Reduced basis methods and high performance computing. Applications to non-linear multi-physics problems

Christophe Prud'homme
prudhomme@unistra.fr

Cemosis - http://www.cemosis.fr
IRMA
Université de Strasbourg

15 avril 2014

Collaborators on the framework

- Cecile Daversin (IRMA - UdS, Strasbourg and CNRS/LNCMI, Grenoble)
- Christophe Prud'homme (IRMA - UdS, Strasbourg)
- Alexandre Ancel (IRMA - UdS, Strasbourg)
- Christophe Trophime (CNRS/LNCMI, Grenoble)
- Stephane Veys (LJK - UJF, Grenoble)

and former collaborators : S. Vallaghe, E. Schenone.

Non-intrusive RB

- Rachida Chakir (LJLL - UPMC, Paris)
- Yvon Maday (LJLL - UPMC, Paris)

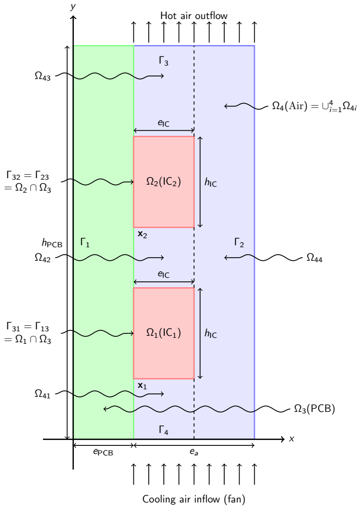
Current Funding

ANR/CHORUS, ANR/HAMM, FRAE/RB4FASTSIM, ANR/Vivabrain, Labex IRMIA, IDEX

Motivations and Framework

OPUS Heat Transfer Benchmark

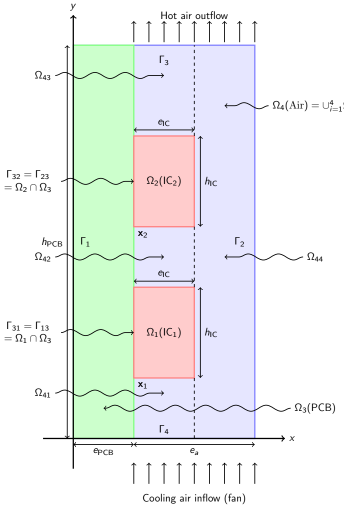
Thermal Testcase Description



Overview

- Heat-Transfer with conduction and convection possibly coupled with Navier-Stokes
- Simple but complex enough to contain all difficulties to test the certified reduced basis
  - non symmetric, non compliant
  - steady/unsteady
  - physical and geometrical parameters
  - coupled models
- Testcase can be easily complexified

Thermal Testcase Description



Heat transfer equation

$$\rho C_i \left(\frac{\partial T}{\partial t} + \mathbf{v} \cdot \nabla T \right) - \nabla \cdot (k_i \nabla T) = Q_i, \quad i = 1, 2, 3, 4$$

Inputs

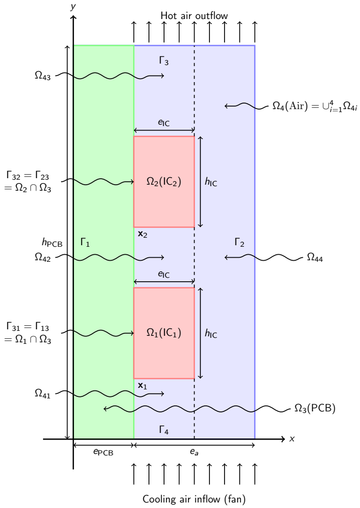
$$\mu = \{e_a; k_{Ic}; D; Q; r\}.$$

Outputs

$$s_1(\mu) = \frac{1}{e_{IC} h_{IC}} \int_{\Omega_2} T$$

$$s_2(\mu) = \frac{1}{e_a} \int_{\Omega_4 \cap \Gamma_3} T$$

Thermal Testcase Description



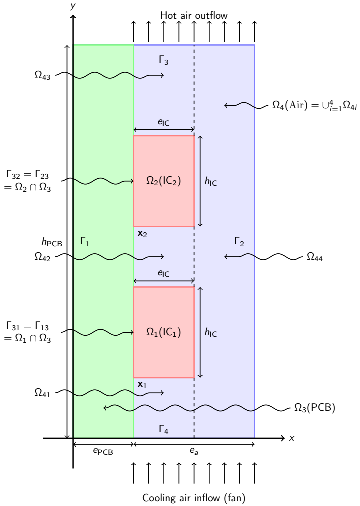
Fluid model

Poiseuille flow or Navier-Stokes flow

Boundary conditions

- on $\Gamma_3 \cap \Omega_3$, a zero flux
- on $\Gamma_3 \cap \Omega_4$, outflow
- on $\Gamma_4, (0 \leq x \leq e_{Pcb} + e_a, y = 0)$ temperature is set
- Γ_1 and Γ_2 periodic
- at interfaces between the ICs and PCB, thermal discontinuity (conductance)
- on other internal boundaries, the continuity of the heat flux and temperature

Thermal Testcase Description



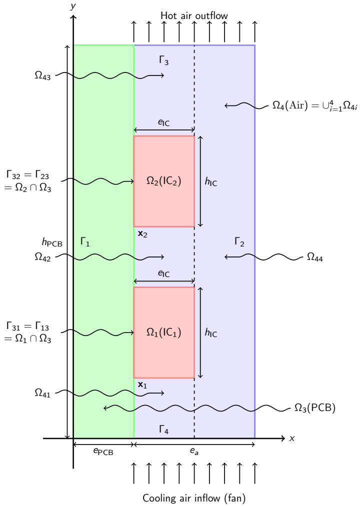
Finite element method

- $\mathbb{P}_k, k = 1, \ldots, 4$ Lagrange elements
- Weak treatment of Dirichlet conditions
- CIP Stabilisation
- Locally Discontinuous FEM functions

Validation

- Comparison between Comsol(EADS) and Feel++
- Extensive testing and comparisons
- Implementation validated, ref. config. max rel error $< 1\%$
- Diff. : mesh, stabilisation, Dirichlet

Thermal Testcase Description



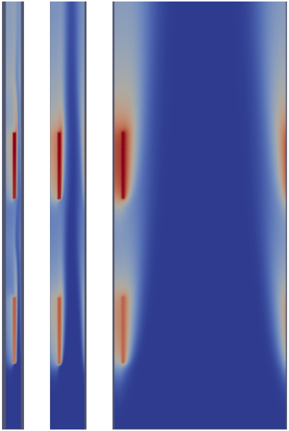


Figure : Temperature plot for $e_a \in \{2.5e-3, 8e-3, 5e-2\}$

Chorus Aerothermal Flow Benchmark

Aerothermic : air conditioning/environment control systems

- Steady Navier-Stokes/Heat transfer problem
- 2 parameters : Grashof and Prandtl number
- Study the average temperature on heated surface with respect to parameters
- Application to aerothermal studies (buildings, cars, airplane cabins,...)

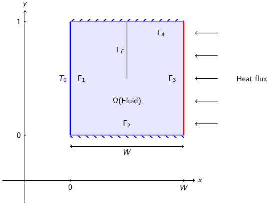
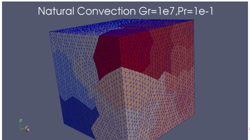
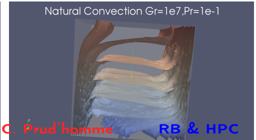
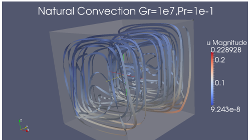


Figure : Geometry of the 2D model. Consider an extrusion of this geometry in 3D case is the extrusion in z axis of length 1.







Aerothermic : air conditioning/environment control systems

- Steady Navier-Stokes/Heat transfer problem
- Coupling 2D/3D mesh based aerothermal model with ECS modelica model
- ECS and A/C design parameters to be optimized

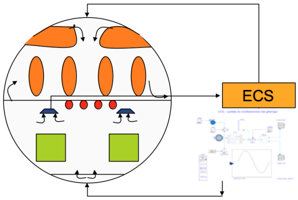
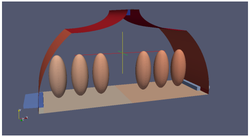
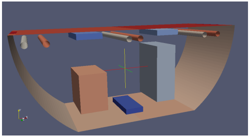


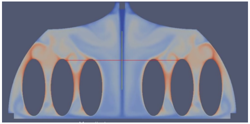
Figure : Design and sizing of thermal control of avionic bay and cabin



(a) Airplane Cabin



(b) Airplane Bay



(c) 2D temperature iso-surfaces

HiFiMagnet project

High Field Magnet Modeling

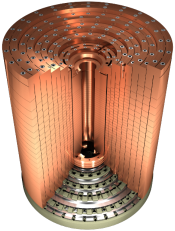
Laboratoire National des Champs Magnétiques Intenses

Large scale user facility in France

- High magnetic field : from 24 T
- Grenoble : continuous magnetic field (36 T)
- Toulouse : pulsed magnetic field (90 T)

Application domains

- Magnetoscience
- Solide state physic
- Chemistry
- Biochemistry



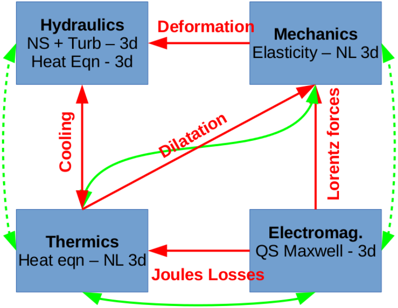
Magnetic Field

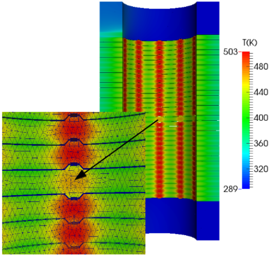
- Earth : $5.8 \cdot 10^{-4}\,T$
- Supraconductors : $24\,T$
- Continuous field : $36\,T$
- Pulsed field : $90\,T$

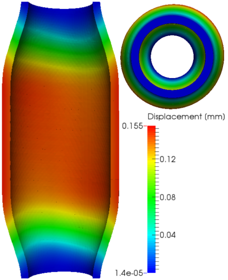
Access

- Call for Magnet Time : 2 $\times$ per year
- $\approx$ 140 projects per year

High Field Magnet Modeling







Why use Reduced Basis Methods ?

Challenges

- Modeling : multi-physics non-linear models, complex geometries, genericity
- Account for uncertainties : uncertainty quantification, sensitivity analysis
- Optimization : shape of magnets, robustness of design

Objective 1 : Fast

- Complex geometries
  - Large number of dofs
- Uncertainty quantification
  - Large number of runs

Objective 2 : Reliable

- Field quality
- Design optimization
  - Certified bounds
  - Reach material limits

An open reduced basis framework

Objectives

- Provide an <u>open</u> framework for certified reduced basis methods
- Provide a rapid prototyping framework using the Feel++ language for the standard finite/spectral element methods
- Provide interfaces to various <u>open</u> "mathematical" programming environments such as Python/OpenTURNS(UQ) or Octave

Where to get it ?

- sources are available at `http://www.feelpp.org`
- available as Debian/Ubuntu packages

Feel++

Features

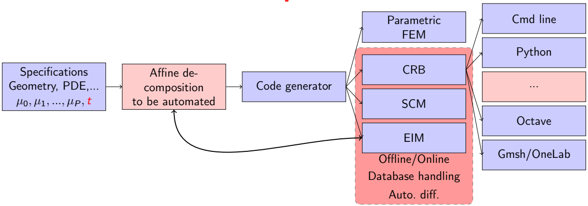
- Galerkin methods (fem,sem, cG, dG) in 1D, 2D and 3D on simplices and hypercubes
- Interfaces to PETSc/SLEPc
- Language embedded in C++ close to variational formulation language that shortens tremendously the "time to results"

```
// $\mathcal{T}_h = \{\text{elements}\}$
auto mesh = loadMesh( new Mesh<Simplex<3> > );
// $X_h = \{v \in C^0(\Omega) | v_K \in \mathbb{P}_2(K), \forall K \in \mathcal{T}_h\}$
auto Xh = Pch<2>(mesh);
auto u = Xh->element(), v = Xh->element();
auto a = form2( _test=Xh, _trial=Xh, );
// $a(u,v) = \int_\Omega \nabla u \cdot \nabla v$
a=integrate(elements(mesh), gradt(u)*trans(grad(v)));
auto b=form2( _test=Xh, _trial=Xh );
// $a(u,v) = \int_\Omega u \ v$
b = integrate( elements(mesh), idt(u)*id(v) );
```

Feel++ Reduced Basis Features

Lower bound for coercivity/inf-sup	OK	90%
CRB Linear Elliptic case	OK	100% (coercive) 90% (non-coercive)
CRB Linear Parabolic case	OK	100%
Automatic differentiation	OK	90%
EIM	OK	100%
CRB Nonlinear case	Ok	80%
CRB automated affine decomposition	Not OK	50%
CRB for multiphysics	OK	80%

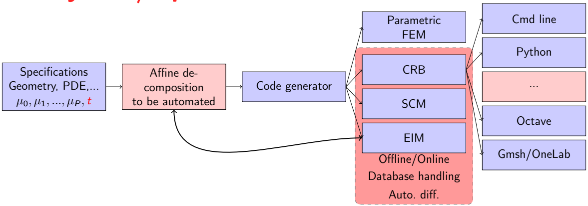
Feel++ Framework : the User point of view




```
class MyModel :
  public ModelBase<ParameterSpace<4>,
     decltype(Pch<5>(Mesh<Simplex<3>>::New()))>{
  ...
  init(){
    auto mesh=loadMesh(_mesh=new Mesh<Simplex<3>>);
    this->setFunctionSpaces( Pch<5>( mesh ) );

    // define bounds for $D^\mu$
    ...
    // affine decomposition here
    ...
  }
```

Wrappers : Python/OpenTURNS

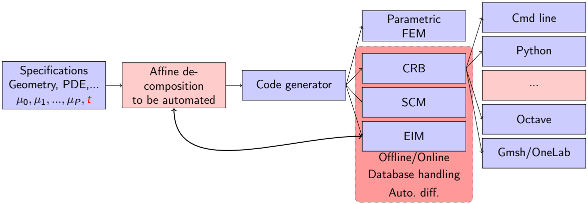


Wrappers are automatically generated by the framework

Python Code (OpenTURNS wrapper for UQ)

```
# fem code
modelfem = NumericalMathFunction("modelfem")
# crb code
modelrb =  NumericalMathFunction("modelrb")
mu[0] = 10
mu[1] = 7e-3
outputfem = modelfem(mu)
outputrb = modelrb(mu)
```

Wrapper : Octave



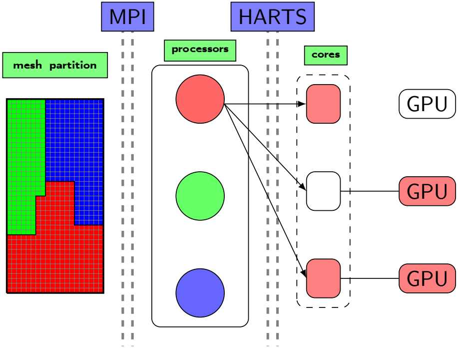
Wrappers are automatically generated by the framework

Octave code

```
# setup parameters
# kIC : thermal conductivity (default: 2)
inP(1) = 1.0e+1;
# D : fluid flow rate (default: 5e-3)
inP(2) = 7.0e-3;
....
for i=1:N
  inP(1)= 0.2+(i-1)*(150-0.2)/N;  D=[D inP(1)];
  s= [s opuseadscrb( inP )];
end
```

High Performance Computing

HPC Strategies



Computing ressources

Objectives :

- Realistic geometries
- Accurate computing

Consequences :

- Memory
- Performance

Technologies

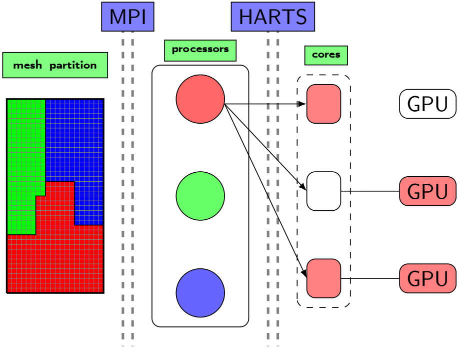
- MPI : Data partitioning
- MT : Global assembly
- GPU : Local assembly

High Performance Computing and RB

- Training parameter sampling
  - Offline : identical on all cores
  - Online : distributed (greedy)
- Parallel in spatial domain
  - RB construction
  - Residual parameter independent terms
  - SCM
- Collective communications
  - Scalar products
  - Outputs
- Opportunities : Robust preconditioners reuse
- Memory hungry RB : matrix free operators

Reconstruction of reduced basis fields : for visualisation or usage in other context might be tricky due to spatial partitioning.

HPC Strategies



Computing ressources

Objectives :

- Realistic geometries
- Accurate computing

Consequences :

- Memory
- Performance

Technologies

- MPI : (Spatial,Parameter)Data partitioning
- (MT,)GPU : Online computations

"Truth" FEM Approximation

Let $I = (0, T_f)$, with T_f is the final time. Let $\mu \in \mathcal{D}^\mu$ and $t \in I$, evaluate

$$s^{\mathcal{N}}(t;\mu) = \ell(t; u^{\mathcal{N}}(\mu)) \ ,$$

where $u^{\mathcal{N}}(t;\mu) \in X^{\mathcal{N}} \subset X$ satisfies

$$m\left(\frac{\partial u^{\mathcal{N}}(\mu)}{\partial t}, v; \mu\right) + a(u^{\mathcal{N}}(\mu), v; \mu) = f(t; v), \quad \forall\, v \in X^{\mathcal{N}} \quad \forall\, t \in I \ .$$

- $a(\cdot,\cdot;\mu)$ and $m(\cdot,\cdot;\mu)$ are bilinear, $f(\cdot;\mu)$ and $\ell(\cdot;\mu)$ are linear
- f and ℓ are bounded

"Truth" FEM Approximation : Inner products and Norms

Let Δt the time step defined by $\Delta t = \frac{T_f}{K}$.
$\forall w, v \in X$ and $1 \leq k \leq K$ we next define the

- energy inner product and associated norm (parameter dependent)

$$\left(\left(\left(w(t^k), v(t^k)\right)\right)\right)_\mu = m(w(t^k), v(t^k); \mu) + \sum_{k'=1}^{k} a_S(w(t^{k'}), v(t^{k'}); \mu)\Delta t$$

$$\left|\left|\left|v(t^k)\right|\right|\right|_\mu = \sqrt{m(v(t^k), v(t^k); \mu) + a_S(v(t^{k'}), v(t^{k'}); \mu)\Delta t}$$

- X-inner product and associated norm (parameter independent)

$$\left(w(t^k), v(t^k)\right)_X = \left(\left(\left(w(t^k), v(t^k)\right)\right)\right)_{\bar{\mu}} \quad \forall w, v \in X, 1 \leq k \leq K$$

$$\left|\left|v(t^k)\right|\right|_X = \left|\left|\left|v(t^k)\right|\right|\right|_{\bar{\mu}} \quad \forall v \in X, 1 \leq k \leq K$$

where a_s denotes the symmetric part of a.

Spaces

Let $\bar{N}$ a postivie number such that $1 \leq \bar{N} \leq N_{\max}$.
Parameter Samples :

$$\text{Sample}: \quad S_{\bar{N}} = \{\mu_1 \in \mathcal{D}^{\mu}, \dots, \mu_{\bar{N}} \in \mathcal{D}^{\mu}\} \quad 1 \leq N \leq \bar{N},$$

with

$$S_1 \subset S_2 \dots S_{\bar{N}} \subset \mathcal{D}^{\mu}$$

Let $Snap(\mu) = \left\{ u^{\mathcal{N}}(t^k, \mu), 1 \leq k \leq K \right\}$ a snapshot set with $\mu \in S_{\bar{N}}$.
Let N_m such that $1 \leq N_m \leq K$, So we have $\bar{N} = \frac{N_{\max}}{N_m}$.
Let $\rho_i(\mu) \in X^{\mathcal{N}}$,$1 \leq i \leq N_m$, eigen modes (associated to μ) selected a Proper Orthogonal Decomposition algorithm

$$\left\{ \rho_i(\mu) \in X^{\mathcal{N}}, 1 \leq i \leq N_m \right\} = POD\Big(Snap(\mu), N_m \Big)$$

$$W_N = \mathrm{span}\left\{ \zeta_n \equiv \rho_i(\mu) \text{ such that } \lfloor n/N_m \rfloor N_m + i \leq n, \mu \in S_{\bar{N}}, n = 1, \dots, N \right\}$$

with

$$W_1 \subset W_2 \dots W_{N_{\max}} \subset X^{\mathcal{N}} \subset X$$

Algorithm

POD algorithm :

Algorithm 1 $\{\rho_i(\mu) \in X^{\mathcal{N}}, 1 \leq i \leq N_m\} = POD(Snap(\mu), N_m)$

Build matrix $\mathcal{M}$ such that $\Big(\mathcal{M}\Big)_{ij} = \Big(u^{\mathcal{N}}(t^i,\mu), u^{\mathcal{N}}(t^j,\mu)\Big)_X$ $1 \leq i,j \leq K$

Solve $\mathcal{M}\ \varphi_i = \lambda_i\ \varphi_i$ for $(\varphi_i \in \mathbb{R}^K, \lambda_i \in \mathbb{R})_{1\leq i\leq N_m}$ associated to N_m larger eigen values of $\mathcal{M}$

Build $\rho_i(\mu) = \sum_{k=1}^{K} \varphi_k\ u^{\mathcal{N}}(t^k,\mu)$ with $1 \leq i \leq N_m$.

A posteriori error estimation

Given $\mu \in \mathcal{D}^\mu$ we define

$$\varepsilon_N(t^k;\mu) = \left|\left| r(u_N(t^k;\mu), v;\mu) \right|\right|_{X'} \ , \ 1 \leq k \leq K.$$

Let $e(t^k,\mu) = \left|\left| u^{\mathcal{N}}(t^k,\mu) - u_N(t^k,\mu) \right|\right|_X$, we can write

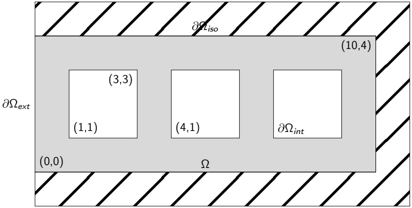
$$e(t^k,\mu) \leq \Delta_N(t^k,\mu) \equiv \sqrt{\frac{\Delta t}{\alpha_{LB}(\mu)} \sum_{k'=1}^{k} \varepsilon_N(t^{k'};\mu)^2} \ , \ 1 \leq k \leq K.$$

$\forall \mu \in \mathcal{D}^\mu$ and $1 \leq k \leq K$ the output error bound is given by

$$\left| s^{\mathcal{N}}(t^k,\mu) - s_N(t^k,\mu) \right| \leq \Delta_N^s(t^k,\mu) \equiv \Delta_N(t^k,\mu) \ \Delta_N^{du}(t^k,\mu).$$

Example Heat Shield : Problem statement

$$\begin{cases} -\Delta u + \frac{\partial u}{\partial t} = 0 & \text{in } \Omega, \\ \text{boundaries conditions} & \text{on } \partial\Omega. \end{cases}$$



Boundaries conditions

$\partial\Omega_{ext}$: heat transfert with $T_{air} = 1$

- $-\nabla u \cdot \mathbf{n} = Biot_{ext}(u - T_{air})$;

$\partial\Omega_{int}$: heat transfert, $T_{air} = 0$

- $-\nabla u \cdot \mathbf{n} = Biot_{int}(u - T_{air})$;

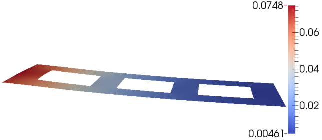
$\partial\Omega_{iso}$: Insulated.

2 parameters

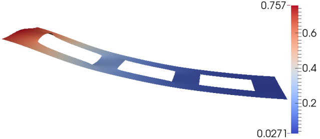
- $Biot_{ext}$ and $Biot_{int}$.

Example Heat Shield

- final time : 20 s ;
- time step : 0.2 s ;
- Minimum parameters values.

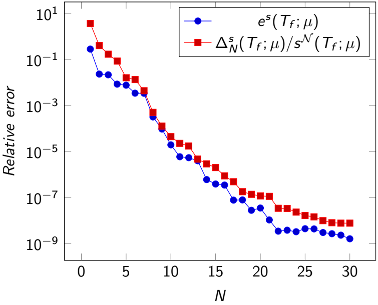


- Maximum parameters values.



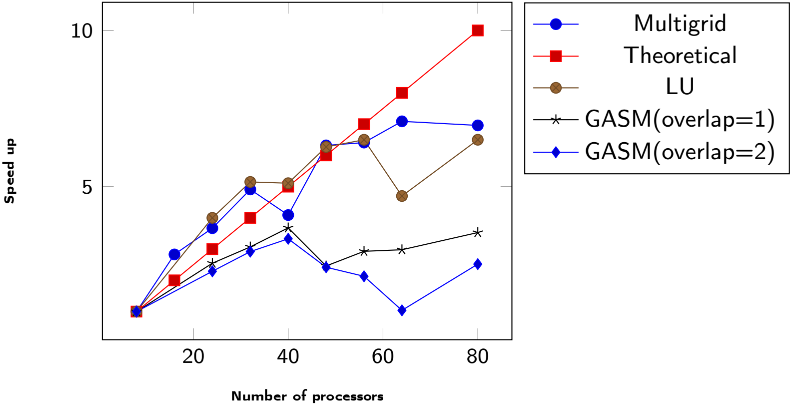
Example Heat Shield

- Configuration :
  - 33 000 dofs ;
  - Preconditioner : LU(MUMPS) – Solver : KSP
  - Ξ : parameter sampling of dimension 430.
- Let $e^s(T_f;\mu) = \dfrac{|s^{\mathcal{N}}(T_f;\mu) - s_N(T_f;\mu)|}{s^{\mathcal{N}}(T_f;\mu)}$, plot $\max_{\mu\in\Xi} e^s(T_f;\mu)$



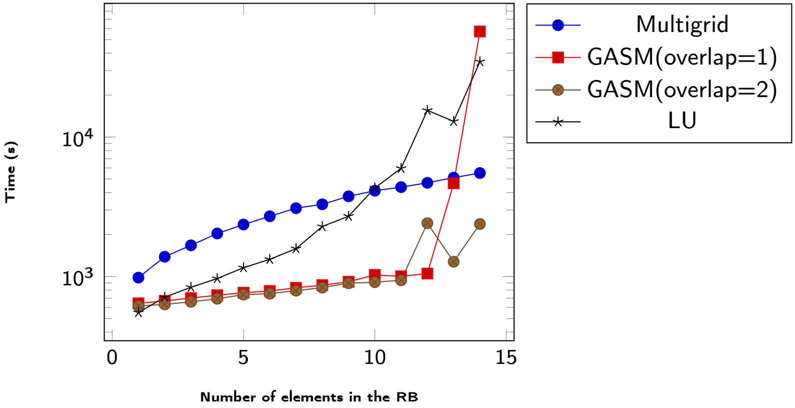
Example Heat Shield : Scalability

- Time to build the first reduced basis
- Configuration : 292 000 dofs for FEM approximation.
- Solver : KSP. Preconditioner : LU(MUMPS), GASM(1 or 2), Multigrid



Example Heat Shield : Basis construction

- Time to build the full reduced basis on 32 procs
- Configuration : 292 000 dofs for FEM approximation.
- Solver : KSP Preconditioner : LU(MUMPS, GASM(1 or 2), Multigrid



Reduced Basis for Non-Linear Problems and Extension to Multiphysics

Notations

NonLinear μ-parametrized PDE

- Set of parameters : $\mu \in \mathcal{D}^{\mu} \subset \mathbb{R}^{p}$,
- Solution of the nonlinear μ-PDE : $u(\mu) \in X \equiv H^1(\Omega \subset \mathbb{R}^d)$,
- PDE weak formulation : We look for $u(\mu) \in X$ such that

$$g(v; \mu, u(\mu)) = 0, \ \forall\, v \in X \ .$$

Bootstrap Truth approximation

- $X^{\mathcal{N}} \subset X$: finite element approximation of dimension $\mathcal{N} >> 1$.
- $u^{\mathcal{N}}(\mu) \in X^{\mathcal{N}}$ is solution of $g(v; \mu, u^{\mathcal{N}}(\mu)) = 0, \ \forall\, v \in X^{\mathcal{N}}$.
- Solution strategies such as Newton or Picard iterations, e.g. given ${}^0u^{\mathcal{N}}$, build the nonlinear iterates ${}^1u^{\mathcal{N}}, \ldots, {}^ku^{\mathcal{N}}, \ldots$

  $$j(\delta^k u^{\mathcal{N}}(\mu), v; {}^k u^{\mathcal{N}}(\mu), \mu) = -g(v; \mu, {}^k u^{\mathcal{N}}(\mu))$$

  where
  $$\delta^k u^{\mathcal{N}}(\mu) = {}^{k+1}u^{\mathcal{N}}(\mu) - {}^k u^{\mathcal{N}}(\mu).$$

  We recover the linear case.
- Equate $u(\mu)$ and $u^{\mathcal{N}}(\mu)$, i.e. $\|u(\mu) - u^{\mathcal{N}}(\mu)\|_X \leq \text{tol}, \ \forall\, \mu \in \mathcal{D}^\mu$.
- Bootstrapping the reduced basis method

Decomposition of the jacobian and residual

Non affine decomposition of g and j

We suppose that we have $\forall v \in X$ and $\forall \mu \in \mathcal{D}^{\mu}$, j reads

$$j(u(\mu), v; \mu, w(\mu)) = \sum_{q=1}^{Q_j} \int_{\omega_q} \sigma_q^j(x, \mu; w(\mu)) \; \mathrm{j}_q(u(\mu), v)$$

and g reads

$$g(v; \mu, w(\mu)) = \sum_{q=1}^{Q_g} \int_{\omega_q} \sigma_q^g(x, \mu; w(\mu)) \mathrm{g}_q(v).$$

where j_q and g_q no longer depend on μ, however σ_q^j and σ_q^g depend on x, μ and u. ω_q denotes a part of the computational domain.

Recovering affine decomposition (Nonlinear-case)

Apply EIM on all σ_q^g and build $g_{AD}\left(u(\mu), v; \mu\right)$ such that

$$g\left(v; \mu, w(\mu),\right) \approx g_{AD}\left(v; \mu, w(\mu)\right) = \sum_{q=1}^{Q_g} \sum_{m=1}^{M_q^g} \beta_g^{qm}(\mu; w(\mu)) \underbrace{\int_{\omega_q} q_m(x) \mathrm{g}^q(v)}_{g^{qm}(v)},$$

and similarly build EIM expansion for σ_q^j and build $j_{AD}\left(u(\mu), v; \mu, w(\mu)\right)$ such that

$$j\left(u(\mu), v; \mu; w(\mu)\right) \approx j_{AD}\left(u(\mu), v; \mu; w(\mu)\right) = \sum_{q=1}^{Q_j} \sum_{m=1}^{M_q^j} \beta_j^{qm}(\mu; w(\mu)) \underbrace{\int_{\omega_q} q_{qm}^j(x) \mathrm{j}^q(u(\mu), v)}_{j^{qm}(u(\mu), v)}, \quad (1)$$

Truth Finite element approximations

- $X^{\mathcal{N}} \subset X$: finite element approximation of dimension $\mathcal{N} >> 1$.
- $u_{AD}^{\mathcal{N}}(\mu) \in X^{\mathcal{N}}$ is solution of $g_{AD}(u_{AD}^{\mathcal{N}}(\mu), v; \mu) = 0, \; \forall\, v \in X^{\mathcal{N}}$.
- Solution strategies such as Newton or Picard iterations, e.g. given ${}^0u_{AD}^{\mathcal{N}}$, build the nonlinear iterates ${}^1u_{AD}^{\mathcal{N}}, \ldots, {}^k u_{AD}^{\mathcal{N}}, \ldots$

$$j_{AD}\left(\delta^k u_{AD}^{\mathcal{N}}(\mu), v; \mu; {}^k u_{AD}^{\mathcal{N}}(\mu)\right) = -g_{AD}\left(v; \mu, {}^k u_{AD}^{\mathcal{N}}(\mu)\right) \;,$$

for the increment $\delta^k u^{\mathcal{N}}(\mu)$ defined by

$$\delta^k u^{\mathcal{N}}(\mu) = \left({}^{k+1}u^{\mathcal{N}}(\mu) - {}^k u^{\mathcal{N}}(\mu)\right) \;. \tag{2}$$

Empirical Interpolation Method [Barrault et al., 2004]

Ingredients

- Training set $\Xi^{\mu}_{train} \subset \mathcal{D}^{\mu}$
- Offline step
  - Sample $S_M = \{\mu_1 \in \Xi^{\mu}_{train}, ..., \mu_M \in \Xi^{\mu}_{train}\}$, Interpolation points $t_1, \ldots, t_M \in \Omega$
  - Approximation space $W_M = span\{q_1(x), \ldots, q_M(x)\}$
    - Residual $r_m(x) = \sigma(x, \mu_m; u^{\mathcal{N}}(\mu_m)) - \sigma_m(x, \mu_m; u^{\mathcal{N}}(\mu_m))$
    - $q_{m+1}(x) = \frac{r_m(x)}{r_m(t_m)}$ (matrix $(B_{i,j}) = q_j(t_i)$ lower triangular)
- Online step : Compute approximation coefficients $\beta_m(\mu; u^{\mathcal{N}}_{AD}(\mu))$

$$\sigma_M(t_i; \mu; u^{\mathcal{N}}_{AD}(t_i, \mu)) = \sum_{m=1}^{M} \beta_m(\mu; u^{\mathcal{N}}_{AD}(t_i, \mu))\, q_m(t_i) = \sigma(t_i; \mu; u^{\mathcal{N}}_{AD}(t_i, \mu))$$

$$\forall i = 1, \ldots, M$$

A language embedded in C++ : EIM expansion

Let u be the solution of $g(u, v; \mu) = 0 \; \forall v \in X^{\mathbb{N}}$ and $\sigma(u)$ the non linear expression involving a field.

```
parameterspace_ptrtype D; parameter_type mu; //μ ∈ D^μ
auto TrainSet = Dmu->sampling();
int eim_sampling_size = 1000;
TrainSet->randomize(eim_sampling_size);

//expression we want EIM expansion
auto sigma = ref(mu(0))/(1+ref(mu(2))*(idv(u)-u0));
//call Feel++ function eim
auto eim_sigma = eim( _model=solve( g(u,v;μ;x) = 0 ),
        _element=u,     // u^N(μ)
        _parameter=mu,  // μ
        _expr=sigma,    // σ(u)
        _space=X_N,
        _name="eim_sigma",
        _sampling=TrainSet );

  //then we can have access to β coefficients
  // of EIM expansion Σ_{m=1}^M β(μ, u^N(μ)) q_m(x)
  std::vector<double> beta_sigma = eim_sigma->beta( mu );
```

Reduced Basis Approximation

- Build $S_N = \{\mu_i, i = 1, ..., N\}$: a parameter sampling
- Build $X_N = \{u_{AD}^{\mathcal{N}}(\mu_i), i = 1, ...N\}$: reduced basis approximation space of dimension $N << \mathcal{N}$.
- $u_{AD}^N(\mu) \in X_N$ is solution of $g_{AD}(u_{AD}^N(\mu), v; \mu) = 0, \ \forall\, v \in X_N$.
- Solution strategies such as Newton or Picard iterations, e.g. given ${}^0u_{AD}^N$, build the nonlinear iterates ${}^1u_{AD}^N, \ldots, {}^ku_{AD}^N, \ldots$

  $$j_{AD}\left(\delta^k u_{AD}^N(\mu), v; \mu; {}^k u_{AD}^N(\mu)\right) = -g_{AD}\left(v; \mu, {}^k u_{AD}^N(\mu)\right) \ ,$$

  with the increment $\delta^k u^N(\mu) = \left({}^{k+1}u_{AD}^N(\mu) - {}^k u_{AD}^N(\mu)\right)$
- EIM Online step : Compute $\beta_m(\mu; u_{AD}^N(t_i, \mu)), \ i = 1, ..., M$

  $$\sigma_M(t_i; \mu; u_{AD}^N(t_i, \mu)) = \sum_{m=1}^{M} \beta_m(\mu; u_{AD}^N(t_i, \mu))\, q_m(t_i) = \sigma(t_i; \mu; u_{AD}^N(t_i, \mu))$$

  where $u_{AD}^N(t_i; \mu) = \sum_{n=1}^N \ u_{AD,n}^N(\mu) u_{AD}^{\mathcal{N}}(t_i; \mu_n)$

Non-affine Non-Linear decomposition : Wrap-up

- Build EIM approximations of non-linear terms using the initial finite element approximation
  - Generate databases of $\mathcal{N}$ independent terms and $\mathcal{N}$ dependent terms
  - Optimisation opportunities in EIM right hand side online step evaluation
    $$\sigma(t_i; \mu; u^{\mathcal{N}|N}(\mu);)$$
    by storing the (FEM or RB) basis functions associated to $u^{\mathcal{N}|N}(\mu)$ at the t_i.
- Build the generalized affine decomposition of the non-linear problem (Newton or Picard iterations)
- Compute the RB approximations (and associated reduced quantities) using the FEM approximation of the generalized affine problem
- Store all the $\mathcal{N}$-independent terms in database (we get rid of the finite element space dimension) and depend solely N, Q and the complexity of the generalized affine expansion.

Affine decomposition in Feel++

given Q_g , Q_j and Q_ℓ the EIM determines $(M_q^g)_{q=1,..,Q_g}$, $(M_q^j)_{q=1,..,Q_j}$ and $(M_q^\ell)_{q=1,..,Q_\ell}$ such that we can write :

$$g_{AD}\left({}^k u(\mu), v; \mu\right) = \sum_{q=1}^{Q_g} \sum_{m=1}^{M_q^g} \beta_g^{qm}(\mu; {}^k u(\mu))\ g^{qm}(v)\ ,$$

$$j_{AD}\left(u(\mu), v; \mu; {}^k u(\mu)\right) = \sum_{q=1}^{Q_j} \sum_{m=1}^{M_q^j} \beta_j^{qm}(\mu; {}^k u(\mu))\ j^{qm}(u(\mu), v)\ ,$$

and

$$\ell_{AD}(v; \mu) = \sum_{q=1}^{Q_\ell} \sum_{m=1}^{M_q^\ell} \beta_\ell^{qm}(\mu)\ \ell^{qm}(v)\ .$$

The standard affine decomposition is in fact a special case of the generalized one.

Reduced basis for Nonlinear Multiphysics

We are able to extend the framework from a single non-linear equation to a system of non-linear equations.

- Monolithic view
  - Support product of function spaces which might be different (scalar vs vectorial, approximation properties,...) or not

$$X = \Pi_{i=1}^{N_{\mathrm{spaces}}} X_i,\ \ u = (u_1, \dots, u_{N_{\mathrm{spaces}}}) \in X,\ \ u_i \in X_i$$

  - Support bilinear and linear forms on product of function spaces

$$\begin{aligned} a : X \times X &\to \mathbb{R}, \\ (u, v) &\to a((u_1, \dots, u_{N_{\mathrm{spaces}}}), (v_1, \dots, v_{N_{\mathrm{spaces}}})) \end{aligned}$$

  - Requires advanced strategies for solvers/preconditioners

HiFiMagnet project

High Field Magnet Modeling

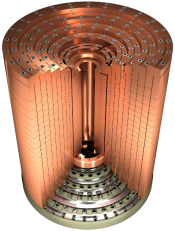
Laboratoire National des Champs Magnétiques Intenses

Large scale user facility in France

- High magnetic field : from 24 T
- Grenoble : continuous magnetic field (36 T)
- Toulouse : pulsed magnetic field (90 T)

Application domains

- Magnetoscience
- Solide state physic
- Chemistry
- Biochemistry



Magnetic Field

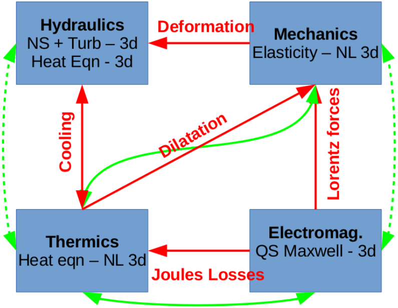
- Earth : $5.8 \cdot 10^{-4}\,T$
- Supraconductors : $24\,T$
- Continuous field : $36\,T$
- Pulsed field : $90\,T$

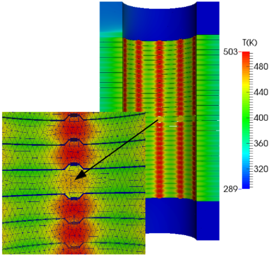
Access

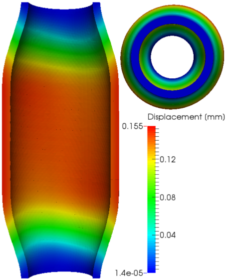
- Call for Magnet Time : $2 \times$ per year
- $\approx$ 140 projects per year

HiFiMagnet

High Field Magnet Modeling







Why use Reduced Basis Methods ?

Challenges

- Modeling : multi-physics non-linear models, complex geometries, genericity
- Account for uncertainties : uncertainty quantification, sensitivity analysis
- Optimization : shape of magnets, robustness of design

Objective 1 : Fast

- Complex geometries
  - Large number of dofs
- Uncertainty quantification
  - Large number of runs

Objective 2 : Reliable

- Field quality
- Design optimization
  - Certified bounds
  - Reach material limits

Electro-thermal model

- V : electrical potential
- T : temperature

$$\begin{cases} -\nabla \cdot (\sigma(T)\nabla V) = 0 \text{ on } \Omega \\ -\nabla \cdot (k(T)\nabla T) = \sigma(T)\nabla V \cdot \nabla V \text{ on } \Omega \end{cases}$$

Boundary conditions

- Applied potential
  - $V = 0$ on *Bottom*
  - $V = V_{Top}$ on *Top*
- Water / Glue electrically isolant
  - $-\sigma(T)\nabla V \cdot \mathbf{n} = 0$
- No thermic exchange with air
  - $-k(T)\nabla T \cdot \mathbf{n} = 0$
- Thermic exchange (h) with cooling water (T_w)
  - $-k(T)\nabla T \cdot \mathbf{n} = h(T - T_w)$

Non-linearity

Electrical conductivity

$$\sigma(T) = \frac{\sigma_0}{1 + \alpha(T - T_0)}$$

- $\sigma_0 = \sigma(ref = 20^\circ C)$
- $T_0 = 20^\circ C$
- α = temperature coeff.

Thermal conductivity

$$k(T) = LT\sigma(T)$$

- L = Lorentz number

Electro-thermal model : Inputs/Outputs

Parameters

Material properties

- Electrical conductivity (σ_0)
- Temperature coeff (α)
- Lorentz number (L)

Operating conditions

- Applied potential (V_D)
- Heat transfert coeff. (h)
- Water temperature (T_w)

$$\mu = (\sigma_0, \alpha, L, V_{Top}, h, T_w)$$

Outputs

$$s(\mu) = \ell(V(\mu), T(\mu))$$

Possibilities for ℓ :

- Mean temperature in the domain
- Magnetic field on specific point (Biot & Savart's law)
- Power of the magnet

Variationnal formulation

$$\begin{cases} \nabla \cdot (\sigma(T)\nabla V) = 0 \text{ on } \Omega_V \\ \nabla \cdot (k(T)\nabla T) = \sigma(T)\nabla V \cdot \nabla V \text{ on } \Omega_T \end{cases}$$

$$\begin{cases} V = V_D \text{ on } D_V \\ -\sigma(T)\nabla V \cdot \mathbf{n} = V_N \text{ on } N_V \end{cases} \qquad \begin{cases} -\sigma(T)\nabla T \cdot \mathbf{n} = 0 \text{ on } N_T \\ -\sigma(T)\nabla T \cdot \mathbf{n} = T_{R1} T + T_{R2} \text{ on } R_T \end{cases}$$

Electrical Potential

Find $V \in X \subset H_1(\Omega)$ such that $\forall\ \phi_V \in X$:

$$\int_\Omega \sigma(T)\nabla V \cdot \nabla \phi_V - \int_{D_V} \sigma(T)(\nabla V \cdot \mathbf{n})\phi_V + \int_{D_V} \sigma(T)(\frac{\gamma}{h_s} V\phi_V - (\nabla\phi_V \cdot \mathbf{n})V)$$
$$- \int_{D_V} \sigma(T)(\frac{\gamma}{h_s} V_D\phi_V - (\nabla\phi_V \cdot \mathbf{n})V_D) = 0$$

Temperature

Find $T \in X \subset H_1(\Omega)$ such that $\forall\ \phi_T \in X$:

$$\int_\Omega k(T)\nabla T \cdot \nabla \phi_T + \int_{R_T} T_{R1} T\phi_T = \int_\Omega \sigma(T)\nabla V \cdot \nabla V\phi_T - \int_{R_T} T_{R2}\phi_T$$

Non-affine parameter dependance

Considering first term of electrical potential formulation :

$$a_v = \int_\Omega \sigma(T) \nabla V \cdot \nabla \phi_V = \int_\Omega \frac{\sigma_0}{1 + \alpha(T - T_0)} \nabla V \cdot \nabla \phi_V$$

As σ_0 and α are input parameters :

$$\nexists \; a_q^v, \theta_q^v \;\; | \;\; a_v(V, T; \mu) = \sum_q \Theta_q^v(\mu) a_q^v(V, T, \phi_V, \phi_T)$$

EIM : Empirical Interpolation Method

Build an affine approximation a_v^{aff} of a_v such that :

$$a_v^{aff} = \sum_q \Theta_q^v(\mu) a_q^v(V, T, \phi_V, \phi_T)$$

exact on a set of interpolation points $\{t_i\}$: $a_v^{aff}(t_i) = a_v(t_i) \; \forall i$.

Electrical potential

$$\int_\Omega \sigma(T)\nabla V\cdot\nabla\phi_V \quad -\int_{D_V}\sigma(T)\left((\nabla V\cdot\mathbf{n})\phi_V+\frac{\gamma}{h_s}V\phi_V-(\nabla\phi_V\cdot\mathbf{n})V\right)$$
$$-\int_{D_V}\sigma(T)V_D\left(\frac{\gamma}{h_s}\phi_V-(\nabla\phi_V\cdot\mathbf{n})\right)=0$$

$$\sigma(T)=\frac{\sigma_0}{1+\alpha(T-T_0)}\longrightarrow\quad\sigma^{aff}(T)=\sum_{m_\sigma=0}^{M_\sigma}\beta_{m_\sigma}(\mu)q_{m_\sigma}(T)$$

Temperature

$$\int_\Omega k(T)\nabla T\cdot\nabla\phi_T+\int_{R_T}T_{R1}T\phi_T=\int_\Omega\sigma(T)\nabla V\cdot\nabla V\phi_T-\int_{R_T}T_{R2}\phi_T$$

$$k(T)=\sigma(T)LT\longrightarrow\quad k^{aff}(T)=\sum_{m_k=0}^{M_k}\beta_{m_k}(\mu)q_{m_k}(T)$$

$$J(V,T)=\sigma(T)\nabla V\cdot\nabla V\longrightarrow\quad J^{aff}(V,T)=\sum_{m_J=0}^{M_J}\beta_{m_J}(\mu)q_{m_J}(V,T)$$

Coupled formulation

Find $(V,T) \in X \times X \subset [H_1(\Omega)]^2$ such that $\forall\ (\phi_V, \phi_T) \in X \times X$:

$$a((V,T),(\phi_V,\phi_T);\mu) = f((\phi_V,\phi_T);\mu) \quad \forall (\phi_V,\phi_T) \in X \times X$$

Affine decomposition

$$\boxed{\sum_{q_a=1}^{Q_a} \Theta_a^q(\mu) a^q((V,T),(\phi_V,\phi_T)) = \sum_{q_f=1}^{Q_f} \Theta_f^q(\mu) f^q((\phi_V,\phi_T))}$$

$$\sum_{m_\sigma=1}^{M_\sigma} \beta_{m_\sigma}(\mu) \left[\int_\Omega q_{m_\sigma}(T) \nabla V \cdot \nabla \phi_V - \int_{D_V} q_{m_\sigma}(T) \left((\nabla V \cdot \mathbf{n}) \phi_V + \frac{\gamma}{h_s} V \phi_V - (\nabla \phi_V \cdot \mathbf{n}) V \right) \right]$$

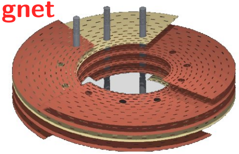
$$- \sum_{m_\sigma=1}^{M_\sigma} \beta_{m_\sigma}(\mu) V_D \int_{D_V} q_{m_\sigma}(T) \left(\frac{\gamma}{h_s} \phi_V - (\nabla \phi_V \cdot \mathbf{n}) \right) + \sum_{m_k=1}^{M_k} \beta_{m_k}(\mu) \int_\Omega q_{m_k}(T) \nabla T \cdot \nabla \phi_T$$

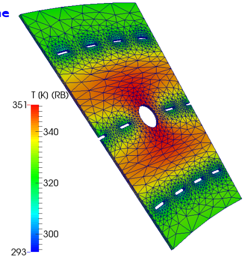
$$+ T_{R_1} \int_{R_T} T \phi_T = \sum_{m_J=1}^{M_J} \beta_{m_J}(\mu) \int_\Omega q_{m_J}(V,T) \phi_T - T_{R_2} \int_{R_T} \phi_T$$

Reduced Electro-thermal model

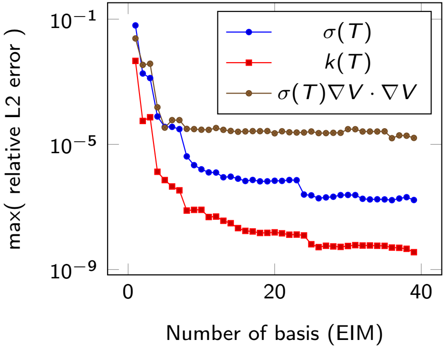
From small towards large simulations

Bitter Magnet

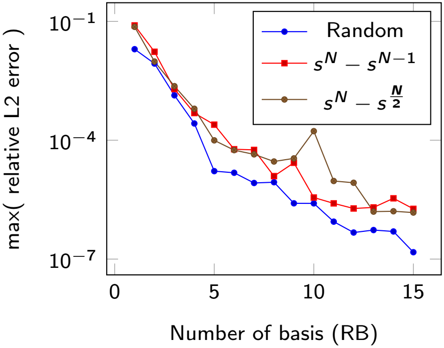




EIM - Convergence study



CRB - Convergence study



Bitter Magnet - Parametric study

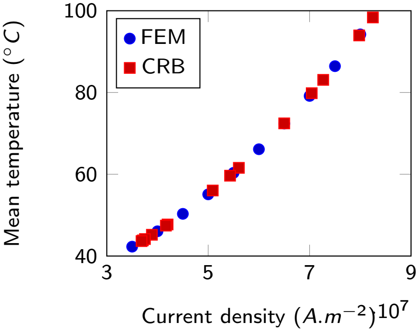
Objective

- Generate higher magnetic field
  - Increase current density $\mathbf{j} = \sigma \nabla V$
  - $\Rightarrow$ Temperature increase !

Question

$Max(\mathbf{j})$ without thermal damages ?

- $\sigma_0 = 58 \times 10^6 S$
- $\alpha = 3.5 \times 10^{-3} K^{-}1$
- $L = 2.5^{-8}$
- $\mathbf{j} \in [30; 90].10^6 A.m^{-2}$
- $h = 80000 W.m^{-2}.K^{-1}$
- $T_w = 293K$



$40\ ^\circ C$ to $60\ ^\circ C$: + 1 Tesla

Bitter Magnet - Sensitivity analysis

Inputs ranges (Uniform distribution)

- $\sigma_0 \in [5.5 \times 10^4, 6 \times 10^4]S$
- $\alpha \in [3.3^{-3}, 3.5 \times 10^{-3}]K^-1$
- $L \in [2.5^{-8}, 2.9 \times 10^{-8}]$
- $\mathbf{j} \in [60e + 6, 70e + 6]A.m^{-2}$
- $h \in [70000, 90000]W.m^{-2}.K^{-1}$
- $T_w \in [293, 313]K$

Temperature Range

Mean of outputs : $T = 332.25K \approx 59.25^\circ C$
Standard deviation : 6.03

$\Rightarrow$ Range for T :
$\mathbf{[326.22; 338.28]K = [53.22; 65.28]^\circ C}$

Sobol indices

$$S_i = \frac{V(E[Y \mid X_i])}{V(Y)}$$

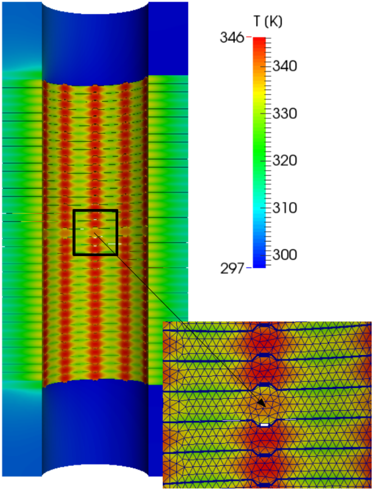
$\boldsymbol{\sigma_0}$	:	**0.022**
$\boldsymbol{\alpha}$	:	$\mathbf{3.6 \times 10^{-5}}$
$\boldsymbol{L}$	:	**0.0042**
$\boldsymbol{j}$	:	**0.16**
$\boldsymbol{h}$	:	**0.044**
$\boldsymbol{T_w}$	:	**0.77**

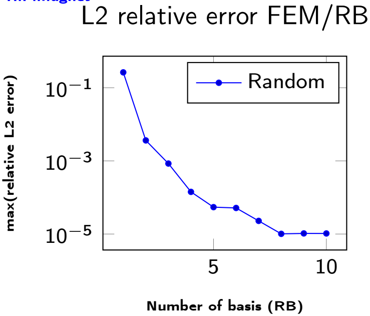
Quantiles

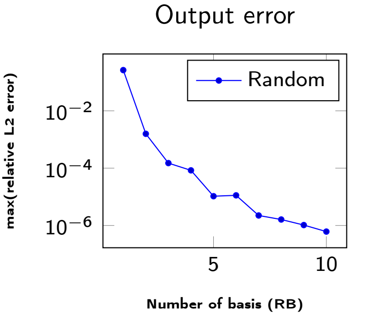
Determine $q(\gamma)$ such that
$P(Y < q(\gamma)) > \gamma$

99.0% : $\mathbf{343K = 70^\circ C}$
80.0% : $\mathbf{336.5K = 63.5^\circ C}$

Helix magnet - Convergence study







Helix magnet - Performances

Simulation characteristics

- Number of dofs $\approx \mathbf{2.4 \times 10^6}$
  - 16 processors
  - Dofs / proc ≈ 155000
- Number of inputs : 6
  - σ_0, α, L, U, h, T_w
- Reduced basis approximation :
  - EIM basis space : 10 basis (sampling size $=$ 100)
  - RB space : 25 basis (sampling size $=$ 1000)

PFEM time

- FEM approx. using affine decomposition
- 16 processors

Mean time $\approx 35min$

RB time

- RB approximation
- For any number of procs

Mean time $\approx 2min$

Gain factor ≈ 17

Perspectives

Ongoing work on electro-thermal model

- Continue investigations with large simulations
  - Increase number of basis
  - Analyse convergence (EIM, RB)
  - ...
- Work on error estimation for such a model
  - Error estimation for EIM approximation
  - Dealing with non-linearity

Towards full reduced model

- Add Linear Elasticity model
- Add Magnetostatic model

Conclusions

- Framework in place, need to add rigor in the nonlinear case if possible
- HPC is definitely required for (non-linear multiphysics) RB but it should be as seamless as possible
- Still some ingredients are missing
  - *hp* framework for eim and rb ;
  - Lego simulation (with domain decomposition) ;
- Another application : Aerothermal problems (Navier-Stokes+Heat Transfer) ;
- Embed advanced analysis tools (automatic differentiation, polynomial chaos, ...)

References

Barrault, M., Maday, Y., Nguyen, N. C., and Patera, A. (2004).
An empirical interpolation method : application to efficient reduced-basis discretization of partial differential equations.
Comptes Rendus Mathematique, 339(9) :667–672.