

# Photochemistry in KROME

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## Aims of this talk

- 1 Understand how photobinning works
- 2 How to include photochemical reactions in KROME
- 3 Get opacity from KROME

## Photochemistry equations (thin)

$$k_{ph} = \frac{4\pi}{h} \int_{E_0}^{\infty} \frac{I(E)\sigma(E)}{E} dE \quad (1)$$

$$\Gamma_{ph} = \frac{4\pi}{h} \int_{E_0}^{\infty} \frac{I(E)\sigma(E)}{E} (E - E_0)\eta(E) dE \quad (2)$$

## Units

$$k_{ph} = [s^{-1}] \quad (3)$$

$$\Gamma_{ph} = \left[ \frac{\text{erg}}{\text{s}} \right] \quad (4)$$

$$E = [\text{eV}] \quad (5)$$

$$I(E) = \left[ \frac{\text{eV}}{\text{cm}^2 \text{ s Hz sr}} \right] = \left[ \frac{\text{eV}}{\text{cm}^2 \text{ sr}} \right] \quad (6)$$

$$\sigma(E) = [\text{cm}^2] \quad (7)$$

## Photochemistry equations (thin)

$$k_{ph} = \frac{4\pi}{h} \int_{E_0}^{\infty} \frac{I(E)\sigma(E)}{E} dE \quad (8)$$

$$\Gamma_{ph} = \frac{4\pi}{h} \int_{E_0}^{\infty} \frac{I(E)\sigma(E)}{E} (E - E_0)\eta(E) dE \quad (9)$$

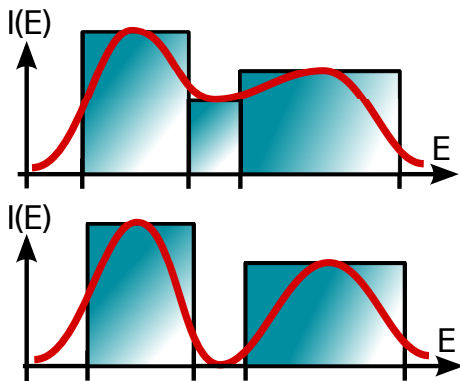
## Bins in KROME

$$k_{ph} = \frac{4\pi}{h} \sum_{i=1}^{N_{bins}} \frac{I_i \sigma_i}{\langle E_i \rangle} (E_i^{right} - E_i^{left}) \quad \langle E_i \rangle > E_0 \quad (10)$$

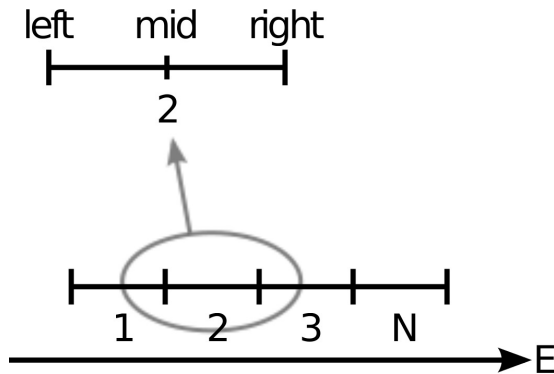
$$\Gamma_{ph} = \frac{4\pi}{h} \sum_{i=1}^{N_{bins}} \frac{I_i \sigma_i}{\langle E_i \rangle} (E_i^{right} - E_i^{left}) (\langle E_i \rangle - E_0) \quad (11)$$

$$\langle E_i \rangle = \frac{E_i^{right} + E_i^{left}}{2} \quad (12)$$

## Binning: why and how



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



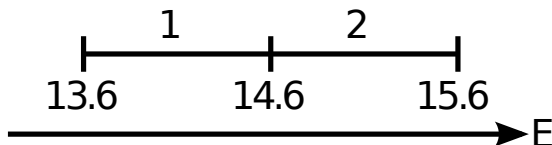
$$\langle E \rangle = E_{\text{mid}} = 0.5(E_{\text{left}} + E_{\text{right}})$$

```
use krome_user
```

```
call krome_set_photoBinE_lr(arrayL(:), arrayR(:))
```

# KROME Bootcamp 2018 - Get / Set

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

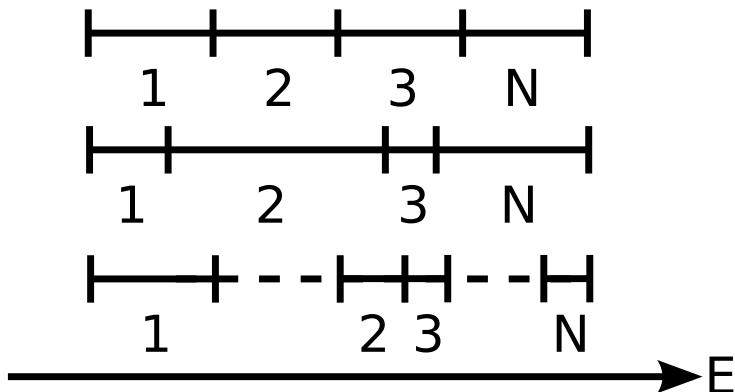


```
use krome_user
real*8::arrayL(krome_nPhotoBins)
real*8::arrayR(krome_nPhotoBins)
arrayL(:) = (/13.6d0, 14.6d0/) !eV
arrayR(:) = (/14.6d0, 15.6d0/) !eV
call krome_set_photobinE_lr(arrayL(:), arrayR(:))
arrayR(:) = krome_get_photoBinE_right()
print *,arrayR(:)
```

```
14.6000000 15.6000000
```

## Why left and right?

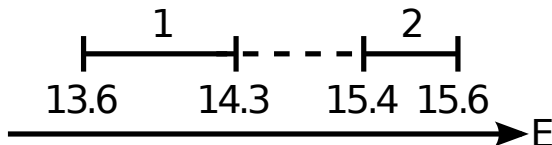
Left / Right allow to customize intervals (including empty)





# KROME Bootcamp 2018 - Custom bins (example)

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



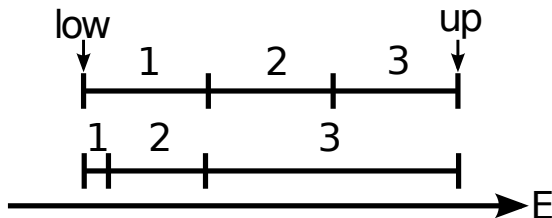
```
real*8::arrayL(krome_nPhotoBins)
real*8::arrayR(krome_nPhotoBins)
arrayL(:) = (/13.6d0, 15.4d0/) !eV
arrayR(:) = (/14.3d0, 15.6d0/) !eV
call krome_set_photobinE_lr(arrayL(:), arrayR(:))
mid(:) = krome_get_photoBinE_mid()
print *,mid(:)
```

```
13.950000000000000
```

```
15.500000000000000
```

# KROME Bootcamp 2018 - Automatic bins (example)

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

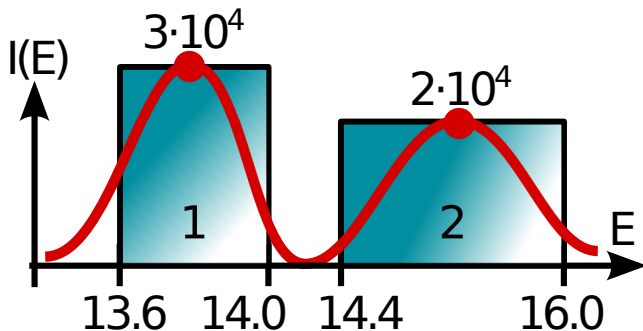


```
low = 1d0, up = 1d3 !eV
```

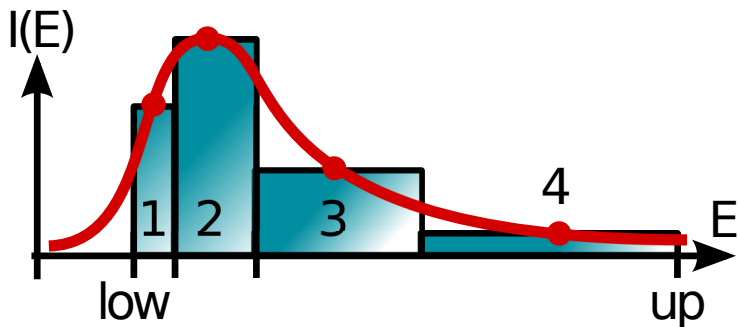
```
call krome_set_photobinE_lin(low, up)
call print *, krome_get_photoBinE_mid()
call krome_set_photobinE_log(low, up)
call print *, krome_get_photoBinE_mid()
```

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

# KROME Bootcamp 2018 - I(E) bins (example)

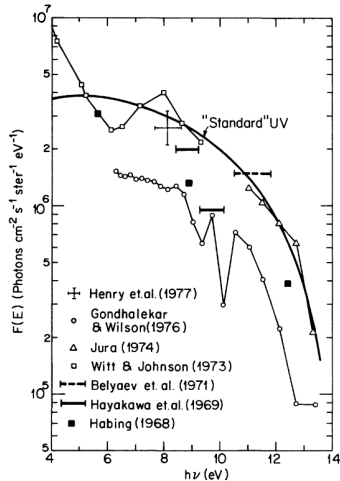


```
arrayL(:) = (/13.6d0, 14.4d0/) !eV  
arrayR(:) = (/14.0d0, 16.0d0/) !eV  
arrayJ(:) = (/3d4, 2d4/) !eV/cm2/sr  
call krome_set_photoBinE_lr(arrayL(:), arrayR(:))  
call krome_set_photoBinJ(arrayJ(:))
```



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

# KROME Bootcamp 2018 - Automatic I(E)/2

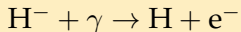


low = 5d0 !eV

up = 12d0 !eV

call krome\_set\_photoBin\_draineLog(low, up)

## How to add a photoreaction to a network file



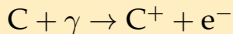
```
@format:idx,R,P,P,Tmin,Tmax,rate
```

```
@photo_begin
```

```
42,H-,H,E,0.755,1d3,2.11d-16*(energy_eV-.755)**(1.5)  
*energy_eV**(-3)
```

```
@photo_end
```

## Automatic $\sigma(E)$



```
@photo_begin
```

```
11,C,C+,E,auto
```

```
@photo_end
```

**NOTE: KROME is not a reaction database (GIGO)!**

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



HOME Photon Spectra How to Use this Website References Contact

Photo Cross Sections Blackbody Radiation Field Interstellar Radiation Field Solar Radiation Field

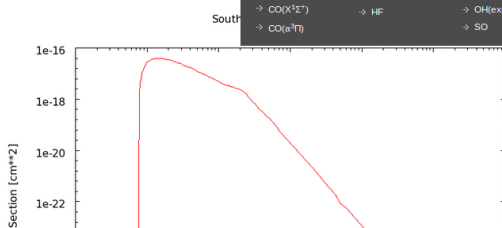
## Photo Cross Sections

### TOTAL AND PARTIAL CROSS SECTIONS

X Axis Value:  Wavelength  Energy

## Cross Sections of H<sup>+</sup>

Total



## Molecule Selection

Atomic Neutrals

Atomic Ions

Diatomics

Triatomics

Tetramomics

Pentatomics

> 5 Atoms

## 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  
  . . .
```

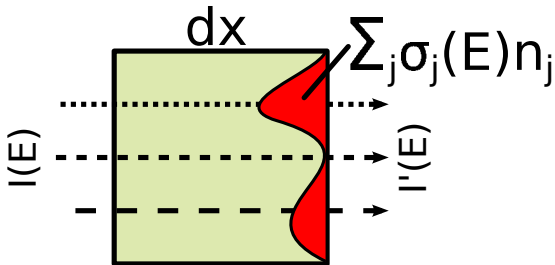


## External cross section (network)

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

## External cross section (data file)

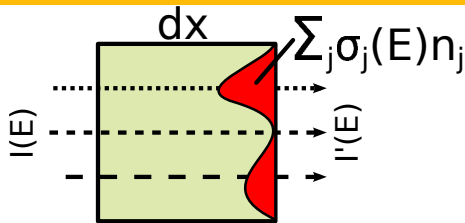
#LEFT (eV)	RIGHT (eV)	XSEC (cm <sup>2</sup> )
14.6	14.8	1.3d-18
20.2	20.5	7.3d-19
...		



## Opacity

$$I'(E) = I(E)e^{-\tau(E, \mathbf{n})}$$

$$\begin{aligned} \tau(E, \mathbf{n}) \rightarrow \tau_j &= \sum_{j \in \text{react}} \sigma_{ij} n_j \Delta x \\ &+ \pi \sum_{j \in \text{dust}} Q_{ij} a_j^2 n_j^d \Delta x \end{aligned}$$



## No size information (assumes geometry)

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

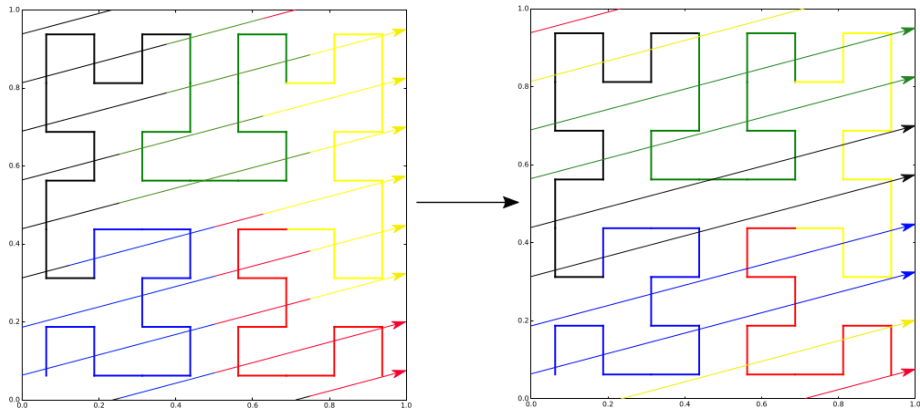
## Use table for dust opacity (size-based)

```
krome_load_opacity_table(fileName)  
krome_get_opacity_size_d2g(n(:), Tgas, dx, dust2gas)
```

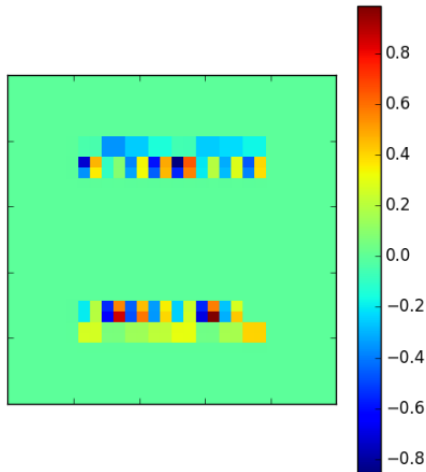
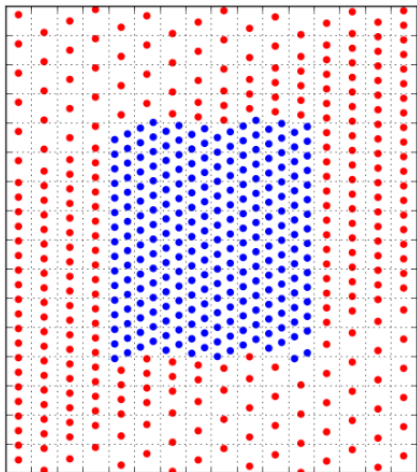
## Fully-consistent (size-based)

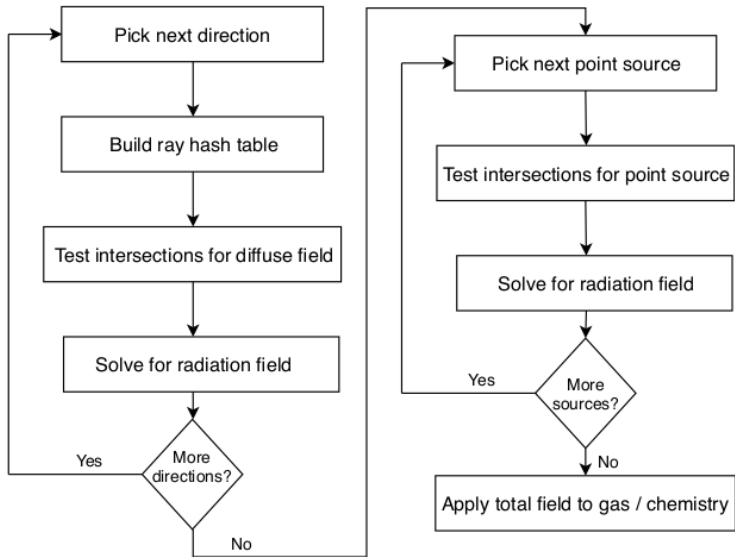
```
krome_get_opacity_size(n(:), Tgas, dx)
```

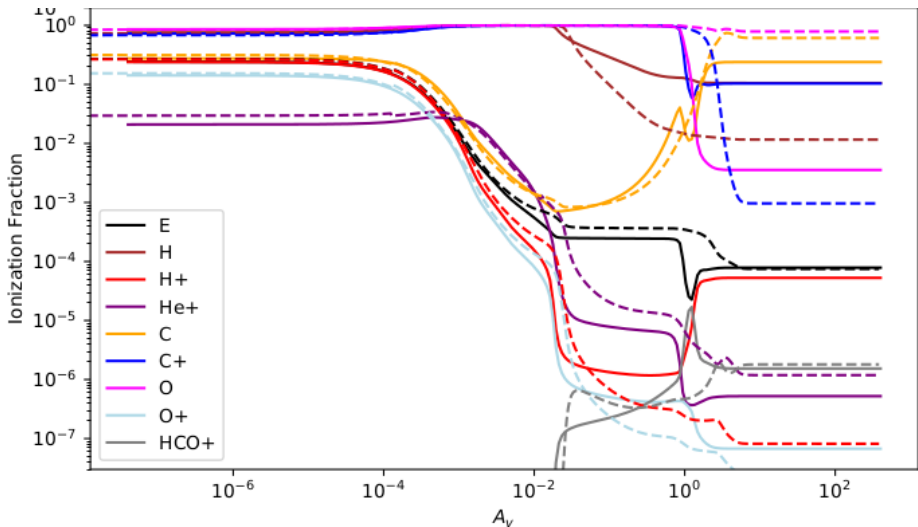
# LAMPRAY (Frostholtm, Haugbølle, & TG, arXiv:1809.05541)



colors are MPI ranks







vs. Richings+2014b, see also Röllig+2007

## What you learned

- 1 KROME photobinning
- 2 Include photochemical reactions in KROME (cross sections)
- 3 How to get opacity from KROME

(Thank you for your attention!)