iPATH USER MANUAL

2018.9

Preface

The iPATH model mainly consists of three parts:
(1)MHD module:a hydrodynamic ZEUS code that simulates the background solar wind (assumed spherically symmetric) and a propagating CME-driven shock.
(2)Acceleration module: an 2D onion shell module where injected particles are accelerated by the DSA mechanism and diffuse between shells within the shock complex.
(3)Transport module:This model is based on the focused transport equation modified with a cross field diffusion term, which we solve using a backward stochastic differential equation method. Specifically, we use a Monte-Carlo approach to track the propagation of quasi-particles.

The iPATH model is portable to LINUX. The compilers gfortran and python2.7 are used to compile our code.(Recommended configuration: ubuntu 16.04 LTS +gfortran+anaconda python 2.7)

Several fundamental packages (Numpy,matplotlib.pyplot,gdal) for scientific computing with Python2.7 are necessary for plotting. Make sure these compilers are installed before you officially start working.

1.Installation for ZEUS-3D version 3.6

First,you need to port ZEUS36 to your Linux computing platform.
(1)Go to the directory iPATH,type:

```
tar -zxvf dzeus36.tar.gz
```

This will create and fill a new directory called zeus_v3.6_ICA in your present working directory.
(2)In the folder zeus_v3.6_ICA ,there are a series of directories. Go to the directory manuals,open the file install_dz36.txt. As you can see,this is a full instructions for installing ZEUS-3D.You just need to follow these steps ,and then finish the installation easily.
(3)after finish step (2),copy backsw and CME into the directory zeus_v3.6_ICA ,you need to compile them first,go to the directory zeus_v3.6_ICA ,type:

```
cd backsw
csh -v dzeus36.s
cd ../CME
csh -v dzeus36.s
```

if there are no error messages , you have compiled these code successfully. Then, move the folders backsw and CME back to the directory iPATH.

2.get initial boundary parameters from ACE satellite data

The Solar Wind Electron Proton Alpha Monitor (SWEPAM) experiment provides the bulk solar wind observations for the Advanced Composition Explorer (ACE).And Magnetic Field Monitor (MAG) experiment records the magnitude of magnetic field in the solar wind.

Go to the directory get-initial,One-hour-average real-time proton density，bulk speed and magnetic field strength data will be downloaded when you run the code download_aces_data.py . Meanwhile,we will average the latest 12h data of proton density,bulk speed and magnetic field strength as the solar wind properties at 1AU.Then we use several functions to get the initial boundary at 0.05AU or 0.1 AU.Alternatively,you can modify this program the get the initial boundary of specified time.

You need to change some parameters in the file download_settings if you want to get the initial boundary your interested.
1) the initial boundary location at 0.05AU or 0.1AU.
2) the span of time you want to average
3) initial boundary perturbing duration
4) Density perturbation amplitude
5) Temperature perturbation amplitude
6) Velocity perturbation amplitude
7) magnetic field perturbation amplitude
9) CME width in degree
other parameters are not needed in the initial boundary inputs.
When you finish these changes,type:

```
python download_aces_data.py
```

the file initial-bndy will generate into directories backSW and CME automatically.

If you want to simulate solar wind and CME condition you interested, we provide programs that you can convert the solar wind properties at 1AU to the initial boundary at 0.05AU or 0.1AU.Type:

```
python convert_initial_bndy-0.1AU.py
or
python convert_initial_bndy-0.05AU.py
```

3.Modeling a stable background solar wind

Go to the directory backsw,there are some basic parameters you need to change in the different files.
Open file dzeus36.s ,you need to understand the meaning of some parameters:
(1)parameters (*in,jn,kn*) set the dimensions of the 3-D “field variables ” (density,velocity,etc), which are the principle determinators of memory requirement of a particular run. The iPATH model’s simulation is based on a spherical polar(RTP) geometry. Parameter *in* is the dimensions of r-direction .Parameter *jn* is the dimensions of θ-direction .Parameter *kn* is the dimensions of φ-direction. Since the iPATH model is a 2D model,the θ-direction is set to be 1.Specifically, *in,kn* contain 5 ghost or boundary zone while the remaining zones are “active” zones in which the equations of MHD are solved.
(2)In the namelist *recon* ,parameter *dtdmp* is the problem time interval between restart dumps,which means the time step of creating a new restart dump(zr0**TW).
(3)In the namelist *ggen1*,parameter nbl set the number of zones of r-direction(*ggen2,ggen3* similarly).Parameter (*x1min,x1max*) set the minimum and maximum extent of the block in coordinate units (*ggen2,ggen3* similarly). *x1min* is the inner boundary to be close at 0.05AU or 0.1AU. *x1max* is the outer boundary to be choosed at 2AU or farther.
(4)In the namelist *pcon*, parameter *nlim* set the cycles to run and tlim set the problem time to stop calcuation.
(5) In the namelist *hdfcon*, parameter *dthdf* set the time interval between hdf files(zhto***TW).

Open file initial-bndy ,you need to know these inputs:
(1)the first row is the inner boundary condition for background solar wind. Five inputs are density(cm^{-3}),proton temperature(MK) ,velocity(km/s, the real solar wind speed should times 52.483),b1 (nT)and b3(nT) respectively.
(2)the second row is the perturbed inner boundary condition for CME Five solar wind inputs multiplied by different perturbation amplitude is the CME input.
(3)the third row is perturb duration and the CME angular width.

We get background solar wind inputs from the ACE database. The specific process have been discussed in the previous section.
If you change these parameters, we need recompile the program and run it,type:

```
rm xdzeus36
csh -v dzeus36.s
./xdzeus36
```

It will take 2-3 hours when this program is completed, you will get a series of restart files(zr0**TW), we copy last but one restart file into the directory CME,type:

```
cp zr0**TW ../CME/
```

4.generate a CME-driven shock , particles accelerate and diffuse within a shock complex

Go to the directory CME,
(1)Open the file dzeus36.s,you need to change ‘*resfile=zr003TW*’（the restart file name you copied from the basksw)in the namelist *recon*. The parameter *tlim* in the namelist *pcon* should change with the restart file’s generate time.(e.g.If *dtdmp*=0.1,zr003TW generated at t=0.3 ,so the *tlim* should equal to 0.3+x, x is shock propagating time. x~0.1 within 2AU.) Other parameters should be same as the file dzeus36.s in the backsw.
(2)Open the file input, there are five inputs related to the acceleration part.
1st input select a specified heavy ion between CNO (now is Oxygen ion)and iron ion.
2nd input controls whether this is a perpendicular shock.
3rd input is a pre-factor for Gordon-Lee's wave intensity.
4th input is a free parameter to adjust seed spectrum.
5th input is a parameter of injection rate.
Use default inputs first.
(3) The file initial boundary have been presented in the section 2 and you just copy this file to the directory CME. The second row can be changed for your specified CME. Distinguishingly, you need to set the CME center along the longitude direction in the file dzeus36.s .
(4)If you have finished these parameters setting, then type:

```
rm xdzeus36
csh -v dzeus36.s
./xdzeus36 < input
```

When this program is completed,you will get a series of output data in the file path_output. These files will be used in the next module transport.

5.Particle transport in the solar wind

This is a independent part that don’t need ZEUS anymore. Message-Passing-Interface(MPI) is introduced for running this module faster. So make sure you have been install openmpi-dev in your own Linux system. Go to the directory transport, you also should set some inputs first.
(1)Open the file assign_common.h, you just need change several parameters.
time_start/time_end: time start is the restart time in the CME part and time_end is equal to parameter tlim you set in the file dzeus36.s (CME). (e.g. If you use file ‘zr003TW’ as a restart file, time_start is equal to 0.3 and time_end is equal to tlim.)
usw : solar wind speed .(m/s)
(We are currently setting up *usw* equal to solar wind speed at 1AU.If you not sure this speed value, you can read this inputs in the file /CME/path_outputs/trspt_params .This file will generate at the beginning when you run CME module.)
br_bnd:radial magnetic field at inner boundary ,which is equal to the value b1 in the file initial boundary.(T)
r0 : observation location expressed by x*AU (m)
r_bnd: initial boundary location expressed by x*AU (m)
cme_center: same as you changed in the file dzeus36
cme_width: same as you changed in the file initial-bndy
phi_e: this is observation longitude position on the ecliptic plane, you could choose the selected longitude of observation(e.g. STEREO-A and STEREO-B.)
(2)Open the file combine.f, the parameter *ranks* sets to be the available core number of your computer or cluster node.
(3)compile transport module, this module has three type of particles using for transport(proton,iron ion,CNO).using proton by default.type:

```
mpif90 -O3 parallel_wrapper.f transport_back_1.09.f -o proton_80.out
gfortran combine.f -o combine.out
mv proton_80.out proton_80_1.09
cp combine.out  proton_80_1.09
cp ../CME/path_output/dist_at_shock.dat proton_80_1.09
cp ../CME/path_output/shock_momenta.dat proton_80_1.09
cp ../CME/path_output/esc_distr_dn.dat proton_80_1.09
cp ../CME/path_output/all_shell_bndy.dat proton_80_1.09
cp ../CME/path_output/dist_all_shl.dat proton_80_1.09
cd ./proton_80_1.09
mpirun -np 4 ./proton_80.out
```

(attention:The number 4 is the available core of your working platform, it should be equal to the input *ranks* in the combine.f.)

```
./combine.out
rm Raw*
```

For convenience, we use a script run_trspt.sh to compile it. So you just type:

```
chmod u+x run_trspt.sh
./run_trspt.sh
```

You will get a final output file named fp_total for plotting time intensity profile and particle spectrum.

6.Plotting

Go to the directory plotting, you will get some results by running these program.

(1)solar wind properties

Open the file swprofile.py, this program will plot solar wind density and solar wind speed along the radial direction. Three parameters deserve attention.

xdims: this input should be same as the parameter $ggen1 *nbl* in the dzeus36.s,which is the number of zones of radial direction.

x1min/x1max: the initial boundary and the outer boundary.

Then, type:

python swprofile.py

(2)CME-density

Open the file plot-density_simple.py, there are five parameters need to be change.

n_start: This is the first HDF file's number.(zhto***TW),default value =1.

n_end:This parameter is decided by the restart time,inputs *tlim* and *dthdf*. You could calculate the results by the equation *n_end* = int((*tlim*-restart time)/*dthdf*).

xdims/x1min/x1max:same as above.

By running this code, you will get a few cartoons of CME propagating over time.Type:

python plot-density_simple.py

(3)shock parameters

Open the file shock_param_overview.py, these inputs deserve attention.

cme_center:same as the value you changed in the dzeus36.

r_bnd: the initial boundary in the unit of m, so it express by 0.05*AU or 0.1*AU.(AU=1.5e11)

time_index:This input decides the shock parameters in some moment you get. we set five time index in this plotting program. So you will get five curves at different time in a figure. The index should to be round number from small to big.

Then type:

python shock_param_overview.py

(4)time intensity profile and particle spectra

Open the file time_intens_new.py, you just need to change some inputs that we have introduced above.

phi_e:this is the observation loction in the longitude direction.

r_e: this is the observation loction in the radial direction.

cme_center: same as above.

energy_index:these indexes represent different energies of .

time_start/time_end: introduced in the previous section.

Then type:

```
python time_intens_new.py
```

you will get three figures ,time intensity, time-integrated-intensity and proton flux respectively.

(5)ESP(energetic storm particle) phase

Open the file ESP_new.py, these parameters settings are same as the file time_intens_new.py.

Then type :

```
python ESP.py
```

you will get a time intensity profile with ESP phase.

7.Full automatic script

The above sections introduce iPATH instruction step by step, however, it may be too cumbersome. If you modify the parameters very skilled,we provide a script run-ipath.sh to run all programs automatically. Ensure that all parameters have been set up correctly,go to the directory ipath,type:

```
chmod u+x run-ipath.sh
./run-ipath.sh
```

If you modify the restart file or parameter *ranks*, you need to modify it in the file run-ipath.sh too.