RMC Run Report	Material: CCl_4 Cfg. Size: 10240 atoms
Data: 1 neutron	RMC Options: FNC
Run Date: March 2002	Code rmc_fi

First steps in RMC with liquid CCl4

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1 A beginner's tale

The initial objective of this series of runs was the study of the effect of various constraints and data ranges on RMC results. But, this being also my first 'hands-on' use of the RMC algorithm and of the **rmc_fi** programme, things did not really go as planned. Nevertheless, there is a positive aspect in this: by identifying what went wrong, I can make sure that I do not make the same mistake twice. It is also possible that, eventually, we learn something about the way RMC works, even though it is not what we were investigating in the first place. In this case, it is the importance of the σ parameter which controls the fit of RMC calculated data to the experimental data.

The material under study was liquid CCl_4, whose molecule can be well defined by FNC's, and for which we had neutron diffraction data measured at the Budapest research reactor[1]: 100 points in a range from 0.55 $Å^{-1}$ to 9.15 $Å^{-1}$.

Our purpose was to discriminate (if possible at all) between effects of algorithmic constraints (such as cut-offs and FNC's) and experimental data (especially the Q-range). For this purpose I defined a 3×3 'constraints grid' with 3 Q-range extensions (9.15, 6.9 and 4.975 $Å^{-1}$) and 3 FNC's (C-Cl allowed distances in the ranges [1.71,1.85], [1.69, 2.00], and [1.69, 2.19]). The comparison of successful RMC runs would, in principle, bring some information about the specific effect of the different constraints.

2 The 9 runs

Common run parameters for all the runs were:

- 10240 atoms (*i.e.* 2048 molecules),
- density: 0.0319 atoms per cubic Angstrom,
- cubic cell size: 1/2 edge= 34.23522 Å,
- r-spacing 0.1 Å,
- move range for all atoms: 0.1 Å.
- cut-offs 3.3, 1.69 and 2.8 Åfor C-C, C-Cl and Cl-Cl respectively
- the σ (data standard deviation) was set to 0.005.

The other run parameters appear in Tab. 1

The starting configuration for the run 1 was obtained from some other RMC run (it was a 'disordered' configuration, 'close enough' to the solution). The starting configuration for all the other runs were the intermediate configuration obtained after 20 hours for the run 1. The asterisk (*) in the duration column indicates that two runs were run in parallel. The computer used was a twin processor 550 Mhz PC.

3 First mistakes

Some *essential* information about the runs has not been noted:

- the total number of generated, tried and accepted moves
- the acceptance ratios of moves
- the evolution of the χ^2

All that I can make out of my logbook notes is the final value of the χ^2, which is not of great use. I would not even bet that the algorithm had reached convergence. I have one excuse there, because this

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was not convenient at all with rmc_fi, whereas now thanks to the .hst 'history' file of RMC++, this is straightforward.

4 Results

Despite the initial mistakes, it would have still been possible to have successful runs. However, it appeared that for all runs, the fit of the calculated data to the experimental data was very poor (see Fig. 1). Since we knew that the data were of good quality, the misfit could only originate in one of the run parameters. Because a wide range of constraints was used (from 'loose' to 'strict'), the discrepancy between observed and calculated data could not be due to the FNC's.
There remained the 'standard deviation' σ which can be adjusted in RMC in order to make the model fit the data (in this sense it does not truely represent the experimental errors).
The 'large' value $\sigma = 0.005$ was the faulty parameter. Subsequent runs with $\sigma = 0.001$ were indeed succesful.

References

[1] Jóvári P. *et al. J. Chem. Phys.* **114**, 18 (2001).

Run	Q_{max} (data points)	C-Cl FNC	duration (hours)
1	9.15 (100)	1.71 - 1.85	24 + 20
2	9.15 (100)	1.69 - 2.00	65*
3	9.15 (100)	1.69 - 2.19	65*
4	6.9 (85)	1.71 - 1.85	20*
5	6.9 (85)	1.69 - 2.00	20*
6	6.9 (85)	1.69 - 2.19	24*
7	4.975 (70)	1.71 - 1.85	24*
8	4.975 (70)	1.69 - 2.00	20*
9	4.975 (70)	1.69 - 2.19	20*

Table 1: Data range, FNC's and duration for the 9 runs.

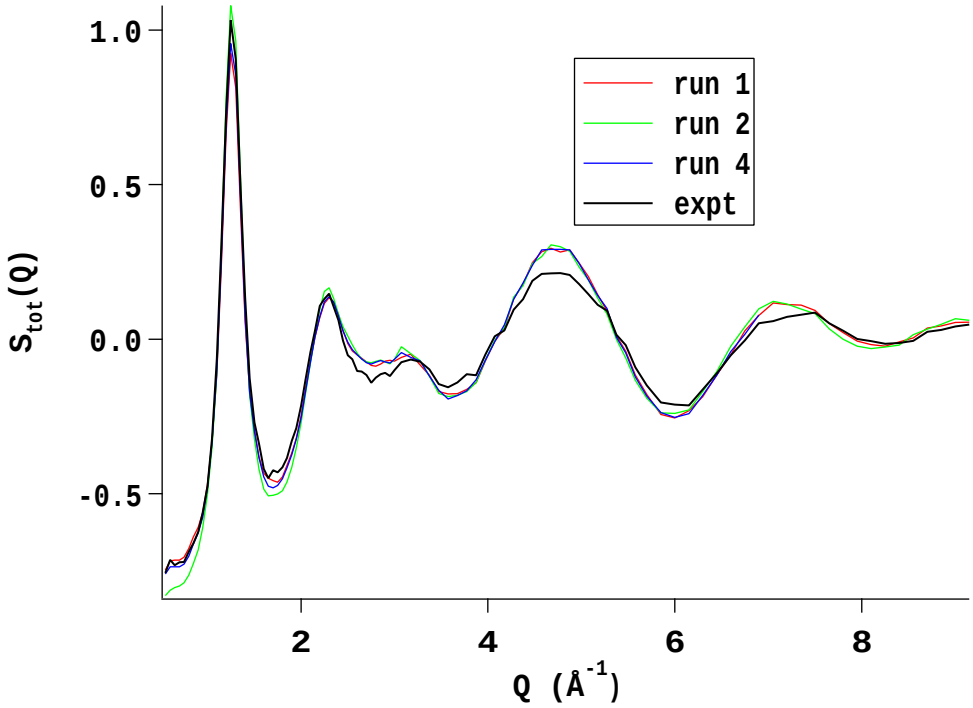

Figure 1: Experimental and RMC structure factors for runs 1, 2 and 4. The fit quality is very poor compared to usual RMC simulations with good data.