Theoretical electron-impact ionization cross sections of P-like ions, W^{17+}, and W^{+}

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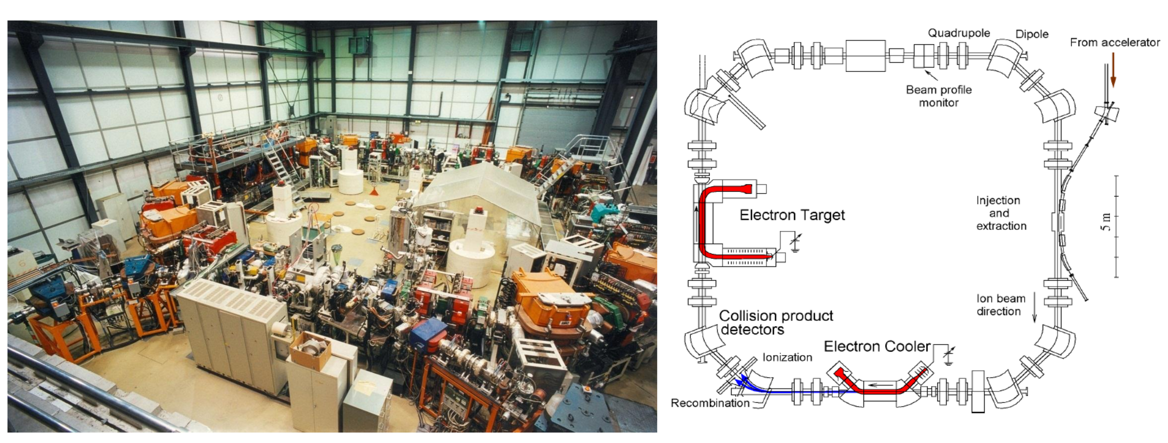
Introduction

- A reliable analysis and modeling of plasma spectra relies on accurate charge state distribution (CSD) calculations. The CSD for collisionally ionized plasma is determined by the balance between electron-impact ionization (EII) and electron-ion recombination.
- Experimental EII cross sections measurements have usually been limited to single pass experiments using ion beams with an unknown population of metastable levels. However, using an ion storage ring one can store many ions long enough so that essentially all of the metastable levels can radiatively decay to their ground states. Recently EII measurements at TSR have been reported for P-like Fe^{11+} [1].

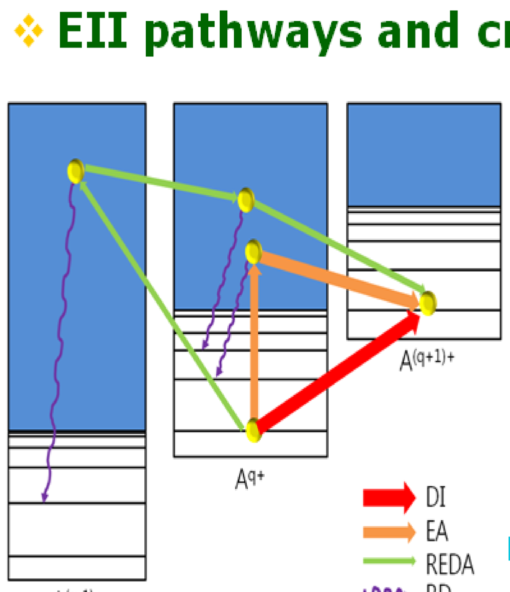


Test Storage Ring (TSR) in Heidelberg for Atomic Data Measurement

- Recent EII calculations for Fe^{11+} by Dere [2], using the flexible atomic code (FAC) [3] based on a distorted wave (DW) approximation, show a discrepancy with the TSR work. The theory falls below the measurement near the 3p direct ionization threshold and lies above the measurement at higher energies.
- We performed an improved FAC-DW calculation helping to resolve much of these discrepancies [4]. In our calculation, we take into account the 3l → nl' (n=3-35) excitation-autoionization (EA) channels near the threshold and the 2l → nl' (n=3-10) EA channels at higher energies, along with their detailed branching ratios [5]. We have extended our EII calculations for Fe^{11+} to P-like ions from P to Zn^{15+} and the total EII Maxwellian rate coefficients for plasma modeling are provided. Similar methods were applied for EII calculations of W^{17+} and W^{+}.
- The calculated total EII cross section including direct ionization (DI) and EA for Fe^{11+} agrees well with recent experiment except for 2l → nl' EA. For this excitation the calculated cross section is larger than experiment. The calculated total EII cross section for W^{+} is about 25% larger than experiments. R-matrix calculations have been carried out for collisional excitation (CE) cross sections of Fe^{11+} and W^{+} ions by debugging and parallelizing R-matrix routines implemented in original FAC which have fatal segmentation fault errors for those complex system calculations and are programmed for single processor. The collisional excitation cross sections calculated by the R-matrix method will be presented and compared with our previous results by the DW method in detail.

EII Calculations (DW)

EII pathways and cross sections



Direct ionization (DI)

$A^{q+} + e \rightarrow A^{(q+1)+} + e' + e''$

Excitation-autoionization (EA)

$A^{q+} + e \rightarrow A^{q+*} + e'$

$\rightarrow A^{(q+1)+} + e' + e''$

Resonant excitation-double autoionization (REDA)

$A^{q+} + e \rightarrow A^{(q-1)+**}$

$\rightarrow A^{q+*} + e'$

$\rightarrow A^{(q+1)+} + e' + e''$

Resonant excitation-auto double ionization (READI)

$A^{q+} + e \rightarrow A^{(q-1)+**} \rightarrow A^{(q+1)+} + e' + e''$

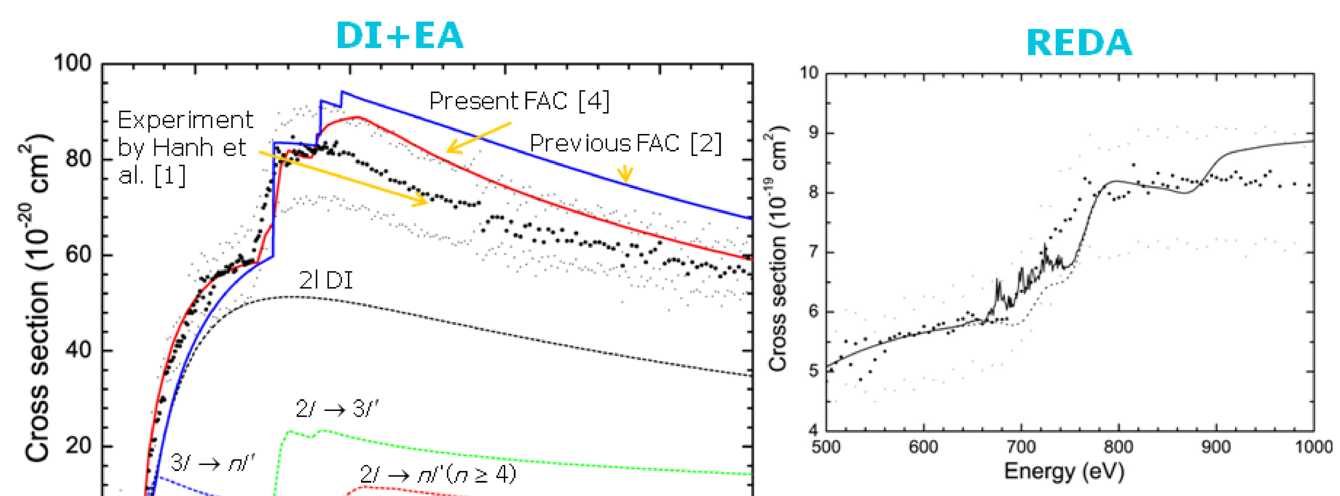
Total EII cross section in an Independent Process-Isolated Resonance (IP-IR) approximation

$$\sigma_{tot} = \sum_i \sigma_i^{DI} + \sum_j \sigma_j^{CE} B_j^a + \sum_k \tilde{\sigma}_k^{DC} B_k^{da}$$

Autoionization (AI) branching ratio (BR) and double AI-BR

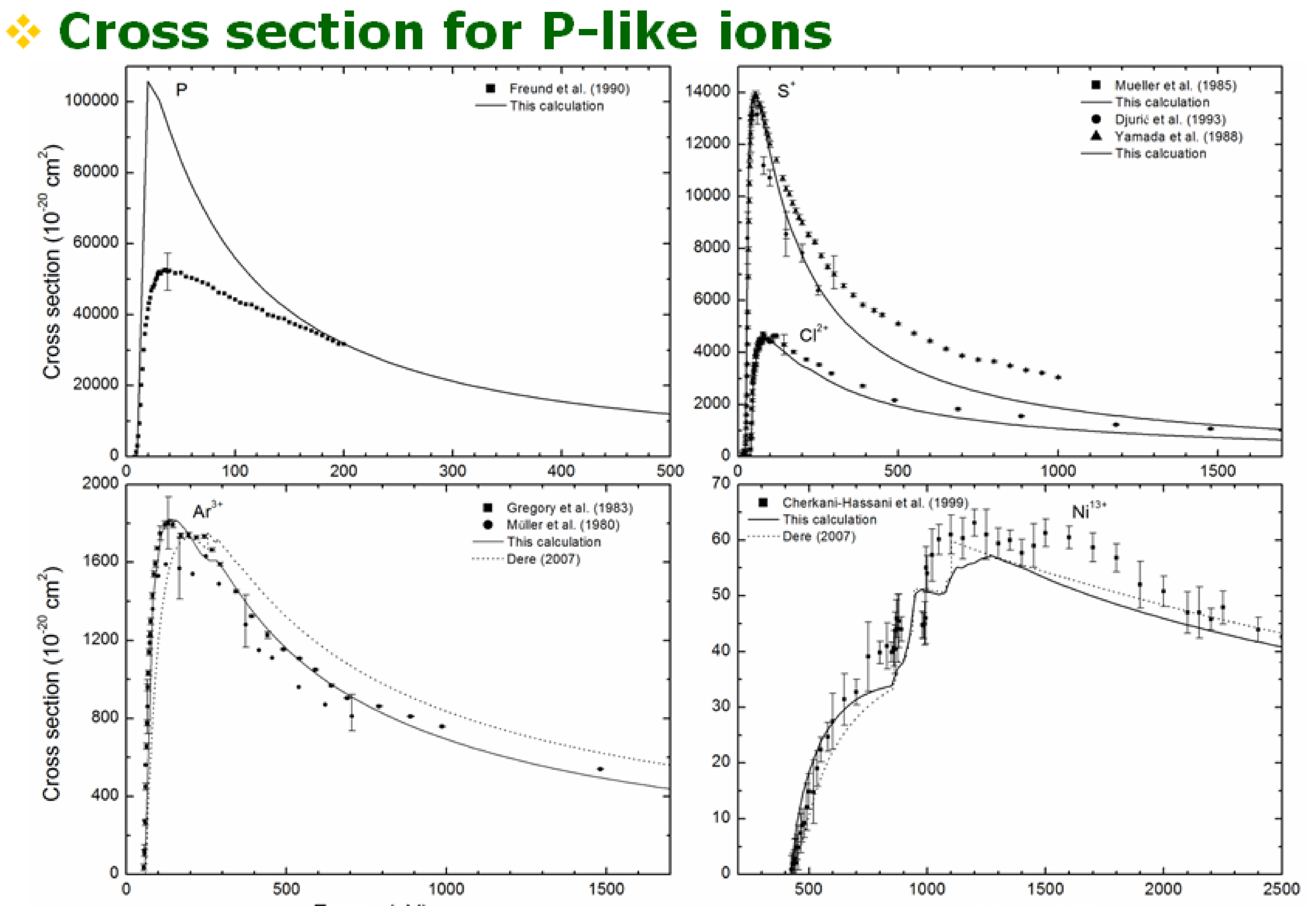
$$B_j^a = \frac{\sum_h A_{jh}^a B_h^r + \sum_f A_{jf}^a B_f^a}{\sum_h A_{jh}^a + \sum A_{jf}^r}, \quad B_k^{da} = \frac{\sum_f A_{kj}^a B_j^a}{\sum_j A_{kj}^a + \sum_{f'} A_{kf'}^r}$$

Cross section for Fe^{11+} ($3s^2\ 3p^3\ {}^4S_{3/2}$)

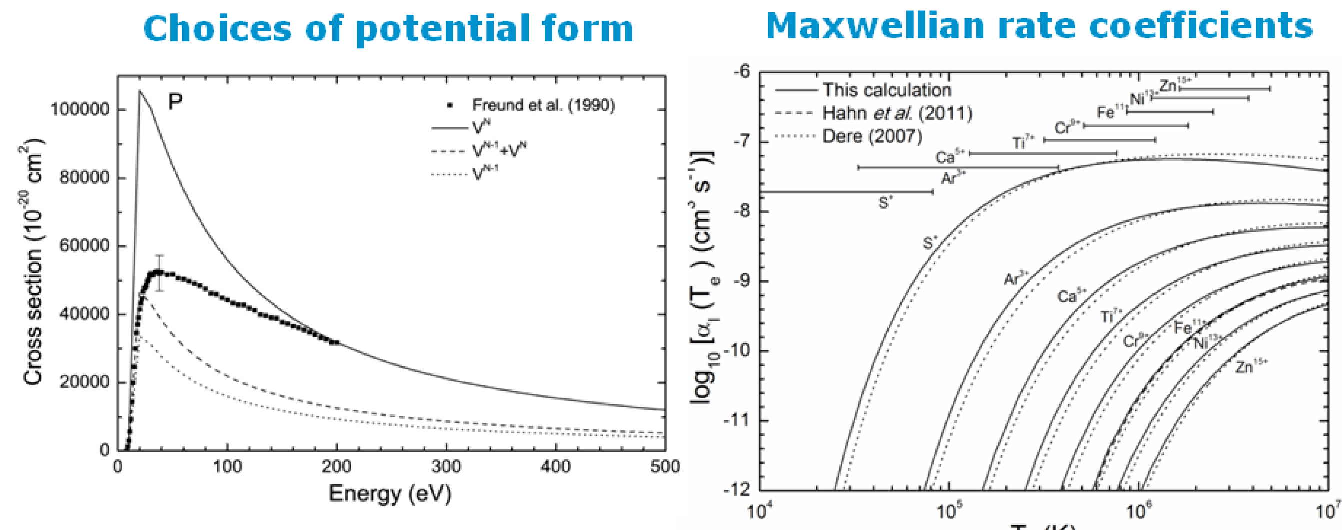


REDA contribution is within about 4% in rate coefficient

Cross section for P-like ions



D.-H. Kwon and D. W. Savin, Astrophys. J **784**, 13 (2014)

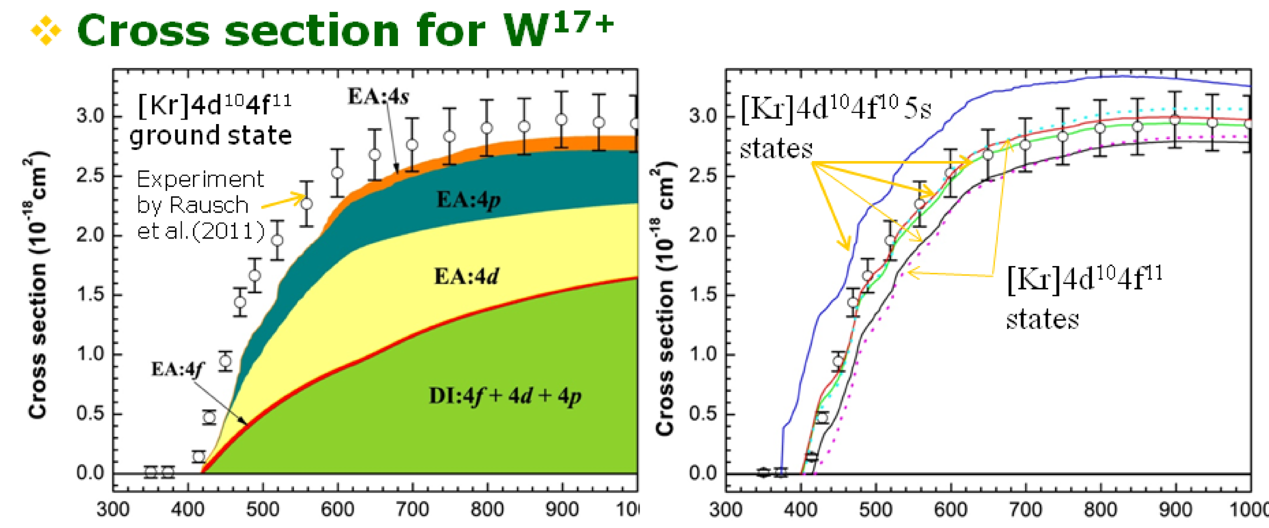


Large sensitivity of DI cross section to potential choices in the case of neutral P

7~50% relative differences from previous FAC results

$$\alpha_I(T_e) = \left[\frac{8k_B T_e}{\pi m_e}\right]^{1/2} \int_{I_0}^{\infty} \sigma(E)\left(\frac{E}{k_B T_e}\right)\exp\left(-\frac{E}{k_B T_e}\right) d\left(\frac{E}{k_B T_e}\right)$$

Cross section for W^{17+}



There are many long lived excited states and parent ion beams are mixed in ground and excited states.

D.-H. Zhang and D.-H. Kwon, J Phys. B **47**, 075202 (2014)

DW vs. R-Matrix calculations for CE

Channels :

$S = S_i + s, \quad L = L_i + l, \quad \pi = (-1)^{\pi_i + l}$

$E = E_i + k^2$

$\Psi_\alpha = \sum_{i,j} c_{ij} A[\Phi_i, \phi_j] + \sum_m d_m \theta_m, \quad H = \sum_i H_D + \sum_{i<j} \frac{1}{r_{ij}}$

$H(N+1)\Psi_\alpha = E_\alpha^{(N+1)}\Psi_\alpha, \quad \Psi_E = \sum_\alpha A_{E\alpha}\Psi_\alpha$

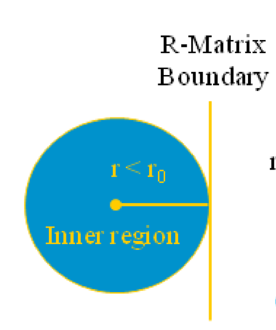
Wavefunction of the scattered electron in channel i

$\begin{pmatrix} P_i(r) \\ Q_i(r) \end{pmatrix} = \sum_\alpha A_{E\alpha} \begin{pmatrix} u_\alpha(r) \\ v_\alpha(r) \end{pmatrix}$

$\frac{Q_i(r_0)}{P_i(r_0)} = \frac{b + \kappa}{2r_0 c}$

$P_i(r_0) = \sum_j R_{ij}\left[2r_0 c Q_j(r_0) - (b + \kappa_j) P_j(r_0)\right]$

$R_{ij} = \frac{1}{2r_0} \sum_\alpha \frac{w_{i\alpha}(r_0) w_{j\alpha}(r_0)}{E_\alpha^{N+1} - E}$



Exchange potential between scattered electron and bound electron is neglected.

Scattering matrices :

$S = (1 - K)(1 - K)^{-1}, \quad S^\dagger S = I$: Unitary condition is satisfied.

$T = I - S$

$\Omega_{ac} = \frac{1}{2} \sum_{J\pi} (2J+1) \sum_{\kappa_a \kappa_c} \left|T_{ac}^{\kappa_a \kappa_c}\right|^2$

DW approximation

$$T = I - S = I - \frac{I + iK}{I - iK} = -\frac{2iK}{I - iK} \simeq -2iK,$$

$$\Omega_{01}^{CE} = 2 \sum_{\kappa_0 \kappa_1} \sum_{J_T} [J_T] \left|\langle K(j_0 \kappa_0, j_1 \kappa_1; J_T)\rangle\right|^2$$

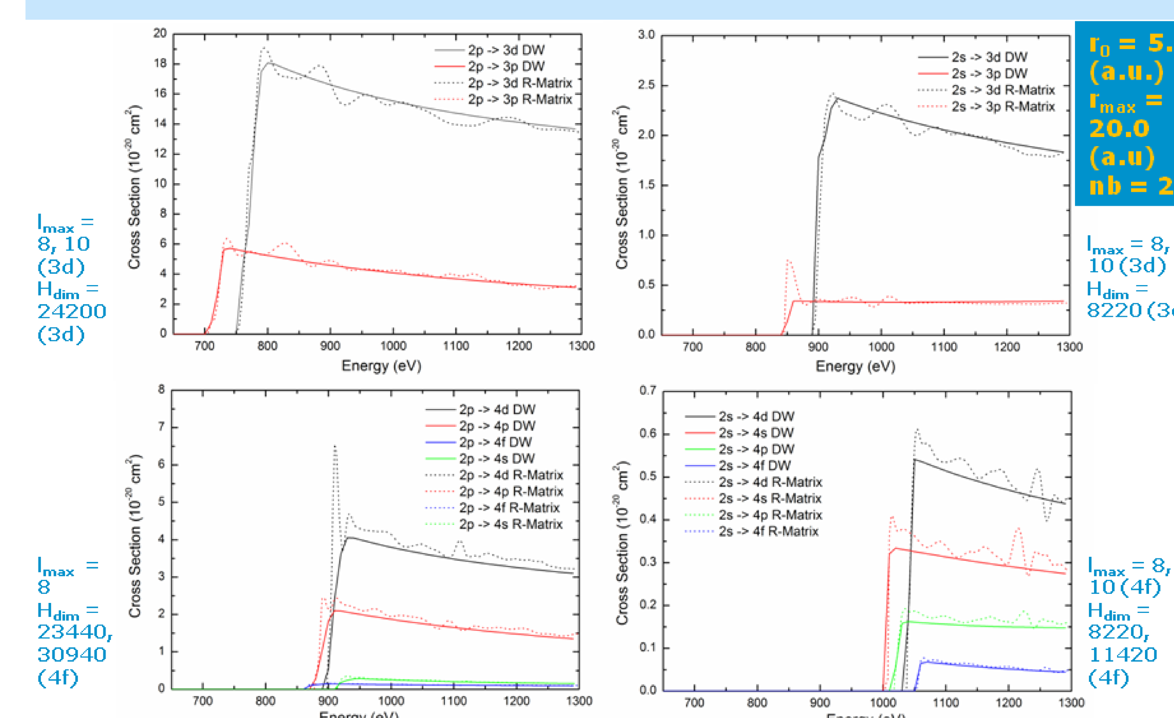
$$= 2 \sum_{\kappa_0 \kappa_1} \sum_{J_T} [J_T] \left|\langle \Psi_0 \kappa_0, J_T M_T \left| \sum_{i<j} \frac{1}{r_{ij}} \right| \Psi_1 \kappa_1, J_T M_T \rangle\right|^2$$

Channels are not coupled. Unitarity is not satisfied.

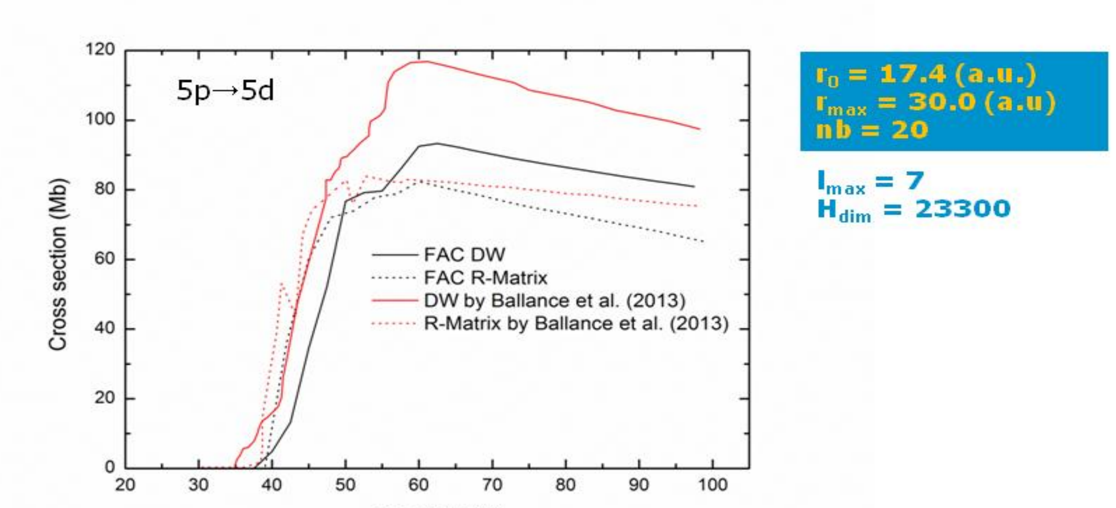
R-Matrix computation

- A terrible segmentation fault in large size R-Matrix calculations of the original fac was debugged by changing 32bit data type to 64bit one.
- Parallelization by channel symmetry in surface amplitudes and by electron energy in collision strengths have been carried out for the R-Matrix routines of the original FAC.
- Computer Resources : Intel Xeon E5-2690 2.90GHz Workstation server (2CPUs, 8cores, 32 Gbyte/core Memory)
- At present just initial and final two states close coupling is considered.

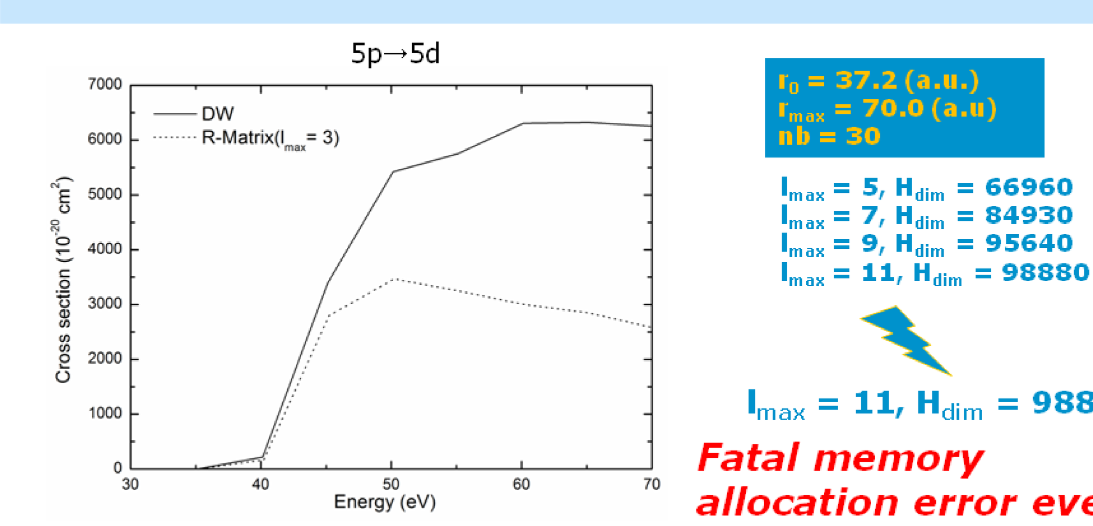
Collisional excitation : Fe^{11+}



Collisional excitation : W^{3+}



Collisional excitation : W^{+}



l_{max} = 11, H_{dim} = 98880

Fatal memory allocation error even in 64bit OS system!

```
wik0 = (double *) malloc(sizeof(double )*max);
```

$H_{dim}^2 \approx max \le 32 \times 10^9$

~10days for surface amplitudes of 29 channel symmetries

Summary and Outlook

- DW-DI cross sections for neutral atom and lowly charged ions show large sensitivity to local central potential form.
- DW-CE cross sections for neutral atom and lowly charged ions show significant discrepancy with R-Matrix calculations.
- Parallelization of FAC will be continued to improve computational efficiency for R-Matrix calculation.
- Unitary correction for DW calculation of FAC will be performed.

REFERENCES

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[2] K. P. Dere 2007, Astron. & Astrophys. , 466, 771
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[5] P. Bryans, E. Landi and D. W. Savin 2009, Astrophys. J., 691, 1540