HBI User's guide

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August 9, 2024

1 Introduction

Fortran90 software `HBI` performs three-dimensional quasi-dynamic numerical simulations of sequences of earthquakes and aseismic slip (SEAS). It can handle arbitrary fault geometry such as branches, step-overs, and rough faults in an elastic half-space. 2D problems can also be solved in the same code. The computation is accelerated by taking advantage of $\mathcal{H}$-matrices. $\mathcal{H}$ACApK, open-source software for $\mathcal{H}$-matrices, is called for constructing and operating $\mathcal{H}$-matrices.

The code has been benchmarked by several SEAS problems under SCEC [Jiang et al., 2022,Erickson et al., 2023], as well as with fully-dynamic codes for 2D nonplanar fault problems [Romanet and Ozawa, 2022].

The latest versions can be found at `https://github.com/sozawa94/hbi`. Feel free to contact So Ozawa (`sozawa@stanford.edu`), if you have any questions.

2 License

This software is freely available under the MIT license. If you write a paper using this code, please cite the following manuscript [Ozawa et al., 2023].

So Ozawa, Akihiro Ida, Tetsuya Hoshino, Ryosuke Ando (2023), "Large-scale earthquake sequence simulations of 3D geometrically complex faults using the boundary element method accelerated by lattice H-matrices on distributed memory computer systems", Geophysical Journal International

3 How to run

Download the source codes from github. Type:

```
git clone http://github.com/sozawa94/hbi
```

To compile and link the code, type

```
make
```

You may need to modify `Makefile` depending on your environment.

To run a simulation, type:

```
./lhbiem (inputfile)
```

or use MPI parallelization;

```
mpirun -np 16 ./lhbiem (inputfile)
```

To run the code in parallel, **the number of MPI processes must be a squared number.**

Several input files, including the benchmark problems of the SEAS project (`https://strike.scec.org/cvws/seas/`), are available in `examples` (see the next section).

3.1 Note on Sherlock users

If you use HBI in Sherlock (cluster in Stanford University), you need to load required modules before make:

```
ml load ifort
ml load impi
```

You also need to switch compiler options by editing `Makefile`. As of June 2024, Intel MPI is not working in Sherlock. I recommend the users to use open MP parallelism.

3.2 Monitoring ongoing jobs

The standard output first shows the information about (lattice) $\mathcal{H}$-matrices (approximated integration kernel). Then, timestep and time (measured by year) are recorded.

`job.log` is a record of the start and normal stop of jobs.

4 Problem setting

4.1 Description of Input file

Various simulations can be performed by modifying the input file, rather than modifying the source code. The input variable list is in Table 1.

4.2 Problem

The list of problems are shown in Table 2.

4.3 Physical variables and constants

Physical variables are in Table 3. The fundamental physical constants are set in `m_const.f90`. The default values are in Table 4.

4.4 Fault Geometry

For 2dp, 2dph, 3dp, and 3dph, fault geometry is set in inputfile. For other problems, an additional `geometry_file` is necessary.

4.4.1 2dp, 2dvs

The fault geometry is uniquely characterized by its element size `ds` and the number of elements `ncellg`.

4.4.2 3dp

The fault geometry is uniquely characterized by its element size `ds` and the number of elements along strike and dip (`imax, jmax`).

4.4.3 2dph

The fault geometry is characterized by its element size `ds`, the number of elements `ncellg`, and dip angle in degree `dipangle`. For nonplanar case, use `2dnh`.

4.4.4 3dph

The fault geometry is characterized by its element size `ds`, the number of elements along strike and dip (`imax, jmax`), and dip angle in degree `dipangle`. See also Figure 1.

Table 1: Parameters for input file

name	type	meaning
filenumber	integer	job number (name of output files)
problem	character	dimension, planar or non-planar, mesh, etc.
ncellg	integer	number of elements (not used in 3dp, 3dph, 3dht,3dnt)
nstep	integer	maximum number of time steps
interval	integer	output & checkpointing every this time steps
dtout	real	output every this time (year)
dtinit	real	initial time step width (s)
geometry_file	character	name of geometry file
parameter_file	character	name of parameter file
parameterfromfile	logical	true if parameters are read from parameter_file
parameter_file_nloc	integer	number of columns in the parameter file
restart	logical	true if restarting a suspended job
backslip	logical	true if loading is added by backslip
vpl	real	the velocity of backslip (m/s) (used if backflip=T)
sr	real	the stressing rate (MPa/s) (used if backslip=F)
tmax	real	maximum time (year)
dtmax	real	maximum time step (second)
sigmaconst	logical	true if normal stress is kept constant
ds	real	element size (km) (used in 2dp, 3dp, 3dph)
imax	integer	the number of elements in slip-parallel direction (used in 3dp, 3dph)
jmax	integer	the number of elements in slip-perpendicular direction (used in 3dp, 3dph)
crake	real	rake angle (deg) in 3D problems (not used if parameterfromfile=T)
dipangle	real	dip angle (deg) used in 3dph and 2dph
evlaw	character	evolution law for RSF ("aging" or "slip', default="aging")
a	real	a in RSF
b	real	b in RSF
dc	real	dc (m) in RSF
f0	real	f0 in RSF
tauinit	real	initial shear stress (MPa)
sigmainit	real	initial normal stress (MPa)
velinit	real	initial slip rate (m/s)
eps_h	real	error allowance in H matrix (default: 1e-4)
eps_r	real	error allowance in Runge-Kutta (default: 1e-4)
velmax	real	computation stop if maximum velocity is above this value (default:1e7)
velmin	real	computation stop if maximum velocity is below this value (default:1e-16)
limitsigma	logical	true if you want to limit normal stress
maxsig	real	maximum normal stress (MPa) (used if limitsigma=T)
minsig	real	minimum normal stress (MPa)(used if limitsigma=T)

Table 2: Problems

problem	description
2dp	2D planar fault in full-space (plane strain)
2dph	2D planar fault in half-space (plane strain)
2dn	2D nonplanar fault in full-space (plane strain)
2dnh	2D nonplanar fault in half-space (plane strain)
25d	2D nonplanar fault in full-space (plane strain) with finite fault width (2.5D approximation)
2dvs	2D vertical strike-slip fault
3dp	3D planar squared elements in full-space
3dph	3D planar squared elements in half-space
3dnr	3D nonplanar squared elements in full-space
3dhr	3D nonplanar squared elements in half-space
3dnt	3D nonplanar unstructured triangular elements in full-space
3dht	3D nonplanar unstructured triangular elements in half-space

Table 3: Units of physical variables

quantity	unit
time	s
location	km
displacement	m
slip velocity	m/s
wave speed	km/s
shear modulus	GPa
stress	MPa

Table 4: Constants and their default values

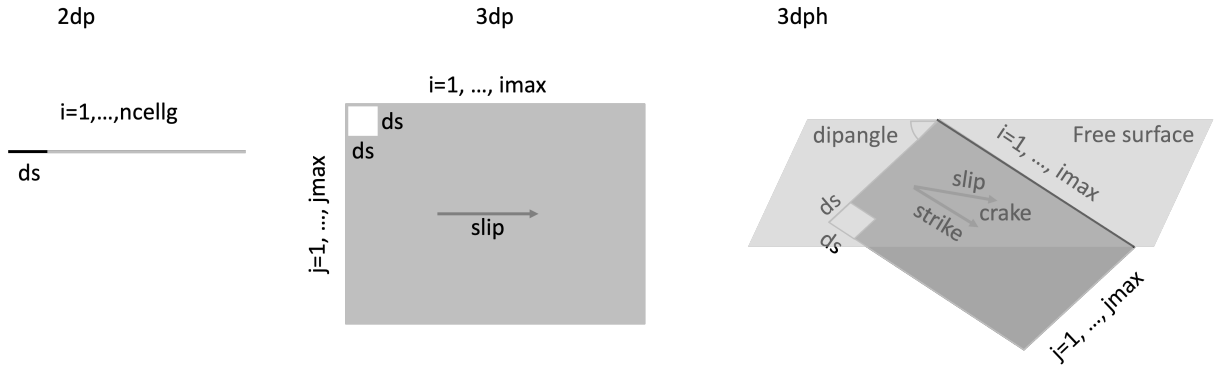| quantity	default value
rigidity	32.04 GPa
P-wave speed	6.000 km/s
S-wave speed	3.464 km/s
reference slip rate on RSF	1μm/s

Figure 1: Fault geometry

4.4.5　2dn, 2dnh, 25d

The coordinates of two edges of a straight line have the geometrical information of an element. `xel<xer` is necessary. `geomerty_file` has the following format:

```
xel(1) xer(1) yel(1) yer(1)
xel(2) xer(2) yel(2) yer(2)
...
```

For 2dnh, the structure `geomerty_file` is the same with 2dn. Here, $y = 0$ is assumed to be the free surface and y-axis is downward (i.e., y is always positive).

4.4.6　3dnt, 3dht

The coordinates of the three edges of a triangle have the geometric information of an element. `geometry_file` should have STL (ASCII) format:

```
facet normal normal_vector(1:3)
  outer loop
    vertex xs1 ys1 zs1
    vertex xs2 ys2 zs2
    vertex xs3 ys3 zs3
  endloop
endfacet
```

This structure repeats `ncellg` times. For `3dht`, $z = 0$ is the free surface and all elements must be located below the free surface (i.e., $z < 0$).

4.4.7　3dnr, 3dhr

Cell size `ds` must be specified in the inputfile. `geometry_file` should have STL (ASCII) format:

```
x(1) y(1) z(1) strike(1) dip(1)
x(2) y(2) z(2) strike(2) dip(2)
...
```

Here, x,y,z are the center of the square, strike and dip are measured in radian.

4.5　Parameters and Initial conditions

The following parameters and initial values are needed for each element.

4.5.1　Rake angle

In 3D problems, it is also necessary to specify the direction of slip (rake angle) for each element. The angle of rake is defined as 90 = reverse faulting, 0 = right lateral strike-slip faulting, and -90=normal faulting. The code does not allow for a time-varying slip direction. In the uniform case, set `crake` in `inputfile`.

Alternatively, rake angle for each element can be calculated from the plate convergence orientation for subduction zone simulations. Users use `rakefromglobal = T`, and set `convangle` for the orientation of the plate (0 degree for west-east (positive in x-axis) direction and anticlockwise). For example, Cascadia subduction zone has `convangle` of 10 - 20 degrees.

2D problems do not use rake values.

4.5.2 Friction parameters

`HBI` uses the regularized version of the rate and state friction law (RSF), which is employed in the SEAS benchmark problems. The friction coefficient are given by

$$\tau/\sigma = a\sinh^{-1}(Ve^{\psi/a}/2V_0). \tag{1}$$

The state evolution is governed either by the aging law

$$\frac{d\psi}{dt} = \frac{bV_0}{d_c}\exp[(f_0 - \psi)/b] - \frac{bV}{d_c}. \tag{2}$$

or the slip law

$$\frac{d\psi}{dt} = -\frac{V_0}{d_c}(f - f_{ss}) \tag{3}$$

$$f_{ss} = f_0 + (a - b)\log\frac{V}{V_0} \tag{4}$$

The evolution law is the aging law as default. Set `evlaw` to `slip` in the inputfile to switch. The values of parameters (a, b, d_c, f_0) are set in `inputfile` in the case of uniform parameters.

4.5.3 Initial conditions

The initial condition is uniquely determined by the value of normal stress, shear stress, and slip rate at each element (the state variable is determined by these three accordingly). In the case of uniform initial values of (σ, τ, V), these values are set in `inputfile` as `sigmainit`, `tauinit`, and `velinit`. Users can also set `muinit` for initial τ/σ, which overwrite `tauinit`.

4.5.4 External loading

To have repeated ruptures on the same fault, external loading is necessary. `taudot` and `sigdot` are the stressing rates for shear and normal stresses, respectively. In the uniform case, `taudot` is `sr` and `sigdot` is zero. the value of `sr` must be specified in `inputfile`.

Alternatively, the code has "backslip" loading option. If `backslip=T`, then the loading is added by slip deficit rate, that is,

$$\dot{\tau}_i = -V_{pl}\sum_j K_{ij} \tag{5}$$

$$\dot{\sigma}_i = -V_{pl}\sum_j L_{ij} \tag{6}$$

where K_{ij} and L_{ij} are kernel matrices for shear and normal stresses, respectively. The value of `vpl` must be specified in `inputfile` or `parameter_file`.

4.5.5 Format of parameterfile

If you want to use non-uniform parameters and/or initial values, set `parameterfromfile T` in `inputfile` and create `parameter_file`. Users have to state how many parameters are non-uniform in the by setting `parameter_file_ncol`.

For example, if users only vary friction parameters and use uniform initial values and loading rate, then parameter file is

```
a b dc f0
a(1) b(1) dc(1) f0(1)
a(2) b(2) dc(2) f0(2)
...
```

and set `parameter_file_ncol = 4` in the input file.

Table 5: Parameters that can be non-uniform in the parameter file

parameter	meaning
a	direct effect
b	evolution effect
dc	state evolution distance
f0	reference friction
tau	shear stress
sigma	normal stress
vel	slip rate
taudot	shear stress loading rate
sigmadot	normal stress loading rate
vpl	backslip rate

4.6 Stop control

The simulation stops when any of the following is satisfied.
1. the time-step reaches `nstep`
2. the maximum slip rate is greater than `velmax` [m/s].
3. the maximum slip rate is smaller than `velmin` [m/s].
4. the physical time reaches `tmax` [year].

4.7 Useful functions

If `sigmaconst=T`, then normal stresses do not change over time as assumed in many studies. If `sigmaconst=F` (as the default value), the normal stress changes with time. The computation can fail if the normal stress becomes very large or small. To avoid this, the user can set limits on the value of normal stress by setting `limitsigma=T`. In this case, `maxsig` and `minsig` are the maximum and minimum normal stresses, which should be stated in `inputfile`.

5 Visualization

For those familiar with Python, Analysis2D.ipynb and Analysis3D.ipynb are some examples for processing and visualizing data.

Here, the structure of the output files is briefly shown. `monitorX.dat` records the following information at every time step.

```
timestep time max(log10(vel)) mean(disp) mean(tau/sigma) max(sigma) min(sigma)
error-of-RK stepwidth wall-clock-time
```

For example, if you want to view the temporal change of the maximum slip rate in **gnuplot**, type

```
pl 'monitorX.dat' u 2:3 w l
```

The earthquake catalog is saved in `eventX.dat`. This file lists the event number, the onset time, and the moment magnitude. //

The field data are saved in binary stream files. `xyzX.dat` is the coordinates of the elements. `velX.dat`, `tauX.dat`, `sigmaX.dat`, and `slipX.dat` are slip velocity, shear stress, normal stress, and slip every `interval` time steps, respectively. These are binary stream files.

5.1 Paraview

(under construction)

name	type	meaning	
kpmax	real	Maximum permeability	unit: m^2
kpmin	real	Initial (minimum) permeability	unit: m^2
kL	real	Permeability evolution distance	unit: m
kT	real	Permeability healing time	unit: s
beta	real	Compressibility	unit: Pa^{-1}
eta	real	Fluid viscosity	unit: Pa s
phi0	real	Porosity	unit: none
bcl	character	Left boundary condition	Dirichlet or Neumann
bcr	character	Right boundary condition	Dirichlet or Neumann
pbcl	real	Fluid pressure at the left BC	Used when bcl=Dirichlet
pbcr	real	Fluid pressure at the right BC	Used when bcr=Dirichlet
q0	real	Flow rate at the boundary	unit: m/s

Table 6: Parameters for HBI-fluid

6 HBI-Fluid (2D)

This is a different version of HBI that allows fault-zone fluid flow and pore pressure evolution. To switch to the fluid version, you have to compile `main_fv.f90` instead of `main_LH.f90`. The fluid version is only available for 2D planar/nonplanar faults (2dp or 2dn) and parallel computation is not yet supported.

6.1 Governing equations

The fluid version of HBI additionally solves the fluid pressure diffusion equation

$$\beta\phi\frac{\partial p}{\partial t} = \frac{\partial}{\partial x}\left(\frac{k}{\eta}\frac{\partial p}{\partial x}\right). \tag{7}$$

The boundary conditions for both ends are either Dirichlet (fixed pressure) or Neumann (fixed flow rate), which can be specified by parameter pbcl and pbcr.

Permeability k evolves as.

$$\frac{\partial k}{\partial t} = \frac{V}{L}(k_{\max} - k) + \frac{1}{T}(k_{\min} - k), \tag{8}$$

where T is the healing time and L is the permeability enhancement distance. Initial permeability is `kpmin`, so setting `kpmax = kpmin` disables permeability evolution.

The fluid pressure is related to the shear stress with the effective stress law

$$\tau = f(\sigma - p). \tag{9}$$

6.2 Setting for 2D

There are several different initial and boundary conditions for fluid models. Users specify one of the following for the parameter `setting` in the inputfile.

6.2.1 injectionp

This is fluid injection at the fault center with constant pressure `pinj` (MPa).

6.2.2 injectionq

This is fluid injection at the fault center with constant flow rate `q0` (m/s). The duration of injection is `tinj` (year). SEAS BP6 can be solved with this setting (see `examples/bp6a.in`).

6.2.3 swarm

This is constant pressure injection at the left end ($x = 0$) of the fault. The injection pressure is `pbcl` (MPa). bcl must be Dirichlet to enforce the injection.

6.2.4 thrust

(under construction)

7 HBI-Fluid (3D)

`main_fv3dp.f90` is for 3D fluid pressure diffusion on a 3D planar fault. MPI parallization is supported. It solves 2D pressure diffusion equation on the fault.

$$\beta\phi\frac{\partial p}{\partial t} = \frac{\partial}{\partial x}\left(\frac{k}{\eta}\frac{\partial p}{\partial x}\right) + \frac{\partial}{\partial y}\left(\frac{k}{\eta}\frac{\partial p}{\partial y}\right) \tag{10}$$

Permeability evolution law is the same with 2D.

Nonuniform friction parameters can be used. Currently, the parameter file has a different strcuture with HBI. Parameter file has friction parameter a, b, dc, f0 at each element, which is ordered like (1,1),(1,2),$\cdots$,(1,jmax), (2,i),$\cdots$,(2,jmax),$\cdots$,(imax, 1),$\cdots$,(max, jmax).

Currently 3D code only has `injectionq` setting, but allows a slightly complicated injection protocol using an external injection file.

The injection file includes:

```
nwells (number of wells)
i j (indexes of the locations of the wells) nq (data of qVals and qTimes)
qVals (injection rate at t=qTimes (m/s))
qTimes (time (s))
```

See examples/wells.dat for an example of injection file, which is used in inputfile `examples/3dinjection2.in`.

8 Troubleshooting

1. Compare the input file with another input file that worked (many errors are due to wrong values in the input file).

```
diff inXXX inYYY
```

2. Check the first line of the monitorXX.dat to see if the initial values were set appropriately.

```
head monitorXX.dat
```

3. Check if the simulation was finalized by looking at job.log (sometimes the simulation worked but the visualization script has a bug).

```
cat job.log
```

9   References

 [Tse and Rice, 1986] and [Rice, 1993] are early examples of earthquake cycle simulations on a planar fault with rate and state friction. For nonplanar fault geometry, [Segall, 2010] is a great reference to the theoretical foundation of the BEM kernel. For the implementation of `2dn`, we use the formula in [Ando et al., 2007]. `3dhr` and `3dph` are based on [?]. `3dnt` and `3dht` are based on the expression of [Nikkhoo and Walter, 2015]. The time-stepping algorithm is based on "Numerical Recipe for Fortran90" [Press et al., 2002].

10   Acknowledgements

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