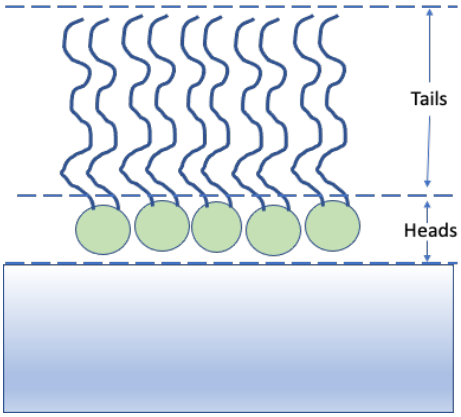
3. An example - a lipid monolayer.

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	
1	"Hydrogenated Heads"	"Heads Thickness"	"Hydrogenated Heads SLD"	"Heads Roughness"	"He
2	"Deuterated Heads"	"Heads Thickness"	"Deuterated Heads SLD"	"Heads Roughness"	"He
3	"Hydrogenated Tails"	"Tails Thickness"	"Hydrogenated Tails SLD"	"Tails Roughness"	<m
4	"Deuterated Tails"	"Tails Thickness"	"Deuterated Tails SLD"	"Tails Roughness"	<m

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        setUse
addBacksPar         addParam            removeParam         setBulkOut          setParamConstr      toStru
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"
```