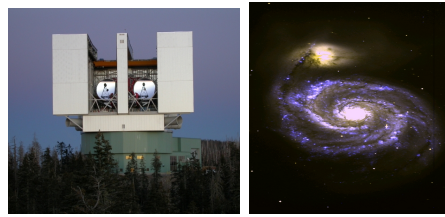




THE OHIO STATE UNIVERSITY



## ”Computational Workshop: Running R-matrix Codes for Atomic Processes

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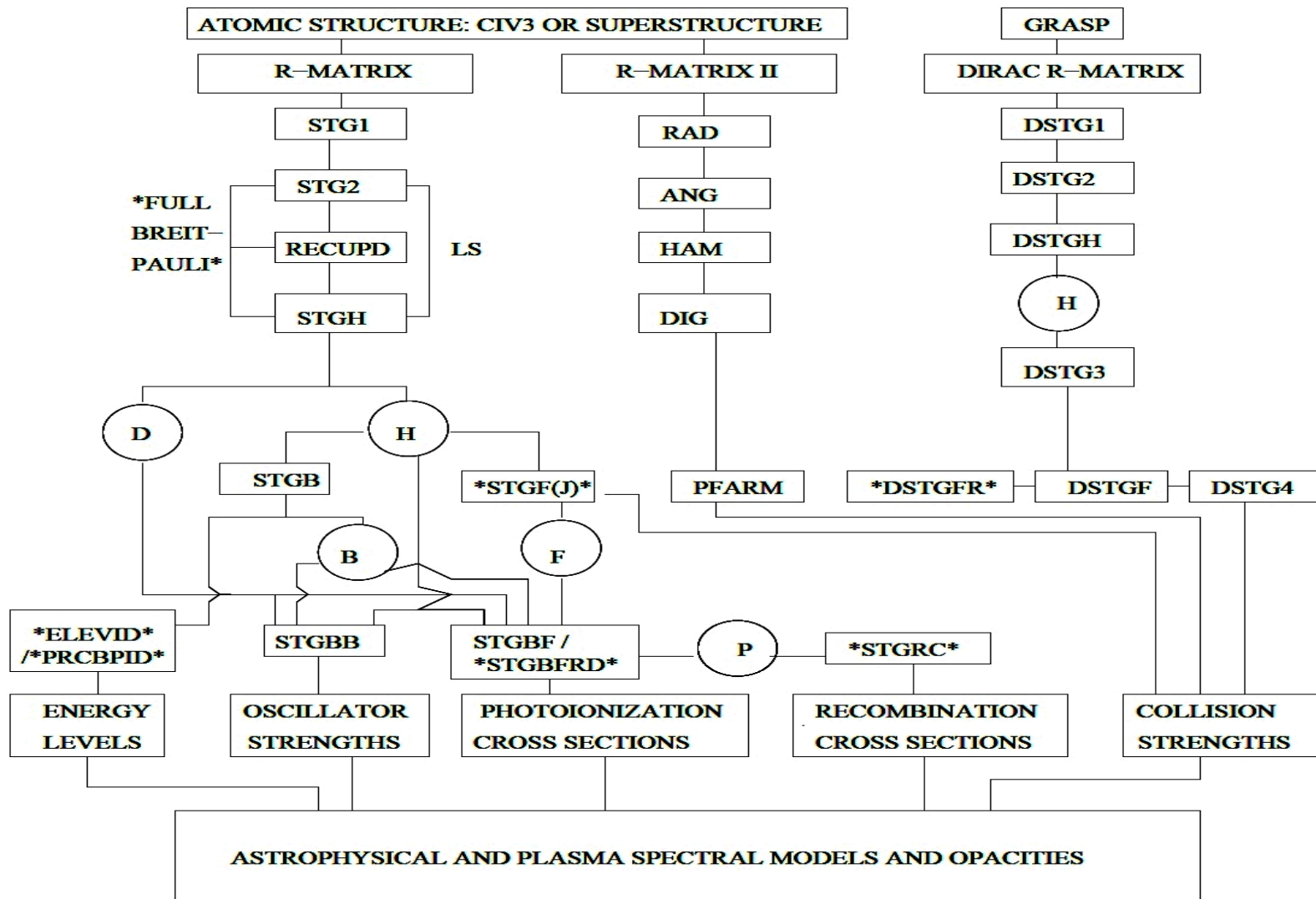
- Textbook: ”Atomic Astrophysics and Spectroscopy” - By A.K. Pradhan and S.N. Nahar (Cambridge University Press, 2011)
- Computation: Ohio Supercomputer Center (OSC)

Notes from workshops given at universities

# THE R-MATRIX CODES

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

## THE R-MATRIX CODES AT OSU



# RUNNING R-MATRIX CODES

- We will calculate collision strengths for O III using R-matrix codes. This is a package of codes. We will use 5-stages of computation - "STG1", "STG2", "RECUPD+RECMOD", "STGH", "STGF". The programs for all stages are named as "rstg1.f", "rstg2.f", "recupd.f" and "recmod.f", "stgh.f", "stgf.f". Starting with STG1, stages run one after the other where output of one is the input for the next.
- "STGLIB", library of routines, is needed from STG2 to STGH. All necessary files for R-matrix computations are in OSC directory "rmtutorial" & also at
  - <http://www.astronomy.ohio-state.edu/~nahar/teaching.html#program>
- Theory and general description of the codes are given in "bprm-cpc95.pdf"
- To run the codes, login to OSC: login: osu0333@oakley.osc.edu, pw:
- cd rmtutorial (to go to directory "rmtutorial")
- mkdir groupn (create your own directory groupn)
- cp \* groupn → to copy all files to your directory
- "cd groupn" to go to your directory

## Compilation of the codes:

- File "psbprm" contains commands to compile and make executable of stages STG1, STG2, RECUPD, and STGH which create the Hamiltonian matrix file "H.DAT". We need "H.DAT" for the atomic processes.
- Use an editor, such as "vi psbprm", to edit the file:
  - Take cursor to command line for compilation of a stage, such for STG1, type "x" key to delete "#" of the command line. Use "i" key for "insert" mode of vi and then type "#" and press < esc > to comment out an unnecessary command line
  - < control > s → to save the modified file
  - :q → to exit vi mode
- type "./psbprm" and hit return to run for compilation

# RUNNING R-MATRIX CODES

## Compilation of the codes:

Otherwise for compilation simply type the command (given inside "psbprm") on-line. For example, to compile and make executable of STG2, type  
ifort -r8 -i8 -o rstg2x rstg2.f stglib.f

- Compile and make executables of STG1, STG2, RECUPD, STGH and name them as "rstg1x", "rstg2x", "recupdx", "rstghx" (already exist in directory "rmtutorial").
- For STGF, the compilation command is in file "psbpas". Type  
./psbpas stgf → 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". 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.

- For Stage 1: Program= "rstg1.f", Compiled executable= "rstg1x", Input files= i) "stg1.inp", ii) "zsspnl".

"zsspnl" is the output file "fort.7" created by SUPERSTRUCTURE

"stg1.inp" has the following contents:

Line 1: "S.S." for SS or "CIV3" for CIV target wavefunctions

Lines 2-3: - STG1 → input for STG1 run

- MAXLS = largest L-value of target or core states

- MAXPW = Maximum 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

# RUNNING R-MATRIX CODES

- IBC = boundary condition, =0 for default R-matrix boundary, = 1 for when a boundary is specified
- LAM=3, KRELOP=7, IZESP=-2 LRANG3=4 for relativistic approximation
- Line 4: RA value if IBC=1, otherwise it is a blank line
- To copy parameter file stg1.inp.eie.o3 to stg1.inp: cp stg1.inp.eie.o3 stg1.inp
- To copy zsspnl.o3 to zsspnl: cp zsspnl.o3 zsspnl
- To run STG1, type: ./rstg1x &
- Use commant "ps" to check the status of the run
- When job is done, open output file: vi stg1.out,
- then type: < shift > g to go to the last line. If it says "END OF STG1" it means job ran fine.
- Type :q to get out of the file
- STG2 computes all angular momentum algebra for the Hamiltonian.
- For 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 these
- 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). 2nd, 3rd, and 4th "1"s indicate inludsiion of relativistic 1-body corrections.
- Line 5: 8 06 +11 +0 0 62 +0 0 1 0 +5 → means 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 core+interacting electron), ignore the rest values

# RUNNING R-MATRIX CODES

- 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: List of core states (total number = NTG=11 as specified above). Each state is specified as L 2S+1  $\pi$  where L and S are orbital and spin angular momenta,  $\pi$  is parity (specify 0 for even, 1 for odd)
- 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. We typically put 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 at the end should stay
- Line 121-182: NLS number of (N+1) states, again in L 2S+1  $\pi$  order
  - ./rstg2x & → to run STG2.
  - Open output file "stg2.out" to check whether the last line is "END OF STG2". It means job ran fine.
  - Programs RECUPD and RECMOD together carry out algebraic transformation from LS coupling to fine structure.

# RUNNING R-MATRIX CODES

- For Stage RECUPD: Programs= "recupd.f", "recmod.f", and "stglib.f", Compiled executable= "recupdx", Input files= "recupd.inp" and output of STG2.

To run RECUPD: cp recupd.inp.eie.o3 recupd.inp

- ./recupdx & → to run RECUPD
  - 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.
- For Stage H: Program= "rstgh.f" and "stglib.f", Compiled executable= "rstghx", Input file= "stgh.inp".

• To run STGH: cp stgh.inp.eie.o3 stgh.inp

- ./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
- Next stage is STGF which computes collision strength for electron impact excitation (EIE), continuam wave functions.

- For Stage F: Program= "stgf.f", Compiled executable= "stgfx", Input files= "stgf.inp", H.DAT.

• To run: cp stgf.inp.eie.o3 stgf.inp

- ./stgfx & → to run STGF
- Open output file stgf.out to check the last line is "COLLISION STRENGTHS WRITTEN TO FILE OMEGA". It means collision strengths have been computed in file OMEGA.
- STGF writes EIE collision strength in file "OMEGA". We repeat STGF many times depending on the need of higher resolution, covering larger energy range, etc.

## RUNNING R-MATRIX CODES

- type: vi OMEGA (to see collision strengths)
- 1st line: NZ (=nuclear charge), NELEC (=number of electrons) in O III
- NT (=number of target states), NE (=number of energies of the colliding electron)
- Target energies (total = NT), first one is ground state energy and rest are excited state energies
- 1st energy, then list of collision strengths for excitations from the all excited states to the ground state, then to 1st excited state and so on
- Collision strength is non-zero when the electron energy is high enough to excite the state.