UK Atomic Energy Authority

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ReMKiT1D Workshop January 2024
Collisional-Radiative Models in ReMKiT1D

Imperial College London

Engineering and Physical Sciences Research Council

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Collisional-Radiative Modelling – the basics

Rate equations of the form $\frac{d\vec{n}}{dt} = \boldsymbol{M}(\vec{n}) \cdot \vec{n} + \vec{\Gamma}$

where n_i are the states being transformed between

Transition rates are encoded in the matrix **M**

The matrix needs to be built for each spatial location!

In general we might have many states/species and transitions

How do we represent species?

Species objects

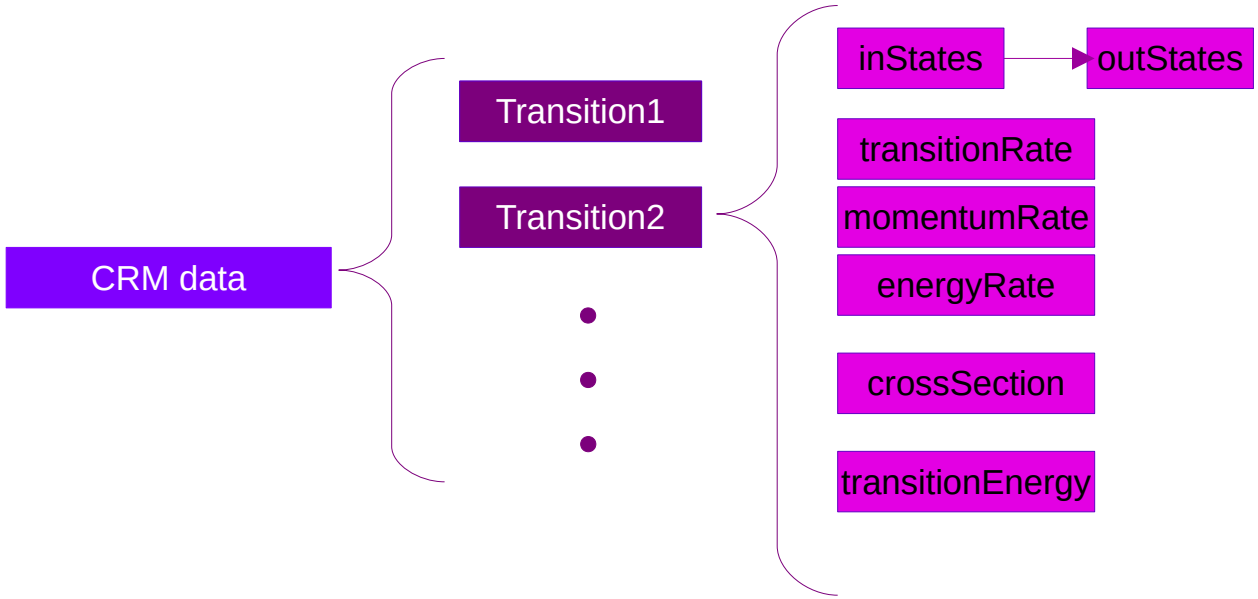
```
rk.addSpecies(name="D+", speciesID= -1, atomicA=2.014, charge=1)
```

Can associate variables to species

How do we represent transitions?

CRM modelbound data

Collisional-Radiative modelbound data



Example: $H + e^- \rightarrow H^+ + e^- + e^-$

IDs: 1 0 -1 0 0

inStates: 1 0
outStates: -1 0 0

transitionEnergy: 13.6eV

rates:
- transitionRate: derivation1
- momentumRate: derivation2
- energyRate: derivation3

Set by the user

Collisional-Radiative modelbound data

When used with kinetic electrons, CRM data enables particle and energy conserving implementations of Boltzmann collision integrals

Note:

Kinetic electron CRMs and Boltzmann collision integrals are beyond the scope of this workshop

ReMKiT1D comes with Fortran-level built-in hydrogen cross-section data

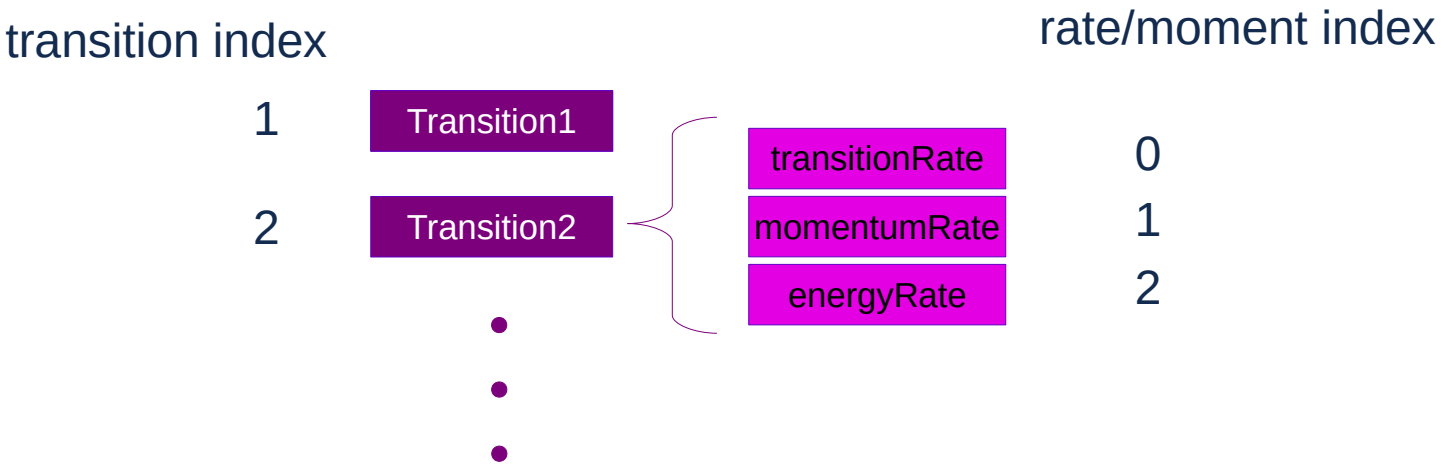
Python routines for using NIST and AMJUEL data are also supplied

crm_support Python module lets you build transitions and CRMs by hand

Term generators – given a CRM modelbound data object will produce all the particle sources/sinks, or Boltzmann integrals

Collisional-Radiative modelbound data

As with variable-like data, the 1D structures in CRM data are available



energyRate of the 5th transition in the CRM data: “rate2index5”

Transitions are indexed in the order they are added to the CRM data

Collisional-Radiative modelbound data

When to use CRM data instead of individual rate variables:

1. When you have many species and transitions between them

2. When using kinetic electrons

Let the term generators worry about which terms to add

Note:

Terms added by term generators are not visible in the Python wrapper!

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Hands-on session