Photochemistry in KROME: a look under the hood

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Aims of this talk

1. Understand that ~~cooling processes~~ photochemistry is a mess
2. Realize that KROME saves your day*

* modulo databases

KROME Bootcamp 2015 - Equations first

Photochemistry process

$$\mathrm{OH} + \gamma \xrightarrow{\sigma_1(E)} \mathrm{OH}^+ + \mathrm{e}^- \quad (1)$$

$$\mathrm{OH} + \gamma \xrightarrow{\sigma_2(E)} \mathrm{O} + \mathrm{H} \quad (2)$$

Photochemistry equations (thin)

$$k_{ph} = \frac{4\pi}{h} \int_{E_0}^{\infty} \frac{I(E)\sigma(E)}{E} \mathrm{d}E \quad (3)$$

$$\Gamma_{ph} = \frac{4\pi}{h} \int_{E_0}^{\infty} \frac{I(E)\sigma(E)}{E} (E - E_0)\eta(E) \mathrm{d}E \quad (4)$$

Photochemistry ODE (RHS)

$$\dot{n}_{\mathrm{OH}} = -k_1\, n_{\mathrm{OH}} - k_2\, n_{\mathrm{OH}} \quad (5)$$

$$\dot{E}_{\mathrm{gas}} = +\Gamma_1\, n_{\mathrm{OH}} + \Gamma_2 n_{\mathrm{OH}} \quad (6)$$

KROME Bootcamp 2015 - Equations first

Photochemistry equations (thin)

$$k_{ph} = \frac{4\pi}{h}\int_{E_0}^{\infty}\frac{I(E)\sigma(E)}{E}\mathrm{d}E \tag{7}$$

$$\Gamma_{ph} = \frac{4\pi}{h}\int_{E_0}^{\infty}\frac{I(E)\sigma(E)}{E}(E-E_0)\eta(E)\mathrm{d}E \tag{8}$$

Units

$$k_{ph} = \left[\mathrm{s}^{-1}\right] \tag{9}$$

$$\Gamma_{ph} = \left[\frac{\mathrm{erg}}{\mathrm{s}}\right] \tag{10}$$

$$E = [\mathrm{eV}] \tag{11}$$

$$I(E) = \left[\frac{\mathrm{eV}}{\mathrm{cm}^2\,\mathrm{s}\,\mathrm{Hz}\,\mathrm{sr}}\right] = \left[\frac{\mathrm{eV}}{\mathrm{cm}^2\,\mathrm{sr}}\right] \tag{12}$$

$$\sigma(E) = \left[\mathrm{cm}^2\right] \tag{13}$$

Photochemistry equations (thin)

$$k_{ph} = \frac{4\pi}{h}\int_{E_0}^{\infty}\frac{I(E)\sigma(E)}{E}\mathrm{d}E \tag{14}$$

$$\Gamma_{ph} = \frac{4\pi}{h}\int_{E_0}^{\infty}\frac{I(E)\sigma(E)}{E}(E-E_0)\eta(E)\mathrm{d}E \tag{15}$$

Bins in KROME

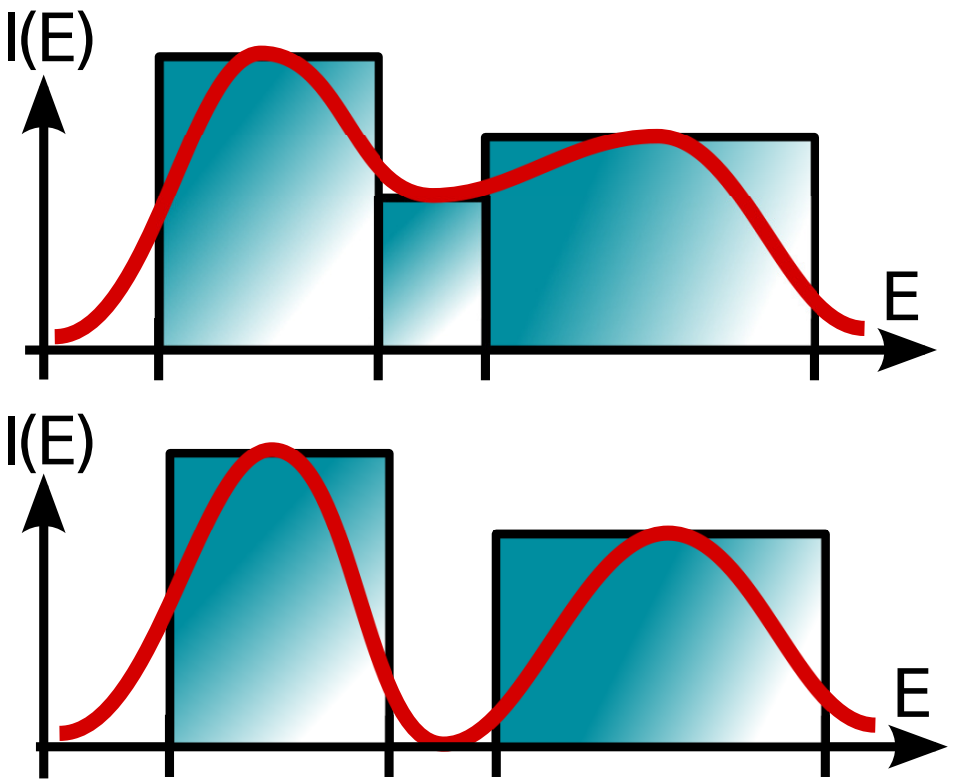
$$k_{ph} = \frac{4\pi}{h}\sum_{i=1}^{N_{bins}}\frac{I_i\sigma_i}{\langle E_i\rangle}(E_i^{right}-E_i^{left}) \qquad \langle E_i\rangle > E_0 \tag{16}$$

$$\Gamma_{ph} = \frac{4\pi}{h}\sum_{i=1}^{N_{bins}}\frac{I_i\sigma_i}{\langle E_i\rangle}(E_i^{right}-E_i^{left})(\langle E_i\rangle - E_0) \tag{17}$$

$$\langle E_i\rangle = \frac{E_i^{right}+E_i^{left}}{2} \tag{18}$$

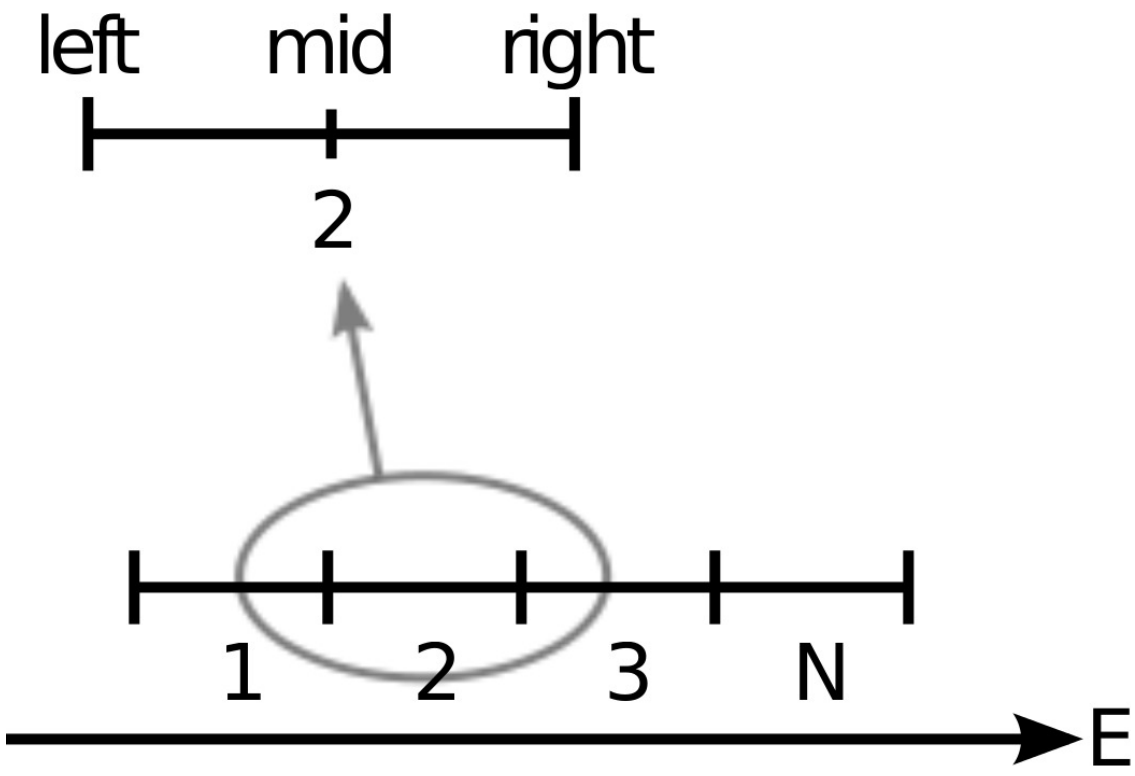
KROME Bootcamp 2015 - I(E) bins

Binning: why and how



$$I(E) = \left[\frac{\mathrm{eV}}{\mathrm{cm}^2\,\mathrm{s}\,\mathrm{Hz}\,\mathrm{sr}}\right] = \left[\frac{\mathrm{eV}}{\mathrm{cm}^2\,\mathrm{sr}}\right]$$

KROME Bootcamp 2015 - Left / Right

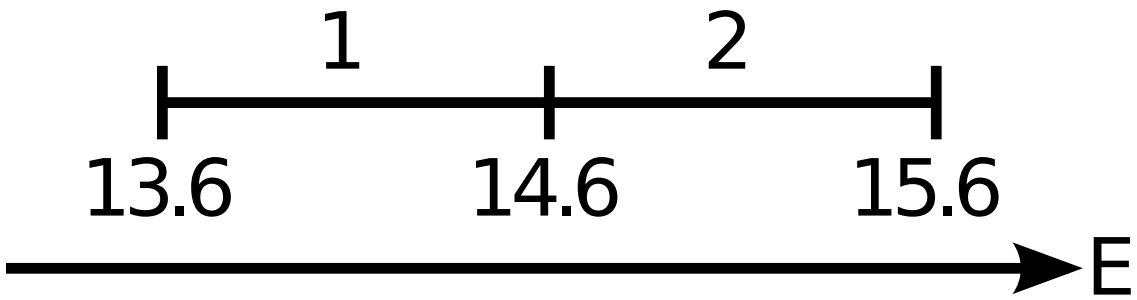


$$\langle E \rangle = E_{\text{mid}} = 0.5\,(E_{\text{left}} + E_{\text{right}})$$

```
use krome_user
krome_set_photoBinE_lr(arrayL(:), arrayR(:))
```

KROME Bootcamp 2015 - Get / Set

```
./krome -n network.ntw -usePhotoBins=2
```

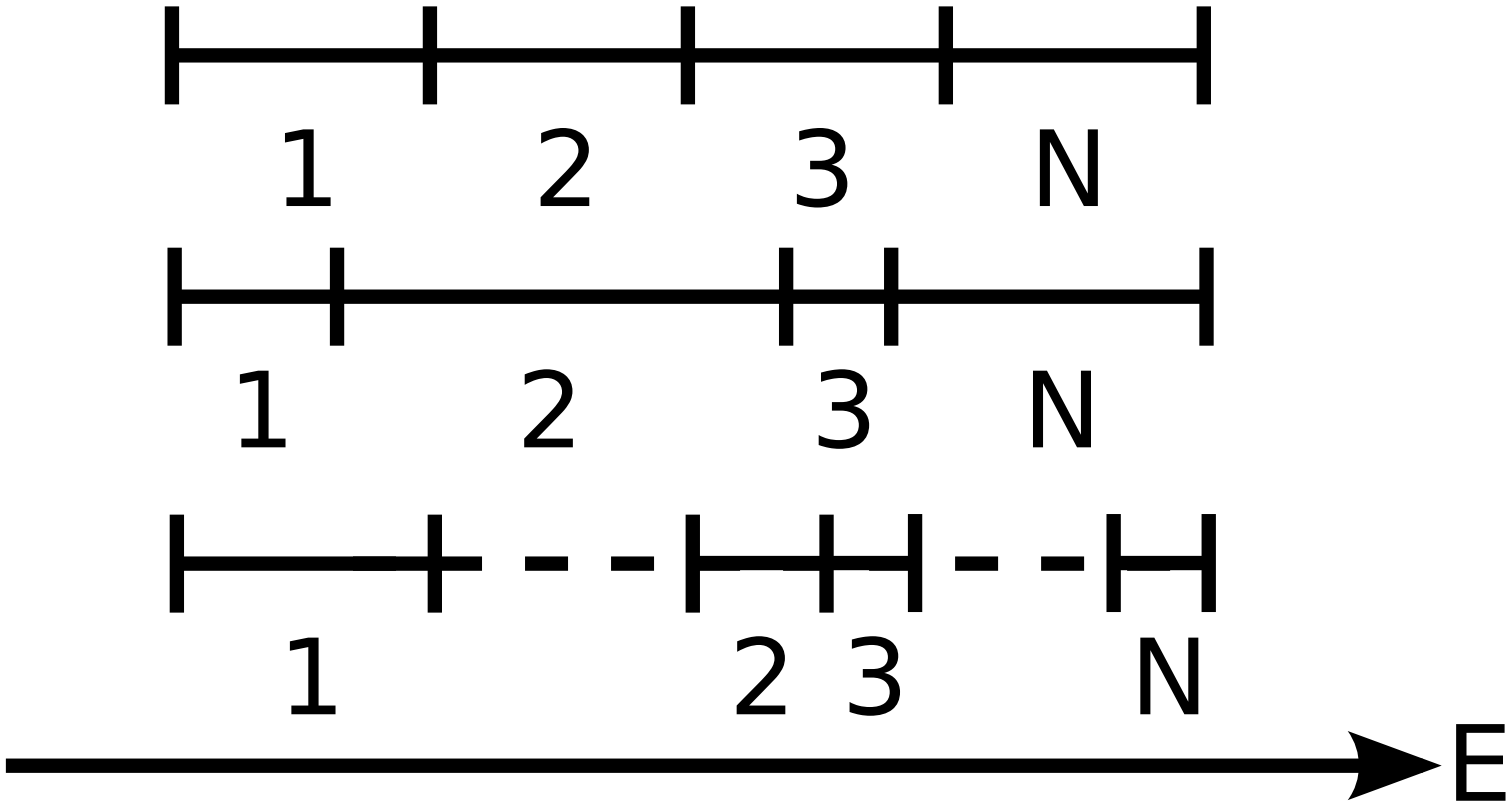



```
use krome_user
real*8::arrayL(krome_nPhotoBins)
real*8::arrayR(krome_nPhotoBins)
arrayL(:) = (/13.6d0, 14.6d0/) !eV
arrayR(:) = (/14.6d0, 15.6d0/) !eV
call krome_set_photobinE_lr(arrayL(:), arrayR(:))
arrayR(:) = krome_get_photoBinE_right()
print *,arrayR(:)
```

```
14.6000000 15.6000000
```

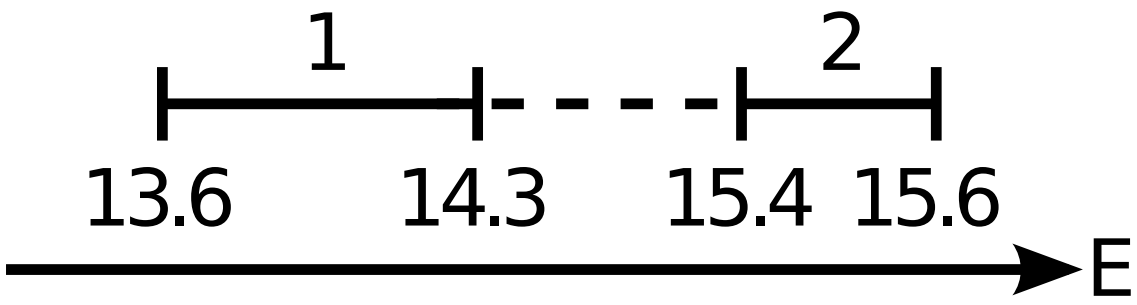
Why left and right?

Left / Right allow to customize intervals (including empty)



KROME Bootcamp 2015 - Custom bins (example)

```
./krome -n network.ntw -usePhotoBins=2
```

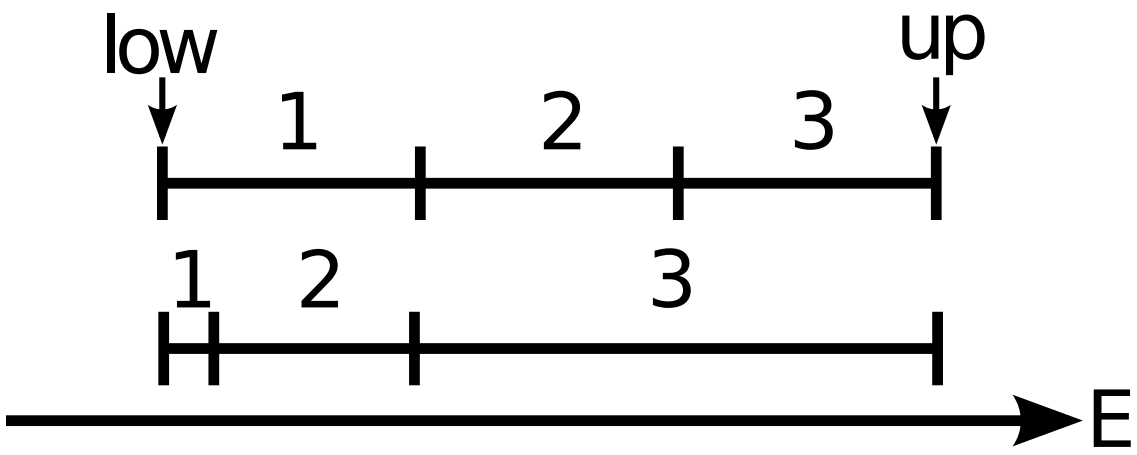



```
real*8::arrayL(krome_nPhotoBins)
real*8::arrayR(krome_nPhotoBins)
arrayL(:) = (/13.6d0, 15.4d0/) !eV
arrayR(:) = (/14.3d0, 15.6d0/) !eV
call krome_set_photobinE_lr(arrayL(:), arrayR(:))
mid(:) = krome_get_photoBinE_mid()
print *,mid(:)
```

```
13.9500000000000    15.5000000000000
```

KROME Bootcamp 2015 - Automatic bins (example)

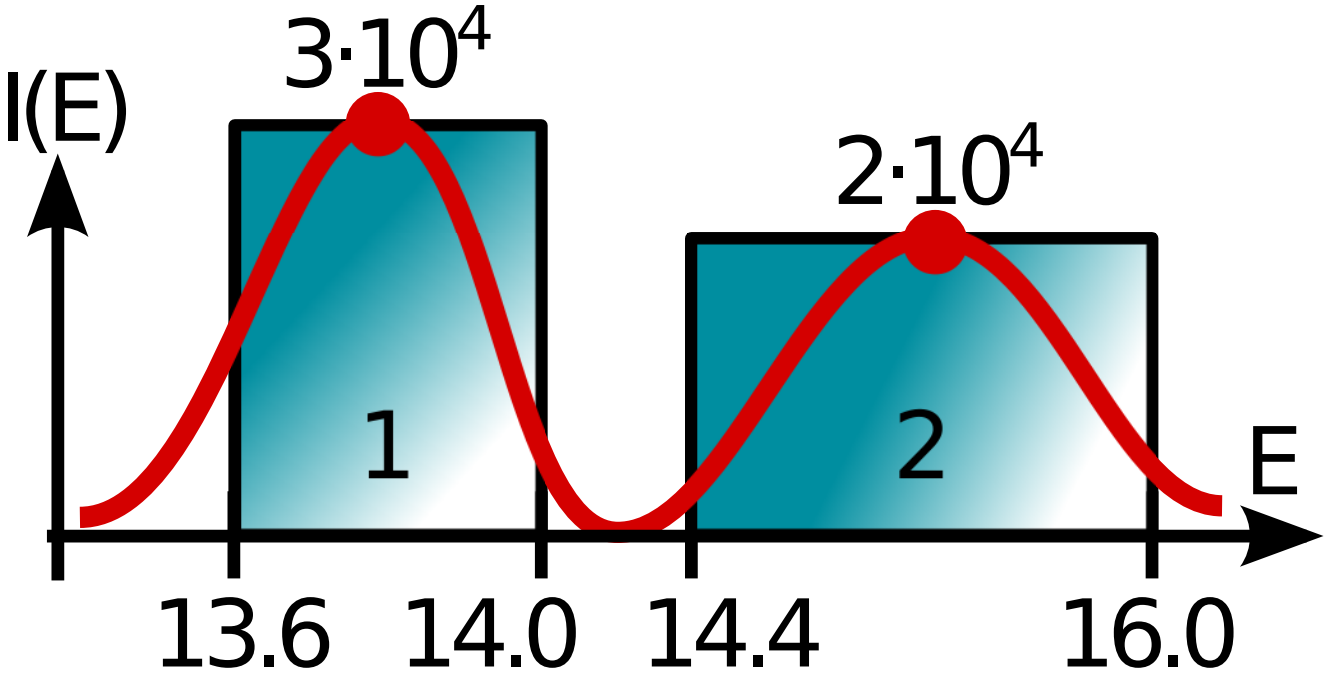
```
./krome -n network.ntw -usePhotoBins=3
```




```
low = 1d0, up = 1d3 !eV
call krome_set_photobinE_lin(low, up)
call print *, krome_get_photoBinE_mid()
call krome_set_photobinE_log(low, up)
call print *, krome_get_photoBinE_mid()
```

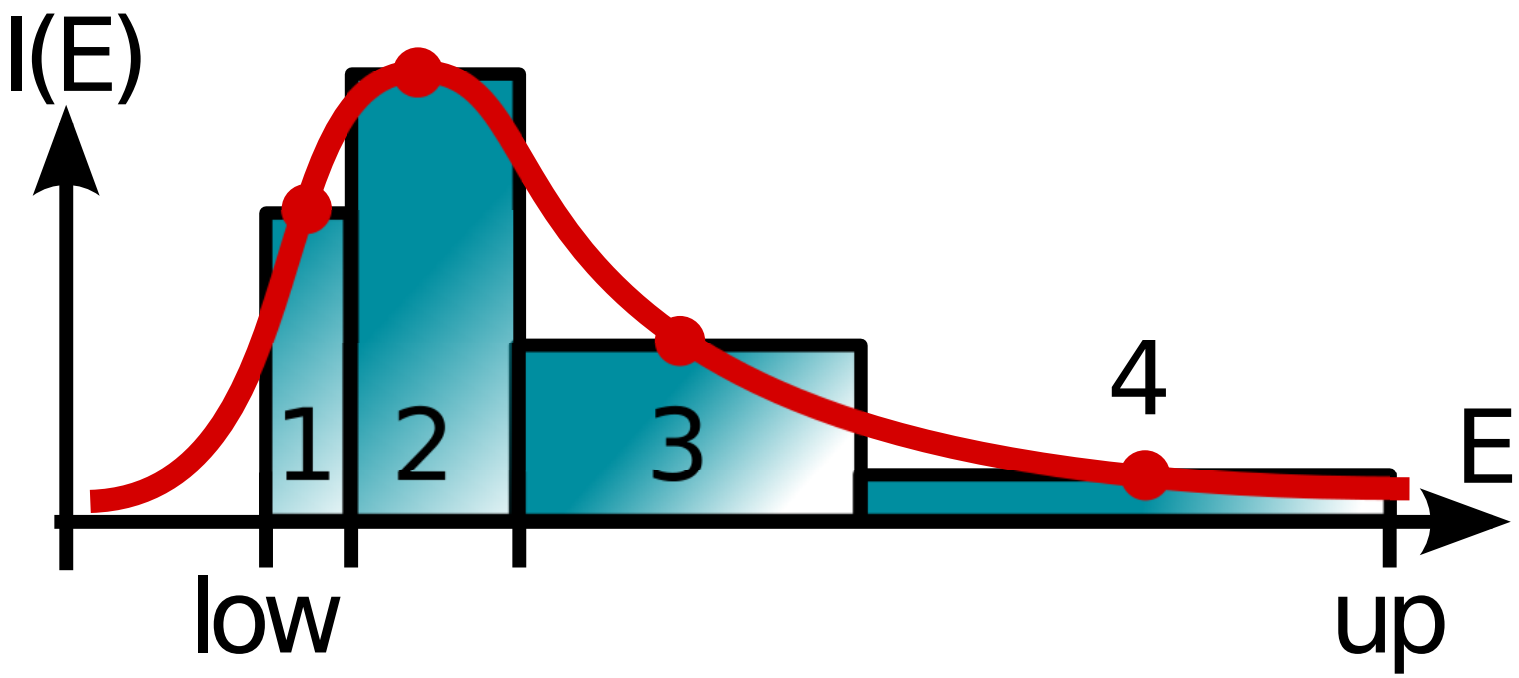
```
167.5000000   500.5000000   833.5000000
5.500000000   55.00000000   550.0000000
```

KROME Bootcamp 2015 - I(E) bins (example)



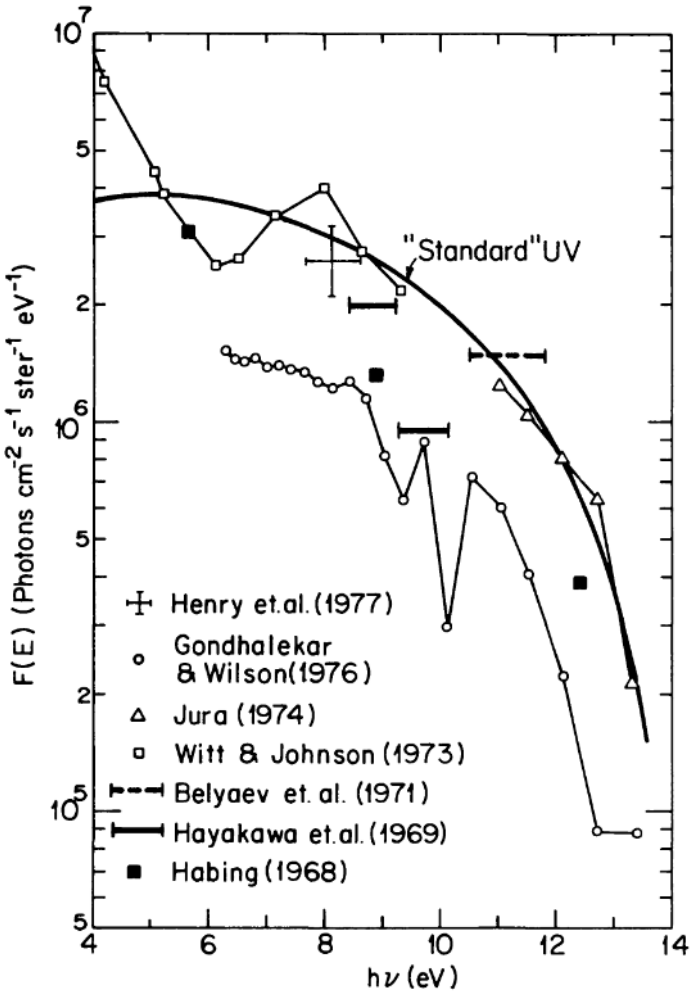

```
arrayL(:) = (/13.6d0, 14.4d0/) !eV
arrayR(:) = (/14.0d0, 16.0d0/) !eV
arrayJ(:) = (/3d4, 2d4/) !eV/cm2/sr
call krome_set_photoBinE_lr(arrayL(:), arrayR(:))
call krome_set_photoBinJ(arrayJ(:))
```

KROME Bootcamp 2015 - Automatic I(E)



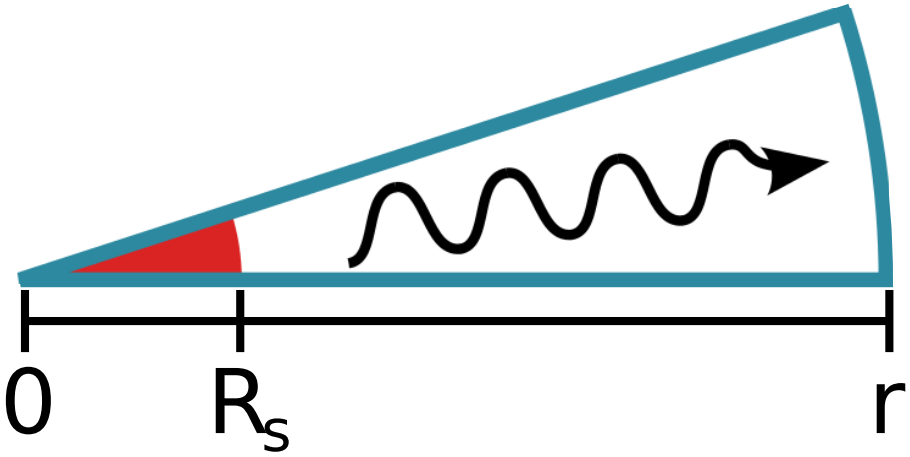

```
low = 5d0 !eV
up  = 2d1 !eV
Tbb = 3d4 !K
call krome_set_photoBin_BBlog(low, up, Tbb)
```

KROME Bootcamp 2015 - Automatic I(E)/2




```
low = 5d0 !eV
up  = 12d0 !eV
call krome_set_photoBin_draineLog(low,up)
```

KROME Bootcamp 2015 - Scaling Example



$$I(E)|_r = \frac{4\pi^2 R_s^2}{4\pi r^2} I(E)|_{R_s}$$

$$k_{ph} = \frac{4\pi}{h} \int_{E_0}^{\infty} \frac{I(E)\sigma(E)}{E} \mathrm{d}E$$

```
low    = 13.6d0     !eV
up     = 20.0d0     !eV
Tbb    = 3d4        !K
Rs     = 1d1*Rsun   !cm
r      = 6d0*pc2cm !cm
iso    = 1d0/(4d0*krome_pi)
call krome_set_photoBin_BBlog(low, up, Tbb)
call krome_photoBin_scale(iso*krome_pi*(Rs/r)**2)
call krome_photoBin_scale_array(xscale(:))
```

KROME Bootcamp 2015 - Cross Sections

$$\mathrm{C} + \gamma \xrightarrow{\sigma(E)} \mathrm{C}^+ + \mathrm{e}^- \tag{19}$$

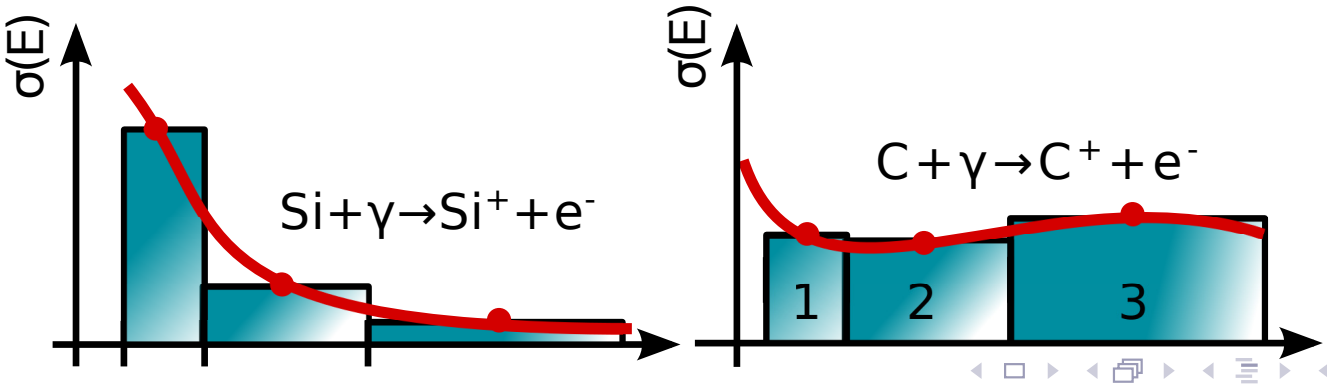
$$\sigma(E) = f(\mathbf{E}, E_0, \sigma_0, y_a, P, y_w, y_0, y_1) \qquad \mathrm{Verner} + 96 \tag{20}$$

$$x = \mathbf{E}/E_0 - y_0 \tag{21}$$

$$y = \sqrt{x^2 + y_1^2} \tag{22}$$

$$F_y = [(x-1)^2 + y_w^2]\, y^{0.5P-5.5}(1 - \sqrt{y/y_a})^{-P} \tag{23}$$

$$\sigma = 10^{-18}\sigma_0\, F_y \quad [\mathrm{cm}^2] \tag{24}$$



How to add a photoreaction to a network file

$\mathrm{H}^- + \gamma \rightarrow \mathrm{H} + \mathrm{e}^-$

```
@format:idx,R,P,P,Tmin,Tmax,rate
@photo_begin
#Wishart+1979
42,H-,H,E,0.755,1d3,2.11d-16*(energy_eV-.755)**(1.5)
                    *energy_eV**(-3)
@photo_end
```

Automatic $\sigma(E)$

$\mathrm{C} + \gamma \rightarrow \mathrm{C}^+ + \mathrm{e}^-$

```
@format:idx,R,P,P,rate
@photo_begin
11,C,C+,E,auto
@photo_end
```

data/database/photoionization.dat

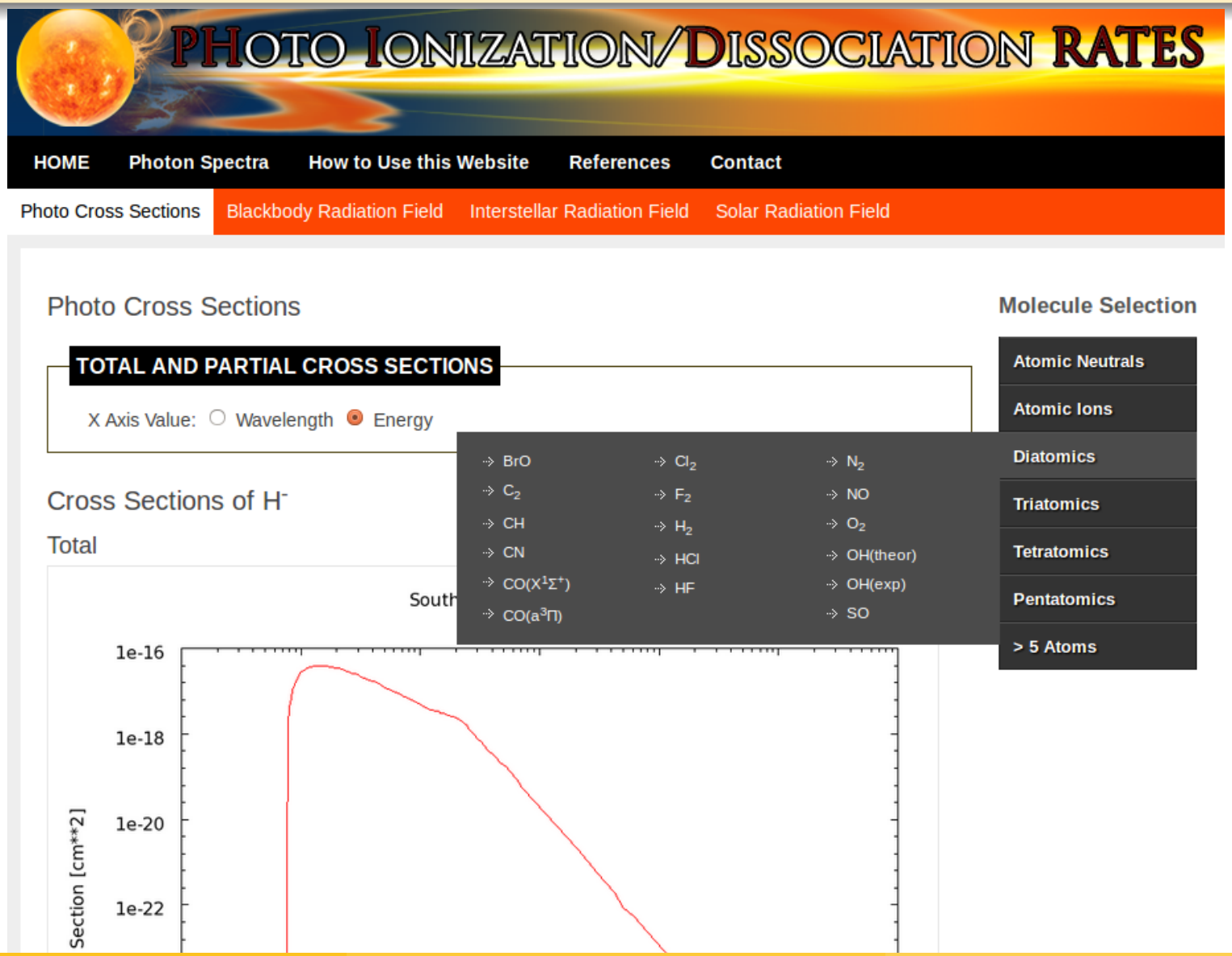
```
#photoionization rate from verner+96
@type: photoion
@reacts: C
@prods: C+, E
@limits: 1.126d+01, 2.910d+02
@rate: sigma_v96(energy_ev, 2.144d+00, ...
```

data/database/radiative_rec.dat

```
#radiative recombination rate from verner+96
@type: radrec
@reacts: He+, E
@prods: He
@limits: 3d0, 1d10
@rate: radrec_v96(Tgas, 3.294d-11, 0.6910d0, ...
```

KROME Bootcamp 2015 - Cross sections (SWRI database)

http://phidrates.space.swri.edu/



External cross section (network)

```
@photo_start
 1,H-,H,H,@xsecFile=SWRI
@photo_end
```

```
data/database/swri_xsecs/H-.dat
```

External cross section (data file)

```
 Branching ratio for H-   Total   2 branches
 Lambda  Total      H+/2e      H/e
    1.0  2.00E-27  0.00E+00  2.00E-27
    5.2  6.11E-25  4.58E-28  6.11E-25
   10.0  5.60E-24  9.00E-27  5.59E-24
   15.5  2.40E-23  6.22E-26  2.39E-23
   20.0  5.53E-23  1.87E-25  5.51E-23
    ...
```

http://home.strw.leidenuniv.nl/~ewine/photo/

N2O cross sections [download]

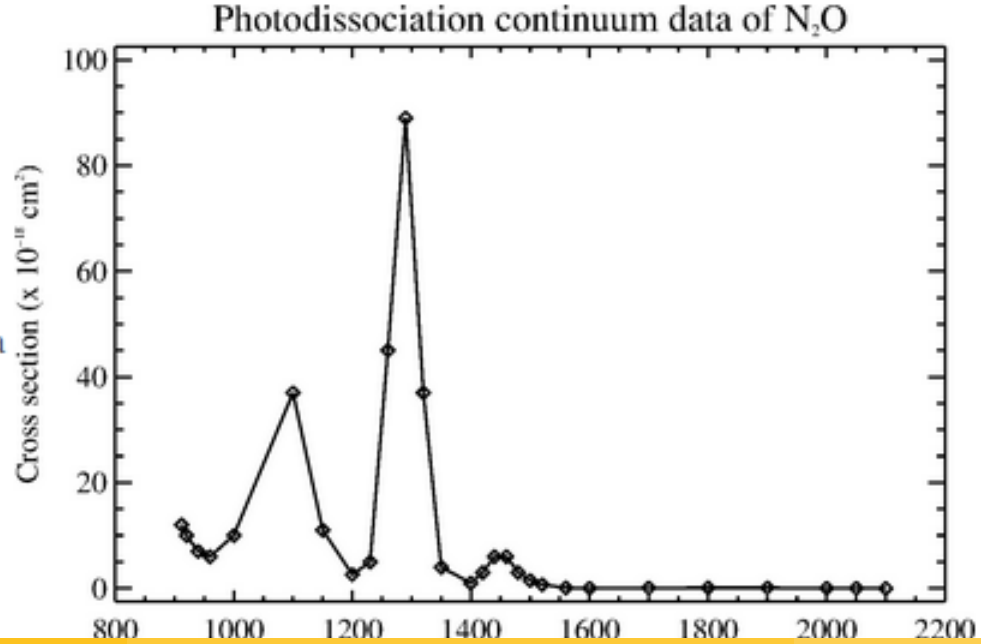
Tabulated photorates [download]

Tabulated photorates in units per second (s^{-1}).

	Draine Field	4000 K	6000 K	10000 K	20000 K
Continuum processes	1.9 (-09)	2.0 (-11)	7.9 (-11)	4.8 (-10)	1.5 (-09)

Figures of cross section versus wavelength [download]

No line data



External cross section (network)

```
@photo_start
 1,N2O,N2,O,@xsecFile=Leiden
@photo_end
```

```
data/database/leiden_xsecs/N2O__N2_O.dat
```

External cross section (data file)

```
 N2O P.D. CF. ZELIKOFF ET AL. ('53)
    0
   28
   -1.
    1    912.0   0.120E-16
    2    920.0   0.100E-16
    3    940.0   0.700E-17
  ...
```

External cross section (network)

```
@photo_start
 1,C,C+,E,@xsecFile=photoC.dat
@photo_end
```

External cross section (data file)

```
#LEFT(eV)  RIGHT(eV)  XSEC(cm2)
14.6       14.8       1.3d-18
20.2       20.5       7.3d-19
...
```

KROME Bootcamp 2015 - Under the hood

```
!loop on energy bins
do j=1,nPhotoBins
   dE = photoBinEdelta(j) !energy interval, eV
   E = photoBinEmid(j) !energy of the bin in eV
   Jval = photoBinJ(j) !intensity eV/s/cm2/sr/Hz
   !loop on reactions
   do i=1,nPhotoRea
      Eth = photoBinEth(i) !reaction energy treshold, eV
      if(E>Eth) then
         kk = 4d0*pi*photoBinJTab(i,j)*Jval/E*dE
         photoBinRates(i) = photoBinRates(i) + kk
         photoBinHeats(i) = photoBinHeats(i) + kk*(E-Eth)
      end if
   end do
end do

photoBinRates(:) = photoBinRates(:) * iplanck_eV !1/s
photoBinHeats(:) = photoBinHeats(:) * iplanck_eV * eV_to_erg !erg/
```

Photochemistry equations (thick)

$$k_{ph} = \frac{4\pi}{h}\int_{E_0}^{\infty}\frac{I(E)\sigma(E)}{E}e^{-\tau(E,\{n\})}\mathrm{d}E \quad (25)$$

$$\tau(E,\{n\}) = \sum_{j\in react}\sigma_{ij}N_j^p + \pi\sum_{j\in dust}Q_{ij}a_j^2N_j^d = \tau_i \quad (26)$$

$$k_{ph} = \frac{4\pi}{h}\sum_{i=1}^{N_{bins}}\frac{I_i\sigma_i}{\langle E_i\rangle}\left(E_i^{right} - E_i^{left}\right)e^{-\tau_i} \quad (27)$$

```
op(:) = krome_get_opacity_size(x(:), Tgas, csize)
```

$$N_j = n_j\, c_{size}$$

```
./krome -n mynetwork.ntw -columnDensityMethod JEANS
op(:) = krome_get_opacity(x(:), Tgas)
```

$$N_j = n_j\, \lambda_j/2$$

Network file

```
@format:idx,R,P,P,rate
@photo_begin
 1,H,H+,E,auto
 2,He,He+,E,auto
 3,C,C+,E,auto
@photo_end
```

```
./krome -n network.ntw -heating=PHOTO
```

$$\Gamma_{ph} = \frac{4\pi}{h}\sum_{i=1}^{N_{bins}}\frac{I_i\sigma_i}{\langle E_i\rangle}(E_i^{right}-E_i^{left})(\langle E_i\rangle - E_0) \quad (28)$$

Conclusions

1. Understand that ~~cooling processes~~ photochemistry is are a mess
2. Realize that KROME saves your day*

* modulo databases

Thank you for your attention!

"and God said, - let there be light! - and
SEGMENTATION FAULT (CORE DUMPED)"
(Anonymous)

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KROME
better science through chemistry

http://kromepackage.org/
http://kromepackage.org/bootcamp