JOURNAL OF APPLIED CRYSTALLOGRAPHY

Volume 53 (2020)

Supporting information for article:

Classifying and analyzing small-angle scattering data using weighted *k* nearest neighbors machine learning techniques

Richard K. Archibald, Mathieu Doucet, Travis Johnston, Steven R. Young, Erika Yang and William T. Heller

S.1 SasView models employed in training and testing

The training and test data were generated using a program written in Python 2.7 using a YAML configuration file that specified the models to be used and the ranges of possible values that the parameters could take. An explanation of the various fields and their hierarchical relationships follow.

- The top-level specification is the name of the model taken from the SasView package
    - The name is repeated in the "name" field
    - The category of the model, taken from the SasView documentation is provided in the "Category" field
    - Most of the remaining items at this level are variables taken from the sasmodels implementations of the models. The values that the variable can take are specified using the following.
        - "**fixed: [value]**" The parameter has the value specified.
        - "**linear: [minimum value, maximum value]**" The parameter is a randomly selected floating point number between the minimum and maximum value.
        - "**log: [minimum value, maximum value]**" A floating point number V between the minimum and maximum values is randomly selected. Then the actual parameter used for calculating the model SAS curve is 10^V.
        - Any "fixed", "linear" or "log" parameter can be "**coupled: [variable name]**" to another parameter specified by [variable name]. If the value of the coupled parameter is selected to be V, the value used for the calculation of the SAS model curve is V multiplied by the value of the named variable.
        - "**polydispersity:**" denotes that the parameter is actually polydisperse. The distribution and widths are specified at the next level
            - "**Distribution_Name: [minimum value, maximum value]**" where Distribution_Name can be SchulzDistribution, GaussianDistribution,

LogNormalDistribution and RectangeDistribution, all of which are implemented in SasView. The width of the distribution is randomly selected floating point number between the minimum and maximum value.

- If a structure factor is desired, it is denoted at this level by adding "Structure_Factor". Within the SasView models implemented in *sasmodels*, several possible structure factors are implemented and are denoted as such with their "Category" tag. Each structure factor therefore has a set of variables that can are specified using the configuration language specified above. In the work presented here, the only structure factor used was the hard sphere structure factor "hardsphere".

S.1.1. Specific model configurations used in the manuscript

The models and parameters sets are listed below. Lines that start with a "#" were disabled for the work presented in the main text. The most commonly disabled parameters were those related to polydispersity for a parameter. The maximum number of polydisperse parameters per model was one to limit the computational cost for any single intensity profile.

```
adsorbed_layer:
   name: adsorbed_layer
   Category: shape-sphere
   scale:
      fixed: [1.0]
   background:
      fixed: [0.001]
   second_moment:
      linear: [5.0, 100.0]
   adsorbed_amount:
      linear: [0.0, 4.0]
   density_shell:
      linear: [0.50, 1.50]
   radius:
      log: [1.0, 3.0]
   volfraction:
      linear: [0.0, 0.25]
   sld_shell:
      linear: [-0.56, 8.00]
   sld_solvent:
      linear: [-0.56, 6.38]


broad_peak:
   name: broad_peak
   Category: shape-independent
   scale:
      fixed: [1.0]
   background:
      fixed: [0.001]
   porod_scale:
      linear: [0.000001, 0.00005]
   porod_exp:
      linear: [2.0, 4.0]
   lorentz_scale:
      linear: [5.0, 100.0]
   lorentz_length:
      linear: [20.0, 100.0]
   peak_pos:
      log: [-2.0, 0.0]
```

```
    lorentz_exp:
      linear: [1.0, 3.0]

core_multi_shell:
    name: core_multi_shell
    Category: shape-sphere
    scale:
      fixed: [1.0]
    background:
      fixed: [0.001]
    sld_core:
      linear: [-0.56, 8.00]
    sld_solvent:
      linear: [-0.56, 6.38]
    radius:
      log: [1.0, 3.0]
      polydispersity:
        SchulzDispersion: [0.0, 0.40]
    n:
      integer: [1, 10]
    thickness1:
      log: [1.0, 3.0]
#       polydispersity:
#         SchulzDispersion: [0.0, 0.40]
    thickness2:
      log: [1.0, 3.0]
#       polydispersity:
#         SchulzDispersion: [0.0, 0.40]
    thickness3:
      log: [1.0, 3.0]
#       polydispersity:
#         SchulzDispersion: [0.0, 0.40]
    thickness4:
      log: [1.0, 3.0]
#       polydispersity:
#         SchulzDispersion: [0.0, 0.40]
    thickness5:
      log: [1.0, 3.0]
#       polydispersity:
#         SchulzDispersion: [0.0, 0.40]
    thickness6:
      log: [1.0, 3.0]
#       polydispersity:
#         SchulzDispersion: [0.0, 0.40]
    thickness7:
      log: [1.0, 3.0]
#       polydispersity:
#         SchulzDispersion: [0.0, 0.40]
    thickness8:
      log: [1.0, 3.0]
#       polydispersity:
```

```
#           SchulzDispersion: [0.0, 0.40]
   thickness9:
      log: [1.0, 3.0]
#      polydispersity:
#         SchulzDispersion: [0.0, 0.40]
   thickness10:
      log: [1.0, 3.0]
#      polydispersity:
#         SchulzDispersion: [0.0, 0.40]
   sld1:
      linear: [-0.56, 8.00]
   sld2:
      linear: [-0.56, 8.00]
   sld3:
      linear: [-0.56, 8.00]
   sld4:
      linear: [-0.56, 8.00]
   sld5:
      linear: [-0.56, 8.00]
   sld6:
      linear: [-0.56, 8.00]
   sld7:
      linear: [-0.56, 8.00]
   sld8:
      linear: [-0.56, 8.00]
   sld9:
      linear: [-0.56, 8.00]
   sld10:
      linear: [-0.56, 8.00]
   Structure_Factor:
      name: hardsphere
      volfraction:
         linear: [0.0, 0.50]

core_shell_sphere:
   name: core_shell_sphere
   Category: shape-sphere
   scale:
      fixed: [1.0]
   background:
      fixed: [0.001]
   sld_core:
      linear: [-0.56, 8.00]
   sld_shell:
      linear: [-0.56, 8.00]
   sld_solvent:
      linear: [-0.56, 6.38]
   radius:
      log: [1.0, 3.0]
      polydispersity:
         SchulzDispersion: [0.0, 0.40]
```

```
   thickness:
      log: [0.0, 2.0]
#       polydispersity:
#          SchulzDispersion: [0.0, 0.40]
   Structure_Factor:
      name: hardsphere
      volfraction:
         linear: [0.0, 0.50]

correlation_length:
   name: correlation_length
   Category: shape-independent
   scale:
      fixed: [1.0]
   background:
      fixed: [0.001]
   lorentz_scale:
      linear: [10.0, 100.0]
   porod_scale:
      linear: [0.000001, 0.000005]
   cor_length:
      linear: [20.0, 100.0]
   porod_exp:
      linear: [2.0, 3.0]
   lorentz_exp:
      linear: [1.8, 3.0]

dab:
   name: dab
   Category: shape-independent
   scale:
      log: [1.0, 3.0]
   background:
      fixed: [0.001]
   cor_length:
      log: [1.0, 3.0]

flexible_cylinder:
   name: flexible_cylinder
   Category: shape-cylinder
   scale:
      fixed: [1.0]
   background:
      fixed: [0.001]
   sld:
      linear: [-0.56, 8.00]
   sld_solvent:
      linear: [-0.56, 6.38]
   radius:
      log: [1.0, 3.0]
#       polydispersity:
```

```
#          SchulzDispersion: [0.0, 0.40]
   length:
      log: [1.0, 5.0]
      polydispersity:
         SchulzDispersion: [0.0, 0.40]
   kuhn_length:
      linear: [0.01, 0.25]
      coupled: [length]
#      polydispersity:
#          SchulzDispersion: [0.0, 0.40]

fractal_core_shell:
   name: fractal_core_shell
   Category: shape-independent
   scale:
      fixed: [1.0]
   background:
      fixed: [0.001]
   sld_core:
      linear: [-0.56, 8.00]
   sld_shell:
      linear: [-0.56, 8.00]
   sld_solvent:
      linear: [-0.56, 6.38]
   volfraction:
      linear: [0.01, 0.10]
   fractal_dim:
      linear: [1.5, 3.0]
   radius:
      linear: [5.0, 50.0]
      polydispersity:
         SchulzDispersion: [0.0, 0.40]
   thickness:
      linear: [5.0, 50.0]
#      polydispersity:
#          SchulzDispersion: [0.0, 0.40]
   cor_length:
      linear: [1.0, 10.0]
      coupled: [radius]

fractal:
   name: fractal
   Category: shape-independent
   scale:
      fixed: [1.0]
   background:
      fixed: [0.001]
   sld_block:
      linear: [-0.56, 8.00]
   sld_solvent:
      linear: [-0.56, 6.38]
```

```
    volfraction:
      linear: [0.01, 0.10]
    fractal_dim:
      linear: [1.5, 3.0]
    radius:
      linear: [5.0, 50.0]
      polydispersity:
        SchulzDispersion: [0.0, 0.40]
    cor_length:
      linear: [1.0, 10.0]
      coupled: [radius]

fuzzy_sphere:
    name: fuzzy_sphere
    Category: shape-sphere
    scale:
      fixed: [1.0]
    background:
      fixed: [0.001]
    sld:
      linear: [-0.56, 8.00]
    sld_solvent:
      linear: [-0.56, 6.38]
    radius:
      log: [1.0, 3.0]
      polydispersity:
        SchulzDispersion: [0.0, 0.40]
    fuzziness:
      linear: [0.25, 2.0]
      coupled: [radius]
    Structure_Factor:
      name: hardsphere
      volfraction:
        linear: [0.0, 0.50]

gauss_lorentz_gel:
    name: gauss_lorentz_gel
    Category: shape-independent
    scale:
      fixed: [1.0]
    background:
      fixed: [0.001]
    gauss_scale:
      log: [1.0, 4.0]
    lorentz_scale:
      log: [1.0, 4.0]
    cor_length_static:
      log: [1.0, 3.0]
    cor_length_dynamic:
      log: [1.0, 3.0]
```

```
guinier:
  name: guinier
  Category: shape-independent
  scale:
    fixed: [1.0]
  background:
    fixed: [0.001]
  rg:
    log: [1.0, 3.0]

lamellar_hg:
  name: lamellar_hg
  Category: shape-lamellae
  scale:
    fixed: [1.0]
  background:
    fixed: [0.001]
  sld:
    linear: [-0.56, 8.00]
  sld_head:
    linear: [-0.56, 8.00]
  sld_solvent:
    linear: [-0.56, 6.38]
  length_tail:
    linear: [5.0, 100.0]
    polydispersity:
      GaussianDispersion: [0.0, 0.40]
  length_head:
    linear: [5.0, 100.0]
#     polydispersity:
#       GaussianDispersion: [0.0, 0.40]

lamellar_stack_paracrystal:
  name: lamellar_stack_paracrystal
  Category: shape-lamellae
  scale:
    fixed: [1.0]
  background:
    fixed: [0.001]
  sld:
    linear: [-0.56, 8.00]
  sld_solvent:
    linear: [-0.56, 6.38]
  Nlayers:
    integer: [10, 1000]
  thickness:
    linear: [5.0, 100.0]
    polydispersity:
      GaussianDispersion: [0.0, 0.40]
  d_spacing:
    linear: [1.1, 10.0]
```

```
      coupled: [thickness]
   sigma_d:
      linear: [0.001, 1.0]
      coupled: [d_spacing]

lamellar:
   name: lamellar
   Category: shape-lamellae
   scale:
      fixed: [1.0]
   background:
      fixed: [0.001]
   sld:
      linear: [-0.56, 8.00]
   sld_solvent:
      linear: [-0.56, 6.38]
   thickness:
      log: [1.0, 2.0]
      polydispersity:
         GaussianDispersion: [0.0, 0.40]

linear_pearls:
   name: linear_pearls
   Category: shape-sphere
   scale:
      fixed: [1.0]
   background:
      fixed: [0.001]
   sld:
      linear: [-0.56, 8.00]
   sld_solvent:
      linear: [-0.56, 6.38]
   radius:
      log: [1.0, 3.0]
   edge_sep:
      linear: [0.01, 25.0]
      coupled: [radius]
   num_pearls:
      integer: [3, 10]

lorentz:
   name: lorentz
   Category: shape-independent
   scale:
      fixed: [1.0]
   background:
      fixed: [0.001]
   cor_length:
      log: [1.0, 3.0]
```

```
mass_fractal:
   name: mass_fractal
   Category: shape-independent
   scale:
      fixed: [1.0]
   background:
      fixed: [0.001]
   radius:
      log: [1.0, 2.0]
   fractal_dim_mass:
      linear: [1.7, 3.0]
   cutoff_length:
      linear: [2.0, 10.0]
      coupled: [radius]

mass_surface_fractal:
   name: mass_surface_fractal
   Category: shape-independent
   scale:
      fixed: [1.0]
   background:
      fixed: [0.001]
   rg_cluster:
      log: [1.0, 2.0]
   rg_primary:
      log: [2.0, 4.0]
      coupled: [rg_cluster]
   fractal_dim_mass:
      linear: [1.7, 3.0]
   fractal_dim_surf:
      linear: [2.0, 3.0]

mono_gauss_coil:
   name: mono_gauss_coil
   Category: shape-independent
   scale:
      fixed: [1.0]
   background:
      fixed: [0.001]
   rg:
      log: [1.0, 3.0]
   i_zero:
      log: [-1.0, 4.0]

multilayer_vesicle:
   name: multilayer_vesicle
   Category: shape-sphere
   scale:
      fixed: [1.0]
   background:
      fixed: [0.001]
```

```
    sld:
      linear: [-0.56, 8.00]
    sld_solvent:
      linear: [-0.56, 6.38]
    radius:
      log: [1.0, 3.0]
      polydispersity:
        SchulzDispersion: [0.0, 0.40]
    thick_shell:
      log: [1.0, 2.0]
#     polydispersity:
#       SchulzDispersion: [0.0, 0.40]
    thick_solvent:
      log: [1.0, 2.0]
#     polydispersity:
#       SchulzDispersion: [0.0, 0.40]
    n_shells:
      integer: [1, 25]
    Structure_Factor:
      name: hardsphere
      volfraction:
        linear: [0.0, 0.50]

onion:
    name: onion
    Category: shape-sphere
    scale:
      fixed: [1.0]
    background:
      fixed: [0.001]
    sld_core:
      linear: [-0.56, 8.00]
    sld_solvent:
      linear: [-0.56, 6.38]
    sld_in1:
      linear: [-0.56, 8.00]
    sld_in2:
      linear: [-0.56, 8.00]
    sld_in3:
      linear: [-0.56, 8.00]
    sld_in4:
      linear: [-0.56, 8.00]
    sld_in5:
      linear: [-0.56, 8.00]
    sld_in6:
      linear: [-0.56, 8.00]
    sld_in7:
      linear: [-0.56, 8.00]
    sld_in8:
      linear: [-0.56, 8.00]
    sld_in9:
```

```
    linear: [-0.56, 8.00]
  sld_in10:
    linear: [-0.56, 8.00]
  sld_out1:
    linear: [-0.56, 8.00]
  sld_out2:
    linear: [-0.56, 8.00]
  sld_out3:
    linear: [-0.56, 8.00]
  sld_out4:
    linear: [-0.56, 8.00]
  sld_out5:
    linear: [-0.56, 8.00]
  sld_out6:
    linear: [-0.56, 8.00]
  sld_out7:
    linear: [-0.56, 8.00]
  sld_out8:
    linear: [-0.56, 8.00]
  sld_out9:
    linear: [-0.56, 8.00]
  sld_out10:
    linear: [-0.56, 8.00]
  A1:
    linear: [-5.0, 5.0]
  A2:
    linear: [-5.0, 5.0]
  A3:
    linear: [-5.0, 5.0]
  A4:
    linear: [-5.0, 5.0]
  A5:
    linear: [-5.0, 5.0]
  A6:
    linear: [-5.0, 5.0]
  A7:
    linear: [-5.0, 5.0]
  A8:
    linear: [-5.0, 5.0]
  A9:
    linear: [-5.0, 5.0]
  A10:
    linear: [-5.0, 5.0]
  radius_core:
    log: [1.0, 3.0]
    polydispersity:
      SchulzDispersion: [0.0, 0.40]
  thickness1:
    linear: [5.0, 100.0]
#     polydispersity:
#       SchulzDispersion: [0.0, 0.40]
```

```
   thickness2:
      linear: [5.0, 100.0]
#       polydispersity:
#         SchulzDispersion: [0.0, 0.40]
   thickness3:
      linear: [5.0, 100.0]
#       polydispersity:
#           SchulzDispersion: [0.0, 0.40]
   thickness4:
      linear: [5.0, 100.0]
#       polydispersity:
#           SchulzDispersion: [0.0, 0.40]
   thickness5:
      linear: [5.0, 100.0]
#       polydispersity:
#           SchulzDispersion: [0.0, 0.40]
   thickness6:
      linear: [5.0, 100.0]
#       polydispersity:
#           SchulzDispersion: [0.0, 0.40]
   thickness7:
      linear: [5.0, 100.0]
#       polydispersity:
#           SchulzDispersion: [0.0, 0.40]
   thickness8:
      linear: [5.0, 100.0]
#       polydispersity:
#           SchulzDispersion: [0.0, 0.40]
   thickness9:
      linear: [5.0, 100.0]
#       polydispersity:
#           SchulzDispersion: [0.0, 0.40]
   thickness10:
      linear: [5.0, 100.0]
#       polydispersity:
#           SchulzDispersion: [0.0, 0.40]

peak_lorentz:
   name: peak_lorentz
   Category: shape-independent
   scale:
      fixed: [1.0]
   background:
      fixed: [0.001]
   peak_pos:
      log: [-3.0, 0.0]
   peak_hwhm:
      log: [-3.0, 1.0]

pearl_necklace:
   name: pearl_necklace
```

```
    Category: shape-cylinder
    scale:
      fixed: [1.0]
    background:
      fixed: [0.001]
    sld:
      linear: [-0.56, 8.00]
    sld_string:
      linear: [-0.56, 8.0]
    sld_solvent:
      linear: [-0.56, 6.38]
    radius:
      log: [1.0, 3.0]
    edge_sep:
      linear: [0.01, 25.0]
      coupled: [radius]
    num_pearls:
      integer: [3, 10]
    thick_string:
      linear: [0.01, 1.0]
      coupled: [radius]
      polydispersity:
        SchulzDispersion: [0.0, 0.40]

poly_gauss_coil:
    name: poly_gauss_coil
    Category: shape-independent
    scale:
      fixed: [1.0]
    background:
      fixed: [0.001]
    i_zero:
      log: [1.0, 4.0]
    rg:
      log: [1.0, 2.8]
    polydispersity:
      linear: [1.0, 2.0]
    Structure_Factor:
      name: hardsphere
      volfraction:
        linear: [0.0, 0.50]
      radius_effective:
        linear: [1.0, 1.5]
        coupled: [rg]

polymer_excl_volume:
    name: polymer_excl_volume
    Category: shape-independent
    scale:
      fixed: [1.0]
    background:
```

```
      fixed: [0.001]
   rg:
      log: [1.0, 3.0]
   porod_exp:
      linear: [1.0, 4.0]
   Structure_Factor:
      name: hardsphere
      volfraction:
         linear: [0.0, 0.50]

power_law:
   name: power_law
   Category: shape-independent
   scale:
      fixed: [1.0]
   background:
      fixed: [0.001]
   power:
      linear: [1.0, 5.0]

raspberry:
   name: raspberry
   Category: shape-sphere
   scale:
      fixed: [1.0]
   background:
      fixed: [0.001]
   sld_lg:
      linear: [-0.56, 8.00]
   sld_sm:
      linear: [-0.56, 8.00]
   sld_solvent:
      linear: [-0.56, 6.38]
   volfraction_lg:
      linear: [0.00, 0.25]
   volfraction_sm:
      linear: [0.0, 0.1]
      coupled: [volfraction_lg]
   surface_fraction:
      linear: [0.0, 0.8]
   radius_lg:
      log: [3.0, 5.0]
      polydispersity:
         SchulzDispersion: [0.0, 0.40]
   radius_sm:
      log: [1.0, 2.5]
   penetration:
      linear: [0.0, 1.0]
      coupled: [radius_sm]
   Structure_Factor:
      name: hardsphere
```

```
      volfraction:
        linear: [ 0.0, 0.50]

sphere:
  name: sphere
  Category: shape-sphere
  scale:
    fixed: [1.0]
  background:
    fixed: [0.001]
  sld:
    linear: [-0.56, 8.00]
  sld_solvent:
    linear: [-0.56, 6.38]
  radius:
    log: [1.0, 3.5]
    polydispersity:
      SchulzDispersion: [0.0, 0.40]
  Structure_Factor:
    name: hardsphere
    volfraction:
      linear: [0.0, 0.50]


spherical_sld:
  name: spherical_sld
  Category: shape-sphere
  scale:
    fixed: [1.0]
  background:
    fixed: [0.001]
  n_steps:
    fixed: [35]
  n_shells:
    integer: [1, 10]
  sld_solvent:
    linear: [-0.56, 6.38]
  sld1:
    linear: [-0.56, 8.00]
  sld2:
    linear: [-0.56, 8.00]
  sld3:
    linear: [-0.56, 8.00]
  sld4:
    linear: [-0.56, 8.00]
  sld5:
    linear: [-0.56, 8.00]
  sld6:
    linear: [-0.56, 8.00]
  sld7:
    linear: [-0.56, 8.00]
```

```
  sld8:
    linear: [-0.56, 8.00]
  sld9:
    linear: [-0.56, 8.00]
  sld10:
    linear: [-0.56, 8.00]
  thickness1:
    linear: [5.0, 50.0]
    polydispersity:
      SchulzDispersion: [0.0, 0.40]
  thickness2:
    linear: [5.0, 50.0]
#     polydispersity:
#       SchulzDispersion: [0.0, 0.40]
  thickness3:
    linear: [5.0, 50.0]
#     polydispersity:
#       SchulzDispersion: [0.0, 0.40]
  thickness4:
    linear: [5.0, 50.0]
#     polydispersity:
#       SchulzDispersion: [0.0, 0.40]
  thickness5:
    linear: [5.0, 50.0]
#     polydispersity:
#       SchulzDispersion: [0.0, 0.40]
  thickness6:
    linear: [5.0, 50.0]
#     polydispersity:
#       SchulzDispersion: [0.0, 0.40]
  thickness7:
    linear: [5.0, 50.0]
#     polydispersity:
#       SchulzDispersion: [0.0, 0.40]
  thickness8:
    linear: [5.0, 50.0]
#     polydispersity:
#       SchulzDispersion: [0.0, 0.40]
  thickness9:
    linear: [5.0, 50.0]
#     polydispersity:
#       SchulzDispersion: [0.0, 0.40]
  thickness10:
    linear: [5.0, 50.0]
#     polydispersity:
#       SchulzDispersion: [0.0, 0.40]
  interface1:
    linear: [5.0, 50.0]
#     polydispersity:
#       SchulzDispersion: [0.0, 0.40]
  interface2:
```

```
    linear: [5.0, 50.0]
#     polydispersity:
#       SchulzDispersion: [0.0, 0.40]
  interface3:
    linear: [5.0, 50.0]
#     polydispersity:
#       SchulzDispersion: [0.0, 0.40]
  interface4:
    linear: [5.0, 50.0]
#     polydispersity:
#       SchulzDispersion: [0.0, 0.40]
  interface5:
    linear: [5.0, 50.0]
#     polydispersity:
#       SchulzDispersion: [0.0, 0.40]
  interface6:
    linear: [5.0, 50.0]
#     polydispersity:
#       SchulzDispersion: [0.0, 0.40]
  interface7:
    linear: [5.0, 50.0]
#     polydispersity:
#       SchulzDispersion: [0.0, 0.40]
  interface8:
    linear: [5.0, 50.0]
#     polydispersity:
#       SchulzDispersion: [0.0, 0.40]
  interface9:
    linear: [5.0, 50.0]
#     polydispersity:
#       SchulzDispersion: [0.0, 0.40]
  interface10:
    linear: [5.0, 50.0]
#     polydispersity:
#       SchulzDispersion: [0.0, 0.40]
  nu1:
    linear: [1.0, 4.0]
  nu2:
    linear: [1.0, 4.0]
  nu3:
    linear: [1.0, 4.0]
  nu4:
    linear: [1.0, 4.0]
  nu5:
    linear: [1.0, 4.0]
  nu6:
    linear: [1.0, 4.0]
  nu7:
    linear: [1.0, 4.0]
  nu8:
    linear: [1.0, 4.0]
```

```
    nu9:
      linear: [1.0, 4.0]
    nu10:
      linear: [1.0, 4.0]
    shape1:
      integer: [0, 4]
    shape2:
      integer: [0, 4]
    shape3:
      integer: [0, 4]
    shape4:
      integer: [0, 4]
    shape5:
      integer: [0, 4]
    shape6:
      integer: [0, 4]
    shape7:
      integer: [0, 4]
    shape8:
      integer: [0, 4]
    shape9:
      integer: [0, 4]
    shape10:
      integer: [0, 4]

star_polymer:
    name: star_polymer
    Category: shape-independent
    scale:
      fixed: [1.0]
    background:
      fixed: [0.001]
    rg_squared:
      log: [1.0, 3.0]
    arms:
      integer: [1, 10]

surface_fractal:
    name: surface_fractal
    Category: shape-independent
    scale:
      fixed: [1.0]
    background:
      fixed: [0.001]
    fractal_dim_surf:
      linear: [1.0, 3.0]
    radius:
      linear: [5.0, 50.0]
      polydispersity:
        SchulzDispersion: [0.0, 0.40]
    cutoff_length:
```

```
      linear: [5.0, 100.0]
      coupled: [radius]


teubner_strey:
   name: teubner_strey
   Category: shape-independent
   scale:
      fixed: [1.0]
   background:
      fixed: [0.001]
   sld_a:
      linear: [-0.56, 8.00]
   sld_b:
      linear: [-0.56, 8.00]
   d:
      log: [1.0, 2.5]
   xi:
      linear: [2.5, 100.0]
      coupled: [d]

two_lorentzian:
   name: two_lorentzian
   Category: shape-independent
   scale:
      fixed: [1.0]
   background:
      fixed: [0.001]
   lorentz_scale_1:
      log: [2.0, 4.0]
   lorentz_scale_2:
      linear: [0.01, 0.10]
      coupled: [lorentz_scale_1]
   lorentz_length_1:
      log: [2.0, 3.0]
   lorentz_length_2:
      log: [0.0, 2.0]
   lorentz_exp_1:
      linear: [1.0, 3.0]
   lorentz_exp_2:
      linear: [1.0, 3.0]

two_power_law:
   name: two_power_law
   Category: shape-independent
   scale:
      fixed: [1.0]
   background:
      fixed: [0.001]
   coefficent_1:
      log: [1.0, 4.0]
```

```
    crossover:
      linear: [0.01, 0.50]
    power_1:
      linear: [1.0, 4.0]
    power_2:
      linear: [1.0, 4.0]

unified_power_Rg:
    name: unified_power_Rg
    Category: shape-independent
    scale:
      fixed: [1.0]
    background:
      fixed: [0.001]
    level:
      integer: [1, 6]
    rg1:
      log: [2.0, 5.0]
    rg2:
      linear: [0.01, 0.99]
      coupled: [rg1]
    rg3:
      linear: [0.01, 0.99]
      coupled: [rg2]
    rg4:
      linear: [0.01, 0.99]
      coupled: [rg3]
    rg5:
      linear: [0.01, 0.99]
      coupled: [rg4]
    rg6:
      linear: [0.01, 0.99]
      coupled: [rg5]
    power1:
      linear: [1.0, 4.0]
    power2:
      linear: [1.0, 4.0]
    power3:
      linear: [1.0, 4.0]
    power4:
      linear: [1.0, 4.0]
    power5:
      linear: [1.0, 4.0]
    power6:
      linear: [1.0, 4.0]
    B1:
      log: [-8.0, -5.0]
    B2:
      log: [-8.0, -5.0]
    B3:
      log: [-8.0, -5.0]
```

```
    B4:
      log: [-8.0, -5.0]
    B5:
      log: [-8.0, -5.0]
    B6:
      log: [-8.0, -5.0]
    G1:
      log: [2.0, 5.0]
    G2:
      linear: [0.01, 0.99]
      coupled: [G1]
    G3:
      linear: [0.01, 0.99]
      coupled: [G2]
    G4:
      linear: [0.01, 0.99]
      coupled: [G3]
    G5:
      linear: [0.01, 0.99]
      coupled: [G4]
    G6:
      linear: [0.01, 0.99]
      coupled: [G5]

vesicle:
    name: vesicle
    Category: shape-sphere
    scale:
      fixed: [1.0]
    background:
      fixed: [0.001]
    sld:
      linear: [-0.56, 8.00]
    sld_solvent:
      linear: [-0.56, 6.38]
    volfraction:
      linear: [0.00, 1.00]
    radius:
      log: [3.0, 5.0]
      polydispersity:
        SchulzDispersion: [0.0, 0.40]
    thickness:
      log: [1.0, 2.0]
#     polydispersity:
#       SchulzDispersion: [0.0, 0.40]
    Structure_Factor:
      name: hardsphere
      volfraction:
        linear: [0.0, 0.50]
```