Minutes of the 19th meeting of the Steering and Overview Committee of the Swiss-Norwegian Beamlines

The meeting took place at Zuerich on 3rd and 4th December 2001.

Present:

SOC Members : **D. N**icholson (Chairman)

C. Baerlocher, D. Banner, H-B. Buergi, E. Hough and H-P.

Weber

Observer: N. Maraas

Technical Advisor: **P. P**attison

Meeting's Secretary: C. Seferiadis-Heurtebise

The Chairman welcomed everyone to this meeting.

1. Approval of the Agenda

the Agenda was approved.

2. A. Approval of the minutes of June 15, 2001 meeting.

The 18th SOC meeting minutes (15th June 2001) were approved.

Since item 18.3.B-50115 Han-Beat Buergi has received one request concerning molecular modeling software. Hans-Beat Buergi then asked Hans-Peter Weber for additional information, but never got an answer.

Item 18.3.D – point 3,namely the subject of salary increases for the SNBL staff is not mentioned on the notes to the budget 2000-2001 but is mentioned although not budgeted for in the medium range budget forecast for 2002/2004 presented at the SOC meeting of June 9^{th} , 2001.

Nils Maraas requested that item 18.3.D - point 1, should be adjusted, namely "Norway agrees to contribute (EURO11000) of the deficit of EURO37,500 of the budget which is approved".

B. Review and results of actions decided at the last meeting.

- Action 17.2.2 Activity report 2000/01 Reissued as 19.8.2
- **Action 17.9.1** Transferring beamline handbook to the web. To be done by SNBL staff. Deadline January 2002. **Reissued as 19.8.1**
- **Action 18.2.1** Ed Hough and David Banner to submit guidelines for proposals in macromolecular crystallography. **Reissued as 19.2.1** See further down
- **Action 18.3.1** Separating SNBL funds from Hans-Peter Weber's personal grant: UNIL will not do it.
- **Action 18.3.2** Hans-Peter Weber & Chantal Seferiadis-Heurtebise to meet the new person at UNIL. Done in November 2001
- Action 18.3.3 Phip Pattison to provide more precise figures. Done
- **Action 18.3.4** Project Director to send letter (re. Salary Policy) to SOC members and then David Nicholson to send answers back to Project Director. **Reissued as 19.2.2**
- **Action 18.3.5** Breakdown the sum for General Equipment in SNBL Budget into additional items. Done
- **Action 18.3.6** Project Director to write a letter to SOC outlining all of UNIL's "hidden" contributions. **Reissued as 19.2.3**
- Action 18.4.1 Experimental Reports requested. Done in August 2001
- **Action 18.5.1** EU citizens applying for a fellowship in Norway. Done. **See action 19.2.4** regarding the SNBL qualifications for Norwegians applicants. Nils Maraas.
- Action 18.5.2 Extension SLS contract for Philip Pattison. Reissued as 19.2.5
- Action 18.6.1 Ed Hough, report from the Standing Committee. Reissued as 19.6.1
- Action 18.7.1 Web pages, SNBL staff on the Web. In progress. Reissued as 19.8.1
- Action 18.8.1 E-mail to Ragnvald Mathiesen giving a list of regular KUMA users. Done
- Action 18.8.2 Letter of encouragement from SOC to Ragnvald Mathiesen. Done
- Action 18.8.3 Hans-Peter Weber to ask Helge Larsen to take over from Ragnvald. Done
- **Action 18.8.4** Ed Hough. Information re: request for a CCD dectector. Being done.

Action 18.8.6 David Nicholson to coordinate work directed at defining specifications of the EXAFS upgrade. Done

Action 18.8.7 Philip Pattison to report on upgrading beamline optics (medium and long term). Done

Action 18.9.1 Hans-Peter Weber to e-mail Users (summary of SOC meeting, mentioning the Powder Service). Done

Action 18.10.1 David Nicholson to investigate meetings in Norway for SOC meeting June 2003. **Reissued as 19.12.1**

Action 18.12.1 Choice of referees for proposals submitted from Hans-Peter Weber and Philip Pattison. Done. (Comment from Hans-Peter Weber: return from referees "poor").

Action 18.12.2 Reports attached to proposals. Done

Action 18.13.1 Summary of talks with Swiss funding agencies and SLS to be sent to Norwegian side by the Project Director. Not done as Project Director was not party to these discussions. See later (...)

Action 18.13.2 SNBL staff to be present at SLS Users Meeting. Done

Action 18.14.1 In House Research on next agenda. Done

Action 18.14.2 A list of contracts to be provided for next SOC meeting. Such a list was presented orally by Hans-Peter Weber.

Hans-Peter Weber mentioned that contract with NOVARTIS is to be signed. Helijet contract with Rennes: not signed as too many disagreements (Rennes made it impossible to sign). Gervais Chapuis is interested in this contract: namely meaning getting 10 days each year for a duration of three years. Approved by SOC.

Reminder for Chantal Seferiadis-Heurtebise :Send a copy of the contract (CH-N) to CB.Chantal Seferiadis-Heurtebise. Deadline : ASAP.(done)

19.2.1 Send circular to Users regarding macromolecular crystallography new procedures
 Ed Hough + David Banner - Deadline 17/12/01(done January 2002)

19.2.2 Refers to 18.3.4 (Project Director to send a letter, re. SNBL salaries, to SOC members and then David Nicholson to send answers back to Project Director). *Reminder : Content of letter : history of salaries, salary policy, projection of salaries; medium and long term prospectives.* - Hans-Peter Weber Deadline : 15/12/01

19.2.3 Refers to 18.3.6 (Project Director to write a letter to SOC outlining all of UNIL's "hidden" contributions. SOC chairman to respond with a letter to UNIL acknowledging all of these essential contributions). Hans-Peter Weber. Deadline 30/01/2002.

19.2.4 Regarding recruitment of SNBL staff, the following should be taken into account when considering qualification: "given comparable qualifications, preference is to be given to the Norwegian applicant" – Nils Maraas.

19.2.5 Refers to 18.5.2 SLS contract of Philip Pattison. Philip Pattison to contact Gervais Chapuis regarding the extension to either 31st July 2002 or to 30th September 2002. Deadline: 15/12/01

3. Budgetary Matters.

A Accounting at UNIL + Grenoble. Final recommendations.

Nils Maraas suggested that if SNBL make less demands on UNIL's Account Department, the working relationship with UNIL should be improved.

Hans-Beat Buergi commented that:

- the work of UNIL is reduced because an end of the year "bilan" (balance) is no longer asked for, but only a "compte d'exploitation" as the expenses have to be checked anyway.

Hans-Peter Weber informed SOC that although we now have access to UNIL's accounting for the SNBL on the Web, information as to the actual amount in the bank account is not given.

Hans-Peter Weber suggests returning to the "mode standard" of Pierre Wyss. An exact definition of this "mode standard" will be requested from UNIL and transmited to SOC members' for comments (see action below)

The accounts as of 30th September of each year should include those invoices still to be paid or reimbursed. At UNIL this will appear in an account called "transitoires", at ALLSN, this will be shown in "subventions à venir".

19.3.1 Letter to be written by SOC Chairman to UNIL Accounting. Mr. Wyss will be reminded of SNBL's organizational structure (Project Director + Executive Assistant) are the interface between SNBLC and UNIL Accounting. Mr. Wyss will also be asked to give a clear definition of what he means by "mode standard". SOC need to know the deadlines for payment or reimbursement of invoices. Deadline 15/12/01.

B Annual account 1999-2000 and letter from the auditors.

The Financial Report 1999/2000 from Hans-Beat Buergi was approved by SOC (see Appendix N° 1). SOC thanked Hans-Beat Buergi for this work.

19.3.2 Chairman to write letter to Nils Maraas stating that the Financial Report 99/00 has been approved by SOC. David Nicholson. Deadline 15/12/01

Final Draft 07/02/2002

C. Spending as of 30th September 2001.

The overview of the spending has improved. There seems to be a small deficit which may be due to the incorrect currency rate (currency fluctuations) being used in the ALLSN Excel program.

19.3.3 Letter to UNIL, Pierre Wyss, requesting confirmation of expected income. (SNBL provides a list and UNIL checks the amounts). Hans-Peter Weber. Deadline 15/12/01

Letter to UNIL, Pierre Wyss, regarding the Users' Credit (amount reimbursed to SNBL by ESRF): SOC is in favour of using a single account number so as to find this amount quickly and without any misunderstanding. Suggestion from Hans-Beat Buergi: put this amount in an account number "various subventions". Hans-Peter Weber. Deadline 15/12/01

19.3.4 An explanation has to be given regarding the deviation from the allotted General Expenses in the budget . Reasons for deviations larger than CHF10,000 must be accounted for in the Financial Report. Hans-Peter Weber. Deadline 31/01/2002

D. Budget of Oct. 1, 2001 to Sept. 30, 2002.

The budget was approved by SOC. The CHF90.000 left over from last year is to be used to cover any deficit. The remainder will be kept in reserve.

David Nicholson suggested that NOK71.000 donated from his group at NTNU to SNBL is meant as support for the EXAFS Upgrade and is additional to the contractual requirement from Norway and accordingly will appear in the budget as such.

E. An outlook on the CH-N budget after Sept 30, 2002

19.3.5 Budget for 2002/2003 to be presented in the same format as in the Excel sheet presented at the 19.SOC meeting of December 01. Hans-Peter Weber and Hans-Beat Buergi. Deadline 31/01/02

F. Letter from Swiss Office of Education and Science (see Appendix N° 2)

Hans-Beat Buergi mentioned that the various Swiss contributions will be grouped together into a single block.

G. The future (Sept. 2002 – 2003) 50:50 CH: N budget.

For the year 2002/2003, Norway will contribute 3.5 million NOK. Nils Maraas mentioned that the distribution of the total SNBL-budget, to be shared 50/50 by NSR and SUG-SNBL could be :

- Operational Budget €800 000
- Capital Equipment Budget 70.000€

NOK 400.000 (EURO50.000) that Ed Hough applied for from the Research Council of Norway, will be channelled through NSR to SNBL and is to be spent on Equipment as soon as possible in the budget year 2001-2002.

Nils Maraas and Ed Hough mentioned that the new contract for 2002-2003 will contain explicit deadlines for:

- Activity Report SOC of June the following year after the accounts are closed.
- Accounting Report SOC of June the following year after the accounts are closed.

For details, see Appendix 3 (Annual Financial Report).

4. Legal Matters

A. The CH-N Contract. The contract for the period 2001-2002 has been renewed with modifications.

19.4.1 Hans-Beat Buergi asked Nils Maraas to provide him with the amendments to the CH-N contract in writing.

B. Any other Legal matters.

None were suggested.

C. SNBL Contracts with Third Parties.

This item is dealt with in **Action 18.14.2.**

5. Manpower

Hans-Peter Weber informed SOC that SNBL is still understaffed as compared to a typical ESRF beamline.

6. SNBL/ESRF: future Prospects

A. SNBL Vision.

Ed Hough will contact the users again to get more information as to their future scientific plans and also he would like to get more information.

19.6.1 Refers to 18.6.1 (Ed Hough has commenced a sabbatical at the ESRF this Autumn and promises to work hard on the report from the Standing Committee). Ed Hough to send a new e-mail to Users.Deadline: next SOC meeting in June 02

B. EXAFS Upgrade.

David Nicholson informed SOC about the Zurich meeting in August 2001 in which various upgrades of the EXAFS experiment were discussed. The meeting resulted in the

decision to send an application for funding (CHF556 000) to the Swiss National Foundation. Title of the application : see the enclosed title sheet. Total cost CHF700.000 to be divided as follows :

- 2/3rd from Switzerland
- 1/3rd from Norway

Manpower has still not been evaluated for the implementation of the EXAFS upgrade. Philip Pattison does not envisage the additional workload as being too heavy.

If the application to the Swiss National Fondation is successful, then an application for the remaining 1/3 will be sent to the Norwegian Research Council by David Nicholson, The deadline for this is 15. June 2002. If the application to the Swiss National Foundation is not successful, then the Swiss side will re-submit by March 2002.

SOC notes that this upgrade will nicely complement the EXAFS facility planned by SLS.

7. Operational Status of SNBL, 2nd semester 2001.

Philip Pattison presented the Operational Status. See his presentation in Appendix 4.

It was suggested that a patent should be requested for the work done by Hermann Emerich, Wouter Van Beek and Marc Pissard for the beam condensor. Philip Pattison pointed out that there is no novelty in the device. It was then suggested that a licence should be applied for. C. Barloecher offered assistance from ETHZ regarding the procedures to follow for licencing/patenting.

Nils Maraas asked for Philip Pattison's presentation to be e-mailed to him.

19.7.1 Philip Pattison to send a copy of his transparencies by e-mail to Nils Maraas. Deadline: 15/12/01 (*done*)

The goal and aim for SNBL is to get data and scientific results. Philip Pattison underlines that funding is necessary to purchase appropriate software. It was also mentioned that staff training on all the different software was not possible and that the Users will have to be responsible for their own training.

8. Publicity.

A. SNBL Web site.

19.8.1 See Action 17.9.1 regarding transferring the Beamline handbook which should be on the Web. Deadline: February 2002

And Action 18.7.1 Updating SNBL Web pages. Deadline: February 2002

B. Activity Report

19.8.2 Activity Report to be done by Hans-Peter Weber. Deadline: February 2002 – **See action 17.2.2**

C. SNBL Staff addresses on publications.

David Banner suggested that links on the SNBL Web pages to the SLS and vice versa be implemented.

It was also mentioned that SNBL Staff should attend Chemical and Physical Meetings in CH to increase the awareness of the SNBL in this country.

9. Instrumentation.

A. Single-Crystal diffractometer.

- Control software upgrade. Ken Knudsen's report.

Commissioning has been an extremely exhausting period for SNBL team who had to combine commissioning time with experiment time.

Philip Pattison is under the impression that the company has run out of time. He is afraid of further changes to the software as they could affect other presently working functions. Philip Pattison mentioned the possibility of comparing KUMA measurements with measurements on other diffractometers, at this time this is not possible.

19.9.1 Hans-Peter Weber, Philip Pattison and Ken Knudsen to work out a line of actions. re.SNBL's answer to KUMA's commissioning Deadline : ASAP

Send it to Hans-Beat Buergi for comments who is to transmit this to Chairman. Deadline : ASAP

Chairman to write then a letter to KUMA. Deadline 15/12/01

- CCD detector. Ed Hough applied to the Research Council of Norway. It is not possible to indicate at this stage whether the money will be granted. The decision is to be made in December 2001.

A Quotation and a Technical specification have been asked from five companies

Recommendation from SOC: there should be at least three companies in competition. A precise specification should be requested from the companies as to exactly what they will provide.

c. Helijet commissioning.

This has been done.

19.9.3 Period of commissioning time (referring mainly to CCD) to be discussed at next SOC meeting. Philip Pattison. Deadline: SOC June 02

A more detailed discussion on the policy on commissioning time will be put on the Agenda for the next (20) SOC meeting..

10. Powder Diffraction Service.

One PhD student (Denis Machon) has been trained by Wouter Van Beek. He is now collecting data for SNBL users. SNBL charges CHF250 per shift for this service.

The powder diffraction service could be extended to the Mar but needs to be carefully considered first.

11. In-House Research.

In-house research has not been used up to the limiting 10% level. The main reason is that some staff members have had substantial beamtime through regular SNBL or ESRF channels. Another reason is that the staff has to spend much time preparing experiments. This is the usual conflict "User service vs Own Research".

In-house research has been carried out by the following staff members: Silvia Capelli used 9 shifts of beamtime in the spring

Vladimir Dmitriev + Oleksii Kuznetsov + Denis Machon used 8 shifts of buffer time in August, when no users could be found, to train themselves on the use of the ETHZ furnace

Hermann Emerich 25-30 shifts of mostly single-bunch beamtime to test his focusing condensor.

12. SNBL Highlights Meeting 2003 in Norway, June 2003.

19.12.1 David Nicholson to investigate the different meetings taking place (in Norway...) so as to decide to which meeting the SNBL highlights will attach itself to in June 2003. Deadline June 2002

13. Other Matters.

None were submitted.

14. Discussion of Proposals.

Schedule of SNBL Feb 02 to July 02 – See appendix 5

It was agreed that all proposals getting a B rate, would get beamtime.

19.14.1 In the circular to Users to be mentioned that Long Term Proposals are encouraged. Mention also that Users should also apply to ESRF on SNBL. Hans-Peter Weber. Deadline December 01

15. Cooperation with SLS.

A member of SLS, Mr. Bruce Patterson, was present during discussion of proposals, and this proved to be very useful. This is in agreement with the minutes of the 18th SOC meeting.

Swapping experiments between SLS and SNBL is seen by SOC as a positive outcome of the SLS-SNBL contact.

16. Summary of Actions to Be Taken.

The summary was approved.

19.16.1 Actions to be reissued in the current minutes so as to avoid having old actions mixed up together with new ones.

Actions reissued are as follows:

Action 17.2.2 Activity Report 2000/01. Reissued as 19.8.2.

Action 17.9.1 Transferring beamline handbook to the web. To be done by SNBL staff. Deadline January 2002. **Reissued as 19.8.1**

Action 18.2.1 EH and DB to submit guidelines for proposals in macromolecular crystallography. **Reissued as 19.2.1** – See further down

Action 18.3.4 Project Director to send letter (re. Salary Policy) to SOC members and then DN to send answers back to Project Director. **Reissued as 19.2.2**

Action 18.3.6 Project Director to write a letter to SOC outlining all of UNIL's "hidden" contributions. **Reissued as 19.2.3**

Action 18.5.1 EU citizens applying for a fellowship in Norway. Done. **See action 19.2.4** regarding the SNBL qualifications for Norwegians applicants. Nils Maraas.

Action 18.5.2 Extension SLS contract for Philip Pattison. Reissued as 19.2.5

Action 18.6.1 Ed Hough, report from the Standing Committee. Reissued as 19.6.1

Action 18.7.1 Web pages, SNBL staff on the Web. In progress. Reissued as 19.8.1

Action 18.8.4 Ed Hough. Information re: request for a CCD dectector. Being done. **Reissued as 19.9.2**

Action 18.10.1 DN to investigate meetings in Norway for SOC meeting June 2003. **Reissued as 19.12.1**

17. Next SOC Meeting (added on the Agenda during the meeting)

19.17.1 The next SOC meeting will be either just before or just after Sunday 2nd June 2002. **Deadline for decision : January 2002.**