QDYN

Quasi-DYNamic earthquake simulator

V 1.1

User's Manual

github.com/ydluo/qdyn

Developers

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1 Introduction

1.1 Summary

QDYN is a boundary element software to simulate earthquake cycles (seismic and aseismic slip on tectonic faults) under the quasi-dynamic approximation (quasi-static elasticity combined with radiation damping) on faults governed by rate-and-state friction and embedded in elastic media.

QDYN includes various forms of rate-and-state friction and state evolution laws, and handles non-planar fault geometry in 3D and 2D media, as well as spring-block simulations. Loading is controlled by remote displacement, steady creep or oscillatory load. In 3D it handles free surface effects in a half-space, including normal stress coupling. The medium surrounding the fault is linear, isotropic and elastic, and may be uniform or (in 2D) contain a damaged layer.

QDYN implements adaptive time stepping, shared-memory parallelization, and can deal with multi-scale earthquake cycle simulations with fine details in both time and space. It is equipped with a user-friendly Matlab interface and graphical output utilities.

1.2 Main features

- Rate-and-state friction, with velocity cut-offs, aging and slip laws
- Arbitrarily heterogeneous frictional properties
- Slow and fast, aseismic and seismic slip transients (adaptive timestep)
- Non-planar faults (currently limited to variable dip, rectangular elements)
- 3D, 2D and 1D (spring-block)
- Steady and oscillatory loads
- Normal stress coupling
- Faults surrounded by damaged zones
- Matlab wrapper and graphic output display utilities
- Parallelized for shared memory systems (OpenMP)
- Parallelized for distributed memory systems (MPI)
- Fully coupled with SPECFEM3D via QSB (QDYN-SPECFEM Bridge)

1.3 Documentation

Documentation for QDYN is available through the following resources:

- This User's Manual. Click here to access the most recent version.

- The `examples` directory contains several examples, some have a `README` file
- The Matlab tools provided with the QDYN package are documented through Matlab's help. For instance `help qdyn` provides an overview of the usage of the `qdyn` Matlab interface.
- The `ToDo` file contains a list of known issues and features that we plan to implement in the future.

1.4 Support

The QDYN development team offers online support to users who report bugs, installation problems, documentation issues, feature requests, or questions about QDYN usage by submitting "issues" at https://github.com/ydluo/qdyn/issues.

In particular, please do not contact the QDYN developers directly by email. Before submitting an issue please make sure that:

- you have read the QDYN documentation (see section 1.3)
- you are running the most recent version of QDYN (see sections 2.2 and 2.4)
- your problem has not been treated in previous issues. You can browse and search the list of closed issues

New issues are submitted via https://github.com/ydluo/qdyn/issues/new. Please include all information needed to reproduce your problem: input files, operating system, compiler, QDYN version.

1.5 License

This software is freely available for academic research purposes. If you use QDYN please include proper attributions to its authors and cite one of the references in section 1.7 in your scientific papers and reports.

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1.6 Acknowledgements

1.6.1 Code contributions

QDYN outgrew from a 2D code written by Allan Rubin (Princeton University) in the early 2000s. The main developers are Jean Paul Ampuero and Yingdi Luo. Bryan Riel contributed the double-FFT version. Percy Galvez contributed to the MPI parallelization. Martijn van den Ende contributed code fixes for Octave. Benjamin Idini implemented damaged fault zones.

The subroutines implementing Okada's formulas were provided by Shinichi Miyazaki (Kyoto University). They include subroutines written by Y. Okada.

The FFT subroutines are based on the General Purpose FFT Package written by Takuya Ooura (Kyoto University).

1.6.2 Funding

The development of QDYN has been supported by the US National Science Foundation, the Southern California Earthquake Center and Japan's Nuclear Regulation Authority (formerly Japan Nuclear Energy Safety Organization).

1.7 Suggested references

Y. Luo, J. P. Ampuero (2011), Numerical Simulation of Tremor Migration Triggered by Slow Slip and Rapid Tremor Reversals, AGU Fall Meeting 2011 Abstract S33C-02

Y. Luo, J. P. Ampuero (2012), Simulation of Complex Tremor Migration Patterns, AGU Fall Meeting 2012 Abstract S44B-02

Y. Luo, J. P. Ampuero, K. Miyakoshi and K. Irikura (2017) *Surface effects on earthquake moment-area scaling relations* PAGEOPH, Topical Volume on *"Best Practices in Physics-based Fault Rupture Models for Seismic Hazard Assessment of Nuclear Installations",* doi:10.1007/s00024-017-1467-4

Y. Luo, J. P. Ampuero, P. Galvez, M. Ende and B. Idini. (2017). *QDYN: a Quasi-DYNamic earthquake simulator (v1.1) [Data set]*. Zenodo. doi:10.5281/zenodo.322459

2 Installation

2.1 Requirements

- Make and Subversion or GIT facilitate code installation and updates. Both are standard Linux tools.
- A Fortran compiler.
- MPI (e.g. MPICH, Open MPI) linked to your Fortran compiler (mpif90).
- Python, Matlab or Octave.
- For Windows 10 users, Linux tools can be acquired and run natively through a Linux subsystem

We mostly develop and use QDYN with Linux, the Intel Fortran compiler (ifort) and Matlab. The code has been successfully compiled and used on Windows or Mac, with gfortran and Octave.

2.2 Download QDYN

QDYN is hosted on GitHub. You have several options to download it:

2.2.1 Stable versions

You can download stable versions from the releases page.

2.2.2 Development version

You can download development versions of QDYN. These usually contain bug fixes and new features, but they may not be fully tested yet (use it at your own risk and please report issues - see section 1.4).

QDYN is managed under a version control system compatible with both Subversion (SVN) and Git. You can choose either option. In GitHub, Git is the recommended, native version control system. SVN is provided through an interface (Git-SVN bridge) that does not implement all the features of SVN. To switch between Git and SVN you need to checkout the code again from scratch.

To download for the first time the latest development version of QDYN execute the following SVN command:

```
svn checkout https://github.com/ydluo/qdyn qdyn-read-only
```

or the following GIT command:

```
git clone https://github.com/ydluo/qdyn qdyn-read-only
```

This creates a directory `qdyn-read-only` which contains the whole QDYN package. You can create a directory with a different name.

2.2.3 Pre-compiled executables

You can download pre-compiled QDYN executables for Windows or Mac OS directly from this link. However, these may not be most recent versions and they may run slower than if you compile the code by yourself.

2.3 Install QDYN

1. Move to the `src` directory
2. Modify the section "User Settings" of file `Makefile` following the instructions and examples therein:
    a. In section 1, set the variable `EXEC_PATH = [the path to your executable file]`. If you leave the default value (recommended) the executable file `qdyn` is placed in the `src` directory. If you change this variable (not recommended), you must set the `EXEC_PATH` input variable accordingly when you call `qdyn.m`.
    b. In section 2, adjust your Fortran compiler settings: set the variables `F90 = [your compiler name]`, `OPT = [your compiler optimisation flags]` and `PREPROC = [your compiler option to enable preprocessing]`. Intel Fortran (ifort) is the default compiler, but settings for several commonly used compilers are provided. Note that specific optimisation flags need to be set to enable parallelization through OpenMP (see section 4.2.1).
3. Set the parameters in the section "User Settings" of `constants.f90` following the instructions therein
4. Run `make`
5. If in step 2 you changed the path or name of the executable file, modify accordingly the line `status = system('~/bin/qdyn')` of file `qdyn.m`

2.4 Update QDYN

If you are using the development version, after the first-time checkout you can update the package by executing the following command in your `qdyn-read-only` directory:

```
svn update
```

Any source file that you have modified will be flagged as "conflicted" by SVN, and you will be prompted to select a conflict resolution method. You can preserve your modifications by selecting the option `mc` ("mine-conflict"). This is particularly useful to preserve your user settings in `Makefile` and `constants.f90` (otherwise you would need to repeat the steps in the "Install QDYN" section). For that purpose, the following command eliminates the interactive prompt:

```
svn update --accept mc
```

If you are using GIT instead of SVN, update QDYN with the following command:

```
git fetch
```

GIT automatically marks conflicts and you have to fix them manually following the instructions in the GITHUB help pages.

2.5 Additional notes for Windows 10 users

As of 2017, Windows 10 officially supports a bash command line environment by installing a Linux subsystem (as of writing, Ubuntu and OpenSUSE are currently offered in the Windows Store). Within a subsystem, Unix-compiled executables can be run natively, and the user has access to the Canonical software repository (`apt-get install [package]`). Running QDYN in a Linux subsystem is done as follows:

1. Install your preferred Linux subsystem, see this instruction page
2. Install make, gfortran, and Open MPI as:
   `sudo apt-get install make gfortran libopenmpi-dev`
3. Download QDYN as instructed above. Note that Windows does not have access to the Linux file system, so in order to exchange files between the subsystem and Windows, it is recommended to download QDYN to (and run simulations from) a local Windows directory (e.g. C:\Users\bob\qdyn). The Windows file system can be accessed in the Linux subsystem as: `cd /mnt/c/Users/bob/qdyn`
4. Navigate to the QDYN `src` directory and compile QDYN as described above
5. In the case that the required Python or command line Matlab/Octave packages are installed on the Linux subsystem, QDYN can be called

directly from a wrapper. If none of these software packages are available, generate a `qdyn.in` file in Windows (e.g. through a Matlab wrapper), navigate within the subsystem to the location of `qdyn.in` (e.g. `cd /mnt/c/Users/bob/test_simulation`) and run: `/mnt/c/Users/bob/qdyn/src/qdyn`

6. QDYN should now be running within the Linux subsystem, creating output files in C:\Users\bob\test_simulation that can be accessed by Windows for further processing.
7. The Python wrapper (`pyqdyn.py`) also has built-in functionalities to call the subsystem directly from a Windows 10 environment. In order to set-up and run QDYN simulations from the Python wrapper, set `qdyn.W10_bash = True`. When doing so, the wrapper will automatically switch between the Windows and Linux environments.

3 Model assumptions

3.1 Model geometry

QDYN handles the following geometries:

- "0D fault", a spring-block model
- "Finite 1D fault" embedded in a 2D unbounded elastic medium. The fault is straight and actually infinitely long, but its frictional part is confined to a segment of finite length L, $x \in [-L/2,\ L/2]$.
- "Periodic 1D fault" embedded in a 2D unbounded elastic medium. The fault is infinitely long but has a spatially periodic distribution of friction parameters, normal stress and slip with spatial period L. The modeled segment is $x \in [-L/2,\ L/2]$. We account approximately for a characteristic length of the slip distribution in the third dimension (the axis normal to the modeled 2D medium) by assuming slip has a sinusoidal pattern over a length W in the third dimension. This is effectively a 1.5D approximation, in which W is a proxy for the seismogenic width of a 2D fault.
- 1D fault bisecting an elastic slab
- 2D fault embedded in a 3D elastic space or half-space. The fault surface has fixed strike, but possibly depth-dependent dip. The fault is infinite but only a finite area is frictional.

Periodic 1D faults can be embedded in a homogeneous medium or in a damaged fault zone model. The latter is a heterogeneous medium composed of two materials: a layer of damaged material with constant thickness in contact with the fault embedded in an intact material.

3.2 Boundary conditions

Spring-block models are loaded by an imposed load-point velocity. On continuum faults, the frictional segment is loaded by slip imposed along the remaining, non-frictional part of the fault. In all cases, the imposed loading is composed of a steady velocity and an oscillatory component.

The fault shear strength equals the normal stress times the friction coefficient. In rate-and-state friction, the fault shear stress is always equal to the strength.

In the quasi-dynamic approximation adopted in QDYN, fault stresses are the sum of static elastic stresses induced by slip and a radiation damping stress. The latter approximates the effect of wave radiation: it represents exactly the stresses induced by waves radiated in the direction normal to the fault but not the complete elastodynamic stresses.

3.3 Friction laws

The friction coefficient is governed by one of the following rate-and-state laws:

- Conventional rate-and-state
$$\mu(V,\theta) = \mu^* + a\ln(V/V^*) + b\ln(\theta V^*/D_c)$$
- Rate-and-state with cut-offs
$$\mu(V,\theta) = \mu^* - a\ln(1 + V_1/V) + b\ln(1 + \theta V_2/D_c)$$

The state variable follows one of the following evolution equations:

- Aging law
$$d\theta/dt = 1 - \theta V/D_c$$
- Slip law
$$d\theta/dt = -\theta V/D_c \ln(\theta V/D_c)$$

All frictional properties can be spatially heterogeneous.

4 Running a simulation

4.1 The Matlab wrapper

The core of QDYN is a Fortran code. While the format of its input and output files is well defined, we find it more convenient to set up the input parameters, perform simulations and read the output data within the Matlab environment through the wrapper function `qdyn.m`. You first need to set in Matlab the full path to the `src` directory, for instance:

```
addpath ~/qdyn-read-only/src
```

Tip for Mac users: if you get an error message related to gfortran libraries (e.g. `libgfortran.3.dylib`) when running `qdyn` in Matlab, do:

```
setenv('DYLD_LIBRARY_PATH', '/usr/local/bin/')
```

The second argument should be the path to your gfortran libraries (sometimes `/opt/local/lib/libgcc`).

The general usage syntax is:

```
[pars,ot,ox] = qdyn(mode,[parsin],['Property',Value,...])
```

The default input values can be listed by executing:

```
pars = qdyn('set')
```

The input parameters are:

mode	One of the following execution modes: 'set' Outputs the default parameter structure (*pars*) or overrides it with fields present in the structure *parsin* or with *Property/Value* pairs 'write' Sets parameters and writes the qdyn input file 'run' Sets parameters, writes the input file and runs a simulation 'read' Reads parameters and outputs from a previous simulation
parsin	Parameter structure to override the default parameters (see section 3.2 for details)

'Property'	Name of a field to be set in the parameter structure (see section 3.2)
Value	Value to override the default value and the value in *parsin*

The output variables are:

pars	Structure containing the parameters (see section 3.2)
ot	Structure containing time series outputs, global or at selected points (see section 3.3)
ox	Structure containing snapshot outputs, i.e. quantities over the whole fault, output at selected times (see section 3.3)

4.2 Simulation parameters structure (pars)

The parameters in the structure *pars*, that can be set through 'parsin' or 'Prop/Value' pairs are:

Parameters defining the geometry of the problem and loading:

MESHDIM	Dimension of the problem: 0 = Spring-block model 1 = 1D fault in a 2D elastic medium 2 = 2D fault in a 3D elastic medium 4 = Same as 2 but fault stresses computed via 2D-FFT (works only if the grid spacings and dip angle are uniform)
FAULT_TYPE	Fault loading geometry: 1 Strike-slip (right-lateral) -1 Strike-slip (left-lateral)

	2 Thrust -2 Normal
SOLVER	ODE solver mode: 1 Bulirsch-Stoer 2 Runge-Kutta-Fehlberg
MU	Shear modulus (Pa)
LAM	Elastic modulus lambda for 3D simulations (Pa)
VS	Shear wave speed (m/s). If *VS=0*, radiation damping is turned off
V_PL	Plastic loading velocity (e.g. plate velocity; m/s)
D	Damage level = 1 - (damaged shear modulus) / (intact shear modulus) Currently implemented only for MESHDIM=1 and FINITE=0
H	If D>0, half-thickness of the fault damage zone (m) If D=0, half-thickness of an elastic slab bisected by a fault Currently implemented only for MESHDIM=1 and FINITE=0
L	If *MESHDIM=1*, L is the fault length (or spatial period) If *MESHDIM=0*, *MU/L* is the spring stiffness
FINITE	Boundary conditions when *MESHDIM=1* 0 = Periodic fault: the fault is infinitely long but slip is spatially periodic with period L, loaded by steady displacement at distance W from the fault 1 = Finite fault: the fault is infinitely long but only a segment of length L has rate-and-state friction, the rest has steady slip. If running the code with this option gives the error message “kernel file src/kernel_I.tab is too short”, you should create a larger “kernel file” with the matlab function *TabKernelFiniteFlt.m*

	2 = Symmetric periodic fault: like option 0 but slip is symmetric relative to the first element 3 = Symmetric finite fault: like option 1 but slip is symmetric relative to the first element. This can be used to set a free surface next to the first element
W	Distance between displacement loading and fault, only if MESHDIM=1 and FINITE=0
DIP_W	Fault dip angle (degree) if MESHDIM=2 or 4. If depth-dependent, values must be given from deeper to shallower depth.
Z_CORNER	Fault bottom depth (m, negative down) if MESHDIM=2 or 4
SIGMA_CPL	Normal stress coupling: 0 = disable, 1 = enable
APER	Amplitude of additional time-dependent oscillatory shear stress loading (Pa)
TPER	Period of oscillatory loading (s)

Simulation features (only available via Python wrapper):

QDYN offers various non-standard simulation features. Set the following parameters to 1 to enable, or 0 to disable:

FEAT_STRESS_COUPL	Normal stress coupling
FEAT_LOCALISATION	CNS only: Shear localisation
FEAT_TP	High-velocity dynamic weakening by thermal pressurisation

Rate-and-state friction (RSF) parameters:

A	Direct effect coefficient
B	Evolution effect coefficient

DC	Characteristic slip distance (m)
MU_SS	Reference steady-state friction coefficient
V_SS	Reference steady-state slip velocity (m/s)
TH_SS	Reference steady-state state (s). The default is *TH_SS=DC/V_SS*.
RNS_LAW	Type of rate-and-state friction law: 0 = original 1 = with cut-off velocities V1 and V2
V1	Cut-off velocity of direct effect (m/s)
V2	Cut-off velocity of evolution effect (m/s), controls the transition from weakening to strengthening when a<b. V2 should be ≤ V1.
THETA_LAW	Type of evolution law for the state variable: 0 = ageing law in the "no-healing" approximation 1 = ageing law 2 = slip law

***Chen-Niemeijer-Spiers* (CNS) model parameters (only available via Python wrapper):**

THICKNESS	Total thickness of gouge zone (m)
<u>Granular flow parameters</u>	
A_TILDE	Coefficient of logarithmic rate-dependence of grain-boundary friction (-)
MU_TILDE_STAR	Reference grain-boundary friction at Y_GR_STAR (-)
Y_GR_STAR	Reference strain rate corresponding with MU_TILDE_STAR (1/s)

H	Dilatancy geometric factor (-)
Porosity parameters	
PHI_C	Critical state porosity (-)
PHI0	Lower cut-off velocity (e.g. percolation threshold; -)
PHI_INI	Simulation initial porosity (-)
Creep mechanisms (power-law form)	
N_CREEP	Number of (power-law) creep mechanisms
A	Kinetic parameter for each creep mechanism
N	Stress exponent for each creep mechanism
M	Porosity exponent for each creep mechanism

Initial conditions:

SIGMA	Initial effective normal stress (Pa). Remains constant unless *SIGMA_CPL =1*
TAU	CNS only: Initial shear stress (Pa)
V_0	RSF only: Initial slip velocity (m/s)
TH_0	RSF: Initial state (s) CNS: Initial porosity (-)

Discretization and accuracy parameters:

N	Number of fault elements if MESHDIM=1
NX	Number of fault elements along-strike, in 3D
NW	Number of fault elements along-dip, in 3D
NPROCS	Number of processors if running in parallel with MPI (only implemented for MESHDIM=2 and FFT_TYPE=1)
DW	Along-dip length (m) of each element, from deep to shallow

TMAX	Threshold for stopping criterion: Final simulation time (s) when NSTOP=0 Slip velocity threshold (m/s) when NSTOP=3
NSTOP	Stopping criterion 0 = Stop at t=TMAX (s) 1 = Stop at end of slip localization phase 2 = Stop soon after first slip rate peak 3 = Stop when slip velocity exceeds TMAX (m/s)
DTTRY	First trial timestep (s)
DTMAX	Maximum timestep (0=unrestricted)
ACC	Solver accuracy

Output control parameters:

OX_SEQ	Type of snapshot outputs 0 = All snapshots in a single output file (fort.19) 1 = One output file per snapshot (fort.1001, ...)
NXOUT	Spatial interval for snapshot outputs (in number of elements)
NTOUT	Temporal interval (in number of time steps) for snapshot outputs
OX_DYN	Output specific snapshots of dynamic events defined by thresholds on peak slip velocity DYN_TH_ON and DYN_TH_OFF (see below) 0 = Disable 1 = Enable outputs for event #i: Event start: fort.19998+3i Event end: fort.19999+3i Rupture time: fort.20000+3i

NXOUT_DYN	Spatial interval (in number of elements) for dynamic snapshot outputs
DYN_TH_ON	Peak slip rate threshold (m/s) to define the beginning of a dynamic event
DYN_TH_OFF	Peak slip rate threshold (m/s) to define the end of a dynamic event
IC	Index of selected element for time series outputs
IOT	Indices of elements for additional time series outputs: set `IOT(i)=1` to enable time series outputs at the i-th element. By default, `IOT(i)=0` and this output is not done. Each element has a separate output file named `fort.xxxxx`, where `xxxxx` is an index (different than `i`) that starts at `10001` and is incremented by 1 for each selected element. For instance, if `IOT=[0 0 1 1]`, the output of elements `i=3` and `i=4` are in files `fort.10001` and `fort.10002`, respectively.
IASP	Auxiliary flags for elements (will not affect outputs, identification purpose only. e.g you can set elements of the VS part to -1 and VW to 0 and particular points of interests like asperities to numbers you want to use)

Parameters for integration with dynamic code:

DYN_FLAG	Integration with dynamic code 0 = Disable 1 = Enable: stop QDYN at the DYN_SKIP+1-th event with seismic moment > DYN_M
DYN_M	Target seismic moment of a dynamic event
DYN_SKIP	Number of dynamic events to skip (warm up cycles)

4.3 Output structures (ot, ox)

The outputs are:

pars	Structure containing the same fields as *parsin* (see above) plus the positions of the fault elements (X,Y,Z)
ot	Structure of time series outputs, with the following fields: t — Output times (s) locl — Localization length (distance between stressing rate maxima) cl — Crack length (distance between slip rate maxima) p — Seismic potency pdot — Seismic potency rate Outputs at the fault location with maximum slip rate: xm — Location of maximum slip rate v — Maximum slip rate th — State variable theta om — (slip rate)*theta/DC tau — Shear stress d — Slip Outputs at selected fault element with index IC: vc — slip rate thc — state variable omc — (slip rate)*theta/DC tauc — shear stress dc — slip
ox	Structure of snapshot outputs, with the following fields: x — fault coordinates

	t	output times
	v	slip rate
	th	state variable theta
	vd	slip acceleration
	dtau	shear stress relative to initial stress
	dtaud	shear stress rate
	d	slip
	sigma	effective normal stress

4.4 Examples

4.4.1 A simple 2D example

This example is in directory `examples/uniform_slip`. It's a 2D run with uniform slip and initial velocity slightly above steady state. In Matlab:

```
% get default parameters:
p = qdyn('set');
% reset some parameters:
p.N = 16; p.TMAX = 6e9; p.V_0=1.01*p.V_SS;
% run:
[p,ot,ox] = qdyn('run',p);
```

The estimated simulation time is shorter than 10 s on a single thread machine. Let's plot some outputs. Slip velocity as a function of time:

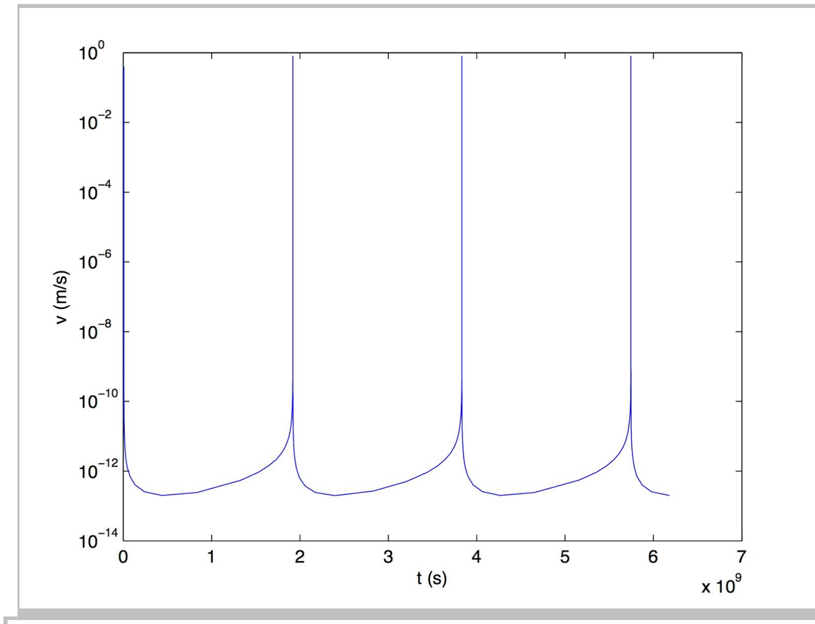
```
semilogy(ot.t,ot.v); xlabel('t (s)'); ylabel('v (m/s)')
```

Plot shear stress as a function of time:

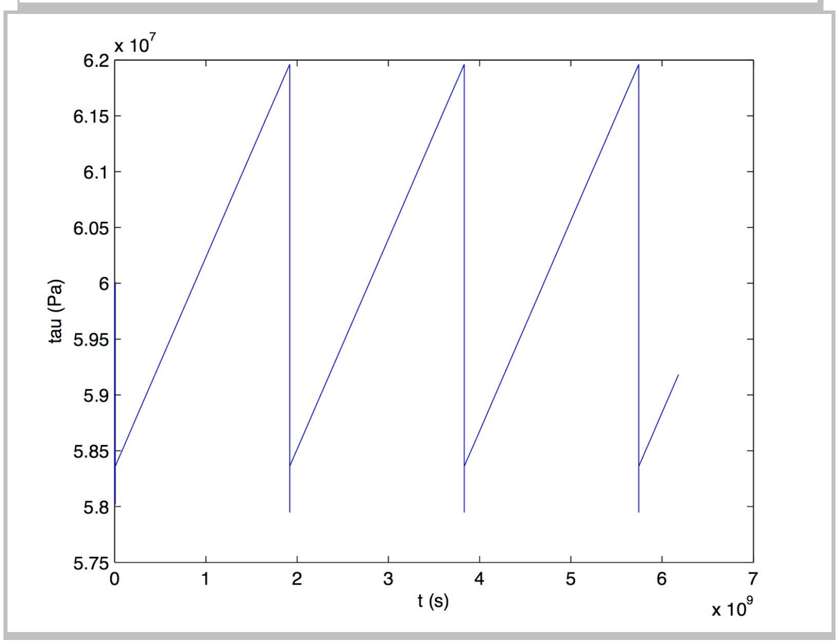
```
plot(ot.t,ot.tau); xlabel('t (s)'); ylabel('tau (Pa)')
```

Visualize the convergence to a limit cycle in a state-velocity plot:

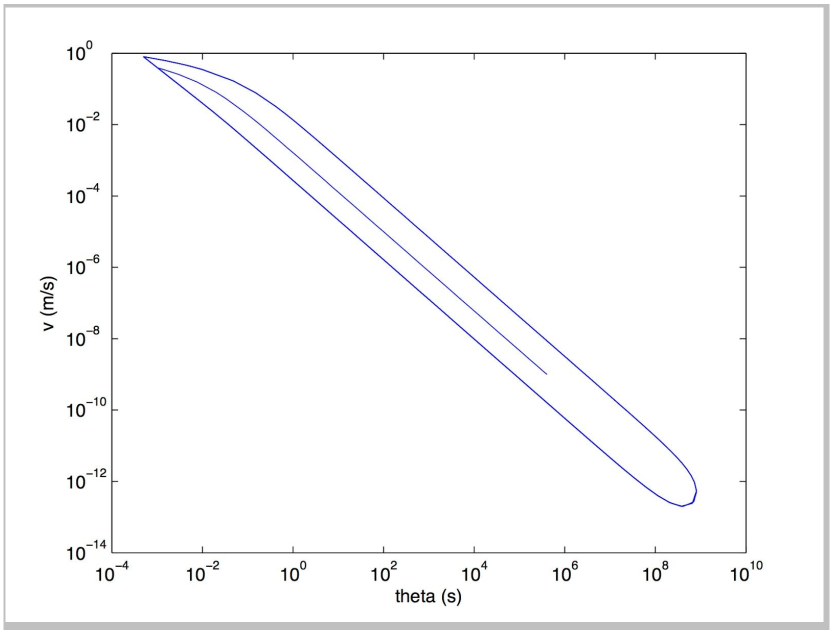
```
loglog(ot.th,ot.v); xlabel('theta (s)'); ylabel('v (m/s)')
```



10^0
10^-2
10^-4
10^-6
10^-8
10^-10
10^-12
10^-14
v (m/s)
0
1
2
3
4
5
6
7
t (s)
x 10^9

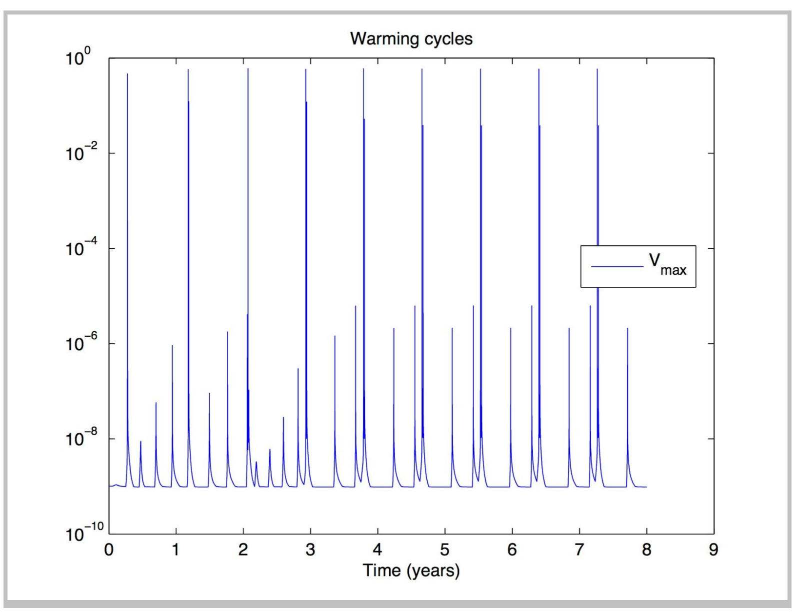


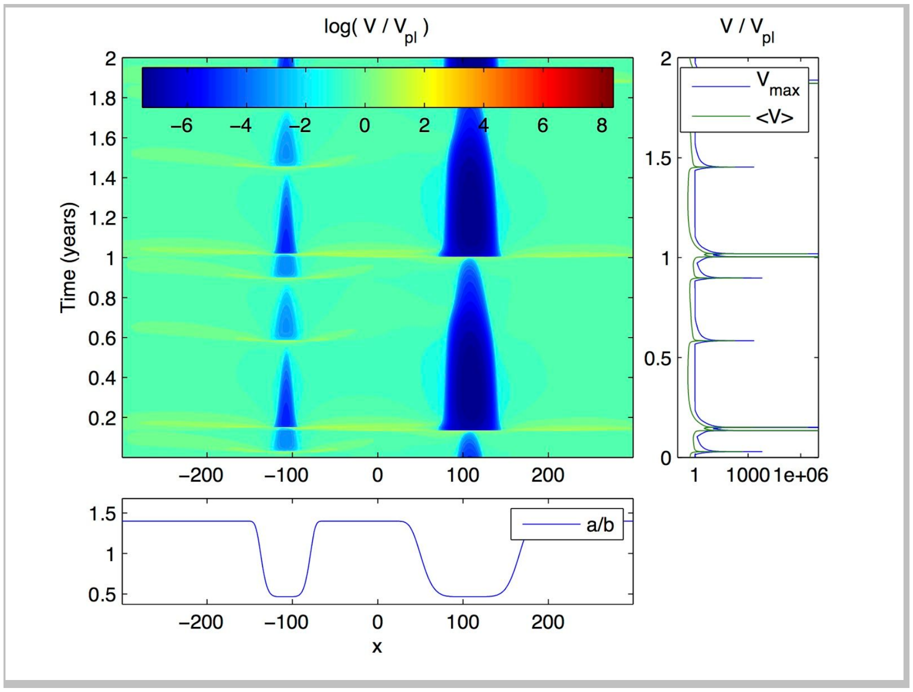
x 10^7
6.2
6.15
6.1
6.05
6
5.95
5.9
5.85
5.8
5.75
tau (Pa)
0
1
2
3
4
5
6
7
t (s)
x 10^9



4.4.2 Two asperities interacting

This example is in directory `examples/double_asperities`. A velocity-weakening asperity interacts with a smaller asperity. Both are embedded in a velocity-strengthening (creeping) fault. When the large asperity breaks, its post-seismic slip propagates bi-laterally and triggers rupture of the small asperity. During the interseismic period of the large asperity, the smaller asperity breaks twice with a decreasing recurrence interval. The estimated simulation time is about 6 mins on a single thread machine.

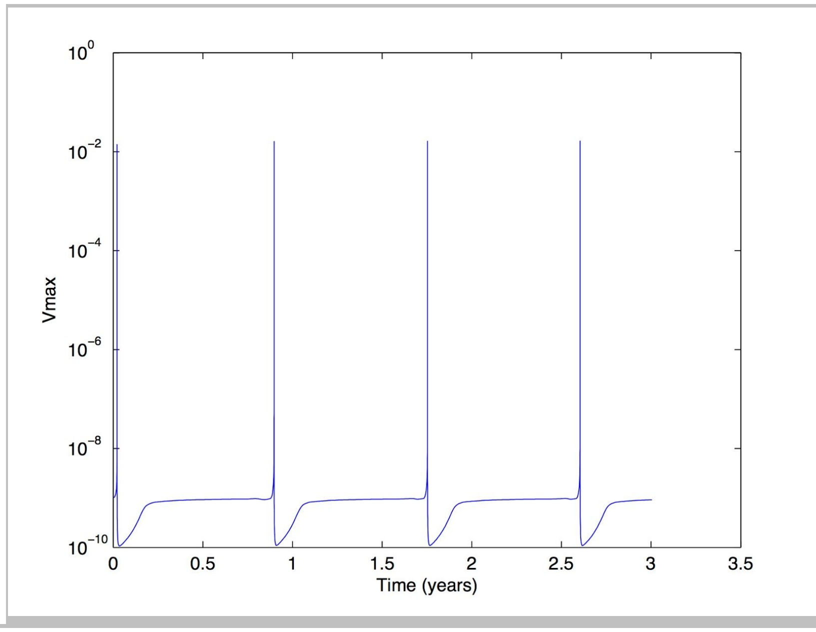


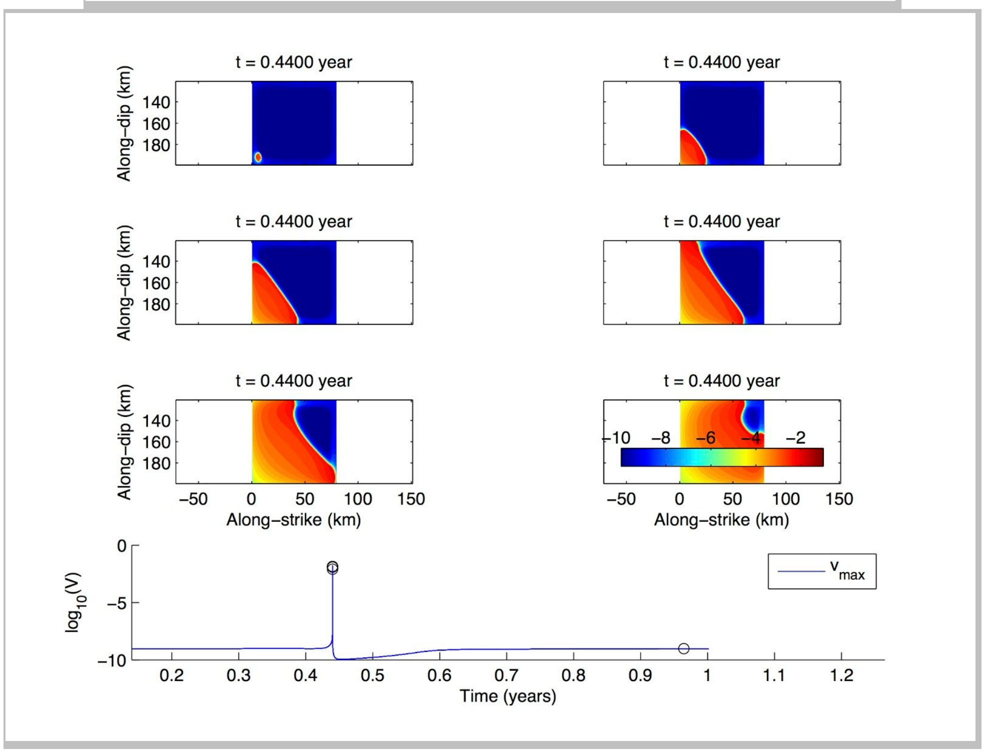


4.4.3 3D simulations

An upper-layer Matlab wrapper for the base-layer Matlab wrapper qdyn.m is recommended for complicated simulations. We have included some examples for reference:

a) A 3D simulation: `examples/3d_fft/test_3dfft.m`
The estimated simulation time is about 10 mins on a single thread machine for the first earthquake cycle. The figures shown below are for a complete multi-cycle simulation, comprising 4 warm-up cycles and one cycle output.





b) A simplified model for the Tohoku earthquake (2D along-dip and 3D simulations): `examples/Tohoku`

For more examples and real-world applications please refer to the wiki pages on the QDYN website.

5 Optimizing Performance

5.1 Running simulations outside the Matlab environment

To run simulations outside the Matlab environment, e.g. when computing on an HPC cluster: run first the Matlab wrapper only to generate the input file qdyn.in, then run the qdyn executable outside Matlab.

5.2 Managing parallel computing

5.2.1 OpenMP

For 3D simulations on 2D faults (`MESHDIM=2` or `4`), QDYN is parallelized for shared memory multi-processor systems with OpenMP. Before compiling the code, you should set the specific compiler optimisation flags that enable OpenMP, as described in the `Makefile` (see step 2.b in section 2.3). Before performing parallel simulations, you should set the following environment variable:

```
setenv OMP_NUM_THREADS 8
```

This command allows QDYN to run on 8 threads, which will roughly speed up calculations by a factor of 8. The number of threads should be set according to demand. In general, set this value to the maximum number of threads available on your shared memory system.

5.2.2 MPI

For 3D simulations with `MESHDIM=2`, QDYN can run in parallel in distributed memory clusters with MPI. The number of processors must be set in the variable `p.NPROCS`.

5.3 Managing outputs of large simulations

QDYN by default outputs results as a single ASCII file (fort.19). In most multi-cycle 3D simulations this file is very large. It is then helpful to set `OX_SEQ = 1` when calling `qdyn.m`, to generate separate “ox” files outputs for each snapshot (fort.1001, ...). Also, setting `OX_DYN = 1` will automatically detect seismic events (according to parameters `DYN_TH_ON` and `DYN_TH_OFF`) and generate 3 snapshots for each event.

6 Visualizing simulation results

The QDYN software package includes several Matlab scripts to visualize simulation results in directory `utils/post_processing`. These scripts are all self-documented:

plot_default.m	Plots slip rate of a 2D problem (along-strike)
plot2d_slip.m	Plots slip of a 2D problem (along-dip)
plot3d_m.m	Plots a sequence of snapshots of slip rate of a 3D simulation
plot3d_faultview_3.m	Plots several snapshots of slip rate for 3D simulation in a single figure

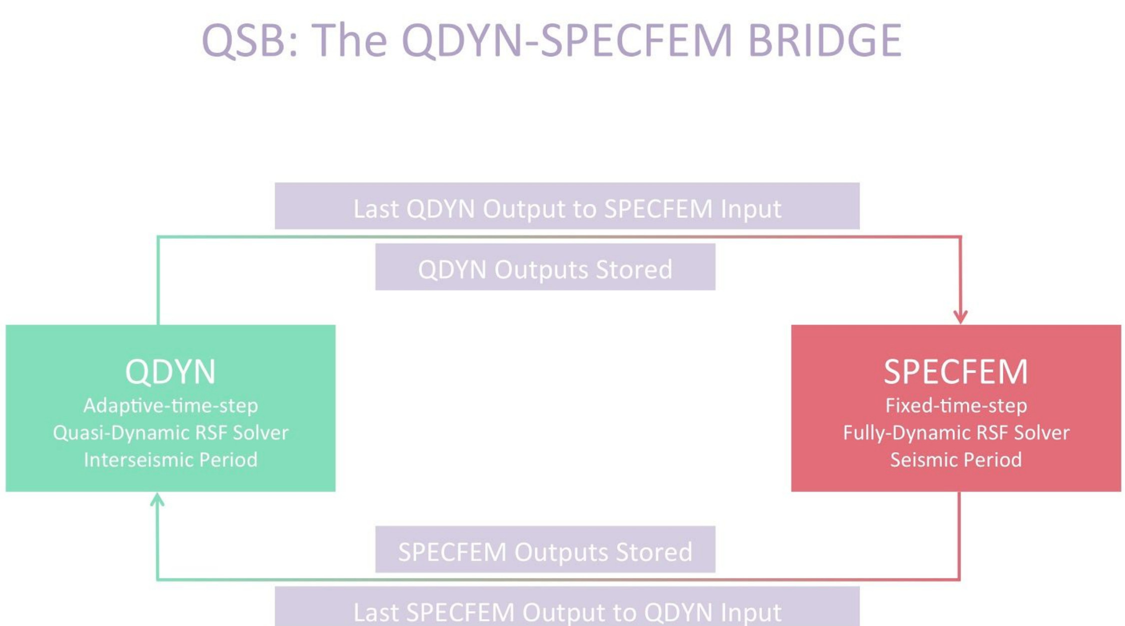
7 Coupling with the dynamic rupture code SPECFEM3D

7.1 The QDYN-SPECFEM Bridge (QSB)

SPECFEM3D is a software for dynamic rupture simulations. It is fully dynamic, i.e. it accounts for inertial effects that are important during earthquakes. However, it is based on a solver with fixed time-step, which cannot be applied to interseismic and postseismic periods involving slow, quasi-static (aseismic) deformation.

QDYN is a software for quasi-dynamic earthquake cycle simulations. It is based on the quasi-dynamic approximation and an adaptive time-step solver. These features are accurate and efficient during periods of aseismic slip, but their accuracy degrades during seismic slip, especially in the presence of severe fault weakening mechanisms at high slip rates.

QSB, the QDYN-SPECFEM3D Bridge module, is a two-way interface between the QDYN and the SPECFEM3D softwares. QSB employs each of these codes in its optimal usage conditions to enable efficient and accurate simulations of multiple earthquake cycles containing periods of both seismic (SPECFEM3D) and aseismic (QDYN) slip. The figure below summarizes the QSB workflow and its pattern of data communication between the two codes.



7.2 Pre-requisites

- Obtain a copy of the development version of SPECFEM, which includes a rate-and-state friction solver,using the following git command: `git clone https://github.com/geodynamics/specfem3d.git -b devel`.
- Obtain a copy of the QDYN package on [GITHUB] following the instructions described in the [QDYN online manual]. The QSB module is made of Bash and Matlab scripts contained in directory `QSB/` of the QDYN package.

7.3 The master QSB Bash Script

`QDYN_SPECFEM_bridge.sh` is the master script of the QSB. It utilizes the matlab script `QDYN_to_SEM_RSF_f.m` to convert the output of QDYN right before an earthquake into a SPECFEM3D input and the matlab script `SEM_to_QDYN_RSF.m` to convert the output of SPECFEM3D right after an earthquake into a QDYN input.

The control variables in `QDYN_SPECFEM_bridge.sh` are:

N_core_allco	Number of cores in the SPECFEM simulations
N_loop	Number of earthquakes to be simulated
QDYN_dir_work	QDYN working directory
QDYN_dir_out_store	Directory to store QDYN outputs. Data for each earthquake is stored in a separate sub-directory named *QDYN_dir_out_store/run{i}* where *i = 1,2,...* is the earthquake index
SPECFEM_dir_work	SPECFEM working directory
SPECFEM_dir_in	Directory where QDYN will place output data for SPECFEM input
SPECFEM_dir_out	Directory where SPECFEM will place output data for QDYN input
SPECFEM_dir_out_store	Directory to store SPECFEM outputs. Data for each earthquake is stored in a separate sub-directory named *SPECFEM_dir_out_store/run{i}* where *i = 1,2,...* is the earthquake index

7.4 The job request script for clusters with job scheduling system

In most High Performance Computing clusters, job requests are submitted through a job scheduling system to better utilize computational resources. The sample job request script `QSB/run_bridge_sh` should serve on most clusters. The script may need slight modifications to adapt it to your job scheduler; please contact your system administrator to get the most accurate information.

To submit your QSB job, edit the control variables in `run_bridge_sh`, then run the following command:

```
qsub run_bridge_sh
```

The control variables in the request script `run_bridge_sh` are:

#PBS -l nodes=[nodes]	Number of cores requested, set to the same value as *N_core_allco*
#PBS -l walltime=[time]	Total walltime requested, process will be terminated briefly after exceeding the requested walltime total queue time is in general assessed over cluster load and [nodes]*[time]
#PBS -m bae	Get notifications at the beginning, end and if an error occurs
#PBS -M [email]	Notification will be sent to [email]
./QDYN-SPECFEM_bridge.sh > [output]	Submit job QDYN-SPECFEM_bridge.sh, simulation progress stores (and overwrites previous existing) outputs file [output]

7.5 How to run fully coupled QDYN-SPECFEM simulations

Step 1: Setup the control variables in the script `QDYN_SPECFEM_bridge.sh`. For most variables you can keep the default settings found in the script.

Step 2: Setup a QDYN simulation and generate first-run input file `qdyn.in`

Step 3: Setup the SPECFEM simulation:
- Set switch `RATE_AND_STATE = .true.` and `RSF_HETE = .true.` in `src/specfem3D/DATA/Par_file_faults`
- Generate a spectral element mesh with same fault geometry (length, width and dip angles) as the QDYN mesh. The average spacing of the GLL nodes on the fault in the SPECFEM mesh should be similar to the grid spacing in QDYN. If the coordinates of the SPECFEM mesh have different starting values, set the values of `x_off` , `y_off` and `z_off` in `QDYN_to_SEM_RSF_f.m` and `SEM_to_QDYN_RSF.m` accordingly.
- Partition the mesh into `N_core_allco` processors. Please refer to the SPECFEM3D manual for further details.
- Set values in `DATA/Par_file` , `DATA/Par_file_faults` and `DATA/FAULT_STATIONS` accordingly. You can find sample files in `EXAMPLES/fault_examples/tpv103/DATA`. Set the 6 components of CMT source in file `CMTsolution` to 0. Please refer to the SPECFEM3D manual for further details.
- Set the `t_dyn` = [SPECFEM target simulation time] in `QDYN_to_SEM_RSF_f.m`
- Store the coordinates of the fault nodes in file `nodesonfault`, a text file with five columns, IX IZ X Y Z, where IX and IZ are node indices (actually not used) and X, Y and Z are fault node coordinates with units of meters. An example is provided in `QSB/nodesonfault`.You can create it by making a test run of SPECFEM and then running the provided matlab script `SEM_write_nodesonfault.m`.

Step 4: Run the Bash script `QDYN_SPECFEM_bridge.sh`, or, on a cluster with scheduler, submit the request script `run_bridge_sh`. You can modify `run_bridge_sh` to change the name of the progress monitoring file (default is `QSB/output.txt`) and your email notification address (see previous section)

Step 5: Monitor the simulation progress in file `QSB/output.txt`. Once the simulation of `N_loop` earthquakes is over, an email notification will be sent

Step 6: Process the outputs, matlab scripts `plot_QDYN_seq.m` and `plot_SEM_seq.m` are provided for your convenience to visualize QDYN and SPECFEM outputs, respectively.

7.6 QSB Example: fully-dynamic earthquake cycle simulation on a heterogeneous fault

Step 1: We want to run SPECFEM with 108 cores and simulate 2 earthquakes, so we set `N_core_allco=108`, and `N_loop=2` in the script `QDYN_SPECFEM_bridge.sh`. We keep the default values for other variables.

Step 2: We prepare the example `hete_3d_ss.m` to run QDYN simulations on a 3D strike-slip fault with 50 km depth and 512 km length and heterogeneous frictional properties. In the script we set `p.OX_SEQ=1`, `p.OX_DYN=1` and `p.DYN_TH_ON=0.1` to generate a snapshot output `fort.20001` when the maximum slip rate reaches 0.1 m/s. We also set `p.NSTOP=3` and `p.TMAX=0.1001` to stop QDYN soon after, when maximum slip rate reaches 0.1001 m/s.

Step 3: We generate a SPECFEM mesh matching the QDYN mesh and store the nodes coordinates in `nodesonfault`. In SPECFEM we set the time step to 0.005 s (as dictated by the mesh) and run 60000 steps with a total target simulation time of 300 s, which is sufficient to allow an event to nucleate and rupture the whole 512 km fault from one side to another (extreme scenario). Accordingly, we set `t_dyn` = 300 s in `QDYN_to_SEM_RSF_f.m`

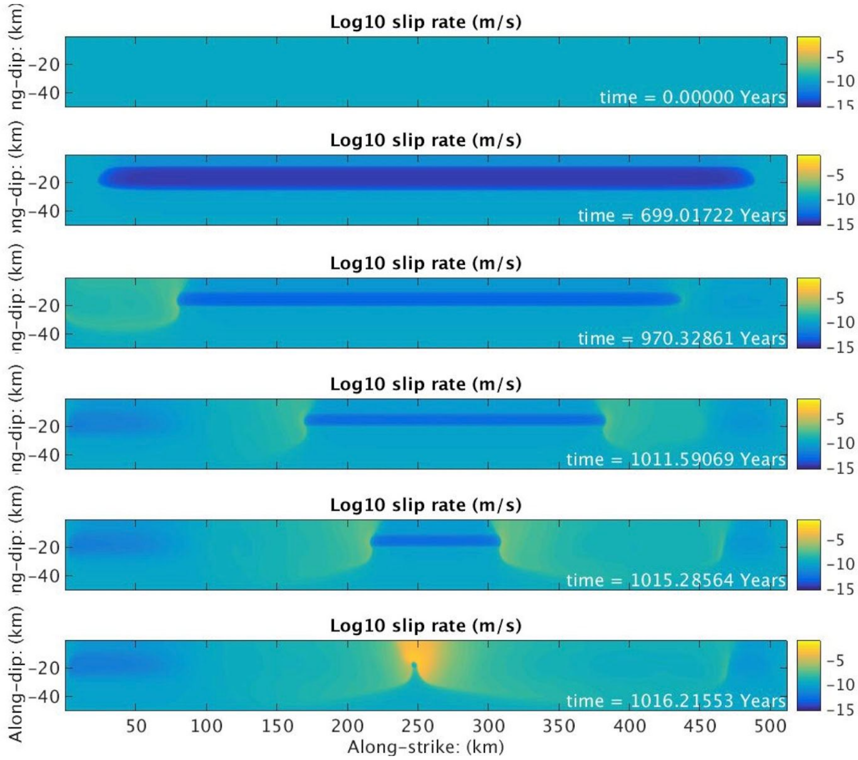
Step 4: We run the script `QDYN_SPECFEM_bridge.sh` on our cluster with command `qsub run_bridge_sh`

Step 5: The monitoring file shows typically this:

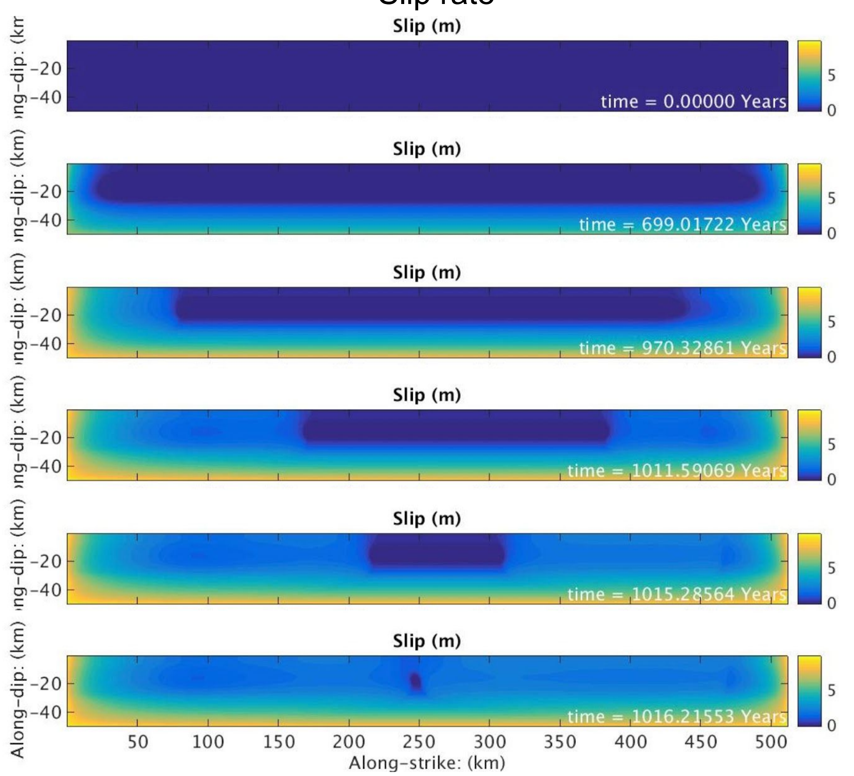
```
N_core_allco = 108
N_loop = 2
Tue Aug  4 03:01:49 PDT 2015
QSB: run no. 1
QSB: run no. 1 QDYN simulation …
…
…
…
```

Step 6: Once the simulation of the 2 earthquakes is over, we process the outputs using matlab scripts `plot_QDYN_seq.m` and `plot_SEM_seq.m`. The figures below show results of a simulation comprising two earthquake cycles. They include the QDYN simulation of the two interseismic periods and the SPECFEM3D simulation of two earthquakes. We show also the results of the first earthquake computed by QDYN only, to highlight the differences introduced by the fully dynamic effects.

QDYN run Event # 1 Interseismic

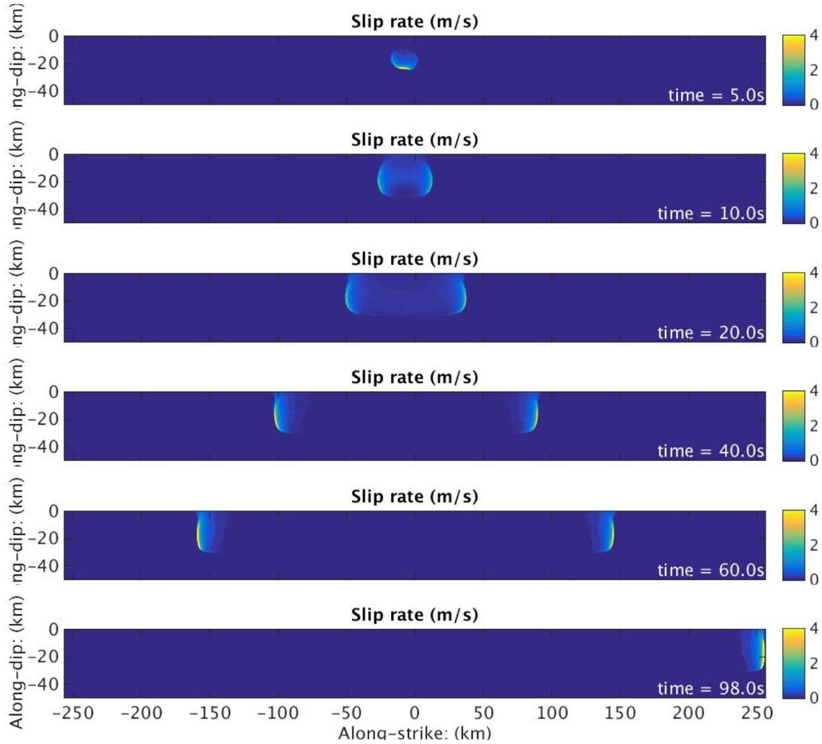


Slip rate

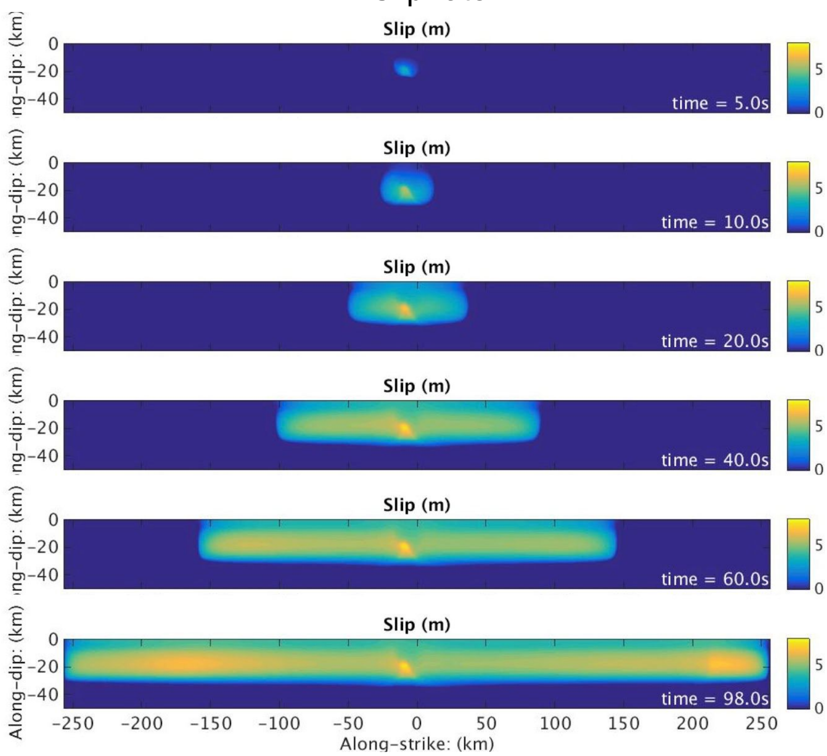


Slip

SPECFEM run Event # 1 Seismic

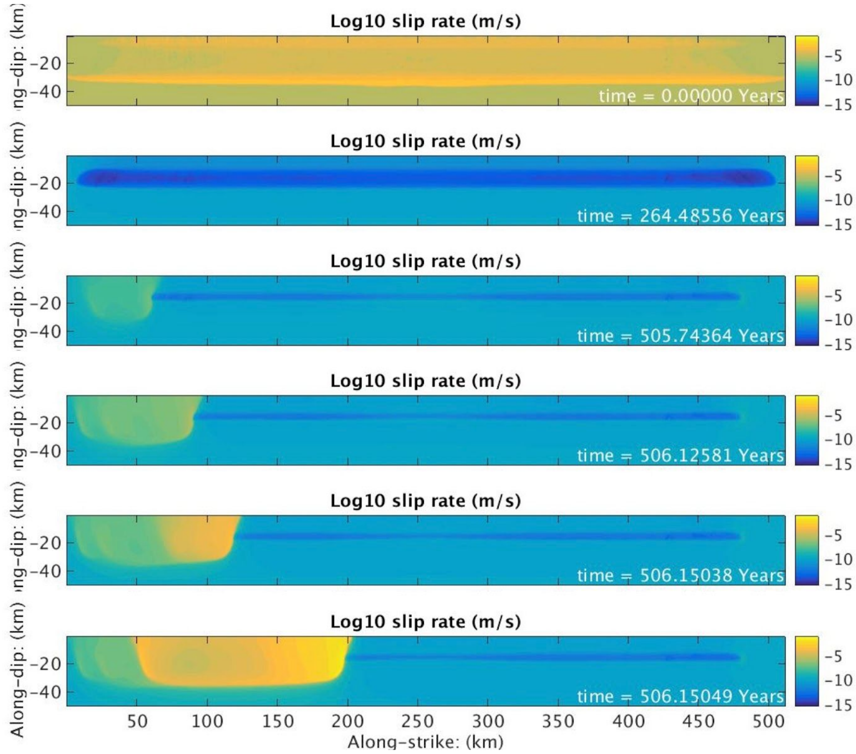


Slip rate

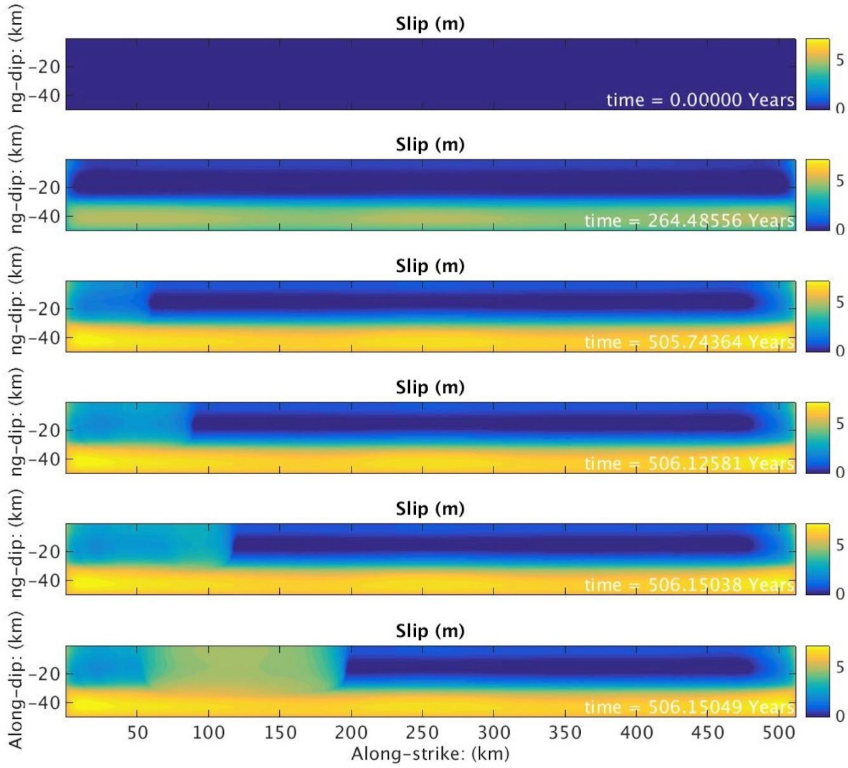


Slip

QDYN run Event # 2 Interseismic

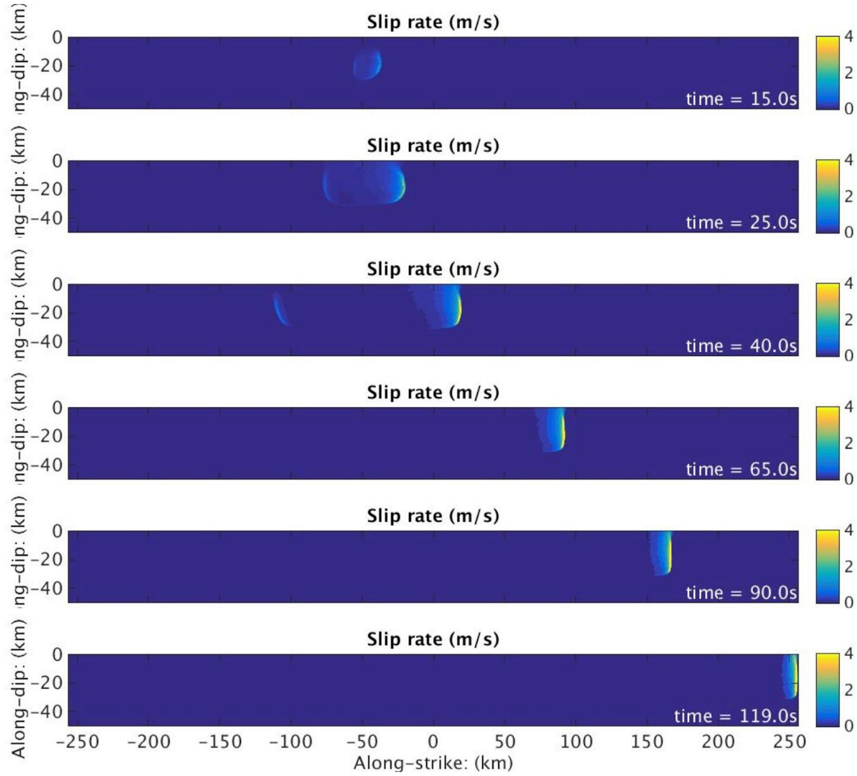


Slip rate

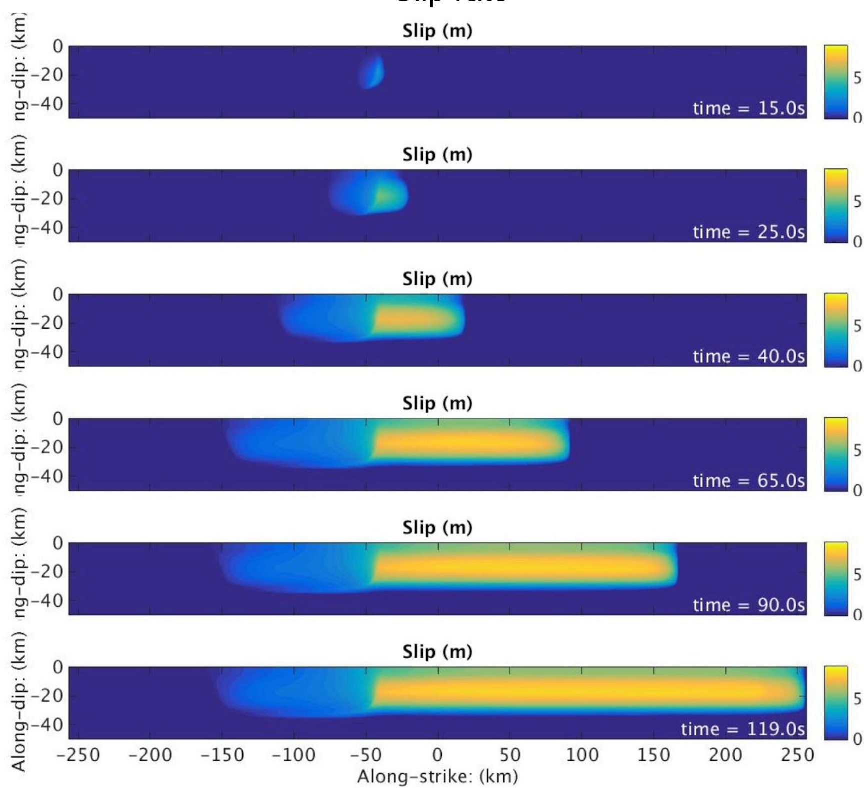


Slip

SPECFEM run Event # 2 Seismic

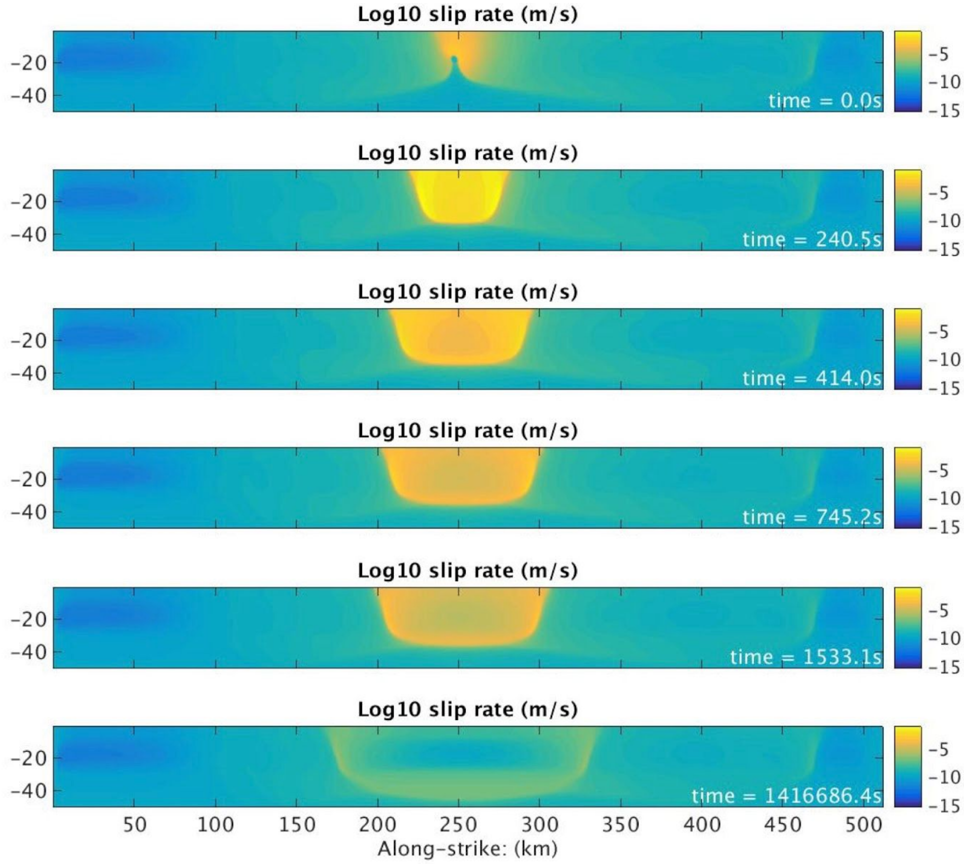


Slip rate



Slip

QDYN run Event # 1 Seismic



Slip rate