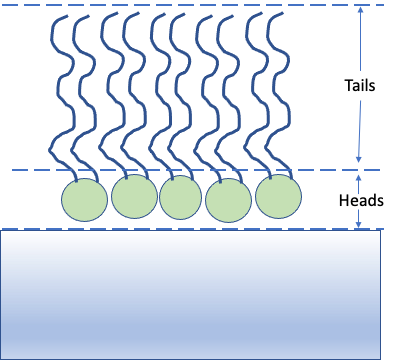
# 3. An example - a lipid monolayer.

In the next chapter, we'll look in detail how to set up the problem definition for a given situation. Initially though, it's useful to take a pre-prepared problem definition, and to see how this is then used in RAT. As an example, we'll use some neutron reflectivity data for a lipid monolayer, collected at various deuterations, which we want to analyse simultaneously.

In terms of reflectivity, the interface we want to model (i.e. a monolayer at an air-water interface) is usually well modeled by two layers: the hydrophobic tail regions of the lipids, which locate outside the bulk water interface, and the hydrophilic heads wich are adjacent (or embedded) in the bulk aqueous phase.

In our example, the layers can be either deuterated of hydrogenated, and the bulk water can either be D2O or ACMW.



The way this kind of model is set up for RAT should be familliar to anyone who has used RasCAL, in that we identify which parameters we need to describe the model, group these into layers, and then group the layers along with data into contrasts. The advantage pf this approach is that it's simple to share parameters beytween layers, so a layer representing deuterated headgroups should share the same thickness and roughness parameters as a layer representing hydrogenated heads, but they should differ from each other in their SLD.

The problem definition in RAT is done by making an instance of a problemDef class, and then using the class methods to then set the layers and so on. But for now, we'll look at a pre-prepared example.

% Load in a pre-made problemDef class

problem = load('twoContrastExample.mat');

problem = problem.problem;

% Have a look at what we have

disp(problem)

ModelType: 'Standard Layers'

experimentName: 'DSPC monolayers'

Geometry: 'air/substrate'

Parameters: ----------------------------------------------------------------------------------------------

**p** **Name** **Min** **Value** **Max** **Fit?**

**\_\_** **\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_** **\_\_\_\_\_\_** **\_\_\_\_\_\_\_** **\_\_\_\_\_** **\_\_\_\_\_**

1 "Substrate Roughness" 2 3 13 true

2 "Tails Thickness" 10 20 30 true

3 "Heads Thickness" 3 11 16 true

4 "Tails Roughness" 2 5 9 true

5 "Heads Roughness" 2 5 9 true

6 "Deuterated Tails SLD" 4e-06 6e-06 2e-05 true

7 "Hydrogenated Tails SLD" -6e-07 -4e-07 0 true

8 "Deuterated Heads SLD" 1e-06 3e-06 8e-06 true

9 "Hydrogenated Heads SLD" 1e-07 1.4e-06 3e-06 true

10 "Heads Hydration" 0 0.3 0.5 true

Layers: --------------------------------------------------------------------------------------------------

**p** **Name** **Thickness** **SLD** **Roughness** **Hydration** **Hydrate with**

**\_** **\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_** **\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_** **\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_** **\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_** **\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_** **\_\_\_\_\_\_\_\_\_\_\_\_**

1 "Hydrogenated Heads" "Heads Thickness" "Hydrogenated Heads SLD" "Heads Roughness" "Heads Hydration" "bulk out"

2 "Deuterated Heads" "Heads Thickness" "Deuterated Heads SLD" "Heads Roughness" "Heads Hydration" "bulk out"

3 "Hydrogenated Tails" "Tails Thickness" "Hydrogenated Tails SLD" "Tails Roughness" <missing> "bulk in"

4 "Deuterated Tails" "Tails Thickness" "Deuterated Tails SLD" "Tails Roughness" <missing> "bulk in"

Bulk In: --------------------------------------------------------------------------------------------------

**p** **Name** **Min** **Value** **Max** **Fit?**

**\_** **\_\_\_\_\_\_\_\_\_** **\_\_\_** **\_\_\_\_\_** **\_\_\_** **\_\_\_\_\_**

1 "SLD Air" 0 0 0 false

Bulk Out: -------------------------------------------------------------------------------------------------

**p** **Name** **Min** **Value** **Max** **Fit?**

**\_** **\_\_\_\_\_\_\_\_\_\_** **\_\_\_\_\_\_\_** **\_\_\_\_\_\_\_\_** **\_\_\_\_\_\_\_\_** **\_\_\_\_\_**

1 "SLD D2O" 6.2e-06 6.35e-06 6.35e-06 false

2 "SLD ACMW" -1e-06 0 1e-06 true

Scalefactors: -------------------------------------------------------------------------------------------------

**p** **Name** **Min** **Value** **Max** **Fit?**

**\_** **\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_** **\_\_\_\_** **\_\_\_\_\_** **\_\_\_\_** **\_\_\_\_\_**

1 "Scalefactor 1" 0.02 0.23 0.25 true

Backgrounds: -----------------------------------------------------------------------------------------------

(a) Background Parameters:

**p** **Name** **Min** **Value** **Max** **Fit?**

**\_** **\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_** **\_\_\_\_\_** **\_\_\_\_\_\_\_** **\_\_\_\_\_** **\_\_\_\_\_**

1 "Backs value ACMW" 1e-07 5.5e-06 1e-05 true

2 "Backs Value D2O" 1e-08 2.8e-06 1e-05 true

(b) Backgrounds:

**p** **Name** **Type** **Value 1** **Value 2** **Value 3** **Value 4** **Value 5**

**\_** **\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_** **\_\_\_\_\_\_\_\_\_\_** **\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_** **\_\_\_\_\_\_\_** **\_\_\_\_\_\_\_** **\_\_\_\_\_\_\_** **\_\_\_\_\_\_\_**

1 "Background ACMW" "constant" "Backs Value ACMW" "" "" "" ""

2 "Background D2O" "constant" "Backs Value D2O" "" "" "" ""

Resolutions: ---------------------------------------------------------------------------------------------

(a) Resolutions Parameters:

**p** **Name** **Min** **Value** **Max** **Fit?**

**\_** **\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_** **\_\_\_\_** **\_\_\_\_\_** **\_\_\_\_** **\_\_\_\_\_**

1 "Resolution par 1" 0.01 0.03 0.05 false

(b) Resolutions:

**p** **Name** **Type** **Value 1** **Value 2** **Value 3** **Value 4** **Value 5**

**\_** **\_\_\_\_\_\_\_\_\_\_\_\_\_\_** **\_\_\_\_\_\_\_\_\_\_** **\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_** **\_\_\_\_\_\_\_** **\_\_\_\_\_\_\_** **\_\_\_\_\_\_\_** **\_\_\_\_\_\_\_**

1 "Resolution 1" "gaussian" "Resolution par 1" "" "" "" ""

Data: ------------------------------------------------------------------------------------------------------

**Name** **Data** **Data Range** **Simulation Range**

**\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_** **\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_** **\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_** **\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_**

"Simulation" "No Data" "-" "[ 0.0050 , 0.7000 ]"

"H-tail / D-head / ACMW" "Data array: [51 x 3]" "[ 0.0518 , 0.5888 ]" "[ 0.0050 , 0.7000 ]"

"D-tail / H-head / D2O" "Data array: [51 x 3]" "[ 0.0518 , 0.5888 ]" "[ 0.0050 , 0.7000 ]"

Custom Files: ------------------------------------------------------------------------------------------------------

**Name** **Filename** **Language** **Path**

**\_\_\_\_** **\_\_\_\_\_\_\_\_** **\_\_\_\_\_\_\_\_** **\_\_\_\_**

"" "" "" ""

Constrasts: ----------------------------------------------------------------------------------------------

**p** **1** **2**

**\_\_\_\_\_\_\_\_\_\_\_\_\_** **\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_** **\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_**

"name" "D-tail/H-Head/D2O" "H-tail/D-Head/ACMW"

"Data" "D-tail / H-head / D2O" "H-tail / D-head / ACMW"

"Background" "Background D2O" "Background ACMW"

"Bulk in" "SLD air" "SLD air"

"Bulk out" "SLD D2O" "SLD ACMW"

"Scalefactor" "Scalefactor 1" "Scalefactor 1"

"Resolution" "Resolution 1" "Resolution 1"

"Model" "Deuterated tails" "hydrogenated tails"

"" "Hydrogenated heads" "deuterated heads"

% Make an instance of a projectClass:

problem = projectClass('test');

% Check what type our class is...

class(problem)

ans = 'projectClass'

% Have a look at its class methods..

methods(problem)

Methods for class projectClass:

addBackground addLayerGroup removeData setBulkIn setModelType setUsePriors

addBacksPar addParam removeParam setBulkOut setParamConstr toStruct

addBulkIn addParamGroup setBackgroundName setContrast setParamFit

addBulkOut addQzshift setBackgroundValue setContrastModel setParamName

addContrast addScalefactor setBacksPar setCustomFile setParamPrior

addCustomFile getAllAllowedNames setBacksParConstr setData setParamValue

addData projectClass setBacksParName setGeometry setParameter

addLayer removeBacksPar setBacksParValue setLayerValue setScalefactor

Methods of projectClass inherited from handle.

% Check our empty project class:

disp(problem)

ModelType: 'Standard Layers'

experimentName: 'test'

Geometry: 'air/substrate'

Parameters: ----------------------------------------------------------------------------------------------

**p** **Name** **Min** **Value** **Max** **Fit?**

**\_** **\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_** **\_\_\_** **\_\_\_\_\_** **\_\_\_** **\_\_\_\_\_**

1 "Substrate Roughness" 1 3 5 true

Layers: --------------------------------------------------------------------------------------------------

**Name** **Thickness** **SLD** **Roughness** **Hydration** **Hydrate with**

**\_\_\_\_** **\_\_\_\_\_\_\_\_\_** **\_\_\_** **\_\_\_\_\_\_\_\_\_** **\_\_\_\_\_\_\_\_\_** **\_\_\_\_\_\_\_\_\_\_\_\_**

0 0 0 0 0 0

Bulk In: --------------------------------------------------------------------------------------------------

**p** **Name** **Min** **Value** **Max** **Fit?**

**\_** **\_\_\_\_\_\_\_\_\_** **\_\_\_** **\_\_\_\_\_** **\_\_\_** **\_\_\_\_\_**

1 "SLD Air" 0 0 0 false

Bulk Out: -------------------------------------------------------------------------------------------------

**p** **Name** **Min** **Value** **Max** **Fit?**

**\_** **\_\_\_\_\_\_\_\_\_** **\_\_\_\_\_\_\_** **\_\_\_\_\_\_\_\_** **\_\_\_\_\_\_\_\_** **\_\_\_\_\_**

1 "SLD D2O" 6.2e-06 6.35e-06 6.35e-06 false

Scalefactors: -------------------------------------------------------------------------------------------------

**p** **Name** **Min** **Value** **Max** **Fit?**

**\_** **\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_** **\_\_\_\_** **\_\_\_\_\_** **\_\_\_\_** **\_\_\_\_\_**

1 "Scalefactor 1" 0.02 0.23 0.25 false

Backgrounds: -----------------------------------------------------------------------------------------------

(a) Background Parameters:

**p** **Name** **Min** **Value** **Max** **Fit?**

**\_** **\_\_\_\_\_\_\_\_\_\_\_\_\_** **\_\_\_\_\_** **\_\_\_\_\_** **\_\_\_\_\_** **\_\_\_\_\_**

1 "Backs par 1" 1e-07 1e-06 1e-05 false

(b) Backgrounds:

**p** **Name** **Type** **Value 1** **Value 2** **Value 3** **Value 4** **Value 5**

**\_** **\_\_\_\_\_\_\_\_\_\_\_\_\_\_** **\_\_\_\_\_\_\_\_\_\_** **\_\_\_\_\_\_\_\_\_\_\_\_\_** **\_\_\_\_\_\_\_** **\_\_\_\_\_\_\_** **\_\_\_\_\_\_\_** **\_\_\_\_\_\_\_**

1 "Background 1" "constant" "Backs Par 1" "" "" "" ""

Resolutions: ---------------------------------------------------------------------------------------------

(a) Resolutions Parameters:

**p** **Name** **Min** **Value** **Max** **Fit?**

**\_** **\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_** **\_\_\_\_** **\_\_\_\_\_** **\_\_\_\_** **\_\_\_\_\_**

1 "Resolution par 1" 0.01 0.03 0.05 false

(b) Resolutions:

**p** **Name** **Type** **Value 1** **Value 2** **Value 3** **Value 4** **Value 5**

**\_** **\_\_\_\_\_\_\_\_\_\_\_\_\_\_** **\_\_\_\_\_\_\_\_\_\_** **\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_** **\_\_\_\_\_\_\_** **\_\_\_\_\_\_\_** **\_\_\_\_\_\_\_** **\_\_\_\_\_\_\_**

1 "Resolution 1" "gaussian" "Resolution par 1" "" "" "" ""

Data: ------------------------------------------------------------------------------------------------------

**Name** **Data** **Data Range** **Simulation Range**

**\_\_\_\_\_\_\_\_\_\_\_\_** **\_\_\_\_\_\_\_\_\_** **\_\_\_\_\_\_\_\_\_\_** **\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_**

"Simulation" "No Data" "-" "[ 0.0050 , 0.7000 ]"

Custom Files: ------------------------------------------------------------------------------------------------------

**Name** **Filename** **Language** **Path**

**\_\_\_\_** **\_\_\_\_\_\_\_\_** **\_\_\_\_\_\_\_\_** **\_\_\_\_**

"" "" "" ""

Constrasts: ----------------------------------------------------------------------------------------------

**p**

**\_\_\_\_\_\_\_\_\_\_\_\_\_**

"name"

"Data"

"Background"

"Bulk in"

"Bulk out"

"Scalefactor"

"Resolution"

"Model"