Debian for Simulation and Numerical Modeling

Applications to High Magnetic Field Magnets Design

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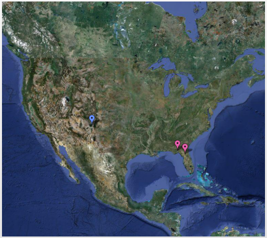
[2] Laboratoire Jean Kuntzmann, Grenoble

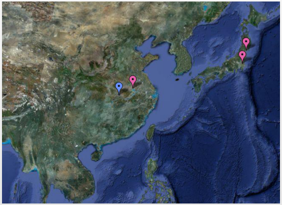


United States

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

Europe

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



Asia

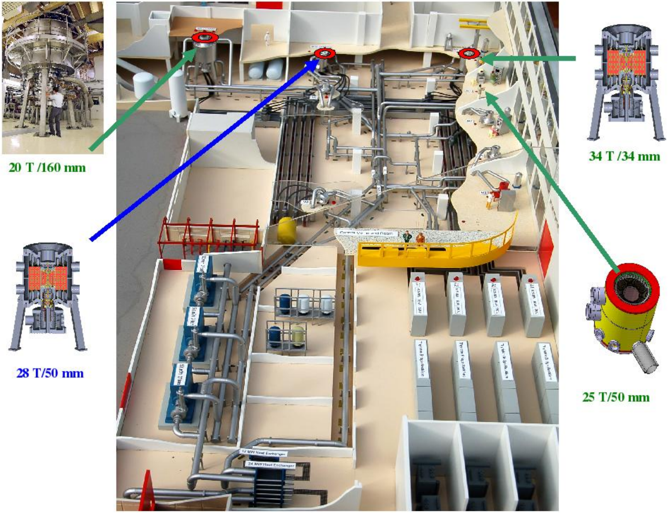
- Tsukuba (Japan)
- Sendai (Japan)
- Hefei (China)
- Wuhan (China)

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

Installations (LNCMI-G)

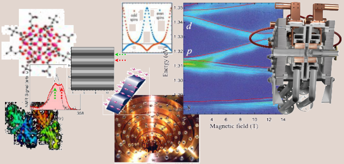


Refroidissement des aimants

LNCMI

Research

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



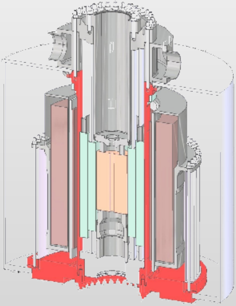
Facilities (10000 hours / year)

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

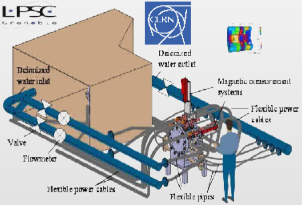
Access

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

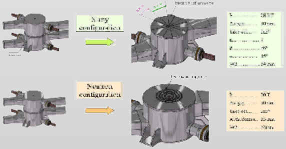
Projets



Hybrid Magnet : 43 T

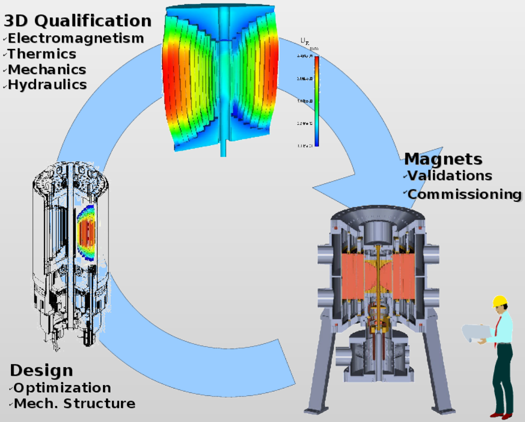


ECR Ion source (Euro ν)



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, $< T >$, 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 Librairies/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/librairies 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://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)

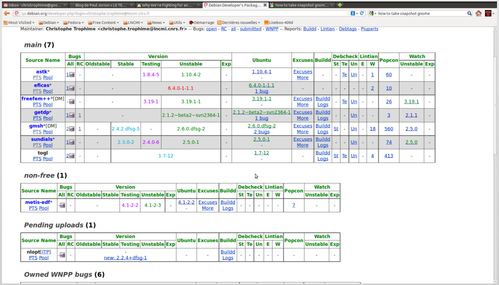
National(/European) facilities

- 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 - 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)



qa.debian.org/developer.php?login=christophe.trophime@lncmi.cnrs.fr

Maintainer: **Christophe Trophime <christophe.trophime@lncmi.cnrs.fr>** -- Bugs: open - RC - all - submitted - WNPP -- Reports: Buildd - Lintian - Debtags - Piuparts

***main* (7)**

Source Name	Bugs		Version					Ubuntu	Excuses	Buildd	Debcheck			Lintian		Popcon	Watch	
	All	RC	Oldstable	Stable	Testing	Unstable	Exp				St	Te	Un	E	W		Unstable	Exp
astk* PTS Pool	1	-	-		1.8.4-5	1.10.4-2	-	1.10.4-1 -	Excuses More	-	-	Te	Un	-	1	60	-	-
eficas* PTS Pool	1	-	-		6.4.0-1-1.1		-	6.4.0-1-1.1 1 bug	-	-	-	-	-	-	2	10	-	-
freefem++*[DM] PTS Pool	-	-	-		3.19-1	3.19.1-1	-	3.19.1-1 -	Excuses More	Buildd Logs	-	Te	Un	-	-	26	3.19.1	-
getdp* PTS Pool	1	1	-			2.1.2~beta2~svn2364-1	-	2.1.2~beta2~svn2364-1 1 bug	Excuses More	Buildd Logs	-	-	Un	-	-	3	2.1.1	-
gmsh*[DM] PTS Pool	2	1	-	2.4.2.dfsg-5	-	2.6.0.dfsg-2	-	2.6.0.dfsg-2 2 bugs	Excuses More	Buildd Logs	St	-	Un	-	18	560	2.5.0	-
sundials* PTS Pool	1	-	-	2.3.0-2	2.4.0-6	2.5.0-1	-	2.5.0-1 -	Excuses More	Buildd Logs	-	-	Un	-	-	74	2.5.0	-
togl PTS Pool	2	-	-	1.7-12			-	1.7-12 -	-	Buildd Logs	St	Te	Un	-	4	413	-	-

***non-free* (1)**

Source Name	Bugs		Version					Ubuntu	Excuses	Buildd	Debcheck			Lintian		Popcon	Watch	
	All	RC	Oldstable	Stable	Testing	Unstable	Exp				St	Te	Un	E	W		Unstable	Exp
metis-edf* PTS Pool	-	-	-		4.1-2-2	4.1-2-3	-	4.1-2-2 -	Excuses More	Buildd Logs	-	-	-	-	-	7	-	-

***Pending uploads* (1)**

Source Name	Bugs		Version					Ubuntu	Excuses	Buildd	Debcheck			Lintian		Popcon	Watch	
	All	RC	Oldstable	Stable	Testing	Unstable	Exp				St	Te	Un	E	W		Unstable	Exp
nlopt[ITP] PTS Pool	-	-	- new: 2.2.4+dfsg-1					-	-	Buildd Logs	-	-	-	-	-	-	-	-

***Owned WNPP bugs* (6)**

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

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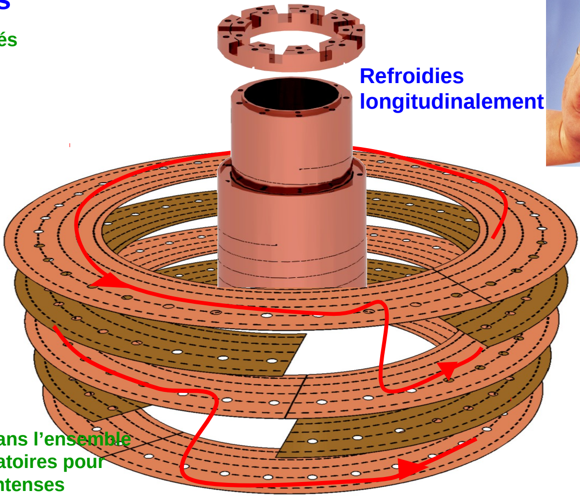
Technologies des aimants

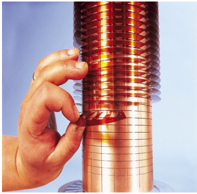
Helices

Développés

Au CNRS



Refroidies longitudinalement



Refroidies radialement

Bitter

Utilisés dans l'ensemble des laboratoires pour champs intenses

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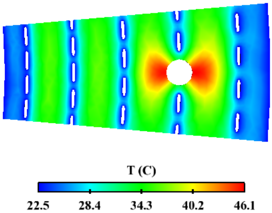
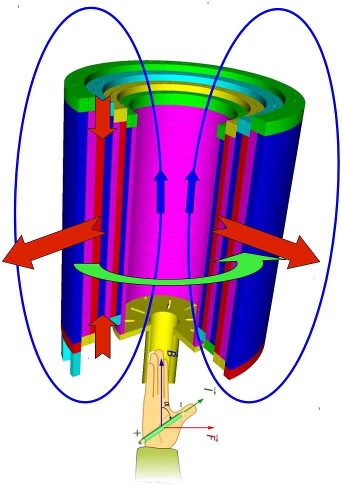
Défis pour la conception

- Efforts magnétiques
- Pertes Joules
- Refroidissement
- Homogénéité ou Profil de champs





Conception des aimants à haut champ (G. Aubert)

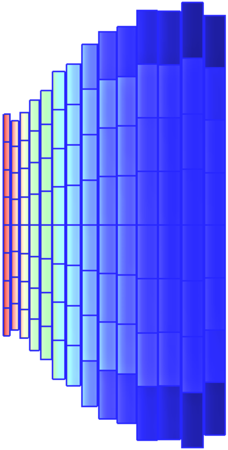
SCOTS® Design

- Ligne de courant hélicoïdale,
- $pas/R_{Interne} \ll 1$
  $\Longrightarrow \mathbf{B}_z \approx \mathbf{B}_z(\mathbf{j}_\theta = j_0\, \rho_0/\rho)$
- Géométrie axisymétrique,

Optimisation sous contraintes

Trouver $j_i \in \mathbb{R}^n$: $max(\sum_i B_i j_i)$ avec

$$\begin{cases} P = \sum_i P_i j_i^2, \\ T_i \leq T_c, \\ r\ j_i\ B(r) \leq \sigma_e. \end{cases}$$



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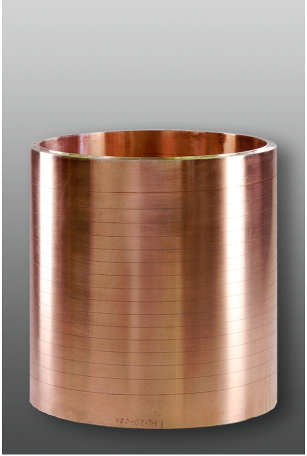
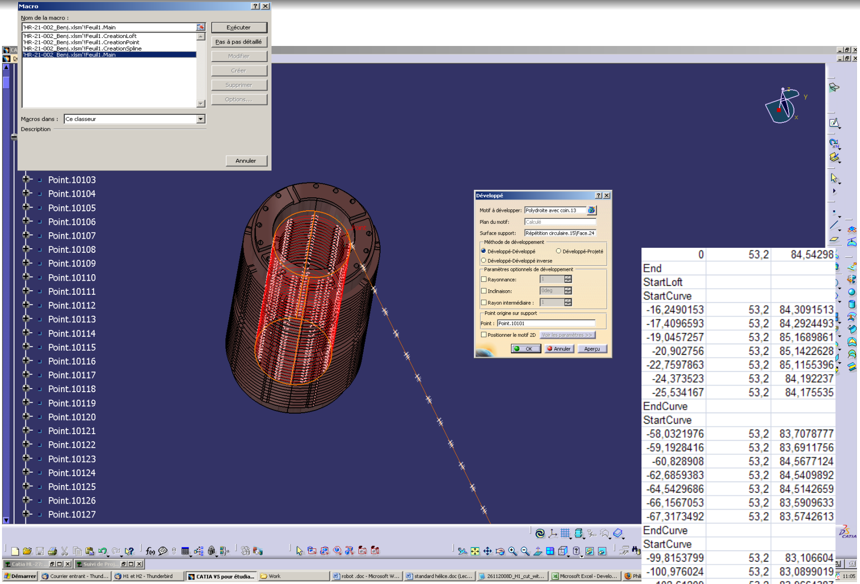
  $\Longrightarrow \mathbf{B}_z \approx \mathbf{B}_z(\mathbf{j}_\theta = j_0\,\rho_0/\rho)$
- Géométrie axisymétrique,
- Optimisation sous contraintes,
- Rapide et précis,

De l'Axi au 3D

- $pas = \Delta z_i \frac{I_{max}}{I_i}$,
- $n_{tours} = \Delta z_i / pas$.



De l'optimisation à la CAO/FAO



0	53,2	84,54298
End		
StartLoft		
StartCurve		
-16,2490153	53,2	84,3091513
-17,4096593	53,2	84,2924493
-19,0457257	53,2	85,1689861
-20,902756	53,2	85,1422628
-22,7597863	53,2	85,1155396
-24,373523	53,2	84,192237
-25,534167	53,2	84,175535
EndCurve		
StartCurve		
-58,0321976	53,2	83,7078777
-59,1928416	53,2	83,6911756
-60,828908	53,2	84,5677124
-62,6859383	53,2	84,5409892
-64,5429686	53,2	84,5142659
-66,1567053	53,2	83,5909633
-67,3173492	53,2	83,5742613
EndCurve		
StartCurve		
-99,8153799	53,2	83,106604
-100,976024	53,2	83,0899019
-102,61209	53,2	83,9664387
-104,469121	53,2	83,9397155
-106,326151	53,2	83,9129922

LNCMI

Qualification 3D

Calcul 3D

- CAO → Maillage (gmsh, Catia, Ghs3d),
- Conduction électrique, Thermique, Magnétostatique,

  → Modélisation Elements Finis (getdp, feel++),

Calcul de structure 3D

- Calcul du champ dans les aimants :

  Biot-Savart → Elements d'arêtes,
- Couplage avec Mécanique (Forces de Laplace, Thermique),
- Interface avec un logiciel de Calcul de structure (Samcef)

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Modèle du Thermistor

Electro-thermique dans Ω

$$\begin{aligned} -\operatorname{div}(\sigma(T)\nabla\phi) &= 0 \\ -\operatorname{div}(\kappa(T)\nabla T) &= \sigma(T)(\nabla\phi)^2 \end{aligned}$$

Propriétés des Matériaux

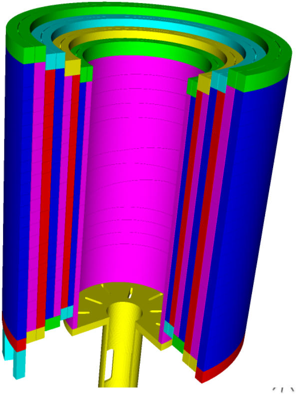
$$\begin{aligned} \sigma(T) &= \frac{\sigma(T_0)}{1+\alpha(T-T_0)} \\ \kappa(T) &= C\sigma(T)T. \end{aligned}$$

Conditions aux limites sur $\partial\Omega$

$$\begin{aligned} \sigma(T)\nabla\phi\cdot\mathbf{n} &= g \\ \kappa(T)\nabla T\cdot\mathbf{n} &= h(T-T_0) \end{aligned}$$

Densité de courant dans Ω

$$\mathbf{j} = -\sigma(T)\nabla\phi$$



GHMFL

Calcul du Champ Magnétique

Densité de courant dans Ω

$$\mathbf{j} = \sigma(T)\nabla\phi$$

Magnétostatique dans $\mathbb{R}^3$

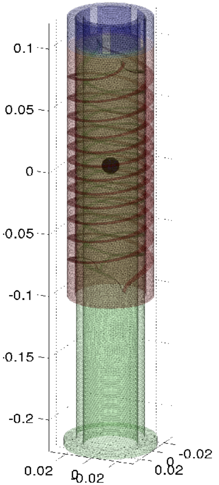
$$\begin{aligned} \operatorname{curl} \mathbf{H} &= \mathbf{j} \\ \operatorname{div} \mathbf{B} &= 0 \\ \mathbf{B} &= \mu_0 \mathbf{H} \end{aligned}$$

Comportement à l'infini

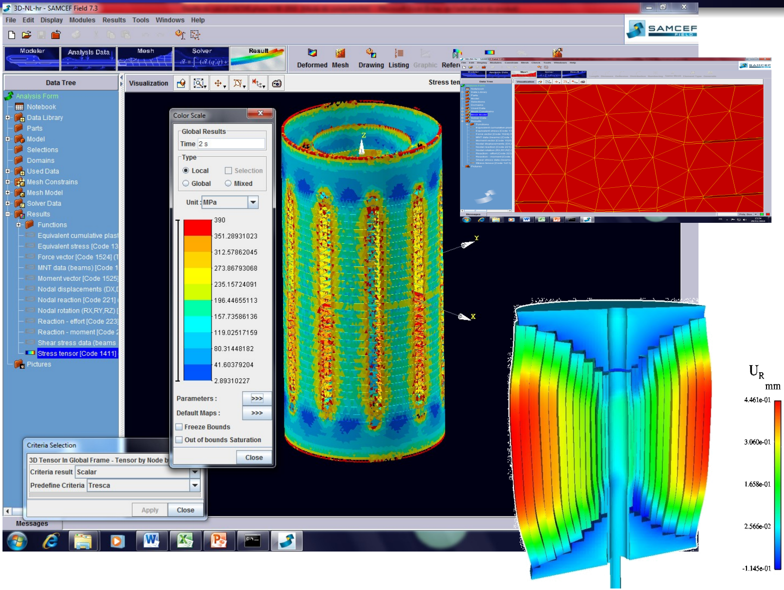
$$|\mathbf{B}| = \mathcal{O}\left(\frac{1}{|x|^2}\right) \quad \text{as} \quad |x| \to \infty$$

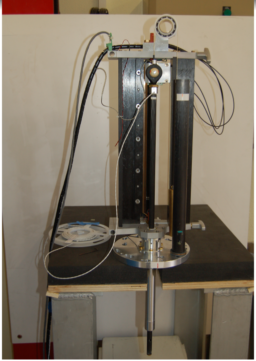
Solution de Biot-Savart

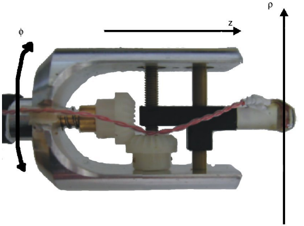
$$d\mathbf{B}_0 = \mu_0 \frac{\mathbf{j} \times \mathbf{r}}{4\pi|\mathbf{r}|^3} dL$$



Calcul de Structure







Caractérisation par "Pickup Coil"

- Détermination du profil de champ sur axe,
- Précision moindre que RMN.

Caractérisation par Sonde RMN

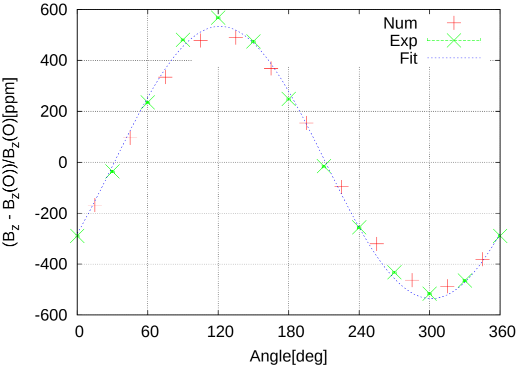
- 20-30 s par point de mesure,
- Précision $+/-4ppm$.

Controle commande

- Puissance dissipée,
- Mesures de tension électrique.
- ΔT dans l'eau, Débit,

LNCMI

Profil de champ magnétique suivant ϕ $(\rho = 8mm)$



Ordre $(2, 2)$

n	F_{n0} $[\frac{ppm}{mm^n}]$	F_{n1} $[\frac{ppm}{mm^n}]$	ϕ_{n1} [deg]
1	-1.65	61.7	33.8
	-	66.7	31.5
2	-2.24	0.1	37.8
	-2.34	-	-

GHMFL

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, $< T >$, stress, ...),
- Uncertainties quantifications

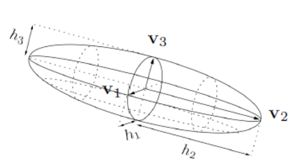
Metric based mesh adaptation [Alauzet and Loseille, 2011]

Metric tensor

Set of quantities that define **geometric properties** of a space

Unit ball of $\mathcal{M}$: $\mathcal{B}_{\mathcal{M}}(\mathbf{a}) = \{\mathbf{x} \in \mathcal{V}(\mathbf{a}) \mid \ \| \mathbf{x} - \mathbf{a} \|_{\mathcal{M}} = 1\}$

- Axes aligned to eigenvectors of $\mathcal{M}$
- Size in direction $\mathbf{v}_i$: $h_i = 1/\sqrt{\lambda_i}$

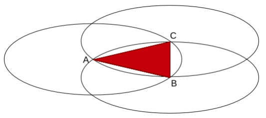


Adaptative mesher

- Several softwares use metric-based adaptation (BAMG, MMG3D, ...)
- Generate a unit mesh in a specific metric space

All elements are **quasi-unit** :

$$\forall\ K\ \forall\ e \in edges(K),\ \ \| e \|_{\mathcal{M}} \in \left[\frac{1}{\alpha};\alpha\right]$$



Hessian based metric tensor

$$\boxed{e(u) = \| u - \pi_h u \|_{L^p(\Omega)} \quad \text{where } \pi_h \text{ is interpolation operator}}$$

Build interpolation error majoration using a metric tensor :

$$|(e(u))(\mathbf{x})| \leqslant \frac{1}{2} \max_{\mathbf{y} \in K} {}^t(\mathbf{a} - \mathbf{x}) \, | H_u(\mathbf{y}) | \, (\mathbf{a} - \mathbf{x})$$

$$\Leftrightarrow \quad \boxed{|(e(u))(\mathbf{x})| \leqslant \frac{1}{2} \left(\frac{d}{d+1} \right)^2 \max_{\mathbf{y} \in K} \max_{v \subset K} {}^t\mathbf{v} \, | H_u(\mathbf{y}) | \, \mathbf{v} \quad = \epsilon}$$

$\Rightarrow$ Control interpolation error $\Leftrightarrow$ Control length of the mesh edges

Metric for mesh adaptation

Build unit mesh such that $\forall \, \mathbf{e} \in \mathcal{H}$:

$$\frac{1}{2} \left(\frac{d}{d+1} \right)^2 \| \mathbf{e} \|_{|H_u|} = \epsilon$$

$$\boxed{\mathcal{M}(x_i) = \frac{1}{2\epsilon} \left(\frac{d}{d+1} \right)^2 | H_u | (x_i)}$$

- Impose h_{min} (limit accuracy)
- Impose h_{max} (avoid $\lambda_i = 0$ cases)

Mesh adaptation algorithm (Feel++ and GMSH)

--> Build initial mesh

```
gmsh_ptrtype desc_geo;
desc_geo=geo(_filename=name_geo,_dim=Dim,_order=G_order,_h=meshSize,
             _files_path="./geofiles",_depends=geo_depends);
mesh = createGMSHMesh( _mesh = new mesh_type,_desc = desc_geo);
```

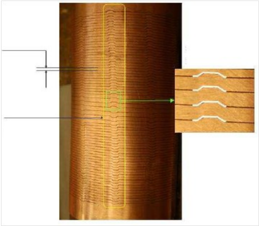
```
--> First resolution on initial mesh, estimation of error
while{ estimated error > error tolerance }
{
      -> Project Hessian matrix on nodes
      -> Compute the metric
      -> Build associated POS file
      -> Give GEO + POS files to GMSH ==> New mesh
```

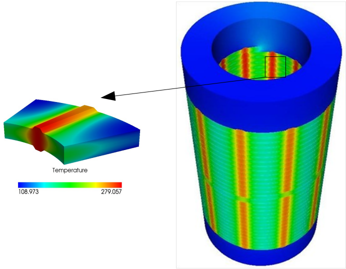
```
mesh=loadGMSHMesh(_mesh = new mesh_type, _filename=new_mesh);
```

```
     -> Resolution on new mesh
     -> Update error estimation
     -> Reduce geometric error tolerance
}
```

Un exemple complet

- Pré-Design (Optimisation Axi semi-analytique),
- Qualification du design 3D (Modélisation 3D),
- Validation expérimentale





Anisotropic meshing on simple 3D geometry

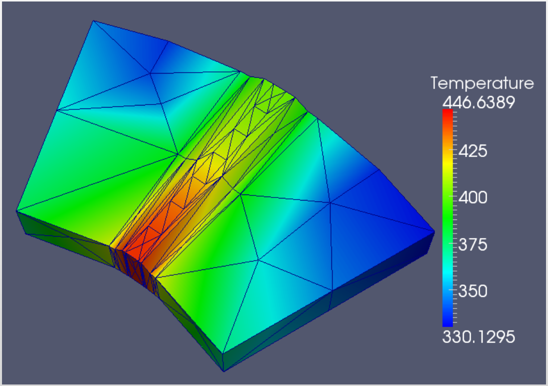


Figure: Initial mesh

Anisotropic meshing on simple 3D geometry

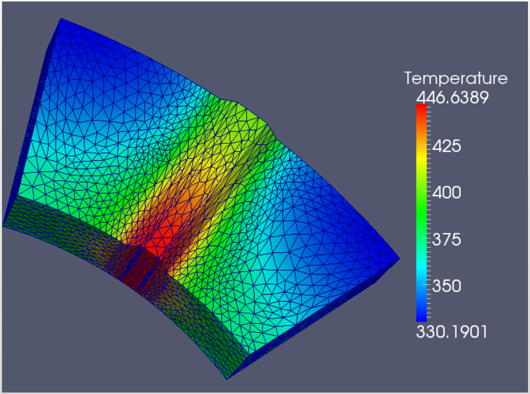


Figure: Third iteration

Anisotropic meshing on more complex geometry

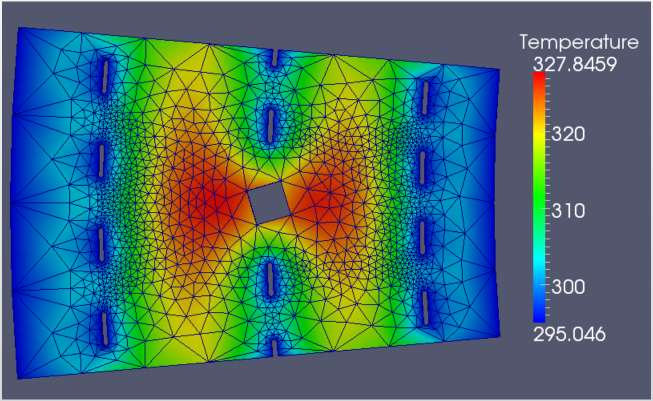


Figure: Initial mesh

Anisotropic meshing on more complex geometry

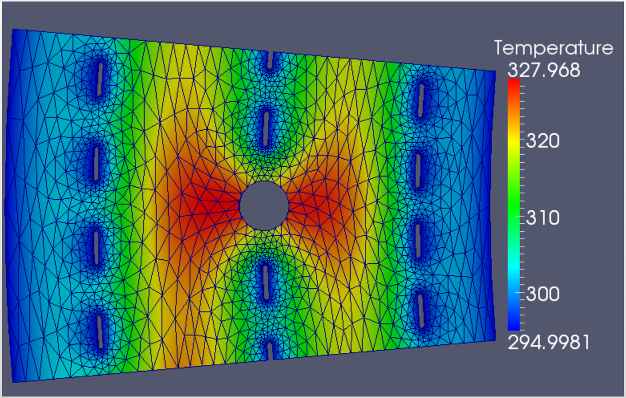


Figure: Third iteration

Needs

- 2D/3D Numerical Modeling
- Fast and reliable methods
- Control of quantity of interest
- Uncertainties quantifications

Challenges

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

Reduced basis methods

Reduced Basis Method [Prud'homme et al., 2002]

Ingredients

- Set of parameters : $\mathcal{D}^{\boldsymbol{\mu}}$
- FEM "truth" approximation
  - $X^{\mathcal{N}}$: finite element approximation of dimension $\mathcal{N} >> 1$
  - $u^{\mathcal{N}}(\boldsymbol{\mu}) \in X^{\mathcal{N}}$ is solution of $a(u^{\mathcal{N}}(\boldsymbol{\mu}), v; \boldsymbol{\mu}) = f(v; \boldsymbol{\mu}) \ \ \forall v \in X^{\mathcal{N}}$
- RB approximation
  - Sample : $S_N = \{\boldsymbol{\mu}_1 \in \mathcal{D}^{\boldsymbol{\mu}}, ..., \boldsymbol{\mu}_N \in \mathcal{D}^{\boldsymbol{\mu}}\}$
  - Approximation space : $W_N = span\{u^{\mathcal{N}}(\boldsymbol{\mu}_1), ..., u^{\mathcal{N}}(\boldsymbol{\mu}_N)\}$ with $N << \mathcal{N}$
  - Galerkin projection on W_N to determine RB coefficients

Computational opportunities

- If the parameter dependance can be expressed as an affine decomposition : $a(u, v; \boldsymbol{\mu}) = \sum_q^{Q_a} \theta_q^a(\boldsymbol{\mu}) \ a_q(u, v)$ and $f(v; \boldsymbol{\mu}) = \sum_q^{Q_f} \theta_q^f(\boldsymbol{\mu}) \ f_q(v)$
  - Strategy : Offline-Online decomposition
    - computationnally intensive initial preprocessing
    - greatly reduced marginal cost

Electro-heat model

Magnet conception (materials, design) requires accurate prediction of temperature
$\Rightarrow$ Electro-heat coupled model

Input parameters

Design

- Material properties
  - Conductivities : $\sigma(T), k(T)$
  - Lorentz number : L
- Ratio $\frac{\text{resistivity}}{\text{temperature}}$: α

In-the-field

- Applied potential : V_D
- Water temperature : T_w
- Heat transfert coefficient : h

$$\boldsymbol{\mu} = (\sigma_0, k_0, \alpha, L, V_D, h, T_w) \subset \mathbb{R}^7$$

Output of interest

- Mean temperature

Sensitivity analysis

Determine :

- Influence of parameters on the output
- A threshold for the output (quantile)

Non linearity treatment : EIM

Properties of the problem

- Coupled equations
  - Electrical potential
  - Heat
- Non linear
- Non affine parameters dependence

Non linear terms

- We need to apply EIM to :
  - $\sigma\left(\boldsymbol{\mu};\mathbf{x};\,T^{\mathcal{N}}(\boldsymbol{\mu})\right)=\dfrac{\sigma_0}{1+\alpha(T^{\mathcal{N}}(\boldsymbol{\mu})-T_0)}$
  - $k\left(T^{\mathcal{N}}(\boldsymbol{\mu})\right)=L\,\sigma\left(\boldsymbol{\mu};\mathbf{x};\,T^{\mathcal{N}}(\boldsymbol{\mu})\right)\,T^{\mathcal{N}}(\boldsymbol{\mu})$
  - $\sigma\left(\boldsymbol{\mu};\mathbf{x};\,T^{\mathcal{N}}(\boldsymbol{\mu})\right)\nabla V^{\mathcal{N}}(\boldsymbol{\mu})\cdot\nabla V^{\mathcal{N}}(\boldsymbol{\mu})$

To recover affine decomposition : EIM

The EIM provides the approximation

$$\sigma_M(\boldsymbol{\mu};\mathbf{x};\,T^{\mathcal{N}}(\boldsymbol{\mu}))=\sum_{m=1}^{M}\beta_m(\boldsymbol{\mu};\,T^{\mathcal{N}}(\boldsymbol{\mu}))\;g_m(\mathbf{x}) \qquad (1)$$

with $\sum_{m=1}^{M}\beta_m(\boldsymbol{\mu};\,T^{\mathcal{N}}(\boldsymbol{\mu}))g_m(\mathbf{x}_i)=\sigma(\boldsymbol{\mu};\mathbf{x}_i;\,T^{\mathcal{N}}(\boldsymbol{\mu}))$ for $i=1,\ldots,M$

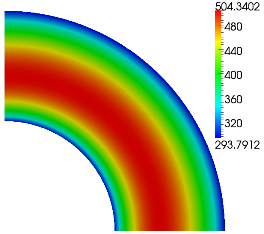
Numerical approximations

Approximations (Feel++ crb)

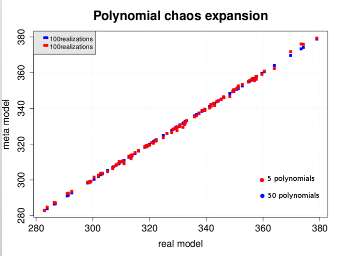
- FEM:
  - Dimension of FEM space : 2 312 (P1)
  - Picard iterations $\approx$ 20 (relative tol 10^{-8})
- RB :
  - Dimension of RB space : 40
  - Picard iterations $\approx$ 20 (relative tol 10^{-8})
  - EIM terms $\approx$ 40 (relative tol 10^{-10})

Meta model (Openturns)

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



Temperature (K)



CRB model vs meta-model

Sobol indices and quantiles

Parameters range

- $\sigma_0 \in [43.5.10^6, 58.10^6](S.m^{-1})$
- $k_0 \in [300, 400](W.m^{-1}.K^{-1})$
- $\alpha \in [3.10^{-3}, 4.10^{-3}](K^{-1})$
- $L \in [2.5.10^{-8}, 2.9.10^{-8}]$
- $V_D \in [0.05, 0.2](V)$
- $h \in [6.10^4, 9.10^4](W.m^{-2}.K^{-1})$
- $T_w \in [273, 323](K)$

Mean, Standard deviation

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

Sobol indices

```
--- Sobol 0 = 3.24405836584e-05
--- Sobol 1 = 5.81262321421e-06
--- Sobol 2 = 3.45831134532e-05
--- Sobol 3 = 0.00242817982199
--- 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

Conclusions

- Hessian-based mesh adaptation :
  - Gradient variations are well detected
  - Anisotropy is well managed
- Reduced Basis method :
  - RB/EIM approximation on a non linear and coupled problem
  - Sensitivity analysis (reduced space dimension)

Perspectives

- Apply these methods on more complex geometries
  - Sensitivity analysis in real cases
  - Optimization of magnet design
- Improve the model
  - Add physics (magnetostatic, elasticity, hydraulic, ...)
  - Transient problem
- Combine these methods : apply RB method on adapted mesh

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