Appendix

An $O(1)$ Orientation Comparison Metric:
The RMSD Between Two Orientations of a Rigid Body.

This section describes a method to calculate the sum-squared-distance between the positions of a rigid set of N points after being rotated and translated in two different ways (the rotations and translations are denoted R, $\vec{T}$ and R', $\vec{T'}$).

Definition: metric, Φ

$$\Phi(R, \vec{T}, R', \vec{T'}) = \sum_{\alpha=1}^{N} |(R\vec{x_\alpha} + \vec{T}) - (R'\vec{x_\alpha} + \vec{T'})|^2 \tag{1}$$

where $\vec{x_\alpha}$ = the position of the αth point in question.

Method:
This metric can be calculated with 17 floating-point multiplies, and 15 additions per comparison, independent of the number of points being rotated.

Proof:

Let $\{\vec{r_\alpha}\}$, be the original set of points $\{\vec{x_\alpha}\}$, only translated and rotated so that the principle axis are now aligned with the $\hat{x}$, $\hat{y}$, and $\hat{z}$ axis, and the centroid is located at the origin. Let $\mathcal{R}$, $\vec{\mathcal{T}}$, $\mathcal{R}'$, $\vec{\mathcal{T}}'$, be the same rotations and translations expressed in this new coordinate system. It turns out to be much easier to calculate Φ using this new data-set, $\{\vec{r_\alpha}\}$. Below is a short detour to review principle axis. It can be skipped without loss of continuity.

Principle-Axis

The principle axis of a set of points, $\{\mathbf{\hat{p}_i}\}$ are defined to be the eigenvectors of the matrix χ, where:

$$\chi_{ij} = \sum_{\alpha=1}^{N} (x_{\alpha i} - x_{cm\ i})(x_{\alpha j} - x_{cm\ j}) \tag{2}$$

where $\vec{x_{cm}}$ is the location of the centriod ($\vec{x_{cm}} \equiv \sum_{\alpha=1}^{N} \vec{x_\alpha}/N$) and $x_{cm\ j}$ is its jth component.

Note χ is a symmetric matrix, so its eigenvectors (the principle axis) form an orthogonal basis. This means it is allways possible to rotate and translate our initial coordinate data $\{\vec{x_\alpha}\}$, to a new orientation so that the principle-axis are aligned with the $\hat{x}$, $\hat{y}$, and $\hat{z}$ axis, and the centroid at the origin. We rename the rotated, translated data $\{\vec{r_\alpha}\}$.

The transformation between these two sets of data is:

$$\vec{x_\alpha} = P\vec{r_\alpha} + \vec{x_{cm}} \tag{3}$$

where P is a 3x3 pure rotation matrix (determinant 1) storing the 3 normalized principle-axis as column vectors P $\equiv [\hat{\mathbf{p_1}}, \hat{\mathbf{p_2}}, \hat{\mathbf{p_3}}]$ We go to all this trouble because this new set of points $\{\vec{r_\alpha}\}$ has the following desireable properties: (which you can verify by substituting Eq.(3) into Eq.(2))

$$\sum_{\alpha=1}^{N} \vec{r_\alpha} = \vec{0} \tag{4}$$

$$\sum_{\alpha=1}^{N} r_{\alpha i} r_{\alpha j} = \lambda_i \delta_{ij} \tag{5}$$

where $r_{\alpha j}$ = the jth component of $\vec{r_\alpha}$, where δ_{ij} is the Kronecker-Delta function, ($\delta_{ij} \equiv 1$ if $i = j$, and 0 otherwise) and λ_1, λ_2, and λ_3 are the eigenvalues corresponding to $\hat{\mathbf{p_1}}$, $\hat{\mathbf{p_2}}$, $\hat{\mathbf{p_3}}$.

In order to express Φ, in terms of $\{\vec{r_\alpha}\}$, instead of $\{\vec{x_\alpha}\}$ we need to modify R, $\vec{T}$, R', and $\vec{T'}$. in order to compensate for the rotation and translation we just applied. Substituting Eq.(3) into Eq.(1) yeilds:

$$\Phi = \sum_{\alpha=1}^{N} |(\mathcal{R}\vec{r_\alpha} + \vec{\mathcal{T}}) - (\mathcal{R}'\vec{r_\alpha} + \vec{\mathcal{T}'})|^2 \tag{6}$$

where:

$$\mathcal{R} \equiv RP$$
$$\mathcal{R}' \equiv R'P$$
$$\mathcal{T} \equiv P\vec{x_{cm}} + \vec{T}$$
$$\mathcal{T}' \equiv P\vec{x_{cm}} + \vec{T}'$$

Calculating Φ

Suppose
$\Delta\vec{r_\alpha}$ = the displacement vector of the αth point between the two orientations and $\Delta r_{\alpha\nu}$ is its νth component.
Re-expressing Eq.(6) in terms of components, we get:

$$\Phi = \textstyle\sum_{\alpha=1}^{N} \sum_{\nu=1}^{3} (\Delta r_{\alpha\nu})^2$$

where

$$(\Delta r_{\alpha\nu})^2 = \left(\sum_{i=1}^{3} (\mathcal{R}_{\nu i} r_{\alpha i} + \mathcal{T}_\nu) - (\mathcal{R}'_{\nu i} r_{\alpha i} + \mathcal{T}'_\nu) \right) \left(\sum_{j=1}^{3} (\mathcal{R}_{\nu j} r_{\alpha j} + \mathcal{T}_\nu) - (\mathcal{R}'_{\nu j} r_{\alpha j} + \mathcal{T}'_\nu) \right) \tag{7}$$

When we expand the square, we can exploint the property that the centroid is at the origin, Eq.(4). This enables us to throw away the terms with odd powers of $r_{\alpha i}$, (for example: $\mathcal{R}_{\nu i} r_{\alpha i} \mathcal{T}_\nu$) since they will be annihilated when we eventually sum over α. Making these changes and collecting equivalent terms, Eq.(7) reduces to:

$(\Delta r_{\alpha\nu})^2 = \sum_{i,j=1}^{3}(\mathcal{R}_{\nu i}\mathcal{R}_{\nu j}r_{\alpha i}r_{\alpha j} - 2\mathcal{R}_{\nu i}\mathcal{R}'_{\nu j}r_{\alpha i}r_{\alpha j} + \mathcal{R}'_{\nu i}\mathcal{R}'_{\nu j}r_{\alpha i}r_{\alpha j}) + (\mathcal{T}_\nu - \mathcal{T}'_\nu)^2$

Summing over ν:

$$\sum_{\nu=1}^{3}(\Delta r_{\alpha\nu})^2 = \sum_{i,j=1}^{3}(\delta_{ij}r_{\alpha i}r_{\alpha j} - 2\sum_{\nu=1}^{3}\mathcal{R}_{\nu i}\mathcal{R}'_{\nu j}r_{\alpha i}r_{\alpha j} + \delta_{ij}r_{\alpha i}r_{\alpha j}) + \sum_{\nu=1}^{3}(\mathcal{T}_\nu - \mathcal{T}'_\nu)^2 \tag{8}$$

In this last step, we exploited the orthonormality of the rotation matrices $\mathcal{R}$ and $\mathcal{R}'$)

Now, by summing Eq.(8) over α, and exploiting Eq.(5), we can simplify Eq.(6) to get:

$$\begin{aligned}\Phi &= \textstyle\sum_{i,j=1}^{3}(2\delta_{ij}\lambda_i\delta_{ij} - 2\sum_{\nu=1}^{3}\mathcal{R}_{\nu i}\mathcal{R}'_{\nu j}\lambda_i\delta_{ij}) + N\sum_{\nu=1}^{3}(\mathcal{T}_\nu - \mathcal{T}'_\nu)^2 \\ &= 2\sum_{i=1}^{3}\lambda_i(1 - \sum_{\nu=1}^{3}\mathcal{R}_{\nu i}\mathcal{R}'_{\nu i}) + N\sum_{\nu=1}^{3}(\mathcal{T}_\nu - \mathcal{T}'_\nu)^2 \end{aligned} \tag{9}$$

$\square$

Property:

RMSD($\sqrt{\Phi/N}$) obeys the
Triangle Inequality:

$$\sqrt{\Phi(R,\mathbf{T},R'',\mathbf{T}'')/N} \leq \sqrt{\Phi(R,\mathbf{T},R',\mathbf{T}')/N} + \sqrt{\Phi(R',\mathbf{T}',R'',\mathbf{T}'')/N} \tag{10}$$

Proof: Let
$\mathbf{X}_\alpha \equiv R\mathbf{x}_\alpha + \mathbf{T}$
$\mathbf{X}'_\alpha \equiv R'\mathbf{x}_\alpha + \mathbf{T}'$

Notice that the set of values $\{X_{\alpha\nu}\}$ (ie. the set of all components of $\mathbf{X}_\alpha$) itself forms a "vector" in a $3N$ dimensional space, and:

$$\Phi = \textstyle\sum_{\alpha,\nu}(X_{\alpha\nu} - X'_{\alpha\nu})^2$$

So $\sqrt{\Phi(R,\mathbf{T},R',\mathbf{T}')}$ is simply a straight evenly weighted Euclidian-length of the differences between the primed and unprimed versions of $X_{\alpha\nu}$, all the components of all the vectors. For any finite-dimensional space of real numbers, Euclidian length, obeys the triangle innequality.