ITC – Project 2009 – FZJ part

s.wiesen@fz-juelich.de

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Contents

I   Introduction

This report summarises the code developments on EIRENE (a Monte-Carlo kinetic solver for neutrals [1]) used witihn JINTRAC as part of the 2009 ITC code development project at JET.

EIRENE has been introduced into JINTRAC as part of EDGE2D under the auspices of the ITC-project in 2005. Later on, EIRENE has been coupled also into JETTO (for modelling the cold neutral distribution in the plasma core) and AS-COT (for creating the fast-ion birthprofile distributions) [2] and EIRENE is now regarded as the main neutral particle distribution solver within JINTRAC.

At FZJ EIRENE has been and is being developed and kept at a high standard with respect to reliability, backwards compatibility and numerical performance. Hence, to profit from new features of EIRENE available and to have a proper way to keep EIRENE at JET updated as good as possible also in the future, the most current EIRENE release has been taken from FZJ (the origin of EIRENE).

The following participants were actively collaborating for this part of the project:

Sven Wiesen (FZJ)
Petra Boerner (FZJ)
Gerard Corrigan (JET)

consultants:
Detlev Reiter (FZJ)
Laura Taroni (JET)
Vassili Parail (JET)

II Updating EIRENE within JINTRAC

The most current EIRENE version has been taken from FZJ's subversion system (October 2009) and only a few modifications were necessary to update the EIRENE version available within JINTRAC. Essentially, the central parts of the EIRENE code have been unaffected and it was obvious that JINTRAC already uses a recent version of EIRENE. Therefore, future updates of EIRENE seem to be uncritical and easy to pursue. Nevertheless, EIRENE at JET has been updated to the most current EIRENE version from FZJ (October 2009).

III Activation of EIRENE MPI parallel support

One criticial issue when using a Monte-Carlo procedure is the performance of the kinetic evaluation of the neutrals distribution. With such a method many geometric details and plenty of molecular and atomic physics can be included and thus the demand for good performance of the numerics is essential and growing. Compared to a fluid-approximation for the plasma the kinetic discription of the neutrals is the critical bottleneck in the modelling per se.

The EIRENE code as it comes from FZJ is already parallelised using MPI standard. It is also capable, knowing the total workload per EIRENE call, to redisribute the available wall-clock time equally to the available processing nodes in order to have as few as possible processing units in idle mode.

EIRENE is capable of running in stand-alone mode using MPI support. But in combination with EDGE2D, where actually EDGE2D is the controlling program to execute EIRENE (at the time when it is necessary to update the source terms), EIRENE is not allowed to initialise the MPI library by itself anymore. Instead, the main subroutine of EDGE2D has to initialise and finalize MPI.

The procedure is the following (cf. figs 1 and 2): EDGE2D is running only on a single node mype=0. The remaining available nodes (npes-1) are sent into idle mode until EDGE2D decides in the fluid-time step loop to activate EIRENE by calling the subroutine call_eirene. The idling is realised by using blocking MPI communication using mpi_bcast: the idling npes-1 nodes are waiting for the execution of mpi_bcast with a valid EIRENE timestep (dteir larger or equal zero). This happens when the main node mype=0 is arriving at the corresponding mpi_bcast and then all npes nodes are running sunchronously in parallel to execute EIRENE. After EIRENE has been executed succesfully and after calling mpi_barrier to synchronise all nodes, npes-1 nodes are sent back into idle mode, waiting for the next execution of EIRENE (blocking mpi_bcast). If the main subroutine of EDGE2D decides to quit, then a non-valid dteir < 0 is sent via mpi_bcast from the main routine to tell the idling nodes to quit. After returning of all nodes back in the main subroutine of EDGE2D, mpi can be finalized and the program exits.

Now the overall performance should increase already since most of the computing time of a combined EDGE2D-EIRENE run is spent in EIRENE anyway and a small overhead of idling processors occurs only at the time when EDGE2D is solving the plasma fluid equations and in most cases this overhead can be neglected. (Although if EDGE2D is ought to model many charge states, for example in the case of unbundled tungsten impurities (Z=74), EDGE2D execution time might be of similar order).

IV   Revision of vessel description within EIRENE in prospect of ILW, introduction of W and Be vessel material

In the past it was only possible to have a single wall material availble in EIRENE, ie. in the modelling only a single intrinsic impurity like carbon or beryllium could be sputtered from the combined main-chamber and divertor wall. For the case of the ILW the main-chamber wall will be made out of beryllium and plasma facing components in the divertor and target plates will be made out of tungsten coated CFC or bulk tungsten material. Hence, EIRENE should be able to have different sputtering and wall reflection models available at different locations.

A full revision of the wall vessel geometry is envisaged for later and to keep things simple for the time being it is now possible to select differnt materials for either the target plates, the lower lying divertor tiles and the higher lying main-chamber wall tiles. To be exact, the main-chamber is defined to be the upper part of vessel segments which are not in direct contact with the parallel plasma flow seen in EDGE2D (ie the target plate representing vessel segments in the model). Similarly, the divertor is regarded as the vessel segments below target segments which are not in direct contact with the parallel flow. Hence, the poloidal extent of main-chamber and divertor segments in the model depend solely on the plasma grid provided by the grid generating code GRID2D.

In the Extra Namelist of EDGE2D one can now select different materials for the divertor and the main-chamber wall. For backwards compatibilty the default is the material chosen for the target plates (ie by the respective configuraion panel in JAMS). If one would like to specify a different divertor material, one should set:

IZDIVERT=Z_{divert}

where Z_{divert} is the charge number of the matrial selected (eg Z=6 for carbon, Z=74 for tungsten, Z=4 for beryllium). Similarly, for the main-chamber we have:

IZMAINCH=Z_{mainch}

for the charge number for the main-chamber material.

EIRENE will then select the corresponding dataset in the wall-reflection TRIM database (when a material for a given Z is not existing, TRIM will interpolate to the nearest Z element available, taking into account mass ratios). Also, the physical sputtering will depend on the selected Z-number.

V Revision of molecular and atomic physics model for the bulk plasma in EDGE2D-EIRENE

By introducing a separate switch in EDGE2D-EIRENE it is now possible to switch to a different atomic and molecular physics model for the main ions and neutrals. This new A&M model is currently the most sophisticated model used also within ITER design studies. Specifically, for high density discharges the neutral pressure in the divertor needs to be treated in an optimal way. Otherwise, the modelling of a divertor operation in detached mode (relevant for ITER and some ILW scenarios) might be unsuitable and it becomes difficult to derive correct pumping efficiencies and particle contents.

This "standard" A&M model consists of the following processes (the specifier in brackets are reference in [1]):

- $D + e \longrightarrow D^+ + 2e$, ionisation (AMJUEL 2.1.5)

- $D + D^+ \longrightarrow D^+ + D$, charge exchange (HYDHEL 3.1.8)

- $D^+ + e \longrightarrow D$, recombination (AMJUEL 2.1.8)

- $D_2 + e \longrightarrow D + D + e$, dissociation (AMJUEL 2.2.5)

- $D_2 + e \longrightarrow D + D^+ + 2e$, dissoc. ionisation (AMJUEL 2.2.10)

- $D_2 + e \longrightarrow D_2^+ + 2e$, molec.ionisation (AMJUEL 2.2.9)

- $D_2 + D^+ \longrightarrow D_2 + D^+$, elastic coll. (AMJUEL 0.3T)

- $D_2 + D^+ \longrightarrow D + D_2^+$, molec. charge exch. (AMJUEL 3.2.3)

- $D_2^+ + e \longrightarrow D^+ + D^+ + 2e$, (AMJUEL 2.2.11)

- $D_2^+ + e \longrightarrow D + D^+ + e$, (AMJUEL 2.2.12)

- $D_2^+ + e \longrightarrow D + D$, (AMJUEL 2.2.14)

Most importantly now the elastic collisions of neutral molecules with bulk ions are included and also the molecular charge exchange which initiates molecular assisted processes via decaying molecuar ions are considered (electrons removed for clarity):

molecular assisted ionisation (MAI):
$$D_2 + D^+ \longrightarrow D + D_2^+ \longrightarrow D + D^+ + D^+$$

molecular assisted dissociation (MAD):
$$D_2 + D^+ \longrightarrow D + D_2^+ \longrightarrow D + D + D^+$$
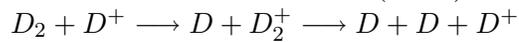
molecular assisted recombination (MAR):
$$D_2 + D^+ \longrightarrow D + D_2^+ \longrightarrow D + D + D$$

Specifically, these new processes are crucial with respect to the neutral pressure build-up in the high density divertor. Currently, the new model can only be switched on via EDGE2D Extra Namelist Editor by setting:

EIR_AM_FUEL=3.

Since EDGE2D by default is applying a source linearisation scheme using an outdated A&M physics database, the source linearisation scheme needs to be switched off explicitly by setting:

LINDEN=F
LINMOM=F
LINSQE=F
LINSQI=F

in the Extra Namelist editor. Now EIRENE will provide EDGE2D with the full set of sourceterms for particle, momentum and temperature equations solved. A general availablity of the new A&M database through the JAMS interface (avoiding to switch special flags in the extras namelist of EDGE2D) is foreseen and implemented later into JAMS.

References

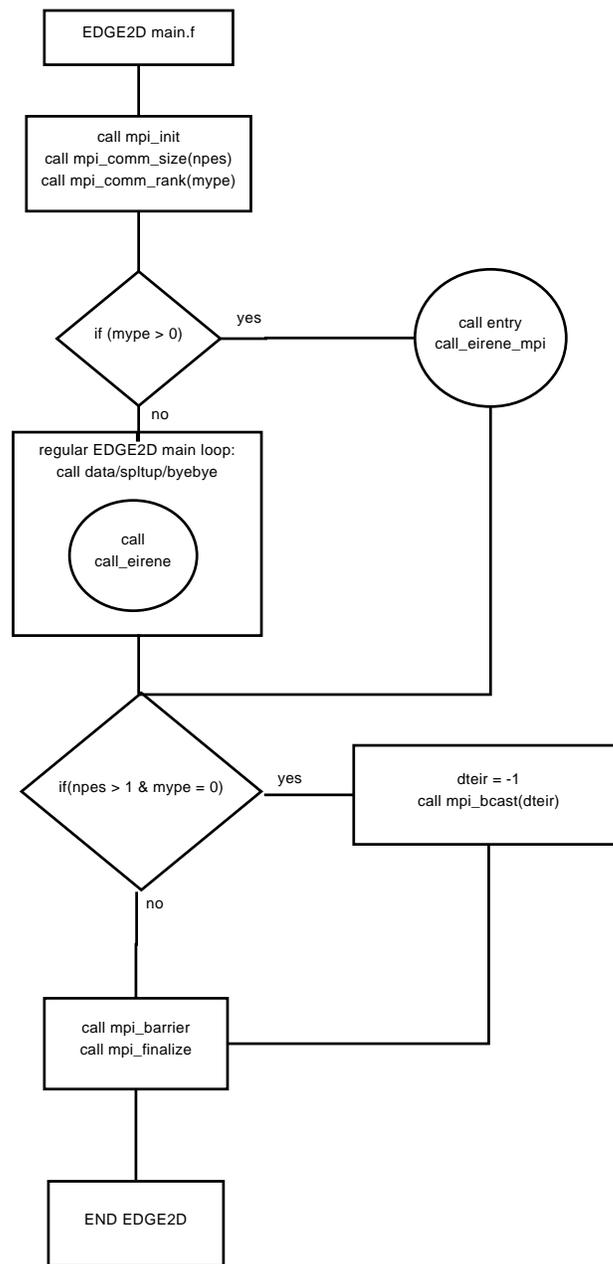[1] http://www.eirene.de

[2] ITC-project JET report 2008, S. Wiesen

Figure 1: Flowchart of EDGE2D main routine with MPI support included. npes is the number of available cpu cores whereas mype is the rank (cpu core number) of the running process. EDGE2D is running on mype = 0 whereas all other cpus with mype > 0 are in wait-state until EIRENE is actually called. dteir normally defines the current EIRENE time-step (or zero when run in time-independent mode) but here dteir < 0 tells the main-routine to finalize and quit the program.
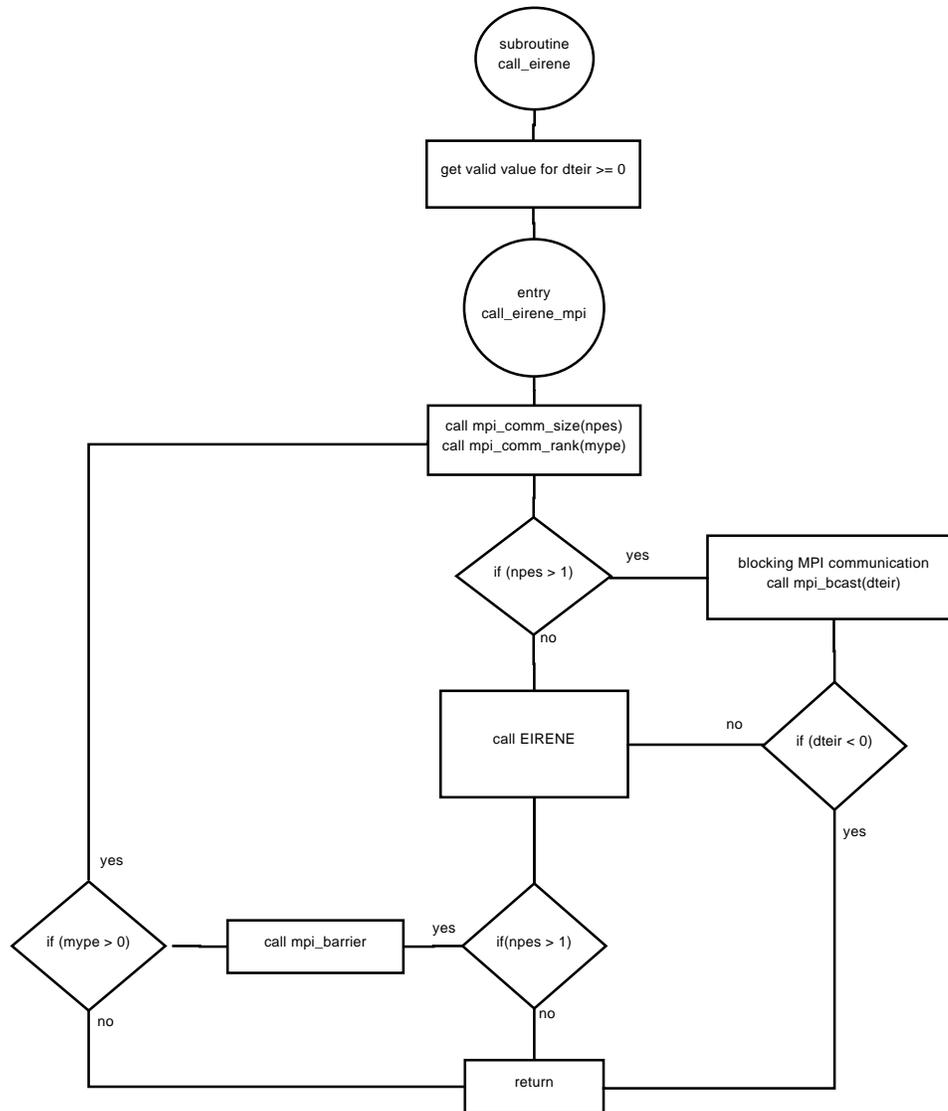
Figure 2: Flowchart of EIRENE driver routine called by EDGE2D with MPI support included. Definitions for mype, npes and dteir as in fig. 1. All cpus are active until EIRENE exits succesfully. Cpus with mype > 0 are idling as long as the outer EDGE2D main-routine is executed.