



Debian for Simulation and Numerical Modeling

Applications to High Magnetic Field Magnets Design

C. Daversin¹, C. Prudhomme², C. Trophime¹ and S. Veys²

¹ Laboratoire National des Champs Magnétiques Intenses, Grenoble

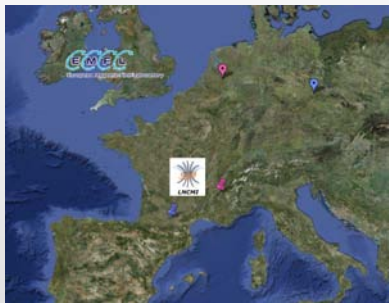
² Laboratoire Jean Kuntzmann, Grenoble





United States

- Thallahassee (FL)
- Los Alamos (NM)
- Gainesville (FL)



Europe

- Grenoble / Toulouse
- Nijmegen (Netherlands)
- Dresden (Germany)



Asia

- Tsukuba (Japan)
- Sendai (Japan)
- Hefei (China)
- Wuhan (China)



LNCMI a User Facility run by the CNRS

Pulsed field installation TOULOUSE : 14 MJ, 24 kV, 1 GW, 80 Tesla



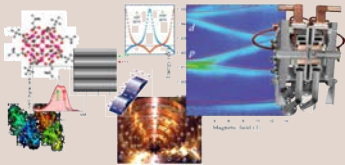
Continuous field installation GRENOBLE : 24 MW, 35 Tesla





Research

- Condensed matter
- Chemistry and Biochemistry
- Applied Superconductivity
- MagnetoSciences
- Magnet development
- Instrumentation under B



Facilities (10000 hours / year)

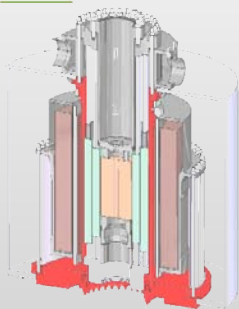
- High Pressure
- EPR, NMR
- Lasers
- Low Temp. : down to 20 mK
- High Temp : up to 1600 Å°C

Access

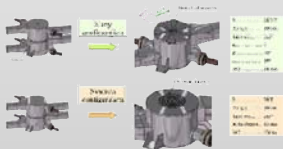
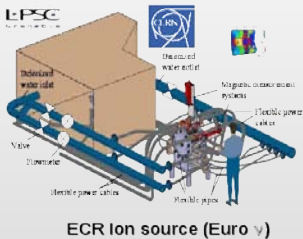
- Call for Magnet Time / 2 x year
- 140 projects / year



Projets



Hybrid Magnet : 43 T

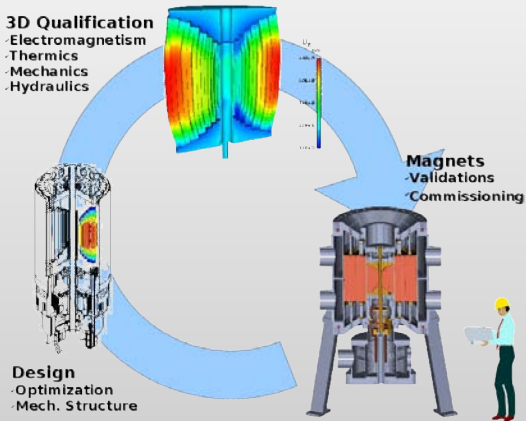


Scattering under Magnetic Field





From Design to Commissioning





High Field Magnet Design

Challenges

- Multiphysics Modeling,
- Non-Linearities and Coupling,
- Complex geometries,
- Optimization

Needs

- 3D Numerical Modeling,
- Fast and reliable methods,
- Control Quantity of Interest (B , $\langle T \rangle$, stress, ...),
- Uncertainties quantifications



Our choice

- Use open source software (“state-of-the-art”),
- Use Linux as a platform for development and computation,
- Need for HPC (from meso centers to national centers).

First attempts

- Use of RedHat/Fedora,
- Few Libraries/Software for numerical modeling,
- (Re)build packages for used/tested software,
- Difficult to get new packages into distribution,
- Difficult System Upgrade.



Why Debian ?

Debian

- Large choice of software/libraries for numerical modeling in Debian,
- Easier to get new packages into distribution,
- Easier system upgrade.
- Bring full programming and runtime environments for science in minutes

Debian for Numerical Modeling and Simulation

- Debian Scientific Computing Project (scicomp) (C. Prudhomme et al.),
- Debian Science (S. Ledru et al.),
- Most scicomp packages have now been merged into Debian science



Debian - A Large offer

General Finite Element Analysis (FEA)

- General Finite Element Analysis (FEA),
- Numerical libraries,
- Pre- and post-processing frameworks and tools

See

- <http://pkg-scicomp.alioth.debian.org/>
- <http://wiki.debian.org/DebianScience>



Debian - HPC ressources

CIMENT meso center (Grenoble)

- 3000 cores (> 5000 in 2013),
- 40 % using Debian,
- Storage grid running Debian.



Grid5000 (Grenoble)

- Heavy Debian user (services and grid nodes)



National(/European) facilities

- Rely unfortunately on poor programming environments : eventually requires compiling down to the compilers, often requires to recompile the numerical libraries stack when one uses modern software
- Suggest Debian@Genci and Debian@Prace



Debian - HPC Ressources

Active development of HPC SysAdmin in Grenoble

- OAR batch scheduler administration tools package
- Taktuk efficient, large scale, parallel remote execution of commands,
- CiGri grid manager tool (to be packaged)
- Xkaapi Lib for parallel programming targeting Hybride archs (CPUs/GPUs)

Contributors (imag.fr)

- CIMENT / CiGri : Bruno.Beznik
- Grid5000 : Pierre.Neyron
- OAR : Olivier.Richard
- Taktuk : Guillaume.Huard
- Parrain debian : Vincent.Danjean
- DD Philippe.Le-Brouster
- Xkaapi : Thierry.Gautier



Debian - How to contribute ?

How and why I became a DM ?

- Use/test some new libraries / software
- (Re)build / Update the packages (eg : gmsh, mumps, petsc, ...)
- Capitalize my efforts by submitting the package (eg : getdp)

The screenshot shows the Debian Package Tracker (DPT) interface. It displays several sections:

- main (7)**: A table listing packages in the main repository. The table has columns for Source Name, Build, Version, Architecture, Size, Milestone, Architecture, Distribution, and Status. Packages listed include 'xapc', 'xfig', 'xfig2pdf', 'xfig2ps', 'xfig2ps2', 'xfig2ps3', 'xfig2ps4', 'xfig2ps5', 'xfig2ps6', 'xfig2ps7', 'xfig2ps8', 'xfig2ps9', 'xfig2ps10', 'xfig2ps11', 'xfig2ps12', 'xfig2ps13', 'xfig2ps14', 'xfig2ps15', 'xfig2ps16', 'xfig2ps17', 'xfig2ps18', 'xfig2ps19', 'xfig2ps20', 'xfig2ps21', 'xfig2ps22', 'xfig2ps23', 'xfig2ps24', 'xfig2ps25', 'xfig2ps26', 'xfig2ps27', 'xfig2ps28', 'xfig2ps29', 'xfig2ps30', 'xfig2ps31', 'xfig2ps32', 'xfig2ps33', 'xfig2ps34', 'xfig2ps35', 'xfig2ps36', 'xfig2ps37', 'xfig2ps38', 'xfig2ps39', 'xfig2ps40', 'xfig2ps41', 'xfig2ps42', 'xfig2ps43', 'xfig2ps44', 'xfig2ps45', 'xfig2ps46', 'xfig2ps47', 'xfig2ps48', 'xfig2ps49', 'xfig2ps50', 'xfig2ps51', 'xfig2ps52', 'xfig2ps53', 'xfig2ps54', 'xfig2ps55', 'xfig2ps56', 'xfig2ps57', 'xfig2ps58', 'xfig2ps59', 'xfig2ps60', 'xfig2ps61', 'xfig2ps62', 'xfig2ps63', 'xfig2ps64', 'xfig2ps65', 'xfig2ps66', 'xfig2ps67', 'xfig2ps68', 'xfig2ps69', 'xfig2ps70', 'xfig2ps71', 'xfig2ps72', 'xfig2ps73', 'xfig2ps74', 'xfig2ps75', 'xfig2ps76', 'xfig2ps77', 'xfig2ps78', 'xfig2ps79', 'xfig2ps80', 'xfig2ps81', 'xfig2ps82', 'xfig2ps83', 'xfig2ps84', 'xfig2ps85', 'xfig2ps86', 'xfig2ps87', 'xfig2ps88', 'xfig2ps89', 'xfig2ps90', 'xfig2ps91', 'xfig2ps92', 'xfig2ps93', 'xfig2ps94', 'xfig2ps95', 'xfig2ps96', 'xfig2ps97', 'xfig2ps98', 'xfig2ps99', 'xfig2ps100'.
- non-free (1)**: A table listing packages in the non-free repository. The table has columns for Source Name, Build, Version, Architecture, Size, Milestone, Architecture, Distribution, and Status. Packages listed include 'xapc', 'xfig', 'xfig2pdf', 'xfig2ps', 'xfig2ps2', 'xfig2ps3', 'xfig2ps4', 'xfig2ps5', 'xfig2ps6', 'xfig2ps7', 'xfig2ps8', 'xfig2ps9', 'xfig2ps10', 'xfig2ps11', 'xfig2ps12', 'xfig2ps13', 'xfig2ps14', 'xfig2ps15', 'xfig2ps16', 'xfig2ps17', 'xfig2ps18', 'xfig2ps19', 'xfig2ps20', 'xfig2ps21', 'xfig2ps22', 'xfig2ps23', 'xfig2ps24', 'xfig2ps25', 'xfig2ps26', 'xfig2ps27', 'xfig2ps28', 'xfig2ps29', 'xfig2ps30', 'xfig2ps31', 'xfig2ps32', 'xfig2ps33', 'xfig2ps34', 'xfig2ps35', 'xfig2ps36', 'xfig2ps37', 'xfig2ps38', 'xfig2ps39', 'xfig2ps40', 'xfig2ps41', 'xfig2ps42', 'xfig2ps43', 'xfig2ps44', 'xfig2ps45', 'xfig2ps46', 'xfig2ps47', 'xfig2ps48', 'xfig2ps49', 'xfig2ps50', 'xfig2ps51', 'xfig2ps52', 'xfig2ps53', 'xfig2ps54', 'xfig2ps55', 'xfig2ps56', 'xfig2ps57', 'xfig2ps58', 'xfig2ps59', 'xfig2ps60', 'xfig2ps61', 'xfig2ps62', 'xfig2ps63', 'xfig2ps64', 'xfig2ps65', 'xfig2ps66', 'xfig2ps67', 'xfig2ps68', 'xfig2ps69', 'xfig2ps70', 'xfig2ps71', 'xfig2ps72', 'xfig2ps73', 'xfig2ps74', 'xfig2ps75', 'xfig2ps76', 'xfig2ps77', 'xfig2ps78', 'xfig2ps79', 'xfig2ps80', 'xfig2ps81', 'xfig2ps82', 'xfig2ps83', 'xfig2ps84', 'xfig2ps85', 'xfig2ps86', 'xfig2ps87', 'xfig2ps88', 'xfig2ps89', 'xfig2ps90', 'xfig2ps91', 'xfig2ps92', 'xfig2ps93', 'xfig2ps94', 'xfig2ps95', 'xfig2ps96', 'xfig2ps97', 'xfig2ps98', 'xfig2ps99', 'xfig2ps100'.
- Pending uploads (1)**: A table listing packages that are pending uploads. The table has columns for Source Name, Build, Version, Architecture, Size, Milestone, Architecture, Distribution, and Status. Packages listed include 'xapc', 'xfig', 'xfig2pdf', 'xfig2ps', 'xfig2ps2', 'xfig2ps3', 'xfig2ps4', 'xfig2ps5', 'xfig2ps6', 'xfig2ps7', 'xfig2ps8', 'xfig2ps9', 'xfig2ps10', 'xfig2ps11', 'xfig2ps12', 'xfig2ps13', 'xfig2ps14', 'xfig2ps15', 'xfig2ps16', 'xfig2ps17', 'xfig2ps18', 'xfig2ps19', 'xfig2ps20', 'xfig2ps21', 'xfig2ps22', 'xfig2ps23', 'xfig2ps24', 'xfig2ps25', 'xfig2ps26', 'xfig2ps27', 'xfig2ps28', 'xfig2ps29', 'xfig2ps30', 'xfig2ps31', 'xfig2ps32', 'xfig2ps33', 'xfig2ps34', 'xfig2ps35', 'xfig2ps36', 'xfig2ps37', 'xfig2ps38', 'xfig2ps39', 'xfig2ps40', 'xfig2ps41', 'xfig2ps42', 'xfig2ps43', 'xfig2ps44', 'xfig2ps45', 'xfig2ps46', 'xfig2ps47', 'xfig2ps48', 'xfig2ps49', 'xfig2ps50', 'xfig2ps51', 'xfig2ps52', 'xfig2ps53', 'xfig2ps54', 'xfig2ps55', 'xfig2ps56', 'xfig2ps57', 'xfig2ps58', 'xfig2ps59', 'xfig2ps60', 'xfig2ps61', 'xfig2ps62', 'xfig2ps63', 'xfig2ps64', 'xfig2ps65', 'xfig2ps66', 'xfig2ps67', 'xfig2ps68', 'xfig2ps69', 'xfig2ps70', 'xfig2ps71', 'xfig2ps72', 'xfig2ps73', 'xfig2ps74', 'xfig2ps75', 'xfig2ps76', 'xfig2ps77', 'xfig2ps78', 'xfig2ps79', 'xfig2ps80', 'xfig2ps81', 'xfig2ps82', 'xfig2ps83', 'xfig2ps84', 'xfig2ps85', 'xfig2ps86', 'xfig2ps87', 'xfig2ps88', 'xfig2ps89', 'xfig2ps90', 'xfig2ps91', 'xfig2ps92', 'xfig2ps93', 'xfig2ps94', 'xfig2ps95', 'xfig2ps96', 'xfig2ps97', 'xfig2ps98', 'xfig2ps99', 'xfig2ps100'.
- Owned WPP bugs (6)**: A table listing bugs owned by the user. The table has columns for Bug ID, Package, Version, and Status. Bugs listed include 'xapc', 'xfig', 'xfig2pdf', 'xfig2ps', 'xfig2ps2', 'xfig2ps3', 'xfig2ps4', 'xfig2ps5', 'xfig2ps6', 'xfig2ps7', 'xfig2ps8', 'xfig2ps9', 'xfig2ps10', 'xfig2ps11', 'xfig2ps12', 'xfig2ps13', 'xfig2ps14', 'xfig2ps15', 'xfig2ps16', 'xfig2ps17', 'xfig2ps18', 'xfig2ps19', 'xfig2ps20', 'xfig2ps21', 'xfig2ps22', 'xfig2ps23', 'xfig2ps24', 'xfig2ps25', 'xfig2ps26', 'xfig2ps27', 'xfig2ps28', 'xfig2ps29', 'xfig2ps30', 'xfig2ps31', 'xfig2ps32', 'xfig2ps33', 'xfig2ps34', 'xfig2ps35', 'xfig2ps36', 'xfig2ps37', 'xfig2ps38', 'xfig2ps39', 'xfig2ps40', 'xfig2ps41', 'xfig2ps42', 'xfig2ps43', 'xfig2ps44', 'xfig2ps45', 'xfig2ps46', 'xfig2ps47', 'xfig2ps48', 'xfig2ps49', 'xfig2ps50', 'xfig2ps51', 'xfig2ps52', 'xfig2ps53', 'xfig2ps54', 'xfig2ps55', 'xfig2ps56', 'xfig2ps57', 'xfig2ps58', 'xfig2ps59', 'xfig2ps60', 'xfig2ps61', 'xfig2ps62', 'xfig2ps63', 'xfig2ps64', 'xfig2ps65', 'xfig2ps66', 'xfig2ps67', 'xfig2ps68', 'xfig2ps69', 'xfig2ps70', 'xfig2ps71', 'xfig2ps72', 'xfig2ps73', 'xfig2ps74', 'xfig2ps75', 'xfig2ps76', 'xfig2ps77', 'xfig2ps78', 'xfig2ps79', 'xfig2ps80', 'xfig2ps81', 'xfig2ps82', 'xfig2ps83', 'xfig2ps84', 'xfig2ps85', 'xfig2ps86', 'xfig2ps87', 'xfig2ps88', 'xfig2ps89', 'xfig2ps90', 'xfig2ps91', 'xfig2ps92', 'xfig2ps93', 'xfig2ps94', 'xfig2ps95', 'xfig2ps96', 'xfig2ps97', 'xfig2ps98', 'xfig2ps99', 'xfig2ps100'.



Debian - How to contribute ?

My experiences / advices

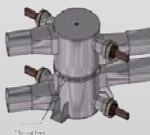
- Try to package libraries / software,
- Upload your work into Debian Science svn/git,
- Fill Bug reports, Provide patches,
- Share your work,
- Simple, Save time, May help other,
- Benefits



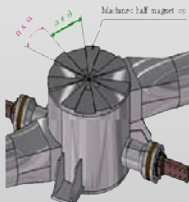
Magnet Development for ESRF



Started with « ESRF Up » FP7



X-ray configuration

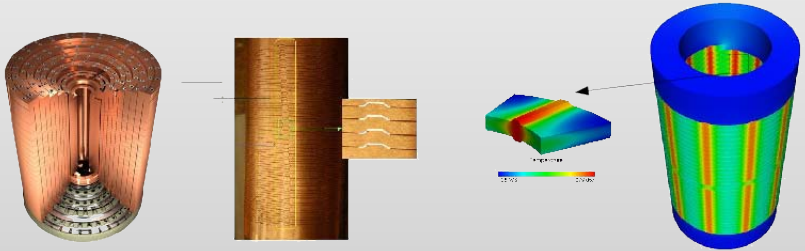


B	28.8 T
Air gap	10 mm
Take off	2x3°
n	7
δ	56°
α	15°
WB	34 mm



High Field Split Magnet Design

- Radially cooled helices insert,
- Temperature within each helices,
- Huge attraction forces.





Thermo-Electrical model and Field calculation with gmsh/getdp

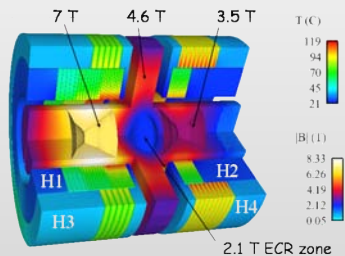
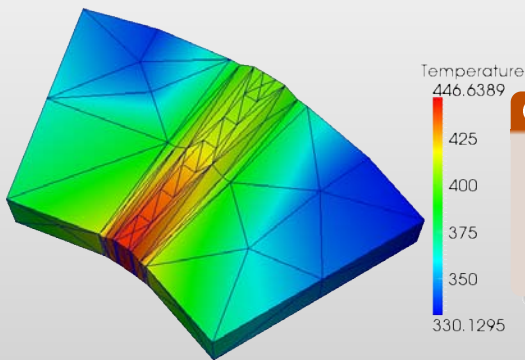


Figure: Initial mesh



Anisotropic mesh Adaption with Feel++ and Gmsh



Control Interpolation error

- Estimate of Hessian (based on grad recovery tech.)
- Hessian-based metric adapt. Control length of mesh edges

Figure: Initial mesh



Anisotropic mesh Adaption with Feel++ and Gmsh

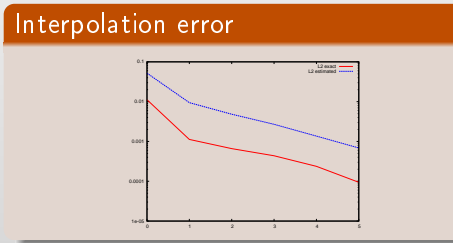
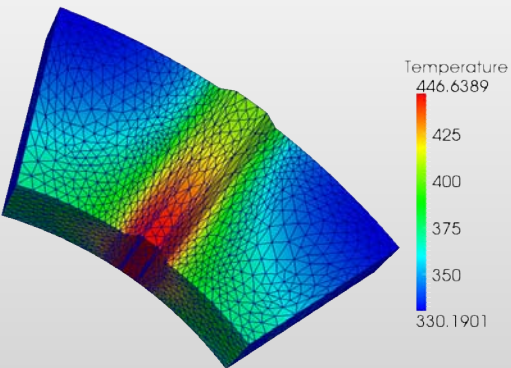


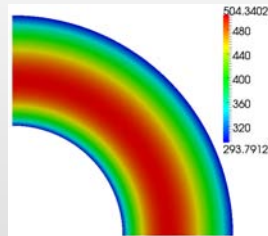
Figure: 3rd iteration



Model order reduction with Feel++ and OpenTurns

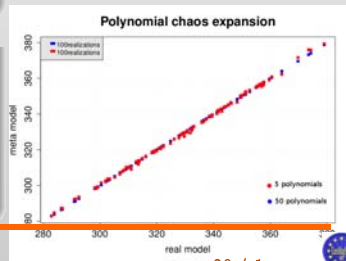
Approximations

- FEM :
 - Dimension of FEM space : 2 312 (P1)
 - NL iterations ≈ 20 (rel. tol 10^{-8})
- RB :
 - Dimension of RB space : 40
 - NL iterations ≈ 20 (rel. tol 10^{-8})
 - EIM terms ≈ 40 (rel. tol 10^{-10})



Meta model

- $Y = F(X)$
 - X and Y are stochastic variables
 - X follows uniform distribution
 - use polynomial chaos expansion





Sobol indices and quantiles with Openturns

Parameters range

- $\sigma_0 \in [...]$
- $k_0 \in [...]$
- $V_D \in [0.05, 0.2](V)$
- $h \in [6.10^4, 9.10^4](W.m^{-2}.K^{-1})$
- $T_w \in [273, 323](K)$

Mean, Standard deviation

```
-- Mean = [328.473]  
-- Standard deviation = 22.0728297966
```

Sobol indices

```
...  
-- Sobol 4 = 0.633300283167 ( $V_D$ )  
-- Sobol 5 = 1.76545493422e-05  
-- Sobol 6 = 0.362812453403 ( $T_w$ )
```

Quantiles

Determine a threshold $q(\gamma)$ such that $P(Y_i < q(\gamma)) > \gamma$

99.0 -quantile = [374.123]

80.0 -quantile = [354.55]



Conclusions and Perspectives

From Debian view point

- Add specific packages to Debian
- Contribute to packaging efforts (code-aster)
- Enlarge offer for Engineering and Design

From a scientific view point

- Improve our numerical model (error control, uncertainty quantification)
- Apply model reductions to our problem,
- Include more physics
- More complex geometries (from a complete helix to an insert)