

BULLETIN DU GROUPEMENT

d'informations mutuelles

AMPERE



SE CONNAÎTRE, S'ENTENDRE, S'ENTRAIDER

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If you would like to become a member of the AMPERE Group, you can register online under: **www.ampere-society.org**

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Editorial

Dear AMPERE colleagues,

Summer is over and it was hot in Europe, certainly so during the EUROMAR conference in Prague in the beginning of August. If you have not been there, you have missed a lot: exciting scientific talks and posters, a beautiful city, and a nice dinner by the side of river Vltava. We are very grateful to Vladimír Sklánař and his team for the very smooth organization and the pleasant atmosphere that they provided.

Next year you might expect somewhat cooler weather for EUROMAR in the second largest city of Denmark, Aarhus. Please mark your calendars: EUROMAR will take place from July 3rd to July 7th 2016. EUROMAR 2017 will take place in Warsaw (Poland) from July 2nd to July 6th.

In Prague, Bureau AMPERE also decided to establish a new subdivision that organizes schools for Biological Solid-State NMR (see page 25). If you want to organize a symposium, conference, or school under the auspices of AMPERE, you may be interested in reading the Guidelines for such events starting on page 26.

At EUROMAR in Prague the Raymond Andrew Prize 2015 was awarded to Jean-Philippe Demers for his thesis "From Slow to Ultra-fast MAS: Structural Determination of Type-Three Secretion System Bacterial Needles and Inorganic Materials by Solid-State NMR" at Georg-August University School of Science (GAUSS) in Göttingen (Germany). If you want to nominate one of your students for the Raymond Andrew Prize 2016, you find the call for nominations on page 11.

A new column in the Bulletin reports on new tools (software, pulse sequences, etc.) that may be of interest for the community. The first article by Stephan Pribitzer from my own group describes SPIDYAN, a software package for simulating experiments with arbitrary wave excitation (p. 12). If you want to contribute such a column, please contact us at contact@ampere-society.org.



Gunnar Jeschke
Secretary General of Groupement AMPERE

Minutes of the Meeting of the AMPERE Bureau

in Zürich, on March 27, 2015

Members Present:

B. Blümich, A. Böckmann, B. Meier, G. Jeschke, J. Dolinsek, L. Frydman (via Scopia), J. van Duynhoven (via Scopia), Christina Redfield (via Scopia), Christoph Arns (via Scopia), Michael Johns (via Scopia), Vladimir Sklenar (via Scopia), M. Ernst

Excused:

H.-W. Spiess, St. Jurga, T. Vosegaard

Agenda:

1. Preparation for EUROMAR 2015 (V. Sklenar)
2. Report EUROMAR Division (L. Frydman)
3. Report on Prizes (B. Meier)
4. Financial Report EUROMAR (C. Redfield)
5. Approval of the minutes of the AMPERE Bureau Meeting in Zurich June 30, 2014
6. Report on the state of the AMPERE Society (B. Blümich)
7. Financial Report (G. Jeschke)
8. Final reports past meetings
 - FOODMR 2014, Cesena, Italy (J. van Duynhoven)
 - AMPERE NMR School Zakopane (Poland) 2014 (G. Jeschke)
 - NMRCM 2014 (V. Chizhik or G. Jeschke)
 - EUROMAR 2014 Zürich (Switzerland) (G. Jeschke)
 - EF-EPR 2014 (G. Jeschke)
 - EBSA Solid-State NMR School München (B. Meier)
9. Future meetings 2015-2016:
 - AMPERE NMR School Zakopane 2015 (G. Jeschke)
 - EUROMAR 2015, Prague July 5- July 11 (V. Sklenar)
 - 13th ICMRM, München, Germany August 2-6 (M. Johns)
 - 9th Alpine Conference September 13-17, Chamonix (B. Meier)
 - EUROMAR 2016, Aarhus July 3-7 2016 (T. Vosegaard)
10. Student grants: Allocation of funds and selection procedure
11. Guidelines for organizing AMPERE events (B. Blümich)
12. Policy on membership fee payment, new homepage (G. Jeschke)
13. Varia
14. Date of the next meeting

At 11:10 hours G. Jeschke opened the meeting. The agenda was modified to discuss the EUROMAR topics first and was approved unanimously.

Ad 1.

The preparations for EUROMAR 2015 in Prague are well on track. The website is active and registration has started. There are not too many people registered yet but this is expected to peak at the oral abstract deadline (April 15) and at the poster deadline (May 11). The location is very good and a strong participation is expected. Visa letters will only be issued to registered participants. There will be additional mass emails sent out before the two abstract deadlines. The student grants by EUROMAR and AMPERE will be awarded following the same scheme as in Zurich. At the EUROMAR in Prague there will also be a lunch-break meeting on Wednesday to discuss a subdivision for Hyperpolarization techniques. This discussion will be organized by J. Matysik.

Ad 2.

The EUROMAR division is doing very well and the selection and preparation for the future conferences are well underway. The last EUROMAR in Zurich went very well and was also a financial success. As just discussed, Prague will host the EUROMAR 2015 and the 2016 EUROMAR will be held in Aarhus. For the EUROMAR 2017 there is a proposal to hold it in Warsaw (organized by Stefan Jurga and Wiktor Kosminski) in the old university campus. This is a very good proposal and Warsaw is well connected. For EUROMAR 2018 there is a proposal by Nantes (organized by Patrick Girardeau) which would fit in alternating the EUROMAR between the eastern and the western part of Europe. In 2019 the ISMAR will again be held in Europe and it is planned to have a joined EUROMAR/ISMAR conference. There are two proposals (Berlin, Hartmut Oschkinat) and (Lille, Olivier Lafon) and the decision will be made at this years ISMAR meeting in Shanghai. All members of the EUROMAR board that are present in Shanghai should participate in the discussion and decision process. The Dutch NMR community is interested in hosting the EUROMAR 2020 but this will not be discussed until 2017. There are 4-5 members stepping down from the EUROMAR board and the board is looking for candidates to replace them.

Ad 3.

Beat Meier reports on a discussion with Richard Ernst and Werner Maas (Bruker Biospin) about prizes at EUROMAR. Werner Mass/Bruker propose to establish a new Richard R. Ernst prize at the EUROMAR which should be awarded on a yearly basis and should replace the AMPERE prize and the Russel Varian prize that have recently been awarded in alternating years. Bruker has indicated that they will no longer support the AMPERE prize since they are not connected to AMPERE. The AMPERE Bureau discussed

several options: keeping the AMPERE prize in its current form, changing the focus of the AMPERE prize to early stage scientists, or abolishing the AMPERE prize. The Bureau came to the conclusion that the AMPERE prize is important for the visibility of the society at the EUROMAR conferences. It was, therefore, decided that AMPERE will continue funding the AMPERE prize internally. The Andrew prize will be given for a PhD thesis, the (annual) AMPERE prize to a early career scientist (less than 10 years past his PhD), and the Richard R. Ernst prize can be given for well established scientists. AMPERE will not be involved directly into the Richard R. Ernst prize which will be the responsibility of the EUROMAR subdivision. Bruker would like to start the Richard R. Ernst prize already at the EUROMAR 2015 in Prague which was viewed as very ambitious by the AMPERE Bureau. There are not yet any guidelines and no selection committee. The AMPERE Bureau suggests to EUROMAR that Bruker presents their ideas and plans to the EUROMAR board in Prague so that an informed decision can be taken. It is very important to ensure that the prize will be awarded independent from any interests of Bruker. In addition, it was noted that the Russel Varian prize will be awarded at the EUROMAR 2015 despite the fact that Agilent is no longer supporting it.

The selection of the Andrew prize winner is well underway. There were 20 good proposals and the prize committee is discussing and evaluating the proposals.

Ad 4.

The finances of EUROMAR are quite healthy which is partially due to the transfer of 50 kEuro form the EUROMAR 2014 in Zurich. The current balance is 135 kEuro. It is planned to reserve again 25 kEuro for student travel stipends for the upcoming EUROMAR in Prague. The remainder will be kept as a safety net for future conferences.

Ad 5.

The minutes of the AMPERE Bureau meeting in Zurich, June 30, 2014, published in the AMPERE Bulletin 254/255, were approved unanimously.

Ad 6.

B. Blümich delivered a short report on the state of the Groupement AMPERE. The main project currently is the integration of the national Magnetic Resonance societies with AMPERE. This will require some changes to the statutes which will be discussed along with the revised guidelines for holding AMPERE conferences (topic 11). Otherwise, the AMPERE group is healthy with many subgroups doing excellent work.

Ad 7.

G. Jeschke explained the current status of the finances of AMPERE. The major expenses are the student grants for the EUROMAR and the AMPERE school. The sudden change of the exchange rate between CHF and EUR had a strong impact on the balance of the accounts. See page 8.

Ad 8.

The reports for the past meetings were accepted. The AMPERE Bureau thanks all the scientific and local organizers for their time and effort.

- FOODNMR 2014, Cesena, Italy (J. van Duynhoven): This meeting was held near Bologna and was very well attended with about 140 participants. Compared to the 70 participants some years ago this is an impressive increase in interest. The next meeting in this series will be held in Karlsruhe (Germany) from June 6-10 2016.
- NMR School 2014 Zakopane (St. Jurga): The meeting was, as always, very successful with 20 teachers and 80 students. It combines tutorial-style lectures with current research results. This meeting is very well connected with AMPERE.
- EUROMAR 2014 Zurich (G. Jeschke): The meeting was very successful with about 700 participants. The talks were very diverse and well attended. The organizers made a profit of 87 kEuro half of which goes back to the EUROMAR board.
- NMRCM 2014 St. Petersburg (G. Jeschke): Last years meeting went very well but the future of the meetings is unclear. The meeting will not take place in 2015 but V. Chizhik is working on organizing it again in the future.
- EF EPR meeting 2014, Marseille (G. Jeschke): The meeting was very good and the next meeting will be held either in 2016 or 2017. The Italian EPR community did not feel well integrated but this problem has been addressed and will be taken into account for the future.
- Advanced Solid-State NMR School, Munich (B. Meier): The 5th edition of the advanced solid-state NMR school worked very well with 50 students attending. The school is now organized biannually and has a very broad range of topics.

Ad 9.

Future meetings for 2015-2016

NMR School Zakopane 2015 (G. Jeschke): The planning goes well and the summer school will be held with the same general outline as in the past.

- EUROMAR 2015 Prague (V. Sklenar): discussed under point 1.- 13th ICMRM, Munich (M. Johns): The meeting will take place on Campus Area Garching (Technische Universität München). An advertisement

video and a flyer have been distributed (see also <http://www.ICMRM2015.com>).

- 9th Alpine Conference on Solid-State NMR, Chamonix (B. Meier): The conference preparations are well on track. The conference is very well established with about 200 people attending biannually.
- EUROMAR 2016 Aarhus (L. Frydman): The preparations are going well and the program committee will be established during the meeting in Prague. Since Thomas Vosegaard was not able to join the AMPERE Bureau meeting for technical reasons, there will be a separate teleconference (T. Vosegaard, L. Frydman, C. Redfield, B. Blümich) next week to discuss the detailed status of the preparations.

Ad 10.

The AMPERE Bureau decided to give again 10 student grants of Euro 500.- each for the EUROMAR 2015 and for the AMPERE Summer School in Zakopane.

Ad 11.

The guidelines for AMPERE events need to be updated to reflect the changes from the Congress AMPERE to the EUROMAR conferences. This will also require a change of the statutes of AMPERE since the Congress AMPERE is mentioned there. We plan to discuss the required changes at the Bureau meeting in Prague such that we can get the process started for changing the statutes at the general assembly in 2016 in Aarhus. Besides the mentioning of the Congress AMPERE, we also plan to change the statutes to limit the membership in the AMPERE committee to two terms with four years each. This will allow us to periodically rejuvenate the AMPERE committee. In addition, the presidents of the national magnetic-resonance groups should become members *ex officio* of the AMPERE committee besides members who are elected. The idea is that the Bureau proposes new members for the committee that are then approved by the general assembly.

The new guidelines need to be worked out in detail for the Bureau meeting in Prague. We will propose them then to the EUROMAR board and make them mandatory for other conferences organized as part of the AMPERE activities. The AMPERE Bureau suggests to include the following requirements: AMPERE logo has to be displayed on the webpage, AMPERE tree needs to be included in the book of abstracts, one year AMPERE membership fees included in conference fee and discounts for AMPERE members. The details will be fixed in the new guidelines.

Ad 12.

Gunnar Jeschke proposes a change in the way how membership fees are handled. They will now be valid for 12 months and no longer for a calendar year. There will be an automatic reminder with a request for renewal. People who do not answer to the reminders will be deleted from the list of members. There was a proposal to exempt retired members from paying the membership fee. This is currently not practical because we do not have records of birthdays or employment. We will include a statement on the annual bill that retired members can be exempt from paying the annual fee. The Bureau will decide such requests.

In the future, the AMPERE Bulletin will be published in three issues on fixed dates. Unfortunately, there is often not enough material available. The Bureau reminds the conference organizers that they should deliver a report for all the conferences (see point 11) organized under the name of AMPERE. G. Jeschke also suggested other topics like reports about the research of prize winners, subdivision portraits, conference portraits, or NMR center portraits. One could also ask younger members for a portrait of their research. This request could be included in the next editorial.

G. Jeschke is currently setting up a new webpage for AMPERE. The current content of the webpage will be transferred but if there are suggestions for new content, this would be very welcome. The AMPERE tree will be put on the homepage to illustrate the diversity of the events organized under the umbrella of AMPERE. The webserver could also be used as an archive for conference websites which are currently lost after the conference. The AMPERE Bureau will propose this to the EUROMAR board.

Ad 13.

Varia: There were no points discussed under Varia

Ad 14.

The next annual meeting of the AMPERE Bureau will be on April 1, 2016 in Zurich. The Bureau meeting during the EUROMAR in Prague will be during the lunch break on Monday July 6, 2015.

At 13:25 hours G. Jeschke closed the meeting and thanked all the present members for their time and effort.

Zürich, 27.3.2015

Matthias Ernst

Financial Situation

Fortune of the Society per March 19th 2015

AMPERE Accounts (CHF)	CHF	Euro
Savings Account	30,907.55	
Current Account	7,778.78	
Security Depot	0.00	
Savings Account Andrew	33,348.20	
Security Depot Andrew	94,233.39	
Total	166,267.92	
Accounts of subdivisions (CHF)		
NMR school (AMPERE)		€ 7,027.31
MRPM	24,228.80	
Savings Account SMRM	27,887.40	
Savings Account EUROMAR	61,455.05	
Current Account EUROMAR	26,219.31	€ 24,760.38
DNP	0.00	
EPR	7,414.20	
FOOD NMR	3,647.25	
Total	158,293.38	
Grand Total CHF	322,688.31	
1 Euro = 1.0589069 CHF		

Our «Lühike jalg»¹ to Europe

A remembrance of the Estonian physicist and chemist Endel Lippmaa

A. V. Kessenikh, Vavilov Institute for the History of Science and Technology, Russian Academy of Sciences, Moscow

Endel Lippmaa died 30 of July 2015 in Tallinn. He was born in Tartu (Estonia) on the 15th of September 1930 as a son of the well-known Estonian biologist professor Theodor Lippmaa, who tragically has perished during the hostilities in 1944 as a result of an air bombing of Tartu. Endel graduated in 1953 from the Tallinn Engineering Institute, and in 1956 he received the degree „candidate (Ph. D.) of technical sciences“ for work on chromatography. Lippmaa soon decided to devote himself to the development of the new physico-chemical method of nuclear magnetic resonance (NMR). Due to the embargo and the de facto prohibition of foreign trips during the USSR period he had almost no possibility to use the latest achievements of his foreign colleagues, but with his own experimental equipment, self-made in his laboratory, together with own pupils he was able to master the new method and make important contributions to many fields of applications of NMR. In 1961 the Lippmaa laboratory became the Physic Sector of the Institute of Cybernetics of the Estonian Academy of Sciences. In 1969 Lippmaa received degree “doctor of Science (physics and mathematics)” from the Institute of Chemical Physics (Moscow). His dissertation theme was on the “Nuclear-nuclear Overhauser effect and the structure of organic compounds”. In 1975 Lippmaa became a member of Estonian Academy Sciences. There he was the head of the division of astronomy and physics from 1977 to 1982. In 1980 he became director and founder of new Institute of Biological and Chemical Physics. From 1980 on Lippmaa became more and more active in political affairs concerning the independence of Estonia, but he also continued his scientific work, for example as the head of one of CERN laboratories.

In the 1960ies Lippmaa gained limited ability to communicate with chemists of the German Democratic Republic, Finland and Sweden, and established strong ties with the Soviet chemists. His laboratory was one of three in the world to create a database for carbon NMR (1965). From the 1970ies to

¹ Lühike jalg (Estonian) – short way, literally “short leg”. This is how Tallinn people named the shortest ascent to the upper part of the city.

the 1990ies Lippmaa with his disciples E. Kundla, A. Samoson, T. Saluvere et al. have made seminal contributions in the field of solid-state NMR. They developed methods for observing the NMR signals from ^{29}Si , ^{27}Al and other nuclei in powder and polymer samples. For these innovations Lippmaa was honored by the Groupement AMPERE in 1994.

Endel Lippmaa lived the most part of his life in the USSR period of Estonia. He was the outstanding expert of the Soviet scientific community in the fields of NMR, all of Chemical Physics and on many other chemical phenomena. We remember his respectful and friendly attitude to the Soviet colleagues. In 1967 at the general meeting of the Division of General and Technical Chemistry of the Soviet Academy of Sciences Lippmaa demonstrated the possibilities of NMR of carbon, oxygen and nitrogen isotopes and of double-resonance NMR to study the structure of chemical compounds. In the same year Lippmaa met the Soviet NMR experts at the All-Union Symposium on Nuclear Magnetic Resonance in Tallinn and we had the opportunity to get acquainted with the original equipment set up in his laboratory. Many times Lippmaa organized meetings in Tallinn with the participation of foreign scientists. The most memorable of the meetings are the Symposium on Chemically Induced Nuclear Polarization (1972), the Congress on Molecular Spectroscopy (1973), and the Congress AMPERE (1978). Endel Lippmaa's outstanding reputation in the international scientific community enabled others Soviet spectroscopists in magnetic resonance and related phenomena to join the international exchange of knowledge in their fields.

We remember Lippmaa as a friendly and affordable opponent, reviewer and consultant. The last event at the all-union scale, the School of NMR in Chemistry and Petrochemistry was carried out by Lippmaa in 1988. His brilliant lecture on NMR in solids had a great impact on many professionals. We express our deepest condolences to Jaak and Mikki Lippmaa and all the Estonian colleagues. The bright memory of Endel Lippmaa is inseparable from the memories of friendly meetings in the beautiful land of Estonia.

Raymond Andrew Prize 2016 Call for nominations

Call for Nominations for the Raymond Andrew Prize for an outstanding PhD thesis in the field of magnetic resonance:

For the Raymond Andrew Prize 2016 the AMPERE Prize Committee is seeking your help in searching for qualified candidates who completed their dissertation during the period of 2014/2015. The prize will be presented during the EUROMAR in Aarhus (Denmark) from July 3rd to July 7th 2016.

You are kindly invited to submit nominations by e-mail to;
andrewprize@nmr.phys.chem.ethz.ch

Suggestions must be received by 15th February 2016 and should include the following documents:

- Nomination letter
- Curriculum vitae
- List of publications and presentations at conferences
- PhD thesis in PDF

The thesis should be written in English. In exceptional cases, the thesis may also be submitted in triplicate as a hardcopy to the AMPERE Secretariat. Please note that the nomination letter cannot be written by the candidate herself or himself.

Submissions that arrive too late will automatically be transferred to the next year. The prize committee will reconsider excellent contributions for two years in a row.

For a list of past Andrew Prize winners see: <http://www.ampere-society.org/index.php?page=andrewprice>

Sincerely yours,

Gunnar Jeschke

SPIDYAN

A new MATLAB library for simulating pulse EPR

Stephan Pribitzer

Laboratory of Physical Chemistry, ETH Zurich, Switzerland

Short rectangular microwave pulses in pulse electron paramagnetic resonance (EPR) spectroscopy can cover bandwidths of about 100 MHz. But the spectral width of nitroxides and in particular paramagnetic transition metal complexes usually exceeds 1 GHz. This restricts sensitivity and the application of common pulse EPR sequences on such compounds. Partially, this can be overcome by shaped frequency modulated pulses generated with arbitrary waveform generators (AWG). Those can usually cover a substantial fraction of typical EPR spectra, which led to development and deployment of new experimental schemes with amplitude- and phase modulated pulses.

The recent advances in the field of AWGs made sampling rates in the GS/s range accessible at a reasonable price. Thus it has become possible to extend the excitation bandwidth further, up to and beyond 500 MHz, into the ultra-wide band (UWB) regime¹. AWGs allow for excitation with frequency-swept pulses, which provide effective flip angles between 0 and π .

In need of a package for simulation of frequency swept pulses the free and open-source SPIn DYNamic ANalysis (SPIDYAN) library was developed, which runs in the MATLAB environment. Some functionality of the current version of SPIDYAN depends on the MATLAB Signal Processing Toolbox and for improved performance the Parallel Computing Toolbox is recommended. A detailed documentation, including a short tutorial, a quick reference sheet and some example files are provided on the download page*. The first release of SPIDYAN can treat one-spin and two-spin systems with arbitrary spin quantum numbers. At the current stage of development of EPR spectroscopy with shaped pulses, this appears appropriate. In future releases this will be extended to arbitrary spin systems.

The previously mentioned passage pulses are well known and studied in NMR spectroscopy, but their effects are not yet fully understood in EPR spectroscopy, where formally forbidden transitions are often weakly allowed and systems of several coupled spins with arbitrary spin quantum numbers are of interest. During such a pulse the magnetization is locked to an effective field ω_{eff} . With the sweep rate $k = d\omega/dt$, the amplitude of the irradiation field ω_1 and the resonance offset $\Delta\omega = \omega - \omega_0$ it is possible to

*www.epr.ethz.ch/software

define the adiabaticity factor as

$$Q(t) = \frac{(\omega_1^2 + \Delta\omega^2)^{1/2}}{d\theta/dt} = \frac{\omega_{\text{eff}}}{d\theta/dt} .$$

For a linear sweep, $Q(t)$ approaches its minimum when the isochromate is on resonance, which results in the critical adiabaticity

$$Q_{\text{crit}} = \frac{\omega_1^2}{k} = \frac{\omega_1^2 t_p}{2\pi\Delta f}$$

where t_p is the pulse length and Δf the sweep bandwidth.

Adiabatic inversion requires Q_{crit} to be much larger than unity, which can usually be achieved by reducing the sweep rate. Pulses with $Q_{\text{crit}} < 1$ are known as fast passage pulses.

The inversion efficiency $I = (1 - \langle S_z \rangle / 2)$ of a variety of passage pulses can be described with

$$I = 1 - \exp(-\pi Q_{\text{crit}} / 2) .$$

This equation is based on the Landau-Zener formula which describes the transition probability at a level anti-crossing.

An equivalent flip angle can now be defined by:

$$\beta = \arccos[2 \exp(-\pi Q_{\text{crit}} / 2) - 1]$$

Starting from initial polarization, maximum coherence ($\beta = \pi/2$) is therefore achieved through a pulse with $Q_{\text{crit}} = 2 \ln(2)\pi$. The equivalent flip angle approaches its maximum $\beta = \pi$ for large Q_{crit} .

SPIDYAN

Like other MATLAB libraries (EasySpin, SPINACH) that can be used for EPR spectroscopy simulations, SPIDYAN is command line controlled. The program allows the user to quickly write a complex pulse sequence, which is defined in terms of events (pulses, delays, detection periods) of given durations that are further specified by auxiliary parameters. Pulses can be created from microwave amplitude, flip angle, or critical adiabaticity factors. SPIDYAN includes routines for phase cycling and computation of rectangular and linearly frequency-swept pulses. To account for bandwidth limiting effects, as they occur in UWB EPR spectroscopy, SPIDYAN can model resonators through a simple RLC circuit. If relaxation can be neglected, the program uses propagators to evolve spin density matrices in Hilbert space. For simulations explicitly considering relaxation effects,

the program solves the quantum mechanical master equation in Liouville space.

For propagation, SPIDYAN builds the system Hamiltonians from resonance frequencies, spin quantum numbers and interaction parameters. Non-supported interactions can be added manually by the user. By adapting pulse and system parameters accordingly, SPIDYAN can also be used for simulating NMR experiments. A broad variety of detection operators is included for detailed analysis of spin dynamics during any time of the experiment. This includes transition selective operators, which are useful for high-spin ($S > 1/2$) simulations.

Applications

By default, SPIDYAN calculates expectation values for all time steps. The program returns an $n \times k$ -dimensional matrix, where n is the number of selected detection operators and k the number of time steps. The corresponding time axis and the final state after propagation are returned as well.

The time evolution of $\langle S_z \rangle$ of a single spin $S = 1/2$ for an inversion pulse with $Q_{\text{crit}} = 5$ is displayed on the left side of Figure 1. The 3D plot on the right is obtained by applying $\langle S_x \rangle$, $\langle S_y \rangle$ and $\langle S_z \rangle$. This illustrates the efficiency of adiabatic inversion for pulses with large Q_{crit} and highlights the difference

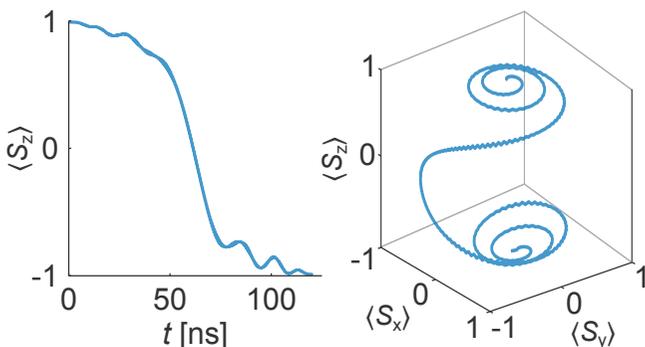


Figure 1: Trajectory of a single spin $S = 1/2$ during a chirp with $Q_{\text{crit}} = 5$.

in spin dynamics compared to common rectangular pulses.

Most EPR experiments use pulse sequences that create spin echoes. Figure 2 shows the normalized signal of a $\pi/2 - \tau - \pi$ chirp pulse sequence, which is also used for the two-pulse electron spin echo envelope modulation (ESEEM). To successfully reproduce a spin echo, the simulation has to

be carried out with the same pulse parameters for a distribution of spin packets. In this case SPIDYAN was looped over a Gaussian distribution of the resonance frequencies of the spin packets. For detection the raising operator \hat{S}^+ was used. The signal of each spin packet was stored and, after completion of the loop, summed up, resulting in the depicted time trace. The spin echo can be further processed, just as experimental data. Example MATLAB scripts for the spin echo and the inversion pulse can be found online.

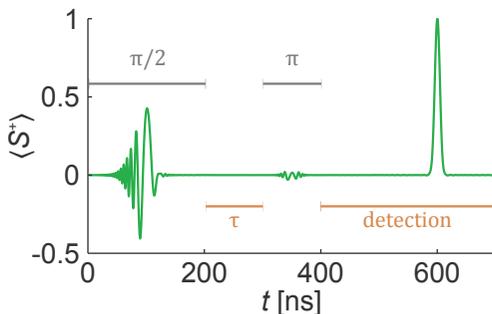


Figure 2: Spin echo of a $\pi/2 - \tau - \pi$ - echo sequence. Simulated using a Gaussian distribution of the resonance frequency of spin packets.

By exciting electron spin echoes with frequency-swept pulses on a home-built UWB EPR spectrometer, based on an AWG with a sampling rate of up to 12 GS/s, we measured ESEEM spectra on single crystals of γ -irradiated malonic acid and Cu^{2+} in TiO_2 (rutile)². Through recording the entire echo it is possible to correlate the ESEEM spectrum to the EPR spectrum³, resulting in two-dimensional spin echo correlation spectra. Related simulations were carried out on a desktop PC, running Windows 7 on an Intel i7-4770 processor using the MATLAB parallel computing toolbox.

In the malonic acid system, formally forbidden transitions which drive ESEEM, arise from the hyperfine interaction between the electron spin $S = 1/2$ and the nucleus $I = 1/2$:

$$\hat{H} = \Omega_s \hat{S}_z + \omega_I \hat{I}_z + A \hat{S}_z \hat{I}_z + B \hat{S}_z \hat{I}_x$$

The experimental EPR/two-pulse ESEEM correlation spectrum is displayed in Figure 3a. For the simulation with SPIDYAN we extracted the hyperfine coupling parameters from the experimental data and were able to reproduce the experiment very well, Figure 3b. Here we used two monochromatic pulses with lengths of 3.25 ns and 6.5 ns. The experiment was recorded in

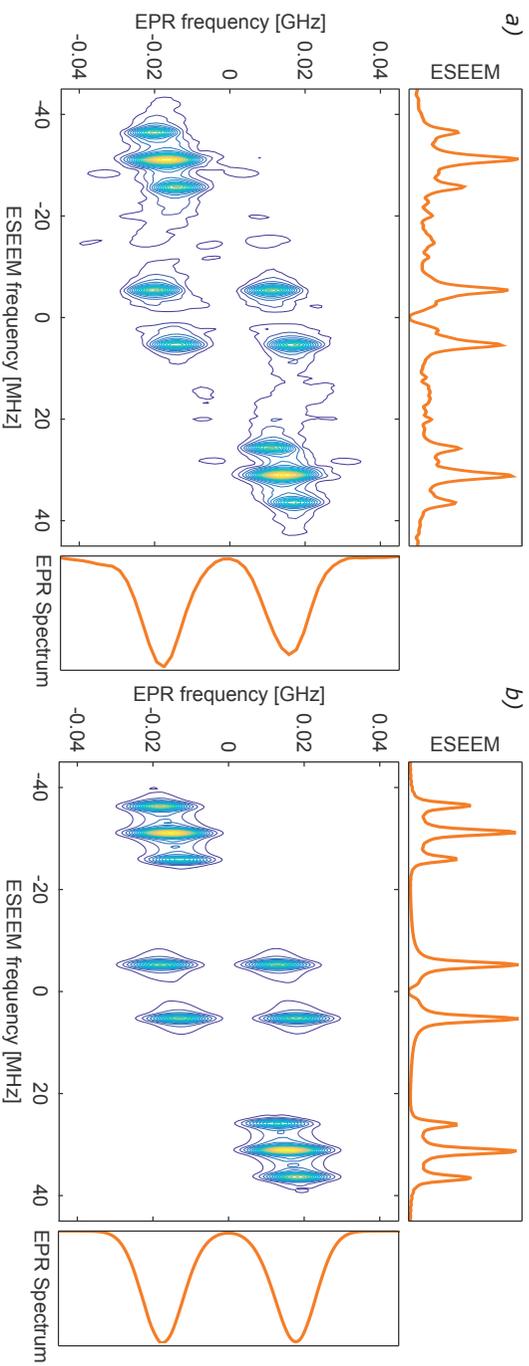


Figure 3: 2D EPR/two-pulse ESEEM spectrum of γ -irradiated malonic acid crystal, recorded with a two-pulse sequence of 3.25 ns and 6.5 ns monochromatic rectangular pulses. a) Experimental spectrum. b) Simulated spectrum.

5 minutes, while the simulation took about 2 hours.

For a system with larger ESEEM frequencies we chose to study Cu(II) ions in a TiO₂ (rutile) crystal. The Hamiltonian now also includes the nuclear quadrupole interaction P of the high spin copper ($I = 3/2$).

$$\hat{H} = \Omega_s \hat{S}_z + \omega_I \hat{I}_z + A \hat{S}_z \hat{I}_z + B \hat{S}_z \hat{I}_x + IPI$$

Since the quadrupole interaction and the hyperfine interaction have comparable magnitude, a number of formally forbidden transitions become significant. To excite the complete spectrum, chirp pulses with a sweep width of 500 MHz were required. These had lengths of 128 ns and 64 ns with $Q_{\text{crit}} = 0.6$ and $Q_{\text{crit}} = 4.6$.

The experimental 2D EPR/two-pulse ESEEM of Cu(II) in rutile is shown in Figure 4a. In the experiment the rutile crystal (110) surface was approximately aligned perpendicular to the magnetic field. For the simulation (Figure 4) we used parameters as determined by Brant et al.⁴ and considered both Copper isotopes (⁶³Cu and ⁶⁵Cu). Best agreement with the experiments was achieved by a frame rotation of 1.8° around the (001) axis from the (110) orientation. The experimental acquisition time was 12 hours, while the simulation was completed in 2 hours.

We then simulated the 2D EPR/three-pulse ESEEM for a hypothetical powder of Cu²⁺ in rutile (see Figure 5). For the $\pi/2 - \tau - \pi/2 - T - \pi/2 - \tau$ -echo sequence we applied a $[(+ (+x) - (-x))]$ phase cycle to the first pulse combined with a $[(+ (+x) - (-x))]$ pulse on the second pulse, to remove combination and difference frequencies. The spectrum was obtained simulating a total of 40 orientations in 1 day. To excite the entire spectrum we used pulse lengths of 500 ns – 250ns – 250 ns and a sweep width 1.7 GHz. While such a large sweep width may not be feasible experimentally, one should note most of the information in the correlation spectrum is contained in the perpendicular singularity of the copper spectrum. For such a spectral window, Fourier-Transform techniques are experimentally feasible⁵.

Conclusion

We introduced the new MATLAB library SPIDYAN, which can be used to simulate frequency-modulated pulses in EPR experiments, in particular in UWB EPR spectroscopy. The program can help to investigate the effect of frequency-swept pulses on commonly used EPR experiments. Such simulations can be used to predict effects, which are specific to chirp pulses, as demonstrated for EPR/ESEEM correlation spectroscopy of Cu(II) centers² and population transfer in high-spin Gd(III)-ions⁶. In the future, SPIDYAN could become a tool for optimizing and designing new UWB methods and for understanding the underlying spin dynamics.

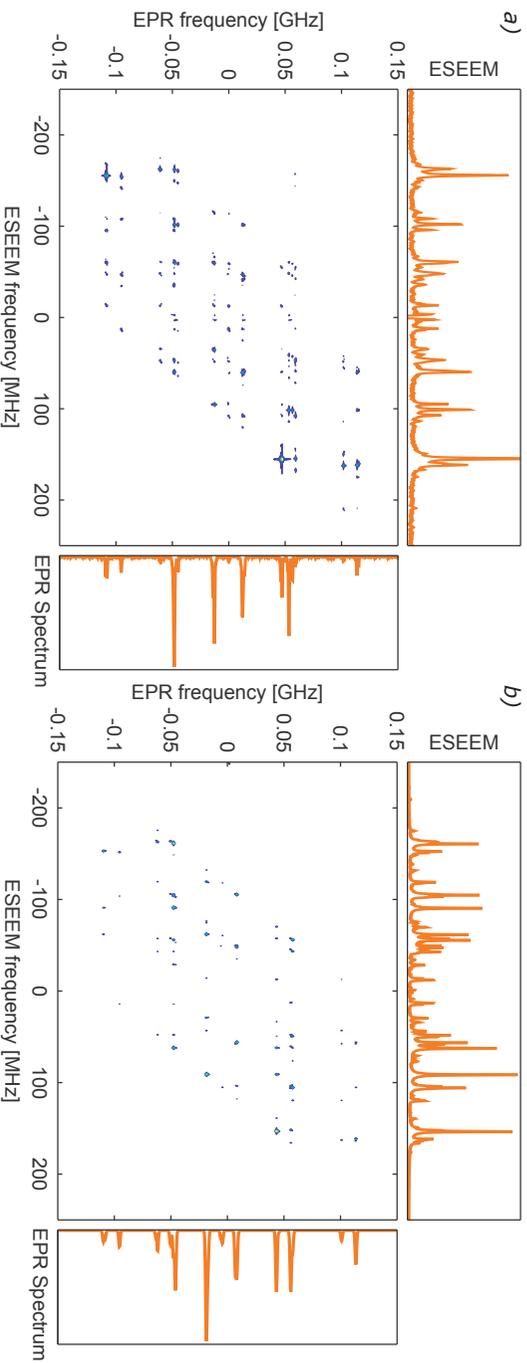


Figure 4: 2D EPR/two-pulse ESEEM spectrum of Cu^{2+} impurities in TiO_2 (rutile). Two-pulse sequence with 128 ns and 64 ns duration over a sweep range of 500 MHz. a) Experiment, the rutile crystal (110) surface was approximately aligned perpendicular to the magnetic field. b) Simulation, the system parameters for ^{63}Cu and ^{65}Cu were taken from Brant et al.⁴ and a rotation of 1.8° around the (001) crystal axis was applied.

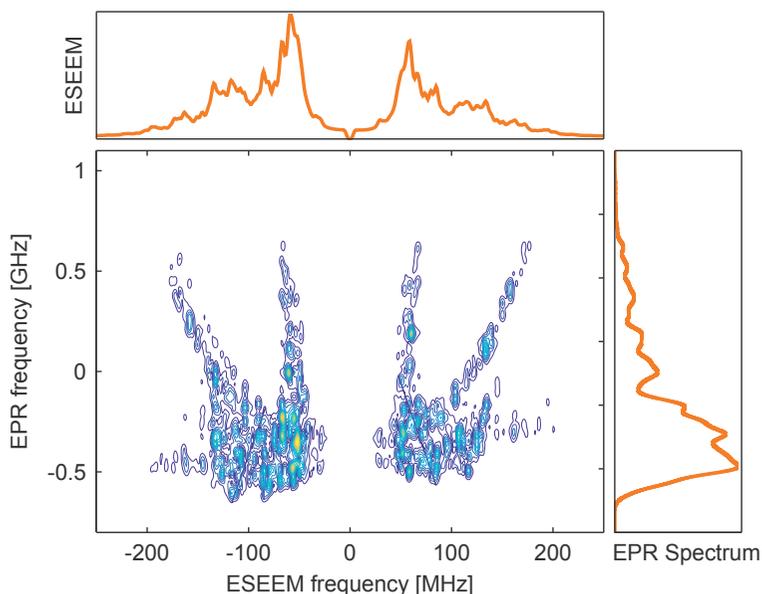


Figure 5: Simulation of a 2D EPR/three-pulse ESEEM correlation spectrum of a hypothetical powder of rutile with Copper impurities. Used were a total of 400 orientations. Pulses in three-pulse ESEEM sequence had durations of 500 ns - 250 ns - 250 ns and a sweep width of 1.7 GHz.

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Minutes of the Meeting of the Ampere Bureau

in Prague, on July 7, 2015

Members Present:

B. Blümich, A. Böckmann, B. Meier, G. Jeschke, J. Dolinsek, L. Frydman, C. Redfield, S. Jurga, M. Ernst

Excused:

C. Arns, J. van Duynhoven, F. Stallmann, H.W. Spiess

Agenda:

1. Proposed changes in AMPERE statutes, to be voted upon in Aarhus 2016 (B.Blümich)
2. Procedures and Guide-Lines for the Organization of AMPERE events (B.Blümich)
3. Inclusion of national magnetic resonance societies in the AMPERE Committee
4. Improving visibility of AMPERE
5. Future of the AMPERE Prize
6. New subdivision "Biological solid-state NMR"
7. Varia
8. Date of the next meeting: April 1 2016

At 13:05 hours G. Jeschke opened the meeting. The agenda was modified and approved unanimously.

Ad 1.

It is planned to update the statutes of the Groupement AMPERE at the next General Assembly at the EUROMAR 2016 in Aarhus. This requires that all members are informed about the changes three months before the General Assembly. The AMPERE Bureau discussed the changes in detail which are given in the appendix to the minutes. The most important change is the reform of the AMPERE Committee. Committee members are now elected for a 4 year term with a limit to two successive terms. The Committee members will be elected by the General Assembly.

Ad 2.

The AMPERE Bureau discussed a draft for the guidelines for the organization of AMPERE events. The AMPERE Bureau voted unanimously to accept the new guidelines. All the AMPERE subdivisions and the chairs of AMPERE events will be informed about these new rules by the Secretary General. The guidelines are given on page 19.

Ad 3.

It is the intention of the AMPERE Bureau to strengthen the link to the national MR societies by proposing the presidents of the national MR societies to be elected into the AMPERE Committee to the General Assembly. For the next EUROMAR conference in Aarhus, we plan to have a meeting with representatives from the national MR societies. For the Bureau meeting in March 2016, the list of national MR societies and the contact persons needs to be updated. At the next Bureau meeting we will also draft a first suggestion for a list of new Committee members.

Ad 4.

The visibility of the AMPERE society at the EUROMAR 2015 was quite good. The pen and sponsored tutorial worked well. The new guidelines discussed under topic 2 will also help to make AMPERE better visible at other AMPERE events. It was also suggested to make a webpage that links to the national MR societies and also ask them to include the AMPERE logo with a link to the AMPERE webpage on their sites.

Ad 5.

The new Richard R. Ernst prize sponsored by Bruker was discussed at the EUROMAR board of trustees. It will most likely be awarded for the first time at the next EUROMAR in Aarhus. It will be given for a "development that leads to new applications of magnetic resonance". The AMPERE group will continue to award the AMPERE Prize but will shift the focus and give it for work done by an early-stage independent researcher. It will be a lump sum of 3000.- Euro plus free registration at the EUROMAR. Nominations should consist of a short two-page summary and up to five publications. Self nominations will not be accepted.

Ad 6.

Beat Meier proposed a new subdivision "Biological solid-state NMR" with the main purpose of organizing the summer school on "biological solidstate NMR". The details of the proposal are given on page 23. The AMPERE Bureau voted in favor of the new subdivision with one abstention.

Ad 7.

Bernhard Blümich informed that there will be a meeting on Wednesday July 8 to discuss the formation of an AMPERE subdivision "Hyperpolarization". This will be organized by Jörg Matysik.

At 14:35 hours G. Jeschke closed the meeting and thanked all the present members for their time and effort. Zürich, 7.7.2015, Matthias Ernst

Statutes of the Groupement AMPERE

- Draft -

To be approved by the AMPERE Committee on July 4, 2016 at the EUROMAR Congress in Aarhus

Paragraph I: Definition, Domicile, Expiry

1. Under the name of „Groupement AMPERE“ a European association has been constituted which is corporatively organized under the rules of the paragraphs 60 (and following paragraphs) of the Swiss Civil Code and of the statutes presented here.
2. The time, for which the association is constituted, is not limited.
3. Its domicile is in Zürich, Switzerland.

Paragraph II: Purpose

The purpose of the association is to contribute to the progress of radio spectroscopy, magnetic resonance and related phenomena. This is done

1. by means of congresses and specialized „Colloques“;
2. by means of symposia, summer institutes, schools, and workshops;
3. by means of a bulletin acting as a link between the members to be published at least twice a year (electronically and/or on paper);
4. by means of prizes that honor outstanding contributions to the progress of the fields covered by the purpose of the association.

Paragraph III: Members

The association consists of individual members (natural persons) and associated members: laboratories and companies (civil entities). Documentation centers and libraries can subscribe to the Bulletin AMPERE without having the status of a member.

Applications for new membership of the Groupement AMPERE have to be addressed to the secretary general who will submit doubtful cases to the executive committee (AMPERE Bureau).

The membership implies the full consent (without any restriction) with the statutes presented here, as well as with the decisions taken or to be taken legally by the organs or by the officers of the association.

The members cannot be made individually responsible for the debts of the association. These fall entirely under the responsibility of the secretariat.

The membership to the Groupement AMPERE will end

1. with a resignation, submitted in a written form, for the end of the civil year, announced at least six months ahead;
2. with death of individual members or a dissolution of an associate member;

3. with exclusion which can be pronounced by the AMPERE Committee at the normal session;
4. with failure to pay the membership fees after two reminders.

Paragraph IV: Organization

The organs of the association are

1. the General Assembly;
2. the AMPERE Committee;
3. the AMPERE Bureau;
4. the secretariat.

Paragraph V: General Assembly

1. The General Assembly is the supreme power of the association.
2. The General Assembly executes all rights, which are not delegated to another organ by the present statutes.
3. The meeting of the General Assembly takes place annually at the EUROMAR conference.

Paragraph VI: AMPERE Committee

The AMPERE Committee is the organ, which is responsible for executing all the power, which is normally executed by the General Assembly of an association. It decides on the general policy of the Groupement AMPERE. The AMPERE Committee consists of the members of the AMPERE Bureau, one or more representatives of each European country of members, and of some eminent scientists.

The members of the AMPERE Committee are elected by the General Assembly for four years. They can be reelected once in succession.

The AMPERE Committee meets usually at the occasion of every EUROMAR conference. It elects the executive officers for a period of two years. Furthermore it elects a maximum of three honorary members of the AMPERE Bureau for a period of four years. Honorary members can be reelected twice.

The AMPERE Committee can also elect honorary members of the AMPERE society for a lifelong term. The election is by simple majority of present and voting members and by secret ballot.

Paragraph VII: AMPERE Bureau

The AMPERE Bureau consists of

1. the executive officers: the president, the secretary general, the vice presidents, the past president, and the executive secretary, the chairperson and financial officer of the EUROMAR Board of Trustees, and one representative of each other subdivision;

2. the temporary members: the chairpersons of the last and the immediate next AMPERE events;
3. the chairpersons of major scientific conferences where AMPERE participates;
4. the chairperson of the AMPERE prize committee;
5. the honorary members: (elected by the AMPERE Committee) who are entitled to attend the meetings of the AMPERE Bureau.
6. The AMPERE Bureau governs the association and in particular takes decisions during the time between the meetings of the Committee. It meets at least once a year.

Paragraph VIII: Secretariat

The Secretariat consists of the president and the secretary general. It is responsible for the management, administration and finances. It resides in Zürich, Switzerland.

Paragraph IX: Resources

The Groupement AMPERE is financed by

1. fees of individual members and subscribers to the Bulletin;
2. grants and donations;
3. contributions of associated members.

Paragraph X: Modification of statutes and dissolution

1. Any suggestion for modification of the statutes has to be communicated to all members of the Groupement AMPERE, via the secretary general, at least three months before the session of the AMPERE Committee which will treat this suggestion.
2. Any modification of the statutes has to be approved by a majority of two thirds of the attending and voting members of the AMPERE Committee.
3. The dissolution of the Groupement AMPERE is pronounced by the general assembly, on proposition of the AMPERE Committee, which is based on a majority of two thirds of the attending and voting members. It has to be approved by a majority of two thirds of the attending and voting members of the general assembly.
4. In case of dissolution of the Groupement AMPERE the remaining active property will be transferred to one or several associations with similar purposes.

A new AMPERE sub-division «Biological solid-state NMR»

An application by the European Solid-state NMR school organizers for the creation of an AMPERE subdivision «Biological solid-state NMR» has been approved in the last AMPERE Bureau meeting. The main activity of the subdivision will be the organization of the biannual biological solid-state NMR summer school, which shall then be renamed to «AMPERE biological solid-state NMR school».

The biological solid-state NMR school is organized since 2007 on a biannual basis (Brueckentinsee, Germany; Sonderborg, Denmark; Leiden, Holland; Brno, Czechia; Munich, Germany). It was initiated and organized since 2007 by Hartmut Oschkinat and Beat H. Meier, joined by a local organizer. The school aims at providing an advanced course in biological solid-state NMR, from spin dynamics to biological applications.

The school aimed at becoming a subdivision of AMPERE in order to create a solid basis for future school organizations, and to ensure optimal handling of resources.

The subdivision will be run by a collegial Board of at least three Trustees, presently Prof. Hartmut Oschkinat, Prof. Beat H. Meier, Prof. Matthias Ernst and Dr. Anja Böckmann. New trustees will be appointed by the Board.

The Board agrees on a location for the forthcoming conference and appoints a local organizer who is, together with the board, responsible for organizing the scientific program. The subdivision has no subscription or annual membership fee; as it is a subdivision of AMPERE, all AMPERE members are entitled to a reduced conference fee. Non-AMPERE members will obtain a one-year membership on registration. The corresponding member fees shall be transferred to AMPERE.

The topics of the school typically include: Specific elements of spin quantum mechanics; anisotropic interactions; time-dependent Hamiltonians; Decoupling/recoupling; Electrons and nuclei: DNP and other interactions; Relaxation in solids; Structure determination: from spectra to structure; NMR hardware; sample preparation.

The next school will take place in fall 2016.

Procedures and Guidelines for the Organization of AMPERE events

Approved by the AMPERE Bureau
on 7 July 2015 in Prague

1. Preamble

The Groupement AMPERE is the largest association of the magnetic-resonance community in Europe. Its incorporation as a non-profit organization (Verein) under Swiss law results in financial stability, and the tax exemption allows AMPERE to keep accounts, and to assure that the finances linked to conference organizations, awards and schools can be kept and used under the best possible conditions. The organization of the Groupement AMPERE is spelled out in the Statutes of the society.

AMPERE events are organized by different subdivisions of the Groupement AMPERE, whereby the Groupement AMPERE is the umbrella organization, which coordinates the events over the years, provides long-term stability, experience, and quality assurance, and administers their finances.

2. Definition

An AMPERE event is a periodically occurring congress, colloque, school, symposium or workshop, which has been approved by the AMPERE Bureau and which is organized by one of the AMPERE subdivisions.

The guidelines stated below apply to all of these events.

Other meetings can be approved by the AMPERE Bureau to obtain the label "Organized under the auspices of AMPERE". They shall comply with the guidelines stated below, with exception of point 4 (Finances). The principal AMPERE event is the EUROMAR conference. It follows the AMPERE guidelines with amendments determined by the EUROMAR Board of Trustees.

3. Applications

a) Applications to obtain the label "Organized under the auspices of AMPERE" can be submitted to the Groupement AMPERE at any time and can be voted on by e-mail by the AMPERE Bureau.annual or biannual events.

b) Applications for the organization of AMPERE events need to be submitted to the Secretariat of the Groupement AMPERE 2 years in the case of the principal event or 6 months for colloques, symposia, summer schools, and workshops before the event is to take place unless they are recurring annual or biannual events.

c) The AMPERE Bureau will discuss and approve applications during its next regular meeting and decide on whether further information, including a local inspection, is needed.

d) If the proposal is accepted, the chairperson appointed by the AMPERE Subdivision will become a temporary ex officio member of the AMPERE Bureau according to Section VII of the statutes. The chairperson has the full responsibility for the organization and the program of the meeting. The chairperson reports regularly on the progress of the organization at the occasion of the sessions of the AMPERE Bureau and the AMPERE Committee.

4. Finances

a) The finances of an AMPERE event are the sole responsibility of the local organizer. The Groupement AMPERE does not take financial responsibility.

b) The local organizers should aim at the lowest possible conference fees. If possible, fixed costs such as the rent of lecture halls should be covered by grants or sponsorships.

c) AMPERE members will receive a discount on the registration fee corresponding to a one-year membership fee. For non-members, the one-year AMPERE membership fee (full/student) should be included in the full/student registration fee. The local organizers will detail numbers of member and non-member registrations in their financial report. The Groupement AMPERE is entitled to transfer the corresponding amounts from the division to the AMPERE account. If registration numbers are not provided, they will be estimated by the AMPERE Bureau.

d) The local organizing committee shall present a financial report within 12 months to the AMPERE Subdivision. In case of a financial surplus, the chair of the local organizing committee will transfer 50% to the account of the Subdivision of the Groupement AMPERE in support of future events.

5. Announcements

a) The first announcements of AMPERE events are to be sent to all members of the Groupement AMPERE except for small events as e.g. workshops with a restricted number of participants (<50) via the secretary of the Groupement AMPERE.

b) Every AMPERE event will be advertised in the AMPERE Bulletin along with all relevant data such as title of the event, deadlines, and address for further information.

c) The web page of the event shall display the AMPERE logo with a link to the AMPERE web page. The AMPERE web page will link back to the conference web page from the list of conferences. It is the responsibility of the local organizer to provide the AMPERE secretariat (contact@ampere-society.org) with the link to the web page.

d) The 'AMPERE tree' page available via contact@ampere-society.org should be included into the conference program to create awareness for the Groupement AMPERE.

e) The AMPERE web page will list all recurring conferences even before the date of the conference is known. The conference organizers will inform the Secretary of the Groupement AMPERE when the conference date is fixed so that it can be published on the AMPERE web page.

6. EUROMAR conferences

a) Vendors are an important part of EUROMAR. They should be placed in good locations with high traffic in participants. Vendors should be given the option to inspect the location prior to the event.

b) To attract visitor flow to the vendors, it is recommended to organize coffee breaks in the vendor area and to organize a vendor raffle for conference participants.

c) The EUROMAR organizers are encouraged to visit the vendor suites during the conference to ensure satisfaction.

d) Organizational meetings of the Groupement AMPERE and the EUROMAR Subdivisions shall be publicly announced during the conference so that members are reminded to attend and conference attendees are reminded that they are being cared for.

e) Suggested time line for EUROMAR conferences

-4 years: Call for conference proposals detailing location, conference chair, budget, accommodation, venue, lecture halls, poster space, vendor space, support by national funding agencies as well as the city and possibly the university, general time table of sessions and events.

-3 years: Decide on conference location and date.

-2 years: Finalize local organizing committee and international organizing committee.

-18 months: Collect suggestions for session titles, chairs, plenary and invited speakers. Setup webpage

-12 months: Advertise conference in journals, mailing lists, and the Bulletin AMPERE. Attract sponsors. Contact vendors for sponsoring and vendor space.

7. Proceedings

a) The local organizers decide on whether or not and in which form they will publish proceedings of the event.

b) If proceedings are to be published they should be made available also to scientists who did not attend the meeting, by publishing them on the webpage of the conference. For periodically organized conferences, the AMPERE Subdivision will attempt to maintain internet access to the proceedings from all past conferences.

c) A PDF copy of the proceedings or of the book of abstracts is to be sent to the AMPERE secretariat for documentation and archiving.

8. Final report

A final report of the conference in electronic form suitable for reproduction in the AMPERE Bulletin should be sent to the secretariat. It should contain the highlights of the conference, number of participants etc., and in particular information about the proceedings.

Executive Officers and Honorary Members of the AMPERE Bureau

The AMPERE BUREAU includes the executive officers (which take the responsibility and the representation of the Groupement between the meeting of the committee), the honorary members of the Bureau and the organizers of forthcoming meetings.

Executive Officers 2014 - 2015

President	B. Blümich
Vice Presidents	J. Dolinšek A. Böckmann
Secretary General	G. Jeschke
Executive Secretary	M. Ernst
EF-EPR Representative	G. Smith
SRMR Representative	M. Johns
MRPM Representative	C. Arns
MR-FOOD Representative:	J. van Duynhoven
EUROMAR Representative	L. Frydman
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Future conferences

Ampere events

2016

Euromar 2016	Aarhus (Denmark)	July 3-7 2016
Food MR 2016	Karlsruhe (Germany)	June 7-10 2016

2017

Euromar 2017	Warwaw (Poland)	July 2-6 2017
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Other events

2016

ICMRBS 2016	Kyoto (Japan)	August 21-26 2016
57 th ENC	Pittsburgh (USA)	April 10-15 2016

2017

20 th ISMAR conference	Québec City (Canada)	July 23-28 2017
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