GeoPDEs
An Octave/Matlab software for research on IGA

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Motivation

We wanted to share our codes with people interested on IGA.

Starting point: different codes, different problems, different developers.

Primary goal: uniform implementation of our different codes.

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The result is **GeoPDEs**: open and free software for IGA.

The software is implemented in **Octave**, fully compatible with **Matlab**.

- Very **clear** for **teaching** purposes.
- Easy to modify and to use for **fast prototyping**.
- Follows an **abstract setting** to cover many problems and methods.

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Secondary goal: faster and more efficient implementation.

- Important advances in **GeoPDEs 2.0** (last part of the talk).

General description of the software

GeoPDEs consists of a set of interrelated **packages** for different problems:

- **base**: the main package, with examples for Laplace problem.
- **elasticity**: a simple package for linear elasticity problems.
- **fluid**: Stokes' equations, with different choices for the discrete spaces.
- **maxwell**: Maxwell equations, generalization of edge finite elements.
- **multipatch**: extension to multi-patch defined geometries.

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The other packages are based on the structures defined in **base**.

The nomenclature is mostly the same in every package.

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We define IGA in an **abstract way**, to cover as many cases as possible.

IGA in an abstract framework

- Problem to solve at the continuous level.

Abstract framework

$$a(u, v) = (f, v), \quad \forall v \in V.$$

Simple example: Poisson equation

$$\int_\Omega \mathbf{grad}\, u \cdot \mathbf{grad}\, v = \int_\Omega f\, v, \quad \forall v \in H_0^1(\Omega).$$

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- Problem to solve at the continuous level.
- Parametric domain and **parameterization** of the physical domain.

Abstract framework

$$\mathbf{F} : \widehat{\Omega} \longrightarrow \Omega \subset \mathbb{R}^d, \text{ and } \mathbf{F} \text{ is known and computable.}$$

Simple example: Poisson equation

$$\widehat{\Omega} = (0,1)^d, \text{ and } \mathbf{F} \text{ is a NURBS.}$$

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- **Discrete** problem and **spaces** in the parametric and physical domain.

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$$a(u_h, v_h) = (f, v_h), \quad \forall v_h \in V_h.$$

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$$\int_\Omega \mathbf{grad}\, u_h \cdot \mathbf{grad}\, v_h = \int_\Omega f\, v_h, \quad \forall v_h \in V_h.$$

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$$V_h = \{v_h : \iota(v_h) = \widehat{v}_h \in \widehat{V}_h\}, \text{ where } \iota \text{ is a pull-back depending on } \mathbf{F},$$

and $\widehat{V}_h = \mathrm{span}\{\widehat{v}_j\}_{j=1}^{N_h}$ is a finite-dimensional and computable space.

Simple example: Poisson equation

$$V_h = \{v_h : v_h \circ \mathbf{F} = \widehat{v}_h \in \widehat{V}_h\},$$

with $\widehat{V}_h = \mathrm{span}\{R_j\}_{i=1}^{N_h}$ a space of NURBS.

IGA in an abstract framework

- Problem to solve at the continuous level.
- Parametric domain and **parameterization** of the physical domain.
- **Discrete** problem and **spaces** in the parametric and physical domain.
- Construct and solve a **linear system** to find the discrete solution.

Abstract framework

Trial function $u_h = \sum_{i=1}^{N_h} \alpha_i v_i$, and test again every v_j, to get

$$\sum_{i=1}^{N_h} \alpha_i a(v_i, v_j) = (f, v_j),\ j = 1, \ldots, N_h, \quad \text{or} \quad \sum_{i=1}^{N_h} A_{ji} \alpha_i = b_j.$$

Simple example: Poisson equation

Trial function $u_h = \sum_{i=1}^{N_h} \alpha_i R_i$, and test functions R_j:

$$\sum_{i=1}^{N_h} \alpha_i \int_\Omega \mathbf{grad}\, R_i \cdot \mathbf{grad}\, R_j = \int_\Omega f\, R_j, \quad j = 1, \ldots, N_h.$$

IGA in an abstract framework

To numerically compute the integrals, we define a **partition** $\widehat{\Omega} = \cup_{k=1}^{N_e} \widehat{K}_k$, and on each "element" $\widehat{K}_k$ a **quadrature rule**: $\{(\widehat{\mathbf{x}}_{\ell,k}, w_{\ell,k})\}_{\ell=1}^{n_k}$.

$\int_\Omega \phi(\mathbf{x}) = \sum_{k=1}^{N_e} \int_{\widehat{K}_k} \phi(\mathbf{F}(\widehat{\mathbf{x}})) |\det(D\mathbf{F}(\widehat{\mathbf{x}}))|$

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Using the quadrature rule, the **stiffness matrix** is computed as

$$A_{ij} \simeq \sum_{k=1}^{N_e} \sum_{\ell=1}^{n_k} w_{\ell,k}\, \mathbf{grad}\, v_j(\mathbf{F}(\widehat{\mathbf{x}}_{\ell,k})) \cdot \mathbf{grad}\, v_i(\mathbf{F}(\widehat{\mathbf{x}}_{\ell,k}))\, |\det(D\mathbf{F}(\widehat{\mathbf{x}}_{\ell,k}))|$$

And recall that $\mathbf{grad}\, v_i(\mathbf{F}(\widehat{\mathbf{x}}_{\ell,k})) = D\mathbf{F}^{-T}\, \widehat{\mathbf{grad}}\, \widehat{v}_i(\widehat{\mathbf{x}}_{\ell,k})$.

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Summarizing, what we need is

- A partition of $\widehat{\Omega}$ and a **quadrature rule** (nodes and weights).
- The evaluation of **F** and the Jacobian $D\mathbf{F}$ at the quadrature points.
- Value of the **shape functions** at the "mapped" quadrature points.
- A routine to put everything together and compute the matrices.

The main structures of GeoPDEs

GeoPDEs has been implemented following the abstract framework.

The code is based on **three** main **structures**:

- **Geometry**: the parameterization $\mathbf{F}$ and its derivatives.
- **Mesh**: the partition of the domain and the **quadrature rule**.
- **Space**: the **shape functions** of the discrete space V_h.

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- **Space**: the **shape functions** of the discrete space V_h.

Everything is **precomputed** (v.1). Easy to understand and to debug.

As a consequence, the computation of the matrices is very **clear**.

The structures can be used in **different applications** with minor changes.

The parameterization: geometry structure

Computation of the **parameterization** $\mathbf{F}$ and its derivatives.

- **map**: function handle to compute $\mathbf{F}$ at given points in $\widehat{\Omega}$.
- **map_der**: function handle to compute $D\mathbf{F}$, the derivatives of $\mathbf{F}$.

The fields contain the handles to evaluate $\mathbf{F}$, not the values of $\mathbf{F}$.

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For NURBS and B-splines, we make use of the **NURBS toolbox**.

- Based on standard NURBS algorithms (see, e.g., the NURBS book).
- Useful for simple **geometry manipulation** (revolution, extrusion,...)
- It is also used in GeoPDEs for **function evaluation**.

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The computation of the geometry is separated from the shape functions.

- Necessary for **non-isoparametric** discretizations.
- Geometry evaluations can be made in the **coarsest** given **geometry**.

The quadrature rule: mesh structure

Contains information on the **partition** of the domain, $\widehat{\Omega} = \cup_{k=1}^{N_e} \widehat{K}_k$,

and the **quadrature rule** $\{(\widehat{\mathbf{x}}_{\ell,k}, w_{\ell,k})\}_{\ell=1}^{n_k}$.

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Remember the expression for the entries of the stiffness matrix

$A_{ij} \simeq \sum_{k=1}^{N_e} \sum_{\ell=1}^{n_k} w_{\ell,k} \, \mathbf{grad}\, v_j(\mathbf{F}(\widehat{\mathbf{x}}_{\ell,k})) \cdot \mathbf{grad}\, v_i(\mathbf{F}(\widehat{\mathbf{x}}_{\ell,k})) \, |\det(D\mathbf{F}(\widehat{\mathbf{x}}_{\ell,k}))|$

- **nel**: N_e, number of elements of the partition.
- **nqn**: n_k, number of quadrature nodes per element.
- **quad_nodes**: $\widehat{\mathbf{x}}_{\ell,k}$, quadrature nodes in $\widehat{\Omega}$.
- **quad_weights**: $w_{\ell,k}$, quadrature weights.

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- **geo_map**: $\mathbf{x}_{\ell,k} = \mathbf{F}(\widehat{\mathbf{x}}_{\ell,k})$, quadrature nodes in Ω.
- **geo_map_jac**: $D\mathbf{F}(\widehat{\mathbf{x}}_{\ell,k})$, Jacobian matrix evaluated at **quad_nodes**.
- **jacdet**: $|\det(D\mathbf{F}(\widehat{\mathbf{x}}_{\ell,k}))|$, absolute value of the Jacobian.

The discrete space: space structure

Information on the basis functions of the **discrete space**

$$V_h = \mathrm{span}\{v_i\}_{i=1}^{N_h},$$

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- **nsh**: number of non-vanishing functions in each "element".
- **connectivity** (IEN): global indices of non-vanishing basis functions.

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- **connectivity** (IEN): global indices of non-vanishing basis functions.
- **shape_functions**: $v_i(\mathbf{x}_{\ell,k})$, shape functions evaluated at the quadrature points.
- **shape_function_gradients**: $\mathbf{grad}\, v_i(\mathbf{x}_{\ell,k})$, gradients of the shape functions evaluated at the quadrature points.

For NURBS and splines, they are computed with the NURBS toolbox.

Other fields may be necessary (curl, divergence, Laplacian...)

A simple example on how to use GeoPDEs

```
geometry = geo_load('ring_refined.mat');
knots = geometry.nurbs.knots;
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- Create the **geometry** structure, from a NURBS toolbox file.

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[x, y] = deal (msh.geo_map(1,:,:), msh.geo_map(2,:,:));
mat = op_gradu_gradv (space, msh);
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- Map the **mesh** structure to the physical domain, using **geometry**.
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- Build the matrix and right-hand side.

Matrices and vector construction

Remember the expression for the entries of the stiffness matrix
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- Everything is **precomputed** (v.1) in the previous structures.
- To construct the matrices, it is enough to correctly gather the information.
- The computation of the matrices is **simple**, and identical to FEM.

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Let me show an example.

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```
function mat = op_gradu_gradv (space, msh)
for iel = 1:msh.nel
  mat_loc = zeros (space.nsh(iel), space.nsh(iel));
  for idof = 1:space.nsh(iel)
    ishp = space.shape_function_gradients(:,:,idof,iel);
    for jdof = 1:space.nsh(iel)
      jshp = space.shape_function_gradients(:,:,jdof,iel);
      for inode = 1:msh.nqn
        mat_loc(idof,jdof) += ishp(:,inode).*jshp(:,inode) *
         msh.jacdet(inode,iel) * msh.quad_weights(inode,iel);
      endfor %inode
    endfor %jdof
  endfor %idof
  mat(space.connect(:,iel), space.connect(:,iel)) += mat_loc;
endfor %iel
```

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- The computation of the matrices is **simple**, and identical to FEM.

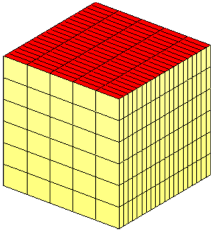
Actually, the efficient Matlab implementation is quite different.

For NURBS, we can also take advantage of the tensor product structure.

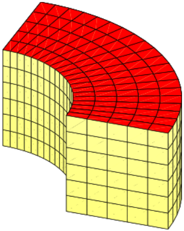
Boundary conditions: the boundary substructures

The structures **mesh** and **space** are completed with the field **boundary**.

These are mesh and space **substructures** of dimension $N-1$.



$\xrightarrow{\mathbf{F}}$



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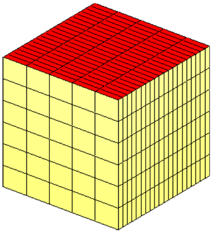
The boundary structures have some particularities:

- **jacdet** contains the area element of the boundary parameterization.
- The **space** structure uses a local numbering for each boundary.
- A new field, **dofs**, is added to recover the global numbering.



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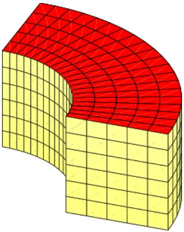

Boundary conditions: the boundary substructures

For **Neumann** conditions, $\frac{\partial u}{\partial n} = g$ on Γ_N, we must compute $\int_{\Gamma_N} g v_j$.

- The integral is computed in the same manner as for bulk forces.
- It is assembled into the global r.h.s. using the field **dofs**.

```
x = msh.boundary.geo_map(1,:,:);
y = msh.boundary.geo_map(2,:,:);
rhs_bnd = op_f_v(space.boundary,msh.boundary,g(x,y));
rhs(space.boundary.dofs) += rhs_bnd;
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For **Dirichlet** conditions, $u = h$ on Γ_D, we must assign the d.o.f. in **boundary.dofs**.

- The needed information should already be in the **boundary** structures.
- As an example we have included the least squares best fit, i.e.

$$\int_{\Gamma_D} uv = \int_{\Gamma_D} hv \quad \forall v.$$

A simple example on how to use GeoPDEs

We have computed all the **structures** and the **linear system**.

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A simple example on how to use GeoPDEs

Apply **boundary conditions** and **solve** the linear system.

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rhs = op_f_v (space, msh, rhs_fun(x, y));
drchlt_dofs = unique ([space.boundary(:).dofs]);
int_dofs = setdiff (1:space.ndof, drchlt_dofs);
u(drchlt_dofs) = 0;
u(int_dofs) = mat(int_dofs, int_dofs) \ rhs(int_dofs);
```

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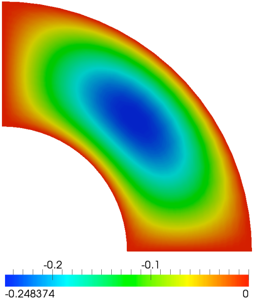
We end up with some **postprocessing**.

```
geometry = geo_load('ring_refined.mat');
knots = geometry.nurbs.knots;
[qn, qw] = msh_set_quad_nodes(knots, msh_gauss_nodes(ngauss));
msh = msh_2d (knots, qn, qw, geometry);
space = sp_nurbs_2d (geometry.nurbs, msh);
[x, y] = deal (msh.geo_map(1,:,:), msh.geo_map(2,:,:));
mat = op_gradu_gradv (space, msh);
rhs = op_f_v (space, msh, rhs_fun(x, y));
drchlt_dofs = unique ([space.boundary(:).dofs]);
int_dofs = setdiff (1:space.ndof, drchlt_dofs);
u(drchlt_dofs) = 0;
u(int_dofs) = mat(int_dofs, int_dofs) \ rhs(int_dofs);
sp_to_vtk (u, space, geometry, [20 20], filename, 'u');
err = sp_l2_error (space, msh, u, exact_solution(x, y));
```

A simple example on how to use GeoPDEs

And the final result is something like this.



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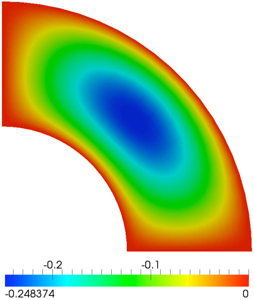

The package contains **several** simple **examples**:

h-,*p*-,*k*-refinement, 2D and 3D, B-splines and NURBS...

The structures can be **easily extended** to solve more **complex problems**.

Linear elasticity problems: the elasticity package

Let us see how to solve the following **linear elasticity** problem:

Find $\mathbf{u} \in V = (H^1_{0,\Gamma_D}(\Omega))^3$ *such that*

$$\int_\Omega (2\mu\,\varepsilon(\mathbf{u}) : \varepsilon(\mathbf{v}) + \lambda\,\mathrm{div}(\mathbf{u})\,\mathrm{div}(\mathbf{v})) = \int_\Omega \mathbf{f}\cdot\mathbf{v} + \int_{\Gamma_N} \mathbf{g}\cdot\mathbf{v} \quad \forall \mathbf{v} \in V,$$

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- The **geometry** and **mesh** are described as in the previous example.
- The basis functions in the **space** structure are now vector-valued.
- A specific **operator** for this problem must be defined.
- Imposing the boundary conditions is similar to the previous problem.

Definition of the vectorial space

We first define one **space** structure for **each component**.

From these we define the vector-valued **space** structure for our problem.

```
spx = spy = spz = sp_nurbs_3d (geometry, msh);
space = sp_vector_3d (spx, spy, spz, msh);
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This command computes the new vector-valued **space** and the numbering.

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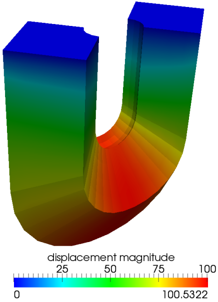
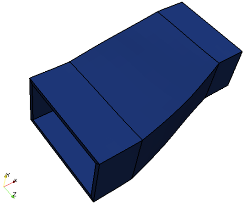


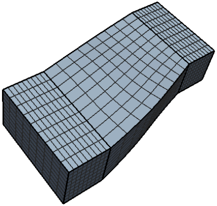
The horseshoe is a courtesy of T.J.R. Hughes' and his group

Electromagnetism: the Maxwell package

An example in electromagnetism:

- Metallic WR-2300 waveguide with a mechanical deformation.
- Consider only the TE_{10} mode at $\simeq 0.35$ GHz.
- Compute relative amplitudes of the transmitted and reflected waves.





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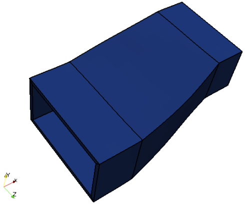

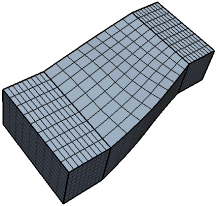

Time-harmonic Maxwell equations in the interior of the waveguide.

Forward (known) and reverse (unknown) traveling waves at Γ_i.

Forward (unknown) traveling wave at Γ_o.

Perfect electrical conductor ($\mathbf{E} \times \mathbf{n} = \mathbf{0}$) on the other boundaries.

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Find $\mathbf{E} \in \mathbf{H}_{0,\Gamma_D}(\mathbf{curl};\Omega)$ *, and* $\alpha_i^r, \alpha_o^f \in \mathbb{C}$ *such that*

$$\int_\Omega (\frac{1}{\mu}\mathbf{curl}\,\mathbf{E} \cdot \mathbf{curl}\,\overline{\mathbf{G}} - \omega^2\varepsilon \mathbf{E} \cdot \overline{\mathbf{G}}) +$$

$$\mathrm{i}\omega(\alpha_i^r \int_{\Gamma_i} \mathbf{H}_\tau^{10} \cdot \overline{\mathbf{G}}_\tau + \alpha_o^f \int_{\Gamma_o} \mathbf{H}_\tau^{10} \cdot \overline{\mathbf{G}}_\tau) = \mathrm{i}\omega\alpha_i^f \int_{\Gamma_i} \mathbf{H}_\tau^{10} \cdot \overline{\mathbf{G}}_\tau,$$

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- Vector-valued **space** with a curl-conserving transform.

The shape functions are given by $\mathbf{E}\circ\mathbf{F} = D\mathbf{F}^{-\top}\widehat{\mathbf{E}}$.

And $(\mathbf{curl}\,\mathbf{E})\circ\mathbf{F} = \frac{1}{\det(D\mathbf{F})}D\mathbf{F}(\widehat{\mathbf{curl}}\,\widehat{\mathbf{E}})$.

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- We need an operator to compute the **curl**-**curl** matrix.
- Vector-valued **space** with a curl-conserving transform.
- For the boundaries, we only store the tangential components.
- Operators to compute the integrals on the boundary are also needed.

Electromagnetism: the Maxwell package

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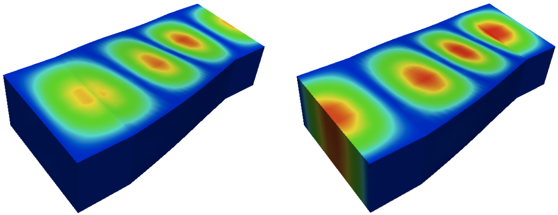

(a) Real part (b) Imaginary part

GeoPDEs 2.0

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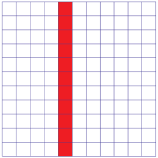

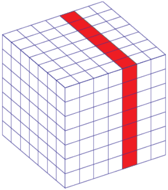

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```
for iel = 1:msh.nel_dir(1)
  msh_col = msh_evaluate_col (msh, iel);
  sp_col = sp_evaluate_col (space, msh_col);
  A = A + op_gradu_gradv (sp_col, msh_col);
end
```

The “column” structures contain the same fields we have seen before.

Conclusions

GeoPDEs is an **open source** and **free** Matlab implementation of IGA.

- Very useful for **teaching** purposes and for new researchers.
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Software download and information

http://geopdes.sourceforge.net

Thanks for your attention!