ADAMANT:
a platform for data users and producers

Romas Kisielius

Institute of Theoretical Physics and Astronomy
Vilnius University, Lithuania

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Outlook

1. **Introduction**
   - ADAMANT
   - Main purpose
   - Developers
2. **Atomic Data**
   - Data Types
   - Data Formats
3. **Important Features**
4. **How it is done**
   - Hardware platform
   - DB structure
5. **How it works**
6. **Summary**

ADAMANT

- Applicable
- DAta
- of Many-electron
- Atom
- eNergies
- and Transitions

Main purpose

- open-access DB
- open-source based development platform
- theoretical high-precision data
- data accuracy assessment
- applicable in plasma modeling
- data user request processing

Team 2015

Dr. R. Kisielius

Dr. Š. Mikolaitis

Dr. P. Bogdanovich

Dr. A. Kupliauskienė

Dr. R. Karpuškienė

G. Valiauga

ADAMANT team 2015

- Data producers:
  - Pavel Bogdanovich
  - Rasa Karpuškienė
  - Romas Kisielius
  - Alicija Kupliauskienė
- Database software development: Šarūnas Mikolaitis
- System manager: Gintaras Valiauga
- Support team: Dr. G. Merkelis, Dr. E. Stonkutė

Atomic Data

- continuously updated and extended
- automated pipeline for updates
- data formats
- *info* files
- accuracy assessment
- website for information and user guide
- user comments and requests

Data Types

A. Spectroscopic parameters

- level energies, level CI wavefunction compositions
- level lifetimes, Lande *g*-factors
- radiative transition wavelengths
- transition probabilities, oscillator strengths, line strengths

B. Electron-ion interaction parameters

- electron-impact excitation X-sections, CS, CR
- electron-impact ionization X-sections, strengths, rates
- level autoionization probabilities
- dielectronic recombination rates (level resolved)

Data Formats

- HTML (formatted)
- ASCII (machine readable)
- ASCII (";" separated values)
- XML VOtable standard
- producer (author) information
- calculation method description (*info* files)
- assessed accuracy (*if available*)
- separate files for each data type
- data files are inter-connected

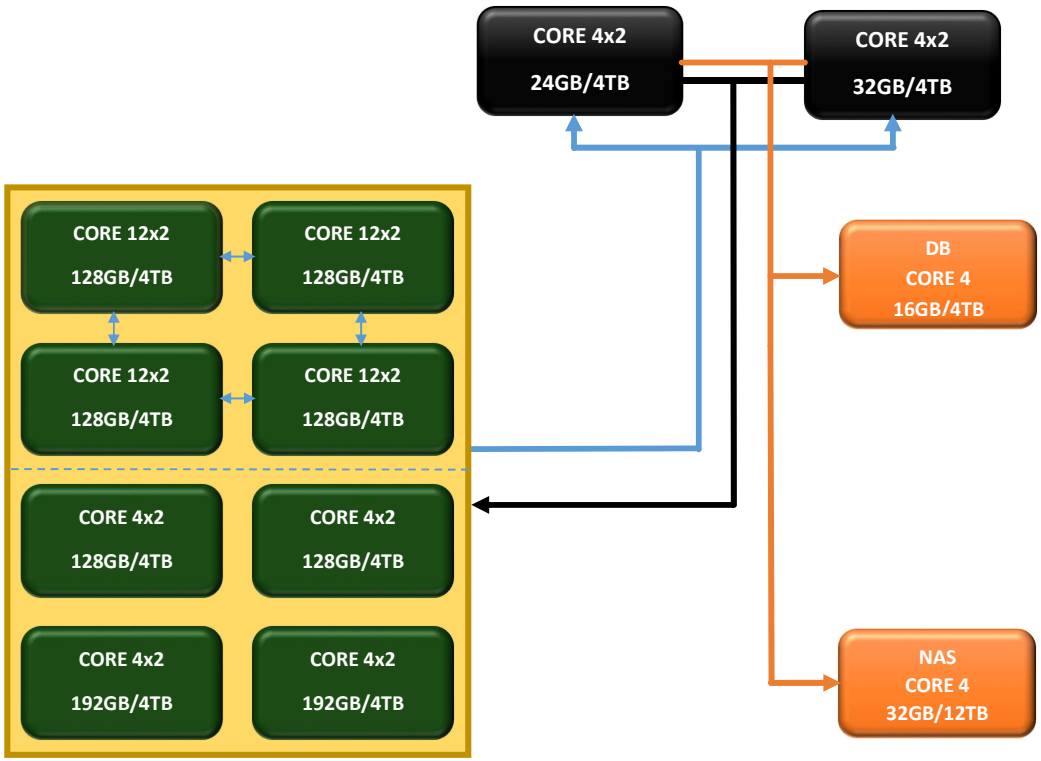
Producer <-> User Interaction

- GUI for data selection
- answers to FAQ
- comments on data accuracy
- requests for new data production
- DB User Guide

Important Features

- same computer code suites
- same approximation for CI and relativistic effects
- identical multireference wavefunction basis
- reduced workload for data application
- simple data parsing for modeling codes

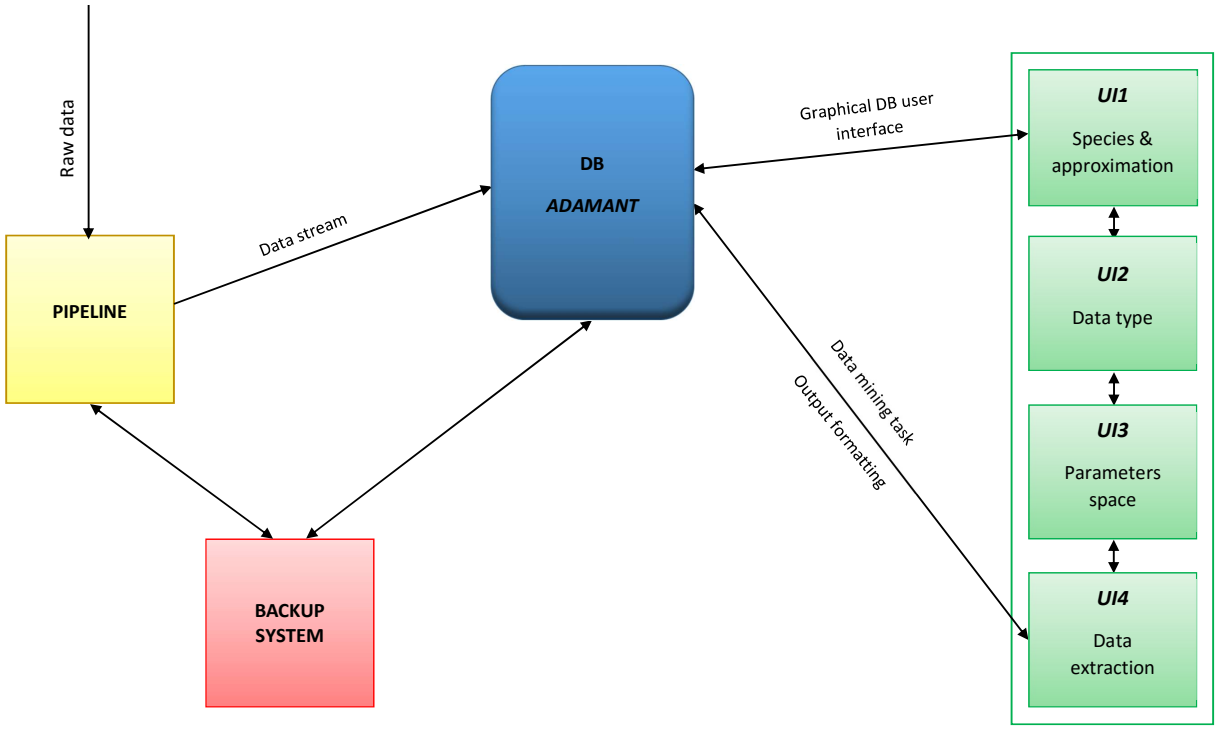
Hardware


CORE 4x2
24GB/4TB
CORE 4x2
32GB/4TB
CORE 12x2
128GB/4TB
CORE 12x2
128GB/4TB
CORE 12x2
128GB/4TB
CORE 12x2
128GB/4TB
DB
CORE 4
16GB/4TB
CORE 4x2
128GB/4TB
CORE 4x2
128GB/4TB
CORE 4x2
192GB/4TB
CORE 4x2
192GB/4TB
NAS
CORE 4
32GB/12TB

Some specifics

- serial vs distributed calculations: QRHF+TRO, HF+TRO
- job size:
  CI: H size $\leq$ 120 000; wavefunction odd/even CSF number $\leq$ 2 000 000
- calculation wall-clock times:
  Cl^{5+} ($3s^2$) 110/19 hrs; Ti^{5+} ($3p^5$) 149/37 hrs;
  W^{34+} ($4d^4$) 56/21 days; W ($5d^4 6s^2$) 70/34 days
- serial calculations: Flexible Atomic Code (FAC) for:
  $Z \leq 30$ inner-shell transitions
  alkaline (Li, Na, K, Rb, Cs) ions

DB data stream



MySQL infrastructure

Data amount: 14 GB of data for $>$ 1100 species
automated data updates/modifications

A. Data types (10)

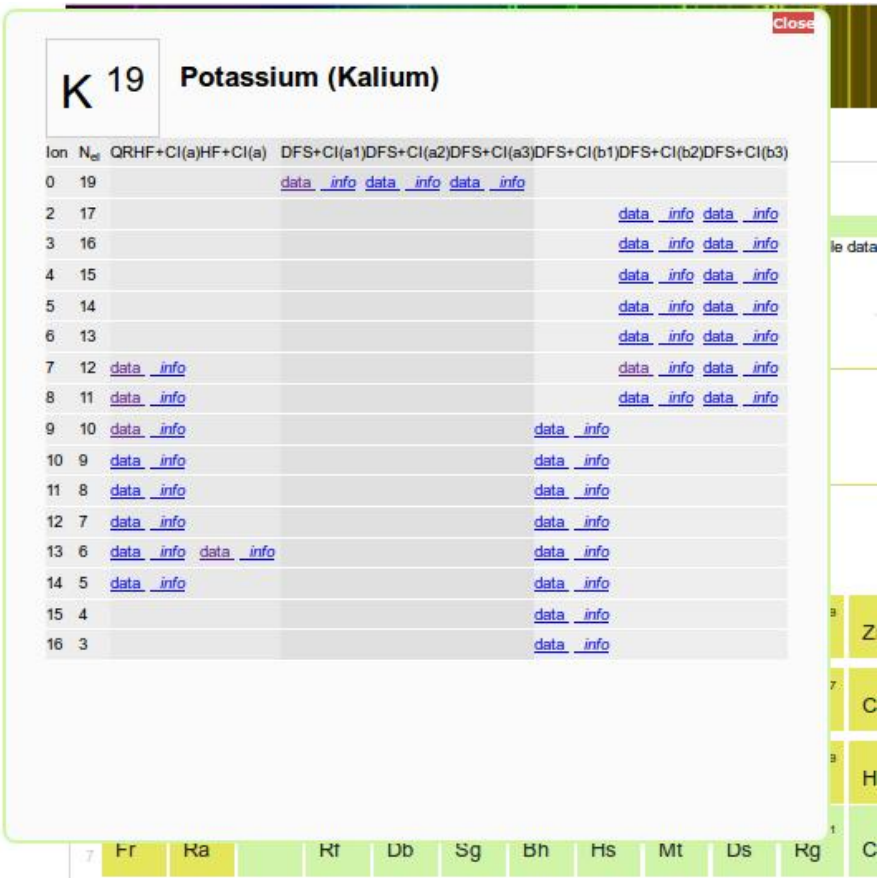
- Energy levels
- Radiative transitions (E1, E2, E3, M1, M2, M3)
- Autoionization
- Dielectronic recombination
- EIE collision strengths; EIE cross-sections; EIE rates
- EII collision strengths; EII cross-sections; EII rates

DB software

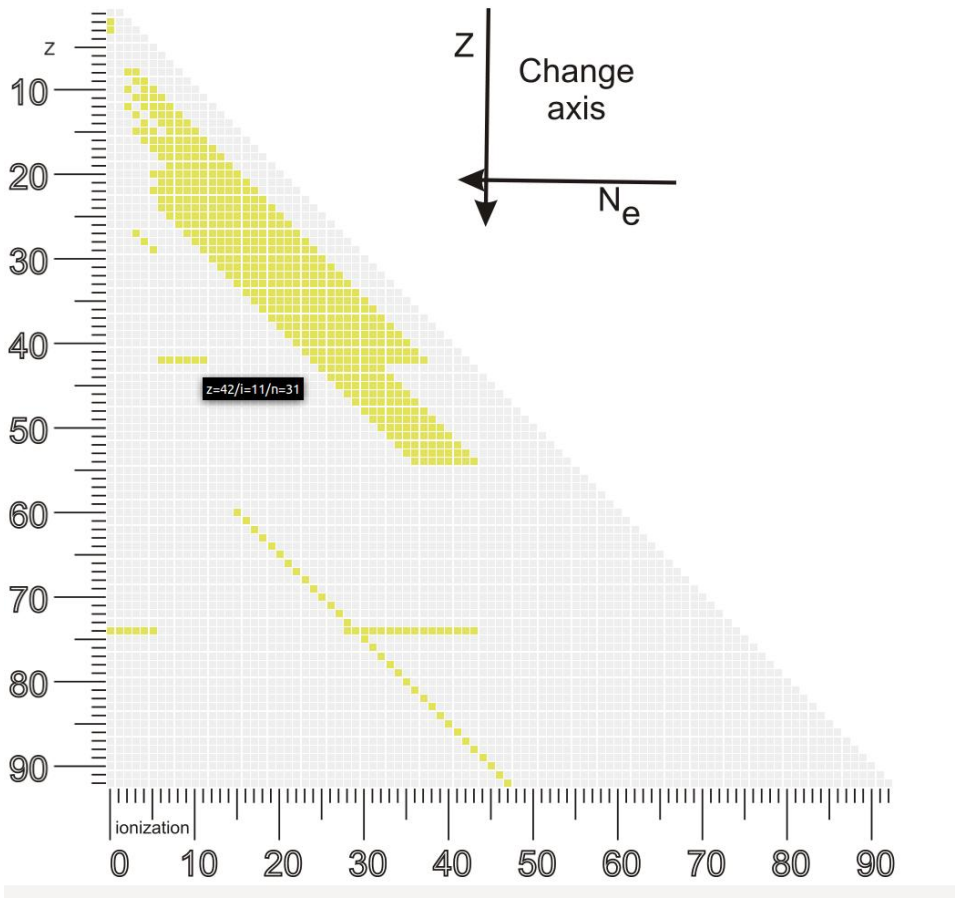
- Linux (openSUSE 13.2) OS
- Apache 2.4.3 HTTP server
- PHP 5.4.10 dynamic programing language
- MySQL 5.6 relational DB management
- javascript
- php5 script
- html/xml script

Ion selection *(UI1)*

Method selection *(UI1)*



Alternative ion+method selection *(UI1)*



Data type selection *(UI2)*

Potassium (Kalium) K VIII									
Data type									
Energy levels	Radiative transitions	Autoionization	Dielectronic recombination	Electron-impact excitation collision strengths	Electron-impact excitation cross-sections	Electron-impact excitation rates	Electron-impact ionization collision strengths	Electron-impact ionization cross sections	Electron-impact ionization rates

Data type selection *(UI3)*

Radiative transitions
Specify parameters

Z:	19
Ion:	7
Approach used:	Quasirelativistic Hartree-Fock + CI (a) Hartree-Fock + CI (a) Dirac-Fock-Slater + CI (a1) Dirac-Fock-Slater + CI (a2) Dirac-Fock-Slater + CI (a3) Dirac-Fock-Slater + CI (a4) Dirac-Fock-Slater + CI (b1) Dirac-Fock-Slater + CI (b2) Dirac-Fock-Slater + CI (b3)
Output type:	HTML table ASCII table ASCII table ; separated values XML VOtable standard
Units:	Å nm μm
Wavelength from:	0.0
Wavelength to:	1.0E+99
gf from:	0.0
gf to:	1.0E+99
Transition probability from:	0.0
Transition probability to:	1.0E+99

Enter

Back

Data output *(UI4)*

Radiative transitions
Potassium (Kalium) (K VIII) > Quasirelativistic Hartree-Fock + CI (a) approach
Go back

info on the table
full info
Click here for level energies and level indexes

Ni	Ji	Nf	Jf	Type	Wavelength (nm)	A(1/s)	gf	S	Z	Ne	Ion
3	1.0	1	0.0	E1	77.314	1.400e+6	3.770e-4	9.590e-4	19	12	7
4	2.0	1	0.0	M2	76.040	3.360e-1	1.460e-10	2.860e+1	19	12	7
4	2.0	3	1.0	M1	4614.670	1.370e-1	2.190e-7	2.500e+0	19	12	7
5	1.0	1	0.0	E1	51.763	9.210e+9	1.110e+0	1.890e+0	19	12	7
6	2.0	3	1.0	E1	58.451	6.690e+7	1.710e-2	3.300e-2	19	12	7
6	2.0	4	2.0	E1	59.201	1.450e+8	3.810e-2	7.420e-2	19	12	7
6	2.0	5	1.0	E1	93.252	5.630e+8	3.670e-1	1.130e+0	19	12	7
7	0.0	3	1.0	E1	56.928	7.680e+9	3.730e-1	7.000e-1	19	12	7
8	1.0	2	0.0	E1	56.206	2.670e+9	3.790e-1	7.010e-1	19	12	7
8	1.0	3	1.0	E1	56.530	1.960e+9	2.820e-1	5.260e-1	19	12	7
8	1.0	4	2.0	E1	57.231	3.150e+9	4.640e-1	8.740e-1	19	12	7
9	2.0	3	1.0	E1	55.787	1.970e+9	4.600e-1	8.450e-1	19	12	7
9	2.0	4	2.0	E1	56.470	5.740e+9	1.370e+0	2.550e+0	19	12	7
10	0.0	5	1.0	E1	60.469	7.710e+9	4.230e-1	8.420e-1	19	12	7
11	1.0	2	0.0	E1	41.634	6.500e+9	5.070e-1	6.950e-1	19	12	7
11	1.0	3	1.0	E1	41.811	4.810e+9	3.780e-1	5.210e-1	19	12	7

Data output *(UI4)*

```
##############################<12.19.qr.tran.txt>##############################
#
#    K  VIII      Potass.
#
#    Z =  19,  Ne = 12,  Ion =   7
#
#    Radiative transition data
#
#    Approach used: QR+CI
#
#    Number of selected transitions            692
#
#    File contains selected transitions
#    with emission probabilities A > Amax * 1.0E-02
#
#===============================================================================
#    Byte-by-byte Description of Data
#-------------------------------------------------------------------------------
#   Bytes  Format Units   Label          Explanation
#-------------------------------------------------------------------------------
#    1 -  6 I6     ---     Ni             Initial (upper) level index
#    7 - 11 F5.1   ---     Ji             Initial level total angular momentum J
#   12 - 17 I6     ---     Nf             Final (lower) level index
#   18 - 22 F5.1   ---     Jf             Final level total angular momentum J
#   26 - 27 A2     ---     Type           Transition type
#   30 - 42 F13.3  nm      Wavelength     Transition wavelength
#   43 - 52 E10.3  1/s     A              Emission transition probability
#   53 - 62 E10.3  ---     gf             Weighted oscillator strength
#   63 - 72 E10.3  ---     S              Line strength
#===============================================================================
#
#    Electron transitions were calculated
#    for such types of transitions:
#    EVEN -> EVEN  M1  E2
#    ODD  -> EVEN  E1  M2  E3
#    ODD  -> ODD   M1  E2
#
#    Author: P. Bogdanovich
#
#    2015-06-02
#
#    See <12.19.qr.elev.txt> for level energies and indexes.
#    See <12.19.qr.info.txt> for full explanation of the calculations.
#
#-------------------------------------------------------------------------------
#   Ni  Ji     Nf  Jf  Type     Wavelength    A         gf        S
#-------------------------------------------------------------------------------
##############################<12.19.qr.tran.txt>##############################
```

Further info

DB location
http:/www.adamant.tfai.vu.lt

- Database
- Forum
- User guide
- Links, contacts, etc.

- comments are welcome - use forum
- data requests (modest) are cautiously welcome
- experimental data inclusion (?)