CRETIN

Session 1

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General info

- Weekly sessions: 2/26, ~~3/5~~, 3/12, ~~3/19~~, 3/26, 4/2 …
- Topics
  - General code usage ← this session
  - Atomic models
  - Radiation transport
  - Postprocessing
  - Physics / Input / Output options
- CRETIN User's Manual is a 200+ page reference guide
- "A Practical Guide to Cretin" is intended as a "how-to" guide
  - Started by Alison Saunders
  - We can all contribute, details to follow

The code and manual are export controlled – do not pass on a copy without checking

General info

- Code + useful materials located in /usr/apps/cretin on LC machines

.../bin	executables
…/doc	references
…/exercises	simple generators
…/examples	more generators
…/radtransport	radiation transport lecture examples
…/tests	regression tests
…/yorick	useful Yorick scripts

- Atomic models are located in /usr/gdata/dca/Models
  - …/2014_03_03 (= …/latest) holds the default set of models
  - …/2017_09_08 holds the recommended set for ”regular” models

Cretin info

- 0-, 1-, 2-, and 3-dimensional non-LTE atomic kinetics / radiation transfer code
  (+ line shapes, temperature evolution, conduction, 1-d hydro, …)
- Arbitrary mixtures of elements
- All physics data derived from collisional-radiative models
- Generates screened-hydrogenic atomic models or uses externally-supplied atomic data

- Used heavily for spectral analysis
- Can be driven by rad-hydro codes (postprocessing)
- Runs on most computers: LC machines to laptops
  parallel on processors and/or threads (not massively parallel)

Cretin kinetics runs in-line in HYDRA, ARES, KULL

Cretin atomic kinetics

- Arbitrary number and mixture of elements
- LTE / steady-state NLTE / time-dependent NLTE
- Fixed mass density or fixed electron density
- Standard set of electron- and photon-driven atomic processes
  (+ options for ion collisions and charge exchange)
- Multiple e^- temperatures and/or arbitrary f_e distribution w/ degeneracy
  (e^- temperatures will equilibrate, f_e not yet)
- Plasma effects
  continuum lowering
  Stark broadening / line shapes

Atomic kinetics calculation is iterated to consistency with all other physical processes

Radiation “flavors” in Cretin

Continuum, lines and spectra are treated separately for efficiency

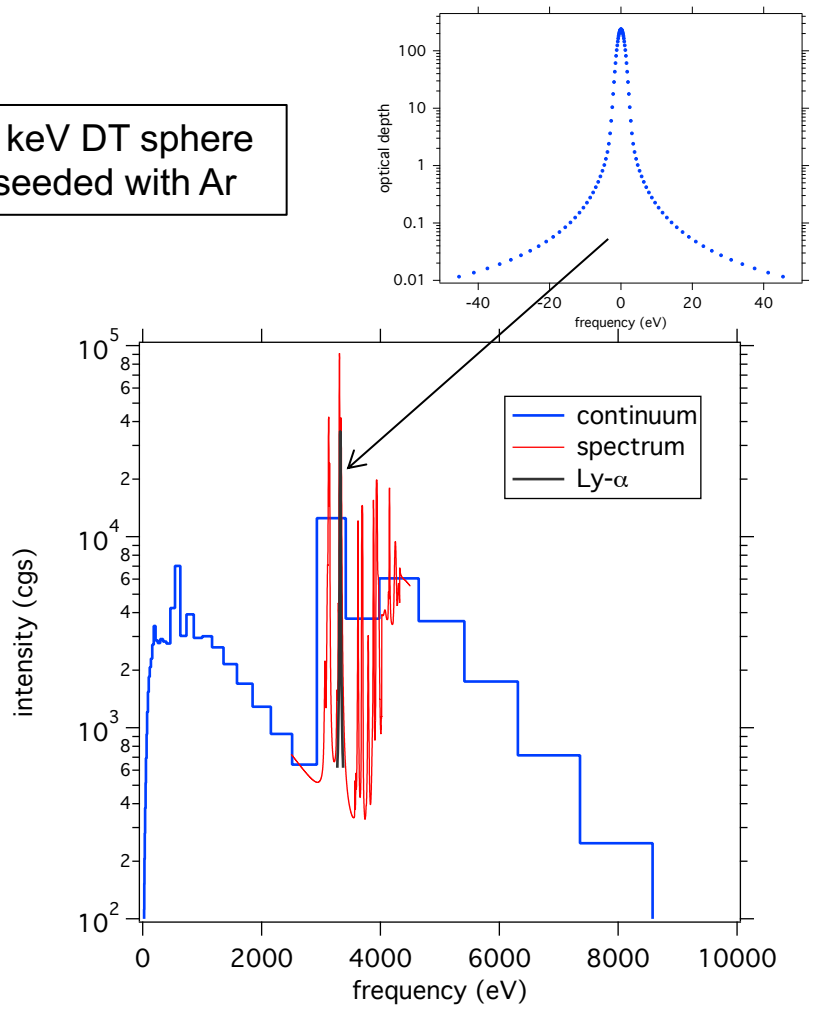
Iterated to consistency with atomic kinetics (and other processes):

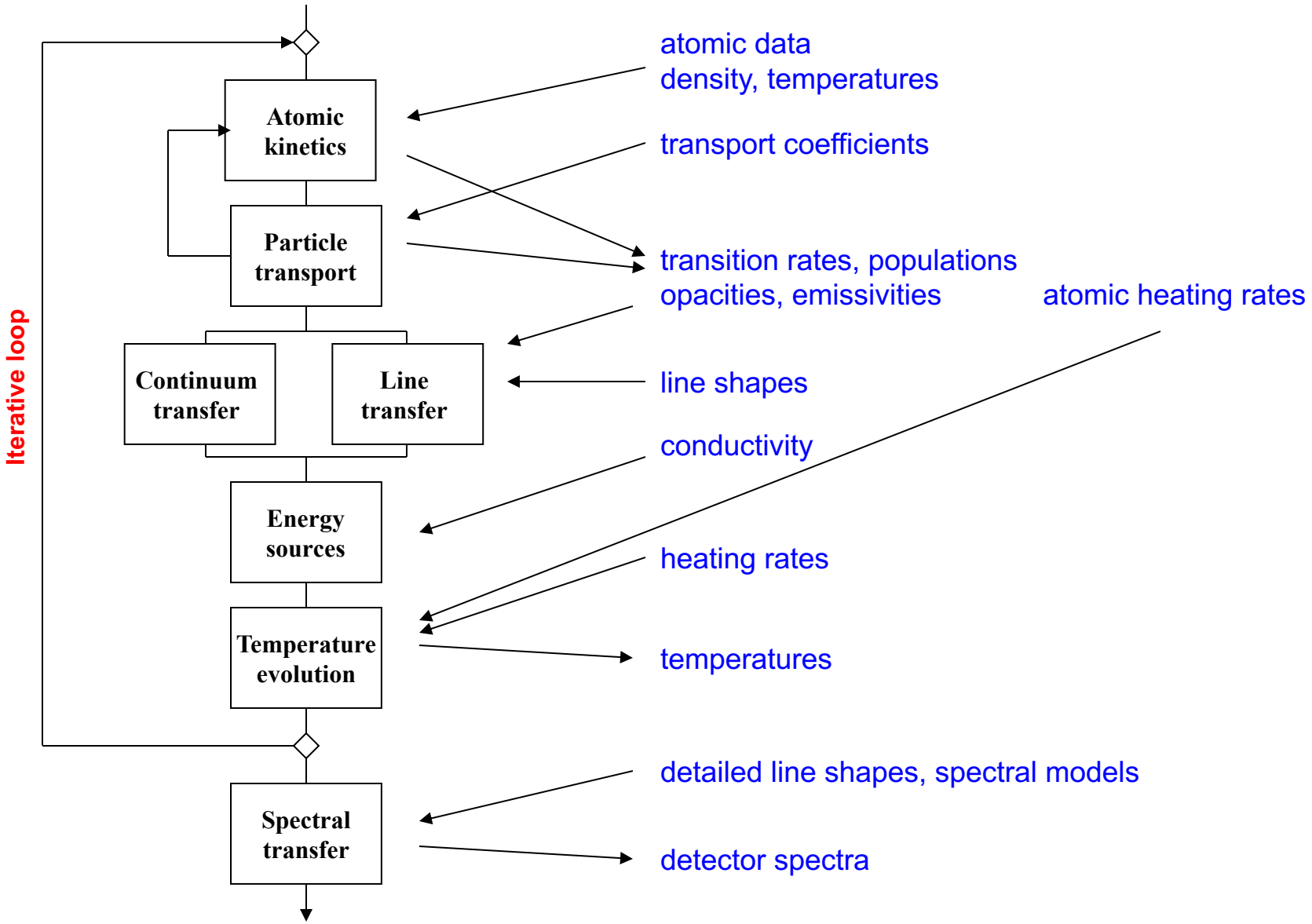
- continuum radiation coarsely-binned over full energy range for evaluating photo rates
- line radiation finely-binned for resolving individual line profiles

Evaluated after convergence:

- spectral radiation at arbitrary energies to resolve features of interest

1 keV DT sphere seeded with Ar




Iterative loop
Atomic kinetics
Particle transport
Continuum transfer
Line transfer
Energy sources
Temperature evolution
Spectral transfer
atomic data
density, temperatures
transport coefficients
transition rates, populations
opacities, emissivities
atomic heating rates
line shapes
conductivity
heating rates
temperatures
detailed line shapes, spectral models
detector spectra

Running Cretin: files

- Generator file e.g. *"ex2.gen"*
  - problem description (spatial mesh, frequency bins, materials, …)
  - physics options
  - desired outputs (edits, dumps)

- Other input files
  - atomic datafile for each element
  - external data files (xfiles)

- Output files
  - *"ex2.tbl"* contains execute line, code info, generator, messages, …
  - edits "*ex2.*plt" is text and can be used with many plotting packages
    "ex2.ult" is PDB and can be viewed with ULTRA or Yorick
  - dumps restart: *"ex2.r00"*, data: *"ex2.d00"* are binary only (PDB or HDF5)

- Environment variables
  - maximum number of threads for execution: OMP_NUM_THREADS

All output (edits and dumps) must be <u>explicitly</u> requested

Running Cretin: command line options

Usage: CRETIN **file** | VERSION | -v [file2]
[**GENERATE**] [SPECTRA] [DRAT] [OUT=file3 | -o file3]
[DEFINE | UNDEFINE var] [ALIAS var value]
[OPACITY | SERVER | TABOP id | TABOPEOS | LRM[S] | JRM]
[DOMAINS=k,l,m] [**PAUSE**]
[TRACE | TRACEMEM | TRACEMSG | TRACEALL]
[SIZE] [GROUPS=ng] [PROCS=np] [THREADS=nt]

Run a simulation

or

CRETIN file SOURCE | RECONST [BINARY/HISTORY/DIRECTORIED]
[KLM=k,l,m] [XYZ=i,j,k]

Work with an xfile

or

CRETIN file HYDROGENIC(iso1:iso2)_n_l symbol [DCA]

Produce an atomic model

or

CRETIN file ATOMS | RECONST[W] | RADLIST [symbol]

Work with an atomic model

Command line arguments can be lower or upper case

Most command line options are for special purpose runs

Running Cretin: command line options

cretin ex2.gen : run generator ex2.gen

cretin ex2.gen generate : run cycle 0 only (and then finish)

cretin ex2.gen pause : initialize run and wait for interactive commands

<u>Interacting with a running job</u>

start with “pause” on command line

-- or --

interrupt with a single Ctrl-C and wait for a response

code will only respond at the end of a timestep

“help” gets a list of possible commands for

running a specified number of cycles or Δt

turning physics or I/O options on or off

querying (or plotting) values of many variables

Generator commands

- Commands are described in the manual grouped by physical process

Materials	Mesh	
Continuum radiation	Spectral radiation	
Lineshapes	Line radiation	
Electron distribution	Laser raytrace	
Edits	Miscellaneous	Macros

- Code options (switches and parameters) are also grouped by process

Atomic kinetics	Atomic models	
Radiation transfer: Continuum radiation		Spectral radiation
Lineshapes		Line Radiation
Escape factors	Electron distribution	
Temperature	Rad transfer / temperature	
Hydrodynamics	Laser raytrace	
Timesteps / convergence	Output	

An ordered listing (with brief descriptions) is also available

Generator construction: *ex2.gen*

```
c       **** 0D Argon kinetics + coarse spectrum ****
c                  w/ hydrogenic model

c ------------------------------------------------------------
c   Aliases
c ------------------------------------------------------------

alias Te        500.        !   [eV]
alias Ni_ar     1.e18       !   [cm-3]


c ------------------------------------------------------------
c   Materials
c ------------------------------------------------------------

atoms hydrogenic ar

region  1 1  Te Te Tr
  element 1 Ni_ar
```

Fields on each line are white space delimited
Order of fields is significant, position is not significant
absent fields have values 0. and " "
Commands should be lower-case

"c" as first field → comment line
"!" comments out remainder of line

"alias" is a macro capability –
straight substitutions + limited mathematical operations
unspecified items have values 0. and " "

Units: cgs for everything except
eV for temperatures, atomic energies

"atoms" assigns an atomic model and index to each element
"hydrogenic" → build a screened hydrogenic model
default index increments for each command (1, 2, 3, …)
index can be assigned with e.g. "atoms iz=18"

"region" assigns nodes [ir1,ir2] and (T_e, T_i, T_r) to each region
"element index #-density" adds an element to the region

1 node → no geometry or spatial mesh

Generator construction: *ex2.gen*

```
c ------------------------------------------------------------
c   Radiation
c ------------------------------------------------------------

ebins 61  1. 1.e4


c ------------------------------------------------------------
c   Controls
c ------------------------------------------------------------

tstart  0.
tquit   0.


c ------------------------------------------------------------
c   Switches and Parameters
c ------------------------------------------------------------

switch  11   1        ! make .plt file
switch  20   1        ! NLTE
switch  28   1        ! initialize in steady-state

switch  44  10        ! number of iterations
switch 120   1        ! show convergence diagnostics
```

”ebins 61” assigns 61 frequency bins
1: [0., 1.] eV
2-61: [1., 10^4] eV w/ logarithmic spacing

“fbins …” for Hz, “wbins …” for cm^{-1}
”rbins”, “pbins” (in keV) are also accepted

Cycle 0 is initialization: t=tstart, $\Delta t=0$.

tquit = tstart → no time evolution → LTE or steady-state

Physical process are turned off by default
except atomic kinetics

Default initialization is LTE

Maximum iterations for each cycle to converge to specified tolerances

Generator construction: *ex2.gen*

```
c -------------------------------------------------------------
c   Edits
c -------------------------------------------------------------

plot "NE, RHO vs zone"
  xvar  n
  yvar  ne
  yvar  rho

plot "TEV, TIV, TRV vs zone"
  xvar  n
  yvar  tev
  yvar  tiv
  yvar  trv

plot "ZBAR vs zone"
  xvar  n
  yvar  zbar

plot "Ar CHARGE STATE DISTRIBUTION"
  xvar  iso         1
  yvar  yisofrac   1 1

plot "EMISSION / ABSORPTION"
  xvar  energy
  yvar  cemis      0 1
  yvar  ckappa     0 1

 plot "EMISSION / ABSORPTION"
  xvar  ebins
  yvar  cemis      0 1
  yvar  ckappa     0 1
```

Edits are composed of
- "plot" command + (optional) title
- 1 – 3 xvars : name + 4 indices + (optional) multiplier
- 1 – n yvars : name + 4 indices + (optional) multiplier

Indices correspond to a "dimension"
- 1st: element / transition
- 2nd: node (spatial or logical)
- 3rd: frequency / isosequence
- 4th: direction / level

"iso" : isosequence (# bound e^-) for specified element
"yisofrac" : fractional population for specified (element,node)

"cemis" : continuum emissivity (erg/cm^2/s/Hz/ster)
"ckappa" : continuum absorption coefficient (cm^{-1})

"energy" : photon energy at bin center
"ebins" : photon energies at bin boundaries (histogram)

Important (but non-obvious) switches / parameters

switch 20	0: LTE , 1: J_ν, 2: $T_r = T_e$, 3: T_r for atomic kinetics
switch 25	0: steady-state kinetics , <>0: time-dependent
switch 28	0: LTE initialization , 1 or 2: steady-state initialization
switch 30	# cycles between edits
switch 44	max # iterations / cycle
switch 58	0: fixed mass density, <0: fixed electron density
switch 36	>0: do continuum transfer
switch 37	>0: do line transfer
param 41	initial timestep
param 42-46	timestep controls
param 55-57	convergence controls

Extended generator

```
atoms iz=1   hydrogenic h
atoms iz=18 dca_18k     ar

region 1 N Te Te Tr
  element   1 1.
  element 18 1.e-2     !  Argon number fraction
  rho           RHO     !  total mass density

geometry sphere

rlin     1 N  R0 R1                    !  equal spacing between R0 R1
rlog     1 N  R0 R1                    !  equal ratio spacing
rgeom 1 N  R0 R1  DRMIN  +/-1  !  equal ratio with specified minimum spacing in +/- direction
r        r0  r1  r2  ….                !  specify individual positions
```

"iz=18": assign element index
"dca_18k": designate atomic datafile

Specify relative number densities
plus total mass density

There are usually multiple methods to specify values on a mesh, either in the generator or with xfiles.

Homework

Go through exercises 2-4

- ex2: 0D Argon kinetics + coarse spectrum w/ hydrogenic model
  a) fine spectrum , b) w/ detailed K-shell model , c) in hydrogen
- ex3: 0D Argon kinetics + spectrum on a temperature grid w/ K-shell model
  a) emission by charge state
- ex4: 1D Argon kinetics + spectrum in planar geometry w/ K-shell model
  a) + escape factors , b) spherical geometry
  c) optically thick , d) w/line transfer

  ch) & dh) use a hydrogenic model