Nuclear Instruments and Methods

José Francisco Salgado

The activities of the Group are concentrated on research, development and technical assistance on the field of nuclear instrumentation, nuclear methods and related fields.
The strategy of the group involves activities in two different lines: *Computational Physics*, and *Instrumentation and Technical Assistance*.

Computational Physics

Numerical modeling represents an important tool to fulfil the objectives of the group and two domains of application are presently covered: *Calculation of radiation fields* and *Modelling of cold plasmas for material processing*. Along with these applications, the group is also involved in improving the available computational capacity with the build up of a Beowulf cluster for parallel computation. This cluster will be used to Monte Carlo simulations, application of genetic algorithms and fluid dynamics.

Calculation of radiation fields

The calculation of radiation fields has a broad range of applications, such as in medical physics, material processing, radiosterilisation, reactor irradiation and radiation transport in superconductors. Currently the group is involved in three of these areas:

Medical physics
The radiation fields (energy spectra and dose profiles) produced by a 6MV linear accelerator have been calculated with application in quality control of treatment planning in radiotherapy and radio-surgery.
Future work will take into account heterogeneities, namely the study of lung-bone interface. It is foreseen to initiate the study of irregular electron beams.

Radiosterilisation
The absorbed dose by irradiated products in the Radiation Technology Unit (UTR) has been calculated, allowing a more efficient exploitation of UTR. Impact of gamma irradiation over the properties of disposable surgical clothing is under study. The optimized arrangement for the refurbishment of UTR with new cobalt sources is characterized too.

Reactor physics
Resonance ephitermal self-shielding factors of Co, Au, Mn, Cu, In and Re have been calculated as a function of the wire diameter or foil thickness. The shielding for two neutron beams at RPI (a multi-purpose neutron beam and that for the SANS instrument) was also calculated.

Other applications
Monte Carlo simulations of the energy loss spectra of ^{187}Re beta decay and ^{55}Fe X-ray irradiation in micrometrically-thick rhenium strips have enabled to understand experimental measurements on these detectors. In the future this work will be extended to other superconductor materials.

Modelling of cold plasmas for material processing

Cold plasmas have a significant impact in material processing and environment applications. The activities have been divided both on fundamental aspects, development of general-purpose software tools and on applications.

An inter-comparison work between Boltzmann equation methods and Monte Carlo simulation has been concluded. A chemical kinetics software library for plasma physics and a code to study the positive column region of discharges in atomic gases have been developed. The last code has been used to study a neon discharge. An experimental and theoretical investigation of optical emission in DC argon-copper discharges has also been conducted. The application of a genetic algorithm to cross section fitting is under way.

In the near future, the code will be extended to molecular gases.

A laboratory plasma discharge gas cleaning system will also be installed to study the degradation of volatile organic compounds.

Instrumentation and Technical Assistance

The main objectives of this activity are the technological support for internal groups, including specific design for nuclear instruments, and technical assistance to industrial companies.

Equipment has been developed for the *HotBird* and *SANS* facilities, among others.

The technical assistance takes mainly the forms of specialized consultant engineering advice, installation of nuclear gauges, including calibration maintenance and repair, supply of locally produced ^{192}Ir sources and recharging of gauges with imported sources.

To achieve the goals of the Group, seven projects are presently running.

Research Team

Researchers

- José Francisco Salgado, Coord. Researcher (**Group Leader**)(70%)
- Frederico G. Carvalho, Coord. Researcher (10%)
- João Manteigas, Aux. Researcher (70%)
- Carlos Oliveira, Aux. Researcher
- Isabel F. Gonçalves, Aux. Researcher
- José Neves, Aux. Researcher
- Carlos Cruz, Aux. Researcher
- Nuno Pinhão, Aux. Researcher

Students

- Adérito Chaves, (**PhD** student)
- Jorge Ambrósio (**MSc** student)
- Lina Cerdeiral (Last year **BSc** student)
- Marisa Silva (Last year **BSc** student)

Technicians

- Tiago Jesus
- Nuno Inácio (85%)

Publications

Journals:	9	and 4 in press
Proceedings:	8	and 5 in press
Conf. Communications:	10	
Book Chapters:	3	
Internal Reports:	1	
Theses:	1	

Funding

	$\times 10^3$ PTE
Research Projects:[(a)]	885
Services:	7671
TOTAL:	8556

(a)

	$\times 10^3$ PTE
- Influência da esterilização nas propriedades e desempenho de materiais e produtos de protecção hospitalar descartáveis (P0037STERITEX) (59 205 $\times 10^3$ PTE; ITN 4454 $\times 10^3$ PTE) (2000-2001) Project Co-ordinator: FAPOMED Partners: ITN (C. Oliveira), Minho Univ. (M.E. Cabeço)	885
- Variable voltage gas discharges for surface treatment (ICCTI 423/OMFB) (1998-2000) Project Co-ordinator: Centro de Física dos Plasmas/IST (M. Pinheiro), Partners: ITN (N. Pinhão), SZFKI, Hungria (Z. Donkó, K. Rózsa, G. Bánó, K. Kutasi)	—
- Precision Measurement of the Decay Spectrum of ^{187}Re - The RELIC Project (CERN/P/FIS/1211) (1999-2001) Project Co-ordinator: CFNUL (T.A. Girard), Partners: ITN, (Carlos Oliveira), GPS-CNRS, Negeev Univ. Israel, Bar-Ilan Univ.- Israel, Technical Univ. of Barcelona	—
- Dynamics of Symmetry-breaking Type I Superconducting Phase Transitions (PRAXISFIS/10033) (1999-2001) Project Co-ordinator: CFNUL (T.A. Girard), Partners: ITN (Carlos Oliveira), GPS-CNRS, Negeev Univ. Israel, Bar-Ilan Univ.- Israel, Technical Univ. of Barcelona	—

Modelling and Simulation of Radiation Fields

I. F. Gonçalves, C. Oliveira, L. Ferreira[1], J. Salgado, E. Martinho[2]

Objectives

Calculation of radiation fields in materials for different reactor applications: neutron irradiation, neutron dosimetry and radiation shielding.

Calculation of absorbed dose in products, which allows a more efficient exploitation of the Radiation Technology Unit (UTR). Impact of gamma irradiation over the properties of disposable surgical clothing. Study of new cobalt sources arrangements, in order to optimise the replacement of the old sources by new ones.

Results

Simulation studies were carried out with the MCNP code, with the following purposes:

(a) to enhance the fast neutron flux to gamma dose ratio in samples irradiated near the core of a pool type nuclear reactor, in order to maximize the absorbed dose due to fast neutrons [1];

(b) to calculate the resonance self-shielding factor, G_{res}. Resonance self-shielding factors of Co, Au, Mn, Cu, In and Re were calculated as a function of the wire diameter or foil thickness [2, 3];

(c) to study the shielding of the multi purpose neutron beam tube installed at the RPI [4];

(d) to study the doses due to neutron and gamma radiation near the neutron selector of the SANS instrument under installation at the RPI [5].

a) to calculate the isodose distributions and dose uniformity in sample carriers of the UTR. The absorbed dose rate, gamma flux per energy interval and average gamma energy were also calculated [6];

b) to calculate the dose distributions, minimum dose and uniformity ratio for several irradiator geometry. The results allow concluding that the dose uniformity for the dynamic process is not very sensitive to the irradiator geometry. For static irradiations, the situation is different [7].

Published (or in press) work

[1] Gonçalves, I. F., Martinho, E., Salgado, J., Monte Carlo calculation of gamma spectra inside a lead hollow cylinder, *Kerntechnik* **65** (5-6) (2000) 236-239.

[2] Gonçalves, I. F., Martinho, E., Salgado, J., Monte Carlo calculation of epithermal neutron resonance self-shielding factors in wires of different materials", *Applied Radiation and Radioisotopes*, in press.

[3] Gonçalves, I. F., Martinho, E., Salgado, J., Monte Carlo calculation of resonance self-shielding factors for epithermal neutron spectra, *8th Int. Symp. on Radiat. Phys.*, Praga, 5-9 Jun 2000 (in press).

[4] Gonçalves, I.F., Ramalho, A.G., Gonçalves, I.C., Salgado, J., MCNP Calculations for the Shielding Design of a Beam Tube to be Installed at the Portuguese Research Reactor, *Proceedings of the International Conference on Advanced Monte Carlo for Radiation Physics, Particle Transport Simulation and Applications, MC2000*, Lisbon, 23-26 Oct. 2000, eds. A. Kling, F. Barão, M. Nakagawa, L. Távora, P. Vaz, Springer Verlag, Berlin, Heidelberg, in press.

[5] Safety report for the installation of the SANS instrument, Part II (in Portuguese).

[6] Oliveira, C. and Salgado, J., Isodose distributions and dose uniformity in the Portuguese gamma irradiation facility calculated using the MCNP code, *Appl. Radiat. Isot.*, in press.

[7] Oliveira, C., Ferreira, L.M. Salgado, J., Monte Carlo studies of the Portuguese gamma irradiation facility. The irradiator geometry and its influence on process parameters, *Proceedings of the International Conference on Advanced Monte Carlo for Radiation Physics, Particle Transport Simulation and Applications, MC2000*, Lisbon, 23-26 Oct. 2000 eds. A. Kling, F. Barão, M. Nakagawa, P. Vaz, Springer Verlag, Berlin, Heidelberg, in press.

Further work

The optimization of the filter material arrangement for a beam tube of the RPI is a problem to be solved by performing more Monte Carlo calculations. At the same time, the calculation of the biological shielding of the tube will be carried out.

The optimization of the performance of the SANS instrument will be carried out.

Also the calculation of self-shielding factors will be continued.

Dose and/or dose uniformity calculations and irradiation planning of new products in the UTR will be carried out.

[1] Radiation Technologies: Processes and Products Group.
[2] Reactor Sector.

Improving dose determinations in radiotherapy through Monte Carlo simulation

C. Oliveira, M. C. Lopes[1] and L. Peralta[2]

Objectives

Calculation of radiation fields produced by a linear accelerator for quality control of the treatment planning systems and radio-surgery.

Results

Simulation studies of a Siemens linear accelerator in 6 MV photon and electron modes, were carried out using the MCNP code. Results were compared with other Monte Carlo codes (EGS4 and GEANT3) and with experimental data.

(a) Energy spectra and other phase-space distributions have been extensively compared in different plans along the beam line of the linear accelerator. The depth dose calculations are, in a certain extent, insensible to some simulation parameters such as electron nominal energy. On the contrary, the dose profiles are more sensible to these parameters [1, 6];

(b) Due to the different chamber characteristics, the build-up region and the dose values at the surface show discrepancies. Monte Carlo calculations were performed to evaluate the accuracy of the measured dose values for each used chamber [4];

(c) Radiosurgery is a high-specialised procedure using narrow photon beams. A high degree of dosimetrical accuracy must be achieved. Energy spectra, output factors and depth dose curves are presented and compared with experimental data [2, 3];

(d) Intercomparison of electron energy spectra, angular and spatial distributions were carried out at beam energies of 10 and 15 MeV. Indirect validation was performed against experimental data (for electron depth doses curves and beam profiles). Monte Carlo isodose lines were reconstructed and compared to those from commercial treatment planning systems and with experimental data [5].

Published (or in press) work

[1] Alves, C., Chaves, A, Fragoso, Lopes, M., C, Lourenço, L., Oliveira C., Peralta, L., Rodrigues, P., Seco, J., and Trindade, A., Simulação Monte Carlo em Radioterapia Externa, 12th National Conference of Physics, Figueira da Foz, 2000.

[2] Chaves, A., Lopes, M. C. Alves, C., Oliveira, C., Rodrigues, P., Trindade, A., and Peralta, L., Monte Carlo Calculations for Output factors of radiosurgery narrow beams, *Proceedings of the International Conference on Advanced Monte Carlo for Radiation Physics, Particle Transport Simulation and Applications, MC2000*, Lisbon, 23-26 Oct. 2000, eds. A. Kling, F. Barão, M. Nakagawa, L. Távora, P. Vaz, Springer Verlag, Berlin, Heidelberg, in press.

[3] Chaves, A., Lopes, M. C. and Oliveira, C., Monte Carlo simulation applied to radiosurgery narrow beams using MCNP-4C code, *Radioprotecção* **1** (8-9) (2000), in press.

[4] Alves, C., Lopes, M. C, Chaves, A., Peralta, L., Rodrigues, P., Trindade, A., and. Oliveira, C., Buildup measurements and calculations for photon beams – search of the effective point of measurement for pinpoint and Markus chambers, *Topical Meeting on Medical Radiation Physics and Engineering – MeRPE 2000*, Lisbon, Nov. 2000.

[5] Trindade, A., Rodrigues, P., Alves, C., Chaves, A., Lopes, M., C., Oliveira, C., Peralta, L., Monte Carlo Simulations of electron beams for radiotheraphy – EGS4, MCNP4b and GEANT3 intercomparison, *Proceedings of the International Conference on Advanced Monte Carlo for Radiation Physics, Particle Transport Simulation and Applications, MC2000*, Lisbon, 23-26 Oct. 2000, eds. A. Kling, F. Barão, M. Nakagawa, L. Távora, P. Vaz, Springer Verlag, Berlin, Heidelberg, in press.

[6] Chaves, A., Alves, C., Lopes, M. C., Oliveira, C., Rodrigues, P., Trindade, A., Fragoso, M., Seco, J. and Peralta L., Caracterização de um acelerador linear de electrões usando o método de Monte Carlo, *VII Jornadas Portuguesas de Protecção contra Radiações*, Lisbon, Nov. 2000.

Further work

Concerning the radiotherapy studies, the work will be oriented to continue the study of narrow beams used in radiosurgery and originated by the interposition of additional collimating systems. Problems related with heterogeneities are of great importance. The future work will take into account these problems, namely the study of lung-bone interface. It is foreseen to initiate the study of irregular electron beams. It requires the simulation of the specific head accelerator components, corresponding to the production of therapeutic electron beams.

[1] Instituto Português de Oncologia Francisco Gentil, Centro Regional de Oncologia de Coimbra
[2] Faculdade de Ciências da Universidade de Lisboa, and LIP.

Superconductor irradiation simulations

C. Oliveira and T. Girard[1]

Objectives

The objective of the superconductor irradiation simulations is to assist in the interpretation of response of the materials, which is of interest in understanding the far out-of-equilibrium flux dynamics of superconductivity, the development of a new class of low temperature detector, and the investigation of symmetry-breaking phase transitions related to cosmological interpretations.

Results

Simulations of the Cd irradiations of Sn superconducting strips indicated an un-anticipated near-100% efficiency of the device, which is in conflict of the basic known physics of the superconductive device response. These studies further indicated that the observed detector response was linear in the deposited energy, and that the energy resolution was primarily due to scattering in the source material, rather than the intrinsic detector -- suggesting immediate improvements in device performance.

The similar simulation results with 6 keV X-rays in both Sn and Re are however not observed, raising serious questions regarding the superconductive response to irradiation and forcing a complete reconsideration of the involved out-of-equilibrium dynamics.

Published (or in press) work

[1] Gomes, M.J., Girard, T.A., Oliveira, C., Jeudy, V., Limage, D, A superconductive measurement of the ^{187}Re beta decay spectrum, *Nucl. Inst. and Meth.* ***A*** **444** (1) (2000) 84-87.

[2] Gomes, M.R., Girard, T.A., Oliveira, C., Jeudy, V., Limagne, D., A superconductive measurement of the ^{187}Re beta decay spectrum: preliminary results, *Nucl. Phys. B Proc. Suppl*. **87** (2000) 493-394.

[3] Gomes, M.J., Girard, T.A., Oliveira, C. and Jeudy, V., Particle detection with geometrically-metastable type I superconducting detectors, *Inst. Phys. Conf. Ser.* **167** (2000) 691-694.

[4] Gomes, M.J., Girard, T.A., Oliveira, C. and Jeudy, V., Measurements of the ^{187}Re beta decay spectrum with a geometrically-metastable superconducting detector, World Scientific, Singapore, 2000, pp. 753.

[5] Gomes, M.R., Girard T.A., Oliveira, C., Jeudy V., Particle Detection with Geometrically-Metastable Type-I Superconductors, Applied Superconductivity 1999, ed. X. Obradors, F. Sandiumenge and J. Fonteuberta (IOP Publishing, Bristol, 2000) pp. 691.

[6] Girard, T.A., Valko, P., Gomes, M.R., Oliveira, C., Direct Neutrino Mass Measurement with a Superconductive Detector, *Proc. Carolina Symposium on Neutrino Physics*, Columbia, SC USA, 12-14 March 2000, in press.

[7] Valko, P., Gomes, M. R., Girard, T.A., Oliveira, C., Measurements of the ^{187}Re Beta Spectrum, *Proc. International Workshop on Non-Accelerator New Physics in Neutrino Observations*, Dubna, Russia, 19-22 July 2000, in press.

Further work

Further work includes simulations of electron/X-ray irradiations of various thicknesses of metallic strips of different type I superconductors (PRAXIS), towards elaborating their far out-of-equilibrium responses.

It also includes simulations of the filtered neutron beam irradiations associated with neutron calibrations of SIMPLE detector.

[1] Centro de Física Nuclear, Universidade de Lisboa

Numerical Modelling of Plasmas for Materials Processing

N. R. Pinhão, Z. Donkó[1], D. Loffhagen[2], M. Pinheiro[3], E.A. Richley[4], K. Kutasi[1], G. Bánó[1]

Objectives

The main objective of this project is the development of competence in low temperature plasmas with special attention to applications in material processing. As research and development in this field is heavily based on numerical modelling, the first goal has been the establishment of a solid experience on numerical modeling. However the launching of an applied experimental and demonstration project has been started and will continue next year.

Results

- **Comparison between Boltzmann equation methods and Monte Carlo simulation.**
  The results of an inter-comparison work coordinated by ITN, have been published in a conference proceedings [1].
- **Development of a chemical kinetics software library for plasma physics - *PLASMAKIN***
  A software library to address common problems in a large range of plasma modeling problems has been under development. The library has been extended to include the evaluation of the photon emission spectra, the energy exchanged in reactions and the inclusion of groups of vibrational levels and reactions involving vibrational levels [2].
- **Analysis of the positive column region of a neon discharge**
  A code to study the positive column region of discharges in atomic gases has been developed. This code is based on the PLASMAKIN library and is valid for a large range of conditions between the free-fall and the ambipolar regimes. It has been applied to a neon discharge using a kinetic model that includes the effect of electron collisions with neon 3s excited levels and transitions between 3s levels [2].
- **Experimental and theoretical investigation of optical emission in a DC argon-copper discharges.**
  The results obtained on a project conducted by SZFKI of Budapest and University of Antwerp, have been published this year [3].

Published (or in press) work

[1] Pinhão N., Donkó Z., Loffhagen D., Pinheiro M. and Richley E. A., Comparison of Monte Carlo and electron Boltzmann equation methods at low and moderate E/N field values, *XVth ESCAMPIG: Abstract of Invited Lectures and Contributed Papers* (2000) 156-157

[2] Pinhão, N., PLASMAKIN: A chemical kinetics package for plasma physics modelling, accepted for publication in Computer Physics Communications and *CPC Program Library*. "Hot-Topic" seminar at XVth ESCAMPIG: Abstract of Invited Lectures and Contributed Papers (2000) 44-45

[3] Bogaerts A., Donkó Z., Kutasi K., Bánó G., Pinhão N., Pinheiro M., Comparison of calculated and measured optical emission intensities in a direct current argon-copper glow discharge, *Spectrochimica Acta, part B* 55 (2000) 1465-1479 and *XVth ESCAMPIG: Abstract of Invited Lectures and Contributed Papers* (2000) 200-201

Further work

- **Analysis of the positive column region of neon-chlorine discharge**
  The previously develop code for the analysis of the positive column region of gas discharges will be extended to support molecular gases and the effect of electron-electron collisions. This code will be used to study the positive column region of neon-chlorine and argon-chlorine discharges with interest for semiconductor etching.
- **Application of a Genetic Algorithm to electron collision cross sections fitting**
  The use of a "deconvolution" method to fit the electron collision cross section using the experimentally measured macroscopic parameters is standard in low temperature plasma physics. The idea behind this project is to associate a genetic algorithm with the electron Boltzmann equation to optimize and automate this fitting.
- **Simulation of CN and CN_x thin films production in a N_2 glow discharge with a carbon cathode.**
  The synthesis of carbon nitride CN_x thin films is an active field of research due to the possibility of realization of the “diamond-like” superhard β-C_3N_4 phase. The modeling of a glow discharge for CN production, in collaboration with IST and SZFKI, Budapest, is in progress. Comparison with optical emission measurements will be used for model validation. Results are expected in the first quarter of 2001.
- **Gas cleaning system for the "Treatment and valorization of plastic waste" project**
  A laboratory plasma discharge gas cleaning system will be installed to study the degradation of volatile organic compounds. This system is currently been projected and will use an atmospheric pressure corona discharge for the production of chemical active plasma. This task is included in the project "Treatment and valorization of plastic waste".

[1] SZFKI, Hungary.
[2] Institut fur Niedertemperatur–Plasmaphysick, Germany.
[3] Centro de Física dos Plasmas. IST, Portugal.
[4] Silva Court, USA.

Technical Assistance in the Field of Engineering Applications of Radiation and Radioisotopes

J.B. Manteigas, J. Neves, C. Cruz, C. Oliveira, J. Salgado, N. Pinhão, F.G. Carvalho

Objectives

The main objectives are the technological support to internal groups, including specific design of nuclear instrumentation and assistance to industrial companies. The technical assistance takes mainly the forms of specialized consultant engineering advice, installation of nuclear gauges, including calibration maintenance and repair, supply of locally produced ^{192}Ir sources and recharging of gauges with imported sources.

Results

Considerable work was carried out through technical assistance, design and construction of electronic instrumentation for other ITN groups. A summary of the more relevant work is:

(i) Design and construction of:
an alarming and signaling system aimed to instrument's safe operation (High-temperature X-ray Diffractometer [1]);
an electro-mechanical device for the automatic opening and closing of the neutron beam. This device has a back-up power supply and several circuits for signaling and alarming (SANS instrument);
an "alarm dialler system" (working with the Siemens EDPABX Icom300E to maintain the facility operator, under telephone contact if needed).

(ii) analysis and design optimization of the *HotBird* High-temperature X-ray Diffractometer;

(iii) General maintenance, repair and test of all electronics (ETV and UTR);

(iv) Disassembling, transferring and installation of a Cobalt 60 Gammacell (20 ton, 115 Ci). Design of a new electronic control system is under tests for research groups to operate with the Gammacell safely;

(v) Electronic maintenance of some spectrometers (DPRSN and RPI);

A summary of the more relevant services rendered in 2000 is presented below in **12. Services**.

Published (or in press) work

[1] Sequeira, A.D. , Franco, N., Neves., J., High-Resolution and High-Temperature Double-Crystal X-ray Diffractometer for in-situ Studies - the Hotbird, *Mat. Sci. Forum* 6pp., Accepted for publication.

[2] Margaça, F.M., Pinhão, N.R. and Sequeira, A.D.. Design Optimisation of a High-temperature X-ray Diffractometer for in-situ Residual Stress Analysis and Lattice Mismatch Determination. *Materials Science Forum* **322** (2000) 168.

Further work

In the near future, the Group will be engaged in assisting ITN internal groups and in providing technical support for industrial companies.

Services

A summary of the more relevant services rendered in 2000 is presented below in the Table.

Activity	Quantity	Client
Supply of Personal Dosimeters RAD X 100	2	ITN/Reactor
	7	RITAGRA
Supply of ^{192}Ir gamma sources	24	Siderurgia Nacional
Supply of plating electrode disks	500	ITN/DPSRN
Laboratory equipment for the determination of radioactive element traces by electrodeposition	1	TULANE (USA)
	1	Neurotech, Inc. (USA)
	1	ITN/DPSRN
Supply of gamma level detector units	4	CIMPOR/Souselas
Repair of depleted uranium balance weights	3	TAP Air Portugal
Measuring and control of sources activity	1	PORTUCEL/Cacia
	1	TECNISIS
	26	SOPORCEL/F.Foz
Transfer and storage of radioactive sources	1	Portucel/Cacia
	24	CIMPOR/Alhandra
Supply of ^{60}Co gamma sources	1	SOLVAY Portugal
Supply of source containers	6	Siderurgia Nacional
	1	SOLVAY Portugal
Consulting	1	PROASTELA, SA
Technical assistance	1	SOLVAY Portugal
	1	CMP/Maceira Liz
	1	SOPORCEL
	1	TECNISIS
	1	ISA
	1	Portucel/Tejo
	1	Inst. Geológico e Mineiro
Upgrade and calibration of equipment	1	LNEC