Code Centres Network meeting at IAEA の報告

Fumihiro Koike, Kitasato University

December

Dec 01 Dec 02	Nuclear Security Coordination Meeting	J0-TM-35658	VIC C07 V AUS	Mr Andrews, Timothy John * Ms Lieskovsky, Katerina	20
Dec 01 Dec 02	TM on country nuclear fuel cycle profiles	T1-TM-35290	Fukui JPN	Mr Chayama, Hidekazu * Ms Roch-Braeuer, Jolanta	10
Dec 01 Dec 03	RCM of the CRP on Improving outcomes in radiotherapy using novel biotechnologies: modification of tissue reactions and the use of stem cell therapeutics	E3-RC-1109.1	VIC C0453 AUS	Mr Wondergem, Jan * Ms Soysa, Chandra	15
Dec 01 Dec 04	3rd RCM on Development of harmonized QA/QC procedures for maintenance and repair of nuclear instruments	F1-RC-1004.3	Mexico City MEX	Ms Muelhauser, Francoise * Ms Bojdo, Rozanne	8
Dec 01 Dec 05	RCM for assessment of research results from modelling and analysis of so	J7-RC-1081.2	VIC A0478	Mr Willers, Andrew	15
Dec 01 Dec 05	First RCM on Benchmark ag thermalhydrau and safety ana				20
Dec 01 Dec 05	SAGSI Plena				17
Dec 01 Dec 05	Advanced Detection Equipment	J0-TR-35683	Kiev	Mr Rukhlo, Vladimir	25
Dec 01 Dec 05					
Dec 01 Dec 05	Technology		AUS	* Ms Gomez Nunez, Maria de Las Merce.	
Dec 01 Dec 06	International Conference on "Water Scarcity, Global Changes, and Groundwater Management, Management Responses"	330-N4.10.1; FX.0-USA	Irvine, CA USA	Mr Haji-Saeid, Seyed Mohammad * Ms Obauer-de Bruyker, Myriam	
Dec 02 Dec 03	International Code Centres Network	F4-TM-34563	VIC A0523 AUS	Mr Clark, Robert Edward Holmes * Mr Sheikh, Khalid	12

Dec 02 International Code Centres Network
Dec 03
F4-TM-34563 VIC A0523 AUS Mr Clark, Robert Edward Holmes * Mr Sheikh, Khalid

IAEA, Vienna International Centre, Atomic and Molecular Data Unit

http://www-amdis.iaea.org/

Agenda year 2008

- IAEA Workshop on “Challenges in Plasma Spectroscopy for Future Fusion Research Machines”, Jaipur, India, 20-22 February 2008
- **Code Center Network (CCN)**
- XML Meeting, April and October 2008
- XML Workshop on “A+M/PSI Data”, May 2008
- IFRC Subcommittee Meeting, June 2008
- Final RCM on “A+M Data for Plasma Modelling”, November 2008
- 1st RCM on “Size, Composition and Formation of Dust in Tokomaks”

Technical Meeting on “International Code Centres Network” at IAEA

- 第1回:
  2005年　5月23日～25日
  R.E.H. Clark, D. Stotler, I. Bray, A. Dubois, I. Rabadan, J. Abdallah, Jr., M. Capitelli, D. Reiter, D. Kato, F. Koike, V. Lisitsa, Y. Ralchenko, L. Vainshtein
- 第2回:
  2008年　12月2日～3日
- Will be held every two years

Meeting Agenda (1)

- **Technical Meeting on "International Code Centres Network"**
- 2-3 December, 2008, IAEA Headquarters, Vienna, Austria
- Scientific Secretary: R.E.H. Clark
- Tuesday, 2 December
- 09:30 - 09:45 A. Nichols, R.E.H. Clark Welcoming remarks, Adoption of Agenda
- *Session 1: Reports on current status*
- **Chairman: L. Vainshtein**
- 09:45 - 10:15 I. Bray
- 10:15 - 10:45 F. Koike
- 10:45 - 11:15 *Coffee Break*
- 11:15 - 11:45 I. Rabadan
- 11:45 - 12:15 A. Dubois
- 12:15 - 12:45 M. Capitelli
- 12:45 - 14:00 *Lunch*
- *Session 2: Reports on current status II*
- **Chairman: F. Koike**
- 14:00 - 14:30 A. Kukushkin
- 14:30 - 15:00 L. Vainshtein
- 15:00 - 15:30 D. Reiter
- 15:30 - 16:00 *Coffee Break*
- 16:00 - 16:30 J. Abdallah, Jr.
- 16:30 – 17:00 Y. Ralchenko
- 17:00 - 17:30 D. Stotler

Meeting Agenda (2)

- Wednesday, December 3
- *Session 3: Summary of current status and available tools*
- **Chairman: D. Reiter**
- 09:00 – 10:30 All participants: Summary of current status
- 10:30 - 11:00 *Coffee Break*
- *Session 3: Continued*
- 11:00 - 12:00 All participants: Summary of available codes
- 12:00 - 13:30 *Lunch*
- *Session 4: Establishment of Code Centre*
- **Chairman: Y. Ralchenko**
- 13:30 – 15:00 All participants: Discussion of operation of code centre
- 15:00 - 15:30 *Coffee Break*
- *Session 4: Continued*
- 15:30 – 17:00 All participants: Formulation of conclusions and recommendations
- 17:00 - *Adjournment of Meeting*

Web calculation tools

IAEA

- Cross sections of bare nuclei on hydrogenic ions

  http://www-amdis.iaea.org/HEAVY/

  New process : ionization, Pablo Fainstein and Alain Dubois
- *Average approximation for electron impact excitation of atomic ions*

  http://www-amdis.iaea.org/AVERAGE/
- *Results from collisional radiative calculations of plasmas are available, as carried out with the Los Alamos modelling codes*

  http://www-amdis.iaea.org/RATES/

LANL

- Los Alamos atomic physics codes: an interface is available to run several Los Alamos atomic physics codes to calculate atomic structure and electron impact excitation and ionization cross sections (fine structure levels and configuration average)

  http://aphysics2.lanl.gov/tempweb/

http://www-amdis.iaea.org/ (1)

International Atomic Energy Agency
Nuclear Data Section/Atomic and Molecular Data Unit
Vienna, Austria

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NDS Atomic and Molecular Data Unit

The Atomic and Molecular Data Unit operates within the Nuclear Data Section of the International Atomic Energy Agency, Vienna, Austria.

The primary objective of the Atomic and Molecular Data Unit is to establish and maintain internationally recommended numerical databases on atomic and molecular collision and radiative processes, atomic and molecular structure characteristics, particle-solid surface interaction processes and physico-chemical and thermo-mechanical material properties for use in fusion energy research and other plasma science and technology applications.

- ICTP-IAEA Workshop on "Atomic and Molecular Data for Fusion" *new!*
  20-30 April, 2009, ICTP, Trieste, Italy
  The A+M Data Unit is pleased to announce a joint ICTP-IAEA workshop on atomic and molecular data for fusion to be held on 20-30 April, 2009 at the ICTP facility in Trieste, Italy. The workshop is meant to be a training workshop to young researchers with an interest to expand their knowledge of A+M data relevant to fusion. See the URL for more information and online application to the workshop.

- **Databases on Atomic and Molecular Data for Fusion.**
  1. **ALADDIN**
  2. The bibliographical database **AMBDAS**
  3. **Rovibronic energy levels for triplet electronic states of molecular deuterium** (December 2007)
     B. P. Lavrov and I. S. Umrikhin, Faculty of Physics, St.-Petersburg State University
     Numerical data and report
  4. **Franck-Condon Factors, Transition Probabilities and Radiative Lifetimes for Hydrogen Molecules and their Isotopomeres**, U. Fantz, D. Wünderlich (May 2004).
     Numerical data and report (INDC (NDS) 457)

- **GENIE** for GENeral Internet search Engine allows a multiple search on different databases on the web for spectral and collisional atomic data for fusion and atomic physics research. The new version includes requests for dielectronic recombination data.

- **Online Computing**
  1. **Heavy Particles collisions** Cross sections for excitation and charge transfer for collisions between hydrogenic targets and bare ions can be calculated online. Potential users are asked to request a user name and password.
  2. **Los Alamos atomic physics codes** An interface is available to run several Los Alamos atomic physics codes for calculation of atomic structure, electron impact excitation, as well as ionization processes
  3. **Average Approximation** is an interface to average approximation cross sections for calculating electron impact cross sections for atomic ions. This is expected to be useful in generating cross sections of reasonable accuracy when more accurate cross section data is not available.
  4. **Rate coefficients** Results from collisional radiative calculations of plasmas carried out with the Los Alamos modeling codes are available. Interpolations allow the user to obtain total radiated power, average ion charge, and relative ionization populations in a steady state plasma.

- **XSAMS**: XML Schema for Atoms, Molecules and Solids *new!*

The IAEA Atomic and Molecular Data Unit achieves its objectives by coordinating the activities of the **International Atomic and Molecular Data Center Network** (DCN), initiation and conducting international **Coordinated Research Projects** (CRP), organization of various types of Expert's Meetings, and using other forms (research contracts, research agreements, consultancies) for stimulation of the generation, collection and critical assessment of the required atomic, molecular (A+M) and plasma-material interaction (PMI) data information.

The activity of the IAEA Atomic and Molecular Data Unit is supervised and biennially reviewed by the Subcommittee on Atomic and Molecular Data for Fusion of the International Fusion Research Council (IFRC A+M Subcommittee), an advisory body to the Agency's Director General.

The A+M Data Unit staff

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For problems or questions regarding this web contact the A+M Data Unit.

Candidates of the Code

- **Institution:** Curtin University
- **Contact:** I. Bray
- **Codes:** CCC and RCCC
- **Institution:** NIFS
- **Contact:** F. Koike http://dpsalvia.nifs.ac.jp/~katomasa/crmtest/
- **Codes:** CR model
- **Institution:** Universidad Autonoma de Madrid, Spain
- **Contact:** I. Rabadán
- **Codes:** MELDF*-TCAM, QUAN, SEIKON, CTMC
- **Institution:** France, U. Pierre Marie Curie
- **Contact:** A. Dubois, P. Fainstein, http://www-amdis.iaea.org/HEAVY/
- **Codes:** CDW, VPN
- **Institution:** University Bari, Italy
- **Contact:** M. Capitelli
- **Codes:**
- **Description:** The semi-classical impact parameter method is used to calculate vibrationally resolved cross section for excitation and dissociation for spin − allowed transitions.
- **Institution:** Kurchatov Institute, Moscow
- **Contact:** A. Kukushkin, V.S. Lisitsa
- **Codes:**
- **Description:** Calculation of n,l collisional radiative kinetics of Rydberg atomic states and line intensities can be carried out.) is available.
- **Institution:** Lebedev Physical Institute, Moscow
- **Contact:** L. Vainshtein
- **Codes:** ATOM, ATOM − AKM, GKU
- **Institution:** Forschungzentrum Juelich
- **Contact:** D. Reiter
- **Codes:** HYDKIN
- **Institution:** Los Alamos National Laboratory, USA
- **Contact:** J. Abdallah, Jr.
- **Codes:** LANL codes
- **Institution:** National Institute of Standards and Technology, USA
- **Contact:** Y. Ralchenko http://nlte.nist.gov/FLY/
- **Codes:** MCHF, GRASP2K, FLYCHK, NOMAD
- **Institution:** Princeton Plasma Physics Laboratory, USA
- **Contact:** D. Stotler, http://w3.pppl.gov/degas2
- **Codes:** DEGAS databases
- **Description:** The H and He collisional radiative data are available as tables online

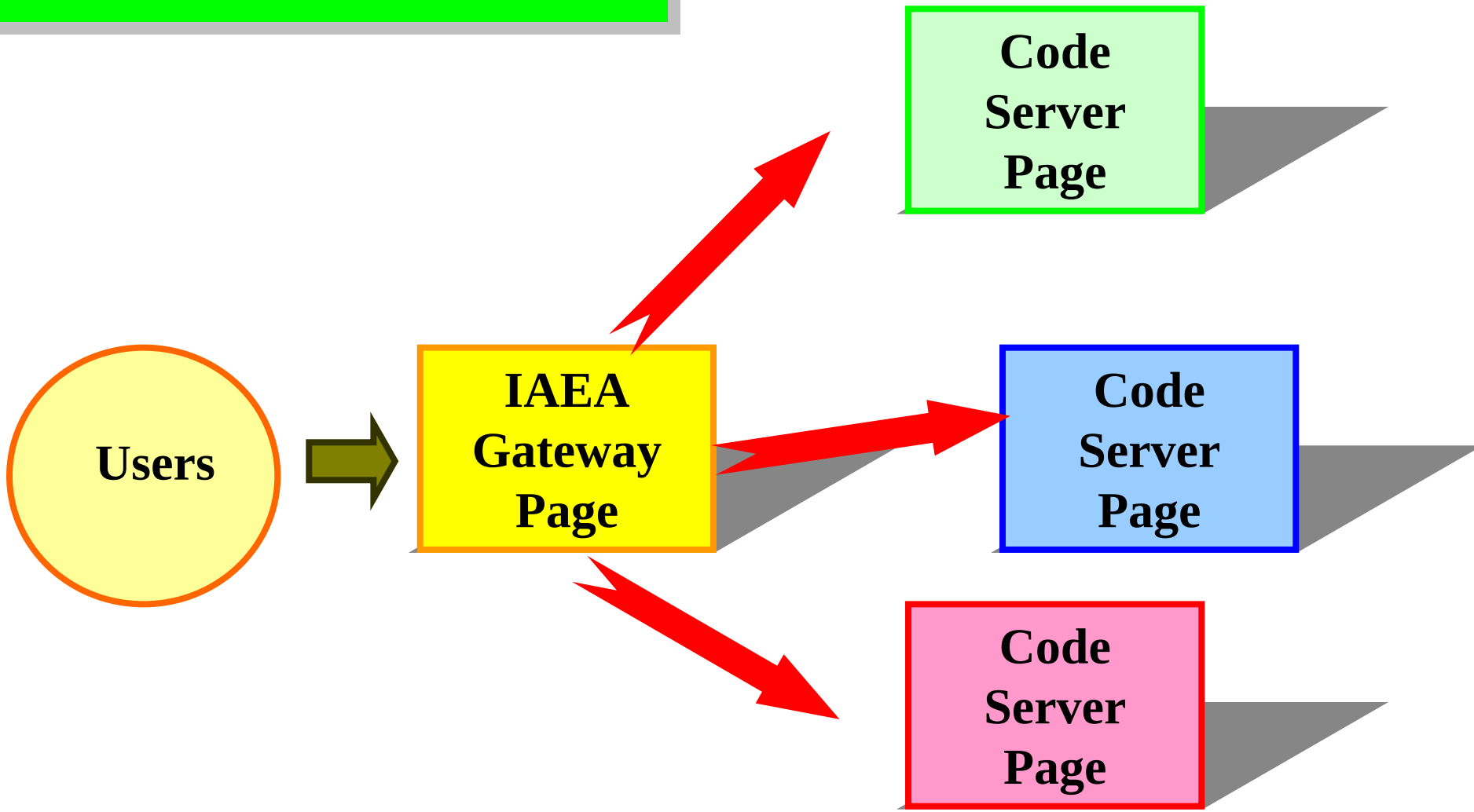
Formulation of a uniform format

- Further discussion focused on formulating a uniform format for each participant to use for an initial web page. It was agreed that the following information should be included:
- Name of code
- Responsible person – contact data
- Description of code (including approximations & accuracy) & applications.
- References & recent applications.
- Link(s)
- Reference to Code Center Network
- Logo / link to Code Center Network

Agreed Recommendations

- An IAEA web page should be created including the basic information from the summaries of the current code capabilities.
  - The A+M Unit will create individual web pages as per the above guidelines. The Unit will contact contributors annually requesting updates to information to these web page(s).
  - Participants will create more extensive pages at their home institutions as needed with links on the A+M Unit page.
  - After a one year trial period, contact should be initiated with other code and data providers (specifically the R-matrix community, the PMI community, Auburn University, P. Krstic at ORNL, the group at Belfast, Biemont, HULLAC, FAC, etc.)
- Code authors will make an attempt at assessing the accuracy of their calculations similar to the numerical database estimate (e.g., graded as “A”, “B”, “C”).
- Code authors and data users should begin utilizing the XSAMS XML format for transmission and exchange of data.
- This group should meet periodically, e.g., every two years, to monitor progress and identify future needs.
- The Network should try to make the broader fusion community aware of the capabilities represented by this group (e.g., via presentations at fusion oriented conferences).

Code Network



GRASP2K will become available on line at NIST

Larger Calculations have been made possible.

New code for angular part calculations

P. Jönsson, X. He, C. Froese Fischer, and I.P. Grant, Computer Physics Communications Volume 177, Issue, 1 October 2007, Pages 597-622

Conclusion of the Meeting

- The following conclusions were reached:
- This meeting was extremely productive and informative, both for the participants and the A+M Data Unit.
- The meeting will lead to substantial new collaborations between the participants.
- The basis for the code center network web page was established.
- It was agreed that the code center network will be an informal federation to permit flexible membership.