (A.15) gives us the solution of $\ddot{\mathbf{q}}$, the spectral acceleration. The constraint spectral force can be computed as:

$$\mathbf{f}_q = \tilde{\mathbf{J}}^{\mathrm{T}}\boldsymbol{\lambda}. \tag{A.16}$$

The corresponding force in spatial domain is:

$$\mathbf{f} = \beta h^2\mathbf{E}^{\mathrm{T}}\boldsymbol{\lambda}. \tag{A.17}$$

The corresponding constraint forces in spectral and spatial domains are related by: $\mathbf{f}_q = \mathbf{\Phi}^{\mathrm{T}}\mathbf{R}^{\mathrm{T}}\mathbf{f}$.

APPENDIX B

Proof of Lemma and Theorem

Proof of Lemma

By Equation (A.13), the changes of velocity at time-steps t, $t+1$, and $t+k$, for $k \geq 2$ can be obtained as follows:

$$\dot{\mathbf{q}}^{\mathrm{t}} - \dot{\mathbf{q}}^{\mathrm{t-1}} = \mathrm{h}(\tfrac{1}{2}(\ddot{\mathbf{q}}^{\mathrm{t-1}} + \ddot{\mathbf{q}}^{\mathrm{t}})), \quad \text{(A.18)}$$

$$\dot{\mathbf{q}}^{\mathrm{t+1}} - \dot{\mathbf{q}}^{\mathrm{t}} = h(\tfrac{1}{2}(\ddot{\mathbf{q}}^{\mathrm{t}} + \ddot{\mathbf{q}}^{\mathrm{t+1}})), \quad \text{(A.19)}$$

$$\dot{\mathbf{q}}^{\mathrm{t+k}} - \dot{\mathbf{q}}^{\mathrm{t+k-1}} = h(\tfrac{1}{2}(\ddot{\mathbf{q}}^{\mathrm{t+k-1}} + \ddot{\mathbf{q}}^{\mathrm{t+k}})). \quad \text{(A.20)}$$

It follows from Equations (A.18) and (A.19) that the acceleration at time-step t, i.e., $\ddot{\mathbf{q}}^{\mathrm{t}}$, contributes to the change of velocity from $t-1$ to t and from t to $t+1$. Further, Equation (A.20) shows that the change of velocity from $t+k-1$ to $t+k$, for $k \geq 2$, is determined by only the accelerations of its current and previous time-step, i.e., $\ddot{\mathbf{q}}^{\mathrm{t+k}}$ and $\ddot{\mathbf{q}}^{\mathrm{t+k-1}}$ for $k \geq 2$, and hence is independent of $\ddot{\mathbf{q}}^{\mathrm{t}}$.

This completes the proof of Lemma. ■

Proof of Theorem

Suppose the acceleration at any time-step t, $\ddot{\mathbf{q}}^{\mathrm{t}}$, is lost, and we directly set it as zero without any prediction, i.e., $\ddot{\mathbf{q}}^{\mathrm{t}} = 0$. Using Equations (A.13) and (A.19), we can derive the velocity distortion at time-step t, $\Delta\dot{\mathbf{q}}^{\mathrm{t}}$, as:

$$\Delta\dot{\mathbf{q}}^{\mathrm{t}} = \tfrac{1}{2}h\ddot{\mathbf{q}}^{\mathrm{t}}, \quad \text{(A.21)}$$

and the velocity distortion at any subsequent time-step as:

$$\Delta\dot{\mathbf{q}}^{\mathrm{t+k}} = h\ddot{\mathbf{q}}^{\mathrm{t}}, \quad \text{(A.22)}$$

for $k \geq 1$. These are the conclusions from Lemma. By Equation (A.12), the displacement at time-step t is $\mathbf{q}^{\mathrm{t}} = \mathbf{q}^{\mathrm{t-1}} + h\dot{\mathbf{q}}^{\mathrm{t-1}} + \frac{h^2}{2}\left(\frac{1}{2}(\ddot{\mathbf{q}}^{\mathrm{t-1}} + \ddot{\mathbf{q}}^{\mathrm{t}})\right)$. So if the acceleration $\ddot{\mathbf{q}}^{\mathrm{t}}$ is lost, we can then define displacement distortion at time-step t, $\Delta\mathbf{q}^{\mathrm{t}}$, as:

$$\Delta\mathbf{q}^{\mathrm{t}} = \tfrac{1}{4}h^2\ddot{\mathbf{q}}^{\mathrm{t}}. \quad \text{(A.23)}$$

Similarly, from Equation (A.12) we have $\mathbf{q}^{\mathrm{t+1}} = \mathbf{q}^{\mathrm{t}} + h\dot{\mathbf{q}}^{\mathrm{t}} + \frac{h^2}{2}\left(\frac{1}{2}(\ddot{\mathbf{q}}^{\mathrm{t}} + \ddot{\mathbf{q}}^{\mathrm{t+1}})\right)$, and when the acceleration $\ddot{\mathbf{q}}^{\mathrm{t}}$ is lost and by Equation (A.21), the displacement distortion at time-step t+1 is:

$$\Delta\mathbf{q}^{\mathrm{t+1}} = \Delta\mathbf{q}^{\mathrm{t}} + h\Delta\dot{\mathbf{q}}^{\mathrm{t}} + \tfrac{1}{4}h^2\ddot{\mathbf{q}}^{\mathrm{t}} = h^2\ddot{\mathbf{q}}^{\mathrm{t}}. \quad \text{(A.24)}$$

Similarly, using Equation (A.22), the displacement distortion at time-step t+2 is $\Delta\mathbf{q}^{\mathrm{t+2}} = \Delta\mathbf{q}^{\mathrm{t+1}} + h\Delta\dot{\mathbf{q}}^{\mathrm{t+1}} = h^2\ddot{\mathbf{q}}^{\mathrm{t}} + h^2\ddot{\mathbf{q}}^{\mathrm{t}} = 2h^2\ddot{\mathbf{q}}^{\mathrm{t}}$.

By induction, the displacement distortion at any time-step $t+k$, for $k \geq 2$, can be computed as:

$$\Delta\mathbf{q}^{\mathrm{t+k}} = \Delta\mathbf{q}^{\mathrm{t+k-1}} + h\Delta\dot{\mathbf{q}}^{\mathrm{t+k-1}} = kh^2\ddot{\mathbf{q}}^{\mathrm{t}}. \quad \text{(A.25)}$$

The second equality comes from both the induction hypothesis $\Delta\mathbf{q}^{\mathrm{t+k-1}} = (k-1)h^2\ddot{\mathbf{q}}^{\mathrm{t}}$ and Equation (A.22): $\Delta\dot{\mathbf{q}}^{\mathrm{t+k-1}} = h\ddot{\mathbf{q}}^{\mathrm{t}}$.

Therefore, it follows that when the acceleration at time-step t is lost, the displacement distortion from time-step $t+2$ is linear with respect to the change of time (k). ■