Parametric NAFEMS LE10 benchmark

Comparison of resource consumption for different FEA programs

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1 Introduction

This test aims at comparing CPU and memory consumption when solving the same problem with different cloud-friendly finite-element analysis programs. Particularly, it was designed to understand how FeenoX compares to other well-established tools and to understand where and how to optimize the code.

The programs tested are

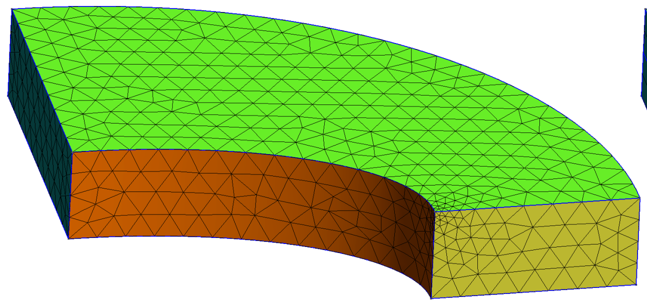
- FeenoX
- Sparselizard
- Code Aster
- CalculiX

The problem being solved is the NAFEMS LE10 problem. It was chosen because

a. It is a well-established benchmark since its publication in 1990
b. It is simple yet has displacement boundary condition on an edge in addition to faces that makes it challenging
c. The reference solution is a single scalar which is easy to compare among different approaches

Each program solves the problem parametrically over a wide range of mesh refinements using two types of Gmsh-generated second-order grids:

1. locally-refined (around point D) unstructured curved tetrahedral grid, and
2. straight incomplete (i.e. hex20) fully-structured hexahedral mesh.


(a) Tetrahedral mesh

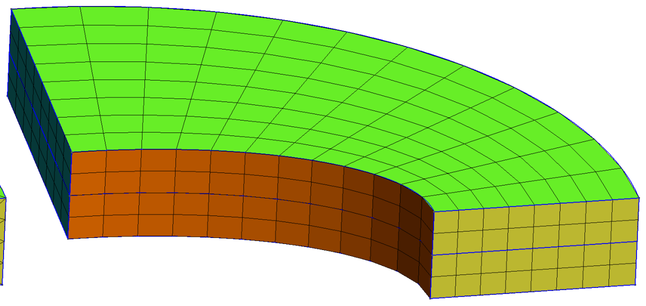

(b) Hexahedral mesh

Figure 1: The two types of meshes used in this test

The NAFEMS LE10 problem asks to compute the normal stress in the y direction at point D that has coordinates $(2000\text{ mm}, 0, 300\text{ mm})$. For each mesh type (tet/hex), a refinement factor $c \in (c_{\text{min}} : 1]$ is applied. Besides σ_y, the wall time, CPU time and memory are recorded for each run so as to create plots of these results vs. c and vs. the total number of degrees of freedom being solved for—which can be different in each code even for the same c, as explained below.

This way of executing FEA programs follows the FeenoX design basis of being cloud-first (and only later desktop-friendly). It is mandatory to be able to control the execution and read the output from an automated script. The reasons for this requirement are explained in the FeenoX documentation, particularly in the SRS and SDS. It might happen that some of the codes tests seem to need to setup and/or read the results in a unnecessarily complex and/or cumbersome way because they were not designed to be either cloud-first and/or script-friendly. It might also happen that the cumbersomeness comes from my lack of expertise about how to properly use the code.

Even though there are some particular comments for each of the code used in this comparison, this test is not about the differences (and eventually pros and cons) each code has for defining and solving a FEA problem. It is about comparing the consumption of computational resources needed to solve the same problem (or almost) in the cloud. The differences about how to set up the problem and considerations about usage, cloud friendliness and scriptability are addressed in a separate directory regarding benchmark NAFEMS LE11, that involves defining a temperature distribution given by an algebraic expression (under preparation at the time of this writing).

1.1 Reference solution

The original problem formulation (which can be found in one of FeenoX' annotated examples) states that the reference solution is -5.38 MPa. This can be confirmed with FeenoX using the input `le10-ref.fee`.

```
$ gmsh -3 le10-ref.geo
[...]
Info    : Done meshing order 2 (Wall 0.456586s, CPU 0.438907s)
Info    : 205441 nodes 59892 elements
Info    : Writing 'le10-ref.msh'...
Info    : Done writing 'le10-ref.msh'
Info    : Stopped on Thu Oct 28 12:03:28 2021 (From start: Wall 1.30955s, CPU 1.44333s)
$ time feenox le10-ref.fee
sigma_y(D) =  -5.3792 MPa

real    1m34.485s
user    1m30.677s
sys     0m10.449s
$
```

This run can also be used to "calibrate" the timing. Just run the `le10-ref.fee` case yourself and see how long FeenoX needs in your server. This figure should help you to scale up (or down) the ordinates of the figures for the parametric results shown here.

1.2 Scripted parametric execution

The driving script is called `run.sh`. Without any arguments, it shows the usage:

```
$ ./run.sh
usage: ./run.sh { tet | hex } c_min n_steps
$
```

The first argument is either `tet` or `hex`. The second is the lower end of the range for the mesh refinement factor $c \in (c_\text{min} : 1]$. In principle there is no problem setting `c_min` to 0 because it will never be reached exactly since the range is open to the left— although the meshes will be insanely large. The last argument is the number of steps.

Note that the range $(c_\text{min} : 1]$ will be swept using a quasi-random number sequence and all the results will be cached until removed by executing `clean.sh`. So if one first runs

```
./run.sh tet 0.1 8
```

and then

```
./run.sh tet 0.1 12
```

the second execution would only run four actual steps, reading the cached values for the first eight. This will hold as long as `c_min` is the same for all invocations of `run.sh`.

To check which of the codes are available in your configuration, run with `--check`:

```
$ ./run.sh --check
FeenoX GAMG:  yes
FeenoX MUMPS: yes
Sparselizard: yes
Code Aster:   yes
CalculiX:     yes
$
```

Run a single step (i.e. $c = 1$, which are the default meshes shown above) for each case to see if everything works.

```
$ ./run.sh tet 1 1
[...]
$ ./run.sh hex 1 1
[...]
$
```

For each c both the geometry and the mesh are created with Gmsh. The refinements are made by setting the `-clscale` command-line parameter equal to $c \in (c_\text{min} : 1]$ to control the elements' size. The actual values taken by c are given by running FeenoX with the input `steps.fee`. This uses a Sobol quasi-random number sequence that starts with $c = 1$ and then fills the interval in subsequent steps. For example, five steps for $c_\text{min} = 0.1$ gives

```
$ feenox steps.fee 0.1 5
1
0.55
0.775
0.325
0.4375
$
```

The first step is the coarsest mesh, which is enforced to be always run. The second one is the middle-range mesh, and the following steps start to "fill" in the blanks without actually reaching $c = c_{\text{min}}$. Since the `run.sh` script caches the results it gets, further steps can be performed by reusing the existing data. So if we now want to run ten steps,

```
$ feenox steps.fee 0.1 10
1
0.55
0.775
0.325
0.4375
0.8875
0.6625
0.2125
0.26875
0.71875
$
```

and the first five steps will use cached data instead of re-running all the codes.

A successful execution of `run.sh` will give files `*.dat` with the following columns:

1. the parameter $c \in (c_{\text{min}} : 1]$
2. the total number of degrees of freedom
3. the stress σ_y evaluated at point D
4. the wall time in seconds
5. the kernel-mode CPU time in seconds
6. the user-mode CPU time in seconds
7. the maximum memory used by the program, in kB

The rows will follow the execution order, so they will be unsorted on the refinement factor (and number of degrees of freedom) so they are not suitable for plotting them directly using lines to connect consecutive data points. There is another script, `report.sh` that will read the data and prepare figures in SVG format (using Gnuplot) and a markdown report with tables with the actual figures:

```
$ ./report.sh tet
[...]
$ ./report.sh hex
[...]
$
```

The report also indicates some data about the host where the test was performed and the versions of the codes used. The SVG files are interactive so they can be opened with a web browser, zoomed in and out and the individual curves can be turned on and off by clicking on the label.

- Results for the unstructured tetrahedral mesh—PDF
- Results for the structured hexahedral mesh—PDF

2 Explanations, comments and caveats

> **Disclaimer**: I am the author of FeenoX so all of my comments are likely to be biased. If you are reading this and feel like something is not true or is indeed way too biased, please contact me and help me to have the fairest comparison possible. There might still be some subjectivity and I apologize in advance for that.

- The objective of this test is to compare consumption of resources for cloud-based computations. It is therefore suggested to run it on a cloud server and not on a local laptop.
- In order to have the most fair comparison possible, even though the codes can measure CPU and memory consumption themselves, all of them are run through the `time` tool (the actual binary tool at `/usr/bin ↩ /time`, not the shell's internal).
- This is a **serial test only** so the variable `OMP_NUM_THREADS` is set to one to avoid spawning OpenMP threads. MPI-based parallel tests across different hosts will come later on. OpenMP will not be the main focus of the scalability study.
- The wall time should thus be equal to the sum of kernel-space CPU time plus user-space CPU time plus some latency that depends on the operating system's scheduler.
- The hex mesh is created as a first-order mesh and then either

  1. converted to a (straight) second-order incomplete (i.e. hex20) mesh, or
  2. the first-order mesh is fed to the code and it is asked to use second-order elements.

  depending on the capabilities of each code (some codes honor the element type in the mesh but others change the order and number of degrees of freedom per element on the fly).
- The second column of the output is the total number of degrees of freedom. In principle for a simple three-dimensional problem like this one it should be equal to three times the number of nodes. But by default Code Aster sets Dirichlet boundary conditions as Lagrange multipliers, increasing the matrix size. On the contrary, CalculiX removes the degrees of freedom that correspond to nodes with Dirichlet boundary conditions resulting in a smaller matrix size. Sparselizard needs complete elements so for order = 2 it assigns an unknown to each node, edge, face and volume of the element, resulting in 27 unknowns per hexahedron. This is equivalent of using hex27 (instead of hex20) elements, resulting in a (much) higher degree-of-freedom count for the hexahedral case.
- Most codes allow to choose the actual linear sparse solver at runtime, maybe depending on the availability of particular solving libraries at compilation time. For these codes, there are many curves, one for each supported preconditioner+solver combination.

- When the mesh is big, chances are that the code runs out of memory being killed by the operating system (if there is no swap partition, which there should be not for efficiency reasons). Code Aster and CalculiX have out-of-core capabilities in which they can run with less memory than the actual requested, at the expense of larger CPU times by using a tailor-made disk-swapping procedure. The other codes are killed by the operating system when this happens and there is no data point for that particular value of c.
- The number of iterations (and thus the CPU time) needed to converge when using iterative solvers depends on the tolerance. In all cases, default tolerances have been used.

2.1 FeenoX

The `run.sh` script calls the executable `feenox` with the `le10.fee` input file as the first argument and `${m}-${c}` ↩ as the second one, resulting in something like `tet-1` or `hex-0.2`. This argument is expanded where the input file contains a `$1`, namely the mesh file name. FeenoX prints the total number of degrees of freedom and the stress σ_y at point D. It does not write any post-processing file (the `WRITE_MESH` keyword is commented out):

```
# NAFEMS Benchmark LE-10: thick plate pressure
PROBLEM mechanical
READ_MESH le10_2nd-$1.msh   # FeenoX honors the order of the mesh

BC upper    p=1      # 1 Mpa
BC DCDC     v=0      # Face DCD'C' zero y-displacement
BC ABAB     u=0      # Face ABA'B' zero x-displacement
BC BCBC     u=0 v=0  # Face BCB'C' x and y displ. fixed
BC midplane w=0      #  z displacements fixed along mid-plane

E = 210e3   # Young modulus in MPa (because mesh is in mm)
nu = 0.3    # Poisson's ratio

SOLVE_PROBLEM   # TODO: implicit

PRINT total_dofs %.8f sigmay(2000,0,300)

# write post-processing data for paraview
# WRITE_MESH le10-feenox-${c}.vtk VECTOR u v w sigmax sigmay sigmaz tauxy tauzx tauyz
```

The mesh file should already contain a second-order mesh. The file `le10-tet.geo` creates tet10 elements, but the `le10-hex.geo` creates hex8 elements that have to be converted to hex20 before FeenoX can use them. This is achieved in the `run.sh` script within the block

```
  if [ ! -e le10-${m}-${c}.msh ]; then
    gmsh -3 le10-${m}.geo -clscale ${c} -o le10-${m}-${c}.msh || exit 1
    gmsh -3 le10-${m}-${c}.msh -setnumber Mesh.SecondOrderIncomplete 1 -order 2 -o le10_2nd-${m}-${c}.msh  ↩
        || exit 1
  fi
```

If the file `le10-${m}-${c}.msh` does not exist (otherwise it would take it as a cached file), Gmsh is first called with either `le10-tet.geo` or `le10-hex.geo` as the input and `-clscale` is set to c to create `le10-${m}-${c}.msh`. Then, this mesh file is explicitly converted to a second-order mesh with `-order 2` and any hex8 is converted to hex20 (instead of hex27 because `Mesh.SecondOrderIncomplete=1`) and saved as `le10_2nd-${m}-${c}.msh`. It is this last mesh file the one that FeenoX needs.

By default, FeenoX uses Mark Adams' Geometric-Algebraic Multigrid Preconditioner provided by PETSc and conjugate gradients as the iterative solver for the mechanical problem. This default corresponds to the "feenox_gamg" curve. One can check the actual options by passing `--ksp_view` as an extra option, e.g.

```
$ feenox le10.fee tet-1 --ksp_view
KSP Object: 1 MPI processes
  type: cg
  maximum iterations=10000, nonzero initial guess
  tolerances:  relative=1e-06, absolute=1e-50, divergence=10000.
  left preconditioning
  using PRECONDITIONED norm type for convergence test
PC Object: 1 MPI processes
  type: gamg
    type is MULTIPLICATIVE, levels=4 cycles=v
      Cycles per PCApply=1
      Using externally compute Galerkin coarse grid matrices
[...]
  linear system matrix = precond matrix:
  Mat Object: K_bc 1 MPI processes
    type: seqaij
    rows=20325, cols=20325, bs=3
    total: nonzeros=1498671, allocated nonzeros=1498671
    total number of mallocs used during MatSetValues calls=0
      has attached near null space
      using I-node routines: found 6775 nodes, limit used is 5
20325   -5.41620113
$
```

If the MUMPS solver is available through PETSc, `run.sh` adds the command-line option `--mumps` to create another curve, "feenox_mumps":

```
$ feenox le10.fee tet-1 --mumps --ksp_view
KSP Object: 1 MPI processes
  type: preonly
  maximum iterations=10000, initial guess is zero
  tolerances:  relative=1e-06, absolute=1e-50, divergence=10000.
  left preconditioning
  using NONE norm type for convergence test
PC Object: 1 MPI processes
  type: cholesky
    out-of-place factorization
    tolerance for zero pivot 2.22045e-14
    matrix ordering: nd
    factor fill ratio given 0., needed 0.
      Factored matrix follows:
        Mat Object: 1 MPI processes
          type: mumps
          rows=20325, cols=20325
          package used to perform factorization: mumps
          total: nonzeros=5974629, allocated nonzeros=5974629
            MUMPS run parameters:
[...]
```

```
               INFOG(39) (after analysis: estimated size of all MUMPS internal data for running BLR out-of- ↩
                    core - sum over all processors): 0
  linear system matrix = precond matrix:
  Mat Object: K_bc 1 MPI processes
    type: seqaij
    rows=20325, cols=20325, bs=3
    total: nonzeros=1498671, allocated nonzeros=1498671
    total number of mallocs used during MatSetValues calls=0
      using I-node routines: found 6775 nodes, limit used is 5
20325   -5.41600874
$
```

2.2 Sparselizard

Thanks to Alexandre Halbach for the discussions about Sparselizard's internals. The following `main.cpp` is used to solve the NAFEMS LE10 benchmark with Sparselizard:

```cpp
// NAFEMS LE10 Benchmark solved with Sparselizard

#include "sparselizard.h"
using namespace sl;

int main(int argc, char **argv) {

  int bulk = 1;
  int upper = 2;
  int DCDC = 3;
  int ABAB = 4;
  int BCBC = 5;
  int midplane = 6;

  double young = 210e3;
  double poisson = 0.3;

  std::string c = (argc > 1) ? argv[1] : "tet-1";
  mesh mymesh("gmsh:../le10-"+c+".msh", 0);
  field u("h1xyz");

  parameter E;
  E|bulk = young;
  parameter nu;
  nu|bulk = poisson;

  u.setorder(bulk, 2);
  u.compy().setconstraint(DCDC); // v=0 @ DCDC
  u.compx().setconstraint(ABAB); // u=0 @ ABAB
  u.compx().setconstraint(BCBC); // u=0 @ BCBC
  u.compy().setconstraint(BCBC); // v=0 @ BCBC
  u.compz().setconstraint(midplane); // w=0 @ midplae

  formulation elasticity;
  elasticity += integral(upper, array1x3(0,0,-1)*tf(u));   // p=1 @ upper
  elasticity += integral(bulk, predefinedelasticity(dof(u), tf(u), E, nu), -2);  // -2 gives an exact  ↩
      integration for up to 4th order polynomial"
  elasticity.generate();
  vec solu = solve(elasticity.A(), elasticity.b(), "cholesky");

  // Transfer the data from the solution vector to the u field:
  u.setdata(bulk, solu);

  double lambda = young * poisson/((1+poisson)*(1-2*poisson));
  double mu = 0.5*young/(1+poisson);

  expression H(6,6,{lambda+2*mu,      lambda,      lambda,  0,  0,  0,
                  lambda,      lambda+2*mu,      lambda,  0,  0,  0,
                  lambda,           lambda, lambda+2*mu,  0,  0,  0,
                       0,                0,           0, mu,  0,  0,
                       0,                0,           0,  0,  mu, 0,
                       0,                0,           0,  0,  0, mu});

  expression sigma = H*strain(u);
//   u.write(bulk, "le10-sparselizard-displ.vtk", 2);
//   comp(1, sigma).write(bulk, "le10-sparselizard-sigmay.vtk", 2);

  field sigmayy("h1");
  sigmayy.setorder(bulk, 2);
  sigmayy.setvalue(bulk, comp(1, sigma));

  std::cout << elasticity.countdofs() << "\t" << sigmayy.interpolate(bulk, {2000, 0, 300})[0] << std::endl;

  return 0;
}
```

The main function takes one argument which should be the same as in FeenoX, i.e. `tet-1`, `hex-0.25`, etc. which is used to read the mesh file as created by Gmsh from the parent directory. The problem order is set to two. The Dirichlet BCs are then set. The Neumann BC is set into the elasticity weak formulation as a surface integral. The volume integral is performed using 2nd-order Gauss points and then the problem is solved for the displacements. The stress tensor field is explicitly computed out of the strain using the linear elastic 6x6 matrix in Voigt notation. The stress at point D is interpolated from a smoothed field over all the elemental contributions to the node and printed into the standard output, along with the total number of degrees of freedom being solved for. Sparselizard uses MUMPS through PETSc. By default, it will use the LU preconditioner. But since the stiffness matrix is symmetric, we choose to use the Cholesky preconditioner.

Note that as already discussed, Sparselizards needs tensor-product elements for the hex case. Therefore, the choice of order equal to two triggers the addition of unknowns at the 12 edges, at the 6 faces and 1 at the volume besides the 8 corners resulting in 27 unknowns (per each of the three degrees of freedom of the problem). The other codes stick to incomplete hex20 elements, so the total number of degrees of freedom is larger for Sparselizard than for the other codes for the same c.

2.3 Code Aster

Thanks to Cyprien Rusu for all the help setting up the code and the input files and to Nicolas Tardieu for an interesting technical discussion about Code Aster's internals.

Even though Gmsh can write the mesh in the very efficient MED format which Code Aster can read, since it is a binary file (it is based on HDF5) the version of the MED library which both Gmsh as Aster are linked with should be the same. Since Code Aster is tricky to compile with custom dependencies and Gmsh uses a newer MED library by default, this option was dismissed.

It was decided to use the text-based (and archaic format UNV). The second-order mesh `le10_2nd-${m}-${c}.msh` is converted to UNV with Gmsh:

```
    if [ ! -e le10_2nd-${m}-${c}.unv ]; then
      gmsh -3 le10_2nd-${m}-${c}.msh -o le10_2nd-${m}-${c}.unv || exit 1
    fi
```

The argument that the Code Aster executable needs in order to run a case is an "export" file that defines some run-time options for the execution (memory and CPU limits, number of MPI instances, etc.) and links Fortran file units (the ones that were introduced in 1954) to actual file system names, like the "comm" (input) file, the mesh file, the output file, etc. Interestingly enough, Code Aster would modify the input export file (sic) and rename relative file paths contained in it to absolute ones. This makes it hard to track export files with Git, but what `run.sh` does is it uses a template export file

```
P actions make_etude
P debug nodebug
P memjob 2097152
P memory_limit 15500.0
P mode interactif
P mpi_nbcpu 1
P mpi_nbnoeud 1
P ncpus 0
P time_limit 9000.0
P tpsjob 16
P version stable
A memjeveux 128.0
A tpmax 9000.0

F comm le10__s_.comm       D  1
F libr le10_2nd-_m_.unv    D  20
F libr le10-_m_.rmed       R  80
F mess message__s_-_m_     R  6
F resu DD-_s_-_m_.txt      R  17
R base base-stage1-_s_-_m_ R  0
```

and then use `sed` would replace `_m_` with `${m}` to have a per-c Git-ignored export file which can be further modified as needed.

The actual problem definition is stored in a "comm" file. There are three variants to solve the NAFEMS LE10 problem with Code Aster, namely

- `le10_default.comm`

  ```
  DEBUT(LANG='EN')
  mesh = LIRE_MAILLAGE(UNITE=20, FORMAT='IDEAS')
  model = AFFE_MODELE(AFFE=_F(MODELISATION=('3D', ), PHENOMENE='MECANIQUE', TOUT='OUI'), MAILLAGE=mesh)

  mater = DEFI_MATERIAU(ELAS=_F(E=210000.0, NU=0.3))
  ```

```
fieldmat = AFFE_MATERIAU(AFFE=_F(MATER=(mater, ), TOUT='OUI'), MODELE=model)

load = AFFE_CHAR_MECA(DDL_IMPO=(_F(DY=0.0, GROUP_MA=('DCDC', )),
                                _F(DX=0.0, GROUP_MA=('ABAB', )),
                                _F(DX=0.0, DY=0.0, GROUP_MA=('BCBC', )),
                                _F(DZ=0.0, GROUP_MA=('midplane', ))),
                      MODELE=model,
                      PRES_REP=_F(GROUP_MA=('upper', ), PRES=1.0))

reslin = MECA_STATIQUE(CHAM_MATER=fieldmat, EXCIT=_F(CHARGE=load), MODELE=model)

reslin = CALC_CHAMP(reuse=reslin,
                    CONTRAINTE=('SIGM_ELGA', 'SIGM_ELNO', 'SIGM_NOEU', 'SIEF_ELGA', 'SIEF_ELNO', ' ↩
                        SIEF_NOEU'),
                    CRITERES=('SIEQ_ELGA', 'SIEQ_ELNO', 'SIEQ_NOEU'),
                    RESULTAT=reslin)

#IMPR_RESU(RESU=_F(RESULTAT=reslin), UNITE=80)

IMPR_RESU(
  FORMAT='RESULTAT',
  RESU=_F(
    GROUP_MA=('DD', ),
    IMPR_COOR='OUI',
    NOM_CHAM=('SIGM_NOEU', ),
    NOM_CMP=('SIYY'),
    RESULTAT=reslin
  ),
  UNITE=17
)

FIN()
```

- `le10_cholesky.comm`

```
DEBUT(LANG='EN')
mesh = LIRE_MAILLAGE(UNITE=20, FORMAT='IDEAS')
model = AFFE_MODELE(AFFE=_F(MODELISATION=('3D', ), PHENOMENE='MECANIQUE', TOUT='OUI'), MAILLAGE=mesh)

mater = DEFI_MATERIAU(ELAS=_F(E=210000.0, NU=0.3))
fieldmat = AFFE_MATERIAU(AFFE=_F(MATER=(mater, ), TOUT='OUI'), MODELE=model)

BC = AFFE_CHAR_CINE(MECA_IMPO=(_F(DY=0.0, GROUP_MA=('DCDC', )),
                                _F(DX=0.0, GROUP_MA=('ABAB', )),
                                _F(DX=0.0, DY=0.0, GROUP_MA=('BCBC', )),
                                _F(DZ=0.0, GROUP_MA=('midplane', ))),
                      MODELE=model,
                      )

load = AFFE_CHAR_MECA(
                      MODELE=model,
                      PRES_REP=_F(GROUP_MA=('upper', ), PRES=1.0))
```

```
reslin = MECA_STATIQUE(CHAM_MATER=fieldmat, EXCIT=(_F(CHARGE=BC),_F(CHARGE=load),), MODELE=model,
                       SOLVEUR=_F(METHODE='GCPC', PRE_COND='LDLT_INC'),
                       )

reslin = CALC_CHAMP(reuse=reslin,
                    CONTRAINTE=('SIGM_ELGA', 'SIGM_ELNO', 'SIGM_NOEU', 'SIEF_ELGA', 'SIEF_ELNO', ' ↩
                        SIEF_NOEU'),
                    CRITERES=('SIEQ_ELGA', 'SIEQ_ELNO', 'SIEQ_NOEU'),
                    RESULTAT=reslin)

#IMPR_RESU(RESU=_F(RESULTAT=reslin), UNITE=80)

IMPR_RESU(
  FORMAT='RESULTAT',
  RESU=_F(
    GROUP_MA=('DD', ),
    IMPR_COOR='OUI',
    NOM_CHAM=('SIGM_NOEU', ),
    NOM_CMP=('SIYY'),
    RESULTAT=reslin
  ),
  UNITE=17
)

FIN()
```

- `le10_mumps.comm`

```
DEBUT(LANG='EN')
mesh = LIRE_MAILLAGE(UNITE=20, FORMAT='IDEAS')
model = AFFE_MODELE(AFFE=_F(MODELISATION=('3D', ), PHENOMENE='MECANIQUE', TOUT='OUI'), MAILLAGE=mesh)

mater = DEFI_MATERIAU(ELAS=_F(E=210000.0, NU=0.3))
fieldmat = AFFE_MATERIAU(AFFE=_F(MATER=(mater, ), TOUT='OUI'), MODELE=model)

BC = AFFE_CHAR_CINE(MECA_IMPO=(_F(DY=0.0, GROUP_MA=('DCDC', )),
                               _F(DX=0.0, GROUP_MA=('ABAB', )),
                               _F(DX=0.0, DY=0.0, GROUP_MA=('BCBC', )),
                               _F(DZ=0.0, GROUP_MA=('midplane', ))),
                      MODELE=model,
                      )

load = AFFE_CHAR_MECA(
                      MODELE=model,
                      PRES_REP=_F(GROUP_MA=('upper', ), PRES=1.0))

reslin = MECA_STATIQUE(CHAM_MATER=fieldmat, EXCIT=(_F(CHARGE=BC),_F(CHARGE=load),), MODELE=model,  ↩
     SOLVEUR=_F(METHODE='MUMPS',))

reslin = CALC_CHAMP(reuse=reslin,
                    CONTRAINTE=('SIGM_ELGA', 'SIGM_ELNO', 'SIGM_NOEU', 'SIEF_ELGA', 'SIEF_ELNO', ' ↩
                        SIEF_NOEU'),
                    CRITERES=('SIEQ_ELGA', 'SIEQ_ELNO', 'SIEQ_NOEU'),
                    RESULTAT=reslin)

#IMPR_RESU(RESU=_F(RESULTAT=reslin), UNITE=80)

IMPR_RESU(
  FORMAT='RESULTAT',
  RESU=_F(
    GROUP_MA=('DD', ),
    IMPR_COOR='OUI',
    NOM_CHAM=('SIGM_NOEU', ),
    NOM_CMP=('SIYY'),
    RESULTAT=reslin
  ),
  UNITE=17
)

FIN()
```

To retrieve the stress at point D, instead of writing the full results into unit 80 (i.e. `le10-${m}.rmed`), only an ASCII file with nodal values of the stress tensor are written for those nodes that belong to the `DD` physical group (the D-D') segment in the original geometry. For some reason, Code Aster won't accept a zero-dimensional physical group (i.e. a point) to write the ASCII result. So the `run.sh` has to parse this ASCII file so as to find the row corresponding to point D and extract the value of σ_y, which is the fifth column:

```
grep "2.00000000000000E+03  0.00000000000000E+00  3.00000000000000E+02" DD-${m}-${c}.txt | awk ↩
    '{print $5}' >> aster_default_${m}-${c}.sigmay
```

The total number of degrees of freedom is taken from the "message" output (unit 6) by grepping the French expression for "degrees of freedom". Luckily UTF-8 works well:

```
grep "degrés de liberté:" message-${m}-${c}  | awk '{printf("%g\t", $7)}' > aster_default_${m}-${c}.sigmay
```

2.4 CalculiX

Thanks Sergio Pluchinsky for all the help to set up the inputs and the mesh files.

As explained below, I just followed his suggestions without understanding them. The way CalculiX input files work will remain unheard of to me for the time being.

The following paragraph explains what `run.sh` does (which is needlessly cumbersome IMHO) to make CalculiX work. It should be noted before the explanation starts that I had to modify the Gmsh UNV writer to handle both "groups of nodes" and "groups of elements" at the same time: https://gitlab.onelab.info/gmsh/gmsh/-/commit/a7fef9f6e8a7c870cf39b8702c57f3e33bfa948d. So make sure the Gmsh version used is later than that commit. Also, there is this `unical.c` conversion tool from UNV to INP that I initially borrowed from https://github.com/calculix/unical1 but had to modify to make it work. The code is included in the test directory and compiled when `run.sh` detects CalculiX is available. For large problems, this conversion procedure takes a non-trivial amount of time (i.e. more than five minutes) which is not accounted for in the resulting curves.

The second-order mesh `le10_2nd-${m}-${c}.msh` is converted to UNV with both options `SaveGroupsOfElements` and `SaveGroupsOfNodes` equal to true. Then, this UNV (which as already explained, needs a Gmsh version later than commit `a7fef9f6` from November 2021 otherwise the next step will fail if there are an odd number of nodes) is read by the slightly-modified tool `unical1` that creates a `.inp` mesh file which can be read by CalculiX:

```
if [ ! -e le10_mesh-${m}-${c}.inp ]; then
  gmsh -3 le10_2nd-${m}-${c}.msh -setnumber Mesh.SaveGroupsOfElements 1 -setnumber  ↩
       Mesh.SaveGroupsOfNodes 1 -o le10_calculix-${m}-${c}.unv || exit 1
  ./unical1 le10_calculix-${m}-${c}.unv le10_mesh-${m}-${c}.inp || exit
fi
```

The main input is a template that reads the appropriate `.inp` mesh file for c and sets successively the Spooles solver ("calculix_spooles"), the internal with diagonal scaling ("calculix_diagonal") and the internal with Cholesky preconditioning ("calculix_cholesky"). There is a reason I still cannot understand that explains why there has to be one template for `tet` and one for `hex`. In effect, Sergio pointed me to section that explains the `DLOAD` keyword (used to set a pressure boundary condition) in the `ccx` manual. It says (casing is verbatim):

> This option allows the specification of distributed loads. These include constant pressure loading on element faces, edge loading on shells and mass loading (load per unit mass) either by gravity forces or by centrifugal forces. For surface loading the faces of the elements are numbered as follows (for the node numbering of the elements see Section 3.1):
>
> for hexahedral elements:
>
> - face 1: 1-2-3-4
> - face 2: 5-8-7-6
> - face 3: 1-5-6-2
> - face 4: 2-6-7-3
> - face 5: 3-7-8-4
> - face 6: 4-8-5-1
>
> for tetrahedral elements:
>
> - Face 1: 1-2-3
> - Face 2: 1-4-2
> - Face 3: 2-4-3
> - Face 4: 3-4-1

So it seems that CalculiX needs some sort of mesh-dependent numbering of the faces of volumetric elements to set surface Neumann boundary conditions (!). This is why I had to blindly rely on Sergio's expertise to handle these `UPPERFn` and `Pn` lines within the `Dload` section below. In any case, the two templates for tets and hexes are, respectively:

- `le10-tet.inp`

  ```
  *include, input = le10_mesh-tet-xxx.inp
  *Material, Name=STEEL
  *Elastic
  200e3, 0.3
  *Solid section, Elset=C3D10, Material=STEEL
  ```

```
*Step
**Static, Solver=PaStiX
**Static, Solver=Pardiso
**Static, Solver=Spooles
**Static, Solver=Iterative scaling
**Static, Solver=Iterative Cholesky
*Boundary, Fixed
ABAB, 1, 1
DCDC, 2, 2
BCBC, 1, 2
MIDPLANE, 3, 3
*Dload
UPPERF1, P1, 1
UPPERF2, P2, 1
UPPERF3, P3, 1
UPPERF4, P4, 1
*Node file
RF, U
*El file
S, E
*End step
```

- `le10-hex.inp`

```
*include, input = le10_mesh-hex-xxx.inp
*Material, Name=STEEL
*Elastic
200e3, 0.3
*Solid section, Elset=C3D20, Material=STEEL
*Step
**Static, Solver=PaStiX
**Static, Solver=Pardiso
**Static, Solver=Spooles
**Static, Solver=Iterative scaling
**Static, Solver=Iterative Cholesky
*Boundary, Fixed
ABAB, 1, 1
DCDC, 2, 2
BCBC, 1, 2
MIDPLANE, 3, 3
*Dload
UPPERF6, P6, 1
*Node file
RF, U
*El file
S, E
*End step
```

These templates are filtered with `sed` that replaces `xxx` with the appropriate mesh and un-comments each of the solver lines successively to have a working input file:

```
sed s/xxx/${c}/ le10-${m}.inp | sed 's/**Static, Solver=Spooles/*Static, Solver=Spooles/' > ⮐
    le10_spooles_${m}-${c}.inp
```

To read the stress at point D, an `awk` file that parses the output `.frd` file and searches for the nodal values of the stress tensor based on the coordinates of the point D had to be written. It has to take into account that this `.frd` file does not have blank-separated fields but fixed-width ASCII columns, such as

```
 -1       371-1.52894E+00 1.19627E+00-5.85388E-02-8.97020E-03 1.73081E-03 7.02901E-01
```

where negative values appear concatenated with the previous one as a single ASCII token in a non-UNIX-friendly way.

```
#!/usr/bin/gawk
{
  # this only works for all-positive coordinates, otherwise we would have to use substr()
  if ($3 == "2.00000E+03" && $4 = "0.00000E+00" && $5 == "3.00000E+02")
  {
    node = $2
  }


  if ($1 == -4 && $2 == "STRESS") {
    stresses = 1
  }

  if (node != 0 && stresses == 1 && found == 0) {
    if (strtonum(substr($0,4,10)) == node) {
      printf("%e\t", substr($0, 26, 12))
      found = 1
    }
  }
}
```

The total number of degrees of freedom is read from the standard output grepping for "number of equations":

```
        grep -C 1 "number of equations" calculix_spooles_${m}-${c}.txt | tail -n 1 | awk '{printf("%d\t",  ↩
            $1)}' > calculix_spooles_${m}-${c}.sigmay
```

3 Setting up the codes

3.1 Gmsh

Both the continuous geometry and the discretized meshes are created with Gmsh. The `run.sh` script will not run if `gmsh` is not a valid command.

It is better to use latest versions instead of the one distributed in the operating system's package repositories. In fact, to run the CalculiX test, version 4.9 or later is needed. Either the official binaries or a compiled-from-scratch version will do.

The no-X binary version can be used. To download and copy it to a system-wide location do:

```
wget http://gmsh.info/bin/Linux/gmsh-nox-git-Linux64-sdk.tgz
tar xvzf gmsh-nox-git-Linux64-sdk.tgz
sudo cp gmsh-nox-git-Linux64-sdk/bin/gmsh /usr/local/bin
sudo cp -P gmsh-nox-git-Linux64-sdk/lib/* /usr/local/lib
```

Alternatively, it can be compile from source (OpenCASCADE is needed to create the LE10's CAD):

```
sudo apt-get install libocct-data-exchange-dev libocct-foundation-dev libocct-modeling-data-dev
git clone https://gitlab.onelab.info/gmsh/gmsh.git
cd gmsh
mkdir build && cd build
cmake ..
make
sudo make install
```

Check it works globally:

```
$ gmsh -info
Version       : 4.9.0-nox-git-701db57af
License       : GNU General Public License
Build OS      : Linux64-sdk
Build date    : 20211019
Build host    : gmsh.info
Build options : 64Bit ALGLIB ANN Bamg Blas[petsc] Blossom Cgns DIntegration Dlopen DomHex Eigen Gmm Hxt  ↩
     Kbipack Lapack[petsc] LinuxJoystick MathEx Med Mesh Metis Mmg Netgen ONELAB ONELABMetamodel OpenCASCADE ↩
      OpenMP OptHom PETSc Parser Plugins Post QuadMeshingTools QuadTri Solver TetGen/BR Voro++  ↩
     WinslowUntangler Zlib
PETSc version : 3.14.4 (real arithmtic)
OCC version   : 7.6.0
MED version   : 4.1.0
Packaged by   : geuzaine
Web site      : https://gmsh.info
Issue tracker : https://gitlab.onelab.info/gmsh/gmsh/issues
$
```

3.2 FeenoX

Not only is FeenoX the docus of the current test, but it also is used to compute the quasi-random sequence of mesh refinements factors c. So it is mandatory to have a working `feenox` command.

The easiest way to set up FeenoX is to download, un-compress and copy a statically-linked binary to a system-wide location:

```
wget https://seamplex.com/feenox/dist/linux/feenox-v0.1.152-g8329396-linux-amd64.tar.gz
tar xvzf feenox-v0.1.152-g8329396-linux-amd64.tar.gz
sudo cp feenox-v0.1.152-g8329396-linux-amd64/bin/feenox /usr/local/bin
```

Instead, it can be compiled from the Github repository using stack PETSc from `apt` (which might be considered "old" in some GNU/Linux distributions). This will also enable the MUMPS solver (so an the extra curve named "feenox_mumps" will be added to the results):

```
sudo apt-get install gcc make git automake autoconf libgsl-dev petsc-dev slepc-dev
git clone https://github.com/seamplex/feenox
cd feenox
./autogen.sh
./configure
```

```
make
make check
sudo make install
```

Custom PETSc versions and architectures are supported as well. The default preconditioner+solver pair gamg+cg is supported with all PETSc configurations. To make the MUMPS direct solver available, PETSc has to be configured and linked properly (i.e. configure with `--download-mumps` or use the PETSc packages from the operating system's repositories). See the compilation guide for further details.

Either way, check it works globally:

```
$ feenox -V
FeenoX v0.1.159-gab7abd8-dirty
a free no-fee no-X uniX-like finite-element(ish) computational engineering tool

Last commit date   : Thu Oct 28 10:43:38 2021 -0300
Build date         : Thu Oct 28 13:52:11 2021 +0000
Build architecture : linux-gnu x86_64
Compiler           : gcc (Ubuntu 9.3.0-17ubuntu1~20.04) 9.3.0
Compiler flags     : -O3
Builder            : ubuntu@ip-172-31-44-208
GSL version        : 2.5
SUNDIALS version   : 3.1.2
PETSc version      : Petsc Release Version 3.12.4, Feb, 04, 2020
PETSc arch         :
PETSc options      : --build=x86_64-linux-gnu --prefix=/usr --includedir=${prefix}/include --mandir=${prefix ↩
    }/share/man --infodir=${prefix}/share/info --sysconfdir=/etc --localstatedir=/var --with-silent-rules=0 ↩
     --libdir=${prefix}/lib/x86_64-linux-gnu --runstatedir=/run --with-maintainer-mode=0 --with-dependency- ↩
    tracking=0 --with-debugging=0 --shared-library-extension=_real --with-shared-libraries --with-pic=1 -- ↩
    with-cc=mpicc --with-cxx=mpicxx --with-fc=mpif90 --with-cxx-dialect=C++11 --with-opencl=1 --with-blas- ↩
    lib=-lblas --with-lapack-lib=-llapack --with-scalapack=1 --with-scalapack-lib=-lscalapack-openmpi -- ↩
    with-mumps=1 --with-mumps-include="[]" --with-mumps-lib="-ldmumps -lzmumps -lsmumps -lcmumps - ↩
    lmumps_common -lpord" --with-suitesparse=1 --with-suitesparse-include=/usr/include/suitesparse --with- ↩
    suitesparse-lib="-lumfpack -lamd -lcholmod -lklu" --with-ptscotch=1 --with-ptscotch-include=/usr/ ↩
    include/scotch --with-ptscotch-lib="-lptesmumps -lptscotch -lptscotcherr" --with-fftw=1 --with-fftw- ↩
    include="[]" --with-fftw-lib="-lfftw3 -lfftw3_mpi" --with-superlu=1 --with-superlu-include=/usr/include ↩
    /superlu --with-superlu-lib=-lsuperlu --with-superlu_dist=1 --with-superlu_dist-include=/usr/include/ ↩
    superlu-dist --with-superlu_dist-lib=-lsuperlu_dist --with-hdf5-include=/usr/include/hdf5/openmpi -- ↩
    with-hdf5-lib="-L/usr/lib/x86_64-linux-gnu/hdf5/openmpi -L/usr/lib/openmpi/lib -lhdf5 -lmpi" -- ↩
    CXX_LINKER_FLAGS=-Wl,--no-as-needed --with-hypre=1 --with-hypre-include=/usr/include/hypre --with-hypre ↩
    -lib=-lHYPRE_core --prefix=/usr/lib/petscdir/petsc3.12/x86_64-linux-gnu-real --PETSC_ARCH=x86_64-linux- ↩
    gnu-real CFLAGS="-g -O2 -fstack-protector-strong -Wformat -Werror=format-security -fPIC" CXXFLAGS="-g - ↩
    O2 -fstack-protector-strong -Wformat -Werror=format-security -fPIC" FCFLAGS="-g -O2 -fstack-protector- ↩
    strong -fPIC -ffree-line-length-0" FFLAGS="-g -O2 -fstack-protector-strong -fPIC -ffree-line-length-0" ↩
    CPPFLAGS="-Wdate-time -D_FORTIFY_SOURCE=2" LDFLAGS="-Wl,-Bsymbolic-functions -Wl,-z,relro -fPIC" ↩
    MAKEFLAGS=w
SLEPc version      : SLEPc Release Version 3.12.2, Jan 13, 2020
$
```

The `PETSc options` line will tell if MUMPS is available or not, so grepping will tell:

```
$ feenox -V | grep -i mumps | wc -l
```

```
1
$
```

3.3 Sparselizard

In order to test Sparselizard, a sub-directory named `sparselizard` should exist in the directory where `run.sh` is, and an executable named `sparselizard` should exist in that sub-directory.

This can be achieved by cloning and compiling the Github repository. It needs a particularly-configured PETSc/SLEPc version, which can be obtained by executing the `install_external_libs/install_petsc.sh` script (which pulls latest PETSc main from the Gitlab repository, configures and compiles it). Also, the Gmsh API is needed to read `.msh` v4, so run `install_external_libsoptional_install_gmsh_api.sh` as well. The `main.cpp` is the file `le10.cpp` provided in the `le10-aster-lizard` directory. Therefore, a symbolic link has to be added in the `sparselizard` directory to point `main.cpp` to `../le10.cpp`:

```
cd feenox/tests/nafems/le10-aster-lizard
git clone https://github.com/halbux/sparselizard/
cd sparselizard/
ln -s ../le10.cpp main.cpp
cd install_external_libs/
./install_petsc.sh
./optional_install_gmsh_api.sh
cd ..
make
cd ..
```

3.4 Code Aster

Code Aster is tricky to compile (and use, at least for me). The following works (only) in Ubuntu 20.04:

```
wget https://www.code-aster.org/FICHIERS/aster-full-src-14.6.0-1.noarch.tar.gz
tar xvzf aster-full-src-14.6.0-1.noarch.tar.gz
cd aster-full-src-14.6.0
mkdir -p $HOME/aster
python3 setup.py --aster_root=$HOME/aster
cd
source aster/etc/codeaster/profile.sh
```

Check it does work globally:

```
$ as_run --getversion
<INFO> Version exploitation 14.6.0 - 11/06/2020 - rev. b3490fa3b76c
$
```

Note that compilation from the repository fails in Debian 11 with gcc10:

```
$ sudo apt-get install mercurial
$ sudo apt-get install gcc g++ gfortran cmake python3 python3-dev python3-numpy tk bison flex dh-exec
$ sudo apt-get install liblapack-dev libblas-dev libboost-python-dev libboost-numpy-dev zlib1g-dev
$ hg clone http://hg.code.sf.net/p/codeaster/src codeaster-src
$ cd codeaster-src
$ ./waf configure
$ ./waf build
checking environment... executing: ./waf.engine build --out=build/std --jobs=4
Waf: Entering directory `/home/gtheler/codigos/3ros/codeaster-src/build/std/release'
[1521/8549] Processing bibfor/echange/lub_module.F90
[2174/8549] Compiling bibfor/prepost/cmqlql.F90
[2175/8549] Compiling bibfor/prepost/cmhho.F90
[2177/8549] Compiling bibfor/prepost/cm1518.F90
[4370/8549] Compiling bibfor/algorith/dtmprep_noli_lub.F90
[6623/8549] Compiling bibfor/algorith/dtmclean_noli_yacs.F90
[7258/8549] Compiling bibcxx/Utilities/GenericParameter.cxx
[7259/8549] Compiling bibcxx/Utilities/CppToFortranGlossary.cxx
[7260/8549] Compiling bibcxx/Utilities/ConvertibleValue.cxx
[7263/8549] Compiling bibcxx/PythonBindings/LoadResultInterface.cxx
In file included from ../../../bibcxx/Utilities/ConvertibleValue.cxx:24:
../../../bibcxx/Utilities/ConvertibleValue.h: In member function ‘const ReturnValue& ConvertibleValue< ↩
     ValueType1, ValueType2>::getValue() ’const:
../../../bibcxx/Utilities/ConvertibleValue.h:69:24: error: ‘’runtime_error is not a member of ‘’std
   69 |             throw std::runtime_error( "Impossible to convert " + _valToConvert );
      |                        ^~~~~~~~~~~~~

In file included from /usr/include/boost/smart_ptr/detail/sp_thread_sleep.hpp:22,
                 from /usr/include/boost/smart_ptr/detail/yield_k.hpp:23,
                 from /usr/include/boost/smart_ptr/detail/spinlock_gcc_atomic.hpp:14,
                 from /usr/include/boost/smart_ptr/detail/spinlock.hpp:42,
                 from /usr/include/boost/smart_ptr/detail/spinlock_pool.hpp:25,
                 from /usr/include/boost/smart_ptr/shared_ptr.hpp:29,
                 from /usr/include/boost/shared_ptr.hpp:17,
                 from ../../../bibcxx/include/astercxx.h:37,
                 from ../../../bibcxx/PythonBindings/LoadResultInterface.h:27,
                 from ../../../bibcxx/PythonBindings/LoadResultInterface.cxx:24:
/usr/include/boost/bind.hpp:36:1: note: ‘#pragma message: The practice of declaring the Bind placeholders ( ↩
     _1, _2, ...) in the global namespace is deprecated. Please use <boost/bind/bind.hpp> + using namespace  ↩
     boost::placeholders, or define BOOST_BIND_GLOBAL_PLACEHOLDERS to retain the current behavior’.
   36 | BOOST_PRAGMA_MESSAGE(
      | ^~~~~~~~~~~~~~~~~~~~
/usr/include/boost/detail/iterator.hpp:13:1: note: ‘#pragma message: This header is deprecated. Use < ↩
     iterator> instead’.
   13 | BOOST_HEADER_DEPRECATED("<iterator>")
      | ^~~~~~~~~~~~~~~~~~~~~~~

Waf: Leaving directory `/home/gtheler/codigos/3ros/codeaster-src/build/std/release'
Build failed
 -> task in 'asterbibcxx' failed with exit status 1 (run with -v to display more information)
$
```

3.5 CalculiX

Thanks Sergio Pluchinsky for all the help to set up the inputs and the mesh files.

CalculiX is available at Debian/Ubuntu repositories, although the versions are not up to date and they only have the Spooles solver and the internal iterative solver with either diagonal or Cholesky preconditioning.

There are sources which come with an already-working makefile (i.e. the don't need configuration). Sadly, the official sources won't compile (and throw millions of warnings) in Debian 11 with gcc10:

```
$ wget http://www.dhondt.de/ccx_2.18.src.tar.bz2
$ tar xf ccx_2.18.src.tar.bz2
$ cd CalculiX/ccx_2.18/src/
$ make
[...]
   21 |      &     nodef,idirf,df,cp,r,physcon,numf,set,mi,ider,ttime,time,
      |                                                             1
Warning: Unused dummy argument ‘’ttime at (1) [-Wunused-dummy-argument]
cross_split.f:101:72:

  101 |      &           *(1.d0-pt2pt1**(1.d0/kdkm1))/r)/dsqrt(Tt1)
      |                                                                        ^
Warning: ‘’a may be used uninitialized in this function [-Wmaybe-uninitialized]
gfortran -Wall -O2 -c cubic.f
gfortran -Wall -O2 -c cubtri.f
cubtri.f:131:18:

  131 |       CALL CUBRUL(F, VEC, W(1,1), IDATA, RDATA)
      |                  1
Error: Interface mismatch in dummy procedure ‘’f at (1): 'f' is not a function
cubtri.f:170:20:

  170 |         CALL CUBRUL(F, VEC, W(1,J), IDATA, RDATA)
      |                    1
Error: Interface mismatch in dummy procedure ‘’f at (1): 'f' is not a function
make: *** [Makefile:11: cubtri.o] Error 1
$
```

So we are sticking with the binaries from the `apt` repository and the default Spooles and internal solvers.