Monolayer 7 contrasts test.

Test of RAT toolbox using new input classes.

To make the problemDef class, first we'll just convert a Rascal1 project instead of making one from scratch..

```
[problem,controls] = r1ToProblemDef('monolayer_7_contrasts_stanLay.mat')
```

```
problem =
  problemDef with properties:

         experimentType: 'standard'
     experimentGeometry: 'air/substrate'
                nParams: 10
                 params: [6.9908 18.7691 6.9356e-06 3.0000 -2.1908e-07 7.0000 5.8551e-06 3.0000 1.8079e-06
              paramNames: {'Substrate Roughness'  'Tails thick'  'Deuterated tails SLD'  'Tails roughness'
             paramConstr: {[3 7]  [12 20]  [5.0000e-06 9.0000e-06]  [3 7]  [-6.0000e-07 -2.0000e-07]  [7 12
          paramFitYesNo: [1 1 1 1 1 1 1 1 1]
           nBackgrounds: 2
            backgrounds: [2.8895e-06 5.1729e-06]
       backgroundNames: {'Background  D2O'  'Background ACMW'}
      backgroundConstr: {[1.0000e-07 7.0000e-06]  [1.0000e-07 7.0000e-06]}
    backgroundFitYesNo: [1 1]
         nScalefactors: 1
          scalefactors: 0.2325
      scalefactorNames: {'Scalefactor 1'}
     scalefactorConstr: {[0.1000 0.4000]}
   scalefactorFitYesNo: 1
             nQzshifts: 1
              qzshifts: 0
         qzshiftNames: {'Qz Shifts 1'}
        qzshiftConstr: {[-0.0300 0.0300]}
      qzshiftFitYesNo: 0
        nbairFitYesNo: 0
              nNbsubs: 2
               nbsubs: [6.3500e-06 3.4929e-08]
           nbsubNames: {'D2O'  'ACMW'}
          nbsubConstr: {[6.3000e-06 6.4000e-06]  [-5.0000e-07 5.0000e-07]}
        nbsubFitYesNo: [1 1]
     numberOfContrasts: 7
          nResolutions: 1
           resolutions: 0.0300
      resolutionNames: {'Resolution 1'}
     resolutionConstr: {[0.0100 0.0500]}
    resolutionFitYesNo: 1
               allData: {[51×3 double]  [51×3 double]  [51×3 double]  [51×3 double]  [51×3 double]  [51×3
           dataPresent: [1 1 1 1 1 1 1]
              resample: [0 0 0 0 0 0 0]
            dataLimits: {[0.0518 0.5888]  [0.0518 0.5888]  [0.0518 0.5888]  [0.0518 0.5888]  [0.0518 0.58
             simLimits: {[0.0518 0.5888]  [0.0518 0.5888]  [0.0518 0.5888]  [0.0518 0.5888]  [0.0518 0.58
         contrastBacks: {[2 1]  [1 1]  [2 1]  [1 1]  [2 1]  [1 1]  [1 1]}
        contrastShifts: [1 1 1 1 1 1 1]
        contrastScales: [1 1 1 1 1 1 1]
          contrastNbas: [1 1 1 1 1 1 1]
          contrastNbss: [2 1 2 1 2 1 1]
           contrastRes: [1 1 1 1 1 1 1]
    contrastRepeatSLDs: {[0 1]  [0 1]  [0 1]  [0 1]  [0 1]  [0 1]  [0 1]}
             modelType: 'layers'
        numberOfLayers: 4
         layersDetails: {4×1 cell}
        contrastLayers: {[1 4]  [1 4]  [2 3]  [2 3]  [1 3]  [1 3]  [2 4]}
controls =
  controlsDef with properties:
```

```
           parallel: 'single'
          procedure: 'calculate'
    calcSldDuringFit: 'no'
```

This gives us the two RAT input classes. Now we just need to make sure we're selecting the right algorithm (simplex), and set any algorithm specific parameters. Also make RAT parallelise across the contrasts..

```
controls.procedure = 'simplex'
```

```
controls =
  controlsDef with properties:

           parallel: 'single'
          procedure: 'simplex'
    calcSldDuringFit: 'no'
            display: 'iter'
               tolX: 1.0000e-06
             tolFun: 1.0000e-06
        maxFunEvals: 10000
            maxIter: 1000
```

```
controls.maxIter = 200;
controls.parallel = 'parallelTF';
[outProb,results] = RAT(problem,controls)
```

```
 Iteration   Func-count     min f(x)         Procedure
     0           1          9.72628
     1          17          9.72628         initial simplex
     2          19          9.72628         contract inside
     3          21          9.72628         contract inside
     4          23          9.72628         contract inside
     5          25          9.72628         contract inside
     6          27          9.72628         contract inside
     7          29          9.72628         contract inside
     8          31          9.72628         contract inside
     9          33          9.72628         contract inside
    10          35          9.72628         contract outside
    11          37          9.72628         contract inside
    12          39          9.72628         contract inside
    13          40          9.72628         reflect
    14          41          9.72628         reflect
    15          43          9.72628         contract inside
    16          45          9.72628         contract inside
    17          47          9.72628         contract inside
    18          48          9.72628         reflect
    19          49          9.72628         reflect
    20          51          9.72628         contract inside
    21          53          9.72628         contract inside
    22          54          9.72628         reflect
    23          55          9.72628         reflect
    24          57          9.72628         contract inside
    25          59          9.72628         contract inside
    26          61          9.72628         contract inside
    27          63          9.72628         contract inside
    28          65          9.72628         contract inside
    29          67          9.72628         contract inside
    30          68          9.72628         reflect
    31          69          9.72628         reflect
    32          71          9.72628         contract inside
    33          72          9.72628         reflect
```

34	74	9.72628	contract inside
35	76	9.72628	contract inside
36	78	9.72628	contract inside
37	80	9.72628	contract inside
38	82	9.72628	contract outside
39	84	9.72628	contract inside
40	86	9.72628	contract outside
41	88	9.72628	contract inside
42	89	9.72628	reflect
43	91	9.72628	contract inside
44	93	9.72628	contract inside
45	94	9.72628	reflect
46	95	9.72628	reflect
47	96	9.72628	reflect
48	98	9.72628	contract outside
49	99	9.72628	reflect
50	100	9.72628	reflect
51	102	9.72628	contract inside
52	104	9.72628	contract inside
53	105	9.72628	reflect
54	107	9.72628	contract inside
55	109	9.72628	contract inside
56	110	9.72628	reflect
57	112	9.72628	contract inside
58	114	9.72628	contract inside
59	115	9.72628	reflect
60	117	9.72628	contract inside
61	119	9.72628	contract inside
62	121	9.72628	contract inside
63	122	9.72628	reflect
64	124	9.72628	contract inside
65	126	9.72628	contract inside
66	128	9.72628	contract inside
67	129	9.72628	reflect
68	130	9.72628	reflect
69	132	9.72628	contract inside
70	133	9.72628	reflect
71	134	9.72628	reflect
72	135	9.72628	reflect
73	137	9.72628	contract inside
74	139	9.72628	contract inside
75	141	9.72628	contract inside
76	142	9.72628	reflect
77	144	9.72628	contract inside
78	146	9.72628	contract inside
79	148	9.72628	contract outside
80	150	9.72628	contract inside
81	151	9.72628	reflect
82	152	9.72628	reflect
83	153	9.72628	reflect
84	155	9.72628	contract inside
85	157	9.72628	contract inside
86	159	9.72628	contract inside
87	160	9.72628	reflect
88	161	9.72628	reflect
89	162	9.72628	reflect
90	164	9.72628	contract inside
91	166	9.72628	contract inside
92	168	9.72628	contract inside
93	170	9.72628	contract inside
94	171	9.72628	reflect
95	173	9.72628	contract inside
96	174	9.72628	reflect
97	175	9.72628	reflect
98	177	9.72628	contract inside

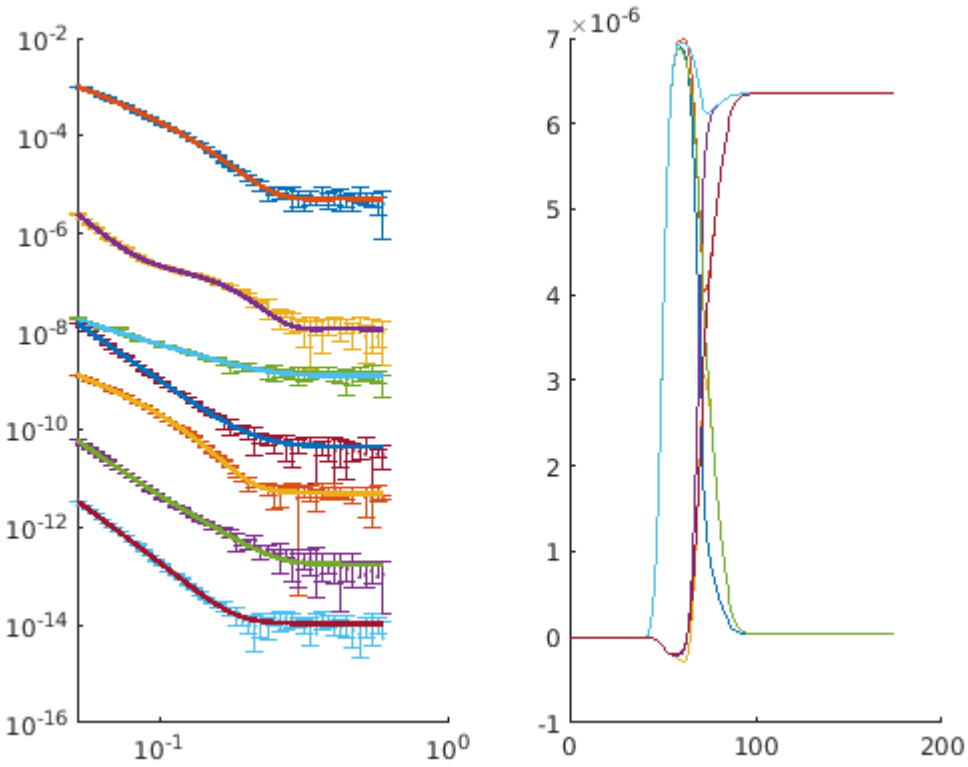
99	179	9.72628	contract inside
100	181	9.72628	contract outside
101	182	9.72628	reflect
102	183	9.72628	reflect
103	185	9.72628	contract inside
104	187	9.72628	contract inside
105	189	9.72628	contract inside
106	191	9.72628	contract inside
107	193	9.72628	contract inside
108	195	9.72628	contract outside
109	197	9.72628	contract inside
110	198	9.72628	reflect
111	200	9.72628	contract inside
112	202	9.72628	contract inside
113	203	9.72628	reflect
114	205	9.72628	contract inside
115	206	9.72628	reflect
116	208	9.72627	contract inside
117	210	9.72627	contract inside
118	212	9.72627	contract inside
119	213	9.72627	reflect
120	215	9.72627	contract inside
121	217	9.72627	contract inside
122	218	9.72627	reflect
123	220	9.72627	contract inside
124	221	9.72627	reflect
125	222	9.72627	reflect
126	224	9.72627	contract inside
127	226	9.72627	contract inside
128	227	9.72627	reflect
129	229	9.72627	contract inside
130	231	9.72627	contract inside
131	233	9.72627	contract inside
132	235	9.72627	contract inside
133	237	9.72627	contract inside
134	239	9.72627	contract inside
135	241	9.72627	contract inside
136	242	9.72627	reflect
137	244	9.72627	contract inside
138	246	9.72627	contract inside
139	248	9.72627	contract inside
140	250	9.72627	contract inside
141	252	9.72627	contract inside
142	253	9.72627	reflect
143	254	9.72627	reflect
144	256	9.72627	contract inside
145	257	9.72627	reflect
146	259	9.72627	contract inside
147	260	9.72627	reflect
148	261	9.72627	reflect
149	263	9.72627	contract inside
150	265	9.72627	contract inside
151	267	9.72627	contract inside
152	268	9.72627	reflect
153	269	9.72627	reflect
154	270	9.72627	reflect
155	272	9.72627	contract inside
156	274	9.72627	contract inside
157	276	9.72627	contract inside
158	277	9.72627	reflect
159	279	9.72627	contract inside
160	280	9.72627	reflect
161	281	9.72627	reflect
162	283	9.72627	contract inside
163	284	9.72627	reflect

```
   164          286          9.72627         contract inside
   165          288          9.72627         contract inside
   166          290          9.72627         contract inside
   167          292          9.72627         contract inside
   168          294          9.72627         reflect
   169          296          9.72627         contract inside
   170          298          9.72627         reflect
   171          299          9.72627         reflect
   172          300          9.72627         reflect
   173          301          9.72627         reflect
   174          303          9.72627         contract inside
   175          305          9.72627         contract inside
   176          306          9.72627         reflect
   177          308          9.72627         contract inside
   178          310          9.72627         contract inside
   179          312          9.72627         contract inside
   180          314          9.72627         contract inside
   181          316          9.72627         reflect
   182          317          9.72627         reflect
   183          318          9.72627         reflect
   184          320          9.72627         reflect
   185          321          9.72627         reflect
   186          322          9.72627         reflect
   187          324          9.72627         contract inside
   188          326          9.72627         contract inside
   189          327          9.72627         reflect
   190          329          9.72627         contract inside
   191          331          9.72627         contract inside
   192          333          9.72627         contract inside
   193          334          9.72627         reflect
   194          335          9.72627         reflect
   195          336          9.72627         reflect
   196          337          9.72627         reflect
   197          339          9.72627         reflect
   198          340          9.72627         reflect
   199          341          9.72627         reflect
   200          342          9.72627         reflect

Exiting: Maximum number of iterations has been exceeded
         - increase MaxIter option.
         Current function value: 9.726274
outProb =
  problemDef with properties:

         experimentType: 'standard'
     experimentGeometry: 'air/substrate'
                nParams: 10
                 params: [6.9909 18.7690 6.9356e-06 3.0000 -2.1907e-07 7.0000 5.8551e-06 3.0000 1.8079e-06
             paramNames: {'Substrate Roughness'  'Tails thick'  'Deuterated tails SLD'  'Tails roughness'
              paramConstr: {[3 7]  [12 20]  [5.0000e-06 9.0000e-06]  [3 7]  [-6.0000e-07 -2.0000e-07]  [7 12
           paramFitYesNo: [1 1 1 1 1 1 1 1 1 1]
            nBackgrounds: 2
             backgrounds: [2.8895e-06 5.1729e-06]
        backgroundNames: {'Background  D2O'  'Background ACMW'}
       backgroundConstr: {[1.0000e-07 7.0000e-06]  [1.0000e-07 7.0000e-06]}
     backgroundFitYesNo: [1 1]
          nScalefactors: 1
           scalefactors: 0.2325
       scalefactorNames: {'Scalefactor 1'}
        scalefactorConstr: {[0.1000 0.4000]}
     scalefactorFitYesNo: 1
               nQzshifts: 1
                qzshifts: 0
            qzshiftNames: {'Qz Shifts 1'}
           qzshiftConstr: {[-0.0300 0.0300]}
```

```
        qzshiftFitYesNo: 0
          nbairFitYesNo: 0
                nNbsubs: 2
                 nbsubs: [6.3500e-06 3.4925e-08]
            nbsubNames: {'D2O'  'ACMW'}
            nbsubConstr: {[6.3000e-06 6.4000e-06]  [-5.0000e-07 5.0000e-07]}
          nbsubFitYesNo: [1 1]
       numberOfContrasts: 7
            nResolutions: 1
             resolutions: 0.0300
          resolutionNames: {'Resolution 1'}
         resolutionConstr: {[0.0100 0.0500]}
       resolutionFitYesNo: 1
                  allData: {[51×3 double]  [51×3 double]  [51×3 double]  [51×3 double]  [51×3 double]  [51×3
              dataPresent: [1 1 1 1 1 1 1]
                 resample: [0 0 0 0 0 0 0]
               dataLimits: {[0.0518 0.5888]  [0.0518 0.5888]  [0.0518 0.5888]  [0.0518 0.5888]  [0.0518 0.58
                simLimits: {[0.0518 0.5888]  [0.0518 0.5888]  [0.0518 0.5888]  [0.0518 0.5888]  [0.0518 0.58
          contrastBacks: {[2 1]  [1 1]  [2 1]  [1 1]  [2 1]  [1 1]  [1 1]}
         contrastShifts: [1 1 1 1 1 1 1]
         contrastScales: [1 1 1 1 1 1 1]
           contrastNbas: [1 1 1 1 1 1 1]
           contrastNbss: [2 1 2 1 2 1 1]
            contrastRes: [1 1 1 1 1 1 1]
       contrastRepeatSLDs: {[0 1]  [0 1]  [0 1]  [0 1]  [0 1]  [0 1]  [0 1]}
                modelType: 'layers'
         numberOfLayers: 4
          layersDetails: {4×1 cell}
         contrastLayers: {[1 4]  [1 4]  [2 3]  [2 3]  [1 3]  [1 3]  [2 4]}
results = struct with fields:
            reflectivity: {7×1 cell}
              Simulation: {7×1 cell}
            shifted_data: {7×1 cell}
               layerSlds: {7×1 cell}
             sldProfiles: {7×1 cell}
               allLayers: {7×1 cell}
      calculationResults: [1×1 struct]
          contrastParams: [1×1 struct]
```

```
plotRefSLD(outProb,results)
```

```
Warning: MATLAB has disabled some advanced graphics rendering features by switching to software
 OpenGL. For more information, click here.
```




```
Warning: Negative data ignored
Warning: Negative data ignored
```