Ion Impact Cross-Sections for ADAS Applications

A new ADAS format and processing for quadrupole transitions induced by ion impact

Matthew Bluteau and the ADAS Team

University of Strathclyde/CCFE Culham/JET

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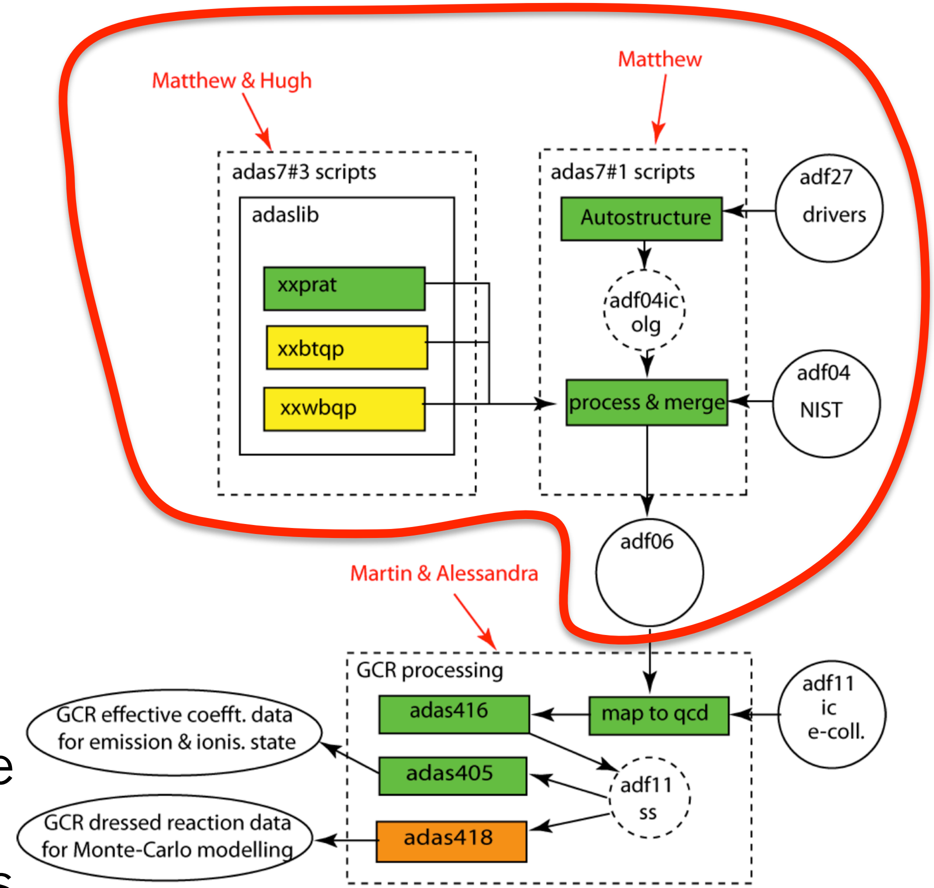
Warsaw

Context

- The bigger picture: ion impact cross-section data is desirable and increasingly relevant in numerous plasma conditions and scenarios
- Focusing questions: how is the data generated (presently and in the future)? What were the guiding considerations when developing the data generation process?
- This presentation will focus on the progress that has been made generating data for ion-impact collisions involving E2 transitions between the low-lying metastables of the target ion



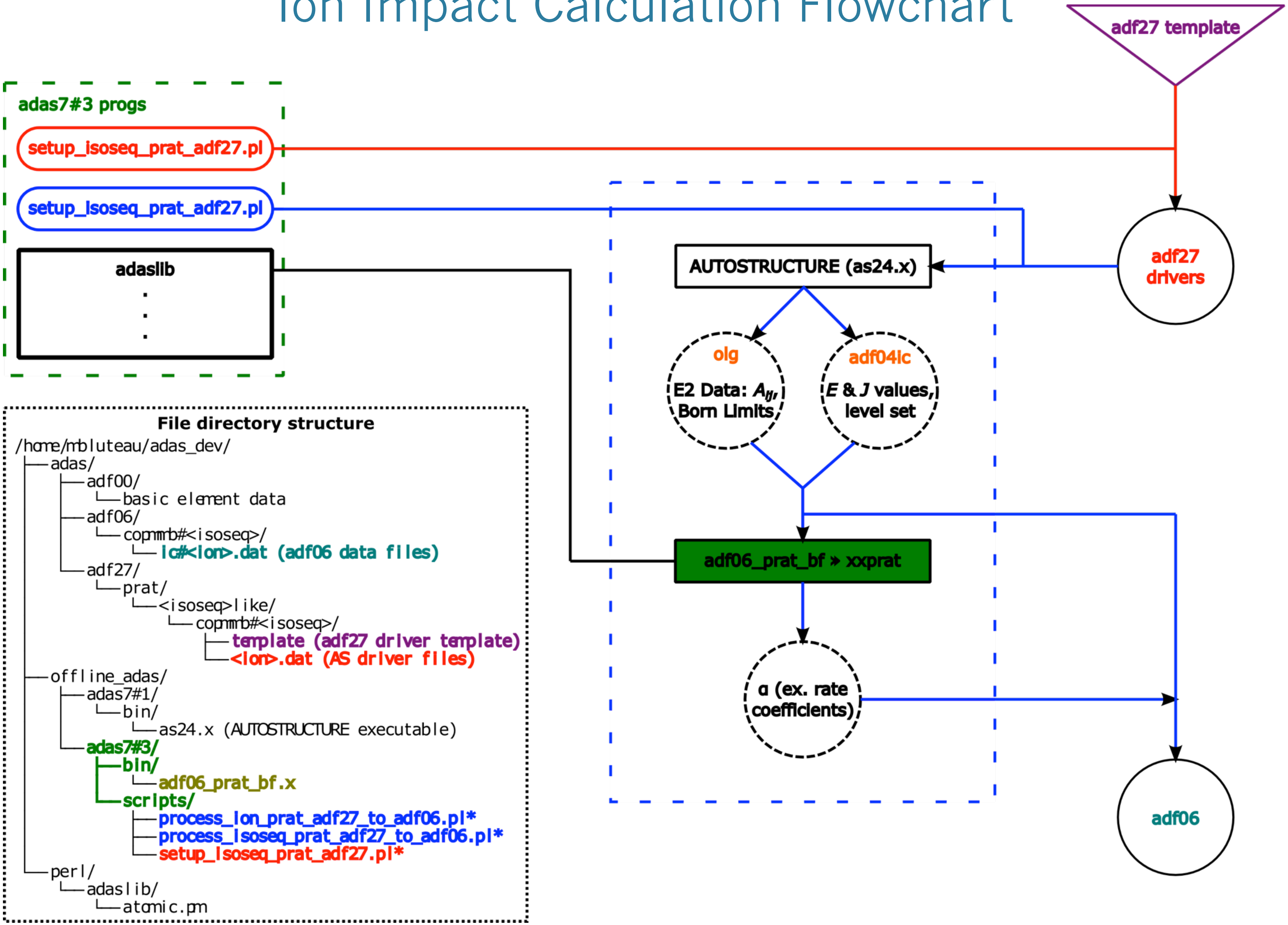
Important Considerations

- Electron collisions have (almost nearly) been the only particle collisions considered in ADAS, so the implementation of new colliders/projectiles must be carefully planned so as to comply with and extend the ADAS framework
- The problem is more complex than in astrophysics where only protons are assumed to be important
  - In fusion plasmas, numerous other ions are present in high enough concentrations to be of relevance (esp. H and He isotopes)
  - Thus, functionality for various projectiles must be incorporated
- However, it is also not worthwhile or prudent to consider all possible ion projectiles

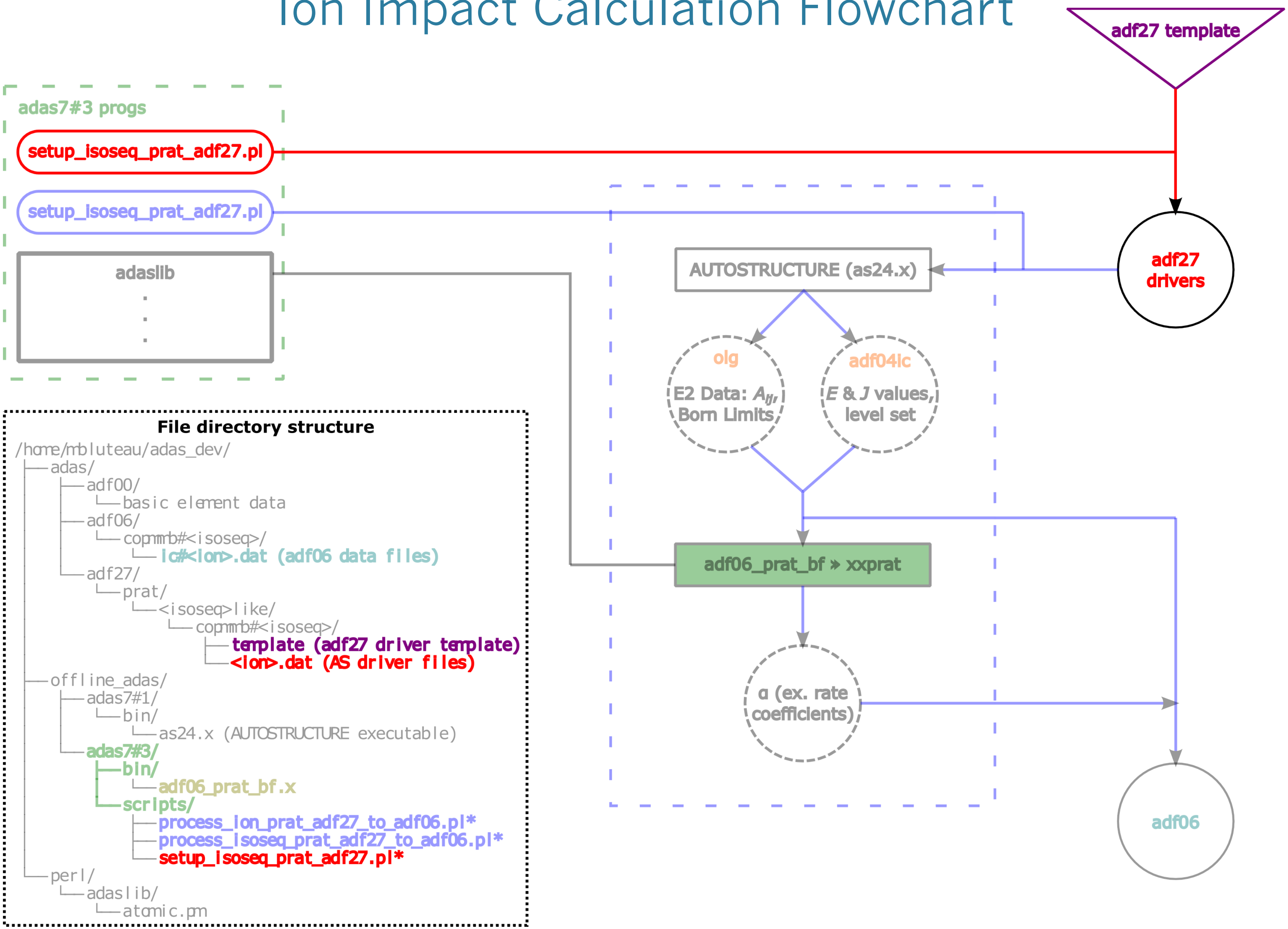
Important Considerations

- Our simplifying assumptions:
  - Only light elements will be relevant as they will have greater velocities and thus larger cross-sections
  - Moreover, fusion plasmas simply cannot tolerate high concentrations of heavier species
  - The light elements will tend to be fully ionized, so we neglect ion-ion collisions where both ions have atomic structure (i.e. we are only considering bare nuclei projectiles)
  - Ne^{10+} is our upper limit (still requires investigation)
- With new devices like ITER pushing energy regimes higher, it is paramount that the high energy behaviour of our cross-sections be correct
  - As mentioned earlier, this relies on correct transition probabilities (quadrupole moments for current applications) and infinite energy Born limits

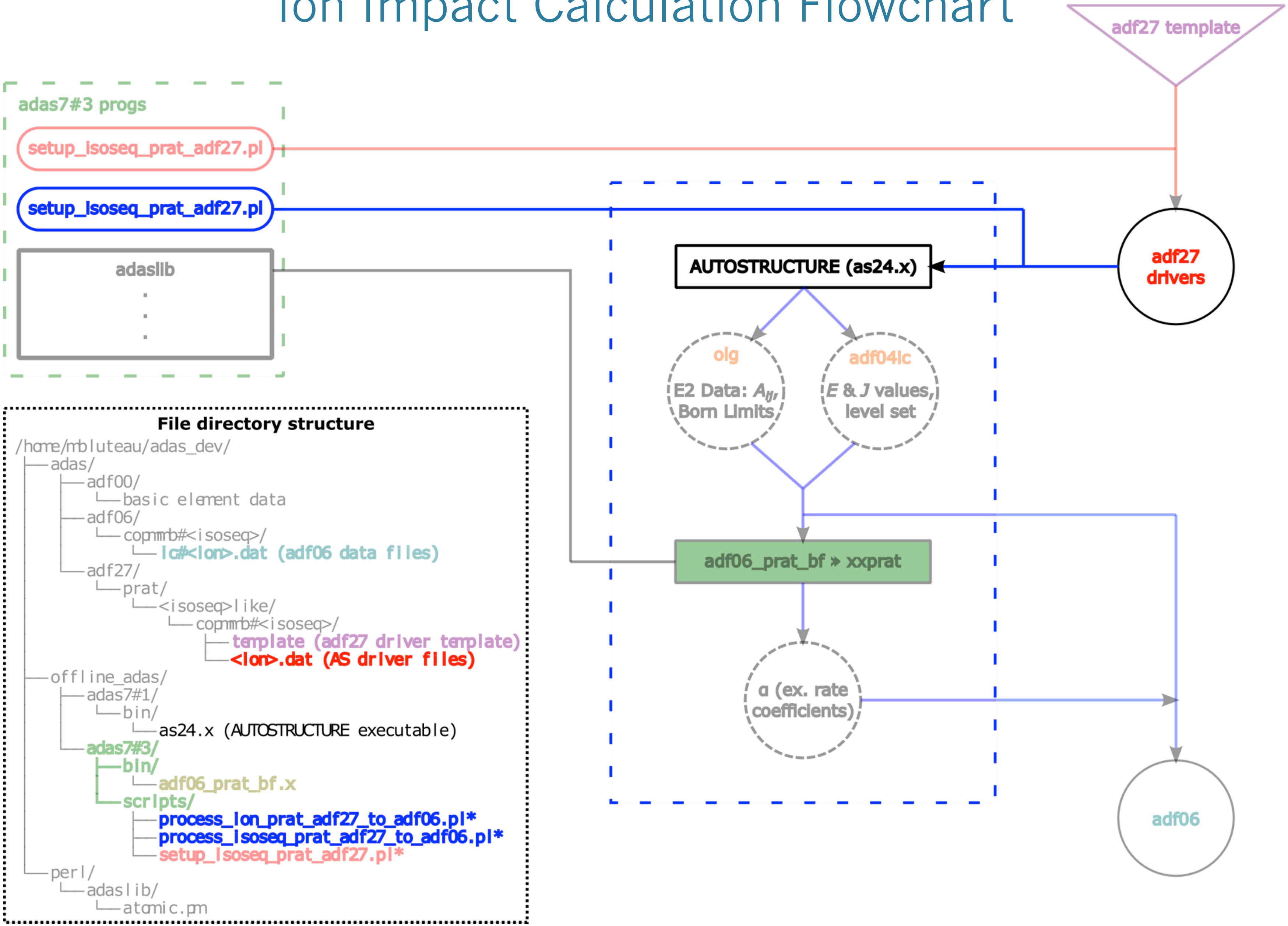
Ion Impact Calculation Flowchart



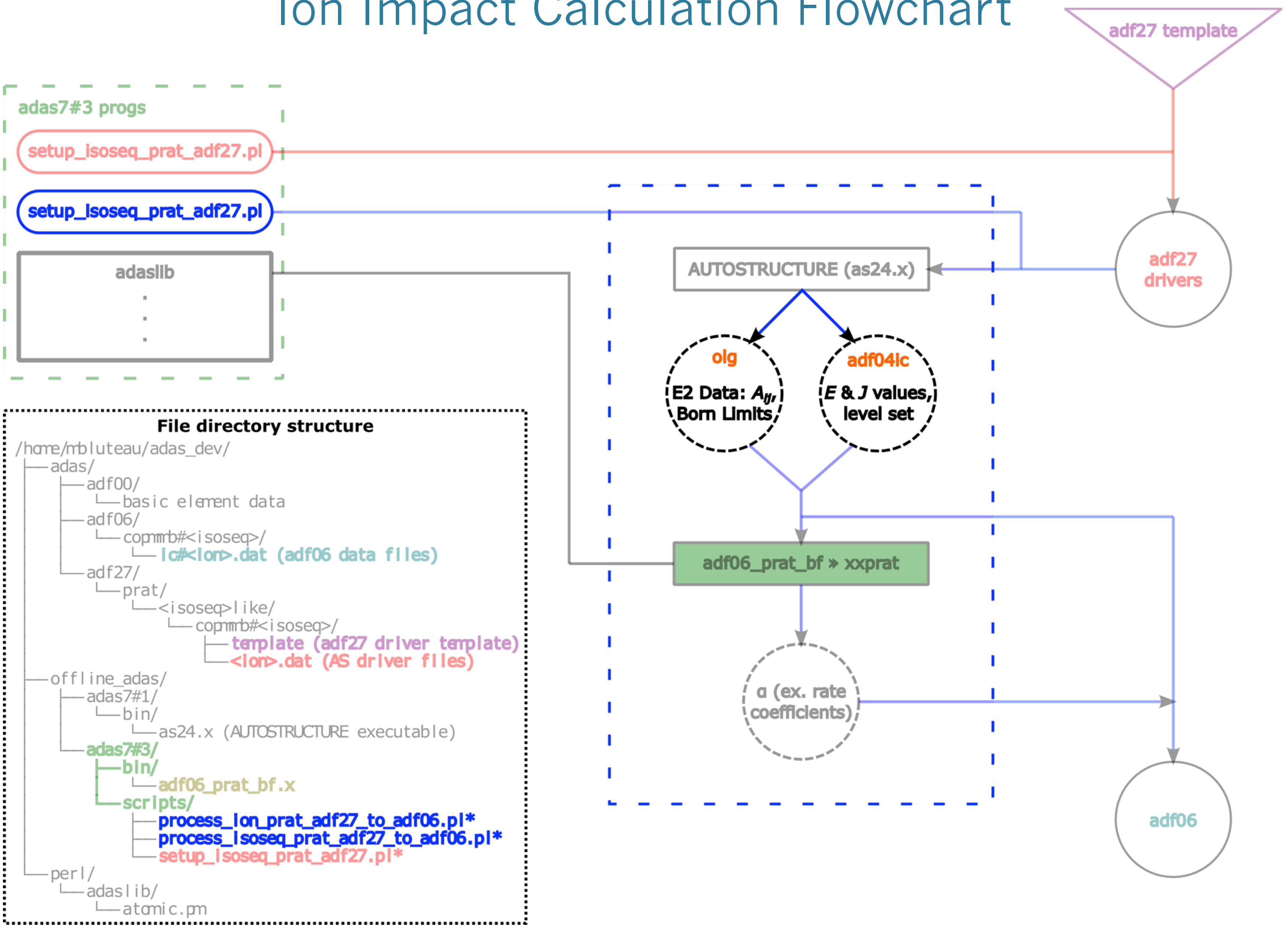
Ion Impact Calculation Flowchart



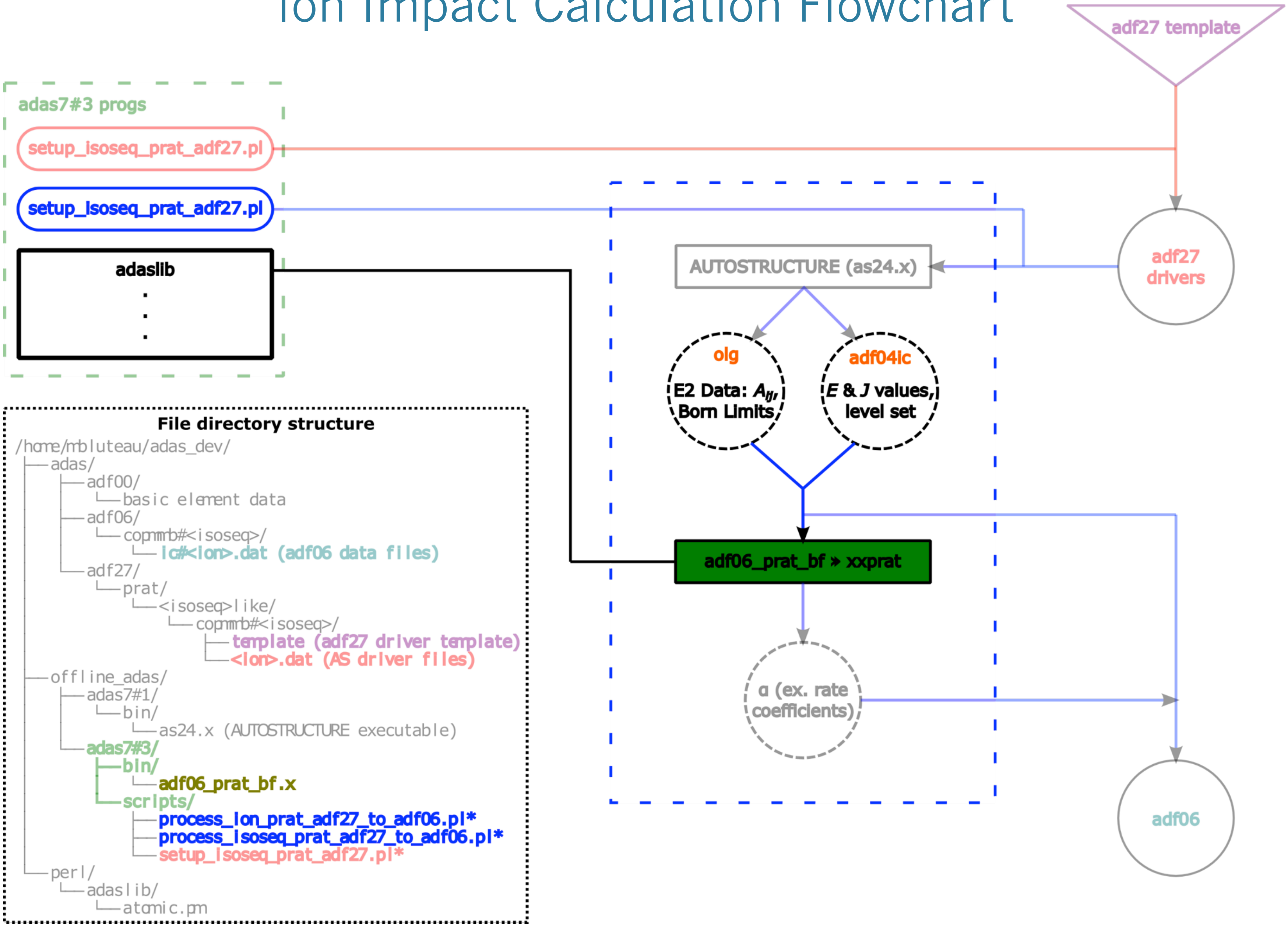
Ion Impact Calculation Flowchart



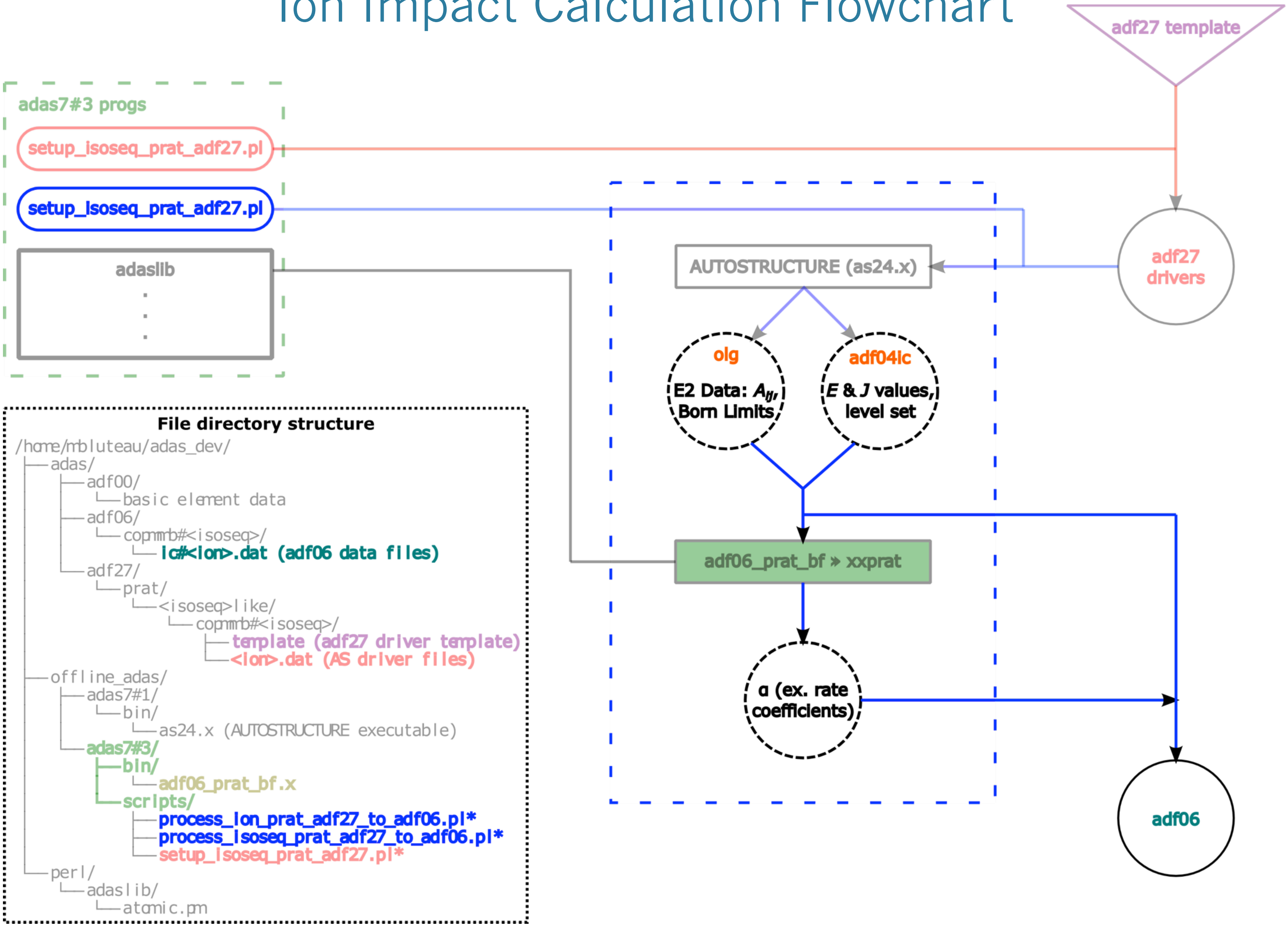
Ion Impact Calculation Flowchart



Ion Impact Calculation Flowchart



Ion Impact Calculation Flowchart



New adf06 File Format

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New adf06 File Format

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Atom+Z

Z+1

Ion. pot. (cm^{-1})

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    2 522513             (2)1( 1.5)          20945.4207
    3 512523             (4)1( 0.5)         229540.1582
    4 512523             (4)1( 1.5)         237549.0935
    5 512523             (4)1( 2.5)         249112.9700
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Index

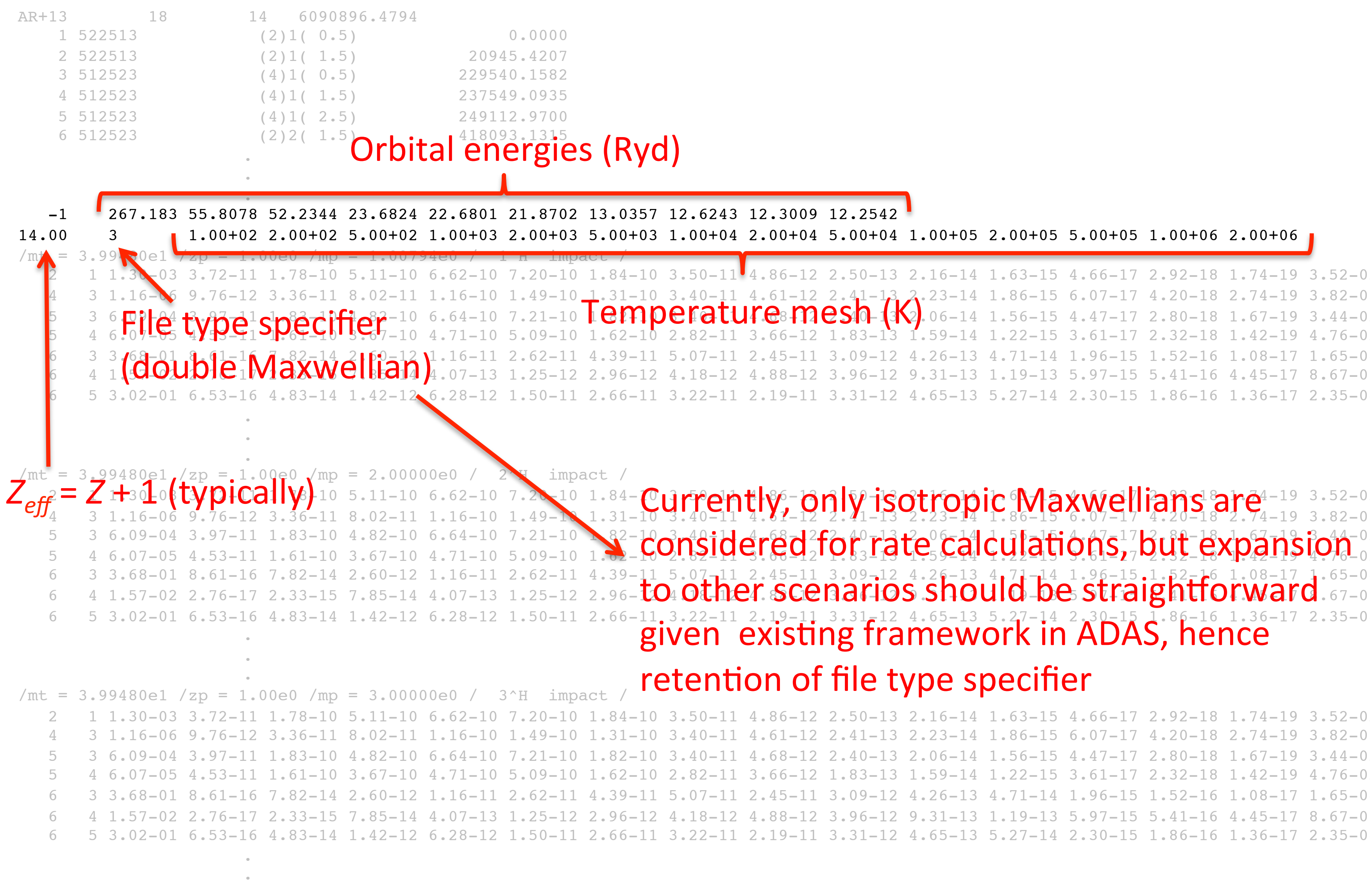
Configuration (Eissner Notation)

(2S+1) L (J)

E rel. to ground (cm^{-1})

Identical to adf04 level specification but truncated to only include levels involved in metastable transitions

New adf06 File Format



New adf06 File Format

New format allows for multiple different colliding ions/projectiles; data for each ion is arranged into blocks with separating headers

Target atom mass (amu)

Projectile ion charge #

Projectile ion mass (amu)

Projectile nuclear specification

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    1 522513            (2)1( 0.5)             0.0000
    2 522513            (2)1( 1.5)         20945.4207
    3 512523            (4)1( 0.5)        229540.1582
    4 512523            (4)1( 1.5)        237549.0935
    5 512523            (4)1( 2.5)        249112.9700
    6 512523            (2)2( 1.5)       [illegible]
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   -1     267.183 55.8078 52.2344 23.6824 22.6801 21.8702 13.0357 12.6243 12.3009 12.2542
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   5   4 6.07-05 4.53-11 1.61-10 3.67-10 4.71-10 5.09-10 1.62-10 2.82-11 3.66-12 1.83-13 1.59-14 1.22-15 3.61-17 2.32-18 1.42-19 4.76-02
   6   3 3.68-01 8.61-16 7.82-14 2.60-12 1.16-11 2.62-11 4.39-11 5.07-11 2.45-11 3.09-12 4.26-13 4.71-14 1.96-15 1.52-16 1.08-17 1.65-04
   6   4 1.57-02 2.76-17 2.33-15 7.85-14 4.07-13 1.25-12 2.96-12 4.18-12 4.88-12 3.96-12 9.31-13 1.19-13 5.97-15 5.41-16 4.45-17 8.67-06
   6   5 3.02-01 6.53-16 4.83-14 1.42-12 6.28-12 1.50-11 2.66-11 3.22-11 2.19-11 3.31-12 4.65-13 5.27-14 2.30-15 1.86-16 1.36-17 2.35-04
                          .
                          .
                          .
```

New adf06 File Format

Block data content is directly analogous to adf04 type 3 (electron collisional data given as Upsilons)

```
AR+13          18          14    6090896.4794
    1 522513              (2)1( 0.5)              0.0000
    2 522513              (2)1( 1.5)          20945.4207
    3 512523              (4)1( 0.5)         229540.1582
    4 512523              (4)1( 1.5)         237549.0935
    5 512523              (4)1( 2.5)         249112.9700
    6 512523              (2)2( 1.5)         418093.1315
                          .
                          .
   -1     267.183 55.8078 52.2344 23.6824 22.6801 21.8702 13.0357 12.6243 12.3009 12.2542
14.00      3       1.00+02 2.00+02 5.00+02 1.00+03 2.00+03 5.00+03 1.00+04 2.00+04 5.00+04 1.00+05 2.00+05 5.00+05 1.00+06 2.00+06
/mt = 3.99480e1 /zp = 1.00e0 /mp = 1.00794e0 /  1^H  impact /
    2    1 1.30-03 3.72-11 1.78-10 5.11-10 6.62-10 7.20-10 1.84-10 3.50-11 4.86-12 2.50-13 2.16-14 1.63-15 4.66-17 2.92-18 1.74-19 3.52-02
    4    3 1.16-06 9.76-12 3.36-11 8.02-11 1.16-10 1.49-10 1.31-10 3.40-11 4.61-12 2.41-13 2.23-14 1.86-15 6.07-17 4.20-18 2.74-19 3.82-03
    5    3 6.09-04 3.97-11 1.83-10 4.82-10 6.64-10 7.21-10 1.82-10 3.40-11 4.68-12 2.40-13 2.06-14 1.56-15 4.47-17 2.80-18 1.67-19 3.44-02
    5    4 6.07-05 4.53-11 1.61-10 3.67-10 4.71-10 5.09-10 1.62-10 2.82-11 3.66-12 1.83-13 1.59-14 1.22-15 3.61-17 2.32-18 1.42-19 4.76-02
    6    3 3.68-01 8.61-16 7.82-14 2.60-12 1.16-11 2.62-11 4.39-11 5.07-11 2.45-11 3.09-12 4.26-13 4.71-14 1.96-15 1.52-16 1.08-17 1.65-04
    6    4 1.57-02 2.76-17 2.33-15 7.85-14 4.07-13 1.25-12 2.96-12 4.18-12 4.88-12 3.96-12 9.31-13 1.19-13 5.97-15 5.41-16 4.45-17 8.67-06
    6    5 3.02-01 6.53-16 4.83-14 1.42-12 6.28-12 1.50-11 2.66-11 3.22-11 2.19-11 3.31-12 4.65-13 5.27-14 2.30-15 1.86-16 1.36-17 2.35-04
```

Upper level, *j*

Lower level, *i*

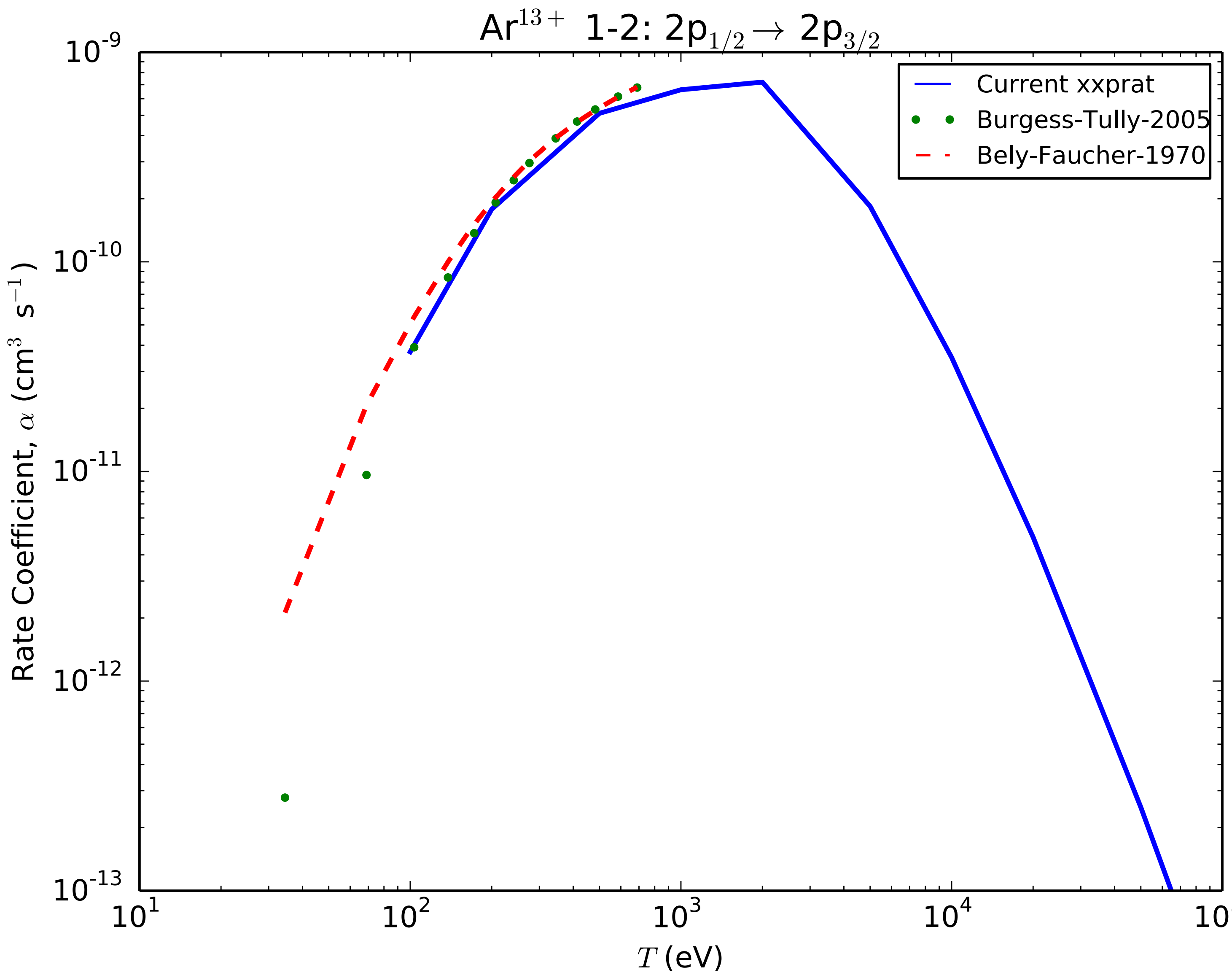
Quadrupole moment, E2

Excitation rate coefficients ($cm^3 s^{-1}$) as a function of $T_i = T_e$

Bethe high energy limit value

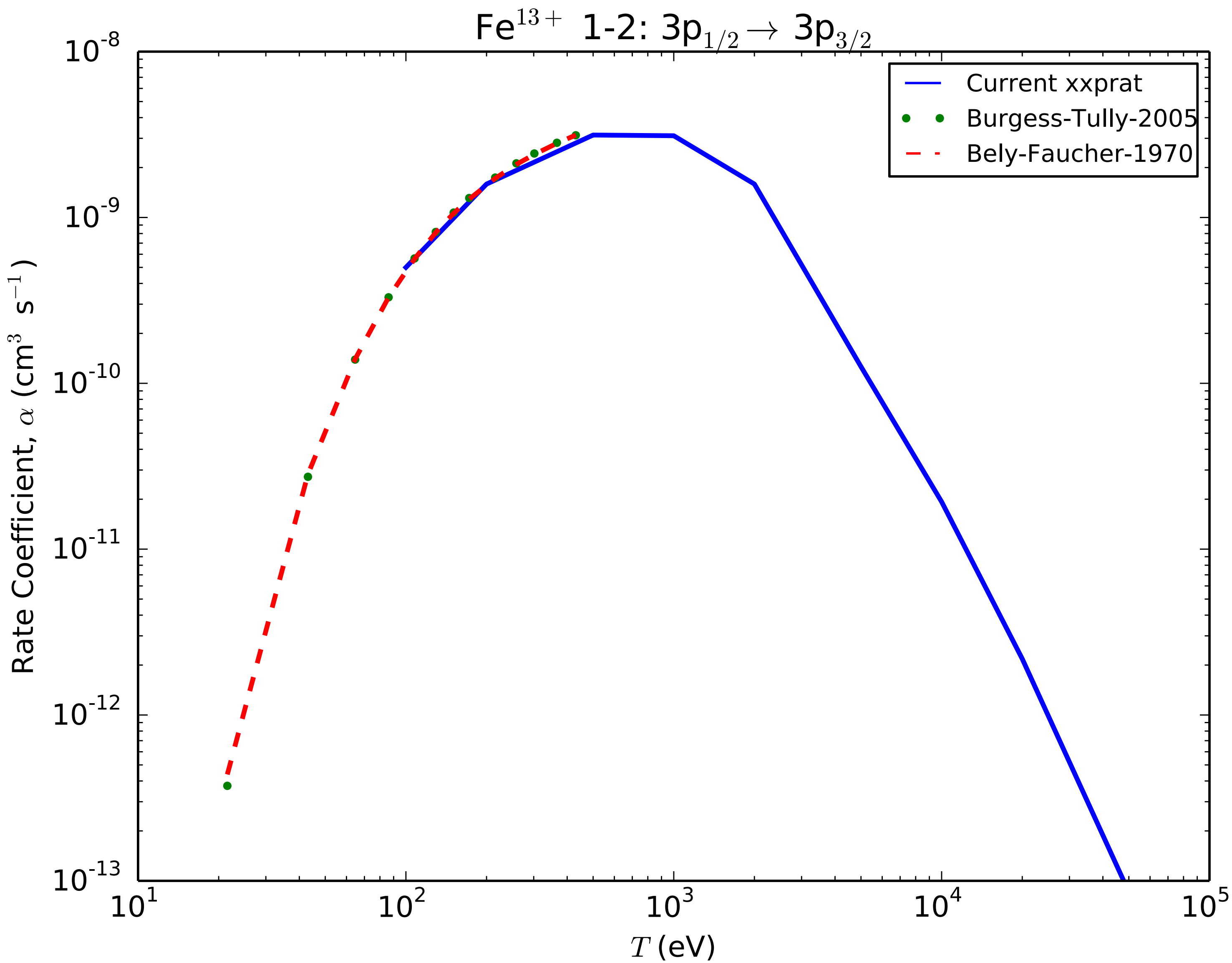
```
                          .
                          .
/mt = 3.99480e1 /zp = 1.00e0 /mp = 2.00000e0 /  2^H  impact /
    2    1 1.30-03 3.72-11 1.78-10 5.11-10 6.62-10 7.20-10 1.84-10 3.50-11 4.86-12 2.50-13 2.16-14 1.63-15 4.66-17 2.92-18 1.74-19 3.52-02
    4    3 1.16-06 9.76-12 3.36-11 8.02-11 1.16-10 1.49-10 1.31-10 3.40-11 4.61-12 2.41-13 2.23-14 1.86-15 6.07-17 4.20-18 2.74-19 3.82-03
    5    3 6.09-04 3.97-11 1.83-10 4.82-10 6.64-10 7.21-10 1.82-10 3.40-11 4.68-12 2.40-13 2.06-14 1.56-15 4.47-17 2.80-18 1.67-19 3.44-02
    5    4 6.07-05 4.53-11 1.61-10 3.67-10 4.71-10 5.09-10 1.62-10 2.82-11 3.66-12 1.83-13 1.59-14 1.22-15 3.61-17 2.32-18 1.42-19 4.76-02
    6    3 3.68-01 8.61-16 7.82-14 2.60-12 1.16-11 2.62-11 4.39-11 5.07-11 2.45-11 3.09-12 4.26-13 4.71-14 1.96-15 1.52-16 1.08-17 1.65-04
    6    4 1.57-02 2.76-17 2.33-15 7.85-14 4.07-13 1.25-12 2.96-12 4.18-12 4.88-12 3.96-12 9.31-13 1.19-13 5.97-15 5.41-16 4.45-17 8.67-06
    6    5 3.02-01 6.53-16 4.83-14 1.42-12 6.28-12 1.50-11 2.66-11 3.22-11 2.19-11 3.31-12 4.65-13 5.27-14 2.30-15 1.86-16 1.36-17 2.35-04
                          .
                          .
                          .
/mt = 3.99480e1 /zp = 1.00e0 /mp = 3.00000e0 /  3^H  impact /
    2    1 1.30-03 3.72-11 1.78-10 5.11-10 6.62-10 7.20-10 1.84-10 3.50-11 4.86-12 2.50-13 2.16-14 1.63-15 4.66-17 2.92-18 1.74-19 3.52-02
    4    3 1.16-06 9.76-12 3.36-11 8.02-11 1.16-10 1.49-10 1.31-10 3.40-11 4.61-12 2.41-13 2.23-14 1.86-15 6.07-17 4.20-18 2.74-19 3.82-03
    5    3 6.09-04 3.97-11 1.83-10 4.82-10 6.64-10 7.21-10 1.82-10 3.40-11 4.68-12 2.40-13 2.06-14 1.56-15 4.47-17 2.80-18 1.67-19 3.44-02
    5    4 6.07-05 4.53-11 1.61-10 3.67-10 4.71-10 5.09-10 1.62-10 2.82-11 3.66-12 1.83-13 1.59-14 1.22-15 3.61-17 2.32-18 1.42-19 4.76-02
    6    3 3.68-01 8.61-16 7.82-14 2.60-12 1.16-11 2.62-11 4.39-11 5.07-11 2.45-11 3.09-12 4.26-13 4.71-14 1.96-15 1.52-16 1.08-17 1.65-04
    6    4 1.57-02 2.76-17 2.33-15 7.85-14 4.07-13 1.25-12 2.96-12 4.18-12 4.88-12 3.96-12 9.31-13 1.19-13 5.97-15 5.41-16 4.45-17 8.67-06
    6    5 3.02-01 6.53-16 4.83-14 1.42-12 6.28-12 1.50-11 2.66-11 3.22-11 2.19-11 3.31-12 4.65-13 5.27-14 2.30-15 1.86-16 1.36-17 2.35-04
                          .
                          .
                          .
```

Sample Results



*Recall, high E behaviour incorrect

Sample Results



*Recall, high E behaviour incorrect

Concluding Remarks

- Groundwork for technical implementation of ion impact data in ADAS has been laid
- Initial data generated for proton impact; preliminary applications possible
- Quadrupole moments and Born limits have been extracted from AUTOSTRUCTURE, and so are available for future improvements (below)
- Improvements/Future work:
  - Implement functionality for other ion projectiles and thus wider applicability
  - Replace xxprat with corrected Burgess Tully (2005) version
  - Finally, employ full close-coupling equations for calculation of excitation rates