Friedrich-Alexander-Universität
Naturwissenschaftliche Fakultät

FAU

DISCUS Workshop

Single crystal PDF 3D-PDF 3D-Δ-PDF

Chemical short range order

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Pair Distribution Function

Intensity: $I(\vec{h}) = F(\vec{h}) \cdot F^*(\vec{h})$

$$\mathcal{F}[I(\vec{h})] = \mathcal{F}[F(\vec{h}) \cdot F^*(\vec{h})]$$

$$= \mathcal{F}[F(\vec{h})] \circ \mathcal{F}[F^*(\vec{h})]$$

$$= \rho(\vec{r}) \circ \rho^*(-\vec{r})$$

$$= \rho(\vec{r}) \circ \rho(-\vec{r}) = P(\vec{u})$$

$$= \textit{Autocorrelation function } P(\vec{u})$$

Intensity is product of Structure factor and conj. complex

Fourier transform to go back to direct space

Convolution of individual Fourier transforms

Back to electron densities real valued function of r

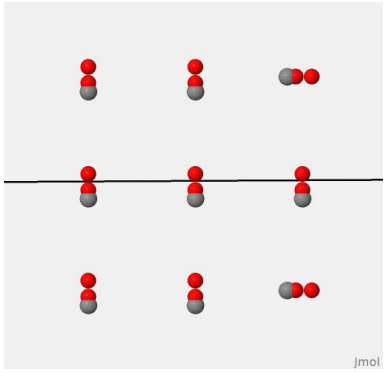
Auto correlation function: peaks at

$$P(\vec{u}) \quad if \quad \rho(\vec{r}) * \rho(\vec{r}+\vec{u}) \gg 0$$

Vectors u that correspond to interatomic vectors

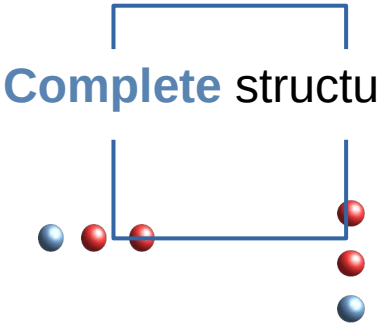
Powder	Pair distribution function	PDF	G(r) , g(r)
	radial distribution function	RDF	RDF(r)
Single crystal	3D-PDF / 3D-Δ-PDF		

Linear **A**-**B**-**B** molecule in two orientations

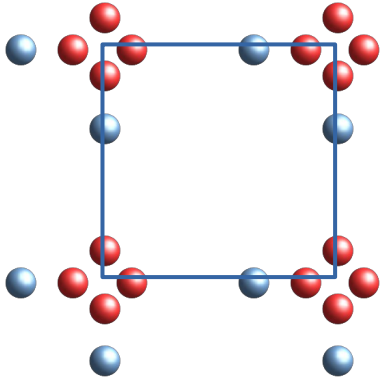


Complete structure

no correlation between molecules

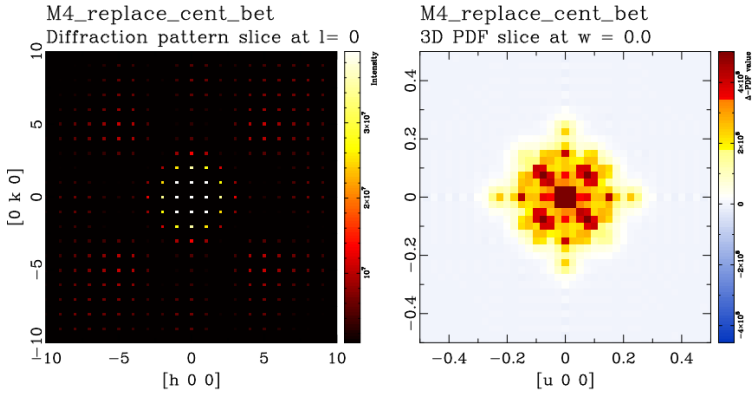


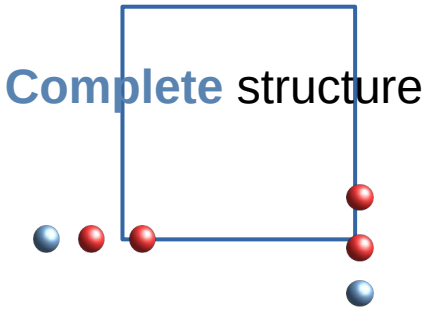
Complete structure



Average structure

3D-PDF

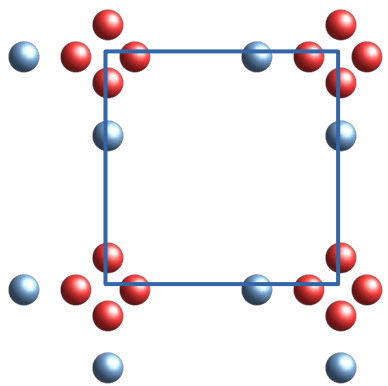




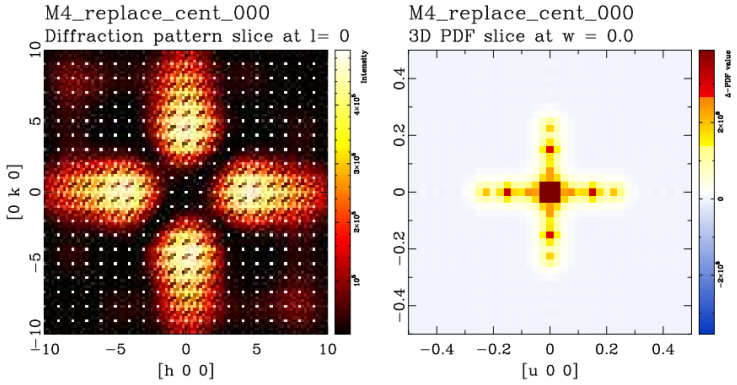
Patterson

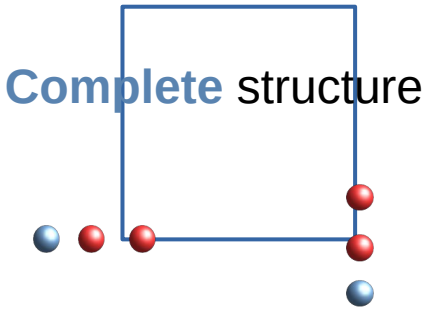
Average structure Patterson

Positive peaks
interatomic vectors in **average** structure



3D-PDF

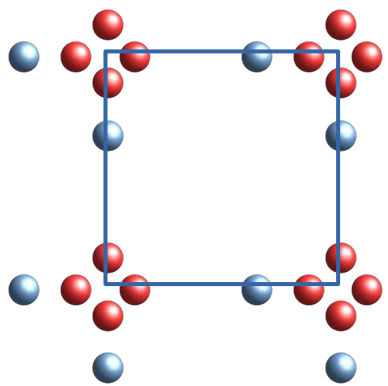




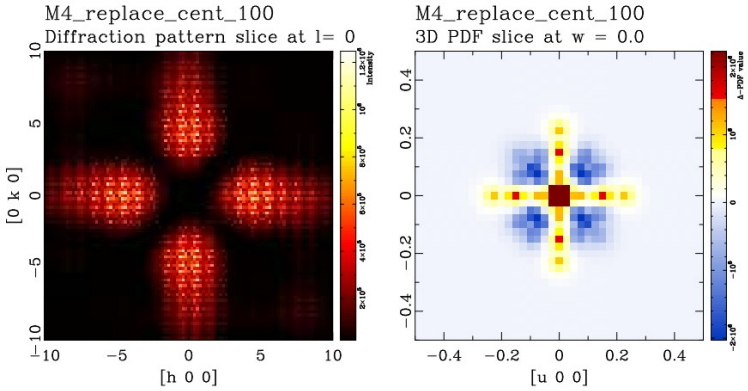
3D PDF

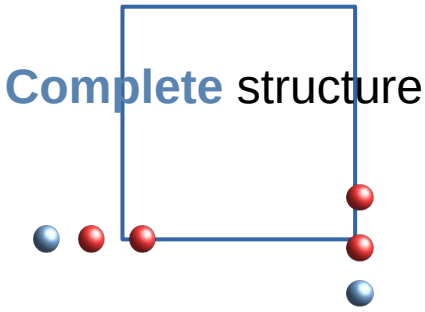
Complete structure Patterson

Positive peaks
interatomic vectors in **actual / complete** structure



3D-PDF



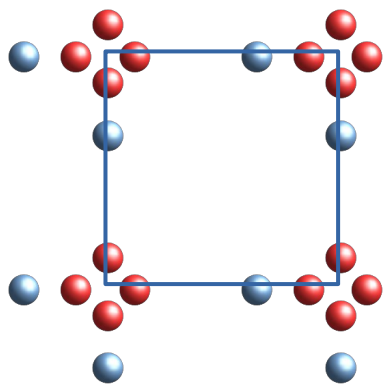


3D - Δ - PDF

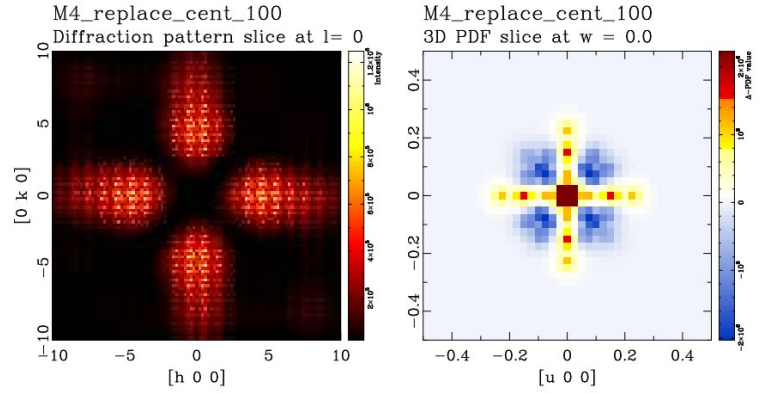
„Local“ structure Patterson

Difference: **Complete** – **Average**

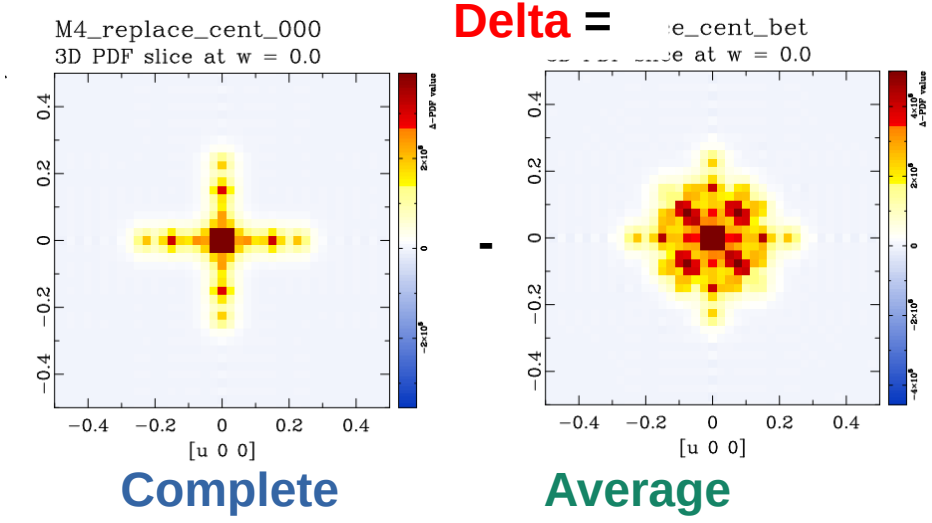
Positive and **Negative** peaks
Deviations of **local** from **average** structure



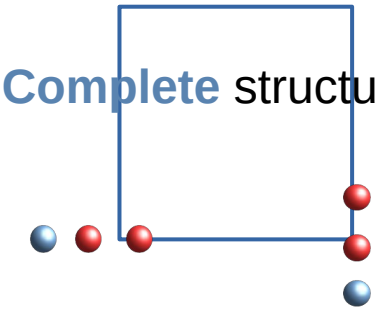
3D-PDF



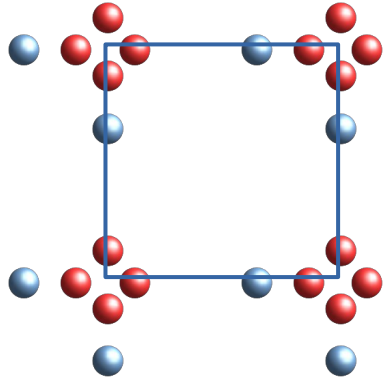
Delta =



Complete **Average**



Complete structure



Average structure

3D-PDF

Patterson

3-D inverse Fourier transform of the **Bragg** scattering

Interatomic vectors periodic

average structure

$$P(\mathbf{u}) = F^{-1} I(\mathbf{hkl})$$

$$P(\mathbf{u}) = F^{-1}\left[F^{*}(\mathbf{hkl})\cdot F(\mathbf{hkl})\right] = \rho(\mathbf{r}) \otimes \rho(-\mathbf{r})$$

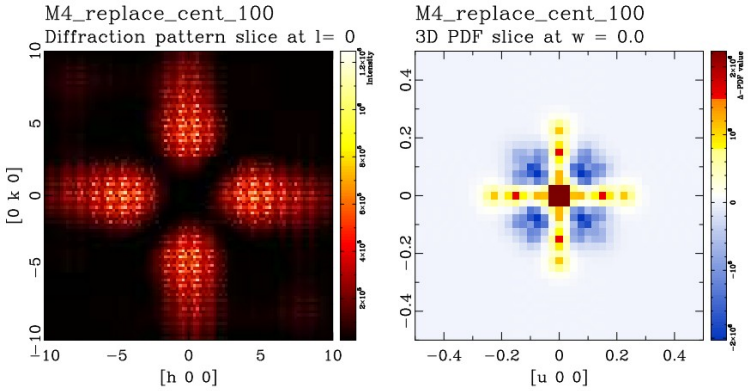
$$P(\mathbf{u}) = F^{-1}\left[F^{*}(\mathbf{hkl})\cdot E(\mathbf{hkl})\right]$$ Sharpened **Patterson**

$$P(\mathbf{u}) = F^{-1}\left[E^{*}(\mathbf{hkl})\cdot E(\mathbf{hkl})\right]$$ Super sharpened **Patterson**

$$PDF(\mathbf{u}) = F^{-1}\frac{I(\mathbf{Q})}{\langle f^{2}\rangle}$$ Super sharpened **3D PDF**

$$E(\mathbf{hkl}) = \frac{F(\mathbf{hkl})}{\sqrt{\langle I(\mathbf{hkl})\rangle_{\Delta\Theta}}}$$

3D-PDF

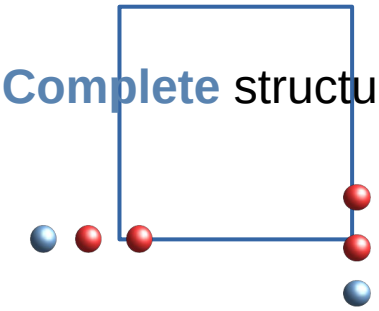


3D - Δ - PDF

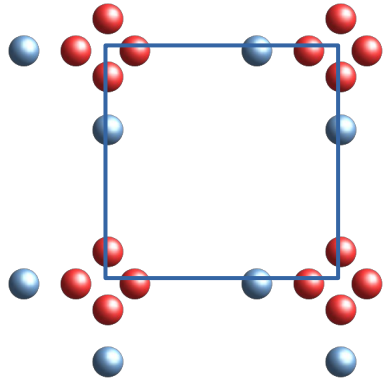
„Local“ structure Patterson

Difference: **Complete** – **Average**

Positive and **Negative** peaks
Deviations of **local** from **average** structure

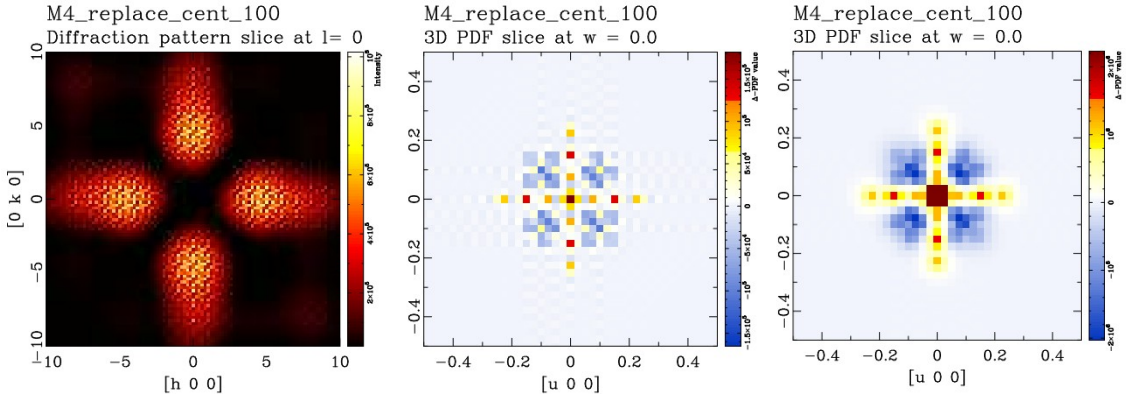


Complete structure



Average structure

3D-PDF

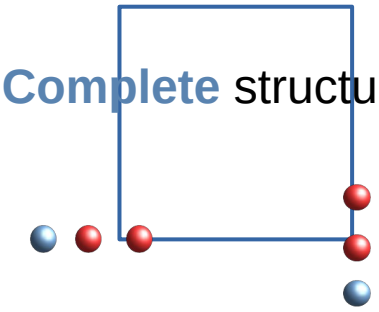


3D - Δ - PDF

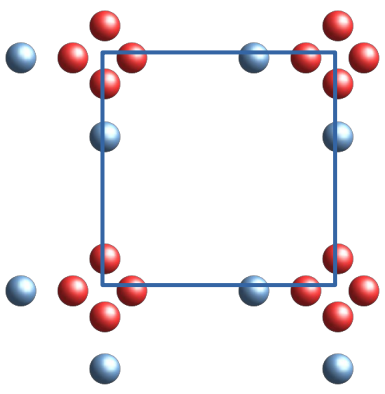
„Local“ structure Patterson

Difference: **Complete** – **Average**

Positive and **Negative** peaks
Deviations of **local** from **average** structure

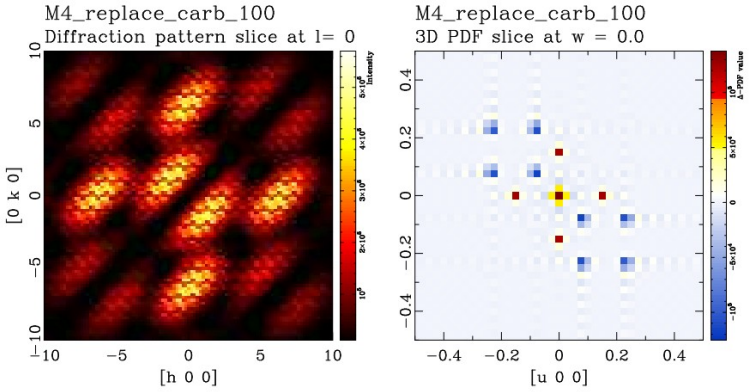


Complete structure



Average structure

3D-PDF



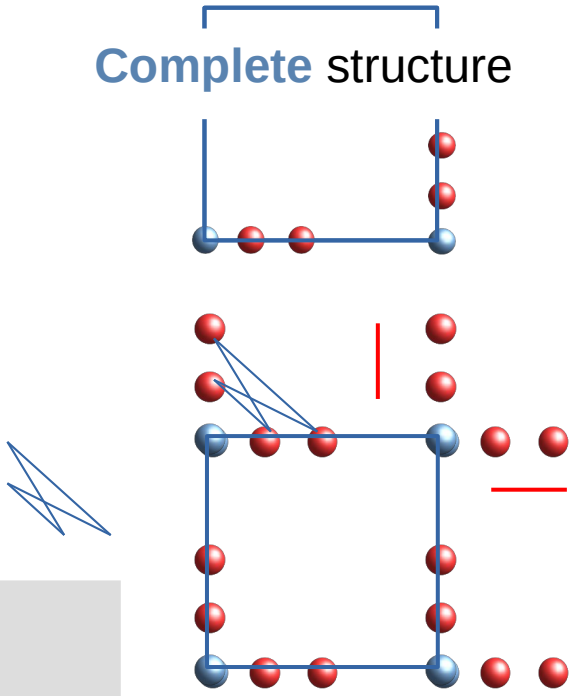
3D - Δ - PDF

„Local“ structure Patterson

Difference: **Complete** - **Average**

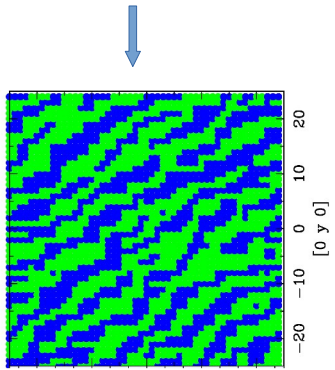
No A..B vectors
in **3D -Δ- PDF**

No positive /negative
Although **disordered**!



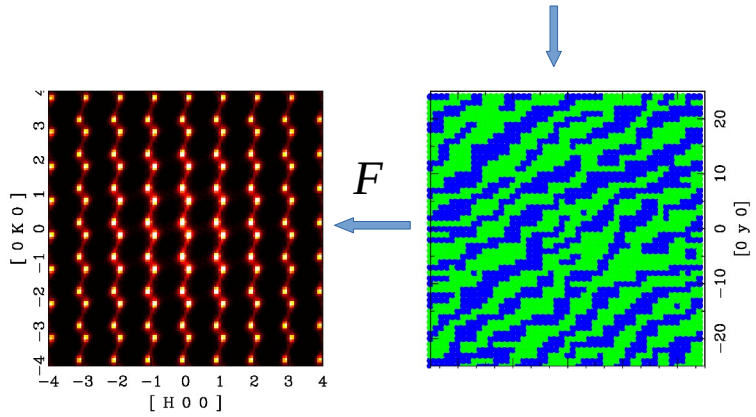
3D-PDF

Simulation / refinement
of disordered structural model



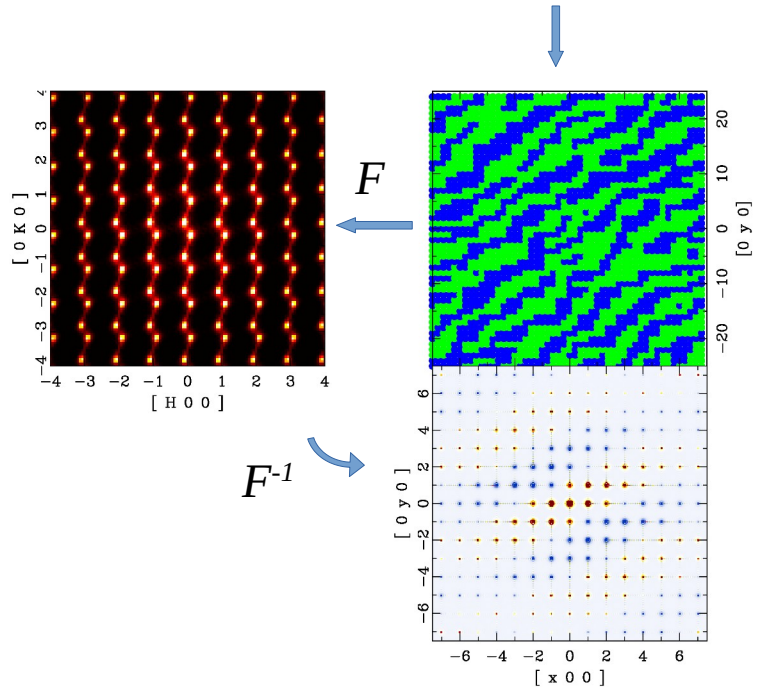
3D-PDF

Simulation / refinement
of disordered structural model



3D-PDF

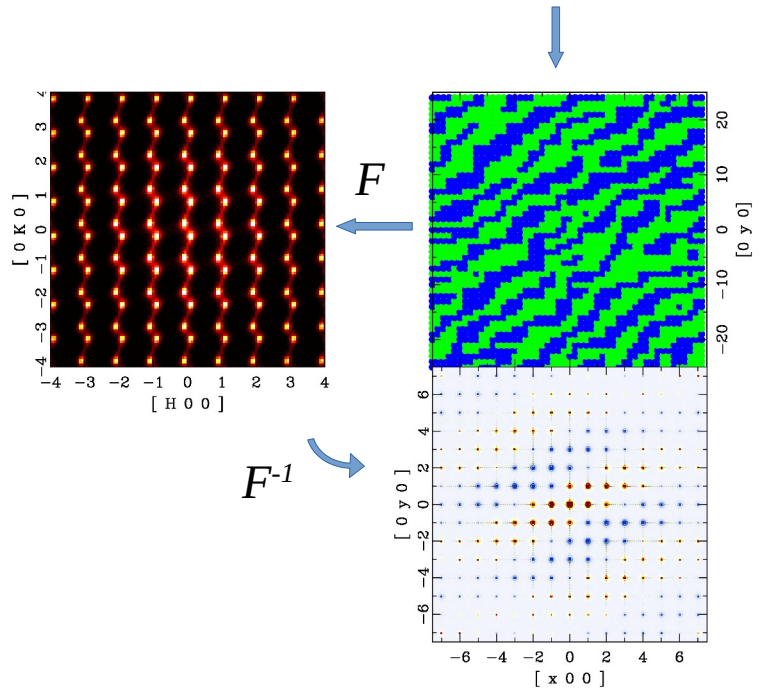
Simulation / refinement
of disordered structural model

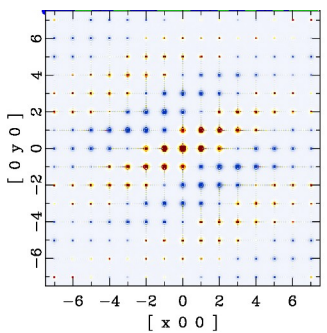


3D-PDF

Simulation / refinement
of disordered structural model

Simulation / refinement
of correlation parameters





DISCUS: www.github.com/tproffen/DiffuseCode

Yell: www.github.com/YellProgram