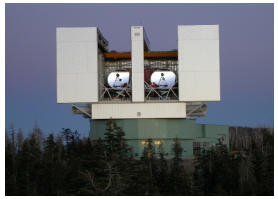
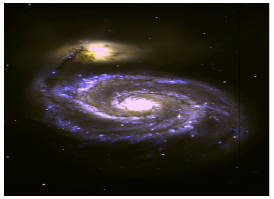
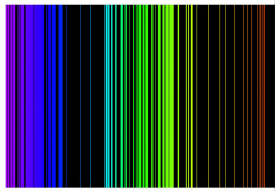

Research based online course:

"Atomic and Molecular Astrophysics and Spectroscopy with Computational workshops on R-matrix and SUPERSTRUCTURE Codes I"

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A.P.J. Abdul Kalam STEM-ER Center
(Indo-US collaboration)

- Organized under the Indo-US STEM Education and Research Center of OSU-AMU, AMU, Aligarh, India, & OSU, Columbus, USA

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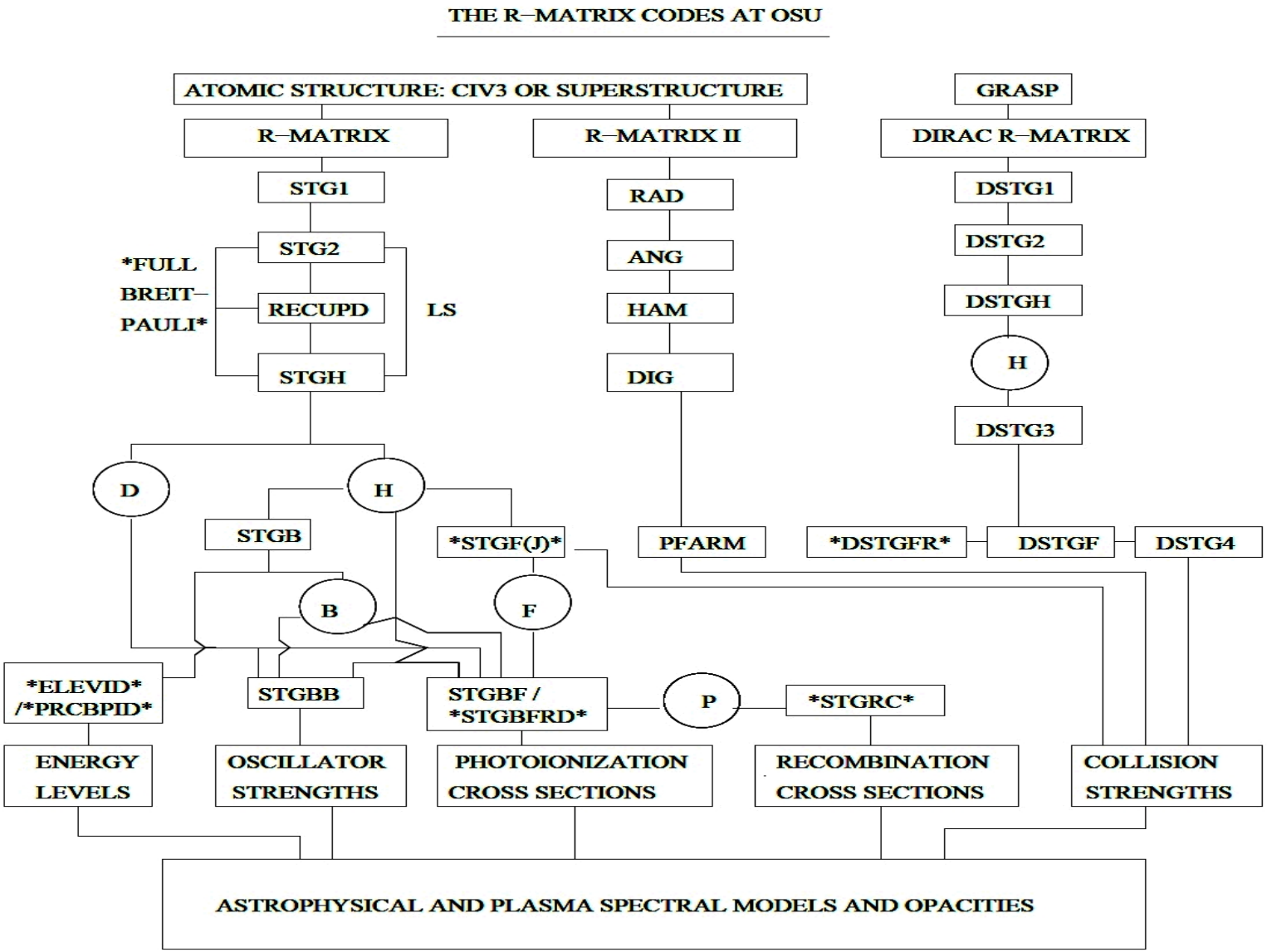
Support: OSU-AMU STEM ER Center, AMU, OSU, OSC

THE R-MATRIX CODES: UNDER THE OP AND IP

- Carry out large-scale calculations for parameters for various atomic processes at the Ohio Supercomputer Center (OSC)
  - Asterisks indicate OSU development
- Results: 1) Energy Levels, 2) Oscillator Strengths, 3) Photoionization Cross sections, 4) Recombination Rate Coefficients, 5) Collision Strengths; - Astrophysical Models



RUNNING R-MATRIX CODES: COLLISION STRENGTHS

• The R-matrix method is the most powerful method to study atomic processes, such as, electron impact excitation (EIE), radiative transitions, photoionization, electron-ion recombination. R-matrix calculations are carried out using the R-matrix package of codes in a number of stages. The programs are written in FORTRAN.

• Stages STG1, STG2, STGLIB, RECUPD, RECMOD, STGH, together called R-matrix computation codes, calculate the Hamiltonian matrix, and diple matrix elemets if radiative transitions are to be computed.

• "STGLIB", library of routines, is needed from STG2 to STGH.

• The stages STGB, STGF, STGBB, PREBF, STGBF together are called the asymptotic codes, that compute various quantities of atomic processes. Asymptotic codes are typically used repeatedly to compute full set of data for various energy ranges and angular symmetries.

• R-matrix calculations begin with the wavefunction expansion of the core ion created by program SUPERSTRUCTURE. It is the file "fort.7" which needs to be renamed to "zsspnl" for BPRM codes. It is an input file for STG1.

• Starting with STG1, other stages run one after the other where output of one stage is used as the input for the next stage. However, each stage needs one parameter file which gives specifics of the computation.

• All necessary files for R-matrix computations are in my OSC directory "/users/PAS0578/osu683/share_PAS1866/rmtutorial" & also at

- http://www.astronomy.ohio-state.edu/nahar.1/teaching.html#program

You will download all files from the website or copy from the OSC directory to your OSC account or laptop

NOTE: i) The actual names of the codes are slightly different but similar to the stages mentioned. E.g. STG1 program is named as "rstg1.f".

• ii) Theory and general description of the codes are given in "bprm-cpc95.pdf"

Login to OSC and get the programs to your account:

• To begin with R-matrix codes, log in to OSC using OSC portal:

Type: ondemand.osc.edu, click on "OSC OnDemand - Ohio Supercomputer Center" which will take you to the login page

• Type in your user name and password in the boxes and click on "log in OSC account" which will

take you to "Ohio Supercomputer Center" page.

• At the top blue bar, click on "Clusters" to see options, click on "Owens Shell Access". This will open up a terminal window and you will be in your home directory.

• Type: mkdir rmtutorial (to create rmtutorial directory only once for the course)

• cd rmtutorial (to go to directory "rmtutorial")

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COLLISION STRENGTHS FOR ELECTRON IMPACT EXCITATION

• We will calculate collision strengths for EIE of O III using R-matrix codes. For EIE, we will use 5-stages of computation - "STG1", "STG2", "RECUPD+RECMOD", "STGH", "STGF". The corresponding programs are named as "rstg1.f", "rstg2.f", "recupd.f" and "recmod.f", "rstgh.f", "stgf.f".

• Type: cp /users/PAS0578/osu683/share_PAS1866/rmtutorial/eie* . (to copy all r-matrix codes and relevant files from my directory to yours)

Compilation of codes:

• Script file "runrm12rh" contains commands, given in sequential order, to compile files rstg1.f, rstg2.f, stglib.f, recupd.f, recmod.f, rstgh.f and make executable for the 4 stages STG1, STG2, RECUPD, and STGH.

• To compile a stage, such as STG1, you will uncomment (which means that erase the # sign) at the beginning of the "ifort" line and type "./runrm12rh" and hit return for compilation of the stage.

You can compile without file "runrm12rh" by typing the command (given inside "runrm12rh") on-line. For example, to compile and make executable of STG2, type

ifort -r8 -i8 -o rstg2x rstg2.f stglib.f

Use vi editor to activate a command for compilation of one STG file and deactive the other commands which are not needed.

• Type: "vi runrm12rh", to edit the file for compilation

- Take cursor to "#" of a command line for compilation of a stage, such for STG1, press "x" key to delete "#". Move the cursor to the beginning of the command line which needs deactivation and press "i" key to be in "insert' mode and type "#" to deactivate the command. Press $<$ esc $>$ key to get out of insert mode.

Press: $<$ control $>$ and key "s" together $\rightarrow$ to save the modifed file

RUNNING R-MATRIX CODES: COLLISION STRENGTHS

Type: :q → to exit vi mode
Type: ./runrm12rh → to run for compilation
• Repeat it for all stages in "runrm12rh". Compiled and executable files of STG1, STG2, RECUPD, STGH are named as "rstg1x", "rstg2x", "recupdx", "rstghx" (already exist in directory "rmtutorial").
• After running all 4 stages, we will have created H.DAT file which is the Hamiltonian matrix file. We will need "H.DAT" file to compute collision strengths.
• STGF is compiled by a separate script file named "runf". "runf" contains one command line to create the executable for STGF, and one to execute for running STGF. You can edit the file making the compilation line active. Type
./runf → to compile and make executable "stgfx".

Running the codes:

• As explained above each stage creates files that become input files for the next stage. Ex: "STG1" creates "RK" file which is an input file for "STG2" and is read automatically.
• But each stage also reads a parameter file, named as "stgn.inp" where "n" in "stgn" indicates the progrm number being used. We need to create ".inp" files for all stages. For O III all ".inp" files are in rmtutorial
• The first stage "STG1" of R-matrix codes calculates radial integrals.
- Stage 1: Program= "rstg1.f", Compiled executable= "rstg1x", Input files= i) "stg1.inp", ii) "zsspnl".
"zsspnl" is the ouput file "fort.7" created by SUPERSTRUCTURE
"stg1.inp" has the following contents:
Line 1: "S.S." for SS or "CIV3" for CIV target wavefunctions
- STG1 → input for STG1 run
- MAXLS = largest L-value of target or core states
- MAXPW = Maximun l-value of the out electron
- MAXE = Highest energy of the interacting or outer electron
- MAXC = largest number of terms in R-matrix basis (typically 12)
- INDATA=14 for Breit-Pauli approximation, IOUT=1, program parameter- IBC = boundary condition, =0 for default R-matrix boundary, = 1 for when a boundary is specified

RUNNING R-MATRIX CODES: COLLISION STRENGTHS

LAM=3, KRELOP=7, IZESP=-2 LRANG3=4 for relativistic approximation
Line 3: RA value if IBC=1, otherwise it is a blank line
• cp stg1.inp.eie.o3 stg1.inp (to copy parameter file stg1.inp.eie.o3 to stg1.inp)
• cp zsspnl.o3 zsspnl
• To run, type: ./rstg1x &
• Open output file: vi stg1.out, then type: < shift > g to go to the last line. If it says "END OF STG1" means job ran fine.
• Type :q to get out of the file
• STG2 computes all angular momentum algebra for the Hamiltonian.
- Stage 2: Programs= "rstg2.f" and "stglib.f", Compiled executable= "rstg2x", Input files= "stg2.inp" and output files of STG1. To run
cp stg2.inp.eie.o3 stg2.inp
• Contents of stg2.inp
- Lines 1 - 3 : parameters, do not change
- Line 4: 0 999 1 1 1 1 → Only last four numbers to be changed. 1st "1"=iopt (=1 for collisional excitation, =2 for radiative processes). 2-4th "1"s are relativistic corrections.
- Line 5: 8 06 +11 +0 0 62 +0 0 1 0 +5 → = NORB=8 (number of orbitals considered in the core configuration list), NELC=06 (no of electrons in the core ion), NTG=+11 (number of core states), 0 0 (parameters), NLS=62 (number of LS states of N+1 electron ion, that is core+interacting electron), ignore rest of the values
- Line 6-7: NORB number of orbitals are specified in numerical form, such as 1 0 2 0 2 1 ... for 1s,2s,2p etc - Line 8: 23=NCFG = number of configurations for the core
- Lines 9: Minimum occupancy number in the 8 orbitals included in the set of configurations
- Lines 10: Maximum occupancy number in the 8 orbitals included in the set of configurations
- Lines 11-33: Configuration list with occupancy numbers. Please note that there is an extra column at the end. Keep it as "0". - Lines 34 - 44: NTG=11 Core states, each state is specified as L 2S+1 π
- Line 45: 73=NCFGF = number of (N+1) electrons configurations
- Lines 46: Minimum occupancy number in the 8 orbitals included in the set of (N+1) electrons configurations
- Lines 47: Maximum occupancy number in the 8 orbitals included in the set of (N+1) electrons

configurations. Note try putting one number larger than those for N core electrons
- Lines 48-120: List of (N+1) electrons configurations. Note that the additional column of 0 should stay
- Line 121-182: NLS number of (N+1) states
• ./rstg2x & → to run STG2.
Open output file stg2.out to check the last line is "END OF STG2". It means job ran fine.
• RECUPD+RECMOD carry out algebraic transformation from LS to fine structure.
- Stage RECUPD: Programs= "recupd.f", "recmod.f", and "stglib.f", Compiled executable= "recupdx", Input files= "recupd.inp" and output of STG2. To run RECUPD:
Type: cp recupd.inp.eie.o3 recupd.inp → copy file
• Contents of recupd.inp
- Line 1 - comment line
- Lines 2 - 3 : parameters, do not change
- Line 4 : JNAST (=Number of levels of the residual levels in the wavefunction expansion), ICHECK (checking option, keep it =-2),IPHOT (radiative parameter not in sue, but leave it =0)
- Line 5 : 2J values of the target levels, total number = JNAST
- Line 6 : parity (0 for even, 1 for odd) of the levels
- Line 7 : IJNAST = number of interested levels of (N+1) electrons system
- Lines 8 - IJNAST+8 : 2J, parity of each level of interest of (N+1) electrons system
./recupdx & → to run RECUPD (may need to submit in batch job due to large computational time
NOTE: In case of end of specified time finishing before end of the job, all information will be lost. So give enough time.
Open output file recupd.out to check the last line is "END OF RECUP". It means job ran fine
• STGH computes the Hamiltonian matrix and dipole matrix elements.
- Stage H: Programs = "rstgh.f" and "stglib.f", Compiled executable = "rstghx", Input files = "stgh.inp" and output files of recupdd+recmod. To run
cp stgh.inp.eie.o3 stgh.inp
• Contents of stgh.inp:
- Line 1 : comment lines
- Lines 2 - 3: parameters (do not change)

RUNNING R-MATRIX CODES: COLLISION STRENGTHS

Lines 4 : i1, i2, iphot (keep i1=i2=0, iphot=1 for collision, =2 for radiative processes)
- Line 5: NBUT,NOT1,NOT2,IDIAG,NAST=23,INAST (NBUT=buttle correction, not1, not2=largest possible number for target states, IDIAG=1, NAST=larget number of the target states in the calculations, INAST=0
- Lines 6 - on: Number of lines listing all target energies in Ryd unit. relative to the ground state.
./rstghx & → to run STGH
Open output file stgh.out to check the last line is "END OF STGH". It means job ran fine.
• "STGH" creates "H.DAT" file which contains the Hamiltonian matrix. After creation of "H.DAT", we do not repeat any previous stages

Run for Electron Impact Excitation collision strength

• STGF computes collision strength for electron impact excitation (EIE), continuuam wave functions.
- Stage F: Program= "stgf.f", Compiled executable= "stgfx", Input files= "stgf.inp", H.DAT. To run
Type: cp stgf.inp.eie.o3 stgf.inp → to copy file
contents of stgf.inp
- -2,0,0,0,0 = IPRINT,IRAD,IPERT,KK,IDR (keep them as they are)
- AC (internal parameter, set it to 0.001 or 0.0001)
- 1 (=rone, do not change) - 1 (leave it unchanged) - npts, E0, DE, 0 (npts=number of energy points, E0=start of electron energy in z-scale = E(Ry)/$(z+1)^2$, DE=energy mesh in z-scale, 0 -leave it unchanged)
- 1 (1=to create F-files for all Jπ specified in recupd.inp, =2 for states specified below this line)
- 0,0,0 (terminator line for the list of Jπ values)
• Type: ./stgfx & → to run STGF
• Open output file "stgf.out" to check that the last printed line is "COLLISION STRENGTHS WRITTEN TO FILE OMEGA". It means that collision strengths have been computed and printed in file OMEGA.
• STGF writes EIE collision strenth in file "OMEGA". We repeat STGF many times depending on the need of higher resolution, covering larger energy range, etc.
• type: vi OMEGA (to see collision strenths)
• Contents of "OMEGA"
- line 1: NZ (=nuclear charge), NELEC (=number of electrons) in O III

RUNNING R-MATRIX CODES: COLLISION STRENGTHS

Line 2: NT (=number of target states), NE (=number of energy points of the colliding electron)

- lines: Target ground and excitation energies (total = NT), 5 energies per line

- Rest of the lines are for set of collision strengths (omega(i,j)) for all possible excitations for each projectile energy (E). Left number is E and right set of numbers is for collision strengths for excitations from the all excited states to the ground state, then to 1st excited state and so on

- **Collision strengtth is non-zero when the electron energy is high enough to excite the state.**