Euler Angle Computation in the CLHEP **Vector** Package

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Version 1.0, April 24, 2003

The naive (though algebraically sound) technique for extracting `HepEulerAngles` from a `HepRotation` is flawed when the `HepRotation` represents a rotation very nearly around the Z axis, in the presence of small round-off induced errors in the values of the rotation matrix components. By flawed, we mean that when the resulting Euler angles are used to reconstruct the `HepRotation`, that reconstructed `HepRotation` may be quite different from the original.

This document will illustrate the mechanism by which this flaw comes up, and will derive and justify a superior algorithm for calculationg the proper euler angles.

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1 The Naive Algorithm

The relation between the Eueler Angles and a `HepRotation` R is given by:

$$\vec{v}.\mathrm{rotate}(\phi,\theta,\psi) \Longrightarrow$$

$$\begin{pmatrix} \cos\psi\cos\phi - \sin\psi\cos\theta\sin\phi & \cos\psi\sin\phi + \sin\psi\cos\theta\cos\phi & \sin\psi\sin\theta \\ -\sin\psi\cos\phi - \cos\psi\cos\theta\sin\phi & -\sin\psi\sin\phi + \cos\psi\cos\theta\cos\phi & \cos\psi\sin\theta \\ \sin\theta\sin\phi & -\sin\theta\cos\phi & \cos\theta \end{pmatrix} \begin{pmatrix} v_x \\ v_y \\ v_z \end{pmatrix} \tag{1}$$

As of CLHEP 1.8, the algorithm for comupting Euler angles (ψ, θ, ϕ), glossing over special cases, was as follows:

1. Find θ by taking $\cos^{-1} R_{zz}$ and $\sin\theta = \sqrt{1 - R_{zz}^2}$. By definition, θ is in quadrant I or II, and $\sin\theta \geq 0$.

2. Knowing the form of $R_{zy} = -\sin\theta\cos\phi$, extract $\cos|\phi| = -R_{zy}/\sin\theta$.

3. Similarly, $\cos|\psi| = +R_{yz}/\sin\theta$.
4. Taking the arc cosine of the expressions just computed gives $|\phi|$ and $|\psi|$. The signs of ψ and ϕ are assigned so as to yield proper signs for R_{zx} and R_{xz} respectively; if one or both of those is zero then demand instead the proper sign for R_{zy} and/or R_{yz}.
5. The case where $R_{zz} = \pm 1$ is treated specially. In that case, there is a freedom to tradeoff values of ψ and ϕ, and an arbitrary rule is imposed: $\psi = R_{zz}\phi$.

2 The Potential Flaw

The above algorithm is analytically correct, but if one perturbs $R_{ij} \to R_{ij} + \epsilon_{ij}$ for some set of $\epsilon_{ij} << 1$, then $\psi \to \psi + \delta\psi$ and $\phi \to \phi + \delta\phi$ where, if $\sin\theta << 1$ then $\delta\psi$ and $\delta\phi$ need not be small.

To illustrate: Say R represents a rotation by angle μ about the Z axis, but R_{zz} is perturbed to be $1-\epsilon$ while none of the other components in the Z row or column–the components with value 0 for a Z rotation–are perturbed. Now a rotation by angle μ about the Z axis falls into the ambiguous case, where any answer with $\theta << 1$ and $\psi + \phi \sim \mu$ would be acceptable.

However, the algorithm described above will assign a tiny *but non-zero* value to $\sin\theta$. So it will decide that the divisions in $\cos|\psi| = -R_{zy}/\sin\theta$ and $\cos|\phi| = +R_{yz}/\sin\theta$ are valid operations. Of course, since the numerators are exactly zero, it does not matter that the denominators are small; these will say that $|\psi| = \pi/2$ and $|\phi| = \pi/2$.

Then the algorithm attempts to determine the signs of ψ and ϕ; and the actual code gets into futher trouble since it knows that $\sin\theta$ is non-zero, thus it is "impossible" (yet true) to have all four of $R_{xz}, R_{yz}, R_{zx}, R_{zy} = 0$. But no matter how clever the algorithm at that point, once it is decided that $|\psi| = |\phi| = \pi/2$ there is no way to recover the proper relationship $\psi + \phi \sim \mu$. And in fact, if you form a `HepRotation` from the computed Euler angles, you will either get something close to the identity matrix, or something close to a 180 degree rotation about the Z axis–neither of which resembles the original matrix in the least!

In general, if the `HepRotation` represents any rotation about some axis making an angle with the Z axis which is smaller than or comparable to the uncertainty in the matrix elements, then the algorithm used in CLHEP 1.8 and earlier is flawed in this way.

3 Deriving The New Algorithm

It is true that for $1 - |R_{zz}|$ small, the exact values of Euler angles depend sensitively on the values of all the matrix components. Thus the problem of extracting Euler angles for such cases is numerically unstable. But this is not fatal; what we want is a set of Euler angles that comes very close to properly representing the rotation matrix, and if other sets of Euler angles would also come close, we don't mind not finding them.

Fortunately, the problem of extracting Euler angles in the presence of perturbations of the matrix elements, such that the reconstructed matrix will match the original up to differences of the same order as those perturbations, is tractable and numerically stable, as we now show.

We start with the observations that

$$R_{xx} + R_{yy} = +\cos(\psi+\phi)(1+\cos\theta) \tag{2}$$
$$R_{xx} - R_{yy} = +\cos(\psi-\phi)(1-\cos\theta) \tag{3}$$

If R_{zz} is non-negative, $(1+\cos\theta) \geq 1$, while if R_{zz} is negative, $(1-\cos\theta) > 1$; so one of the above equations can always be used to determine $|\psi \pm \phi|$ with no risk of division by a small quantity. And if $|R_{zz}|$ is not close to 1, both equations are numerically stable so both combinations can be found.

Still working in the X-Y sector,

$$R_{xy} - R_{yx} = +\sin(\psi+\phi)(1+\cos\theta) \tag{4}$$
$$R_{xy} + R_{yx} = -\sin(\psi-\phi)(1-\cos\theta) \tag{5}$$

We also observe, in the Z sector, that

$$R_{xz}R_{zx} - R_{yz}R_{zy} = +\cos(\psi-\phi)(\sin^2\theta) \tag{6}$$
$$R_{xz}R_{zx} + R_{yz}R_{zy} = -\cos(\psi+\phi)(\sin^2\theta) \tag{7}$$

And

$$R_{xz}R_{zy} + R_{yz}R_{zx} = -\sin(\psi-\phi)(\sin^2\theta) \tag{8}$$
$$R_{xz}R_{zy} - R_{yz}R_{zx} = -\sin(\psi+\phi)(\sin^2\theta) \tag{9}$$

Finally, we note that if we can determine cosine and sine of the sum and the difference of ψ and ϕ in a numerically stable manner, then that determines ψ and ϕ in a stable manner.

All the above relations are all stable except when $1-|R_{zz}| \sim 0$. So except when $1-|R_{zz}| \sim 0$ we can use either the Z sector, or the X-Y sector, or for that matter the simple $R_{xz}/\sin\theta$ and $R_{yz}/\sin\theta$ forms used by the naive algortihm.

When $R_{zz} \sim 1$, the entire Z sector becomes numerically unstable, as do the relations determining $\cos(\psi-\phi)$ and $\sin(\psi-\phi)$ in the X-Y sector. That is not so terrible, since at $R_{zz}=1$ only the value of $\psi+\phi$ is relevant; $\psi-\phi$ is moot.

Similarly, when $R_{zz} \sim -1$, the Z sector is numerically unstable, and the relations determining $\cos(\psi+\phi)$ and $\sin(\psi+\phi)$ in the X-Y sector are useless, but only the value of $\psi-\phi$ is relevant; $\psi+\phi$ is moot.

So what is needed is some method which always gives the correct values for meaningful quantities, and sensible values for the moot quantities. The way to accomplish this is to combine the relations determining sin and cos of the "moot" quantities, so as to find (for the $R_{zz} \sim 1$ case) $\psi-\phi = \tan^{-1}\frac{-(R_{xy}+R_{yx})}{R_{xx}-R_{yy}}$. In this fraction, the factors of $1-\cos\theta$ cancel one another.

Computing $\psi-\phi$ as an arctan would force it to lie between $-\pi/2$ and $\pi/2$. How can we detect when the correct value is outside that range? We could look at the sign of $\sin(\psi-\phi)$, that is to say, the sign of $-(R_{xy}+R_{yx})$. This would tell us whether to use the result of arctan directly or to add or subtract π. On the other hand, it is much easier to use the function *atan2(s/c)*, which does this work for you.

One would expect from the above reasoning that when R is slightly perturbed in a pseudo-random manner, the formulae given would reproduce the original Euler angles more closely than the "naive" formulae described earlier. A bit of mathematical experimentation verifies that this is so–the new formulae are about an order of magnitude less sensitive to fluctuations which violate the orthogonality of R.

Two improvements are tempting, but turn out to be harmful. Both address the issue of attempting to morph smoothly to the action taken when $|R_{zz}|=1$ precisely (in which case we by fiat choose $\psi = R_{zz}\phi$). Sometimes in computing the potentially moot combination of ψ and ϕ, the magnitude of the value computed for $\cos(\psi\pm\phi)(1\mp\cos\theta)$ exceeds $(1\mp\cos\theta)$. It may then be thought that the arithmetic is telling you to consider that denominator as illogically large, and just treat the arctan of that combination as zero (that is, force $\psi = \pm\phi$). This turns out to introduce a flaw in the result (in the sense discussed above) most times that this "improvement" is applied. Similarly, one can check that the sign of the X-Y sector expression for $\sin(\psi \pm \phi)$ matches the sign of the expression for the same $\sin(\psi \pm \phi)$ computed from components in the Z sector, and if they do not match, treat this as an indication that the combination is moot and set $\psi = \pm\phi$. Again, most times this opportunity presents itself, setting $\psi = \pm\phi$ introduces a flaw into the answer.

However, one correction of significance must be applied: The algorithm described will always impute values for $\psi \pm \phi$ which are in the range $(-\pi, \pi]$. But clearly the actual values of ψ and ϕ can can have a sum or difference anywhere in $(-2\pi, 2\pi]$. Getting this wrong will manifest itself as an error by π in the computed values of ψ and ϕ.

This can be dealt with by bringing in information in the Z-sector: If ψ (or ϕ) has the wrong sign relative to that which can be read off the last column or row, then one should add or subtract π from *both* ψ and ϕ. Here, when $|R_{zz}| \sim 1$, there is the potential for numerical instability; fortunately, in such cases only the value of one combination $\psi \pm \phi$ is relevant when re-expressing the rotation matrix. So as long as the correction is applied to both ψ and ϕ or neither, the result (in such a case) is not truly flawed.

There are, of course, four possible terms in the Z-sector to use to ask whether we have the wrong value for ψ and ϕ:

1. R_{xz}: If $\sin\psi > 0$ then $\psi > 0$.
2. R_{yz}: If $\cos\psi > 0$ then $|\psi| < \pi/2$.
3. R_{zx}: If $\sin\phi > 0$ then $\phi > 0$.
4. R_{yz}: If $-\cos\phi < 0$ then $|\psi| < \pi/2$.

The most stable algorithm will use that quantity among those four which is largest in absolute value.

4 The New Algorithm

The algorithm uses only the X-Y sector and R_{zz}. $\cos\theta = R_{zz}$ and this determines θ.
If $R_{zz} \geq 0$ the primary stable quantity is $\psi + \phi$:

1. Compute $\psi + \phi = \tan^{-1}\frac{R_{xy} - R_{yx}}{R_{xx} + R_{yy}}$. With the numerator and denominator in this form we can get the proper value of $\psi + \phi$ (including the proper quadrant) by using the *atan2(s/c)* function.
2. Compute $\psi - \phi = \tan^{-1}\frac{-(R_{xy} + R_{yx})}{R_{xx} - R_{yy}}$.

If $R_{zz} < 0$ the primary stable quantity is $\psi - \phi$:

1. Compute $\psi - \phi = \tan^{-1}\frac{-(R_{xy} + R_{yx})}{R_{xx} - R_{yy}}$. We put the numerator and denominator in this form so that we can get the proper value of $\psi - \phi$ (including the proper quadrant) by using the *atan2(s/c)* function.
2. Compute $\psi + \phi = \tan^{-1}\frac{R_{xy} - R_{yx}}{R_{xx} + R_{yy}}$.

Then, in either case, compute $\psi = \frac{1}{2}\left[((\psi + \phi) + (\psi - \phi)\right]$ and $\phi = \frac{1}{2}\left[((\psi + \phi) - (\psi - \phi)\right]$.
Finally, apply the potential $\pm\pi$ corrections, based on the largest of $|R_{xz}|, |R_{yz}|, |R_{zx}|, |R_{zy}|$:

1. $If R_{xz} > 0$ and $\psi < 0$ then correct ψ and ϕ.
2. $If R_{yz} > 0$ and $|\psi| > \pi/2$ then correct ψ and ϕ.
3. $If R_{zx} > 0$ and $\phi < 0$ then correct ψ and ϕ.
4. $If R_{zy} < 0$ and $|\psi| > \pi/2$ then correct ψ and ϕ.

In each case, to "correct" a quantity means to add π if negative, or to subtract π if positive.

5 Accuracy of a Reconstricted R

Ultimately,if one perturbs $R_{ij} \to R_{ij} + \epsilon_{ij}$ for some set of ϵ_{ij} each of which is of order $\epsilon << 1$, then one has a non-orthogonal matrix. There is no reason to believe that one can perfectly extract Euler angles from such a matrix, and in fact, any manner of approximating the Euler angles will have the following property: A matrix reconstructed from those Euler angles will be perfectly orthogonal (to within achine roundoff errors) and therefore *cannot precisely match the original matrix.*

The naive size of the resulting unavoidable "flaw" is of order ϵ, but in fact (except in special cases such as $\theta \sim \pi/2$) in general the flaw goes as $\sqrt{\epsilon}$. This can easily be seen from the fact that when $R_{zz} = \cos\theta$ is perturbed by ϵ, unless R_{zz} is very small, $\sin\theta$ is perturbed by $O(\sqrt{\epsilon})$. And $\sin\theta$ does appear multiplying terms in the Z row and column, so at least these terms are vulnerable to errors of order $O(\sqrt{\epsilon})$.