BABAR Note #1560, Version 1

New Cluster Splitter/ Photon Finder for the *BABAR* EMC

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August 4, 2006

Abstract

This document describes a scheme under development for photon finding and cluster splitting using a χ^2 fit to incident four-momentum by performing a quasi-analytic integration of a shower shape parameterization in the CsI in three dimensions over the crystal volume.

1 Introduction

This note details a scheme under development for cluster splitting of π^0's and to improve position resolution for photons. It performs a χ^2 fit to incident four-momentum and involves performing a quasi-analytic integration of a shower shape parameterization in the CsI in three dimensions over each crystal volume. The scheme allows for a fit to the shower location and energy; transverse and longitudinal scale parameters; and allows for showers that originate away from the interaction point (e.g. for use in K short reconstruction).

2 The XT_Fitter Class

The XT_Fitter class provides the interfaces for fitting to single photons, composite π^0's or π^0's merged to one or two bumps. It makes initial guesses for the kinematic parameters and performs the χ^2 fit. Each XT_Fitter object performs a minimization of the function:

$$\chi^2(\xi_{[n]}) = \sum_m \left[\frac{E_{[m]} - \left(\sum_n \Delta E_{nm} \right)}{\sigma_{E_{[m]}}} \right]^2 \tag{1}$$

where $E[m]$ is the digi energy in crystal m, and ΔE_{nm} is the calculated energy that would be deposited in crystal m by the n^{th} photon cascade if we assume the cascade is well described by the parameter set:

$$\xi_{[n]} = \left\{ E_{0[n]}, \theta_{t[n]}, \phi_{t[n]}, x_{0[n]}, y_{0[n]}, z_{0[n]}, W_{[n]}, \lambda_{r[n]} \right\} \tag{2}$$

where:

- $E_{0[n]}$ is the hypothesis for incident energy of the n^{th} gamma
- $x_{0[n]}, y_{0[n]}$, and $z_{0[n]}$ give the hypothesis for first hard interaction point in the n^{th} cascade
- $\theta_{t[n]}$ and $\phi_{t[n]}$ are the hyptheses for azimuth and polar angles of the n^{th} gamma momentum axis
- $W_{[n]}$ is a longitudinal shower scale parameter described below
- $\lambda_{r[n]}$ is a transverse shower scale parameter described below.

The details of the evaluation of the χ^2 function are discussed below.

2.1 The interface for XT_Fitter

For a single photon:

$$XT\_Fitter\ the\_XT\_Fitter(EmcCluster * theCluster);$$

Successfully reconstructed photons are flagged by a Boolean:

$the\_XT\_Fitter.valid\_photon$

To split a two bump cluster, as for π^0's merged to two bumps:

$$XT\_Fitter\ the\_XT\_Fitter(map\langle TwoCoordIndex*, EmcBump*, BbrPtrLess\rangle \& theIndexedBumps);$$

Successfully reconstructed π^0's are flagged by a Boolean:

$the\_XT\_Fitter.valid\_Pi0$

and the energy (in MeV) and position of the two photons are given by:

$the\_XT\_Fitter.Photon\_E[0];$
$the\_XT\_Fitter.Photon\_E[1];$
$the\_XT\_Fitter.Photon\_pos[0];$
$the\_XT\_Fitter.Photon\_pos[1];$

And the interface for one π^0's merged to one bump is:

$$XT\_Fitter\ the\_XT\_Fitter(map\langle TwoCoordIndex*, EmcBump*, BbrPtrLess\rangle \& theIndexedBumps, bool\&\ split\_Single);$$

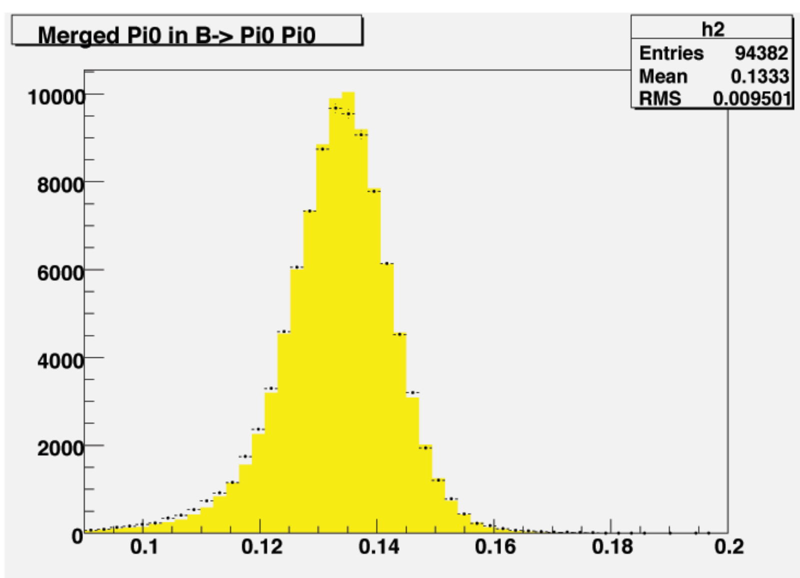

Figure 1: The π^0 mass peak for merged π^0 two bumps in $B \to \pi^0\pi^0$ Monte Carlo. In yellow is the result for this reconstruction algorithm, the tick marks give the mass as determined from production code.

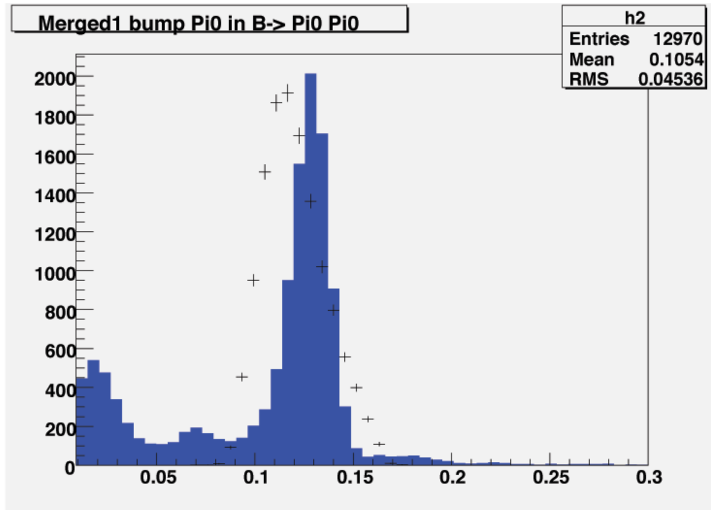

Figure 2: The π^0 mass peak for π^0 merged to one bump in $B \to \pi^0\pi^0$ Monte Carlo. In blue the result this reconstruction algorithm, the tick marks give the mass as determined from second moment analysis (the current production splitter does not split single bumps).

3 The Shower Shape Parameterization

The parameterization of the shower corresponds approximately to that of del Peso and Ros [2] as implemented in ASLUND for the *BABAR* EMC by D. Bernard[3].

To integrate the deposited energy, we assume cylindrical symmetry of the showers and integrate:

$$dE_{dep} = E_0 \; f_z(z) \; f_r(r) \; \tfrac{1}{2\pi} d\phi dz dr \tag{3}$$

The longitudinal shape is the standard one:

$$f_z(z) = \frac{\beta\,(\beta z)^{\alpha-1}\, e^{-\beta z}}{\Gamma\,(\alpha)} \tag{4}$$

and the transverse shower shape is given by:

$$f_r(r) = \frac{\left(\sqrt{\frac{r}{\lambda_r}}\right)^{\alpha_r - 2} e^{-\sqrt{\frac{r}{\lambda_r}}}}{2\lambda_r \Gamma\,(\alpha_r)} \tag{5}$$

.

Here α_r is linear in longitudinal depth z:

$$\alpha_r = \alpha_{0r} + \alpha_r^{/} z \tag{6}$$

so α_{0r}, $\alpha_r^{/}$, and α_r determine the lateral shower shape. In order to facilitate integration, the del Peso and Ros form for transverse shower shape is modeled by a sum of three terms of the Grindhammer type.

$$f_r(r) = \frac{\varepsilon_1 2rR_1^2}{(r^2+R_1^2)^2} + \frac{\varepsilon_2 2rR_2^2}{(r^2+R_2^2)^2} + \frac{(1-\varepsilon_1-\varepsilon_2)\,2rR_3^2}{(r^2+R_3^2)^2} = \sum\nolimits_l \frac{\varepsilon_l 2rR_l^2}{(r^2+R_l^2)^2} \qquad (7)$$

The values for R_l and ϵ_l are determined from fitted polynomials functions of α_r and λ_r which match the del Peso and Ros form of note #476 as closely as possible.

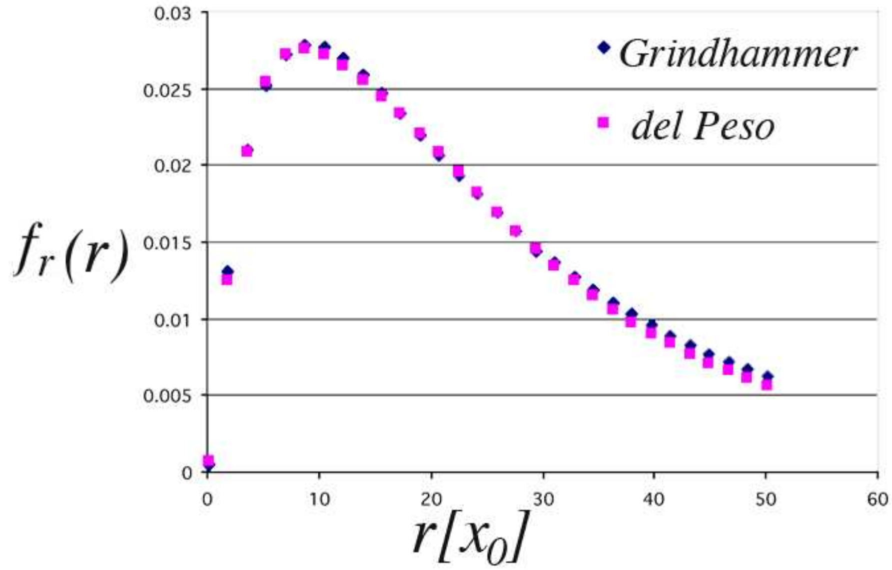

Figure 3: Transverse Energy Distribution of Del Peso (Pink) and Approximation by Grindhammer Sum (Blue).

Figure 3 shows the del Peso transverse distribution in pink and the Grindhammer sum approximation in blue for a particular choice of shower energy and depth.

As implemented for *BABAR*, the product $V = \alpha\beta$ and parameters α_{0r} and $\alpha_r^{/}$ are fixed to their average values as a function of $logE_0$. W is the ratio $W = \alpha/\beta$ where α and β are the parameters used in $f_z(z)$. In a calorimeter with longitudinal segmentation it would be desirable to fit to W at fixed V. In applying this method to *BABAR*, we fix W at its average value.

With longitudinal segmentation the choice of W as a fitting parameter would be motivated by the fact that the longitudinal shower profile depends strongly on the ratio α/β when the product $\alpha\beta$ is held constant, but depends weakly on the product when the ratio is fixed. Figure 4 is reproduced from BaBar note #476. In the lower left $f_z(z)$ is plotted for different values of the product V while the ratio W is held constant. In the lower right $f_z(z)$ is plotted for different values of the ratio while the product is held constant.

4 The Xtl_Con, FP_Set and Xtl_Increment Classes

Three classes have been developed to perform the 3-D integration of the shower shape over the crystal volume: the Xtl_Con, FP_Set, and Xtl_Increment classes. There is one FP_Set object for every cascade and one Xtl_Con object for every affected crystal. The FP_Set class contains the fitting parameters set $\xi_{[n]}$ for one cascade and various quantities derived from them. Xtl_Con contains geometrical information about the individual crystal and performs the summation of crystal energy over all cascades. Xtl_Increment contains the calculated contribution to energy in one crystal due

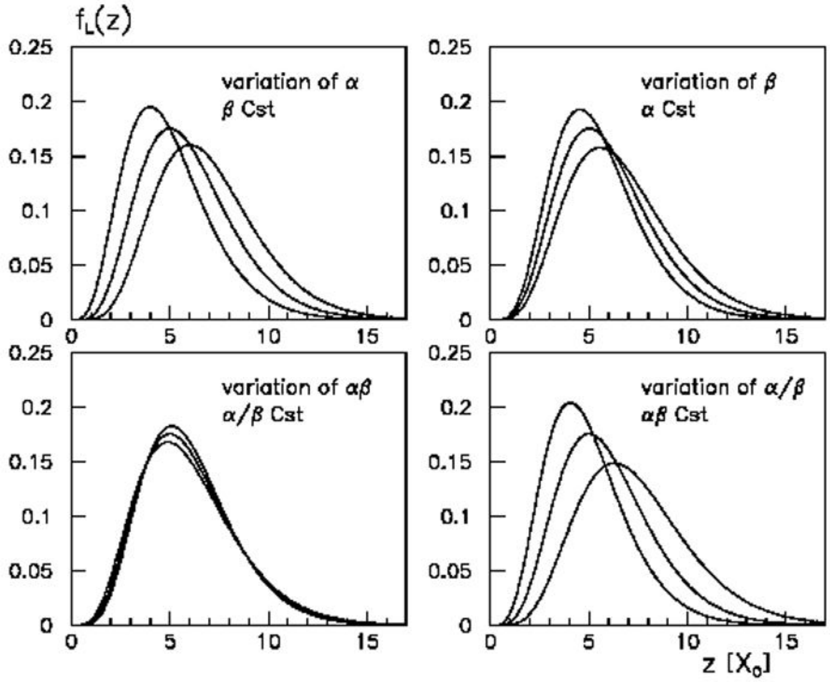

Figure 4: Figure take from *BABAR* note # 476. Longitudinal energy profiles are shown for various choices of α and β. In the upper left the profiles for three different choices of α are shown for the same choice of β. At the upper right, the profiles for three values of β at fixed α. At the lower left three profiles are shown for different values of the product $V = \alpha\beta$ while the ratio $W = \alpha/\beta$
is fixed. At the lower right three profiles are given for different W values for fixed V.

to one cascade, i.e. the contribution to one Xtl_Con object due to one FP_Set object; it is the class which integrates the incremental contribution to the energy in a given crystal when passed a pointer to an object of type FP_Set.

4.1 The Xtl_Increment Class Integration of Crystal Energy

The Xtl_Increment class provides the approximate 3-D integral of the energy shape parameterization over the trapezoidal volume of a CsI crystal in the BaBar EMC. The 3-D integral is approximated by summing over contributions from various layers of depth within the crystal. The position and direction at impact on the crystal face are projected as a ray through the crystal of incidence. Planes perpendicular to this ray are defined at regular intervals in shower depth z as shown in figure Figure 5. The intersection of these planes with the outline of the crystal (as extracted from the EmcXTal::PhysicalOutline routine and stored in Xtl_Con) are determined and the contribution from each slice is given by:

$$\Delta E_{[mn]} = \left[\left(\sum_i dedx_{[in]} \times \sum_{lj} Trans_{[ijlmn]}\right)\right] \times E_{0[n]} \tag{8}$$

where $Trans_{[ijlmn]}$ is defined as the fraction of the energy in the i^{th} plane of cascade n that is contributed by th l^{th} term in the Grindhammer expansion to crystal m by integrating over a triangle defined by three vertices at:

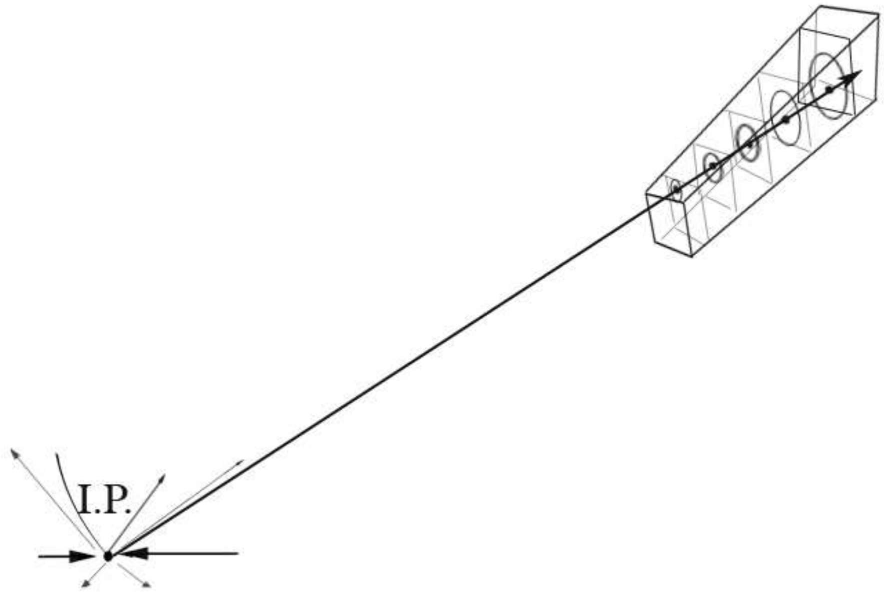

Figure 5: The 3-D integration sums over slices transverse to the projected trajectory.

a) the point where the n^{th} photon trajectory crosses the i^{th} plane of shower n;
b) the point of the intersection of plane i of shower n with the j^{th} edge of the crystal m;
c) the point of intersection between the plane i and the j+1st edge of the crystal m.

The definition of $dEdx_{[in]}$ is the longitudinal weight for the slice i of cascade n:

$$dEdx_{[in]} = \frac{\left(\beta_{[n]} z_i\right)^{\alpha_{[n]}-1} e^{-\beta_{[n]} z_i}}{\sum\limits_j \left(\beta_{[n]} z_j\right)^{\alpha_{[n]}-1} e^{-\beta_{[n]} z_j}} \tag{9}$$

with z_i being the depth beyond the shower origin of the i^{th} slice in radiation lengths as calculated in FP_Set.

The integration over a transverse cross sectional slice through the crystal of incidence is accomplished by dividing the slice into triangles. Figure 6a) represents one such cross sectional slice (viewed from the I.P.), the dot represents the projection of the incident particle trajectory through this slice. The grey shading suggests the transverse energy deposition profile in that slice. Figure 6b) shows the four triangles over which the transverse energy distribution function $f_r\left(r\right)$ need to be integrated and summed over to obtain the value $Trans_{[ijlmn]}$ for this slice. To perform the integration of the transverse profile over a neighboring crystal instead, there would be some combination of integrals over four triangles, some added and some subtracted to form $Trans_{[ijlmn]}$ as in 6c). Each of the four triangles can be rendered as the sum or difference of two right triangles as in figure 6d) and 6e).

This is done because the Grindhammer form can be integrated over an arbitrary right triangle with a corner at the origin as in Figure 7:

$$I(a,b) = \int_{\phi=0}^{\arctan\beta} \int_{r=0}^{a/\cos\phi} \frac{2rR^2}{\left(r^2+R^2\right)^2} dr d\phi \tag{10}$$

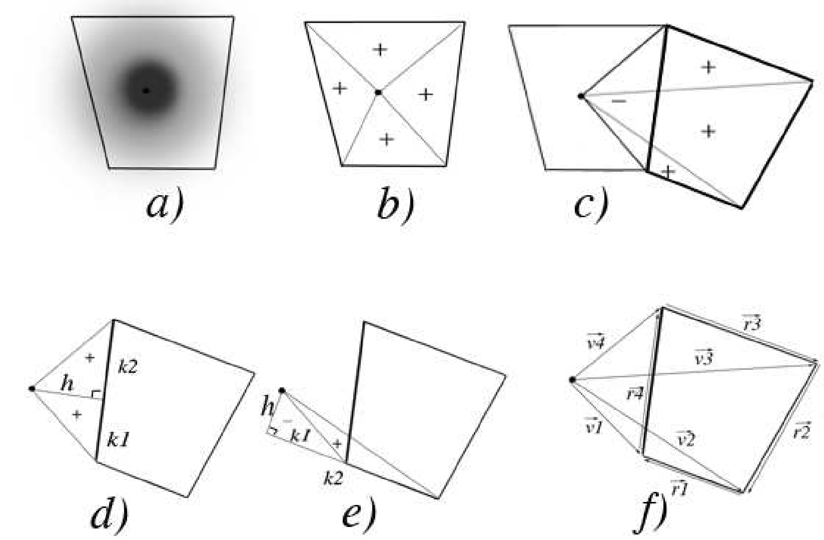

Figure 6:
The analytic integration of the transverse Grindhammer shape is performed over right triangles as described in the text.

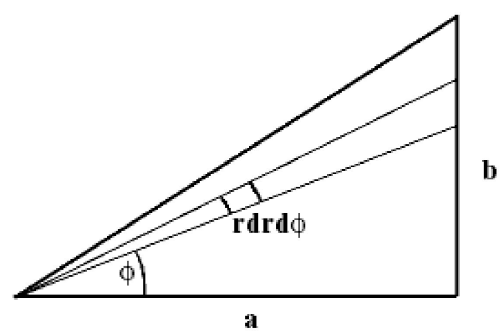

Figure 7: The integration variables.

which evaluates to:

$$I(a,b) = \frac{a}{2\pi\sqrt{a^2+R^2}}\tan^{-1}\left(\frac{b}{\sqrt{(a^2+R^2)}}\right) \tag{11}$$

The integral over each of the four component triangles is calculated as the difference of two right triangles:

$$Trans_{ij} = I(h_{ij}, k1_{ij}) - I(h_{ij}, k2_{ij}) \tag{12}$$

I(a,b) is an odd function of both arguments so that Trans has the same form whether the two right triangles should be added or one subtracted from the other, and whether the projected trajectory traverses this crystal or a neighbor, provided the quantities h, k1, and k2 are properly signed. The full procedure for determining h, k1, and k2 is described below.

4.2 Minimization of Chi-Squared and its Derivatives in XT_Fitter:

Minimization of:

$$\chi^2 = \sum_m \left[\frac{E_{[m]} - \left(\sum_n \left[\left(\sum_i dedx_{[in]} \times \sum_{lj} Trans_{[inmlj]} \right) \right] \times E_{0[n]} \right)}{\sigma^2_{E_{[m]}}} \right]^2 \tag{13}$$

with:

$$\sigma^2_{E_{[n]}} = A + BE_{[n]} \tag{14}$$

is accomplished using the a fitting procedure of the non-linear least-squares type due to Marquardt [1]. The initial guesses for the fitting parameters come from the current production splitter in the case of single photons,

In the case of composite π^0's, or π^0's merged to two bumps:

- $InitialE_{0[n]}$, $x_{0[n]}, y_{0[n]}$, and $z_{0[n]}$ values are derived from the cluster energy and centroid.
- $\theta_{t[n]}$ and $\phi_{t[n]}$ are constrained by the ray from the I.P to $\left(x_{0[n]}, y_{0[n]}, z_{0[n]}\right)$.
- $W_{[n]}$ is constrained to its average value as a function of $lnE_{0[n]}$.
- $\lambda_{r[n]}$ initial value is its average value as a function of $lnE_{0[n]}$.

In the case of the π^0's merged to one bump, XT_Fitter finds an axis along which to split the bump via a scheme using a cluster shape calculation. We minimize:

$$\frac{\partial}{\partial \alpha} \left[\sum_i (\vec{r}_i \bullet \vec{\alpha})^2 E_i^2 \right] = 0 \tag{15}$$

where

$$\vec{r}_i = \vec{x}_i - \langle \vec{x} \rangle \tag{16}$$

is the displacement vector from the shower centroid to the center of the i^{th} crystal, as in figure 8. If we evaluate the dot product with respect to local coordinates with axes corresponding roughly to the crystal theta and phi edges:

$$\sum_i 2E_i^2 \left(r_{ix} \cos\alpha + r_{iy} \sin\alpha \right) \left(-r_{ix} \sin\alpha + r_{iy} \cos\alpha \right) = 0 \tag{17}$$

or:

$$\alpha = \tfrac{1}{2} \arctan \left(\frac{2 \sum_i E_i^2 r_{ix} r_{iy}}{\sum_i E_i^2 \left(r_{iy}^2 - r_{ix}^2 \right)} \right) \tag{18}$$

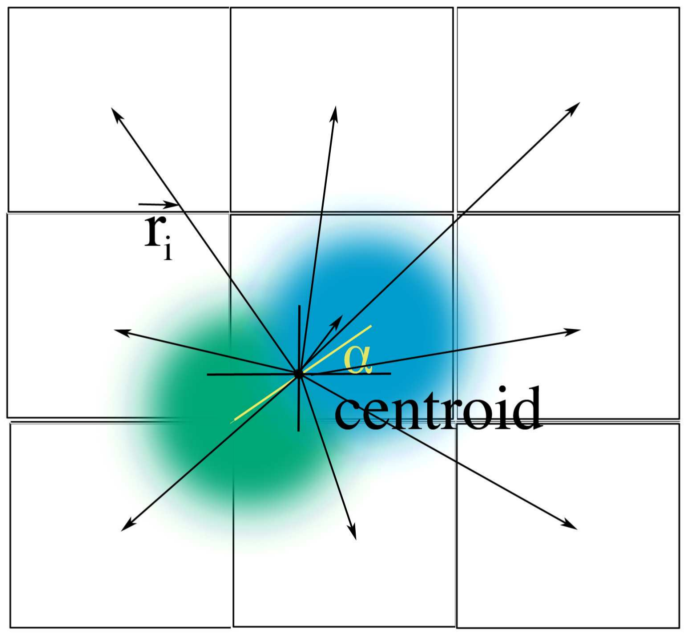

Figure 8: A cluster shape calculation as described in the text finds the axis for splitting the π^0 merged to one bump.

A Detailed Calculations

A.1 Explicit Calculations for the FP_Set Class

a) Find the E dependent Longitudinal Parameters

$$V = 10^{S(\log_{10} E_0)} \tag{19}$$

where:

$$\begin{aligned} s\left(\log_{10} E_0\right) = 2.868129 - 5.256339 * \log_{10}\mathrm{E}_0 + 3.151632 * \left(\log_{10}\mathrm{E}_0\right)^2 \\ -.769710 * \left(\log_{10}\mathrm{E}_0\right)^3 + .068684 * \left(\log_{10}\mathrm{E}_0\right)^4 \end{aligned} \tag{20}$$

the derivative is:

$$\frac{dV}{dE_{0[n]}} = \frac{V}{E_{0[n]}} \times s'\left(\log_{10} E_{0[n]}\right) \tag{21}$$

with:

$$s'\left(\log_{10} E_0\right) = -5.256339 + 6.303264 * \log_{10}\mathrm{E}_0 - 2.30913 * \left(\log_{10}\mathrm{E}_0\right)^2 + .274736 * \left(\log_{10}\mathrm{E}_0\right)^3 \tag{22}$$

$$\bar{W} = \langle \alpha\beta \rangle = 10^{M(\log_{10} E_0)} \tag{23}$$

where:

$$M\left(\log_{10} E_0\right) = -1.936314 + 2.340665 * \log_{10}\mathrm{E}_0 - .712555 * \left(\log_{10}\mathrm{E}_0\right)^2 + .076661 * \left(\log_{10}\mathrm{E}_0\right)^3 \tag{24}$$

and:

$$\frac{d\bar{W}}{dE_0} = \frac{\bar{W}}{E_0} \times M'(\log_{10} E_0) \tag{25}$$

with

$$M'\left(\log_{10} E_0\right) = 2.340665 - 1.42511 * \log_{10}\mathrm{E}_0 + .229983 * \left(\log_{10}\mathrm{E}_0\right)^2 \tag{26}$$

Then find alpha and beta and their derivatives with respect to V and W:

$$\begin{aligned} \alpha_{[n]} &= \sqrt{V_{[n]} W_{[n]}} \\ \beta_{[n]} &= \sqrt{\tfrac{V_{[n]}}{W_{[n]}}} \end{aligned} \tag{27}$$

$$\begin{aligned} \tfrac{\partial \alpha_{[n]}}{\partial W_{[n]}} &= \tfrac{V_{[n]}}{2\alpha_{[n]}} \\ \tfrac{\partial \beta_{[n]}}{\partial W_{[n]}} &= \tfrac{-\beta_{[n]}}{2W_{[n]}} \\ \tfrac{\partial \alpha_{[n]}}{\partial V_{[n]}} &= \tfrac{W_{[n]}}{2\alpha_{[n]}} \\ \tfrac{\partial \beta_{[n]}}{\partial V_{[n]}} &= \tfrac{1}{2W_{[n]}\beta_{[n]}} \end{aligned} \tag{28}$$

b) Calculate the Plane Depths in Radiation Lengths:

$$z_i = i \times \frac{n_{x_0}}{n_{planes}} \tag{29}$$

n_{planes} is the total number of planes and n_{x0} is the total number of radiation lengths in a typical crystal.

c) Calculate dedx for Planes i (and Derivatives):

$$dEdx_{[in]} = \frac{\left(\beta_{[n]} z_i\right)^{\alpha_{[n]}-1} e^{-\beta_{[n]} z_i}}{\sum_j \left(\beta_{[n]} z_j\right)^{\alpha_{[n]}-1} e^{-\beta_{[n]} z_j}} \tag{30}$$

and calculate:

$$\begin{aligned} \frac{\partial\left(dEdx_{[in]}\right)}{\partial \alpha} &= dEdx_{[in]} \left(\ln \beta z_i - \frac{\sum\limits_j \ln \beta z_j (\beta z_j)^{\alpha-1} e^{-\beta z_j}}{\sum\limits_j (\beta z_j)^{\alpha-1} e^{-\beta z_j}} \right) \\ \frac{\partial\left(dEdx_{[in]}\right)}{\partial \beta} &= dEdx_{[in]} \left(\frac{\sum\limits_j z_j (\beta z_j)^{\alpha-1} e^{-\beta z_j}}{\sum\limits_j (\beta z_j)^{\alpha-1} e^{-\beta z_j}} - z_i \right) \end{aligned} \tag{31}$$

and:

$$\begin{aligned} \frac{\partial\left(dEdx_{[in]}\right)}{\partial E_{0[n]}} &= \left(\frac{\partial\left(dEdx_{[in]}\right)}{\partial \alpha} \frac{\partial \alpha}{\partial V} + \frac{\partial\left(dEdx_{[in]}\right)}{\partial \beta} \frac{\partial \beta}{\partial V} \right) \frac{dV}{dE_{0[n]}} \\ &+ \left(\frac{\partial\left(dEdx_{[in]}\right)}{\partial \alpha} \frac{\partial \alpha}{\partial W_{[n]}} + \frac{\partial\left(dEdx_{[in]}\right)}{\partial \beta} \frac{\partial \beta}{\partial W_{[n]}} \right) \frac{d\bar{W}_{[n]}}{dE_{0[n]}} \end{aligned} \tag{32}$$

$$\frac{\partial\left(dEdx_{[in]}\right)}{\partial W_{[n]}}=\left(\frac{\partial\left(dEdx_{[in]}\right)}{\partial\alpha}\frac{\partial\alpha}{\partial W_{[n]}}+\frac{\partial\left(dEdx_{[in]}\right)}{\partial\beta}\frac{\partial\beta}{\partial W_{[n]}}\right) \tag{33}$$

d) Find Z Dependent Transverse Parameters:

$$\begin{aligned}&\alpha_{0[\mathrm{n}]}\left(\log_{10}\mathrm{E}_{0[\mathrm{n}]}\right)=9.102926-7.784449*\log_{10}\mathrm{E}_{0[\mathrm{n}]}+\\&2.241959*\left(\log_{10}\mathrm{E}_{0[\mathrm{n}]}\right)^2-.207938*\left(\log_{10}\mathrm{E}_{0[\mathrm{n}]}\right)^3\end{aligned} \tag{34}$$

$$\begin{aligned}&\alpha'_{0[\mathrm{n}]}\left(\log_{10}\mathrm{E}_{0[\mathrm{n}]}\right)=-7.784449+4.483918*\log_{10}\mathrm{E}_{0[\mathrm{n}]}\\&-.623814*\left(\log_{10}\mathrm{E}_{0[\mathrm{n}]}\right)^2\end{aligned} \tag{35}$$

$$\Phi_{[n]}=10^{-\rho(\log_{10}E_{0[n]})} \tag{36}$$

where:

$$\begin{aligned}&\rho_{[n]}\left(\log_{10}\mathrm{E}_{0[\mathrm{n}]}\right)=-(.510346-.523482*\log_{10}\mathrm{E}_{0[\mathrm{n}]}+.293631*\left(\log_{10}\mathrm{E}_{0[\mathrm{n}]}\right)^2\\&-.070018*\left(\log_{10}\mathrm{E}_{0[\mathrm{n}]}\right)^3+.006082*\left(\log_{10}\mathrm{E}_{0[\mathrm{n}]}\right)^4)\end{aligned} \tag{37}$$

Also:

$$\frac{d\Phi_{[n]}}{dE_{0[n]}}=\frac{\Phi_{[n]}\rho'_{[n]}\left(\log_{10}E_{0[n]}\right)}{E_{0[n]}} \tag{38}$$

with:

$$\begin{aligned}&\rho'_{[n]}\left(\log_{10}\mathrm{E}_{0[\mathrm{n}]}\right)=.523482-2\times.293631*\left(\log_{10}\mathrm{E}_{0[\mathrm{n}]}\right)\\&+3\times.070018*\left(\log_{10}\mathrm{E}_{0[\mathrm{n}]}\right)^2-4\times.006082*\left(\log_{10}\mathrm{E}_{0[\mathrm{n}]}\right)^3\end{aligned} \tag{39}$$

next get:

$$a_{[n]}=\alpha_{[n]}\left(\alpha_{[n]}+1\right)-\Phi_{[n]}\alpha_{[n]}^2 \tag{40}$$

and:

$$\frac{\partial a_n}{\partial E_{0[n]}}=\left(2\alpha_{[n]}(1-\Phi_{[n]})+1\right)\left(\frac{\partial\alpha_{[n]}}{\partial V_{[n]}}\frac{dV_{[n]}}{dE_{0[n]}}+\frac{\partial\alpha_{[n]}}{\partial W_{[n]}}\frac{d\bar{W}_{[n]}}{dE_{0[n]}}\right)-\alpha^2\frac{\partial\Phi_{[n]}}{\partial E_{0[n]}} \tag{41}$$

and:

$$b^*_{[n]}=\left(\alpha_{0[n]}+\tfrac{1}{2}\right)\alpha_{[n]}-\alpha_{0[n]}\alpha_{[n]}\Phi_{[n]} \tag{42}$$

with:

$$\begin{aligned}&\tfrac{\partial b^*_{[n]}}{\partial E_{0[n]}}=\left(\alpha_{0[n]}(1-\Phi_{[n]})+1/2\right)\left(\tfrac{\partial\alpha_{[n]}}{\partial V_{[n]}}\tfrac{dV_{[n]}}{dE_{0[n]}}+\tfrac{\partial\alpha_{[n]}}{\partial W_{[n]}}\tfrac{d\bar{W}_{[n]}}{dE_{0[n]}}\right)-\alpha_{[n]}(1-\Phi_{[n]})\tfrac{\partial\alpha_{0[n]}}{\partial E_{0[n]}}\\&-\alpha_{[n]}\alpha_{0[n]}\tfrac{\partial\Phi_{[n]}}{\partial E_{0[n]}}\end{aligned} \tag{43}$$

and:

$$\frac{\partial b^*_{[n]}}{\partial W_{[n]}}=\left(\alpha_{0[n]}(1-\Phi_{[n]})+1/2\right)\left(\frac{\partial\alpha_{[n]}}{\partial W_{[n]}}\right) \tag{44}$$

$$c_{[n]} = \alpha_{0[n]}(\alpha_{0[n]} + 1) - \Phi_{[n]}\alpha_{0[n]}^2 \tag{45}$$

and:

$$\begin{aligned}\frac{\partial c_{[n]}}{\partial E_{0[n]}} &= \left(2\alpha_{0[n]}(1-\Phi_{[n]}) + 1\right)\left(\frac{\partial \alpha_{[n]}}{\partial V_{[n]}}\frac{dV_{[n]}}{dE_{0[n]}} + \frac{\partial \alpha_{[n]}}{\partial W_{[n]}}\frac{d\bar{W}_{[n]}}{dE_{0[n]}}\right)\\ &-\alpha_{0[n]}^2\frac{\partial \Phi_{[n]}}{\partial E_{0[n]}}\end{aligned} \tag{46}$$

$$\frac{\partial c_{[n]}}{\partial W_{[n]}} = \left(2\alpha_{0[n]}(1-\Phi_{[n]}) + 1\right)\left(\frac{\partial \alpha_{[n]}}{\partial W_{[n]}}\right) \tag{47}$$

get:

$$\alpha^*_{[n]\left\{\begin{matrix}1\\2\end{matrix}\right\}} = \beta_{[n]}\left(\frac{-b^*_{[n]} \mp \sqrt{{b^*_{[n]}}^2 - a_{[n]}c_{[n]}}}{a_{[n]}}\right) \tag{48}$$

and:

$$\begin{aligned}\frac{\partial \alpha^*_{[n]}}{\partial W_{[n]}} &= \frac{\alpha^*_{[n]}}{\beta_{[n]}}\frac{\partial \beta_{[n]}}{\partial W_{[n]}} - \left(\frac{\alpha^*_{[n]}}{a_{[n]}} \mp \frac{\beta_{[n]}c_{[n]}}{2a_{[n]}\sqrt{{b^*_{[n]}}^2 - a_{[n]}c_{[n]}}}\right)\frac{\partial a_{[n]}}{\partial W_{[n]}}\\ &-\frac{\beta_{[n]}}{a_{[n]}}\left(1 \pm \frac{b^*_{[n]}}{\sqrt{{b'_{[n]}}^2 - a_{[n]}c_{[n]}}}\right)\frac{\partial b^*_{[n]}}{\partial W_{[n]}} \pm \frac{\beta_{[n]}}{2\sqrt{{b^*_{[n]}}^2 - a_{[n]}c_{[n]}}}\frac{\partial c_{[n]}}{\partial W_{[n]}}\end{aligned} \tag{49}$$

$$\begin{aligned}\frac{\partial \alpha^*_{[n]}}{\partial E_{0[n]}} &= \frac{\alpha^*_{[n]}}{\beta_{[n]}}\left(\frac{\partial \beta_{[n]}}{\partial V_{[n]}}\frac{dV_{[n]}}{dE_{0[n]}} + \frac{\partial \beta_{[n]}}{\partial W_{[n]}}\frac{d\bar{W}_{[n]}}{dE_{0[n]}}\right) - \left(\frac{\alpha^*_{[n]}}{a_{[n]}} \mp \frac{\beta_{[n]}c_{[n]}}{2a_{[n]}\sqrt{{b^*_{[n]}}^2 - a_{[n]}c_{[n]}}}\right)\frac{\partial a_{[n]}}{\partial E_{0[n]}}\\ &-\frac{\beta_{[n]}}{a_{[n]}}\left(1 \pm \frac{b^*_{[n]}}{\sqrt{{b'_{[n]}}^2 - a_{[n]}c_{[n]}}}\right)\frac{\partial b^*_{[n]}}{\partial E_{0[n]}} \pm \frac{\beta_{[n]}}{2\sqrt{{b^*_{[n]}}^2 - a_{[n]}c_{[n]}}}\frac{\partial c_{[n]}}{\partial E_{0[n]}}\end{aligned} \tag{50}$$

from which we get:

$$\alpha_{r[n]} = \alpha^*_{[n]}z_i + \alpha_{0[n]} \tag{51}$$

and then find R and $_i$ via:

$$\left.\begin{matrix}\alpha_r \leq 2.19\\ 2.99 \geq \alpha_r \geq 2.19\\ \alpha_r \geq 2.99\end{matrix}\right\} \Rightarrow \left\{\begin{matrix}\varepsilon_l = \varepsilon_{la}\\ \varepsilon_l = \varepsilon_{la} + (\alpha_r - 2.19) \times (\varepsilon_{lb} - \varepsilon_{la})\,/\,(2.99 - 2.19)\\ \varepsilon_l = \varepsilon_{lb}\end{matrix}\right. \tag{52}$$

$$\left.\begin{matrix}\alpha_r \leq 2.19\\ 2.99 \geq \alpha_r \geq 2.19\\ \alpha_r \geq 2.99\end{matrix}\right\} \Rightarrow \left\{\begin{matrix}R_l = R_{la}\\ R_l = R_{la} + (\alpha_r - 2.19) \times (R_{lb} - R_{la})\,/\,(2.99 - 2.19)\\ R_l = R_{lb}\end{matrix}\right. \tag{53}$$

where:

$$\begin{aligned}\varepsilon_{1a}(\alpha_r) &= -.004\alpha_r^3 + .0156\alpha_r^2 + .1655\alpha_r + .0223\\ \varepsilon_{2a}(\alpha_r) &= .0253\alpha_r^3 - .2198\alpha_r^2 + .5644\alpha_r - .0092\\ R_{1a}(\alpha_r) &= .1067\alpha_r^3 - .1612\alpha_r^2 + 3.396\alpha_r + 1.428\\ R_{2a}(\alpha_r) &= .0354\alpha_r^3 + .0447\alpha_r^2 + .6659\alpha_r + .234\\ R_{3a}(\alpha_r) &= .0206\alpha_r^3 - .0574\alpha_r^2 + .1322\alpha_r - .0142\end{aligned} \tag{54}$$

and:

$$
\begin{array}{l}
\varepsilon_{1b}(\alpha_r) = -.0114\alpha_r^3 + .111\alpha_r^2 - .1672\alpha_r + .3318 \\
\varepsilon_{2b}(\alpha_r) = .0026\alpha_r^3 - .0464\alpha_r^2 + .135\alpha_r + .3091 \\
R_{1b}(\alpha_r) = \lambda_r\left(.1268\alpha_r^3 - .7988\alpha_r^2 + 6.0648\alpha_r - 1.1216\right) \\
R_{2b}(\alpha_r) = \lambda_r\left(.1416\alpha_r^3 - 1.5713\alpha_r^2 + 7.1756\alpha_r - 6.9898\right) \\
R_{3b}(\alpha_r) = \lambda_r\left(-.2318\alpha_r^5 + 3.6125\alpha_r^4 - 22.514\alpha_r^3 + 69.929\alpha_r^2 - 107.46\alpha_r + 65.588\right)
\end{array} \tag{55}
$$

$$
\left.\begin{array}{c}
\alpha_r \leq 2.19 \\
2.99 \geq \alpha_r \geq 2.19 \\
\alpha_r \geq 2.99
\end{array}\right\} \Rightarrow \left\{\begin{array}{c}
\varepsilon_l'(\alpha_r) = \varepsilon_{la}'(\alpha_r) \\
\varepsilon_l'(\alpha_r) = \varepsilon_{la}'(\alpha_r) + \frac{(\alpha_r - 2.19)}{(2.99-2.19)}\left(\varepsilon_{lb}'(\alpha_r) - \varepsilon_{la}'(\alpha_r)\right) + \frac{(\varepsilon_{lb}(\alpha_r) - \varepsilon_{la}(\alpha_r))}{(2.99-2.19)} \\
\varepsilon_l'(\alpha_r) = \varepsilon_{lb}'(\alpha_r)
\end{array}\right. \tag{56}
$$

$$
\left.\begin{array}{c}
\alpha_r \leq 2.19 \\
2.99 \geq \alpha_r \geq 2.19 \\
\alpha_r \geq 2.99
\end{array}\right\} \Rightarrow \left\{\begin{array}{c}
R_l'(\alpha_r) = R_{la}'(\alpha_r) \\
R_l'(\alpha_r) = R_{la}'(\alpha_r) + \frac{(\alpha_r - 2.19)}{(2.99-2.19)}\left(R_{lb}'(\alpha_r) - R_{la}'(\alpha_r)\right) + \frac{(R_{lb}(\alpha_r) - R_{la}(\alpha_r))}{(2.99-2.19)} \\
R_l'(\alpha_r) = R_{lb}'(\alpha_r)
\end{array}\right. \tag{57}
$$

$$
\begin{array}{l}
\varepsilon_{1a}'(\alpha_r) = -.012\alpha_r^2 + .0312\alpha_r + .1655 \\
\varepsilon_{2a}'(\alpha_r) = .0759\alpha_r^2 - .4396\alpha_r + .5644 \\
R_{1a}'(\alpha_r) = \lambda_r(.3201\alpha_r^2 - .3224\alpha_r + 3.396) \\
R_{2a}'(\alpha_r) = \lambda_r(.1062\alpha_r^2 + .0894\alpha_r + .6659) \\
R_{3a}'(\alpha_r) = \lambda_r(.0618\alpha_r^2 - .1148\alpha_r + .1322)
\end{array} \tag{58}
$$

$$
\begin{array}{l}
\varepsilon_{1b}'(\alpha_r) = -.0342\alpha_r^2 + .222\alpha_r - .1672 \\
\varepsilon_{2b}'(\alpha_r) = .0078\alpha_r^2 - .0928\alpha_r + .135 \\
R_{1b}'(\alpha_r) = \lambda_r(.3804\alpha_r^2 - 1.5976\alpha_r + 6.0648) \\
R_{2b}'(\alpha_r) = \lambda_r(.4248\alpha_r^2 - 3.1426\alpha_r + 7.1756) \\
R_{3b}'(\alpha_r) = \lambda_r(-1.159\alpha_r^4 + 14.45\alpha_r^3 - 67,542\alpha_r^2 + 139.858\alpha_r - 107.46)
\end{array} \tag{59}
$$

$$
\begin{array}{c}
\varepsilon_3 = 1 - \varepsilon_1 - \varepsilon_2 \\
\frac{d\varepsilon_3}{d\alpha_r} = 1 - \frac{d\varepsilon_1}{d\alpha_r} - \frac{d\varepsilon_2}{d\alpha_r}
\end{array} \tag{60}
$$

e) Find the Trajectory Direction in Terms of Fitting Parameters

$$
\begin{array}{c}
\widehat{t}_{[n]} = \left\{\begin{array}{c}
\sin\theta_{t[n]}\cos\phi_{t[n]} \\
\sin\theta_{t[n]}\sin\phi_{t[n]} \\
\cos\theta_{t[n]}
\end{array}\right\} \\
\frac{\partial\widehat{t}}{\partial\theta_t} = \left\{\begin{array}{c}
\cos\theta_t\cos\phi_t \\
\cos\theta_t\sin\phi_t \\
-\sin\theta_t
\end{array}\right\} \\
\frac{\partial\widehat{t}}{\partial\phi_t} = \left\{\begin{array}{c}
-\sin\theta_t\sin\phi_t \\
\sin\theta_t\cos\phi_t \\
0
\end{array}\right\}
\end{array} \tag{61}
$$

A.2 Explicit Calculations for the Xtl_Con Class

a) Extract the Crystal Outline

The normal vector for the j^{th} edge of the m^{th} crystal is given by by :

$$
\widehat{\eta}_{[mj]} = \frac{\vec{x}_{2[mj]} - \vec{x}_{1[mj]}}{\left|\vec{x}_{2[mj]} - \vec{x}_{1[mj]}\right|} \tag{62}
$$

where $X1_{[mj]}$ is the innermost vertex of the j^{th} edge of the m^{th} crystal and $X2_{[mj]}$ is the outermost vertex on the same edge. The outline of the crystal extracted from the EmcXTal::PhysicalOutline routine gives a Hep3VectorD for each of the vertices of the crystal. Normal vectors which follows the direction of each of the four projective edges of the crystal are determined.

b) Find Depth Independent Transverse Parameters:

$$\vec{\Omega}_{[nmj]} = \frac{\widehat{\eta}_{[mj]}}{\widehat{t}_{[n]} \bullet \widehat{\eta}_{[mj]}} \tag{63}$$

Define the following:

$$\vec{x}_{[\Omega jnm]} = \vec{x}_{1[mj]} + \vec{\Omega}_{[nmj]} \left(\widehat{t}_{[n]} \bullet \left(\vec{x}_{0[n]} - \vec{x}_{1[mj]} \right) \right) \tag{64}$$

where:

$$\vec{x}_{0[n]} = \left\{ \begin{array}{c} x_{0[n]} \\ y_{0[n]} \\ z_{0[n]} \end{array} \right\} \tag{65}$$

$$\frac{\partial \vec{x}_0}{\partial x_0} = \left\{ \begin{array}{c} 1 \\ 0 \\ 0 \end{array} \right\} \tag{66}$$

$$\frac{\partial \vec{x}_0}{\partial y_0} = \left\{ \begin{array}{c} 0 \\ 1 \\ 0 \end{array} \right\} \tag{67}$$

$$\frac{\partial \vec{x}_0}{\partial z_0} = \left\{ \begin{array}{c} 0 \\ 0 \\ 1 \end{array} \right\} \tag{68}$$

also define:

$$\begin{aligned} \frac{\partial \vec{v}_{[\Pi jmn]}}{\partial \xi_{[nq]}} &= \vec{\Omega}_{[nmj]} \left\{ \frac{\partial \widehat{t}_{[n]}}{\partial \xi_{[nq]}} \bullet \left[\left(\vec{x}_{0[n]} - \vec{x}1_{[mj]} \right) - \vec{\Omega}_{[nmj]} \left(\widehat{t}_{[n]} \bullet \left(\vec{x}_{0[n]} - \vec{x}1_{[mj]} \right) \right) \right] + \frac{\partial \vec{x}_{0[n]}}{\partial \xi_{[nq]}} \bullet \widehat{t}_{[n]} \right\} - \frac{\partial \vec{x}_{0[n]}}{\partial \xi_{[nq]}} \\ \vec{\Pi}_{[nmjq]} &= \left[\vec{\Omega}_{[nmj]} \left\{ \frac{\partial \widehat{t}_{[n]}}{\partial \xi_{[nq]}} \bullet \vec{\Omega}_{[nmj]} \right\} + \frac{\partial \widehat{t}_{[n]}}{\partial \xi_{[nq]}} \right] \end{aligned} \tag{69}$$

c) Loop over j and i Calculating Energy Contributions From Each Plane

$\vec{x}_{[ijnm]}$ is the intersection of the j^{th} edge of the m^{th} crystal with the i^{th} slice along the trajectory of the n^{th} photon. These positions are represented by the vertices of the trapezoids in Figure 6.

$$\vec{x}_{[ijnm]} = i\Delta\vec{\Omega}_{[nmj]} + \vec{x}_{[\Omega jnm]} \tag{70}$$

$\vec{v}_{[ijnm]}$ is the displacement between the intersection of the trajectory of the n^{th} photon with the i^{th} slice along the the trajectory and the intersection of the j^{th} edge of the m^{th} crystal with the same slice. Figure 6f) shows its orientation (as seen from the I.P.).

$$\vec{v}_{[ijnm]} = \vec{x}_{[ijnm]} - \vec{x}_{0[n]} - i\Delta \widehat{t}_{[n]} \tag{71}$$

$$\frac{\partial \vec{v}_{[ijmn]}}{\partial \xi_{[nq]}} = \frac{\partial \vec{v}_{[\Pi jmn]}}{\partial \xi_{[nq]}} - i\Delta \vec{\Pi}_{[nmjq]} \tag{72}$$

$\vec{r}_{[ijmn]}$ is defined by:

$$\vec{r}_{[ijmn]} = \vec{v}_{[ijmn]} - \vec{v}_{[i(j-1)nm]} \tag{73}$$

It's geometric significance can be read from figure 6f).

$$\frac{\partial \vec{r}_{[ijmn]}}{\partial \xi_{[nq]}} = \frac{\partial \vec{v}_{[ijmn]}}{\partial \xi_{[nq]}} - \frac{\partial \vec{v}_{[i(j-1)nm]}}{\partial \xi_{[nq]}} \tag{74}$$

When each of the four triangles over which the transverse energy distribution must be integrated for a slice is split into a sum or difference of two right triangles, the height of each of the two right triangles is $h_{[ijmn]}$ and the bases of the right triangles are $k1_{[ijmn]}$ and $k2_{[ijmn]}$ respectively. Figure 6f) shows them in relation to the i^{th} slice through the crystal.

$$h_{[ijmn]} = \widehat{t}_{[n]} \bullet \frac{\vec{v}_{[ijmn]} \times \vec{v}_{[i(j-1)nm]}}{\left|\vec{r}_{[ijnm]}\right|} \tag{75}$$

$$\begin{aligned}\frac{\partial h_{[ijmn]}}{\partial \xi_{[nq]}} &= \frac{\partial \widehat{t}_{[n]}}{\partial \xi_{[nq]}} \bullet \frac{\vec{v}_{[ijmn]} \times \vec{v}_{[i(j-1)mn]}}{\left|\vec{r}_{[ijmn]}\right|} + \frac{\widehat{t}_{[n]}}{\left|\vec{r}_{[ijmn]}\right|} \bullet \left[\frac{\partial \vec{v}_{[ijmn]}}{\partial \xi_{[nq]}} \times \vec{v}_{[i(j-1)mn]} + \vec{v}_{[ijmn]} \times \frac{\partial \vec{v}_{[i(j-1)mn]}}{\partial \xi_{[nq]}}\right] \\ &- \frac{\left(\vec{v}_{[ijmn]} \times \vec{v}_{[i(j-1)mn]}\right)}{\left|\vec{r}_{ij}\right|^{3/2}} \left(\frac{d\vec{v}_{[ijmn]}}{\partial \xi_{[nq]}} - \frac{d\vec{v}_{[i(j-1)mn]}}{\partial \xi_{[nq]}}\right) \left(\widehat{t}_{[n]} \bullet \left(\vec{v}_{[ijmn]} \times \vec{v}_{[i(j-1)mn]}\right)\right)\end{aligned} \tag{76}$$

$$k1_{[ijmn]} = \frac{\vec{v}_{[ijmn]} \bullet \vec{r}_{[ijmn]}}{\left|\vec{r}_{[ijmn]}\right|} \tag{77}$$

$$\frac{\partial k1_{[ijmn]}}{\partial \xi_{[nq]}} = \frac{\frac{\partial \vec{v}_{[ijmn]}}{\partial \xi_{[nq]}} \bullet \vec{r}_{[ijmn]} + \vec{v}_{[ijmn]} \bullet \frac{\partial \vec{r}_{[ijmn]}}{\partial \xi_{[nq]}}}{\left|\vec{r}_{[ijmn]}\right|} - k1_{[ijmn]} \frac{\vec{r}_{[ijmn]} \bullet \frac{\partial \vec{r}_{[ijmn]}}{\partial \xi_{[nq]}}}{\left|\vec{r}_{[ijmn]}\right|^2} \tag{78}$$

$$\begin{aligned} k2_{[ijmn]} &= k1_{[ijmn]} - \left|\vec{r}_{[ijmn]}\right| \\ \frac{\partial k2_{[ijmn]}}{\partial \xi_{[nq]}} &= \frac{\partial k1_{ij}}{\partial \xi_{[nq]}} - \frac{\vec{r}_{[ijmn]}}{\left|\vec{r}_{[ijmn]}\right|} \bullet \frac{\partial \vec{r}_{[ijmn]}}{\partial \xi_{[nq]}} \end{aligned} \tag{79}$$

d) Loop over l calculating Grindhammer Contributions to the Sums:

Trans[ijlmn] is defined as the fraction of the energy in plane i of shower n that is contributed by th l^{th} term in the Grindhammer expansion to crystal m by integrating over a triangle defined by three vertices at: a) the point of the intersection of plane i of shower n with the j^{th} edge of the crystal m; b) the point of intersection between the plane i and the j+1st edge of the crystal m; and c) the point where the n^{th} photon trajectory crosses the i^{th} plane of shower n. Taking the relations in the sections above into consideration the calculation for Trans[inmlj] becomes:

$$Trans_{[inmlj]} = \frac{\varepsilon_{[lin]} h_{[ijnm]}}{2\pi\sqrt{h^2_{[ijnm]} + R^2_{[lin]}}} \left\{\tan^{-1}\left[\frac{k1_{[ijnm]}}{\sqrt{h^2_{[ijnm]} + R^2_{[lin]}}}\right] - \tan^{-1}\left[\frac{k2_{[ijnm]}}{\sqrt{h^2_{[ijnm]} + R^2_{[lin]}}}\right]\right\} \tag{80}$$

and its derivatives via:

$$\frac{\partial Trans_{[inmlj]}}{\partial \xi_{[nq]}} = \frac{\partial Trans_{[inmlj]}}{\partial h_{[ijnm]}}\frac{\partial h_{[ijnm]}}{\partial \xi_{[nq]}} + \frac{\partial Trans_{[inmlj]}}{\partial k1_{[ijnm]}}\frac{\partial k1_{[ijnm]}}{\partial \xi_{[nq]}} + \frac{\partial Trans_{[inmlj]}}{\partial k2_{[ijnm]}}\frac{\partial k2_{[ijnm]}}{\partial \xi_{[nq]}} \\ + \frac{\partial Trans_{[inmlj]}}{\partial \varepsilon_{[lin]}}\frac{\partial \varepsilon_{[lin]}}{\partial \xi_{[nq]}} + \frac{\partial Trans_{[inmlj]}}{\partial R_{[lin]}}\frac{\partial R_{[lin]}}{\partial \xi_{[nq]}} \tag{81}$$

with:

$$\frac{\partial Trans_{[inmlj]}}{\partial h_{[ijnm]}} = \frac{Trans_{[inmlj]}}{h_{[ijnm]}} - \frac{h_{[ijnm]}Trans_{[inmlj]}}{\left(h^2_{[ijnm]}+R^2_{[lin]}\right)} \\ - \frac{\varepsilon_{[lin]}h^2_{[ijnm]}}{2\pi\left(h^2_{[ijnm]}+R^2_{[lin]}\right)}\left(\frac{k1_{[ijnm]}}{\left(k1^2_{[ijnm]}+h^2_{[ijnm]}+R^2_{[lin]}\right)} - \frac{k2_{[ijnm]}}{\left(k2^2_{[ijnm]}+h^2_{[ijnm]}+R^2_{[lin]}\right)}\right) \tag{82}$$

$$\frac{\partial Trans_{[inmlj]}}{\partial k1_{[ijnm]}} = \frac{\varepsilon_{[lin]}h_{[ijnm]}}{2\pi\left(k1^2_{[ijnm]}+h^2_{[ijnm]}+R^2_{[lin]}\right)} \\ \frac{\partial Trans_{[inmlj]}}{\partial k2_{[ijnm]}} = \frac{-\varepsilon_{[lin]}h_{[ijnm]}}{2\pi\left(k2^2_{[ijnm]}+h^2_{[ijnm]}+R^2_{[lin]}\right)} \tag{83}$$

$$\frac{\partial Trans_{[inmlj]}}{\partial R_{[lin]}} = -\frac{R_{[lin]}Trans_{[inmlj]}}{\left(h^2_{[ijnm]}+R^2_{[lin]}\right)} \\ - \frac{\varepsilon_{[lin]}h_{[ijnm]}}{2\pi\left(h^2_{[ijnm]}+R^2_{[lin]}\right)}\left(\frac{1}{\left(k1^2_{[ijnm]}+h^2_{[ijnm]}+R^2_{[lin]}\right)} - \frac{1}{\left(k2^2_{[ijnm]}+h^2_{[ijnm]}+R^2_{[lin]}\right)}\right) \tag{84}$$

$$\frac{\partial Trans_{[inmlj]}}{\partial \varepsilon_{[lin]}} = \frac{Trans_{[inmlj]}}{\varepsilon_{[lin]}} \tag{85}$$

$$\Delta E_{[mn]} = \left[\left(\sum_i dedx_{[in]} \times \sum_{lj} Trans_{[inmlj]}\right)\right] \times E_{0[n]} \tag{86}$$

$$\frac{\partial \Delta E_{[mn]}}{\partial \xi_{[n'q]}} = \left[\left(\sum_i dedx_{[in']} \times \sum_{lj} Trans_{[in'mlj]}\right)\frac{\partial E_{0[n']}}{\partial \xi_{[n'q]}} + \\ \left(\sum_i \frac{\partial dedx_{[in']}}{\partial \xi_{[n'q]}} \times \sum_{lj} Trans_{[in'mlj]}\right) \times E_{0[n']} + \left(\sum_i dedx_{[in']} \times \sum_{lj} \frac{\partial Trans_{[in'mlj]}}{\partial \xi_{[n'q]}}\right) \times E_{0[n']}\right] \tag{87}$$

VI. Calculation of f_{leak}

A calculation of the back leakage is available, but is not currently in use because a cluster calibration for this algorithm is first required. Calculation of f_{leak}

f_{leak} is a factor that estimates back leakage of energy beyond the crystal boundary. With the back plane of the crystal is defined by:

$$d_r = \widehat{\alpha}_{pr} \bullet \vec{x} \tag{88}$$

the distance from x0 to the back plane along the t direction is:

$$z_p = \frac{d_r - \widehat{\alpha}_{pr} \bullet \vec{x}_0}{\widehat{\alpha}_{pr} \bullet \widehat{t}} \tag{89}$$

The derivatives with respect to the parameter a_k is:

$$\frac{dz_p}{da_k} = \frac{\left(\widehat{\alpha}_{pr} \bullet \widehat{t}\right) \frac{d\vec{x}_0}{da_k} \bullet \widehat{\alpha}_{pr} - \left(d_r - \widehat{\alpha}_{pr} \bullet \vec{x}_0\right) \frac{d\,\widehat{t}}{da_k} \bullet \widehat{\alpha}_{pr}}{\left(\widehat{\alpha}_{pr} \bullet \widehat{t}\right)^2} \tag{90}$$

where a_k is $x_{0[n]}$, $y_{0[n]}$, $z_{0[n]}$, $\theta_{t[n]}$ or $\phi_{t[n]}$

the factor f_{leak} is determined by:

$$f_{leak} = P(\alpha, \beta z_p) = \frac{\gamma\left(\alpha, \beta z_p\right)}{\Gamma\left(\alpha\right)} \tag{91}$$

where:

$$\gamma\left(\alpha, x\right) = \int_0^x e^{-t} t^{\alpha-1} dt \tag{92}$$

The incomplete gamma function $\gamma\left(\alpha, x\right)$ has a fast converging series expansion for $x < \alpha + 1$:

$$\gamma\left(\alpha, x\right) = e^{-x} x^a \sum_{n=0}^{\infty} \frac{\Gamma(\alpha)}{\Gamma(\alpha+1+n)} x^n \tag{93}$$

and a rapidly converging continuing fraction representation otherwise:

$$\gamma\left(\alpha, x\right) = 1 - e^{-x} x^{\alpha} \left(\frac{1}{x+1-\alpha-} \frac{1(1-\alpha)}{x+3-\alpha-} \frac{2(2-\alpha)}{x+5-\alpha-} \cdots\right) \tag{94}$$

An excellent approximation for Gamma due to Lanczos:

$$\Gamma\left(z\right) \approx \left(z+5.5\right)^{z+\frac{1}{2}} e^{-(z+5.5)} \times \tfrac{2\pi}{z} \left[c_0 + \tfrac{c_1}{z+1} + \tfrac{c_2}{z+2} + \cdots \tfrac{c_6}{z+6}\right] \tag{95}$$

is employed in evaluating f_{leak}.

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