CRETIN

Session 3

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Session topics

- Getting data out of the code
  - edits
  - dumps
- Aliases
- Useful command line options
- Scripting runs

Output options - Edits

Edits are composed of
  "plot" command + (optional) title
  (optional) edit specifications
  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

- Snapshots are edits which do not have time / cycle as an xvar
  - *xvar* possibilities are listed in the manual
  - snapshots are produced as the run progresses
  - snapshot intervals controlled by switch(30) and param(40)

- Time edits are produced only when the run finishes
  - time edits include results from every timestep

- Edits may be integrated / averaged / maximum / minimum
  over time / space / mass / frequency

- Spectral simulations are specialized (and expensive) edits
  - separate controls [switch(72), param(91)] allow better time-integrations

Output options – edit examples

```
plot "YISOFRAC vs ISO"
  xvar  iso           1
  yvar  yisofrac    1 1:-1
```

Charge state distribution snapshot for all nodes

first:last syntax for index

-1 in 2nd index → last node

```
plot "TE vs TIME"
  xvar  time
  yvar  tev         0 1:N:DN
```

Time plot of temperature

first:last:stride syntax for index

```
plot "ZBAR vs R"
  xvar  r
  yvar  zbar
```

Snapshot on 2D mesh

“xvar r” expands to “xvar x2d” + “xvar y2d”

```
plot "ZBAR(1) vs TE"
  xvar  x2d         0  1
  yvar  zbar        1   1:LMAX
```

Snapshot along K-line on 2D mesh

“xvar x2d” requires L index

yvar requires compatible L index

```
plot "TIME-INTEGRATED SPECTRUM"
time-integrated snapshot
  xvar  sp_energy
  yvar  jsparea    0 -1
```

Time-integrated snapshot

appears at each edit interval

w/o ”snapshot” would appear only at conclusion of run

```
plot "INTEGRATED ENERGY vs TIME"
time-integrated
sp-integrated
  xvar  time
  yvar  jsparea    0 -1
```

Time- and energy-integrated

“xvar time” → saved for each cycle

Edit example from homework

- Radiative emissivity
  - cemis = $\eta(\nu)$ erg/cm^3/s/Hz/ster

- Radiative power loss (RPL)   erg/cm^3/s
  - frequency- and angle-integrated emissivity   cemistot = $\int_0^\infty 4\pi\,\eta(\nu)d\nu$

```
plot
 xvar  r
 yvar  cemistot
```

RPL using “cemistot” defined edit quantity

```
plot
energy-integrated
 xvar  r
 yvar  cemis      0  0  0  0  CMULT

alias  CMULT   PI*4.
```

RPL defined using frequency-dependent emissivity “cemis”
integrated over all photon energies
solid angle integration uses multiplier in 5th slot
CMULT defined in “alias” with mathematical expression
PI is a predefined alias

```
plot
energy-integrated  1800.  4000.
 xvar  r
 yvar  cemis      0  0  0  0  4PI
```

M-band RPL
integrated over photon energies ∈ [1.8, 4.0] keV

Output options – restart dumps

- Restart dumps contain everything needed to continue running the problem
  - atomic data, populations, mesh variables
  - controls and options
  - time-dependent edits

- Turned on by “restart” command in generator or interactively
  - familied with suffixes *.r00, .r01, .r02, …*
  - dump intervals controlled by switch(65) and param(87)

- Problem can be restarted [and modified] with

  cretin *problem.r02 [changes.gen]*

  - modifications can include additional edits
  - most modifications can also be done interactively

- Edits (many, but not all) can be reconstructed with

  cretin *problem.r02* edits

Output options – spectral dumps

- Spectral dumps contain everything needed to construct spectra
  - atomic data, populations, some mesh variables

- Turned on by “sdump” command in generator or interactively
  - familied with suffixes *.s00, .s01, .s02, …*
  - multiple timesteps in each dump
  - dump intervals controlled by switch(73) and param(92)

- Spectral dumps are much smaller than restart dumps

- Spectra for all times can be calculated with

  cretin *problem.s00 spectra.gen spectra*

  with spectral frequency mesh and options contained in *spectra.gen*

Spectral postprocessing can be done from either restart dumps or spectral dumps, and is often done multiple times

Output options – data dumps

- Data dumps contain just requested variables
  - mesh, temperatures, densities, populations, radiation, …
  - selected edits (include “send-to-dump” in edit specification)

- Turned on by “dump” command in generator or interactively
  - familied with suffixes *.d00, .d01, .d02, …*
  - multiple timesteps in each dump
  - Yorick time history structure
  - dump intervals match those of edits [switch(30) and param(40)]

Sending edits to dumps is convenient for Yorick users

“Alias” – a basic macro capability

Syntax: **alias** *word value* - sets *word* to *value*

alias *word expression* - sets *word* to evaluation of *expression*

#define *word* - sets *word* to 1

- *value* is interpreted as both a real number and a character string
- *expression* may include numbers, symbols (defined with *alias*), operators, and parentheses, and is evaluated as a real number

Examples:

```
alias  Te        100.
alias  CMULT     4.*PI
alias  Ri        (4.*PI*Ni/3.)^(-1/3)
alias  ILASER   1.e7*ELASER/(TLASER*PI*RSPOT**2)
```

- Evaluations use normal operator precedence
- The position and ordering of **alias** commands is arbitrary
- A *word* which has not been set by an **alias** command has value 0. (and “ “)

“Alias” – a basic macro capability

Syntax: **echo** *word* - prints numerical value assigned to *word* by an alias
echo all - prints numerical values of all aliases

- Predefined aliases (physical constants and sizes):
  PI AVGD CS KB KBEV HP HPEV EMASS PMASS AMASS QELEC
  ABOHR RYD KMAX LMAX MMAX NT NGP
- Operators: + - * / ** ^ sqrt exp ln log sin cos tan asin acos atan int nint

Using aliases:

- Space-delimiting operators - and / avoids some ambiguities
- Defining *word* also defines *word+* and *word-* with values (*word+1*) and (*word-1*)
- Aliases may be redefined or set from the command line

Check that your aliases have been evaluated correctly!

#define – for setting conditionals

Syntax: **#define** *word* - sets value to 1

- Useful for conditional inclusion of commands via structured clauses

```
#ifdef
   …
#elseif   or   #elif
   …
#else
   …
#endif
```

- Variable is considered defined if value is non-zero

From examples/tests/lasfoam/lasfoam.gen:

```
#ifdef SOURCE1

   source laser 4x rate history 1 1. N0 N1

#elif SOURCE2

   source jnu E1 E2 rate history 1 MULT N0 N1

#elif SOURCE3

   source jbndry 1 E1 E2 rate history 1 MULT
   boundary radiation streaming 1. 0. N1 xfile 1 1.

   switch 36 2                    ! turn on continuum transfer

#elif SOURCE4

   source jbndry 1 E1 E2 rate history 1 MULT
   boundary radiation streaming 1. 0. N1 xfile 1 1.

   switch 100  1                  ! use rad package

#elif SOURCE5

   laser 1 4x rate history 1 1.
      lasray 0.11 1. 0. 1.

   switch 45 1                    ! turn on laser ray trace

#endif
```

Some useful command line options

CRETIN file1 [file2] [**OUT**=file3 | **-o** file3]
            [**DEFINE** | **UNDEFINE** word] [**ALIAS** word value]

OUT=file3 or **-o** file3: name output files based on file3

e.g. "cretin ex2.gen –o run5"   produces run5.tbl, run5.plt, …

ALIAS word value: same as "alias" command, but may not be reset
i.e. takes precedence over any definition of word in the generator

DEFINE word: same as "#define word", but may not be reset
UNDEFINE word: ensures "word" is not defined in generator

Examples of command line usage

Varying element and/or atomic model:

```
    alias   ADF   hydrogenic        ← default atomic model
    alias   SYM   kr                ← default element
    atoms  ADF   SYM
```

```
"cretin  problem.gen  -o problem_kr"
"cretin  problem.gen  alias  ADF  dca_54  alias SYM Xe  -o problem_xe"
```

Changing physics options:

```
    region   1  N   Te  Ti  Tr
    element  1  1.

    #ifdef FIXNE
        ne   Ne
        switch 58  -1
    #else
        rho  Rho
    #endif
```

```
"cretin  problem.gen -o problem_rho"
"cretin  problem.gen  define  FIXNE  -o  problem_ne"
```

Scripting runs

Setting aliases from the command line allows automating parameter variations with shell scripts:

```
cretin problem.gen alias Te 1500. -o problem_1500
                              ↓
foreach  i  (500 1000 1500 2000)
   cretin problem.gen alias Te $i -o problem_$i
end
```

```
cretin problem.gen alias P72 1.0 -o problem_1.0.
   param 72  P72      ! autoionization multiplier
                              ↓
foreach  i  (0.1 0.2 0.5 1.0 2.0 5.0 10.0)
   cretin problem.gen alias P72 $i -o problem_${i}.
end
```

Output filenames are based on characters up to the final .

Homework

- Calculate the average charge state <Z> and radiative power loss for Kr as a function of temperature T_e
  - — fixed electron density: n_e = 10^{20} cm^{-3} or 10^{14} cm^{-3}
  - — radiation field: $J_\nu = 0$
  - — temperature range sufficient to cover <Z> from ~neutral to K-shell
  - — radiative power loss = frequency-integrated emissivity: cemistot

Homework generator: physics controls

```
c ----------------------------------------------------------
c   Materials
c ----------------------------------------------------------

atoms dca_36     kr

region  1 n_Te   1. 1. Tr
  element 1 Ni
  ne        Ne


c ----------------------------------------------------------
c   Geometry
c ----------------------------------------------------------

geometry none

rlog  1 n_Te   Te_MIN  Te_MAX

scale  te    1 n_Te   0.   1.  0. 1. 1. 0.


c ----------------------------------------------------------
c   Radiation
c ----------------------------------------------------------

ebins NBINS  E0 E1
```

```
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  55  1        ! continuum lowering
switch  58 -1        ! constant electron density

switch  44 10        ! number of iterations
switch 111  1        ! converge zones independently
switch 120  1        ! show convergence diagnostics
```

Homework generator: aliases + edits

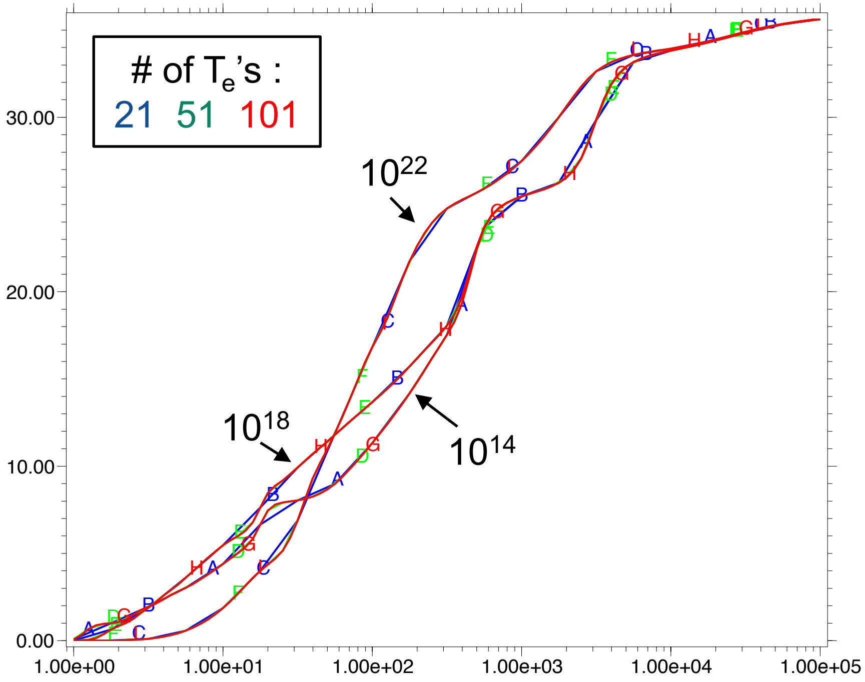
```
c ----------------------------------------------------------
c   Aliases
c ----------------------------------------------------------

alias logNe          20
alias Ne             10.**logNe
alias Ni             Ne / 20.

alias Te_MIN         1.e0
alias Te_MAX         1.e5
alias n_Te           101
alias n_Te5          n_Te-/5

alias E0             1.e0
alias E1             1.e6
alias NBINS          301
```

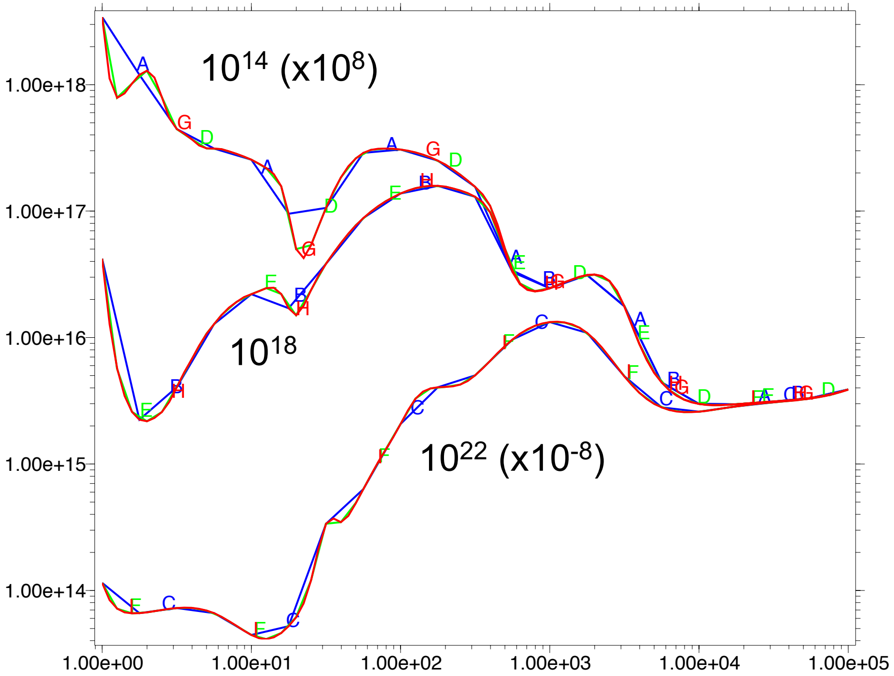
```
c ----------------------------------------------------------
c   Edits
c ----------------------------------------------------------

alias  CMULT  4.*PI

plot "CEMIS"
  xvar  ebins
  yvar  cemis     0 1:-1:n_Te5

plot "RPL vs TE"
energy-integrated
  xvar  r
  yvar  cemis     0 0 0 0 CMULT

plot "RPL vs TE"
  xvar  r
  yvar  cemistot
```

Script for running variations on density + resolution

```
#!/bin/csh -f

foreach  i  (21 51 101)                    ← # of temperatures
   foreach  j  (14 18 22)                  ← log10 electron density
       foreach  k  (61 121 241)            ← # of frequencies

           cretin  hw2.gen  alias  n_Te  $i  alias  logNe  $j  alias  NBINS  $k  -o  hw2_${i}_${j}_${k}

       end
   end
end
```

Results for $N_e = 10^{14}, 10^{18}, 10^{22}$



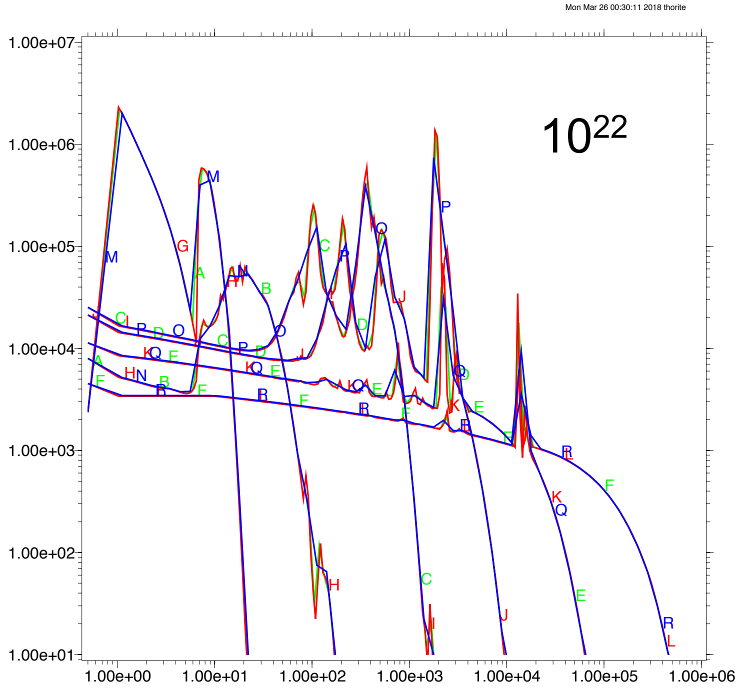


CURVE	LABEL		XMIN	XMAX	YMIN	YMAX	FILE
A	zbar	vs	1.00e+00	1.00e+05	8.17e-02	3.56e+01	hw2_21_14_241.ult
B	zbar	vs	1.00e+00	1.00e+05	1.94e-03	3.56e+01	hw2_21_18_241.ult
C	zbar	vs	1.00e+00	1.00e+05	1.26e-04	3.56e+01	hw2_21_22_241.ult
D	zbar	vs	1.00e+00	1.00e+05	8.17e-02	3.56e+01	hw2_51_14_241.ult
E	zbar	vs	1.00e+00	1.00e+05	1.94e-03	3.56e+01	hw2_51_18_241.ult
F	zbar	vs	1.00e+00	1.00e+05	1.26e-04	3.56e+01	hw2_51_22_241.ult
G	zbar	vs	1.00e+00	1.00e+05	8.17e-02	3.56e+01	hw2_101_14_241.ult
H	zbar	vs	1.00e+00	1.00e+05	1.94e-03	3.56e+01	hw2_101_18_241.ult
I	zbar	vs	1.00e+00	1.00e+05	1.26e-04	3.56e+01	hw2_101_22_241.ult

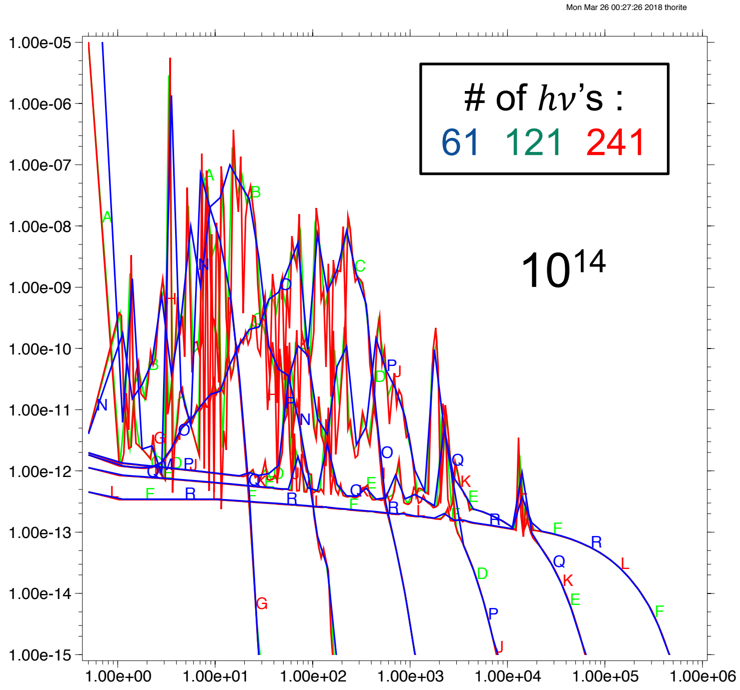
CURVE	LABEL		XMIN	XMAX	YMIN	YMAX	FILE
A	* cemistot	vs	1.00e+00	1.00e+05	2.97e+15	3.43e+18	hw2_21_14_241.ult
B	cemistot	vs	1.00e+00	1.00e+05	2.24e+15	1.58e+17	hw2_21_18_241.ult
C	* cemistot	vs	1.00e+00	1.00e+05	4.44e+13	1.33e+16	hw2_21_22_241.ult
D	* cemistot	vs	1.00e+00	1.00e+05	2.92e+15	3.43e+18	hw2_51_14_241.ult
E	cemistot	vs	1.00e+00	1.00e+05	2.18e+15	1.58e+17	hw2_51_18_241.ult
F	* cemistot	vs	1.00e+00	1.00e+05	4.12e+13	1.33e+16	hw2_51_22_241.ult
G	* cemistot	vs	1.00e+00	1.00e+05	2.92e+15	3.43e+18	hw2_101_14_241.ult
H	cemistot	vs	1.00e+00	1.00e+05	2.18e+15	1.58e+17	hw2_101_18_241.ult
I	* cemistot	vs	1.00e+00	1.00e+05	4.12e+13	1.34e+16	hw2_101_22_241.ult

Integrated quantities like <Z> and RPL are insensitive to resolution

Results for $N_e = 10^{14}, 10^{22}$



```
CURVE    LABEL                                   XMIN      XMAX      YMIN      YMAX      FILE

  A      cemis    (0,1       ) vs                5.00e-01  9.44e+05  0.00e+00  2.21e+06  hw2_101_22_121.ult
  B      cemis    (0,21       ) vs               5.00e-01  9.44e+05  0.00e+00  6.17e+04  hw2_101_22_121.ult
  C      cemis    (0,41       ) vs               5.00e-01  9.44e+05  0.00e+00  4.25e+05  hw2_101_22_121.ult
  D      cemis    (0,61       ) vs               5.00e-01  9.44e+05  0.00e+00  1.28e+06  hw2_101_22_121.ult
  E      cemis    (0,81       ) vs               5.00e-01  9.44e+05  0.00e+00  3.69e+04  hw2_101_22_121.ult
  F      cemis    (0,101       ) vs              5.00e-01  9.44e+05  6.42e-02  6.25e+03  hw2_101_22_121.ult
  G      cemis    (0,1       ) vs                5.00e-01  9.72e+05  0.00e+00  2.31e+06  hw2_101_22_241.ult
  H      cemis    (0,21       ) vs               5.00e-01  9.72e+05  0.00e+00  6.47e+04  hw2_101_22_241.ult
  I      cemis    (0,41       ) vs               5.00e-01  9.72e+05  0.00e+00  5.95e+05  hw2_101_22_241.ult
  J      cemis    (0,61       ) vs               5.00e-01  9.72e+05  0.00e+00  1.37e+06  hw2_101_22_241.ult
  K      cemis    (0,81       ) vs               5.00e-01  9.72e+05  0.00e+00  6.83e+04  hw2_101_22_241.ult
  L      cemis    (0,101       ) vs              5.00e-01  9.72e+05  4.80e-02  8.47e+03  hw2_101_22_241.ult
  M      cemis    (0,1       ) vs                5.00e-01  8.91e+05  0.00e+00  2.02e+06  hw2_101_22_61.ult
  N      cemis    (0,21       ) vs               5.00e-01  8.91e+05  0.00e+00  5.30e+04  hw2_101_22_61.ult
```



```
CURVE    LABEL                                   XMIN      XMAX      YMIN      YMAX      FILE

  A      cemis    (0,1       ) vs                5.00e-01  9.44e+05  0.00e+00  9.86e-06  hw2_101_14_121.ult
  B      cemis    (0,21       ) vs               5.00e-01  9.44e+05  0.00e+00  1.91e-07  hw2_101_14_121.ult
  C      cemis    (0,41       ) vs               5.00e-01  9.44e+05  0.00e+00  1.15e-08  hw2_101_14_121.ult
  D      cemis    (0,61       ) vs               5.00e-01  9.44e+05  0.00e+00  2.64e-10  hw2_101_14_121.ult
  E      cemis    (0,81       ) vs               5.00e-01  9.44e+05  0.00e+00  6.72e-12  hw2_101_14_121.ult
  F      cemis    (0,101       ) vs              5.00e-01  9.44e+05  6.41e-18  6.47e-13  hw2_101_14_121.ult
  G      cemis    (0,1       ) vs                5.00e-01  9.72e+05  0.00e+00  1.01e-05  hw2_101_14_241.ult
  H      cemis    (0,21       ) vs               5.00e-01  9.72e+05  0.00e+00  3.72e-07  hw2_101_14_241.ult
  I      cemis    (0,41       ) vs               5.00e-01  9.72e+05  0.00e+00  1.97e-08  hw2_101_14_241.ult
  J      cemis    (0,61       ) vs               5.00e-01  9.72e+05  0.00e+00  3.72e-10  hw2_101_14_241.ult
  K      cemis    (0,81       ) vs               5.00e-01  9.72e+05  0.00e+00  1.26e-11  hw2_101_14_241.ult
  L      cemis    (0,101       ) vs              5.00e-01  9.72e+05  4.79e-18  8.68e-13  hw2_101_14_241.ult
  M      cemis    (0,1       ) vs                5.00e-01  8.91e+05  0.00e+00  1.83e-05  hw2_101_14_61.ult
  N      cemis    (0,21       ) vs               5.00e-01  8.91e+05  0.00e+00  9.97e-08  hw2_101_14_61.ult
```

Detailed quantities are sensitive to resolution