

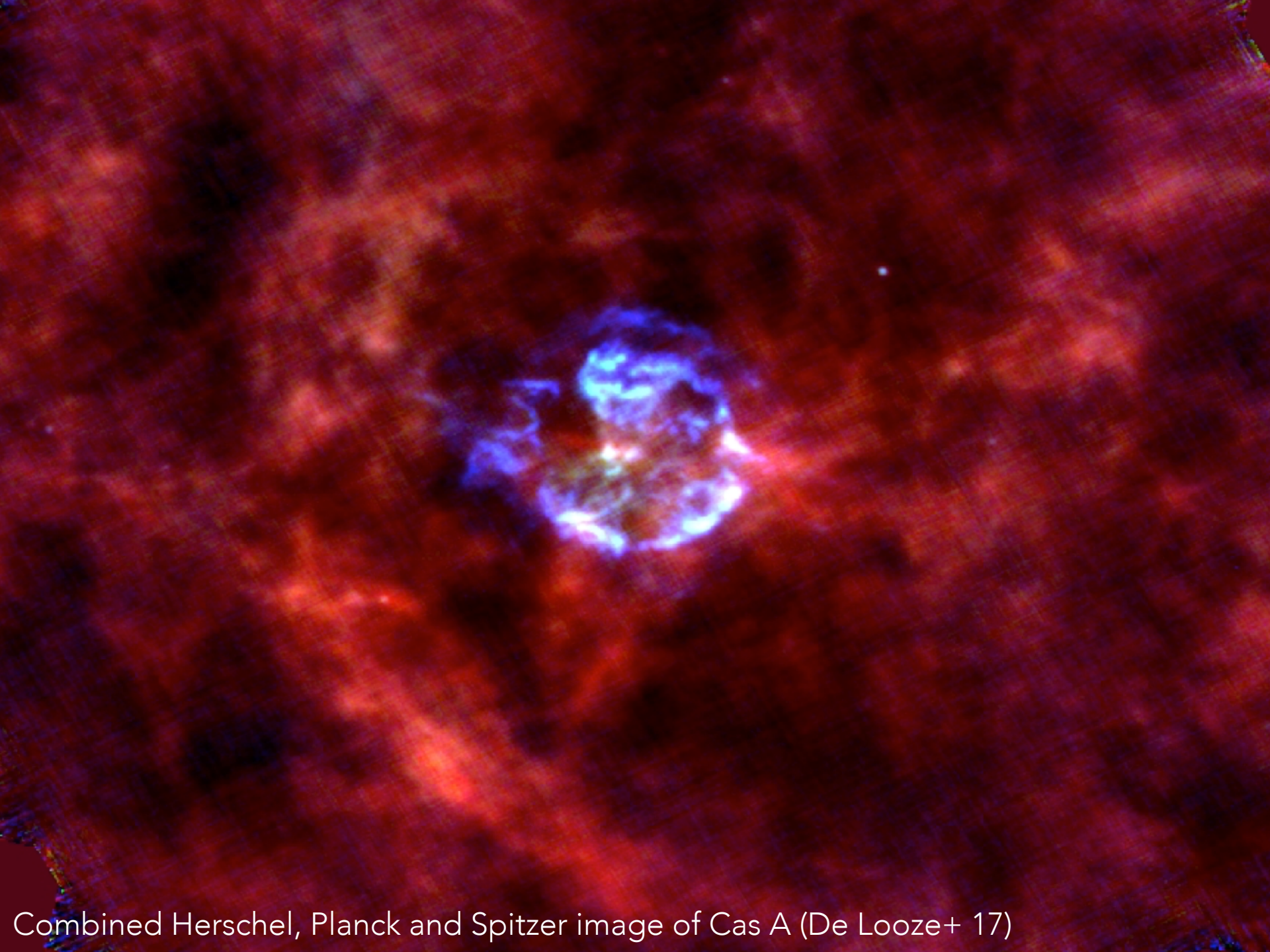
PUTTING THEORY INTO PRACTICE: HOW TO WRITE AN MCRT CODE

Antonia Bevan, UCL

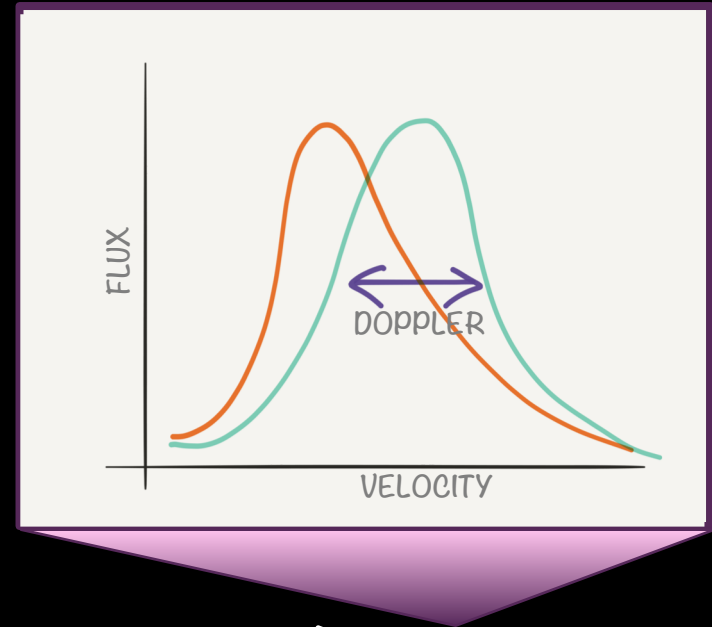
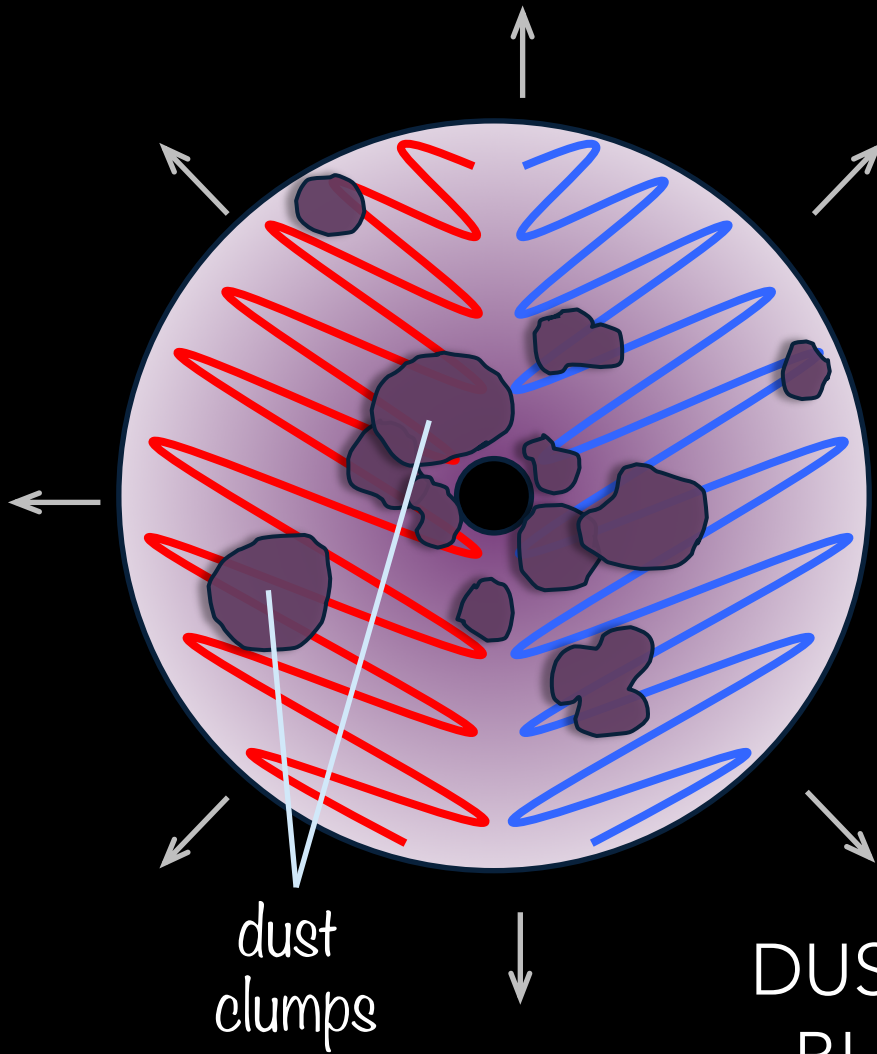
St Andrews Monte Carlo Summer School 2019

Me in October 2012
just after I started my PhD



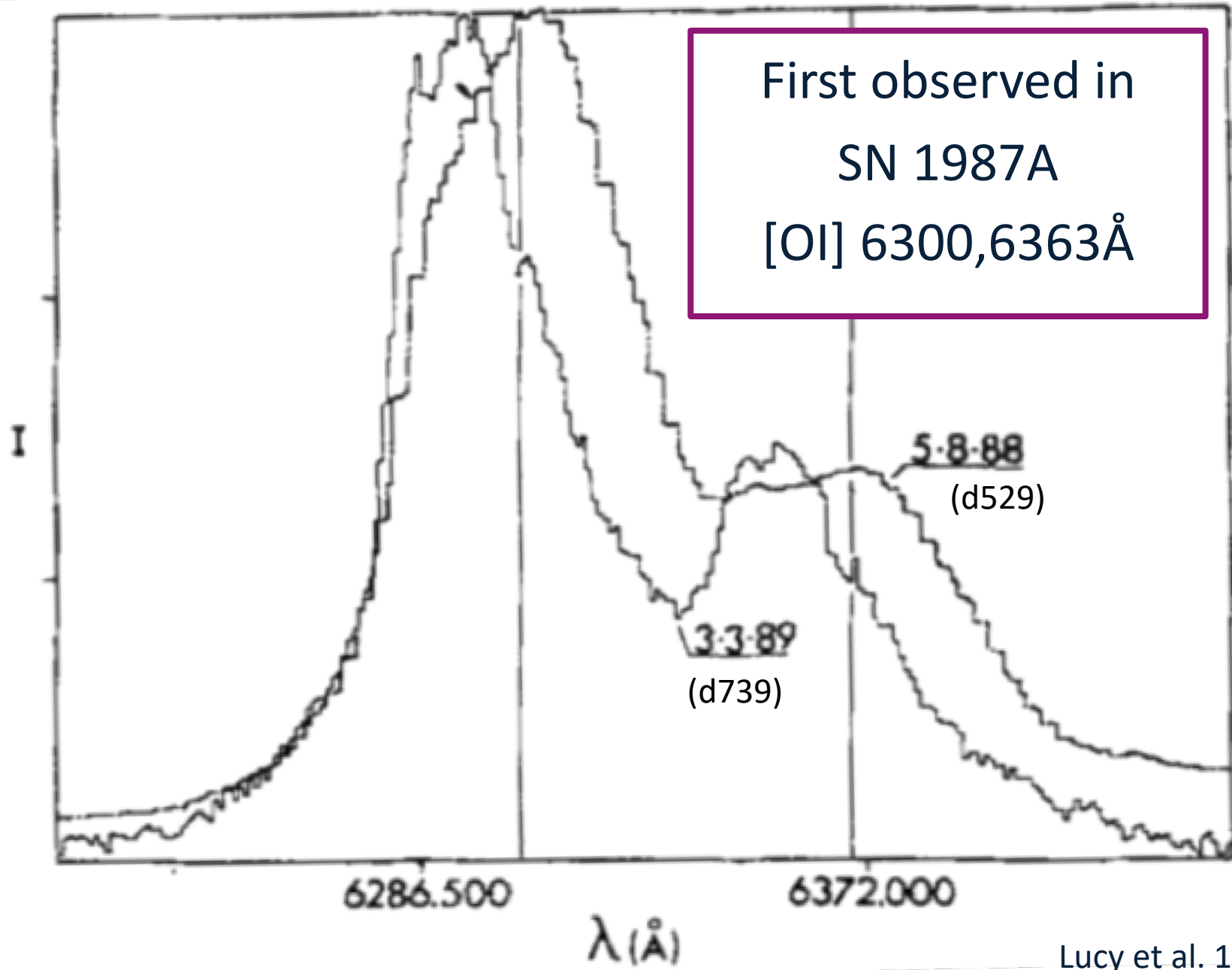


Combined Herschel, Planck and Spitzer image of Cas A (De Looze+ 17)



observer

DUST IN CCSN EJECTA CAUSES
BLUE-SHIFTED EMISSION LINE
PROFILES IN OPTICAL AND IR



CHALLENGE:
WRITE A MONTE CARLO RADIATIVE
TRANSFER CODE THAT WILL...

?

Dust absorption
and scattering

Smooth or
clumped dust
distribution

3D Monte Carlo
radiative transfer
code

Smooth or
clumped
emissivity
distribution

Dust Affected Models Of Characteristic Line Emission in Supernovae

Simple electron
scattering

Velocity field
 $\mathbf{v}(\mathbf{r})$
at fixed time

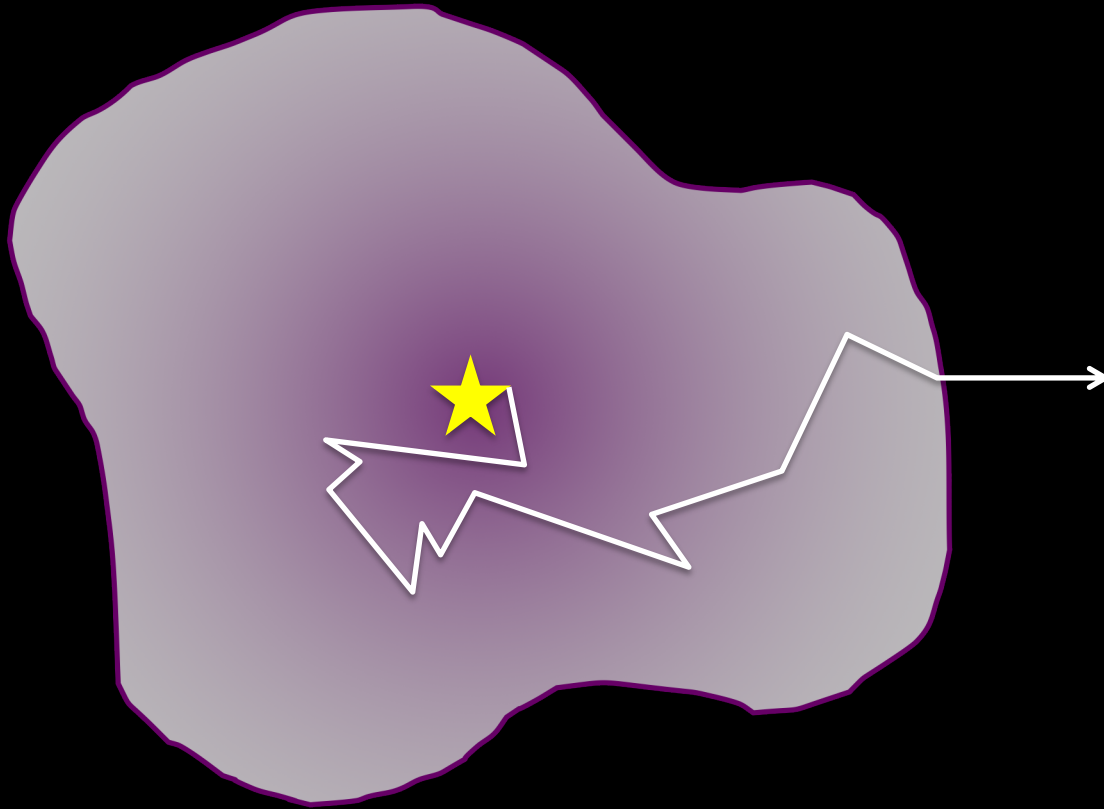
Any dust grain
size distribution

Any combination
of dust species

ASK YOURSELF QUESTIONS...

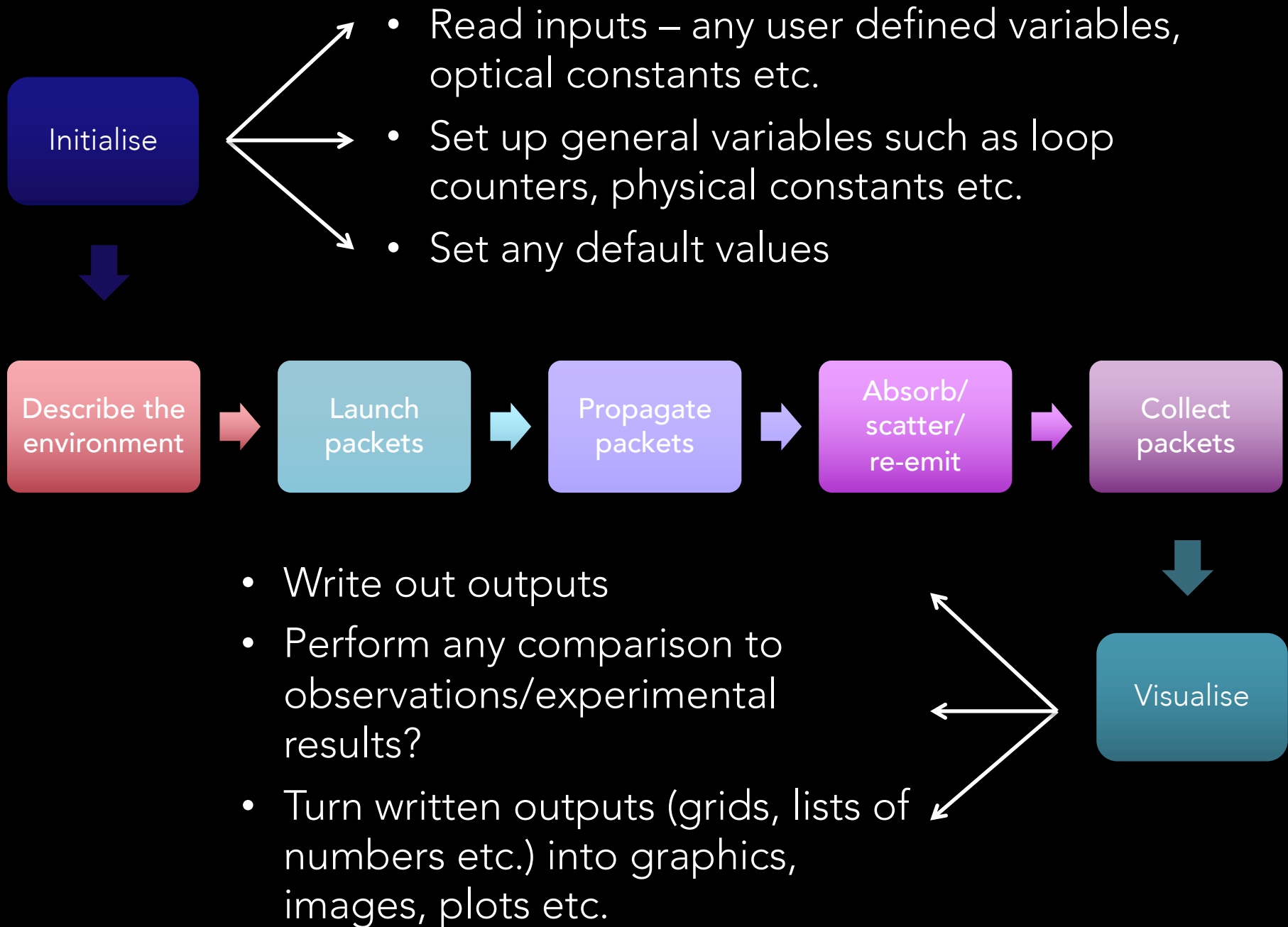
- Where will this go? Will I want to add capacity in future? Is there anything I can do now to make that easier?
- What are the inputs? What are the outputs? What will you do with your outputs?
- Which processes/physics/stats/magic will take you from your inputs to your outputs?
- What can/can't you assume?

MAP OUT YOUR PROBLEM



MCRT codes have the same basic premise but different physics, process and products





INITIALISE

Initialise

Describe the environment

Launch packets

Propagate packets

Absorb/
scatter/
re-emit

Collect packets

Visualise



Initialise

Describe the environment

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QUESTIONS TO ASK

What now?

- You're going to need to make some decisions about your tools
 - Fortran or C or Python or... or... or...?
[you may choose to use multiple]
 - OpenMP or MPI?
 - IDE? text editor?
 - Compiler?
 - Computer...!
 - Which version control – Git, SVN etc.?



USE VERSION
CONTROL



```
graph LR; A[Initialise] --> B[Describe the environment]; B --> C[Launch packets]; C --> D[Propagate packets]; D --> E[Absorb/scatter/re-emit]; E --> F[Collect packets]; F --> G[Visualise];
```

Initialise

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DAMOCLES

DAMOCLES development:

- Fortran 95 + Python
- Tools I use:
 - Eclipse IDE with Photran
 - Sublime Text & emacs for text editing
 - GitHub for version control
 - gcc compilers
 - Develop on my MacBook and run on my MacBook and clusters at UCL

Initialise

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Visualise

my_mcrt_code.f95 *

```
1 program my_mcrt_code  
2  
3 end program
```


Initialise

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my_mcrt_code.f95 *

```
1 program my_mcrt_code
2
3 end program
```

USE
MODULES

```
1 !-----!
2 ! DAMOCLES is a Monte Carlo radiative transfer code to model transfer of !
3 ! a single emission line or doublet through a cartesian grid of dust of !
4 ! multiple species and grain size distributions. !
5 ! !
6 ! Copyright (C) 2017 Antonia Bevan !
7 ! Department of Physics and Astronomy !
8 ! University College London !
9 ! London, WC1E 6BT, UK !
10 ! antoniab@star.ucl.ac.uk !
11 ! !
12 ! This program is free software; you can redistribute it and/or !
13 ! modify it under the terms of the GNU General Public License !
14 ! as published by the Free Software Foundation; either version 2 !
15 ! of the License, or (at your option) any later version. This requires !
16 ! that any changes or improvements made to the program should also be !
17 ! made freely available. !
18 ! !
19 ! This program is distributed in the hope that it will be useful, !
20 ! but WITHOUT ANY WARRANTY; without even the implied warranty of !
21 ! MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE. See the !
22 ! GNU General Public License for more details. !
23 ! !
24 ! DAMOCLES = Dust Affected Models Of Characteristic Line !
25 ! Emission in Supernovae !
26 ! Version 3.0 !
27 !-----!
28
29 !-----!
30 ! the main program is run from here !
31 ! - the driver is included in a module such that it can be run !
32 ! as a function using other languages/script e.g. a python wrapper !
33 !-----!
34 program damocles
35
36 use globals
37 use input
38 use initialise
39 use vector_functions
40 use driver
41
42 implicit none
43
44 character(len=50) :: infile !specified input file
45
46 !check number of input arguments is 1 (the name of the input file)
47 n_args=command_argument_count()
48 if (n_args==1) then
49 call get_command_argument(1,infile)
50
```

Initialise

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Visualise

my_mcrt_code.f95 *

```
1 program my_mcrt_code
2
3 end program
```

globals.f95 *

```
1 module globals
2
3
4
5
6
7
8
9 end module globals
```

my_mcrt_code.f95 *

USE
MODULES

Initialise

Describe the environment

Launch packets

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scatter/
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Collect packets

Visualise

```
my_mcrt_code.f95  global
1  program my_mcrt_code
2
3  use globals
4
5  end program
```

```
globals.f95  my_mcrt_code.f95 *
1  module globals
2
3  !loop variables
4
5  integer :: ii, jj, kk
6
7
8  |!physical constants
9
10 real, parameter :: pi = 3.141592654
11 real, parameter :: c_light = 3.0e8
12
13
14 end module globals
```

USE
MODULES

Initialise

Describe the environment

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Visualise

my_mcrt_code.f95

global

```
1 program my_mcrt_code
2
3 use globals
4
5 end program
```

```
1
2 ! declare here all global variables such as counters, constants etc. !
3 -----
4
5 module globals
6
7   implicit none
8
9   !openmp variables
10  integer,external :: omp_get_num_threads
11  integer,external :: omp_get_thread_num
12  integer          :: thread_id
13  integer          :: num_threads
14
15  !counters
16  integer          :: ii,jj,kk
17  integer          :: ixx,iyy,izz
18  integer          :: ish
19  integer          :: i_dir
20  integer          :: i_spec
21  integer          :: i_doublet
22  integer          :: i_packet
23  integer          :: i_clump
24
25  ! save i_packet
26
27  !dummy counters
28  integer          :: xx,yy,zz
29
30  !identifiers
31  integer          :: ig
32  integer          :: id_theta,id_phi
33  integer          :: id_no
34
35  !random numbers and functions
36  real             :: random(5), ran
37  !real,external  :: r4_uni_01
38  !$OMP THREADPRIVATE(random,ran)
39
40  !constants
41  real, parameter :: pi=3.141592654
42  real,parameter  :: c=3e8                !in si units (m/s)
43
```

USE
MODULES

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my_mcrt_code.f95

input

```
1  program my_mcrt_code
2
3  use globals
4  use input
5
6  call read_input_()
7
8  end program
```

input.f95

*

my_mcrt_code.f95

globals.f9

```
1  module input
2
3  real :: line_frequency
4  real :: minimum_velocity
5  real :: maximum_velocity
6  real :: velocity_power
7
8  contains
9
10     subroutine read_input()
11
12         open(unit = 30, file = 'input_file.in')
13         read(30,*) line_frequency
14         read(30,*) minimum_velocity
15         read(30,*) maximum_velocity
16         read(30,*) velocity_power
17         close(30)
18
19     end subroutine
20
21 end module input
22
```

USE
MODULES

```
graph LR; A[Initialise] --> B[Describe the environment]; B --> C[Launch packets]; C --> D[Propagate packets]; D --> E[Absorb/scatter/re-emit]; E --> F[Collect packets]; F --> G[Visualise];
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RECAP

MODULAR STRUCTURE

- We're building up the program block by block
- 'Program file' – runs the main body of the code calling functions and subroutines
- Break up your code into sections and save them in different files
- FORTRAN – if module A 'uses' module B, then all variables, subroutines and functions declared in module B can be seen and updated by module A
- I put all my variables, subroutines and functions in modules grouped by categories e.g. 'dust'

DESCRIBE THE ENVIRONMENT

Initialise

Describe the
environment

Launch
packets

Propagate
packets

Absorb/
scatter/
re-emit

Collect
packets

Visualise



```
graph LR; A[Initialise] --> B[Describe the environment]; B --> C[Launch packets]; C --> D[Propagate packets]; D --> E[Absorb/scatter/re-emit]; E --> F[Collect packets]; F --> G[Visualise];
```

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QUESTIONS TO ASK

- What is it made of?
 - Dust? Gas? Skin? Rocks?
 - Can I describe how light interacts with it?
- Where is it?
 - Density distribution – Smooth? Clumpy? Layered?
 - Physical extent – how big is it [and how do I want to describe that]?
- How should I describe it?
 - Analytic? Grid?

Initialise

Describe the environment

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Collect packets

Visualise

my_mcrt_code.f95

```
1  program my_mcrt_code
2
3  use globals
4  use input
5  use grids
6  use dust
7
8  call read_input()
9
10 end program
```

dust.f95

```
1  module dust
2
3  integer :: n_dust_species
4  real    :: grain_radius
5  real    :: grain_density
6  real    :: dust_mass
7
8
9  end module dust
```

globals.f95

my_mcrt_

grid.f95

```
1  module grid
2
3  integer :: n_cells
4
5  real    :: x_div, y_div, z_div
6  real,allocatable(:,,:) :: mothergrid
7
8
9  end module grid
```

dust.f95

globals.f95

Initialise

Describe the environment

Launch packets

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Visualise

my_mcrt_code.f95

input.f95

```
1  program my_mcrt_code
2
3  use globals
4  use input
5  use grids
6  use dust
7  |
8  call read_input()
9  call calculate_dust_properties()
10
11 end program
```

grid.f95

my_mcrt_code.f95

dust.f95

```
1  module dust
2
3  integer :: n_dust_species
4  real    :: grain_radius
5  real    :: grain_density
6  real    :: dust_mass
7
8  !...
9
10 contains
11   subroutine calculate_dust_properties()
12
13       !e.g. work out extinction efficiencies
14       !by reading in optical constants
15       !and running a Mie routine
16
17   end subroutine calculate_dust_properties
18
19
20 end module dust
```

USE
LIBRARIES
AND
PACKAGES

Initialise

Describe the environment

Launch packets

Propagate packets

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scatter/
re-emit

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Visualise

my_mcrt_code.f95

input.f95

```
1  program my_mcrt_code
2
3  use globals
4  use input
5  use grids
6  use dust
7  use packet
8
9  call read_input()
10 call calculate_dust_properties()
11 call build_grid()
12
13 end program
```

grid.f95

my_mcrt_code.f95

dust.f95

```
1  module grid
2
3  integer           :: n_cells
4
5  real              :: x_div, y_div, z_div
6  real,allocatable :: mothergrid
7
8  !...
9
10 contains
11
12   subroutine build_grid()
13
14     !this would, say, work out the density
15     !in each cell based on a power law
16     !by looping over the cells in the grid
17
18     !...
19
20   end subroutine
21
22 end module grid
```

USE
LIBRARIES
AND
PACKAGES

Initialise

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Visualise

my_mcrt_code.f95

```
1 program my_mcrt_  
2  
3 use globals  
4 use input  
5 use grids  
6 use dust  
7  
8 call read_input(  
9 call calculate_d  
10  
11 end program
```

```
1 !-----  
2 ! this module declares the dust and dust species derived type objects !  
3 ! dust type includes properties such as extinction, mass, average grain density !  
4 ! species types includes similar properties that are species specific !  
5 ! subroutines include !  
6 ! - calculation of the array describing the dust grain radii !  
7 ! - opacity calculations utilising mie routine !  
8 ! (for each species/wavelength/grain radius combination) !  
9 !-----  
10  
11 module class_dust  
12  
13 use globals  
14 use class_line  
15  
16 implicit none  
17  
18 type species_obj  
19 integer :: id !each species has the following attributes  
20 integer :: nsizes !id number  
21 integer :: n_wav !number of grain sizes  
22  
23 real :: interval !number of wavelengths  
24 real :: amin,amax !spacing of grain sizes  
25 real :: weight !lamin, amax  
26 real :: m_weight !relative weight of species (fractional weighting by area)  
27 real :: v_weight !relative weight of species (fractional weighting by mass)  
28 real :: power !relative weight of species (fractional weighting by volume)  
29 real :: rho_grain !exponent for power law size distribution  
30 real :: av_mgrain !density of a dust grain  
31  
32 :: datafile !average mass of a dust grain for the species  
33  
34 :: radius(:,!) !data file containing optical constants for species  
35  
36 :: mgrain(:,!) !array containing grain sizes (1) and weightings (2)  
37 !weightings are relative abundance by number  
38  
39 :: m_sca(:,!) !mass of grain for each grain size in grams  
40 !array containing scattering extinctions at each wavelength  
41  
42 :: m_ext(:,!) !array containing extinctions at each wavelength  
43  
44 :: g_param(:,!) !array containing g (asymmetry factor) at each wavelength  
45  
46 :: wav(:,!) !array containing the wavelengths  
47  
48 :: albedo(:,!) !array containing albedos for each wavelength  
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```

Initialise

Describe the environment

Launch packets

Propagate packets

Absorb/
scatter/
re-emit

Collect packets

Visualise

my_mcrt_code.f95

```
1 program my_mcrt_
```

```
1 !-----  
2 ! this module declares the dust and dust species derived type objects !  
3 ! dust type includes properties such as extinction, mass, average grain density !  
4 ! species types includes similar properties that are species specific !  
5 ! subroutines include !  
6 ! - calculation of the array describing the dust grain radii !  
7 ! - opacity calculations utilising mie routine !  
8 ! (for each species/wavelength/grain radius combination) !  
9 !-----
```

Exception



No datasets have been created: check the dataset and the OCA rules
in `./xshooter/DataOrganizer`

Because:

No datasets have been created: check the dataset and the OCA rules

Go To Actor

Display Stack Trace

Dismiss

TEST!

AND HANDLE
ERRORS...

```
av_mgrain          !average mass of a dust grain for the species  
:: datafile        !data file containing optical constants for species  
radius(:, :)      !array containing grain sizes (1) and weightings (2)  
                  !weightings are relative abundance by number  
mgrain(:)         !mass of grain for each grain size in grams  
sca(:)            !array containing scattering extinctions at each wavelength  
ext(:)            !array containing extinctions at each wavelength  
g_param(:)        !array containing g (asymmetry factor) at each wavelength  
wav(:)            !array containing the wavelengths  
albedo(:)         !array containing albedos for each wavelength  
  
46 :: n_species     !number of species  
47  
48 :: mass           !total mass of dust (m_sun)
```

```
graph LR; A[Initialise] --> B[Describe the environment]; B --> C[Launch packets]; C --> D[Propagate packets]; D --> E[Absorb/scatter/re-emit]; E --> F[Collect packets]; F --> G[Visualise];
```

Initialise

Describe the environment

Launch packets

Propagate packets

Absorb/
scatter/
re-emit

Collect packets

Visualise

RECAP

- Build up each section of code as you go
- Test each section as you go
 - Use benchmark tests and analytical results
 - Use sense checks and ‘count checks’
 - Consider writing unit tests
- Calculate the properties of your medium in advance and store
- Grids allow for flexibility – properties in a given grid cell are constant

LAUNCH PACKETS

Initialise

Describe the environment

Launch packets

Propagate packets

Absorb/
scatter/
re-emit

Collect packets

Visualise



```
graph LR; A[Initialise] --> B[Describe the environment]; B --> C[Launch packets]; C --> D[Propagate packets]; D --> E[Absorb/scatter/re-emit]; E --> F[Collect packets]; F --> G[Visualise];
```

Initialise

Describe the environment

Launch packets

Propagate packets

Absorb/
scatter/
re-emit

Collect packets

Visualise

QUESTIONS TO ASK

- Frequency distribution $P(\nu) \propto ?$
 - Blackbody? Monochromatic? Continuum?
- Spatial emissivity distribution $i(x,y,z) \propto ?$
 - Proportional to density? Radial distribution? Point source? Arbitrary distribution?
- Propagation direction
 - Isotropic? Non-isotropic? Plane parallel?

Initialise

Describe the environment

Launch packets

Propagate packets

Absorb/
scatter/
re-emit

Collect packets

Visualise

my_mcrt_code.f95

input.f95

```
1  program my_mcrt_code
2
3  use globals
4  use input
5  use grids
6  use dust
7  use packet
8
9  call read_input()
10 call calculate_dust_properties()
11 call build_grid()
12
13 do i = 1,n_packets
14     call launch_packet()
15 end do
16
17 end program
```

my_mcrt_code.f95

packet.f95

inp

```
1  module packet
2
3  use globals
4  use input
5
6  type packet_type
7
8  real :: frequency
9  real :: direction(2)
10 real :: position(3)
11 real :: random(5)
12
13 end type type name
14
15 type(packet_type) packet
16
17 contains
18
19     subroutine launch_packet
20
21         packet%frequency = line_frequency
22
23         !now we need a propagation direction
24         !and an initial position
25
26     end subroutine
27
28 end module packet
```

Initialise

Describe the environment

Launch packets

Propagate packets

Absorb/
scatter/
re-emit

Collect packets

Visualise

Propagation
direction:

e.g.

sample from an
isotropic
distribution

$$\cos \theta = 2\xi - 1$$

$$\phi = 2\pi\xi$$

```
my_mcrt_code.f95      packet.f95      input.f95
1  module packet
2
3  use globals
4  use input
5
6  type packet_type
7
8  real :: frequency
9  real :: direction(2)
10 real :: position(3)
11 real :: random(5)
12
13 end type type name
14
15 type(packet_type) packet
16
17 contains
18
19   subroutine launch_packet
20
21     packet%frequency = line_frequency
22
23     call random_number(2)
24     direction = (/ 2*random(1)-1, 2*random(2)*pi /)
25
26   end subroutine
27
28 end module packet
```

Initialise

Describe the environment

Launch packets

Propagate packets

Absorb/
scatter/
re-emit

Collect packets

Visualise

Position:

e.g. radial power law in 1D

For $P(r) = Cr^n$ where $r \in [r_{\min}, r_{\max}]$

$$r = \left[(r_{\max}^{n+1} - r_{\min}^{n+1})\gamma + r_{\min}^{n+1} \right]^{\frac{1}{n+1}}$$

CARE WITH
RANDOM
NUMBERS

Wolfram MathWorld™ the we
Built with Mathematica Technology

Uniform random numbers in $[0,1)$ can be converted
to other distributions

Initialise

Describe the environment

Launch packets

Propagate packets

Absorb/
scatter/
re-emit

Collect packets

Visualise

my_mcrt_code.f95

```
1  program my_mcrt
2
3  use globals
4  use input
5  use grids
6  use dust
7  use packet
8
9  call read_input
10 call calculate_
11 call build_grid
12
13 do i = 1, n_pack
14   call launch
15 end do
16
17 end program
```

```
!generate an initial propagation direction from an isotropic distribution
!in comoving frame of emitting particle
packet%dir_sph(:)=(/ (2*random(4))-1,random(5)*2*pi /)
packet%dir_cart(:)=cart(acos(packet%dir_sph(1)),packet%dir_sph(2))

!if the photon lies inside the radial bounds of the supernova
!or if the photon is emitted from a clump or cell (rather than shell) then it is processed
if (((packet%pos_sph(1) > gas_geometry%r_min) .and. (packet%pos_sph(1) < gas_geometry%r_max) .and.
& .or. (gas_geometry%clumped_mass_frac==1) &
& .or. (gas_geometry%type == 'arbitrary')) then

!calculate velocity of emitting particle from radial velocity distribution
!velocity vector comes from radial position vector of particle
packet%v=gas_geometry%v_max*((packet%pos_sph(1)/gas_geometry%r_max)**gas_geometry%v_power)
packet%vel_vect=normalise(packet%pos_cart)*packet%v

packet%nu=line%frequency
packet%lg_active=.true.

call lorentz_trans(packet%vel_vect,packet%dir_cart,packet%nu,packet%weight,"emsn")

!identify cell which contains emitting particle (and therefore packet)
!!could be made more efficient but works...
do ixx=1,mothergrid%n_cells(1)
  if ((packet%pos_cart(1)*1e15-mothergrid%x_div(ixx))<0) then !identify grid axis that lies
    packet%axis_no(1)=ixx-1 !then the grid cell id is the
    exit
  end if
  if (ixx==mothergrid%n_cells(1)) then
    packet%axis_no(1)=mothergrid%n_cells(1)
  end if
end do
do iyy=1,mothergrid%n_cells(2)
  if ((packet%pos_cart(2)*1e15-mothergrid%y_div(iyy))<0) then
    packet%axis_no(2)=iyy-1
    exit
  end if
end do
```

PROPAGATE PACKETS & ABSORPTION/SCATTERING/RE-EMISSION

Initialise

Describe the
environment

Launch
packets

Propagate
packets

Absorb/
scatter/
re-emit

Collect
packets

Visualise



```
graph LR; A[Initialise] --> B[Describe the environment]; B --> C[Launch packets]; C --> D[Propagate packets]; D --> E[Absorb/scatter/re-emit]; E --> F[Collect packets]; F --> G[Visualise]; style D fill:#800080,color:#fff
```

Initialise

Describe the environment

Launch packets

Propagate packets

Absorb/
scatter/
re-emit

Collect packets

Visualise

QUESTIONS TO ASK

- What happens to absorbed packets?
- Do I need to use weighted packets?
- With what direction are scattered packets re-emitted?
 - Isotropic? Phase function?
- Are packets re-emitted immediately?
- Do I need to iterate?
 - Update grid properties? Determine thermal balance?

Initialise

Describe the environment

Launch packets

Propagate packets

Absorb/
scatter/
re-emit

Collect packets

Visualise

my_mcrt_code.f95

packet.f95

```
1 program my_mcrt_code
2
3 use globals
4 use input
5 use grids
6 use dust
7 use packet
8
9 call read_input()
10 call calculate_dust_p
11 call build_grid()
12
13 do i = 1, n_packets
14   call launch_packet
15   call propagate_packet
16 end do
```

```
recursive subroutine propagate_packet
```

```
subroutine event_happens()
```

```
call random_number(ran)
```

```
if (ran < albedo) then
```

```
!scattered
```

```
!perform lorentz transform into frame of scatterer
```

```
!sample new scattering direction in scatterer frame
```

```
!lorentz transform back into rest frame
```

```
!frequency updated by lorentz transform
```

```
!update packet weight
```

```
else
```

```
!absorbed
```

```
absorbed = .true.
```

```
end if
```

```
enc
```

```
end moc
```

```
!not applicable in DAMOCLES
```

```
!but might need to re-emit at this point
```

```
!and recalculate frequency
```

```
end subroutine event_happens
```

PARALLEL
WORKS
VERY WELL

Initialise

Describe the environment

Launch packets

Propagate packets

Absorb/
scatter/
re-emit

Collect packets

Visualise

my_mcrt_code.f95

```
1 program my_mcrt_code
2
3 use globals
4 use input
5 use grids
6 use dust
7 use packet
8
9 call read_input()
10 call calculate_dust_pro
11 call build_grid()
12
13 do i = 1, n_packets
14   call launch_packet
15   propagate_pac
```

```
!event occurs when distance travelled (as determined by tau) is < distance to nearest face
!else continues to cell boundary with no event occurring:
```

```
if ((s>s_min)) then
```

```
!packet travels to cell boundary (direction of travel remains the same):
```

```
!position updated to be on boundary with next cell
```

```
!actually moves just past boundary by small factor...
```

```
packet%pos_cart(:)=packet%pos_cart(:)+(abs(s_min)+abs(s_min)*1e-10)*packet%dir_cart(:)
```

```
if (packet%dir_cart(i_min)>0) then
```

```
!if packet travels forwards then advance cell id by 1 in that index
```

```
if (packet%axis_no(i_min) /= mothergrid%n_cells(i_min)) then
```

```
packet%axis_no(i_min)=packet%axis_no(i_min)+1
```

```
else
```

```
!reached edge of grid, escapes
```

```
call check_los()
```

```
return
```

```
end if
```

```
!update id of cell containing packet and update position of packet
```

```
call update_cell_no()
```

```
packet%pos_cart(i_min)=grid_cell(packet%cell_no)%axis(i_min)+((abs(s_min)*1e-10)*pack
```

```
else
```

```
!if packet travels backwards then reduce cell id by 1 in that index
```

```
if (packet%axis_no(i_min) /= 1) then
```

```
packet%axis_no(i_min)=packet%axis_no(i_min)-1
```

```
else
```

```
!reached edge of grid, escapes
```

```
call check_los()
```

```
return
```

```
end if
```

```
!update id of cell containing packet and update position of packet
```

```
call update_cell_no()
```

```
packet%pos_cart(i_min)=grid_cell(packet%cell_no)%axis(i_min)+((abs(s_min)*1e-10)*pack
```

```
end if
```

```
!calculate packet radial position
```

```
packet%r=(sum(packet%pos_cart**2))**.5
```

PARALLEL
WORKS
VERY WELL

Initialise

Describe the environment

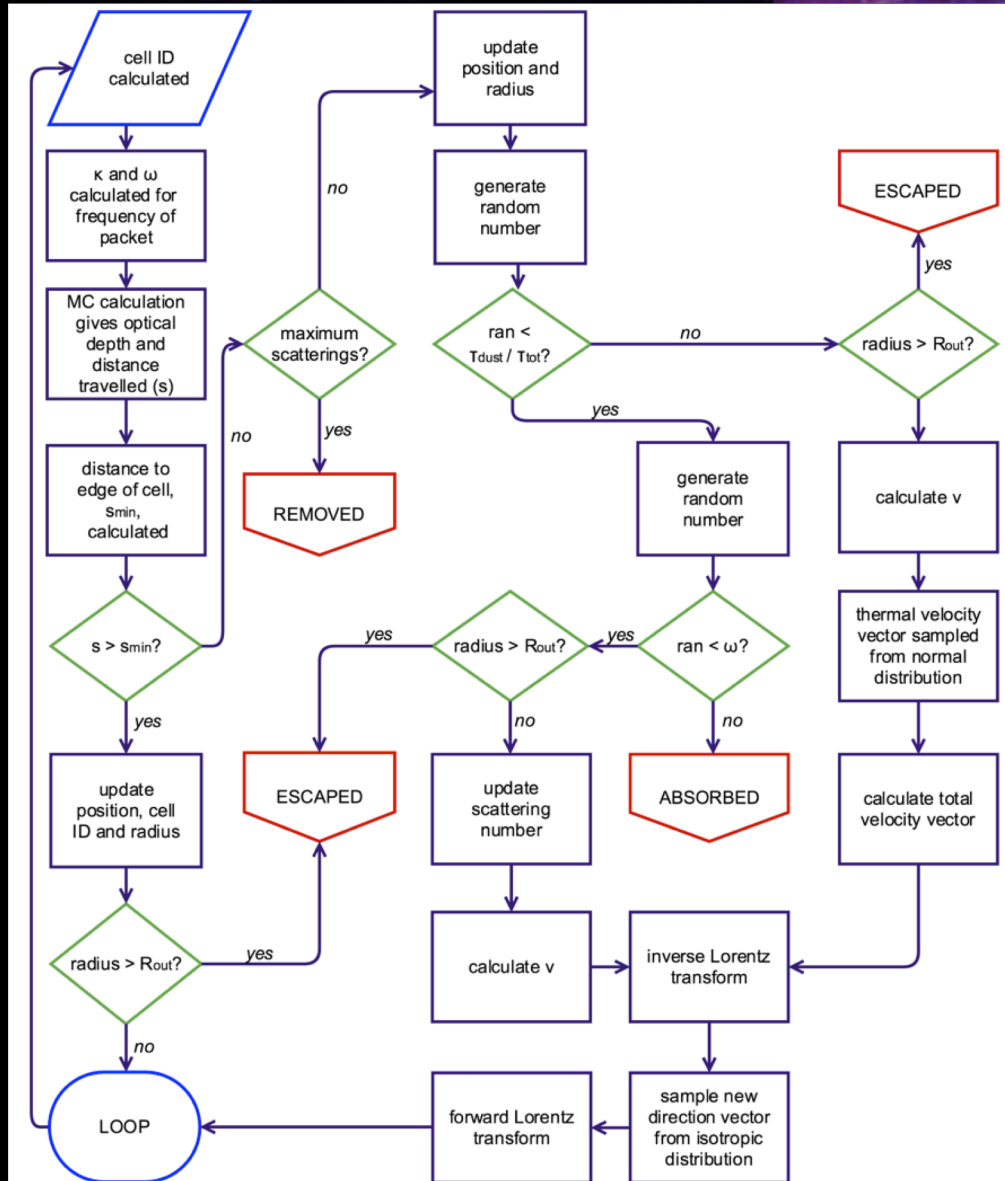
Launch packets

Propagate packets

Absorb/
scatter/
re-emit

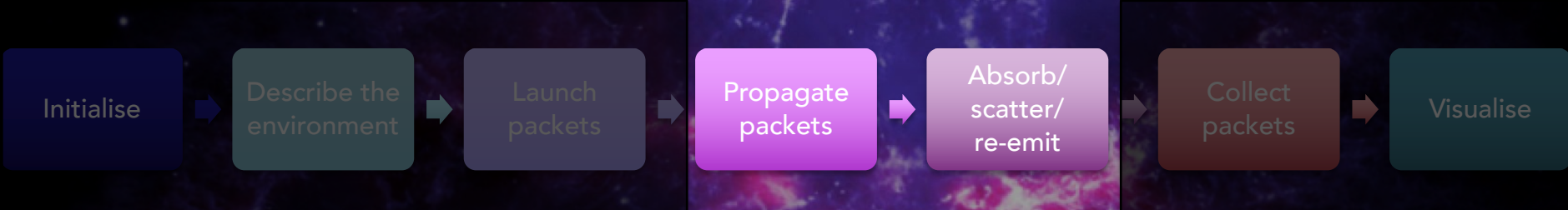
Collect packets

Visualise



A packet's path through the ejecta in DAMOCLES

(note, no re-emission...)



RECAP

- Packets do not interact so...
 - can run multiple at once
- Monte Carlo very, very parallel (and fairly easy to do so)
 - Lots of packets required ($10^4 - 10^9$ typical) means it can be slow so parallelisation helps
- Random numbers determine random walk but also events along the way

COLLECT PACKETS & VISUALISE

Initialise

Describe the
environment

Launch
packets

Propagate
packets

Absorb/
scatter/
re-emit

Collect
packets

Visualise



```
graph LR; A[Initialise] --> B[Describe the environment]; B --> C[Launch packets]; C --> D[Propagate packets]; D --> E[Absorb/scatter/re-emit]; E --> F[Collect packets]; F --> G[Visualise]; style F fill:#f08080
```

Initialise

Describe the environment

Launch packets

Propagate packets

Absorb/
scatter/
re-emit

Collect packets

Visualise

QUESTIONS TO ASK

- What information should be collected?
 - Weights, frequencies, positions, directions...
- How should the information be collated?
 - Binning – what resolution?
- Viewing angles?
- What visualisation/analysis can be used to explore the results of the simulation?
- What graphics/images best represent the model? Convolve to observation?

Initialise

Describe the environment

Launch packets

Propagate packets

Absorb/
scatter/
re-emit

Collect packets

Visualise

my_mcrt_code.f95

packet.f95

```
1  program my_mcrt_code
2
3  use globals
4  use input
5  use grids
6  use dust
7  use packet
8
9  call read_input()
10 call calculate_dust_properties()
11 call build_grid()
12
13 do i = 1, n_packets
14   call launch_packet()
15   call propagate_packet()
16   call collect_packet()
17 end do
18
19 call write_out()
20
21 end program
```

```
subroutine collect_packet()
```

```
    index = minloc(packet%frequency - frequency_array(:,1))
    flux_array(index) = flux_array(index) + packet%weight
```

```
end subroutine collect_packet
```

```
subroutine write_out()
```

```
    open(unit = 31, file = 'line_profile.out')
```

```
    do ii = 1, size(flux_array)
        write(31,*) flux_array(ii)
    end do
```

```
    close(31)
```

```
    !write out any other pieces of information to file
    !e.g. input parameters, calculated quantities
```

```
end subroutine write_out()
```

Initialise

Describe the environment

Launch packets

Propagate packets

Absorb/
scatter/
re-emit

Collect packets

Visualise

my_mcrt_code.f90

```
1  program my_
2
3  use global
4  use input
5  use grids
6  use dust
7  use packet
8
9  call read_
10 call calcul
11 call build
12
13 do i = 1, n
14   call l
15   call p
16   call c
17 end do
18
19 call write
20
21 end program
```

```
module initialise
```

```
  use globals
  use class_line
  use class_geometry
  use class_dust
  use class_grid
  use class_freq_grid
  use input

  implicit none

contains

  subroutine write_to_file()

    if (.not. lg_mcmc) print*, 'writing to file...'

    !real number format, 6 characters, 2dp
    format(a65'   'f10.2)

    !integer format, 4 characters
    format(a65'   'i10)

    !scientific format, 5 characters, 2dp
    format(a65'   'e10.2)

    !create folders dependent on date/time of run if requested
    !otherwise overwrite and store in main output folder
    if (lg_store_all) then
      call date_and_time(date,time)
      run_no_string = time(1:2) // '.' // time(3:4) // '.' // time(5:6)

      call system('mkdir -p output/output_' // date // '/run_' // run_no_string)
      call system('cp input/*.in output/output_' // date // '/run_' // run_no_string // '/')

      !open output files to record resultant modelled line profile, input parameters and properties of m
      open(25,file='output/output_' // date // '/run_' // run_no_string // '/integrated_line_profile.out
      open(26,file='output/output_' // date // '/run_' // run_no_string // '/multiple_los_line_profiles.
```

```
graph LR; A[Initialise] --> B[Describe the environment]; B --> C[Launch packets]; C --> D[Propagate packets]; D --> E[Absorb/scatter/re-emit]; E --> F[Collect packets]; F --> G[Visualise]; style F fill:#f08080
```

Initialise

Describe the environment

Launch packets

Propagate packets

Absorb/
scatter/
re-emit

Collect packets

Visualise

VISUALISATION IS IMPORTANT

- It is how your model is seen by the outside world
- It allows you to easily assess and analyse the results
- Normally worth writing scripts for visualising then packaging with the code
- Many tools and libraries in e.g. Python, matlab

```
graph LR; A[Initialise] --> B[Describe the environment]; B --> C[Launch packets]; C --> D[Propagate packets]; D --> E[Absorb/scatter/re-emit]; E --> F[Collect packets]; F --> G[Visualise]; style F fill:#f08080
```

Initialise

Describe the environment

Launch packets

Propagate packets

Absorb/
scatter/
re-emit

Collect packets

Visualise

RECAP

- Important part of the code
- Normally worth investing time in writing post-processing scripts for visualising results
- Try to collect as many outputs as you might be interested in
- Make an automated output option e.g. automated file names based on date/time or input parameters etc.

Initialise

Describe the environment

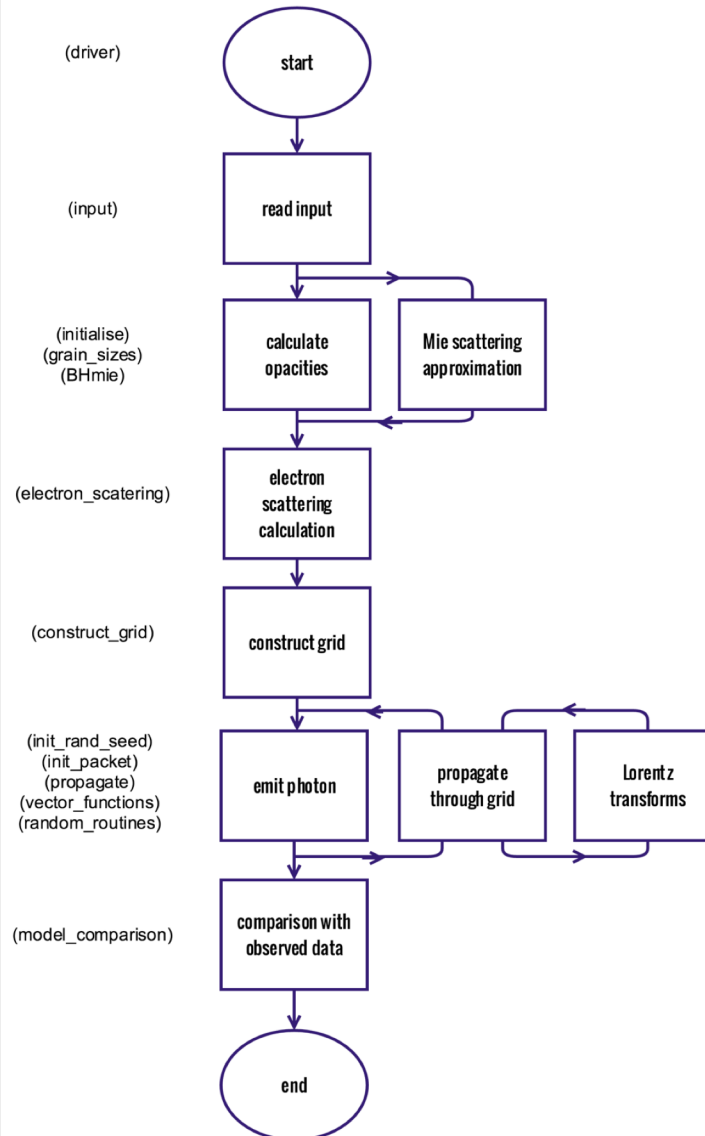
Launch packets

Propagate packets

Absorb/
scatter/
re-emit

Collect packets

Visualise



It didn't quite go like that...

• ~~Spherical grid~~ → Cartesian grid

• Dust absorption

• Dust scattering + electron scattering

• ~~Smooth dust distribution + clumped dust distribution + clumped dust emissivity distribution~~

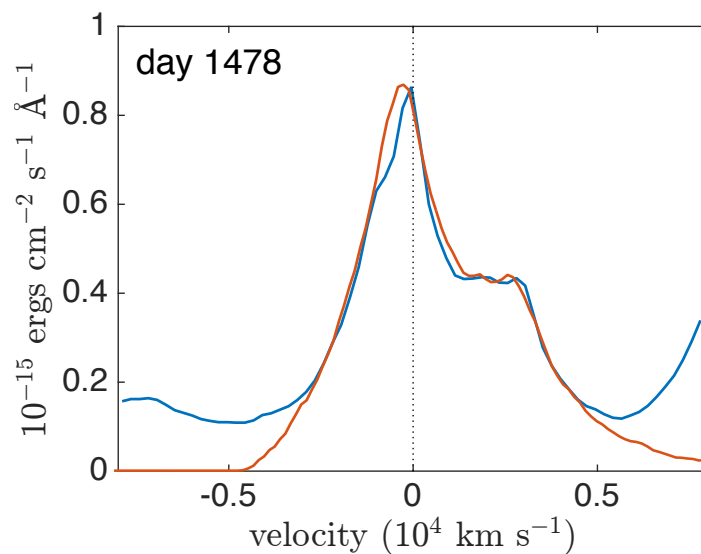
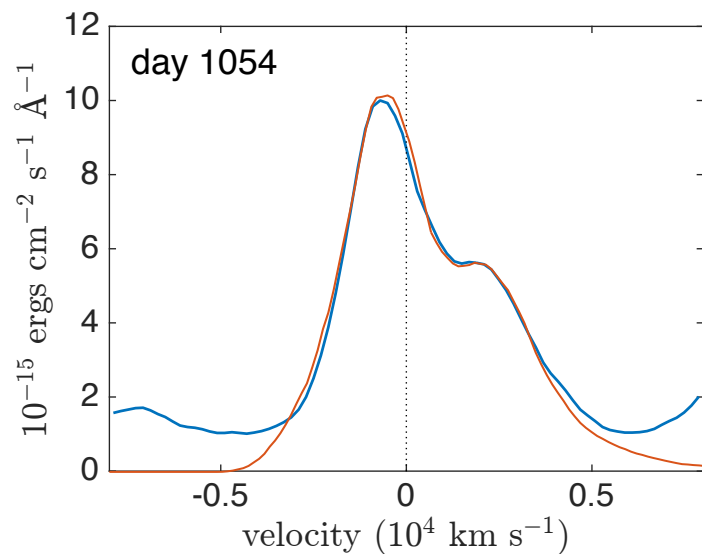
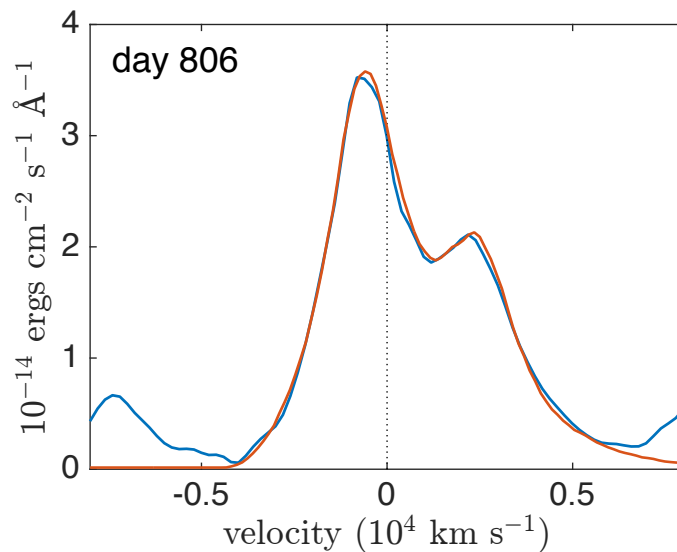
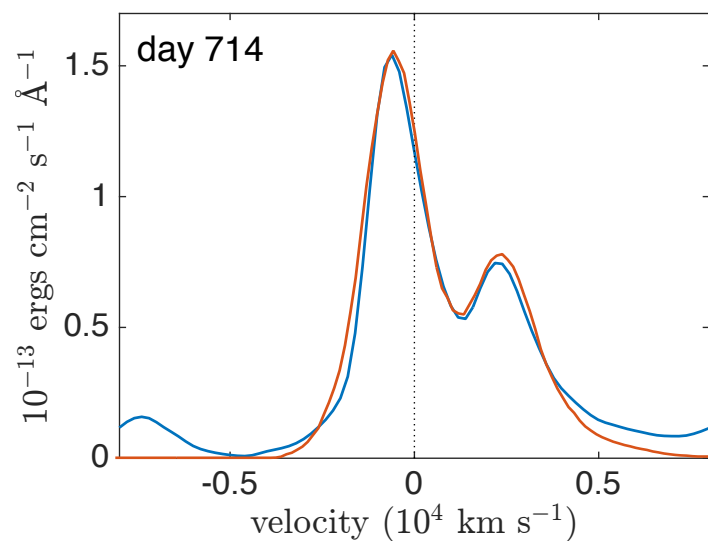
• Monochromatic line packets

BUT ALSO AND
DOUBLETS TRIPLETS...

BAYESIAN MCMC WRAPPER IN PYTHON

END RESULT!

FITS TO THE SN 1987A [O]6300,6363 DOUBLET

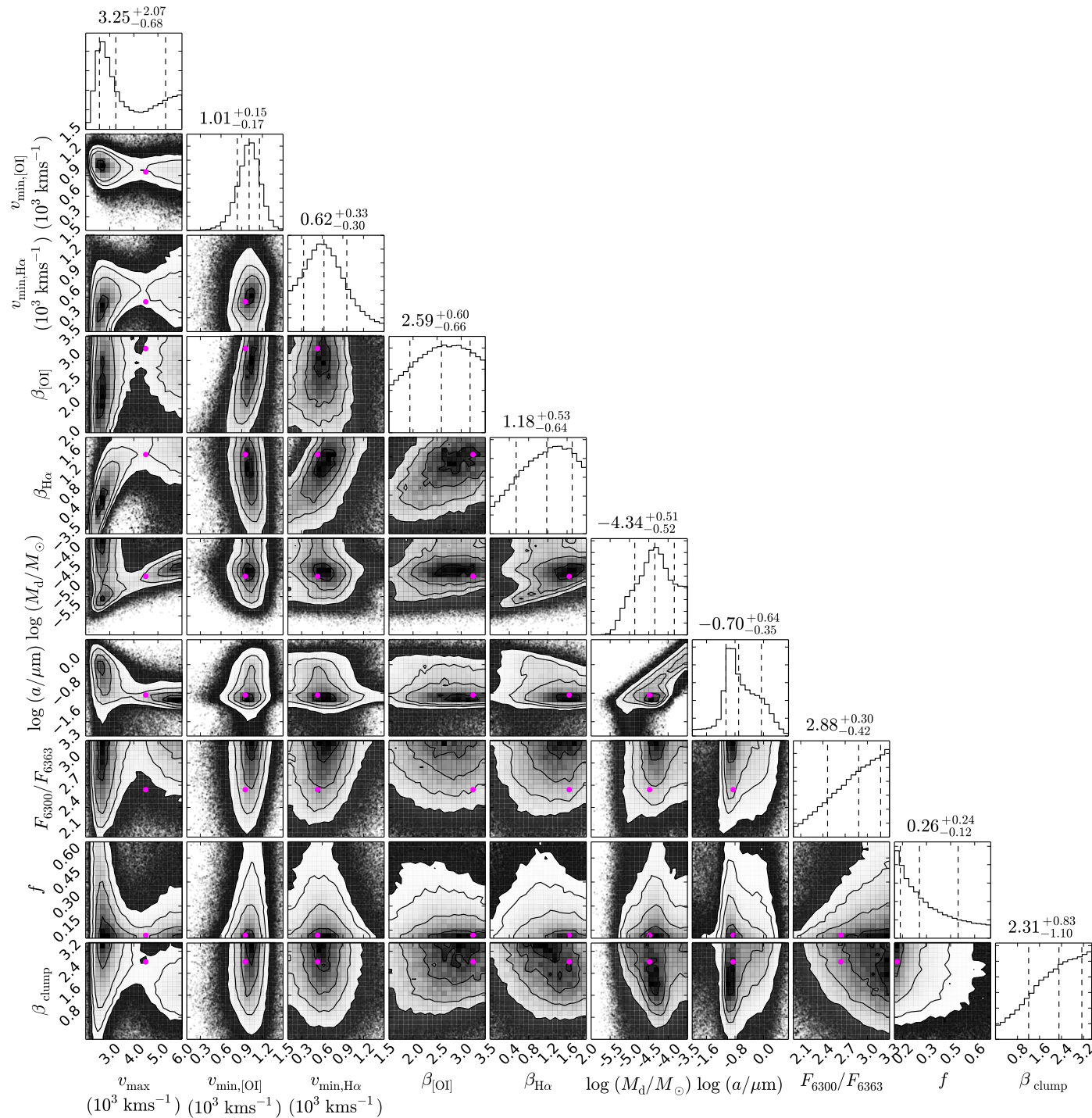


Bayesian Modelling

SN 1987A
H α & [OI]
day 714

smooth

gas & dust
coupled



Best Practices for Scientific Computing

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September 27, 2013

<https://arxiv.org/pdf/1210.0530.pdf>



- Use version control
 - Use modules
 - Use libraries and packages
 - Test twice (at least!)
 - Take care with random numbers
 - Parallelise
-
- Don't assume that only you will be using your code...
 - Comments
 - Clear variable and module names

Ask questions!