Determining the validity of Guinier analysis in slit-smeared small angle scattering data

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Background Information
Small Angle Scattering is a powerful technique for investigating large scale particles or structures.

- **High Q**
  - Smaller length scales
  - Shape of individual particles

- **Low Q**
  - Larger length scales
  - Plateau or peak
  - Overall size and structure
Guinier analysis is a shape independent method for analyzing data

Radius of gyration, $R_g$

Guinier approximation

$$I(Q) - I_{bgd} = I_0 e^{-\frac{1}{3}R_g^2Q^2}$$
Guinier plot $\ln[I(Q)]$ vs $Q^2$

\[ I(Q) - I_{bgd} = I_0 e^{-\frac{1}{3}R_g^2 Q^2} \]

\[ \ln[I(Q) - I_{bgd}] = \ln I_0 - \frac{1}{3} R_g^2 Q^2 \]

\textit{Slope} = -\frac{1}{3} R_g^2 \\
\textit{Intercept} = \ln[I_0]
Slit-smearing is an instrument geometry effect

- Slit geometry enables access to very low Q values
  - USAXS
  - USANS
- Slit geometry causes an effect known as slit-smearing
Approach to evaluating Guinier analysis on slit-smeared data

• Guinier analysis is a useful tool for understanding scattering data

• Slit-smearing causes distortions to data that can influence results from a Guinier fit

• We simulated data from four generic shapes with and without slit-smearing

• Performed Guinier analysis on both data sets and compared fit results and true values defined in the simulation

\[
R_g = \frac{3}{\sqrt{5}} R
\]

\[
R_g = \frac{L^2}{12} + \frac{R^2}{2}
\]

\[
R_g = \frac{1}{6} N b^2
\]

\[
L \gg R
\]

\[
R \gg L
\]
Results
Good agreement between fit $R_g$ and true $R_g$ for spherical model

- Slit-smeread data seems to show good agreement
- Error between 1% – 5%

$$R_g = \sqrt{\frac{3}{5} R}$$
Cylinder seems to have good agreement between fit $R_g$ and true $R_g$ with small aspect ratio.

- Fit results seem to have good agreement
- Error under 10%

$$R_g = \sqrt{\frac{L^2}{12} + \frac{R^2}{2}}$$
Cylinder model has increasing deviation between fit $R_g$ and true $R_g$ value as aspect ratio increases.

- Larger aspect ratios show more deviation
- Error between 15% – 20%

\[
R_g = \sqrt{\frac{L^2}{12} + \frac{R^2}{2}}
\]
Disc model has similar trends as cylinder but with less overall error

- Observed similar trend as cylinder but less deviation
- Error under 10%

\[ R_g = \sqrt{\frac{L^2}{12} + \frac{R^2}{2}} \]
Polymer chain has largest deviation between fit $R_g$ and true $R_g$ out of all models tested

- Large deviation in results
- Increasing deviation as dispersity increases

$R_g = \frac{1}{6} N b^2$
Conclusions

• Evaluated Guinier analysis for slit-smeared data

• Slit-smearing distorts sphere Guinier results the least

• More complex shapes show greater effect of smearing

• Guinier analysis is not ruled out for slit-smeared data, but if using more complex shapes, should be used with caution
• Thanks to Rachel Ford, Yun Liu, Julie Borchers, Joe Dura, Susana Teixeira, and all students for a great SURF 2022

• SASView (https://www.sasview.org/)
Backup Slides (Just in case but not used in presentation)
Shrinking Guinier region shows only slight improvement to cylinder with large aspect ratio.

Percent Error: ~30% to ~24%

Decreasing $Q_{\text{max}}$ used in Guinier plot
Shrinking Guinier shows only slight improvement to cylinder with large aspect ratio.

Percent Error: ~37% to ~31%

Decreasing $Q_{\text{max}}$ used in Guinier plot
Shrinking Guinier allows disc with large aspect ratio to be within a reasonable percent error.

Percent Error: ~12% to ~10%

R >> L
Spherical Model

\[ I(Q) = \frac{\text{scale}}{V} \times [3V(\Delta \rho) \times \frac{\sin(qr) - qr \cos(qr)}{(qr)^2}]^2 + \text{background} \]

\[ R_g = \sqrt{\frac{3}{5}} R \]
Cylindrical Model

\[ R_g = \sqrt{\frac{L^2}{12} + \frac{R^2}{2}} \]

\[ L \gg R \]

\[ P(Q) = \frac{\text{scale}}{V} \int_0^\pi F^2(q, \alpha) \sin \alpha \, d\alpha + \text{background} \]
Disc Model

\[
P(Q) = \frac{\text{scale}}{V} \int_0^\pi F^2(q, \alpha) \sin \alpha \, d\alpha + \text{background}
\]

\[
R_g = \sqrt{\frac{L^2}{12} + \frac{R^2}{2}}
\]

L \gg R
Gaussian Coil Polymer

\[ I(Q) = \text{scale} \times I_0 \times P(Q) + \text{background} \]

\[ P(Q) = 2 \left[ (1 + UZ)^{-1/U} + Z - 1 \right]/(1 + U)^2 \]

\[ U = \left( \frac{M_w}{M_n} \right) - 1 \]

\[ V = \frac{M}{N_A \delta} \]
• Shrinking Guinier plot only slightly improves cylinder and Gaussian polymer coil deviation.
Disc model deviates from true $R_g$ but the effect of slit-smearing is not as drastic in higher aspect ratios.

- Deviation increases as radius increases but the effect of the increasing radius is not as strong.