

*Simulating seismic wave propagation with **SW4***

N. Anders Petersson
Center for Applied Scientific Computing
Computations Directorate

CIG webinar, November 12, 2015

 Lawrence Livermore
National Laboratory



LLNL-PRES-677035

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. Lawrence Livermore National Security, LLC

Outline

- What is implemented in sw4 (seismic waves, 4th order)?
- Setting up the simulation
 - Sources
 - How do I pick the grid size?
 - Topography
 - Material model, visco-elastic modeling
 - Output options
- Running sw4
- Practical suggestions
 - Workflow

The SW4 code solves the time dependent 3D visco-elastic wave equation

- Summation-by-parts finite difference method
 - 4th order accurate in space+time, energy stable
- Cartesian geometry (earth's curvature neglected)
 - Projection from geographical to Cartesian coordinates
- Elastic or visco-elastic material model
 - Isotropic material model ($\mu > 0$, $\lambda > 0$, $\rho > 0$)
 - Quality factors Q_P and Q_S , approx. constant in frequency band
 - Anisotropic materials (21 parameter model)
- Curvilinear coordinates
 - Flat or realistic topography; Mesh generated by SW4
 - Absorbing far-field super-grid layers
- Moment tensor sources or point forces
 - Many pre-defined time functions, or user-specified
 - Complex ruptures: many sources or SRF file (v. 1)
- Output options:
 - Time-series at receivers, solution on 2-D cross-sections, GMT scripts
- Local mesh refinement (coming soon)

Summation by parts discretization mimic integration by parts for finite differences

- Elastic wave equation:

$$\rho \frac{\partial^2 \mathbf{u}}{\partial t^2} = \mathbf{L} \mathbf{u} + \mathbf{f}(\mathbf{x}, t)$$

$$\mathbf{L} \mathbf{u} := \nabla \cdot \mathcal{T}$$

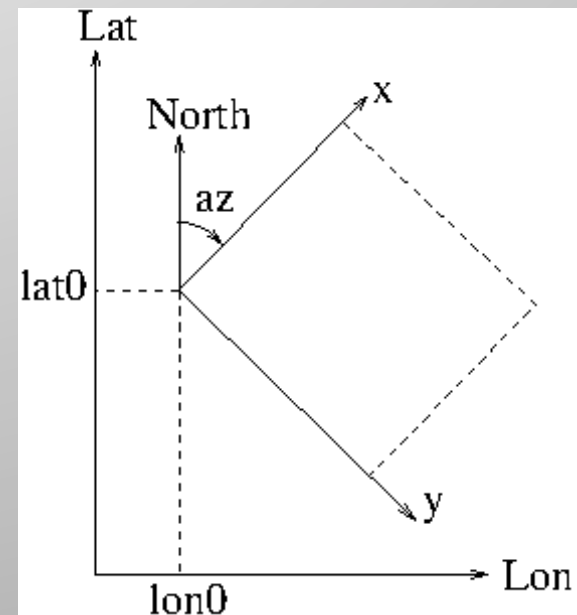
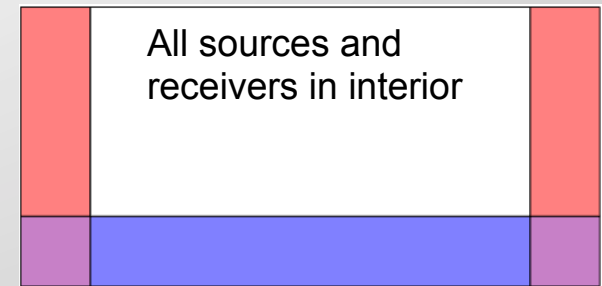
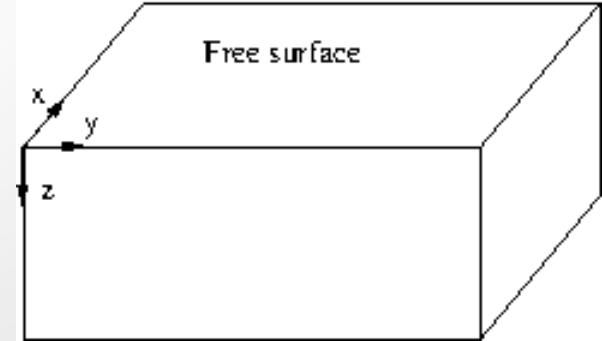
- Discretized in space:

$$\rho \frac{d^2 \mathbf{v}}{dt^2} = \mathbf{L}_h \mathbf{v} + \mathbf{f}(\mathbf{x}, t)$$

- Symmetry and negative definite properties of ‘ \mathbf{L} ’ preserved by summation by parts discretization ‘ \mathbf{L}_h ’
- Numerical scheme is energy stable
- Theory and papers on our web page:
computation.llnl.gov/project/serpentine/

sw4 uses SI-units (MKS), angles in degrees

- Box-shaped computational domain
 - Right-handed system, z positive downwards
- Top surface optionally follows topography
- Free surface boundary condition on top surface
- Super-grid absorbing layers on all other sides
 - SG layers included in computational domain
 - Default thickness: 30 grid points
 - Smallest Cartesian grid: 60x60x30
- Locations in Cartesian or geographic coordinates
- Geographic coordinates are mapped:
 - Default: spheroidal projection
 - Proj.4 library for better accuracy
- Rotate grid with azimuth angle (az)
 - az=0: x-axis = North, y-axis = East



The sw4 simulation is specified by the command file

- `cat seismic1.in`

```
fileio path=lamb-res
```

```
grid x=10e3 y=10e3 z=5e3 h=50
```

```
time t=8.0
```

```
block vp=1.7320508076e+03 vs=1000 rho=1500
```

```
source type=C6SmoothBump x=5e3 y=5e3 z=0 fz=1e13 freq=1 t0=0
```

```
# Time history of solution (comments or blank lines ignored)
```

```
rec x=6e3 y=8e3 z=0 file=v1s
```

```
# Snapshot of solution every 0.5 seconds
```

```
image mode=uz z=0 file=lamb timeInterval=0.5
```

- `mpirun -np 8 sw4 seismic1.in`

SW4 implements two types of kinematic source terms

- Point force:

$$g(t)\mathcal{F}\delta(\mathbf{x} - \mathbf{x}_*)$$

- Moment tensor source:

$$g(t)\mathcal{M}\nabla\delta(\mathbf{x} - \mathbf{x}_*)$$

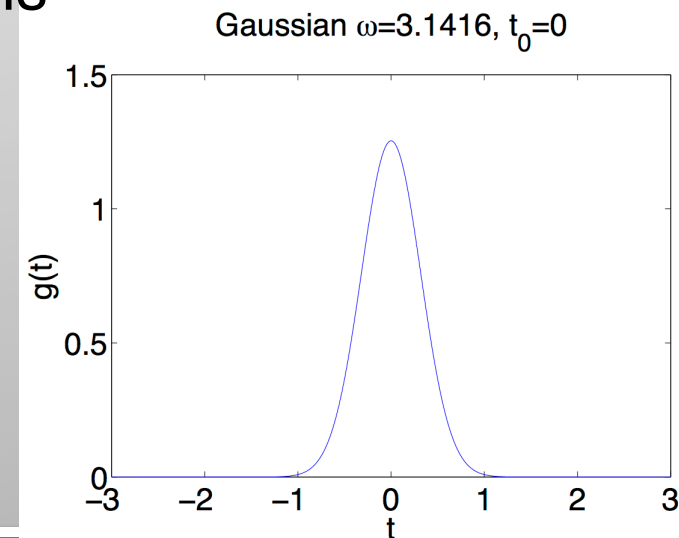
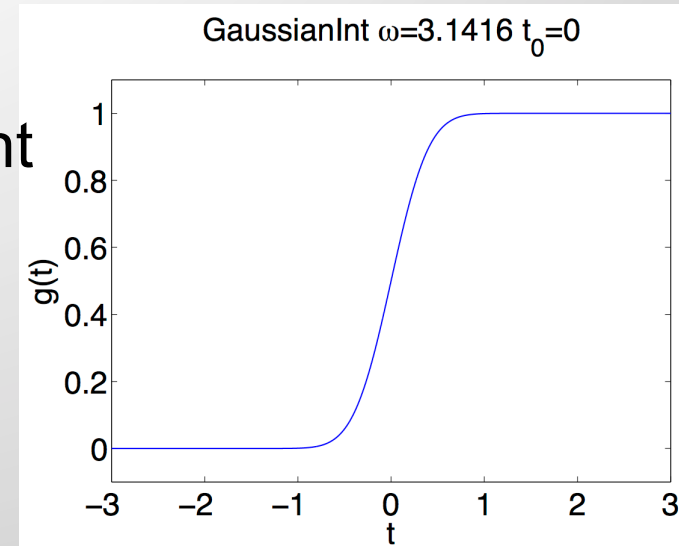
- We discretize the Dirac distribution $\delta(\mathbf{x})$ by imposing moment conditions
 - 6x6x6 point stencil in 3-D
- 4th order accuracy away from the source
- The sources can be located independently of the grid

sw4 provides several options for specifying sources and time-functions

- Any number of point forces or moment tensor sources
 - Forces defined by 3-component vector \mathbf{F}_i
 - Moment tensor (symmetric) defined by 6 components M_{ij} , or
 - Seismic moment (M_0) and strike, dip, rake angles
- 14 pre-defined time functions (Gaussian, Ricker, Liu, ...)
 - Frequency parameter and start/center time
- Dirac delta-distribution: triggers all frequencies on mesh
 - Discrete Green's functions. Motion must be filtered for accuracy
- User defined discrete time function (interpolated by spline)
- Complex ruptures can be specified by using many point sources or through an SRF file (version 1 format)

There are several ways of computing displacements, velocities, or acceleration

- Displacements correspond to source time-functions that tends to a constant (e.g. gaussianInt)
 - Displacements obtained directly
 - Velocities by differentiating once
 - Acceleration by differentiating twice
- Velocities correspond to time-functions that tend to zero but have non-zero integral (e.g. gaussian)
 - Velocities obtained directly
 - Displacements by integrating once
 - Acceleration by differentiating once

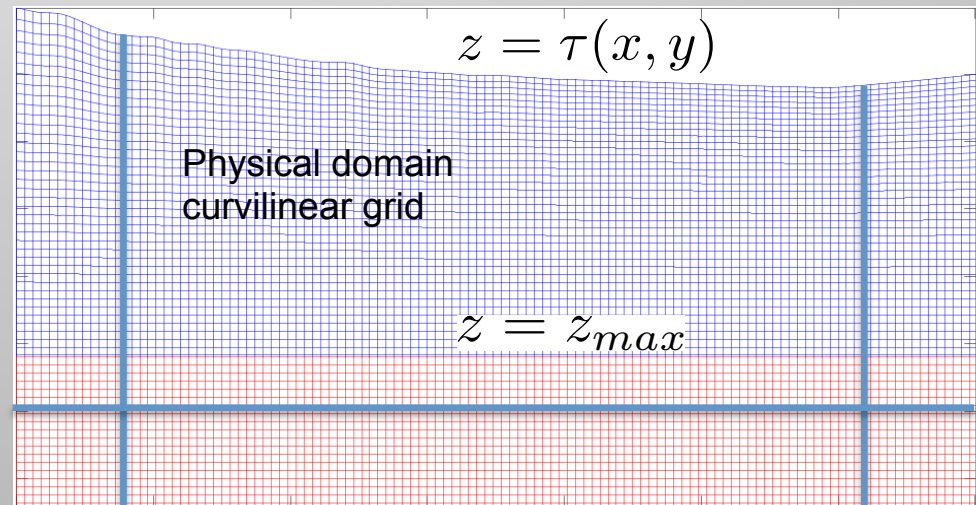
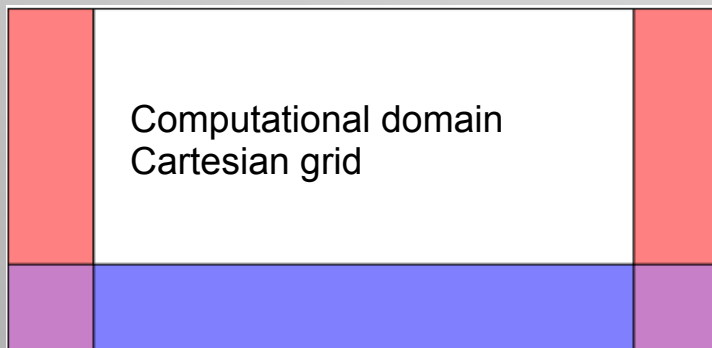


The highest frequency and the lowest wave speed determine the grid size

- Shortest wave length $L_{\min} = \min C_S / f_{\max}$
- Grid points per shortest wave length $P_{\min} = L_{\min} / h$
- Good accuracy when $P_{\min} > 6$ to 10 (depending on distance)
- Several options:
 - Tune f_{\max} in source time function to not trigger unresolved waves
 - Use the `prefilter` command to pre-process all source time fcns
 - Calculate $f_{\max} = \min C_S / (P_{\min} h)$, remove unresolved frequencies afterwards
- Relation between f_{\max} and frequency parameter (`freq`) is different for each time function (see UG 4.4)
- `matlab/octave` scripts for plotting time function and Fourier transform in `...sw4/tools: fcnplot, ftfcnplot`

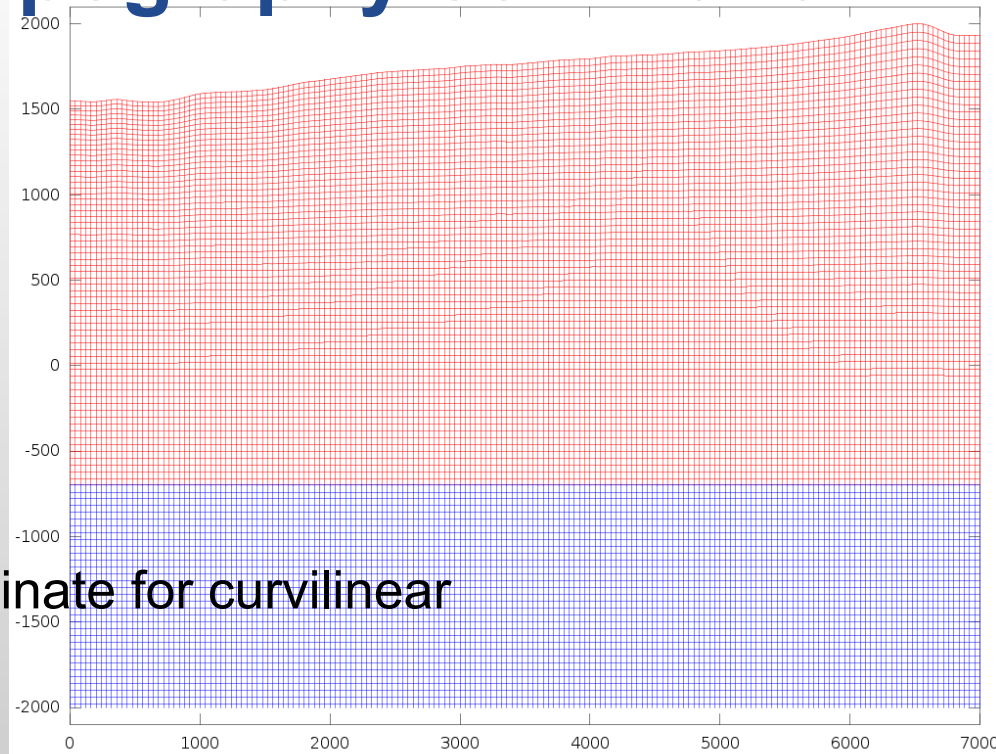
Curvilinear coordinates are used to treat general topography

- Polynomial stretching in vertical direction
 - $z = \tau(x, y) (1 - P(\zeta)) + z_{max} P(\zeta)$
- Transform elastic wave equation to curvilinear coordinates
 - Metric terms similar to anisotropic material properties
- Also used for super-grid absorbing far-field layers



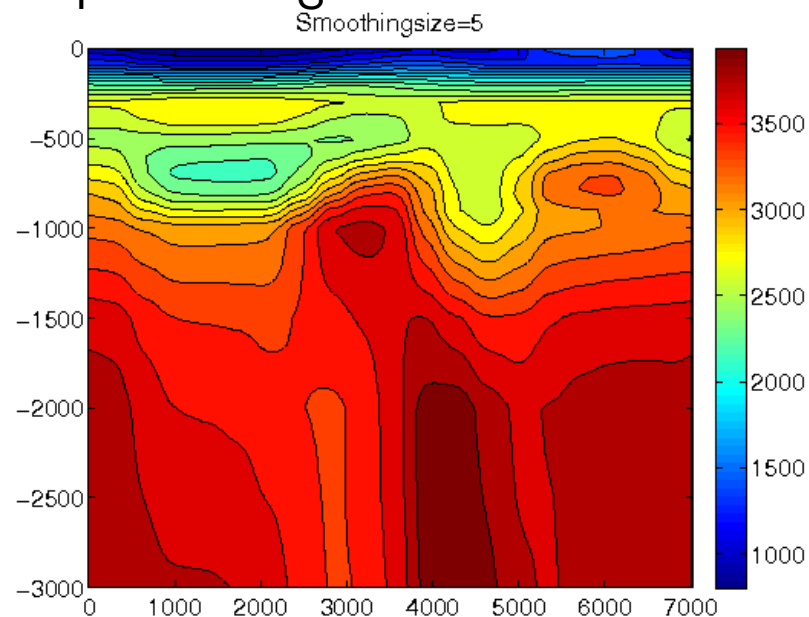
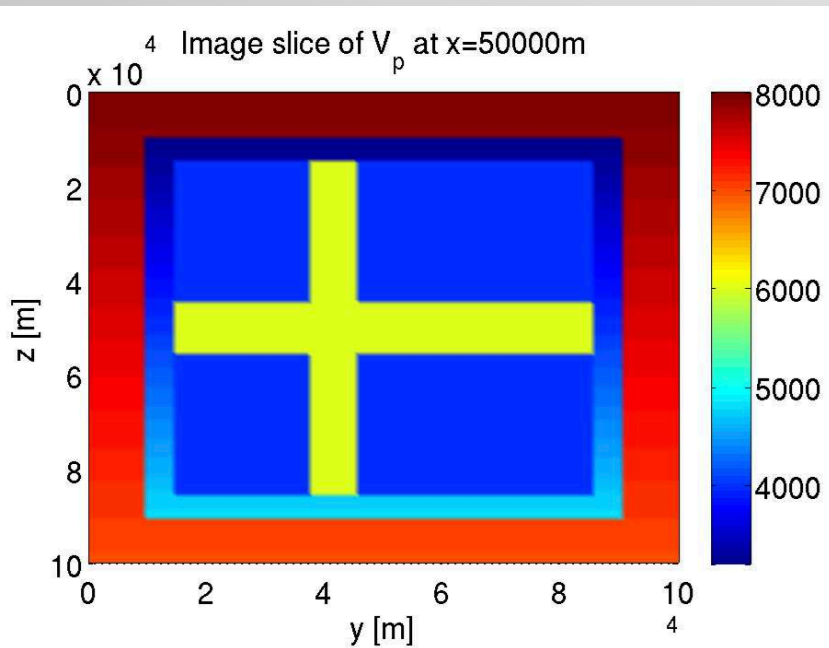
The curvilinear mesh is constructed by sw4 based on the topography command

- 4 ways to specify topography
 - Gaussian hill (testing)
 - Grid file (regular lat-lon lattice)
 - rfile raster file
 - Etree database (SF bay area)
- $z=0$ is mean sea level
- User must pick bottom z-coordinate for curvilinear grid: z_{max}
- Rule of thumb: example:
 - $1500 < \text{elevation} < 2500$ m (positive above sea level)
 - $z_{max} \geq - (1500 - 2 \cdot (2500 - 1500)) = +500$ (positive below sea level)
- `topography input=geographic file=AltaRockSim.topo zmax='700 order=3`



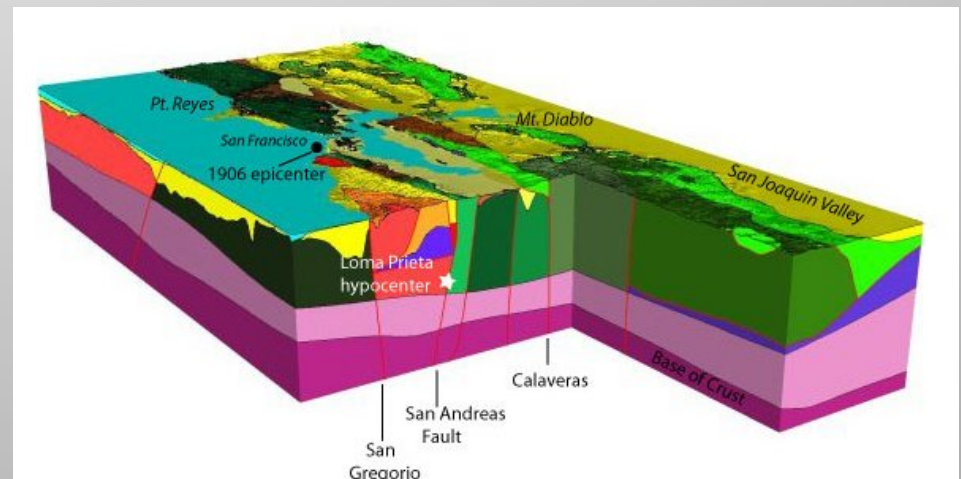
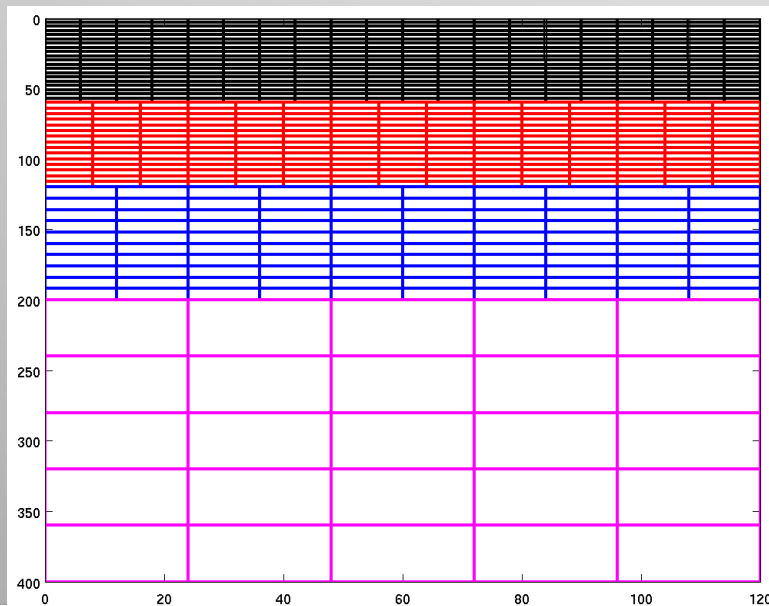
The material model (ρ , C_P , C_S) must be defined at all points in the grid

- One or several material commands can be combined
 - Block, efile, pfile, ifile, rfile
- The order matters (later commands take precedence)
- Visco-elastic modeling triggered by the **attenuation** command: Also need to specify Q_P and Q_S



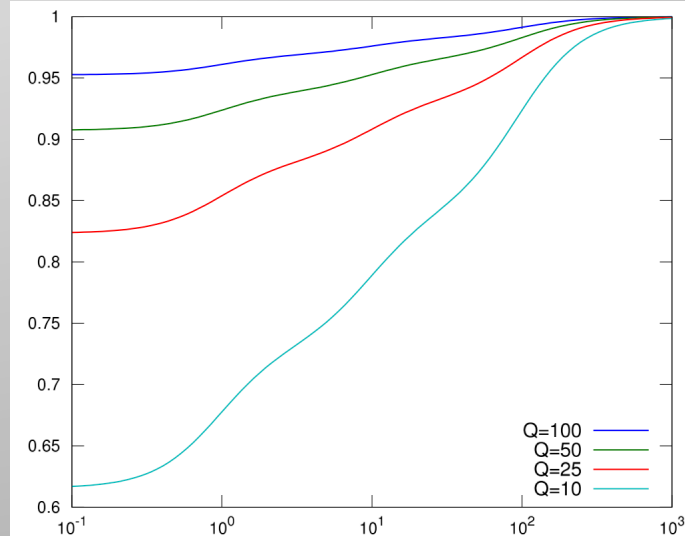
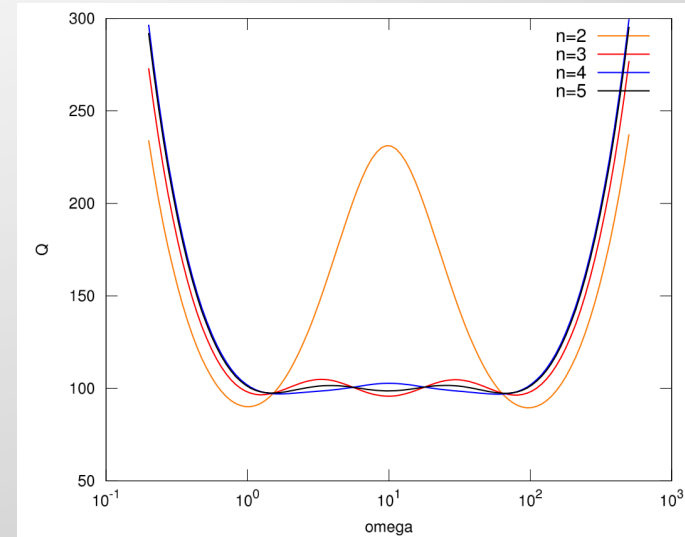
We recommend the binary rfile format for heterogeneous models with topography

- Header + several rectangular blocks of data
- Byte-swapping for mixing Intel/IBM byte ordering
- Parallel I/O allows fast access
- Each core only reads what it needs



Standard linear solid (SLS) mechanisms are used to model anelastic attenuation

- The quality factors (Q_P and Q_S) are approximately constant in frequency band $[0.01 f_{\max}, f_{\max}]$
 - User must specify upper frequency: f_{\max}
 - More mechanisms: less variation in Q , but more calculations. Default $n_{\text{mech}}=3$
- The visco-elastic material is dispersive: phase velocity depends on frequency
 - User must specify phasefreq parameter: frequency where C_P and C_S are accurate.



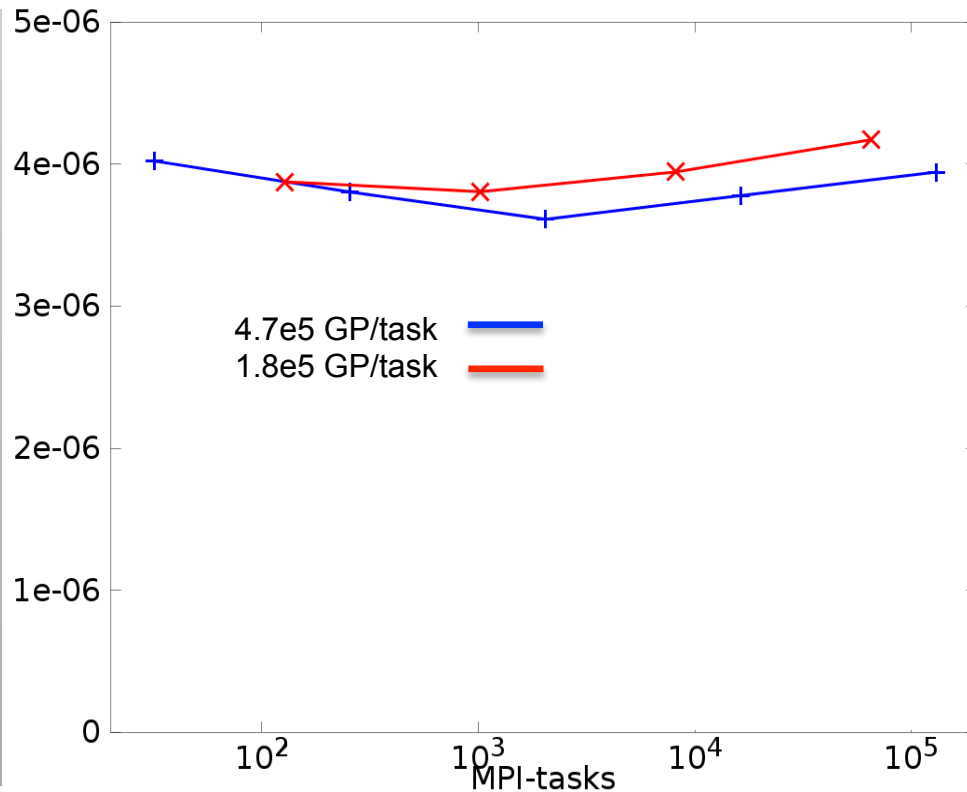
Installing and running sw4

- sw4 can be built on Linux/OSX/Unix machines
 - cmake or make
 - See user's guide appendix A for instructions
- Command file specifies the simulation
 - `srun -ppdebug -n128 sw4 my-input.in`
- Syntax for running MPI-jobs varies:
 - Macs with openmpi: `openmpirun -np 4 sw4 input.in`
 - Linux box with mpich2: `mpiexec -np 8 sw4 input.in`
 - Livermore computing (LC): `srun -n4096 sw4 my-big-job.in`

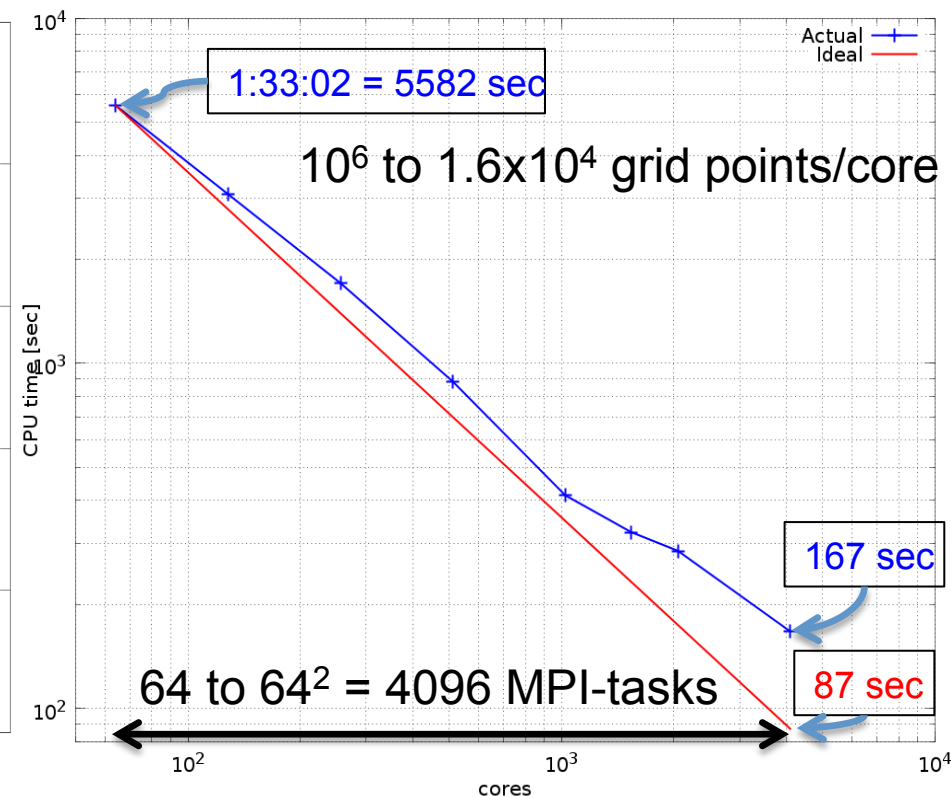
How many cores do I need for running SW4 on a parallel machine?

- The calculation needs to fit in memory (see Appendix C)
- We often use $1e5$ to $1e6$ grid points / core

Weak scaling: 32 to 131,072 cores
Fixed # grid points per core



Strong scaling: 64 to 4096 cores
Fixed problem on more cores



Most SW4 output files can be read with matlab / octave scripts in ../sw4/tools

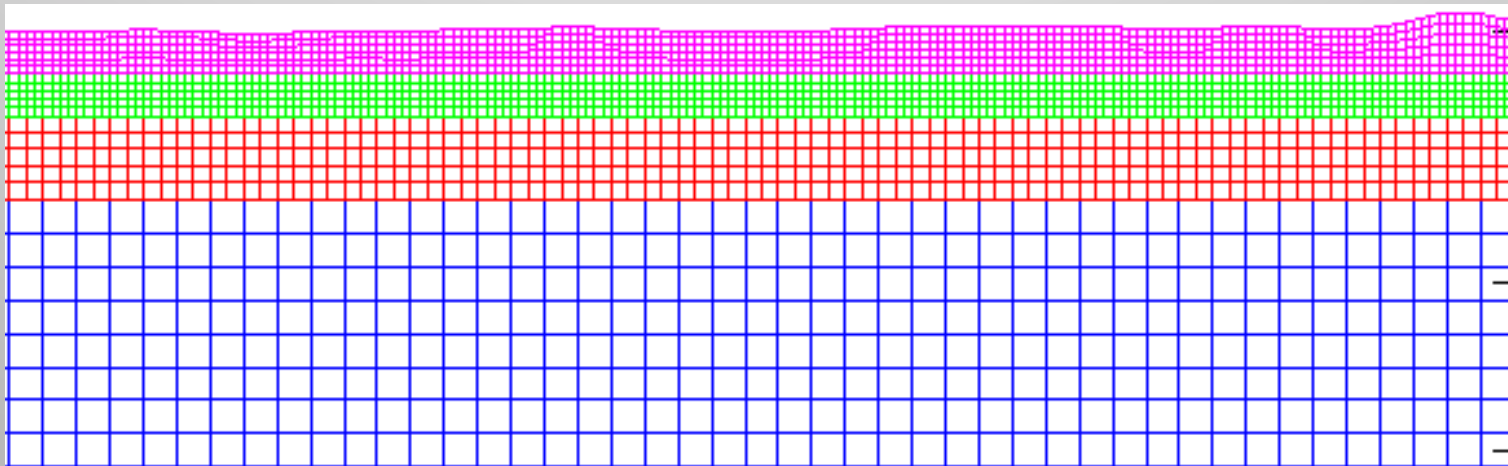
- Synthetic seismograms (sac or usgs txt files): sac or matlab / octave
- 2-D cross-sections (image files): octave / matlab
- Overview on a map (gmt script): gmt programs

General guidelines and scaling

- Check setup on a coarse grid
- Check a few images of the material model
- Check receivers on a map: gmt
- Extrapolate computational resources from coarse run
- Doubling frequency = Halving the grid size = doubling # grid points / dimension
- Doubling # grid points/dimension: 8x grid points, 2x time steps
 - On same number of cores: 8x memory, 16x CPU time
 - On 8x more cores: same memory, 2x CPU time (weak scaling)
 - On 16x cores: $\frac{1}{2}$ x memory, about the same CPU time
- Several examples in `.../sw4/examples`
- Many matlab/octave scripts in `.../sw4/tools`
- SW4 documentation in `.../sw4/doc` and from CIG

Summary and future directions

- SW4 is a documented open source code available from CIG
 - Version 1.1 as tar-ball (Oct-2014)
 - Bleeding edge on github
- Anisotropic materials and curvilinear meshes described in
 - N.A Petersson and B. Sjogreen, J. Comput. Phys. v. 299 pp. 820-841 (2015)
- Local mesh refinement will soon be available



- Currently looking at options for heterogeneous GPU systems

