ICTP − The Abdus Salam International Centre for Theoretical Physics, Trieste, Italy

smr1310/Announcement

SPRING COLLEGE
ON
NUMERICAL METHODS IN
ELECTRONIC STRUCTURE THEORY

7 − 25 May 2001
Miramare, Trieste − Italy

An international course on pseudopotential plane−wave electronic structure calculations will be held at the Abdus Salam International Centre for Theoretical Physics (ICTP), Trieste, Italy, with the co−sponsorship of the Istituto Nazionale per la Fisica della Materia (INFM), Italy, from 7 to 25 May 2001.

DIRECTORS

Stefano Baroni − Scuola Internazionale Superiore di Studi Avanzati (SISSA) and INFM,Trieste, Italy
Andrea Dal Corso − Scuola Internazionale Superiore di Studi Avanzati (SISSA) and INFM, Trieste, Italy
Stefano de Gironcoli − Scuola Internazionale Superiore di Studi Avanzati (SISSA) and INFM, Trieste, Italy

PURPOSE AND NATURE

This College aims at a general introduction to electronic structure calculations within Density Functional Theory and using the plane−wave pseudopotential method. The focus will be on the physical principles and numerical algorithms which underlie the implementation of state−of−the−art computer codes. The course will be opened by a few colloquia given by top scientists on the present status and future perspectives of electronic structure calculations. A series of theoretical lectures will follow, aiming at illustrating how an electronic structure computer code is developed in practice. These lectures will be complemented by hands−on computer sessions where it will be demonstrated how a simple plane−wave pseudopotential computer code is developed, starting from scratch. Finally, in the last part of the course, a state−of−the−art pseudopotential package (PWSCF) will be distributed to the participants and a series of tutorials will be held to illustrate its usage and a number of currently significant applications.

PRELIMINARY LIST OF LECTURERS

Dario Alfe' − University College London, London, UK
Stefano Baroni − SISSA and INFM, Trieste, Italy

Andrea Dal Corso − SISSA and INFM, Trieste, Italy
Stefano de Gironcoli − SISSA and INFM, Trieste, Italy
Giulia Galli − Lawrence Livermore National Laboratory, Livermore, USA
Paolo Giannozzi − Princeton University, Princeton, USA
Steven G. Louie* − University of California, Berkeley, USA
Michele Parrinello − Max−Planck−Institut fur Festkorperforschung, Stuttgart, Germany
Erio Tosatti − SISSA, ICTP and INFM, Trieste, Italy
David H. Vanderbilt − Rutgers University, Piscataway, USA

*To be confirmed

TENTATIVE PROGRAMME

−− Introductory colloquia on the present status and future perspectives of computational condensed matter physics and materials science.
−− Overview of electronic structure theory of atoms, molecules, and solids.
−− Density functional theory, Kohn−Sham equations, and exchange correlation functionals.
−− The plane−wave pseudopotential method.
−− Numerical techniques:
   − Brillouin−zone integration: special points, gaussian smearing, etc.
   − Spectral methods: discrete Fourier transform and its properties, Fast Fourier Transform.
   − Numerical linear algebra: factorization and iterative methods for linear systems and eigenvalue problems.
   − Solving the self−consistent problem: iterative diagonalization vs. global minimization.
−− First derivatives of the total energy. The Hellmann−Feynman theorem. Atomic forces and the stress tensor.
−− Higher order derivatives.
   − Density functional perturbation theory.
   − Phonons.
   − Macroscopic electric fields.
   − The 2n+1 theorem and higher order responses.
−− The quantum theory of electric polarization: the Berry's phase approach.
−− Ab−initio molecular dynamics.
   − Classical molecular dynamics.
   − The Car−Parrinello Lagrangian.
   − Other methods for ab−initio molecular dynamics.
−− Elements of parallel computing.
−− Calculation of selected properties and selected applications.

PARTICIPATION

Students and young scientists from all countries that are members of the UN, UNESCO or IAEA can attend the College. The main purpose of the Centre is to help researchers from developing countries through a programme of training activities within a framework of international co−operation. However, scientists from developed countries are also encouraged to apply. This course is specially meant for strongly motivated graduate students and young post−doctoral scientists. Prior specific training in electronic structure calculations is not strictly required. However, participants are expected to have a good working knowledge of elementary quantum mechanics and solid state physics. Knowledge of FORTRAN and UNIX is a necessary condition. As the College will be conducted in English, participants should have an adequate working knowledge of that language. Due to the

number of PCs available, the total number of participants in the College is limited.

As a rule, travel and subsistence expenses of the participants are borne by their home institutions. However, limited funds are available for some applicants from developing countries, to be selected by the organizers. As scarcity of funds allows travel to be granted only in a few exceptional cases, every effort should be made by candidates to secure support for their fare (or at least half−fare) from their home country. Such financial support is available only to those attending the entire College. There is no registration fee for attending the College. A limited number of grants to support the participation of young Italian scientists belonging to INFM are also available.

The closing date for the receipt of requests for participation is 31 January 2001.

Candidates should complete and sign the "Request for Participation" form, to be found at foot of this Bulletin (also obtainable via e−mail: smr1310@ictp.trieste.it, using as subject "get index", or via WWW Server: http://www.ictp.trieste.it/), and send it to:

the Abdus Salam International Centre for Theoretical Physics
Spring College on
Numerical Methods in Electronic Structure Theory
c/o Ms. Nicoletta Ivanissevich
Strada Costiera 11
I−34014 Trieste, Italy

VERY IMPORTANT:

If you have obtained the following form via e−mail or gopher, please follow these instructions:

1) ABSOLUTELY do NOT modify the form at all!;
2) PRINT it in portrait mode (A4 lengthwise);
3) Fill in the HARD copy of the form, sign it and post it as indicated above.

No forms via e−mail are accepted!

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UNITED NATIONS EDUCATIONAL, SCIENTIFIC AND CULTURAL ORGANIZATION
and
INTERNATIONAL ATOMIC ENERGY AGENCY

the ABDUS SALAM INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS

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I−34014 Trieste Telex: 460392 ICTP I

Italy Telefax: +39−040−224163
E−mail: SMR1310@ictp.trieste.it

REQUEST FOR PARTICIPATION

SPRING COLLEGE ON
NUMERICAL METHODS IN ELECTRONIC STRUCTURE THEORY
7 − 25 May 2001

INSTRUCTIONS
Each question must be answered clearly and completely. Type or print in ink. If more space is required, attach additional pages. This form should be forwarded to: the Abdus Salam International Centre for Theoretical Physics, Spring College on Numerical Methods in Electronic Structure Theory (c/o Ms. N. Ivanissevich), Strada Costiera 11, I−34014, Trieste, Italy, to arrive no later than 31 January 2001.

A recent photograph of the candidate should be attached here,signed legibly on the reverse.

NOTE: This request will be processed only if the permanent address (and present address, if different) is clearly indicated. The ICTP cannot process any visa request, unless all requested personal data are provided.

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P E R S O N A L D A T A

SURNAME/FAMILY Name: MAIDEN Name: First name: Middle name(s): Sex:
For women only (if applicable)

IMPORTANT: PLEASE ALSO COMPLETE THIS SECTION, IF YOUR NAME(S) IN YOUR PASSPORT ARE SPELT DIFFERENTLY FROM THE ABOVE.
SURNAME/FAMILY Name: MAIDEN Name: First name: Middle name(s):
For women only (if applicable)

Place of birth (City and Country): Present nationality: Date of birth:
Year − Month − Day

Full name/address of permanent Institution: Institute: Tel. No.:
Telex/Cable:
Telefax:
Your Office: Tel. No.:
Telefax:
E−mail: *

Full name/address of present Institution : Institute: Tel. No.:
(if different from permanent) Telex/Cable:
Telefax:
Your Office: Tel. No.:

Telefax:
until: Date ..... E−mail: *

Home address: Tel. No.:

Mailing address − please indicate whether:
Permanent __ Present __ Home __

Name and address of person to notify in case of emergency:
Relationship: Tel. No.:

* I agree that my e−mail address(es) may be made public on the ICTP WWW page:
YES __ NO __

EDUCATION (higher degrees)

University or equivalent Name and place	Years attended From	to	Degrees

Seminars, summer schools, conferences or research

Name and place	Year

SCIENTIFIC EMPLOYMENT AND ACADEMIC RESPONSIBILITY

Research Institution or University Name and place	Period of duty From	to	Academic responsibilities

Present employment and duties, and foreseen employment upon return to home country after the activity:

Have you participated in past ICTP activities? If yes, which? Yes__ No__

Are you applying to any other 2001 ICTP activities? If yes, which? Yes__No__

Mention briefly your previous research experience, and explain your reasons for wishing to participate in this activity:

NB: Our Scientific Information System keeps track of all applications made by the candidate to earlier ICTP activities. As a consequence, when the subject of the present activity is far from your previous applications, an explanation (not more than 200 words) of your change of interest should be included.

PRESENT FIELD OF INTEREST (please indicate on the list below your TWO primary fields of interest, in order of priority, 1 and 2.

10. PHYSICS OF CONDENSED MATTER
11. Solid State Physics
12. Atomic and Molecular Physics
13. Materials Science
14. Surfaces and Interfaces
15. Statistical Physics
16. Computational Physics in Condensed Matter

20. PHYSICS OF HIGH AND INTERMEDIATED ENERGIES
21. High Energy and Particle Physics
22. Relativity, Cosmology and Astrophysics
23. Plasma Physics
24. Nuclear Physics

30. MATHEMATICS
31. Applicable Mathematics, including: Mathematical Ecology, System Analysis, Mathematical Economy, Mathematics in Industry
33. Algebra
34. Geometry

35. Topology
36. Differential Equations
37. Analysis
38. Mathematical Physics

40. PHYSICS AND ENERGY
41. Physics of Nuclear Reactors
42. Physics of Controlled Fusion
43. Non−Conventional Energy (Solar, Wind others)
44. Nuclear Energy related technologies

50. PHYSICS AND ENVIRONMENT
51. Solid Earth Geophysics
52. Soil Physics
53. Climatology and Meteorology
54. Physics of the Oceans
55. Physics of Desertification
56. Physics of the Atmosphere, Troposphere, Magnetosphere, Aeronomy
57. Environmental Monitoring and Remote Sensing

60. PHYSICS TEACHING
61. English
62. French
63. Spanish
64. Arabic

80. MISCELLANEOUS
81. Others
82 Digital Communications Computer Networking

90. PHYSICS OF THE LIVING STATE
91. Neurophysics
93. Medical Physics

AO. APPLIED PHYSICS
A1 Physics in industry
A2. Microelectronics
A3. Fibre Optics for Communications
A4. Instrumentation
A5. Synchrotron Radiation
A6. Non−destructive Evaluation
A7. Lasers
AA. Applied Superconductivity

B1. SPACE PHYSICS

Kindly supply a keyword description of your current scientific activities, as follows (strictly within indicated lengths) :

1) Area of research: (e.g. SEMICONDUCTOR PHYS.)

_____
(no more than 15 characters)

2) Specific topic of interest: (e.g. BAND STRUCTURE THEORY)

_____
(no more than 30 characters)

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List your scientific publications including books and articles (authors, title, Journal) in the period 1996–2000 (add a separate page if necessary):

Kindly state any positions you hold in the scientific administration of your Institution or any of the national scientific Institutions.

It would be of assistance to the Selection Committee if this request for participation were accompanied by a letter of recommendation, especially for junior physicists.

Indicate below your proficiency in the English language

Reading:		Writing:		Speaking:	
Good	__	Good	__	Good	__
Average	__	Average	__	Average	__
Poor	__	Poor	__	Poor	__

Indicate below your ability in programming techniques

FORTRAN:		UNIX:	
Excellent	__	Excellent	__
Good	__	Good	__
Average	__	Average	__
Poor	__	Poor	__

APPLICABLE ONLY FOR CANDIDATES FROM DEVELOPING COUNTRIES
(Important: Owing to limited funds, support for travel will be granted only in exceptional cases. Therefore, every effort should be made by applicants to secure support for their fare (or at least a partial contribution) from their home country).

Request for Financial Assistance: (Please tick ONE box only)

__ Full Travel + Subsistence
__ Half Travel + Subsistence
__ Subsistence only
__ No financial support requested

I certify that if granted funds for my
travel, I shall attend the whole activity

.....
Signature

I certify that the statements made by me above are true and complete. If accepted, I undertake to refrain from engaging in any political or other activities which would reflect unfavourably on the international status of the ICTP. I understand that any breach of this undertaking may result in the termination of the arrangements relating to my visit at the Centre.

_____ _____
Signature of applicant Date

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