

QDYN

Quasi-DYNamic earthquake simulator

V 1.1

User's Manual



ydluo.github.io/qdyn/

Developers

Yingdi Luo (http://www.seismolab.caltech.edu/luo_y.html) (Caltech Seismo Lab, USA)
Jean-Paul Ampuero (http://www.seismolab.caltech.edu/ampuero_jp.html)(Caltech Seismo Lab, USA)
Percy Galvez (AECOM, Switzerland)
Martijn van den Ende (Utrecht University, the Netherlands)
Benjamin Idini (University of Chile)

Last modification on 26/02/2017

Click here to access the most recent version

Table of contents

1. Introduction 1.1. Summary 1.2. Main features 1.3. Documentation 1.4. Support 1.5. License 1.6. Acknowledgements 1.6.1. Code contributions 1.6.2. Funding 1.7. Suggested references 2. Installation 2.1. Requirements 2.2. Download QDYN 2.3. Install QDYN 2.4. Update QDYN 3. Running a simulation 3.1. The Matlab wrapper 3.2. Simulation parameters structure (pars) 3.3. Output structures (ot, ox) 3.4. Examples 3.4.1. A simple 2D example 3.4.2. Two asperities interacting 3.4.3. 3D simulations 4. Optimizing Performance 4.1. Running simulations outside the Matlab environment 4.2. Managing parallel computing 4.2.1. OpenMP 4.2.2. MPI 4.3. Managing outputs of large simulations 5. Visualizing simulation results 6. Coupling with the dynamic rupture code SPECFEM3D 6.1 The QDYN-SPECFEM Bridge (QSB) 6.2 Pre-requisites 6.3 The master QSB Bash Script 6.4 The job request script for clusters with job scheduling system 6.5 How to run fully coupled QDYN-SPECFEM simulations 6.6 QSB Example: fully-dynamic earthquake cycle simulation on a heterogeneous fault

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 uniform, linear, isotropic and elastic.

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
- Matlab wrapper and graphic output display utilities
- Parallelized for shared memory systems (OpenMP)
- MPI parallelization
- Normal stress coupling
- Faults surrounded by damaged zones
- 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

Support for QDYN users (reporting bugs, installation problems, documentation issues, feature requests, etc) is available at:

https://github.com/ydluo/qdyn/issues

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 or search the issues database in the <u>closed</u> tag at https://github.com/ydluo/qdyn/issues

New issues are submitted via https://github.com/ydluo/qdyn/issues/new. Please include all information needed to reproduce your problem (input files, name of operating system and compiler, etc).

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.

This program is free software: you can redistribute it and/or modify it under the terms of the GNU General Public License as published by the Free Software Foundation, either version 3 of the License, or (at your option) any later version.

This program is distributed in the hope that it will be useful, but WITHOUT ANY WARRANTY; without even the implied warranty of MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE. See the GNU General Public License for more details.

You should have received a copy of the GNU General Public License along with

this program. If not, see http://www.gnu.org/licenses/.

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.

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 <u>General Purpose FFT Package</u> written by Takuya Ooura (Kyoto University).

Martijn van den Ende (Utrecht University) contributed code fixes for Octave.

1.6.2. Funding

The development of QDYN is partially 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

2. Installation

2.1. Requirements

- <u>Make</u> and <u>Subversion</u> or <u>GIT</u> 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).
- Matlab or Octave.

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 <u>GitHub</u>. It is managed under a version control system compatible with both <u>Subversion</u> (SVN) and <u>Git</u>. 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 get the most current version of QDYN execute the following command on Linux (first time only):

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

or GIT command

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

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

You can also manually download the QDYN source files and pre-compiled executables for Windows or Mac OS directly from this link. However, note that these may not be most up-to-date versions, and that pre-compiled executables may run slower than if you compile the code by yourself.

2.3. Install QDYN

- 1. Move to the qdyn-read-only/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 directory where you are compiling the code, src/. 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] and OPT = [your compiler optimisation flags]. 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

After the first-time checkout, you can update the package by executing the following command in your qdyn-read-only directory:

```
svn update
```

or GIT command

```
git fetch
```

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
```

While with GIT, the version control system will automatically mark the conflicts and you have to fix the conflict manually, for more details, refer to the <u>GITHUB</u> <u>help file</u>.

3. Running a simulation

3.1. 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 th	ne 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)

3.2. 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)
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
Н	Half-thickness of the fault damage zone
	Currently implemented only for MESHDIM=1 and FINITE=0
D	Damage level = 1 - (damaged shear modulus) / (intact shear modulus).
	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 = The fault is infinitely long but slip is spatially periodic with period L, loaded by steady displacement at distance W from the fault
	1 = 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
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)

Rate-and-state friction parameters:

A Direct effect coefficient	
-----------------------------	--

В	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. be="" should="" td="" v1.<="" v2="" ≤=""></b.>
THETA_LAW	Type of evolution law for the state variable: 0 = ageing law in the "no-healing" approximation 1 = ageing law 2 = slip law

Initial conditions:

SIGMA	Initial effective normal stress (Pa). Remains constant unless SIGMA_CPL =1
V_0	Initial slip velocity (m/s)
TH_0	Initial state (s)

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)
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 $\mathtt{IOT}(\mathtt{i}) = \mathtt{1}$ to enable time series outputs at the i-th element. By default, $\mathtt{IOT}(\mathtt{i}) = \mathtt{0}$ and this output is not done. Each element has a separate output file named $\mathtt{fort.xxxx}$, where \mathtt{xxxxx} is an index (different than \mathtt{i}) that starts at $\mathtt{10001}$ and is incremented by 1 for each selected element. For instance, if $\mathtt{IOT} = [0 \ 0 \ 1 \ 1]$, the output of elements $\mathtt{i} = \mathtt{3}$ and $\mathtt{i} = \mathtt{4}$ are in files $\mathtt{fort.10001}$ and $\mathtt{fort.10002}$, 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)	

3.3. Output structures (ot, ox)

The outputs are:

nare	Structure contain	ining the same fields as narein (see above) plus the		
pars	Structure containing the same fields as <i>parsin</i> (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)		
	р	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: fault coordinates Χ t output times ٧ slip rate state variable theta th vd slip acceleration dtau shear stress relative to initial stress dtaud shear stress rate d slip effective normal stress sigma

3.4. Examples

3.4.1. A simple 2D example

This example is in directory <code>examples/uniform_slip</code> 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:

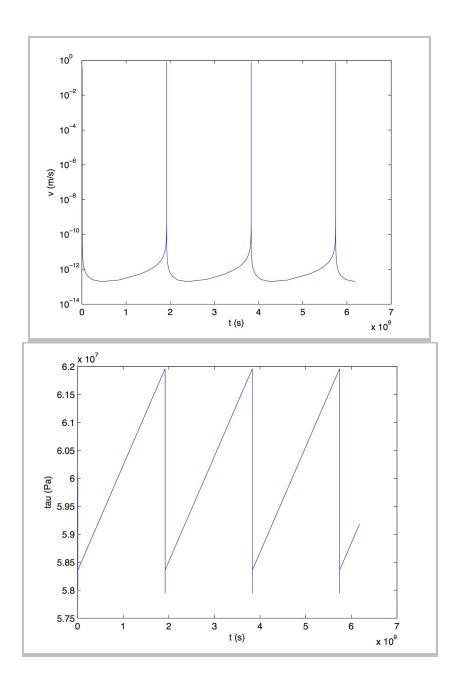
```
semilogy(ot.t,ot.v); xlabel('t (s)'); ylabel('v (m/s)')
```

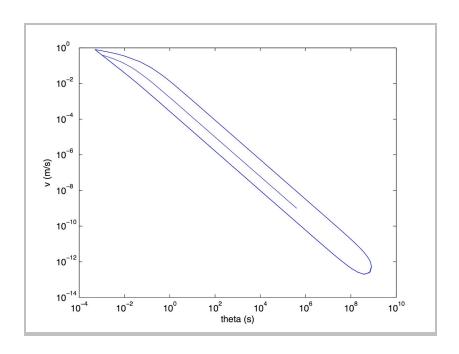
Plot shear stress as a function of time:

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

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

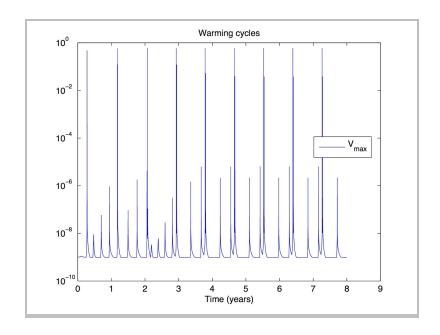
loglog(ot.th,ot.v); xlabel('theta (s)'); ylabel('v (m/s)')

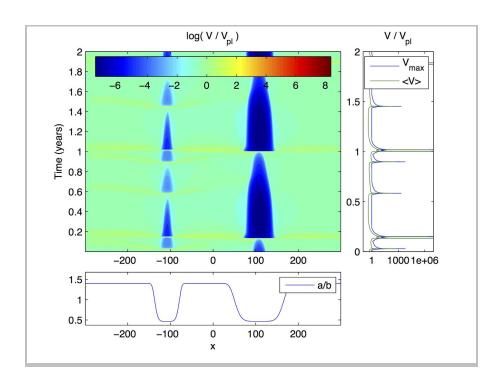




3.4.2. Two asperities interacting

This example is in directory <code>examples/double_asperities</code> 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.



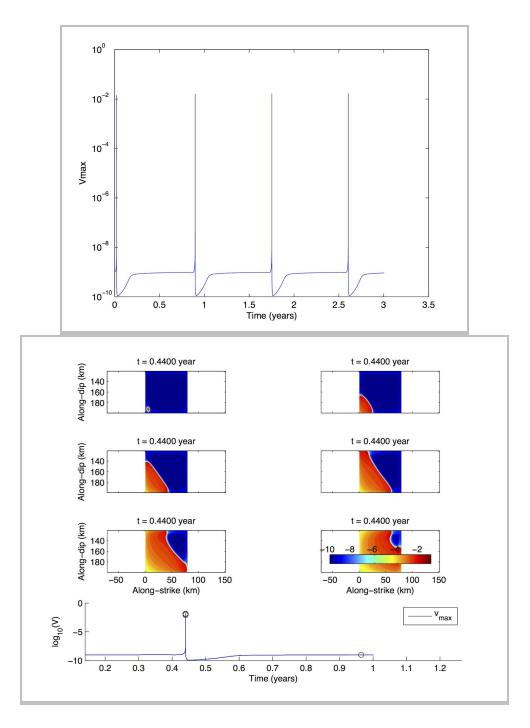


3.4.3. 3D simulations

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 <u>wiki</u> <u>pages on the QDYN website</u>.

4. Optimizing Performance

4.1. Running simulations outside the Matlab environment

Under certain circumstances, you may want to perform simulations outside the Matlab environment (e.g. while computing on a HPC). In this case, use Matlab wrapper separately first to generate an input file (qdyn.in), then run the qdyn executable directly.

4.2. Managing parallel computing

4.2.1. 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.

4.2.2. 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.

4.3. Managing outputs of large simulations

QDYN by default outputs results as a single ASCII file (fort.19) that may be too cumbersome to handle in large simulations. In practice, that is the case for most multi-cycle 3D simulations. 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.

5. 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

6. Coupling with the dynamic rupture code SPECFEM3D

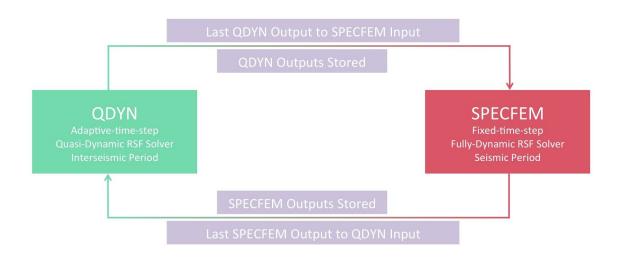
6.1 The QDYN-SPECFEM Bridge (QSB)

<u>SPECFEM3D</u> 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.

QSB: The QDYN-SPECFEM BRIDGE



6.2 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 <u>GITHUB</u> following the instructions described in the <u>QDYN online manual</u>. The QSB module is made of Bash and Matlab scripts contained in directory <u>QSB</u>/ of the QDYN package.

6.3 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

6.4 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 -I nodes=[nodes]	Number of cores requested, set to the same value as <i>N_core_allco</i>
#PBS -I 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_brid ge.sh > [output]	Submit job QDYN-SPECFEM_bridge.sh, simulation progress stores (and overwrites previous existing) outputs file [output]

6.5 How to run fully coupled QDYN-SPECFEM simulations

Step 1: Setup the control variables in the script <code>QDYN_SPECFEM_bridge.sh</code>. 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.

6.6 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_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:

Step 6: Once the simulation of the 2 earthquakes is over, we process the outputs using matlab scripts <code>plot_QDYN_seq.m</code> and <code>plot_SEM_seq.m</code>. 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.

