



EuroMinSci Programme Networking Activity

Scientific Report on the

Workshop on numerical modelling of microstructures

Cadaqués, Spain, February 26-28, 2007

EuroMinSci provided a grant of 7,508 € to organise a workshop on Microstructural Modelling, held in Club Carpe Diem, Cadaqués (Spain) 26-28 February, 2007. The initiative for this workshop was taken by the **MinSubStrDyn** and **MicroMagn** CRPs. The practical organization was carried out by Paul Bons (Tübingen). 21 persons attended (Table 1):

- from 7 different countries (Germany, France, UK, Sweden, Spain, Estonia and Australia)
- 15 male, 6 female
- 8 PhD-students, 6 post-doc or non-permanent staff, and 7 tenured scientists

Table 1: List of participants

EuroMinSci partners ¹	Paul Bons	Tübingen, Germany
	Albert Griera	Toulouse, France
	Daniel Tatham	Liverpool, UK
	Jens Becker	Tübingen, Germany
	Joyce Schmatz	Aachen, Germany
	Marcus Ebner	Mainz, Germany
	Verity Borthwick	Stockholm, Sweden
	Sandra Piazzolo	Stockholm, Sweden
	Daniel Koehn	Mainz, Germany
	Janos Urai	Aachen, Germany
	Mark Jessell	Toulouse, France
EuroMinSci invited ²	Lynn Evans	Melbourne, Australia
	Ondrej Lexa	Strasbourg, France
Non-EuroMinSci ³	Luc Siebenaller	Nancy, France
	Kristjan Urtson	Tallinn, Estonia
	Anne Peschler	Strasbourg, France
	Mark Pearce	Liverpool, UK
	Elena Druguet	Barcelona, Spain
	Mark Peterzell	München, Germany
	Misha Bystricky	Toulouse, France
	Enrique Gómez-Rivas ⁴	Barcelona, Spain

¹ Due to personal circumstances Richard Harrison (MicroMagn CRP) had to cancel at the very last moment.

² Lynn Evans and Ondrej Lexa were invited for their special contributions to the topic. Their expenses were covered by the EuroMinSci grant (except for travel).

³ Non-EuroMinSci attendees paid for their own travel, accommodation and food.

⁴ Enrique Gómez-Rivas was in charge of all shopping, driving, etc. and in return did not have to pay for food and accommodation.



All participants of the workshop in front of the lecture room in Club Carpe Diem in Cadaqués.

Introduction

The 3-day workshop of numerical modelling of microstructures was aimed at a mixed audience from experienced modellers to starting PhD-students, all with an interest in the modelling of microstructures in minerals and other crystalline materials (metals, ceramics). The programme consisted of a mix of lectures, hands-on computer labs and discussions (see Table 2, Programme).

The workshop was held in the Club Carpe Diem bungalow park in Cadaqués, Spain. The venue in the tourist resort was chosen because the bungalow park provided an informal environment with all facilities on-site, except for dinner, which was taken in town, a few minutes away by foot. Cadaqués has the advantage that costs are low in winter and that it is easily reached by low-cost carriers flying into Girona and Barcelona.

The activity

The first day started with an introduction of Sandra Piazzolo of the aims of EuroMinSci and the Mineral Substructure Dynamics (MinSubStrDyn). After this, all attendees briefly introduced themselves, their research and their modelling interests. The morning was closed by Paul Bons, giving an overview of the basics of the main current modelling techniques used for microstructures.

The afternoon was led by Mark Jessell, Jens Becker and Lynn Evans, who introduced the attendees into the modelling platform Elle. Elle is software that is specifically developed to model microstructures (subgrain to multigrain scale) in minerals and rocks. Lynn Evans was invited from Melbourne, because she has been the main programmer of Elle since the start of development in the nineties in Melbourne, Australia. Elle is designed to model simultaneously operating, interacting and competing processes that act on, and modify a microstructure. That aspect makes it unique in earth sciences and mineralogy, as no other single package can model such a wide range of processes as Elle can. This is achieved by a flexible, modular set up where each process is modelled by a separate module. Where possible, existing modelling techniques or even existing software are incorporated into Elle. One of the aims of the workshop was to determine the needs of the community in terms of processes that can be modelled.

Day two was mostly dedicated to practical sessions. Sandra Piazzolo led the first session of modelling static and dynamic recrystallisation and the formation of lattice preferred orientations in minerals during deformation. This provided the attendees to get familiar with Elle as a user. The first session was followed by one on the simulation of fluid-rock interaction, led by Daniel Koehn. Contrary to most current microstructural modelling that uses finite-difference, finite-elements and front tracking techniques, the modelling of Koehn uses a spring-particle code (Latte).

Ondrej Lexa started the afternoon session with a presentation on his GIS-MatLab-based microstructural analysis software. His software could provide a valuable tool to quantify microstructures and provide a link between modelling results and natural microstructures. The rest of the afternoon was dedicated to an "Open Modelling Session". Time was provided for attendees to try out different modelling options in Elle, for which each was supplied with the Elle software and a copy of the manuscript "Microdynamics Simulation" (Bons, Koehn & Jessell, Lecture Notes in Earth Sciences, in prep).

In the early evening, Jens Becker and Albert Griera, both postdocs within the MinSubStrDyn CRP, presented their current modelling projects in detail. Jens Becker led the discussion on modelling microstructures in 3D. Albert Griera explained the novel FFT-technique to model deformation and lattice-preferred orientation development. The advantages and difficulties of linking this software with other Elle modules were discussed.

The third, final day was dedicated to discussions on future developments. The first theme was the integration of numerical modelling with synchrotron experiments. Synchrotron and other tomographic techniques provide rapidly expanding opportunities for 3D analysis of microstructures. Keeping up with these techniques provides a major challenge to modellers. Whereas some single processes can currently be modelled well in 3D (e.g. the FFT-code presented by Albert Griera), no 3D software version of Elle exists yet, which can combine different concurrent processes. It was discussed to which extent the current approach with polyhedral elements (presented by Jens Becker, particularly suited to FEM and front-tracking techniques) should be augmented with Potts, phase-field or general cellular-automaton techniques.

The second theme was the application and development of numerical modelling of microstructures with EuroMinSci. Clearly the absence of representatives of other CRPs (see below) was a drawback, and the discussion therefore mainly focussed on research plans within the MinSubStrDyn CRP in collaboration with the non-EuroMinSci attendees. All material from the workshop can be viewed at the MinSubStrDyn web page: <http://subdynamics.geo.su.se/>.

Table 2: Program.

Monday, 26/02	Day 1
09:00 - 09:15	Paul Bons (Tübingen): "Welcome and practical matters"
09:15 - 09:45	Sandra Piazo (Stockholm): "The Mineral Substructure CRP"
09:45 - 10:15	Richard Harrison (Cambridge): "The MicroMagn CRP" (<i>cancelled, as speaker could not attend</i>)
10:15 - 10:45	Coffee/tea break
10:45 - 12:30	Paul Bons (Tübingen): "Introduction into numerical modelling"
12:30 - 14:30	Lunch
14:30 - 18:00 (*)	Mark Jessell (Toulouse), Jens Becker (Tübingen) & Lynn Evans (Melbourne): "The modelling platform Elle"
20:30	Dinner
Tuesday, 27/02	Day 2
09:00 - 10:30 (*)	Sandra Piazo (Stockholm): "Simulation dynamic recrystallisation and lattice-preferred orientations"
10:30 - 11:00	Coffee/tea break
11:00 - 12:30 (*)	Daniel Koehn (Mainz): "Simulation of fluid-rock interaction with the particle code <i>Latte</i> "
12:30 - 14:30	Lunch
14:30 - 15:00	Ondrej Lexa (Strasbourg): PolyLX analysis of natural and numerical microstructures
15:00 - 18:00 (*)	Open modelling session
18:00 - 18:45	Jens Becker (Tübingen): "Towards 3-dimensional modelling of microstructures"
18:45 - 19:30	Albert Griera (Toulouse): "Integrating the FFT-model into Elle"
20:30	Dinner
Wednesday, 28/02	Business meeting
09:00 - 10:45	Discussion on "The synchrotron experiment", introduced by Sandra Piazo
10:45 - 11:15	Coffee/tea break
11:15 - 13:00	Discussion on "The application of numerical modelling in EuroMinSci"
13:00 - 14:30	Lunch
14:30 - 18:00	Open planning and discussion session
20:30	Dinner

(*) *Practical computer labs*



The lecture room with Mark Jessell leading one of the practical sessions



Jens Becker and Lynn Evans, main programmers of Elle, help out



Discussions and programming continued into the evening



Attendees prepare their lunch

The excursion to Cap de Creus

For those attendees arriving 2 days earlier, an excursion to the nearby Parc Natural de Cap de Creus was provided. Cap de Creus is famous for its excellent exposures of multiply deformed metamorphic turbidites and pegmatite intrusions. The area can be regarded as "type locality" of a range of structures that were first recognised or described here (shear bands, flanking folds, pseudo-boudins, etc.). The excursion provided an excellent way for participants to get to know each other. About half of the attendees took part in the excursion, for which they paid the extra costs (accommodation, food, transport) themselves.



Excursion on the high-grade meta-turbidites and pegmatite intrusions of Cap de Creus, near Cadaqués

Impact of the activity on the EuroMinScl Programme

Numerical modelling is one of the main research tools within EuroMinScl. Several young researchers were introduced into the range of possibilities of numerical modelling. They had the opportunity to discuss their specific problems and research plans with software developers. On the developers level, this workshop provided a chance to take stock, determine needs for further development, and coordinate activities. The subsequent EuroMinScl meeting in Nice clearly showed the interest in the modelling tools presented and discussed during the workshop. Unfortunately, for different reasons, representatives from other CRPs did not attend (see below) and this aspect could not be fully achieved.

Some comments on the planning of a EuroMinScl Networking Activity

The workshop on numerical modelling was originally planned as an activity within the MinSubStrDyn CRP (without additional funding by EuroMinScl). However, several coordinators of other EuroMinScl CRPs expressed their strong interest and indicated that they or other partners in their CRPs would attend. On the base of these oral commitments, the original workshop was expanded to a full EuroMinScl Networking Activity. However, in the end, only one EuroMinScl researcher (Richard Harrison, MicroMagn) from outside MinSubStrDyn took part in the organization of the workshop. One more researcher was seriously interested, but could not come owing to a EU-Marie Curie Summer School that was given higher priority. The delay in the approval of the activity application compounded the problem. Some lessons can be drawn from this and earlier experiences:

- Many have a genuine interest in networking and interdisciplinary activities. However, few actually have the time to actually attend such activities, having to give priority to their own research, management and teaching activities.
- There may be a lack of communication down to the young researchers (PhDs and postdocs) within CRPs who actually have fewer commitments and more time to attend networking activities, but who are not always made aware of the opportunities.
- Applicants for networking activities should be encouraged to submit their applications as early as possible, and the review process should be quick. However, the current 3-month deadline should be maintained to allow for flexibility.
- A solution must be found for the case (like here) where there are a number of expressions of interest on which the activity is based, but followed by only "no shows". By the time it is clear that, because of this, a networking activity does not meet the criteria, the activity cannot be cancelled any more, as many will already have purchased flights and other financial commitments have been made.