AMU/CEA 2022 Report & 2023 work

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Outline – AMU tasks in 2022

- Manage the technical interface with ACH for Eiron :

guidance on relevant mechanisms, on Monte Carlo principles, on how to compare to EIRENE

- Manage the technical interface with ACH on IMAS :

guidance on input/output format, providing test cases

TBD in 2023: coordinate ACH IMAS work with what N. Rivals has done in the framework of his PhD co-funded by ITER

Contribution to EIRENE_unified

- **Remove B2 spill-over into EIRENE** in forks/iter/develop to prepare for the eirene_unified branch (branches species_rescaling_dr3-PB_AMU & compiling_issues_JSON8.2.5_gfortran) after meeting at IO with Xavier Bonnin

- Now merged into EIRENE_unified by Petra

Parallelization of the rate coefficient calculation

- in preparation for the use of CRM models, needed to reduce « overhead » time (preparation of MC calculation in the main loop)
- branch parallel_ColRad_WIP
- so far MPI only

How are collisional radiative model called ?

```
If (my_pe == 0) then
    call input
      call setamd(0)
      ….
      call setamd(1)
    # deal with particle types
    sequentially
        call xsecta
        call xsectm
        call xsecti
        call xsecm
endif ! (my_pe == 0)
```

```
# deal with reaction types
sequentially
call xstei
call xstcx
call xstel
call xstpi
```

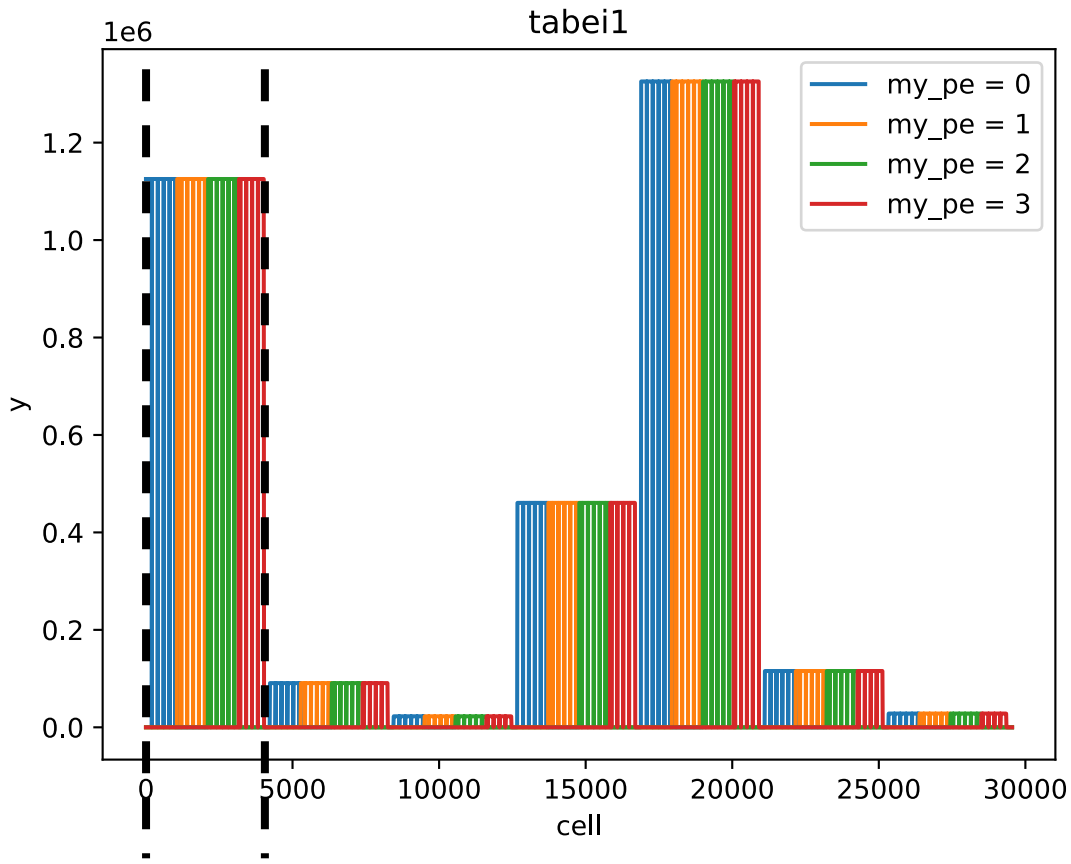
```
do J=1,NSBOX
  call eirene_rate_coeff(…)
enddo
…

do J=1,NSBOX
  call eirene_energy_rate_coeff
enddo
```

```
If (…) then
  call h_colrad(…)
endif
```

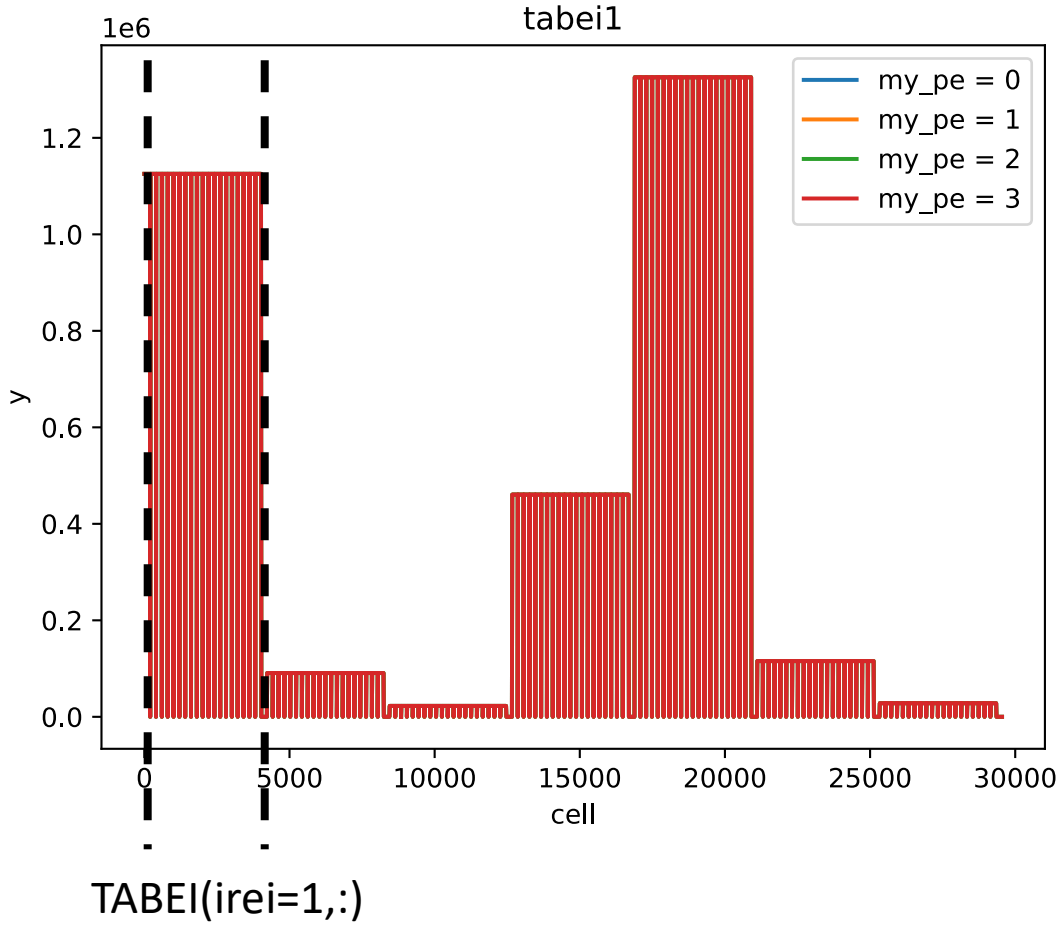
Implementation of MPI parallelisation (1)

- divide the grid in chunks (= ncell/n_processors, not necessarily divisible but make the chunk length as identical as possible) ☑
- call input with all processors, execute most of it with only one processor) ☑
- rate coefficients already broadcasted to all processes, need to adjust initialization/broadcast and so on – that's the dangerous part, lots of potential side effects) ☑
- Modify all loops (explicit or implicit), e.g. replace 1:NSBOX by grid_chunk(1):grid_chunk(2)) ☑
- Each processor has to broadcast his chunk and receive chunks calculated by others) ☑

Implementation of MPI parallelisation (2)



TABEI(irei=1,:)



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- Integrated testing for correctness now ongoing, scaling later on

Parallelization of the rate coefficient calculation next steps

- Decide on control switches for the user (based on scalings, …)
- OpenMP layer for ‘consistency’ with the MC loop (on low level loops)
- Merge into EIRENE unified
- Combination with upcoming domain decomposition ? (same partition or not, since load balancing)

Contributions to EIRENE refactoring

- Revise folneut along the lines proposed (case select) starting from the EIRENE_unified branch (timing w.r.t. free format conversion ?)
- Variable grouping
- Continue on folion, …
- Implementation of MODCOL replacement and testing (feature/MODCOL)

- Time dependent mode ?

Interface to TSVV3

- Major upgrade of SOLEDGE3X interface planned for 2023 (styx2.0; N. Rivals)

  'decouple' interface from EIRENE and move to EIRENE_unified branch

- Demontration of coupled MPI/OpenMP runs of SOLEDGE3X-EIRENE, making use of the memory usage benefit to run finer resolutions
- Improvement of neutral models in SOLEDGE3X ongoing (following TSSV5 work by Horsten et al., PhD V. Quadri)
- Reintegration of hybrid models making use of TSVV5 work, and 1 publication foreseen concluding M. Valentinuzzi's work (exploiting N. Rivals' ITER simulations and enabling further computing time improvements)