Programming and Modelling (week 40)

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   (relevant variables, corresponding conservation equations)

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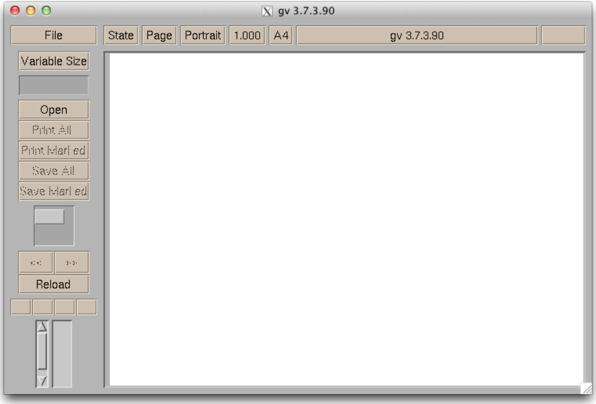
6. fine tune, vary parameters, try end members, push your code
7. produce relevant datas
8. filter/analyse/plot datas
9. discuss figures/graphs

GhostView (1)

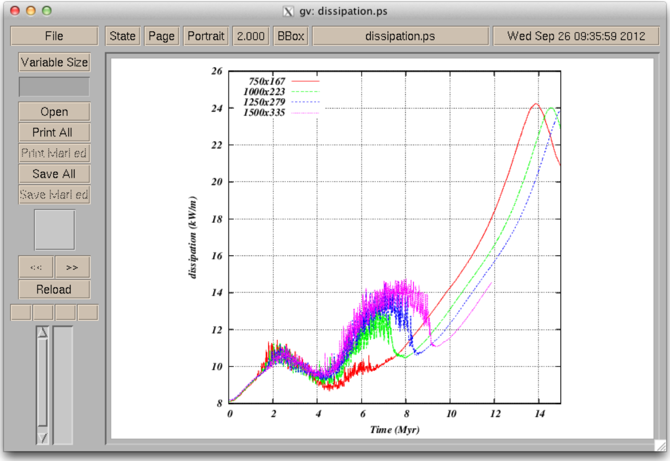
In the terminal:

> gv



GhostView (2)

```
> gv dissipation.eps
```



(press 'Q' to quit the application)

ImageMagick

Postscript (or encapsulated postscripts) isn't a format that text processors (Word, OpenOffice) accept. Here is how to convert plots to different formats:

```
> convert dissipation.ps dissipation.png
> convert dissipation.ps dissipation.jpg
> convert dissipation.ps dissipation.pdf
```

etc...

`convert` is part of ImageMagick , available for Windows, Mac, Linux and even iOS. (www.imagemagick.org)

`> man convert` → lists all options

Makefile (1)

- If your fortran program consists of a unique `.f90` file, compilation is done as follows:

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output_data.f90 module_struc.f90 program.f90
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output_data.f90 module_struc.f90 program.f90
```

What if the code comprises dozens or hundreds of fortran files ?

Makefile (2)

Example: the *elefant* code.

geogarfield — thieulot@gaia:~/ELEFANT/3Dbig/code — ssh — 190×58

```
[thieulot@gaia code]$ ls *.f90
advect_cloud2.f90  define_bc_213.f90  define_bcT_400.f90  material_layout_317.f90  read_exp_226.f90  read_materials_227.f90  stretch_201.f90
advect_cloud.f90  define_bc_214.f90  define_bcT.f90  material_layout_318.f90  read_exp_227.f90  read_materials_228.f90  stretch_205.f90
advect_landscape.f90  define_bc_215.f90  diffuse_surface.f90  material_layout_320.f90  read_exp_228.f90  read_materials_229.f90  stretch_210.f90
advect_lsurface.f90  define_bc_216.f90  diffusion_sp.f90  material_layout_321.f90  read_exp_229.f90  read_materials_230.f90  stretch_211.f90
advect_tracers.f90  define_bc_217.f90  directsolver.f90  material_layout_322.f90  read_exp_230.f90  read_materials_231.f90  stretch_212.f90
advect_vgrid.f90  define_bc_218.f90  elefant.f90  material_layout_400.f90  read_exp_231.f90  read_materials_232.f90  stretch_213.f90
analyse_run.f90  define_bc_219.f90  erosion_232.f90  material_layout_401.f90  read_exp_232.f90  read_materials_233.f90  stretch_215.f90
analytical_solution.f90  define_bc_220.f90  evolve_grid.f90  material_layout.f90  read_exp_233.f90  read_materials_234.f90  stretch_217.f90
bcvel.f90  define_bc_221.f90  find_cell.f90  matrix_profile.f90  read_exp_234.f90  read_materials_235.f90  stretch_218.f90
benchmark.f90  define_bc_222.f90  footer.f90  matrix_setup.f90  read_exp_235.f90  read_materials_300.f90  stretch_224.f90
boundary_cloud_228.f90  define_bc_223.f90  free_memory.f90  modify_grid.f90  read_exp_300.f90  read_materials_301.f90  stretch_228.f90
boundary_cloud_232.f90  define_bc_224.f90  grid_setup.f90  module_structures.f90  read_exp_301.f90  read_materials_302.f90  stretch_232.f90
boundary_cloud.f90  define_bc_225.f90  header.f90  nu_layout_211.f90  read_exp_302.f90  read_materials_303.f90  stretch_301.f90
cailloux_setup.f90  define_bc_226.f90  initialise_mumps_P.f90  nu_layout_232.f90  read_exp_303.f90  read_materials_305.f90  stretch_302.f90
check_cloud.f90  define_bc_227.f90  initialise_mumps_T.f90  nu_layout.f90  read_exp_304.f90  read_materials_306.f90  stretch_303.f90
clean.f90  define_bc_228.f90  initialise_mumps_V.f90  open_files.f90  read_exp_305.f90  read_materials_307.f90  stretch_305.f90
close_files.f90  define_bc_229.f90  interpolate_vel_on_pt2D.f90  output_ascii.f90  read_exp_306.f90  read_materials_315.f90  stretch_306.f90
cloud_setup2.f90  define_bc_230.f90  int_to_char.f90  output_bin.f90  read_exp_307.f90  read_materials_316.f90  stretch_307.f90
cloud_setup.f90  define_bc_231.f90  landscape_setup.f90  output_mats.f90  read_exp_315.f90  read_materials_317.f90  stretch_315.f90
cloud_setup_old.f90  define_bc_232.f90  lsurface_setup.f90  paint_stripes.f90  read_exp_316.f90  read_materials_318.f90  stretch_316.f90
compute_cloudmax.f90  define_bc_233.f90  make_matrix.f90  phase_change_232.f90  read_exp_317.f90  read_materials_320.f90  stretch_317.f90
compute_convergence.f90  define_bc_234.f90  make_matrixT.f90  pslib.f90  read_exp_318.f90  read_materials_321.f90  stretch_318.f90
compute_elemental_values.f90  define_bc_235.f90  material_layout_200.f90  psplot_cloud.f90  read_exp_320.f90  read_materials_322.f90  stretch_400.f90
compute_element_centers.f90  define_bc_300.f90  material_layout_202.f90  psplot_cloud_zoom.f90  read_exp_321.f90  read_materials_400.f90  stretch_401.f90
compute_elsize.f90  define_bc_301.f90  material_layout_203.f90  psplot_grid2D.f90  read_exp_322.f90  read_materials_401.f90  stretch.f90
compute_fluxes.f90  define_bc_302.f90  material_layout_204.f90  psplot_grid2D_zoom.f90  read_exp_400.f90  read_materials.f90  subtiming.f90
compute_heatflux.f90  define_bc_303.f90  material_layout_210.f90  psplot_grid_sandbox.f90  read_exp_401.f90  read_n_compute_parameters.f90  temperature_layout_208.f90
compute_hydr_pressure.f90  define_bc_304.f90  material_layout_211.f90  qshep2d.f90  read_materials_200.f90  renumber_nodes.f90  temperature_layout_209.f90
compute_pressure.f90  define_bc_305.f90  material_layout_212.f90  read_exp_200.f90  read_materials_201.f90  scan_for_arguments.f90  temperature_layout_212.f90
compute_pressure_fem.f90  define_bc_306.f90  material_layout_213.f90  read_exp_201.f90  read_materials_202.f90  set_default_values.f90  temperature_layout_213.f90
compute_qcoords.f90  define_bc_307.f90  material_layout_214.f90  read_exp_202.f90  read_materials_203.f90  smooth_pressure.f90  temperature_layout_225.f90
compute_stress_profile.f90  define_bc_315.f90  material_layout_215.f90  read_exp_203.f90  read_materials_204.f90  SolCx.f90  temperature_layout_232.f90
compute_tensors.f90  define_bc_316.f90  material_layout_216.f90  read_exp_204.f90  read_materials_205.f90  SolKz.f90  temperature_layout_235.f90
compute_timestep.f90  define_bc_317.f90  material_layout_217.f90  read_exp_205.f90  read_materials_206.f90  solve.f90  temperature_layout_303.f90
compute_Trms.f90  define_bc_318.f90  material_layout_218.f90  read_exp_206.f90  read_materials_207.f90  solveP.f90  temperature_layout_305.f90
compute_Trms_old.f90  define_bc_320.f90  material_layout_219.f90  read_exp_207.f90  read_materials_208.f90  solvePfem.f90  temperature_layout_306.f90
compute_viscous_dissipation.f90  define_bc_321.f90  material_layout_220.f90  read_exp_208.f90  read_materials_209.f90  solveT.f90  temperature_layout.f90
compute_volume.f90  define_bc_322.f90  material_layout_221.f90  read_exp_209.f90  read_materials_210.f90  spacer.f90  template.f90
compute_vrms.f90  define_bc_400.f90  material_layout_222.f90  read_exp_210.f90  read_materials_211.f90  spas.f90  time_nl.f90
compute_xyzq.f90  define_bc_401.f90  material_layout_223.f90  read_exp_211.f90  read_materials_212.f90  spline.f90  timevisu_setup.f90
cshep2.f90  define_bc.f90  material_layout_224.f90  read_exp_212.f90  read_materials_213.f90  strain_history_203.f90  tracers_setup_212.f90
define_bc_200.f90  define_bcT_206.f90  material_layout_226.f90  read_exp_213.f90  read_materials_214.f90  strain_history_210.f90  tracers_setup_216.f90
define_bc_201.f90  define_bcT_207.f90  material_layout_228.f90  read_exp_214.f90  read_materials_215.f90  strain_history_211.f90  tracers_setup.f90
define_bc_202.f90  define_bcT_208.f90  material_layout_229.f90  read_exp_215.f90  read_materials_216.f90  strain_history_214.f90  trim_cloud.f90
define_bc_203.f90  define_bcT_209.f90  material_layout_232.f90  read_exp_216.f90  read_materials_217.f90  strain_history_215.f90  trim_landscape.f90
define_bc_204.f90  define_bcT_210.f90  material_layout_233.f90  read_exp_217.f90  read_materials_218.f90  strain_history_301.f90  tshep2.f90
define_bc_205.f90  define_bcT_211.f90  material_layout_234.f90  read_exp_218.f90  read_materials_219.f90  strain_history_302.f90  update_cloud.f90
define_bc_206.f90  define_bcT_213.f90  material_layout_302.f90  read_exp_219.f90  read_materials_220.f90  strain_history_303.f90  vgrid_setup.f90
define_bc_207.f90  define_bcT_225.f90  material_layout_303.f90  read_exp_220.f90  read_materials_221.f90  strain_history_306.f90  write_parameters.f90
define_bc_208.f90  define_bcT_232.f90  material_layout_304.f90  read_exp_221.f90  read_materials_222.f90  strain_history_315.f90
define_bc_209.f90  define_bcT_235.f90  material_layout_305.f90  read_exp_222.f90  read_materials_223.f90  strain_history_316.f90
define_bc_210.f90  define_bcT_303.f90  material_layout_306.f90  read_exp_223.f90  read_materials_224.f90  strain_history.f90
define_bc_211.f90  define_bcT_305.f90  material_layout_315.f90  read_exp_224.f90  read_materials_225.f90  strainweaken.f90
define_bc_212.f90  define_bcT_306.f90  material_layout_316.f90  read_exp_225.f90  read_materials_226.f90  stretch_200.f90
[thieulot@gaia code]$
```

(373 fortran files, 40,000 lines of code)

Makefile (3)

Example: the gravity modelling exercise for this week
The whole programs comprises the following fortran files:

```
write_two_columns.f90
write_three_columns.f90
program.f90
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The whole programs comprises the following fortran files:

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The subroutines are given to you, but you have to write the main program.

Makefile (4)

Compiling all the routines and assembling them all into the executable `grav`:

```
> gfortran write_two_columns.f90
write_three_columns.f90 program.f90 -o grav
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```

- not practical
- if you modify one file, this approach still requires you to recompile all fortran files !

Makefile (5)

We then create the following file: `Makefile` (See appendix C)

```
.SUFFIXES:.out .o .s .c .F .f .f90 .e .r .y .yr .ye .l .p .sh .csh .h

default: code

F90      = gfortran

FLAGS= -c -ffree-line-length-none

OPTIONS =

INCLUDE =

OBJECTS = \
write_two_columns.o\
write_three_columns.o\
program.o

.f90.o:
	$(F90) $(FLAGS) $(INCLUDE) $*.f90
.f.o:
	$(F90) $(FLAGS) $(INCLUDE) $*.f

code:	$(OBJECTS)
	$(F90) $(OPTIONS) $(OBJECTS)  -o grav
```

Makefile (5)

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code:	$(OBJECTS)
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To compile the whole code:

`> make`

Wrapping things up: Key concepts

- data types (integer, real, character, ...)
- data structures (numbers, static arrays, allocatable arrays)
- if then else
- do loop
- subroutines and functions
- intrinsic functions
- modules, formats
- open/close file
- compile vs run
- makefile
- plotting (xmgrace, gnuplot)
- shell commands (ls, cd, pwd, ...)

Things you HAVE to know (for the exam)

How to declare

- an integer, a real
- an array (static, or allocatable)

How to write

- a program
- a subroutine, a function
- a do-loop
- an if-then-else statement

How to

- open a file
- write in a file
- close a file
- call a subroutine/function
- pass an array as argument

salt tectonics(1)

Marine and Petroleum Geology 18 (2001) 779–797

Marine and Petroleum Geology

www.elsevier.com/locate/marpetgeo

Salt diapirs in the Dead Sea basin and their relationship to Quaternary extensional tectonics

Abdallah Al-Zoubi[a,1], Uri S. ten Brink[b,*]

[a]*Woods Hole Oceanographic Institution, Woods Hole, MA 02543, USA*
[b]*US Geological survey, Woods Hole Field Center, 384 Woods Hole Road, Woods Hole, MA 02543, USA*

Received 21 March 2001; received in revised form 23 May 2001; accepted 23 May 2001

salt tectonics(2)

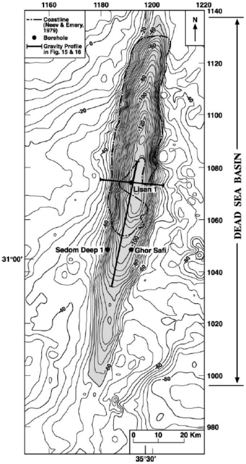
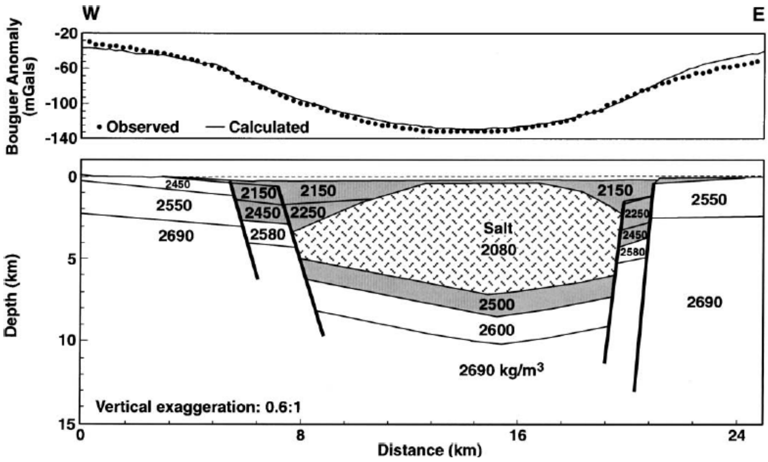


Fig. 14. Bouguer gravity anomaly map of the study area. Contour interval is 3 mGal. Location of the gravity profiles in Figs. 15 and 16. Dashed-dotted line — 1967 coastline of the Dead Sea (after Neev & Hall, 1979). Black dots — location of wells.

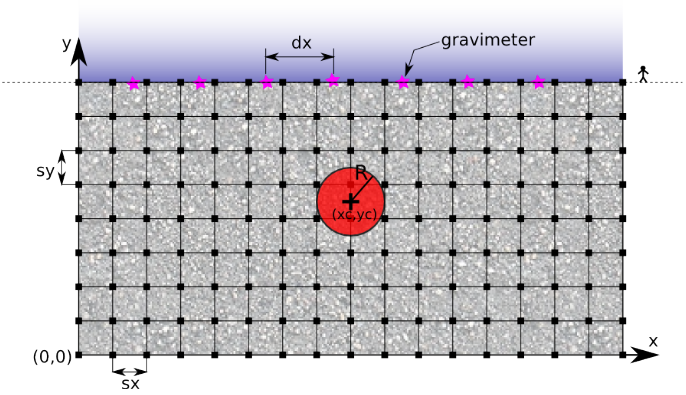
salt tectonics(3)

A. Al-Zoubi, U.S. ten Brink / Marine and Petroleum Geology 18 (2001) 779–797



Grav (1)

The modelling program `grav` computes the gravity anomaly at the Earth's surface of a number of spherical density anomalies in the subsurface.



Grav (2)

A key idea in numerical modelling: **benchmarking**

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- Your code runs and produces beautiful, tangible results 

Grav (2)

A key idea in numerical modelling: **benchmarking**

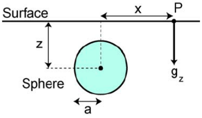
- Your code runs and produces beautiful, tangible results 
- How do you know that you haven't forgotten a minus sign somewhere ? a factor 2 ?

→ You can run your code on typical experiments/problems to which we know an analytical solution
→ You can run your code and a commercial/mature code on the same problem and compare results
→ You can run your code on a problem and compare its results with real life experimental results

Grav (3) - benchmarking the program

A sphere has the same gravitational pull as a point mass located at its centre: it allows us to calculate its gravitational pull.
Simple mathematics (See Turcotte and Schubert) can be used to show that at Point P, the vertical component of g is given by

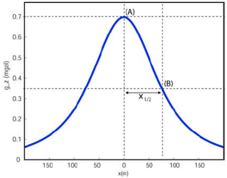
$$g_z = \frac{G M_S z}{(x^2 + z^2)^{\frac{3}{2}}}$$

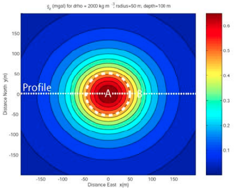


Suppose:

Radius, a	= 50 m	Depth, z	= 100 m
Density contrast , Δρ	= 2000 kg m^{-3}	Excess mass, M_S	= 10^9 kg

The variation in g_z can be plotted on a profile and map





Grav (4) - benchmarking the program