igatools: a TERRIFIC package for Numerical Assembly of Mathematical Operators.

September 1, 2011-August 30, 2014
www.terrific-project.eu

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Call FP7-2011-NMP-ICT-FoF

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SEVENTH FRAMEWORK PROGRAMME

The TERRIFIC toolkit

“Write programs that do one thing and do it well.
Write programs to work together.”

igatools
General Purpose Assembly of Operators

TUKL
Application oriented Solvers using B−Splines and NURBS.

JKU
Feature detection and volume segmentation

INRIA
-geometric modeler
- tools for visualization, interaction and computation.

SINTEF
-geometry and topology
- model exchange
-isogeometric modelling

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OO is the programming paradigm that realize interaction.

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Why OO Software?

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>>> Object obj

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```
>>> Object obj
>>> smth = obj.do_something()
```

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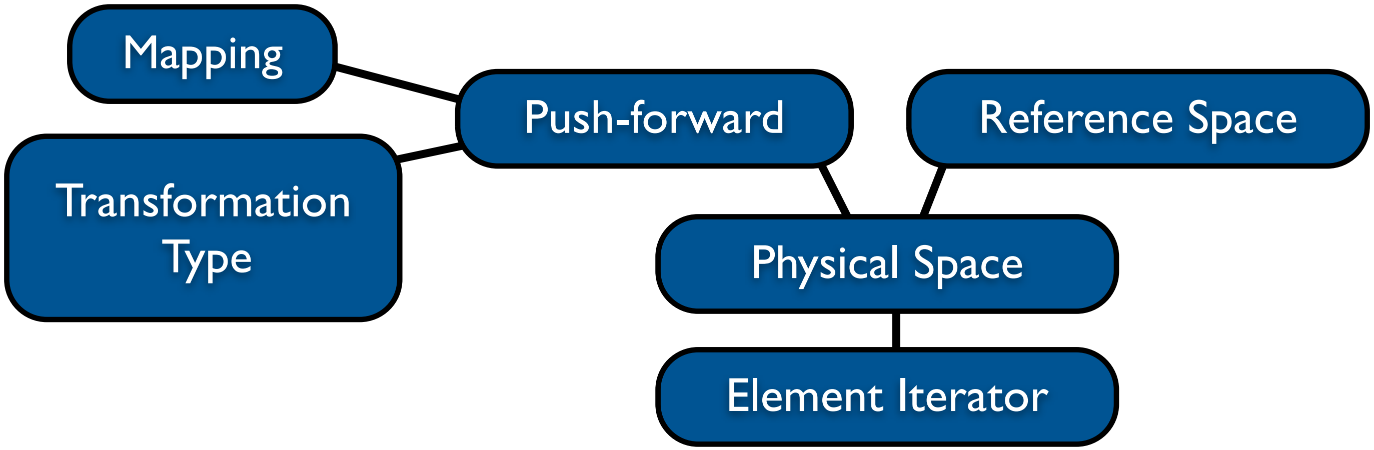
```
>>> Object obj
>>> smth = obj.do_something()
>>> Another anth
>>> cool = anth.do_something_cool(obj.do_something())
```

igatools



$$\int_\Omega \nabla u \cdot \nabla v = \sum_K \int_K \nabla u_j \cdot \nabla v_i = A_{ij}$$

```
element = phys_space->begin();
endc = phys_space->end();

for(; element != endc; ++element) {
    local_dofs = element->get_local_to_global();
    for (q = 0; q < n_qpoints; q++) {
      for (i = 0; i < n_basis; i ++) {
        for (j = 0; j <n_basis; j ++) {
          local_matrix(i,j) += scalar_product(
                element->get_gradient(i,q) ,  element->get_gradient(j,q) )
                * element->get_w_mes(q);  }  }  }
    matrix.add(local_dofs,local_dofs,local_matrix);}
```

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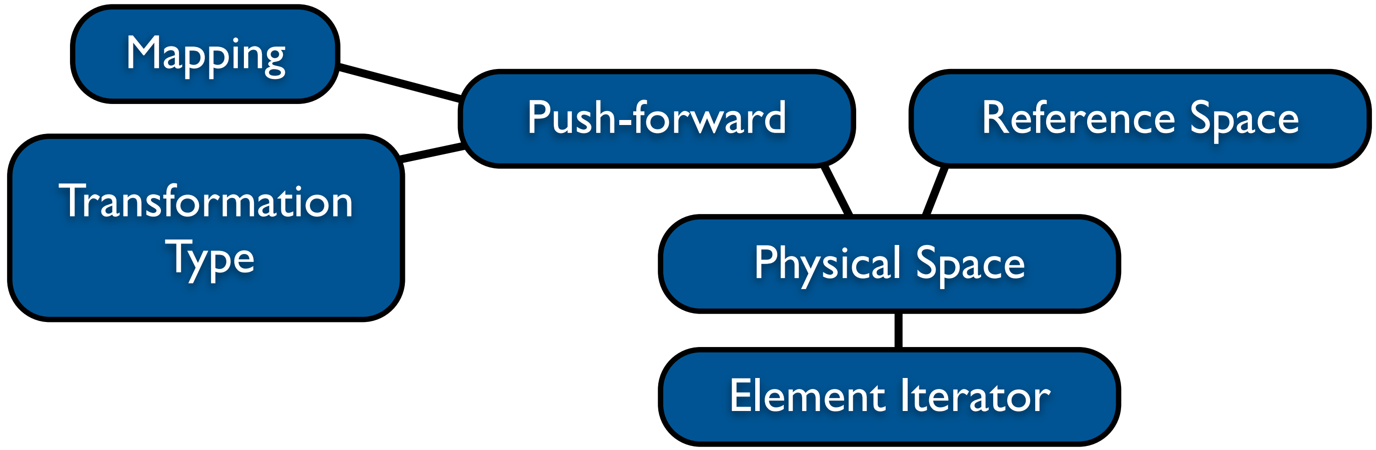


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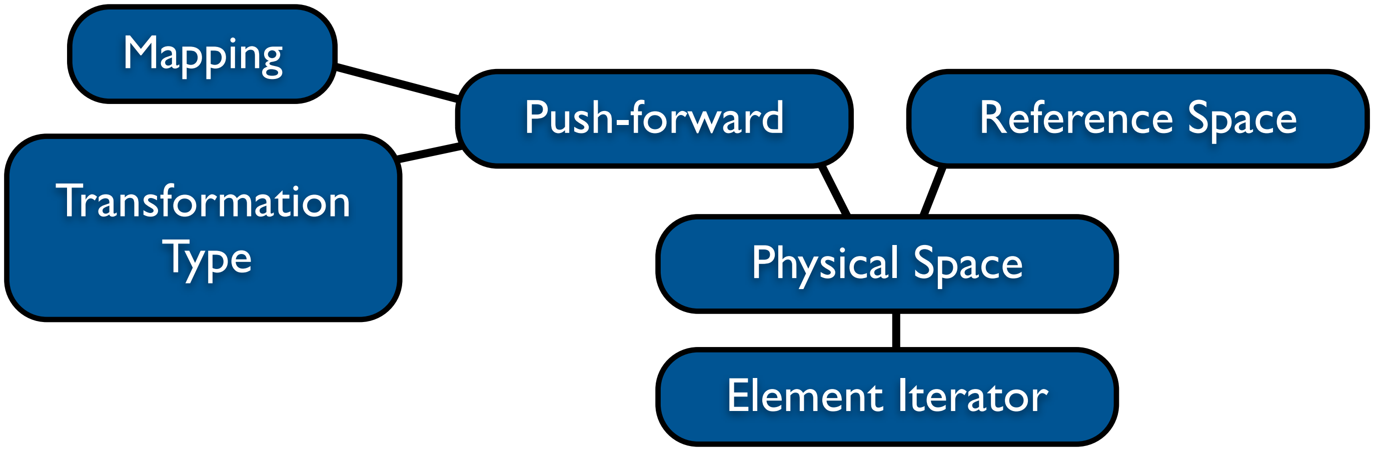

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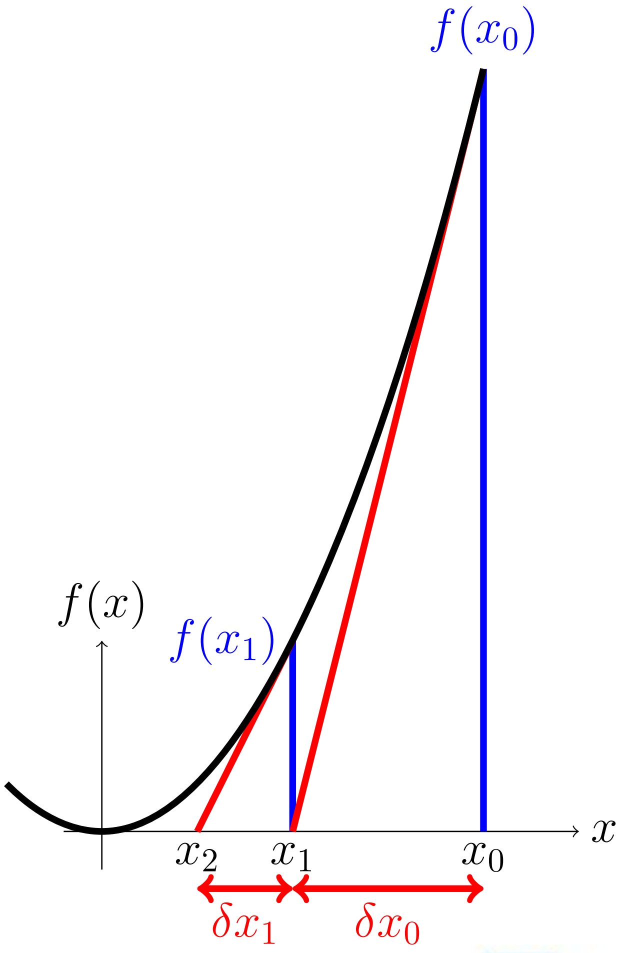
Computational Mechanics



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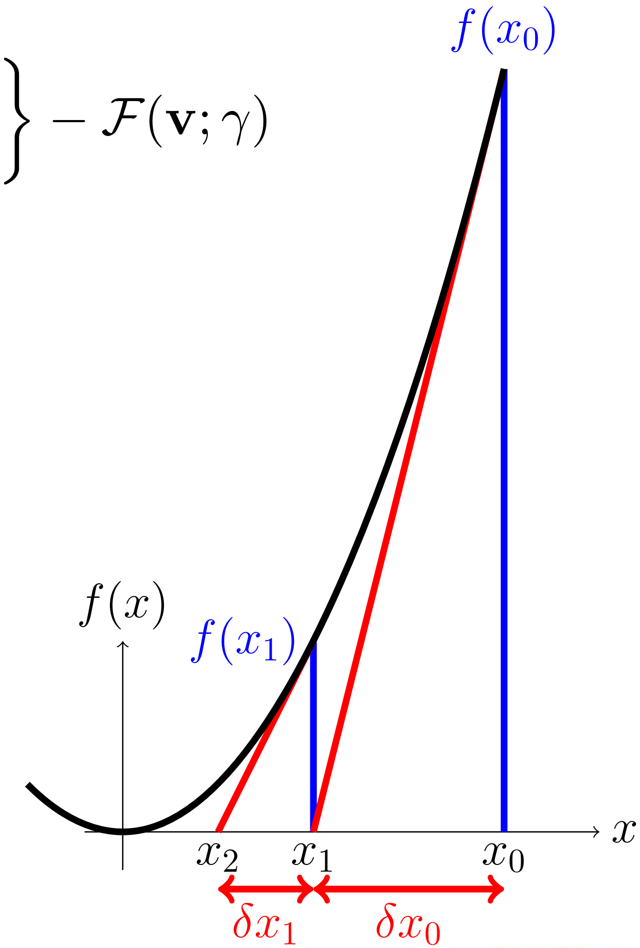
Computational Mechanics

- The Model Equations.

$$\Pi_m^{inc}(\hat{\mathbf{u}}, \hat{p}) = \int_\Omega \left\{ \frac{1}{2}\mu \left[\mathbf{I} : \hat{\mathbf{C}} - 2 \right] - \mu \ln \hat{J} + \hat{p}\ \Theta(\hat{J}) \right\} - \mathcal{F}(\mathbf{v}; \gamma)$$



Computational Mechanics

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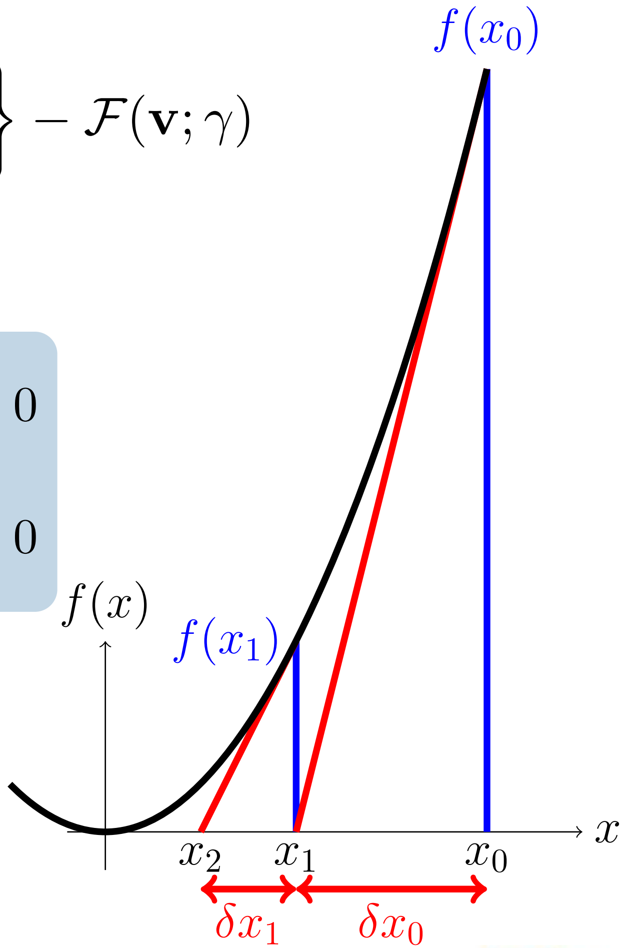
$$\mathrm{d}\Pi_m^{inc}(\hat{\mathbf{u}},\hat{p})[\mathbf{v},q] = 0$$

$$\begin{cases} \mu \displaystyle\int_\Omega [\hat{\mathbf{F}} - \hat{\mathbf{F}}^{-T}] : \nabla\mathbf{v} + \int_\Omega \hat{p}\ \pi(\hat{J})\hat{\mathbf{F}}^{-T} : \nabla\mathbf{v} - \mathcal{F}(\mathbf{v};\gamma) = 0 \\ \displaystyle\int_\Omega \Theta(\hat{J}) q = 0 \end{cases}$$



Computational Mechanics

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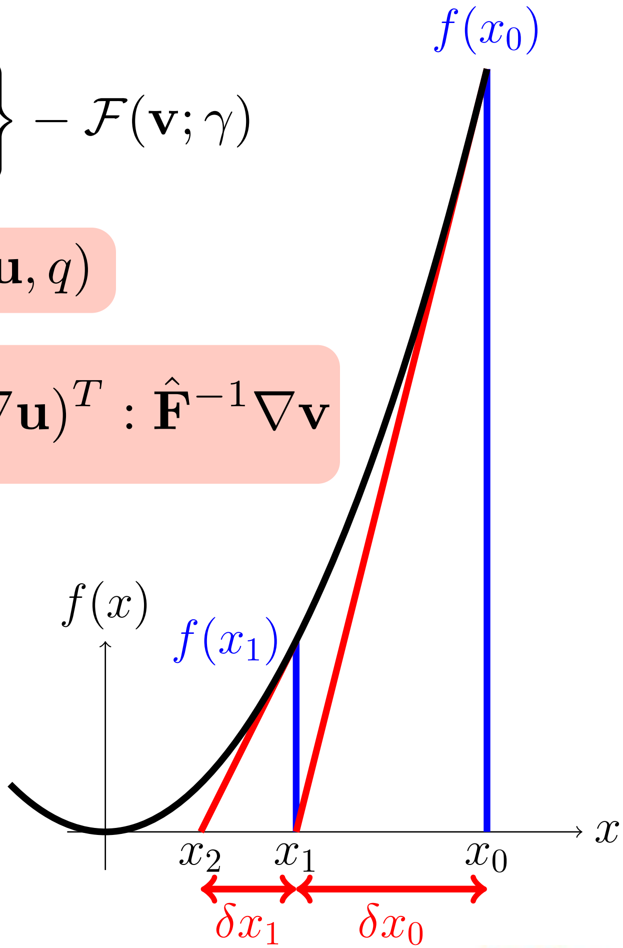
$$\mathrm{d}^2\Pi_m^{inc}(\hat{\mathbf{u}},\hat{p})[(\mathbf{u},p),(\mathbf{v},q)] = a_\gamma(\mathbf{u},\mathbf{v}) + b_\gamma(\mathbf{v},p) + b_\gamma(\mathbf{u},q)$$

$$\begin{cases} a_\gamma(\mathbf{u},\mathbf{v}) := \mu \int_\Omega \nabla\mathbf{u} : \nabla\mathbf{v} + \int_\Omega \left[\mu - \hat{p}\ \pi(\hat{J}) \right] (\hat{\mathbf{F}}^{-1}\nabla\mathbf{u})^T : \hat{\mathbf{F}}^{-1}\nabla\mathbf{v} \\ \qquad + \int_\Omega \hat{p}\ \kappa(\hat{J})(\hat{\mathbf{F}}^{-T} : \nabla\mathbf{u})(\hat{\mathbf{F}}^{-T} : \nabla\mathbf{v}) \\ b_\gamma(\mathbf{v},q) := \int_\Omega q\ \pi(\hat{J})\hat{\mathbf{F}}^{-T} : \nabla\mathbf{v} \end{cases}$$



Computational Mechanics

$$\int_\Omega \hat{p}\ \pi(\hat{J})\hat{\mathbf{F}}^{-T} : \nabla \mathbf{v}$$

- Assembly of the mixed term:

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Computational Mechanics

$$\int_\Omega \hat{p}\ \pi(\hat{J})\hat{\mathbf{F}}^{-T} : \nabla \mathbf{v}$$

- Assembly of the mixed term:

```
T< 1, 1, tensor::cont, Tdouble > prex_q;

T< dim_ref, 1, tensor::cov,
T< dim_phys, 1, tensor::cont, Tdouble > > defgrad_q, defo_grad_q;

for (; defo_elem != defo_end ; ++defo_elem, ++prex_elem){
   for (Index q = 0; q < n_qp; ++q){

      for(Index i = 0; i < defo_loc_ndofs; ++i)
         defo_grad_q += defo_vec(dof) * grad_phi_q[i];

      for(Index i = 0; i < prex_loc_ndofs; ++i)
         prex_q += prex_vec(dof) * prex_phi_q[i];

      defgrad_q = unit_defgrad + defo_grad_q;

      inverse<dim_ref, dim_phys> (defgrad_q,defgrad_inv_q);
      defgrad_invT_q = co_tensor(transpose(defgrad_inv_q));

      for (Index i = 0; i < defo_loc_ndofs; ++i){

         defo_loc_res(i) += mat_mu * prex_q[0] *
            scalar_product(defgrad_invT_q,
                           grad_phi_q[i]) *w[q] ;}}}
```

Listing 1: Assemble of the mixed term in the momentum equation.

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for                                                        lem){
    f



                                                           ];






                                                           inv_q);
                                                           nv_q));




                scalar_product(defgrad_invT_q,
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```

GOAL:
Respect the mathematical formulation of operators, so that any SciCom user can easily assemble sophisticated operators.

Listing 1: Assemble of the mixed term in the momentum equation.

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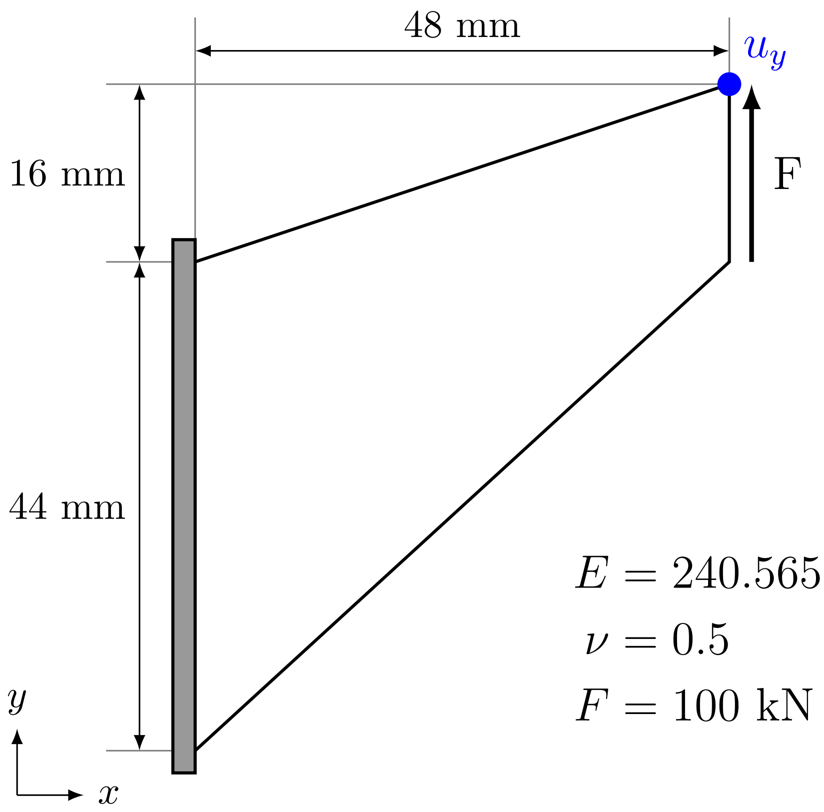
Computational Mechanics

- Benchmark Cook's membrane.



$E = 240.565$ MPa

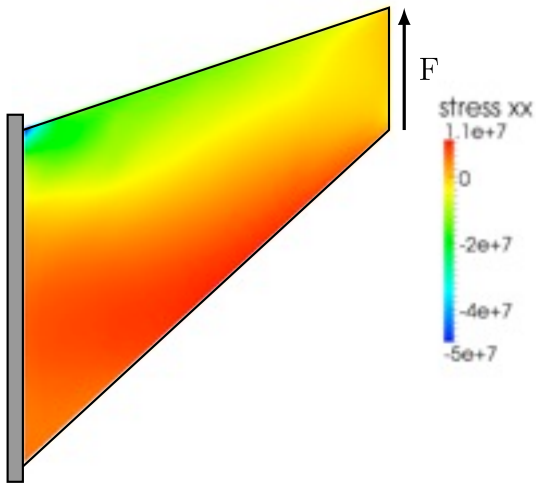
$\nu = 0.5$

$F = 100$ kN

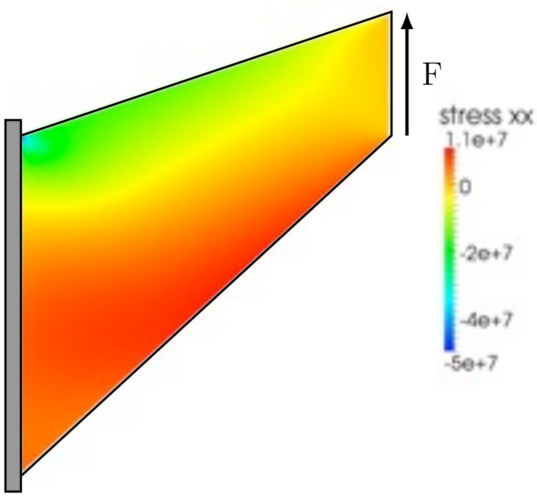
Computational Mechanics

- Benchmark Cook's membrane.

shape functions $= S_3^1/S_2^1$
elements $= 16 \times 16$



shape functions $= S_3^1/S_2^1$
elements $= 4 \times 4$



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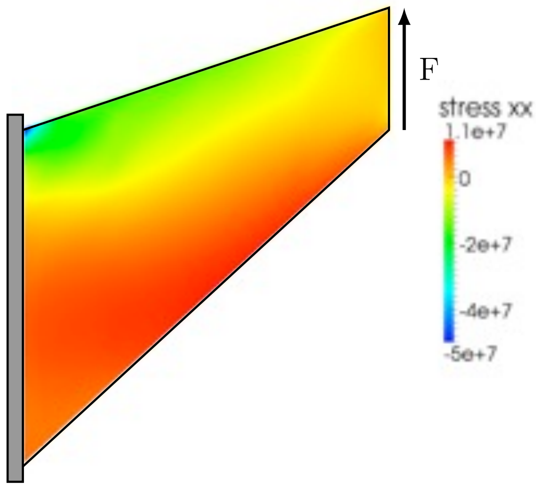
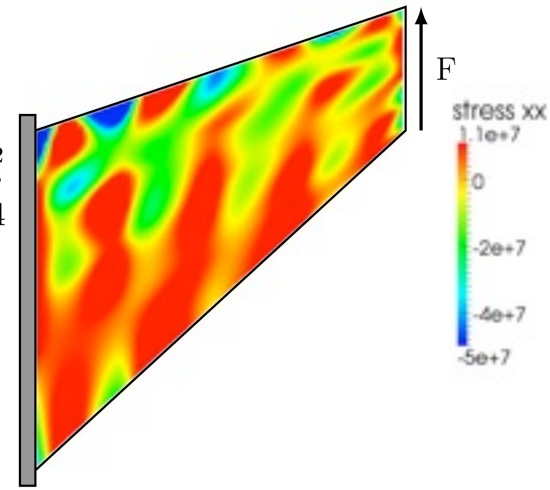


shape functions $= S_3^2$
elements $= 4 \times 4$



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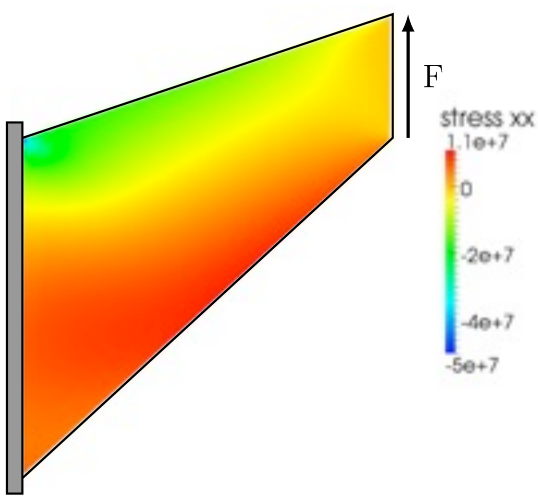

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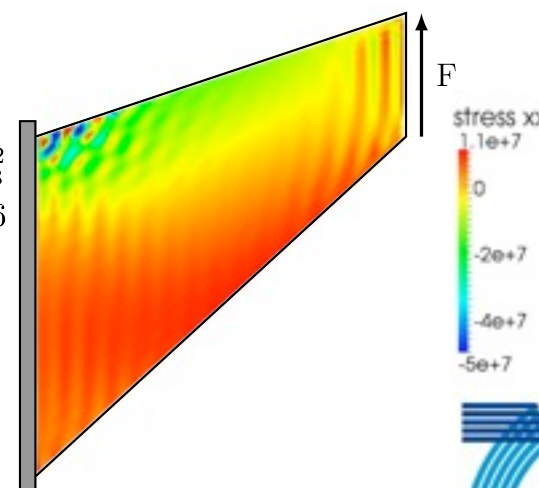

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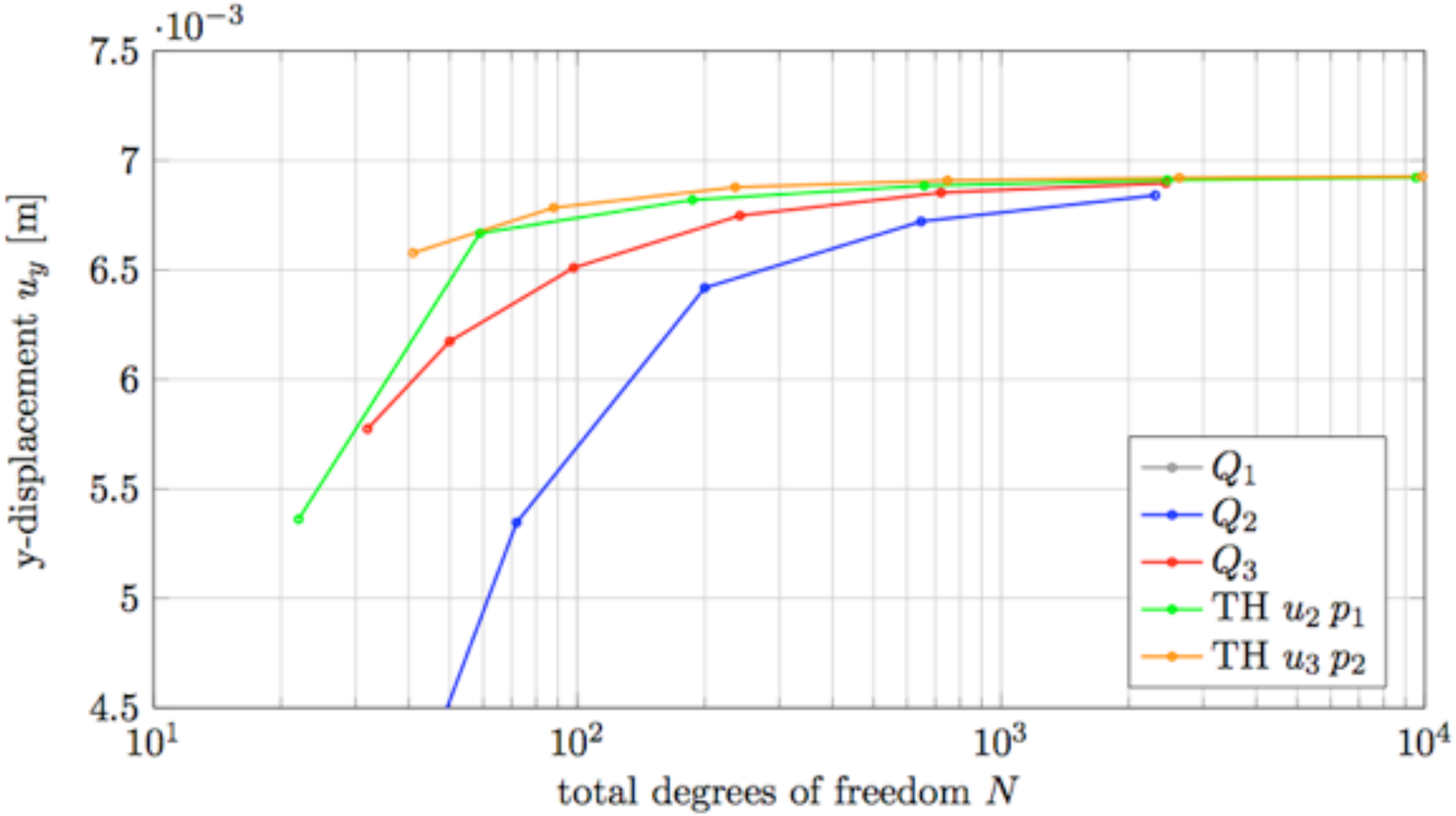

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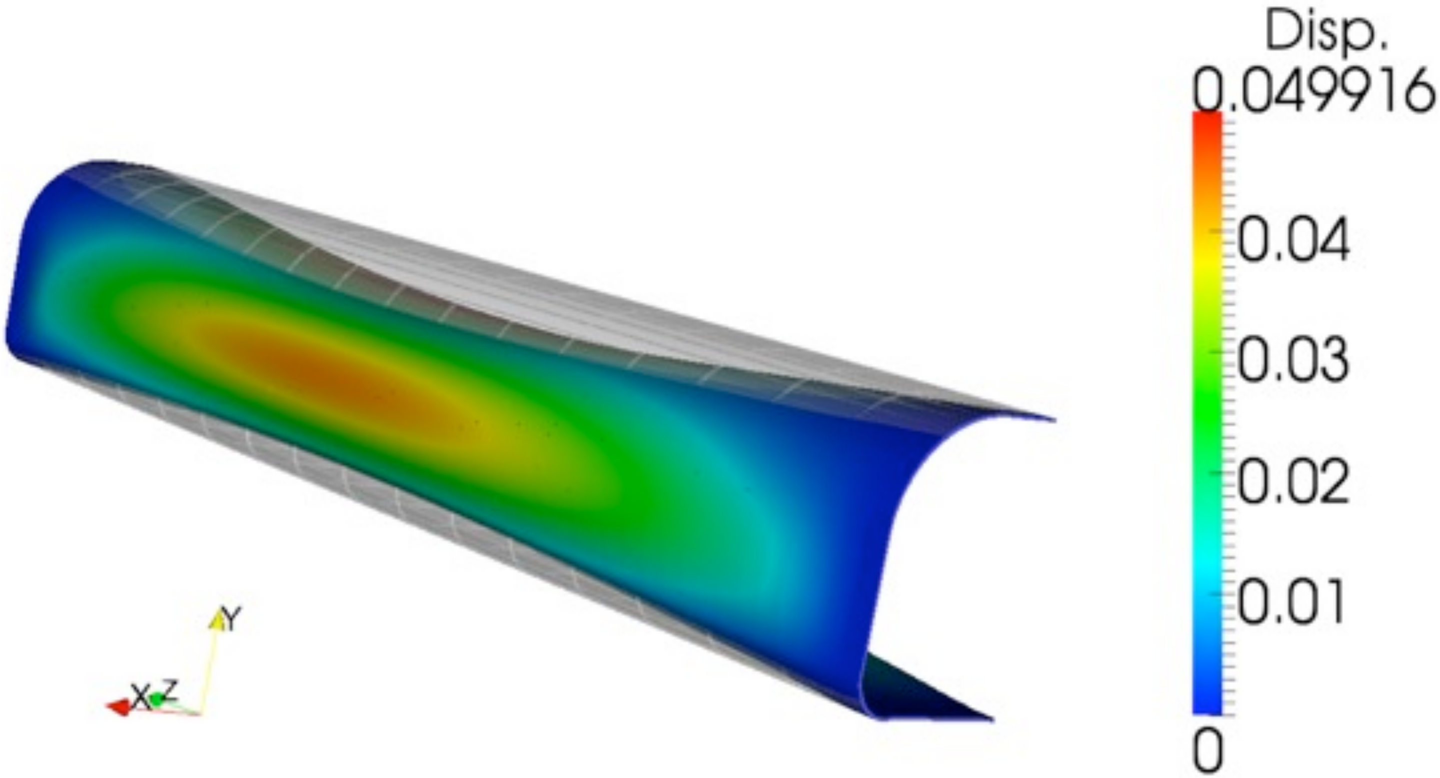
Computational Mechanics

- Industrial Test Case



Computational Mechanics

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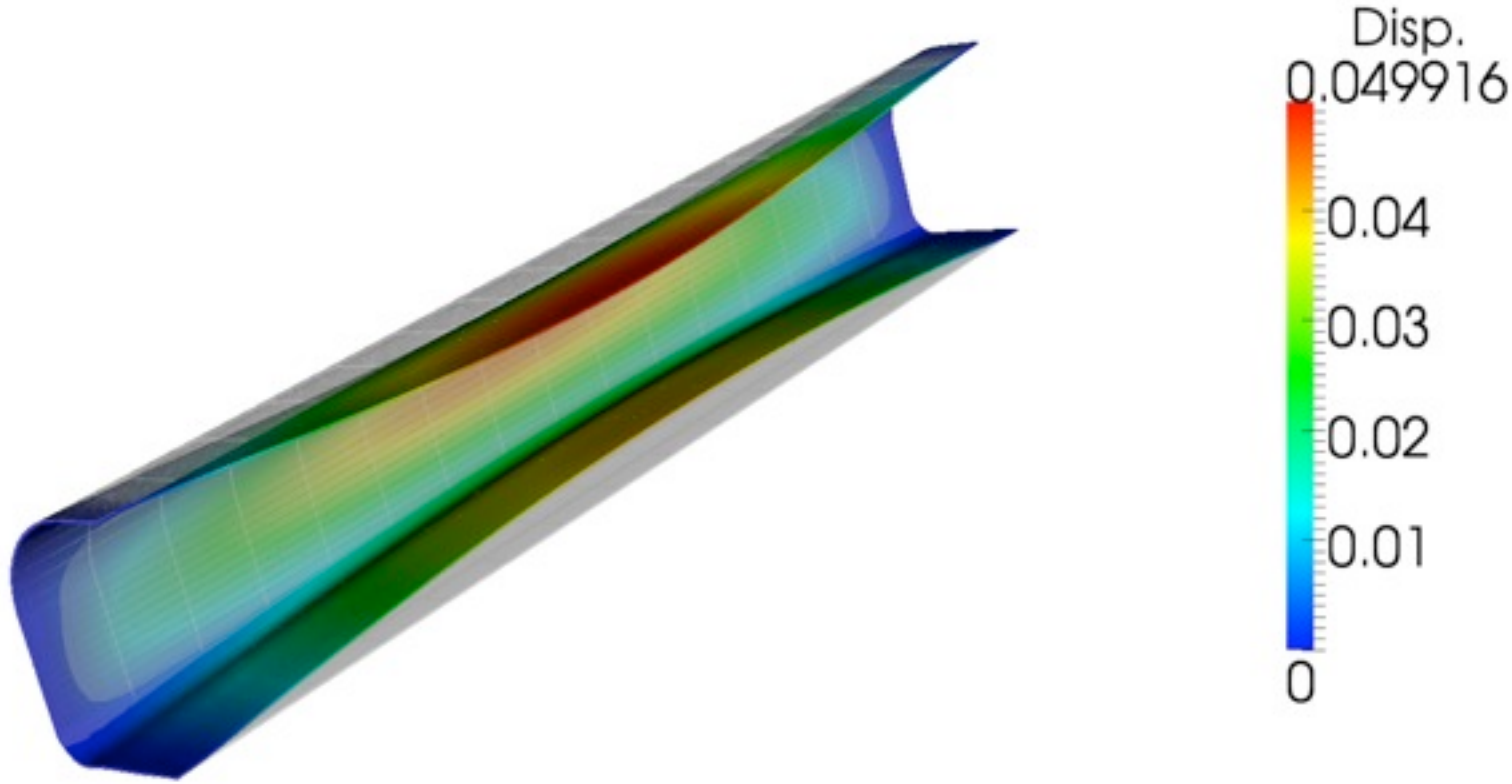

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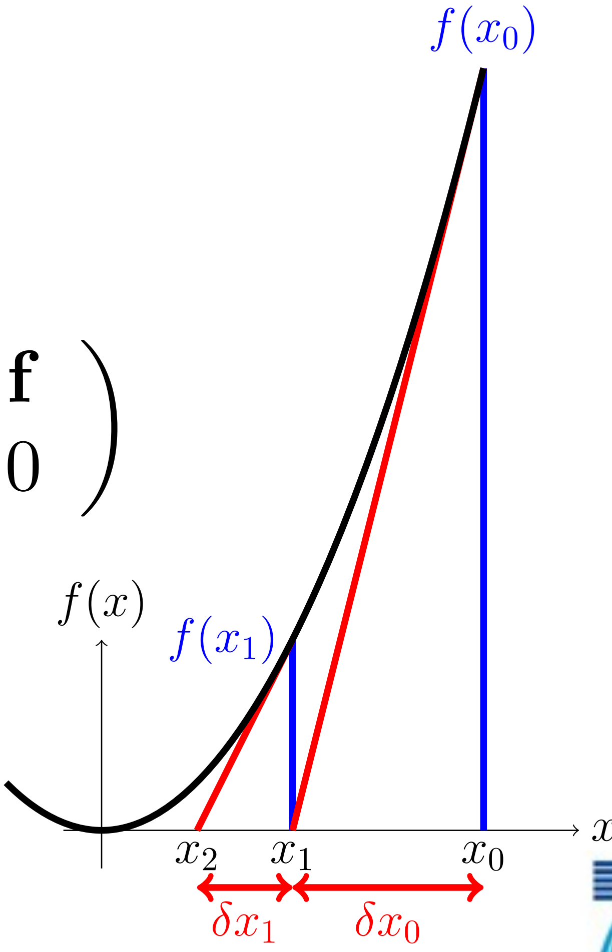
Fluid Dynamics

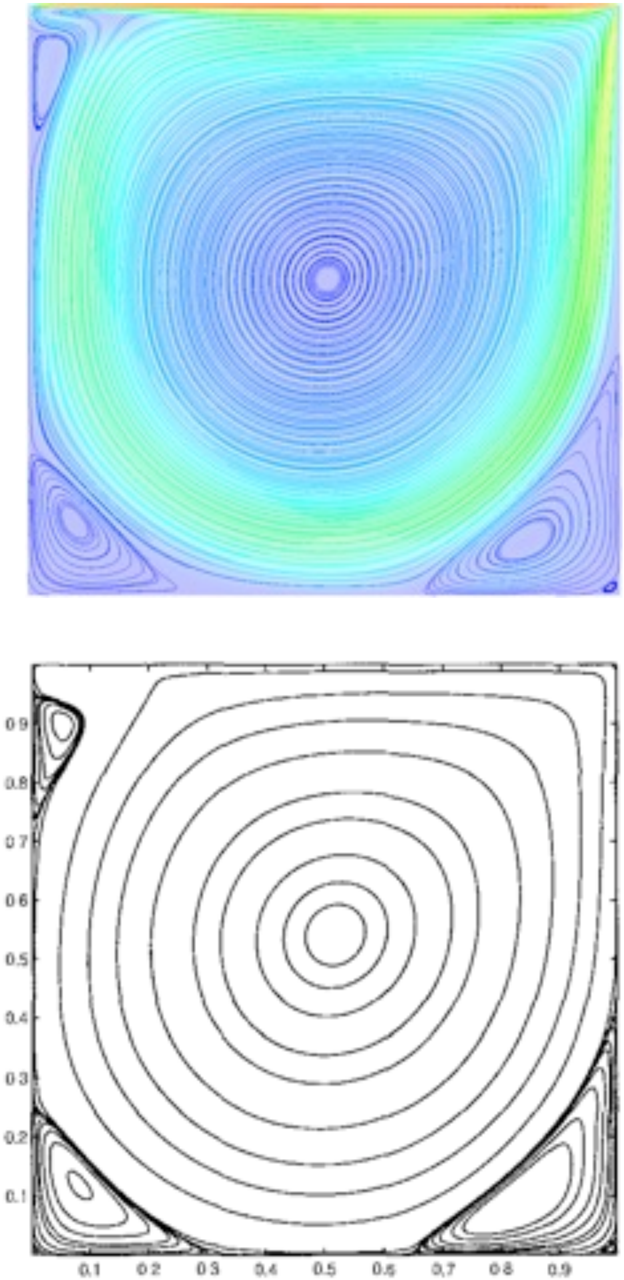
- The Model Equations.

$$\rho\,(\nabla\mathbf{u})\,\mathbf{u} - \mu\nabla^2\mathbf{u} + \nabla p = \mathbf{f}$$
$$\nabla\cdot\mathbf{u} = 0$$

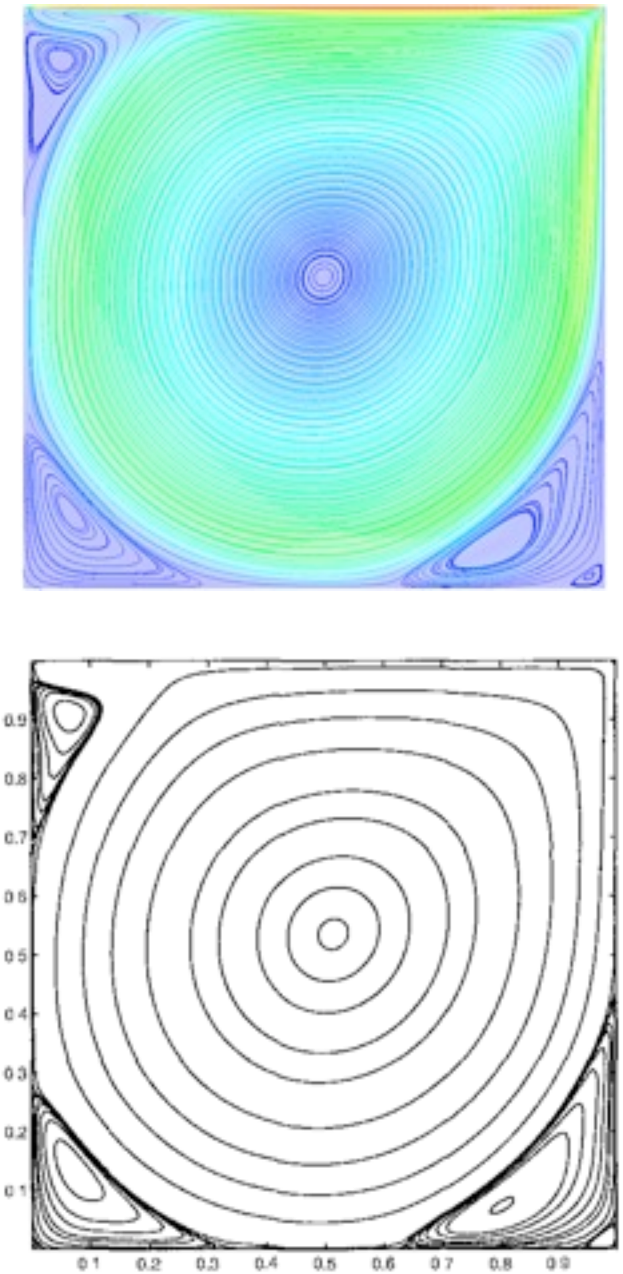
In Matrix Form:

$$\begin{pmatrix} A + N(\mathbf{u}) & B^t \\ B & 0 \end{pmatrix} \begin{pmatrix} \mathbf{u} \\ p \end{pmatrix} = \begin{pmatrix} \mathbf{f} \\ 0 \end{pmatrix}$$





Re = 3200



Re = 5000

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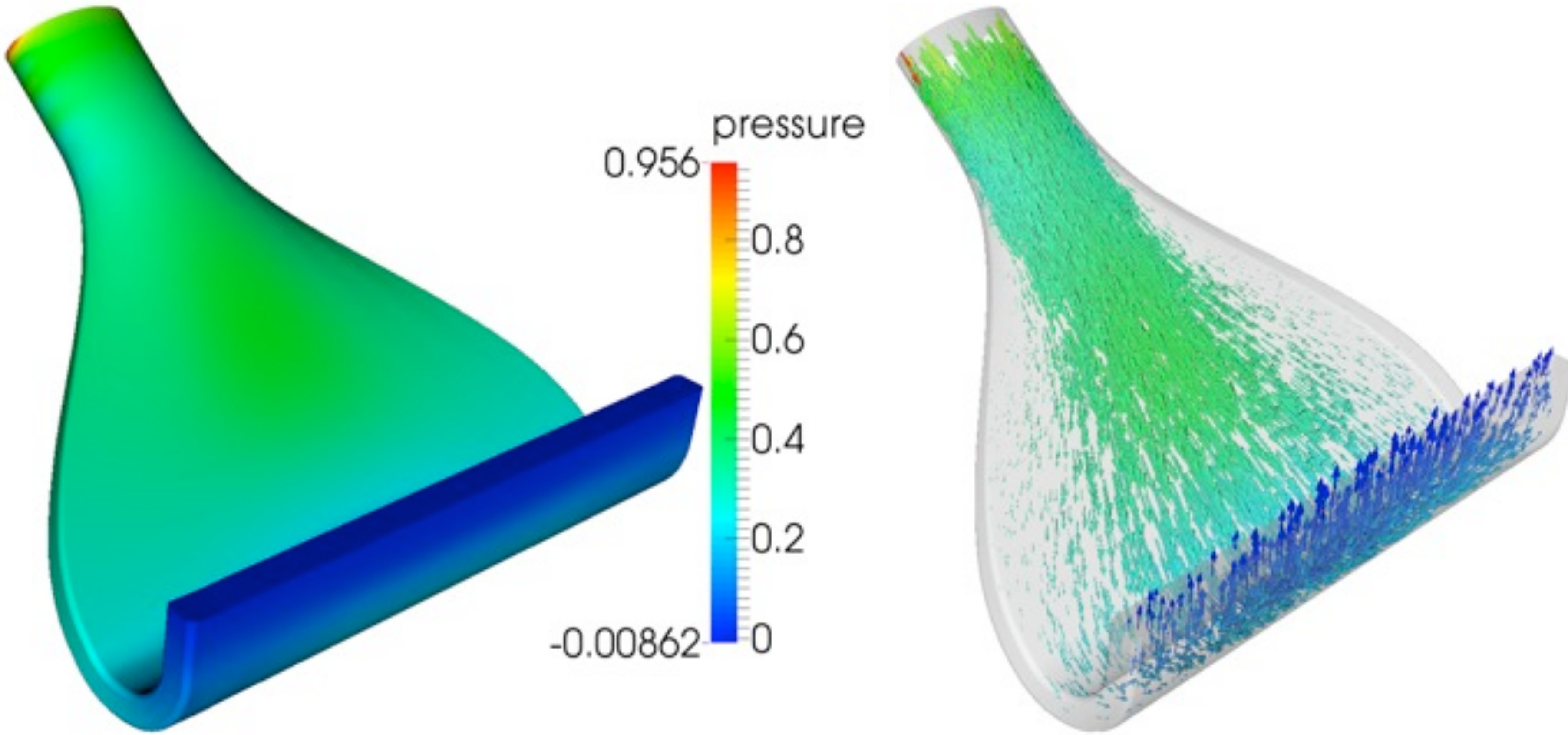

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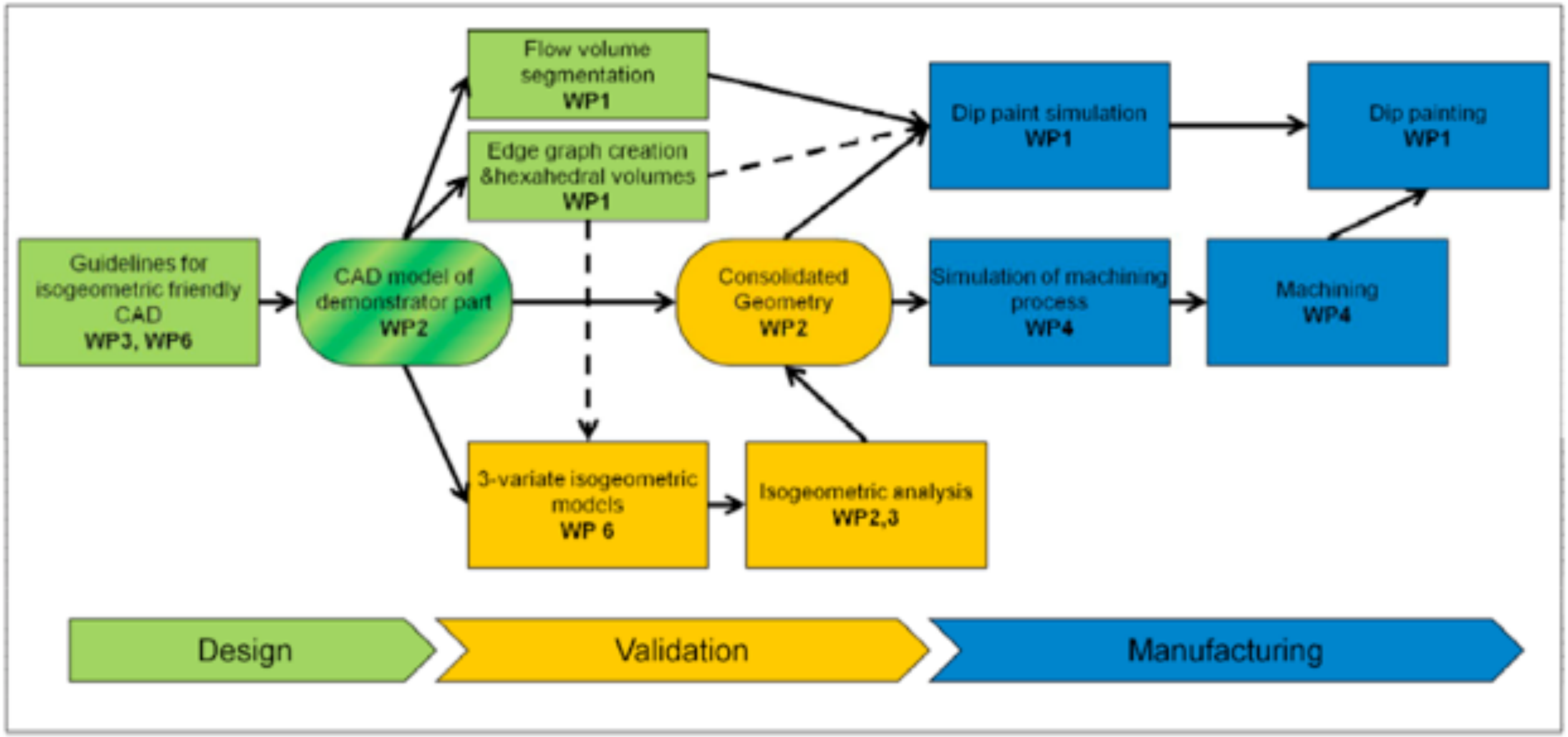
Interplay on The Demonstrator



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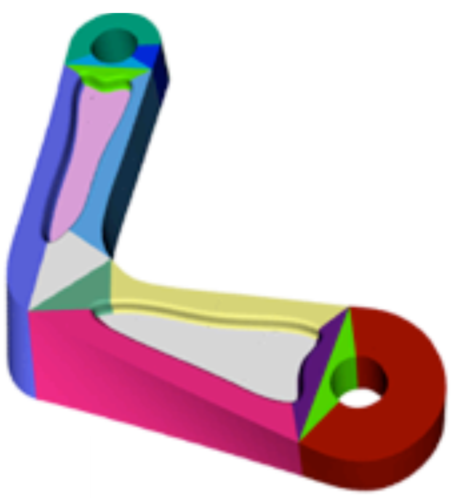

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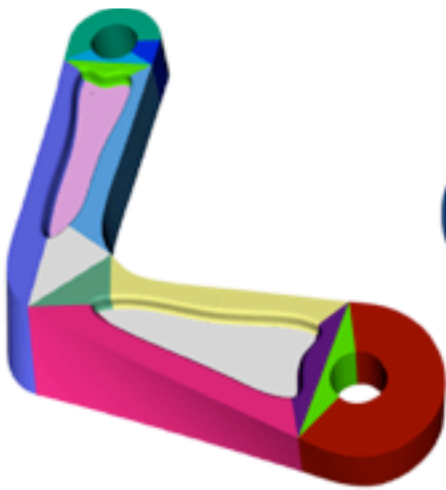

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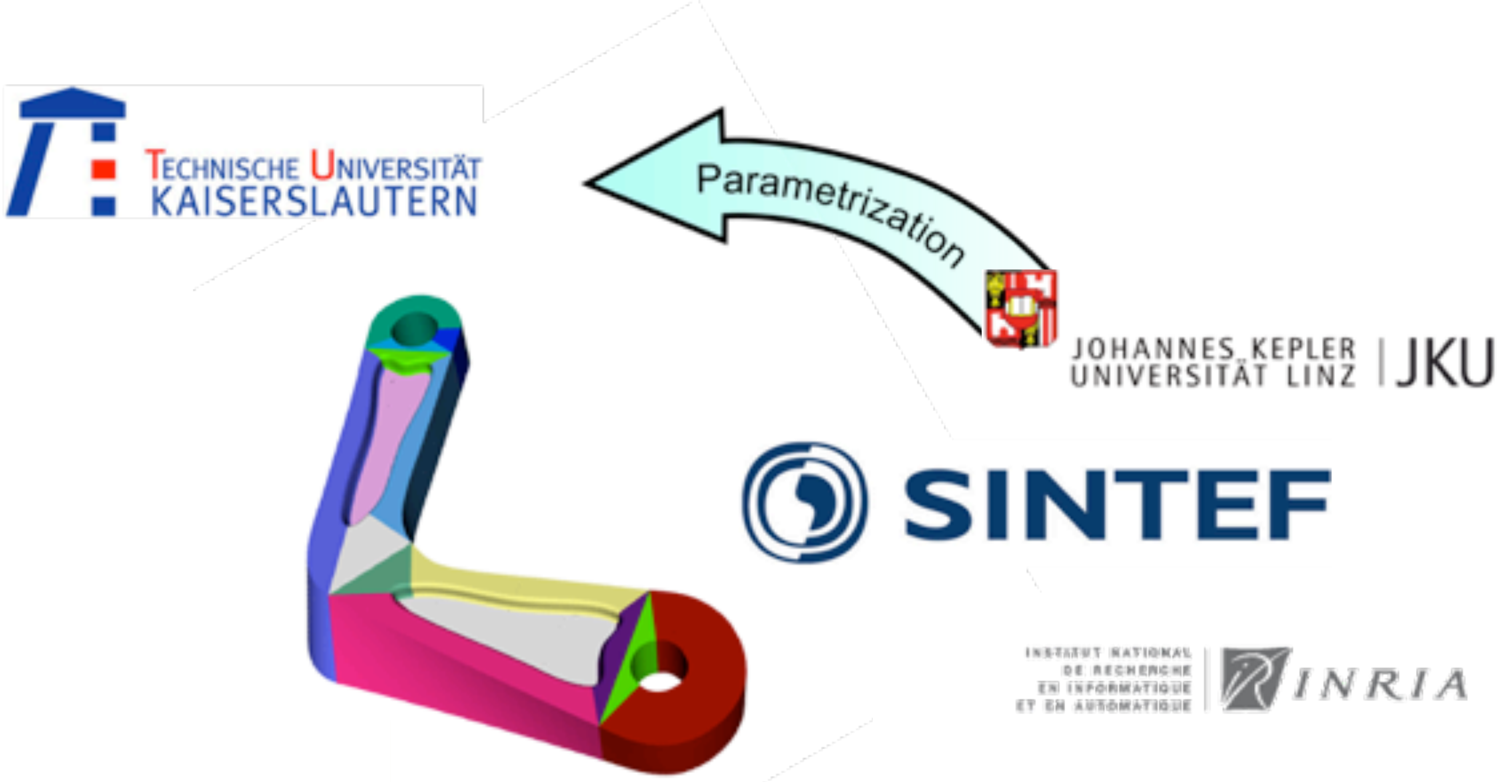

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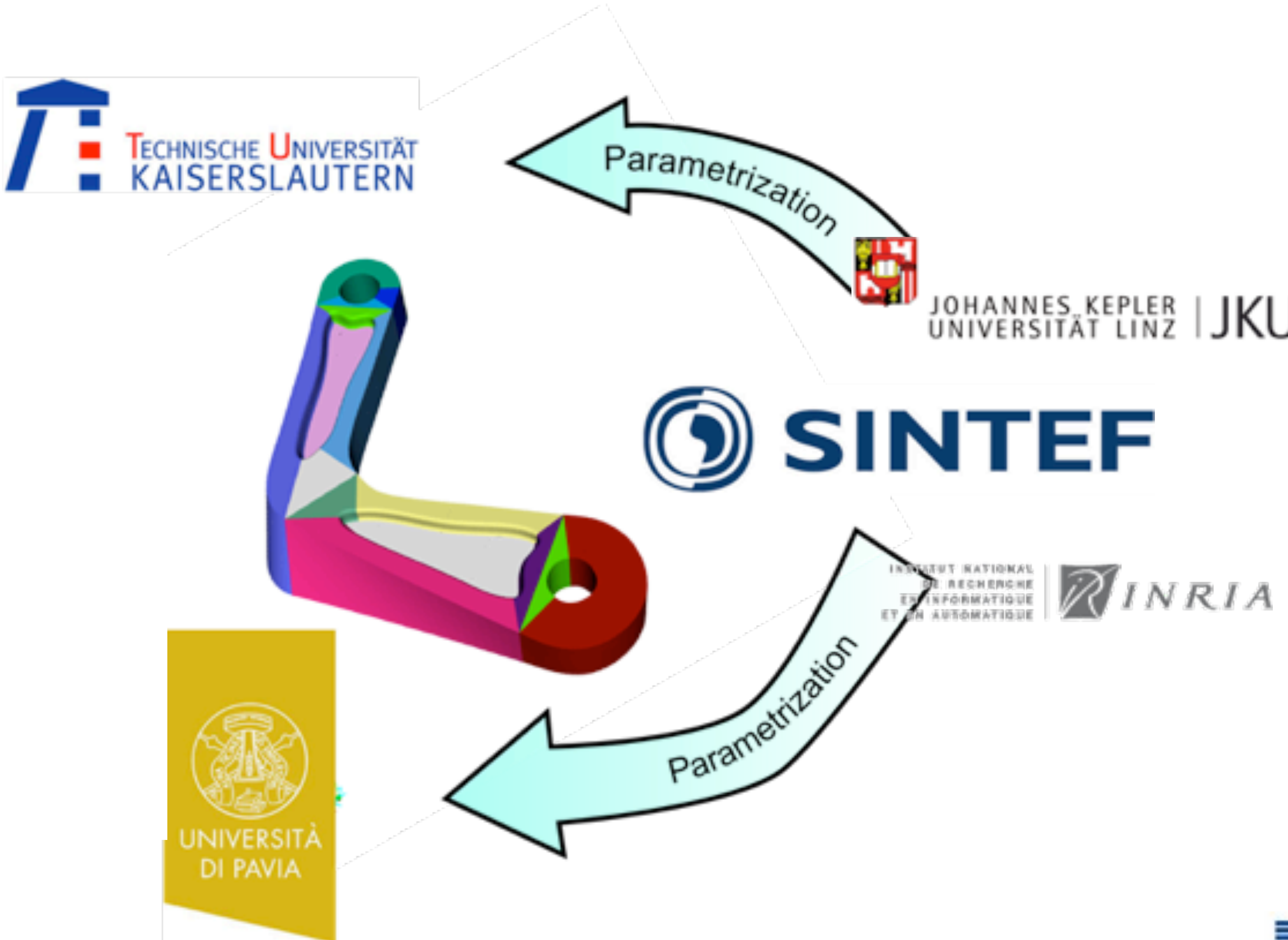

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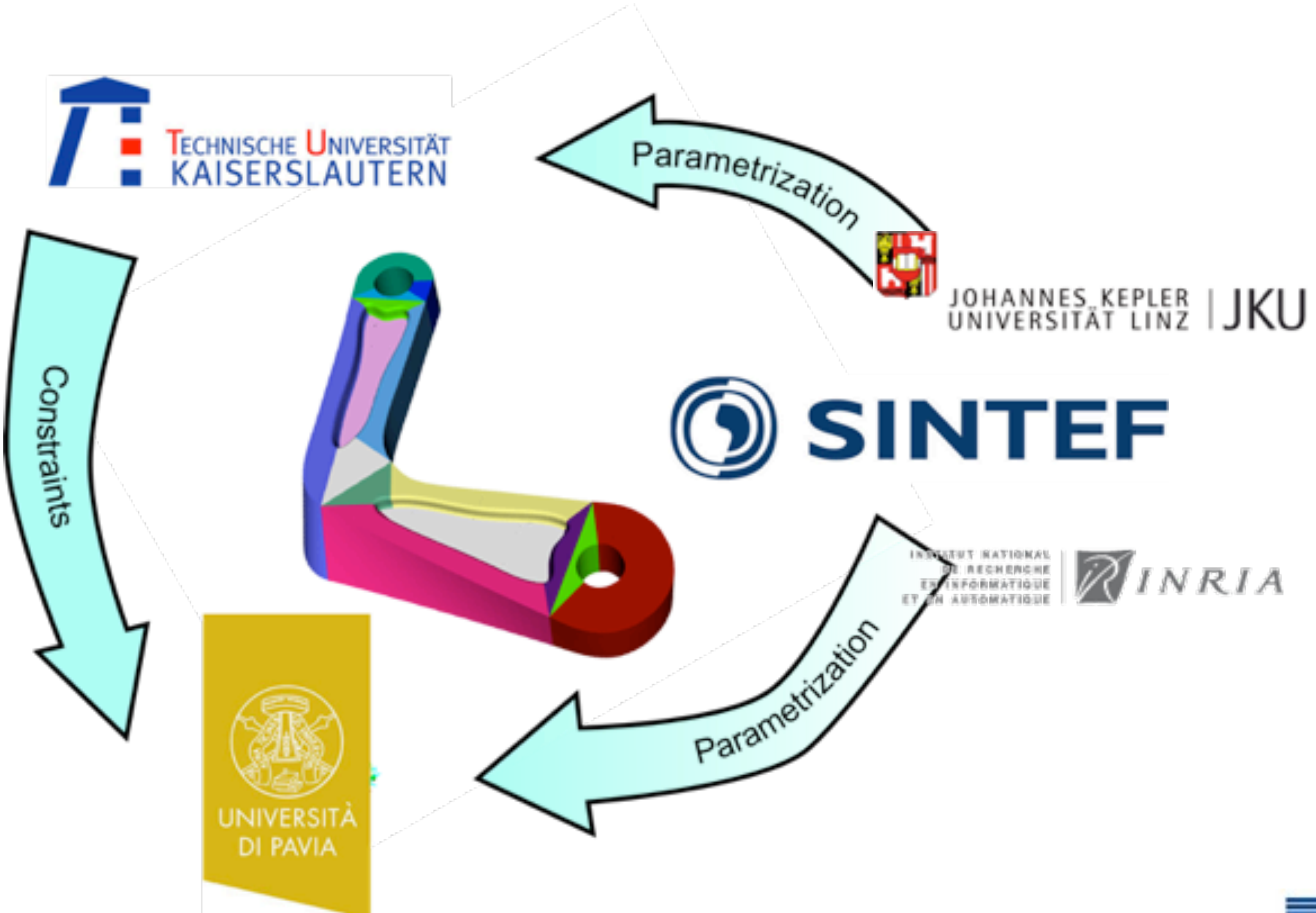

Constraints define the matching of the solution in between patches

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Conclusions

- We developed a modular software that is capable of interfacing with other TERRIFIC modules.
- On the PDE side, this software makes easy the assembly of sophisticated operators.

Fluid Dynamics

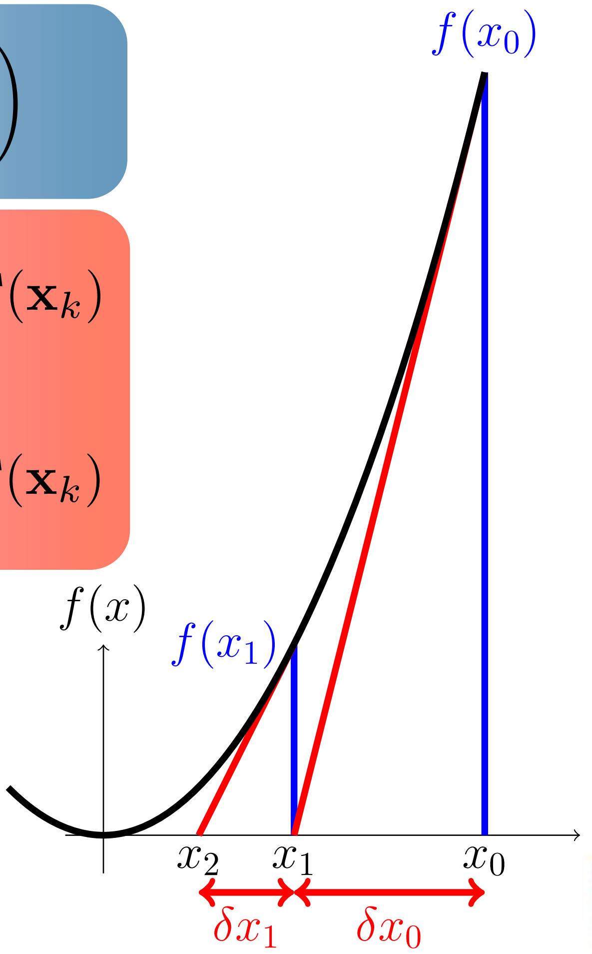
$$\begin{pmatrix} A+N(\mathbf{u}_0) & B^t \\ B & 0 \end{pmatrix} \begin{pmatrix} \mathbf{u} \\ p \end{pmatrix}_k = \begin{pmatrix} \mathbf{f} \\ 0 \end{pmatrix}$$

$$\mathbf{F}(\mathbf{x}_k) = \begin{pmatrix} A+N(\mathbf{u}_k) & B^t \\ B & 0 \end{pmatrix} \begin{pmatrix} \mathbf{u} \\ p \end{pmatrix}_k - \begin{pmatrix} \mathbf{f} \\ 0 \end{pmatrix}$$

$$\begin{pmatrix} A+N(\mathbf{u}_k) & B^t \\ B & 0 \end{pmatrix} \begin{pmatrix} \delta\mathbf{u} \\ \delta p \end{pmatrix}_k = -\mathbf{F}(\mathbf{x}_k)$$

$$\begin{pmatrix} A+N(\mathbf{u}_k)+D(\mathbf{u}_k) & B^t \\ B & 0 \end{pmatrix} \begin{pmatrix} \delta\mathbf{u} \\ \delta p \end{pmatrix}_k = -\mathbf{F}(\mathbf{x}_k)$$

$$\begin{pmatrix} \mathbf{u} \\ p \end{pmatrix}_{k+1} = \begin{pmatrix} \mathbf{u} \\ p \end{pmatrix}_k + \begin{pmatrix} \delta\mathbf{u} \\ \delta p \end{pmatrix}_k$$



$$N_{ij} = \int_\Omega (\nabla \mathbf{u}_j)\,\mathbf{u} \cdot \mathbf{v}_i =$$

$$\int_\Omega \begin{pmatrix} \partial_x u_x & \partial_y u_x \\ \partial_x u_y & \partial_y u_y \end{pmatrix}_j \begin{pmatrix} u_x \\ u_y \end{pmatrix} \cdot \begin{pmatrix} v_x \\ v_y \end{pmatrix}_i$$

```
for (dof_index q = 0; q < quad.get_num_points(); q++)
{
   Tensor<dim_phys, rank, contravariant, double> vel_q;

   for (dof_index i = 0; i <local_ndofs; i ++){
      auto phi = element->get_value(i,q);
      vel_q = vel_q+vel[local_dofs[i]]*phi;}

   for (dof_index i = 0; i <local_ndofs; i ++){
      for (dof_index j = 0; j <local_ndofs; j ++){
         adv_ij = scalar_product(
                  action(element->get_gradient(j,q),vel_q),
                            element->get_value(i,q) )*
                            element->get_w_measures()[q;]}}
}
```

Listing 1: Advection assemble.

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$$D_{ij} = \int_\Omega (\nabla \mathbf{u})\, \mathbf{u}_j \cdot \mathbf{v}_i =$$

$$\int_\Omega \begin{pmatrix} \partial_x u_x & \partial_y u_x \\ \partial_x u_y & \partial_y u_y \end{pmatrix} \begin{pmatrix} u_x \\ u_y \end{pmatrix}_j \cdot \begin{pmatrix} v_x \\ v_y \end{pmatrix}_i$$

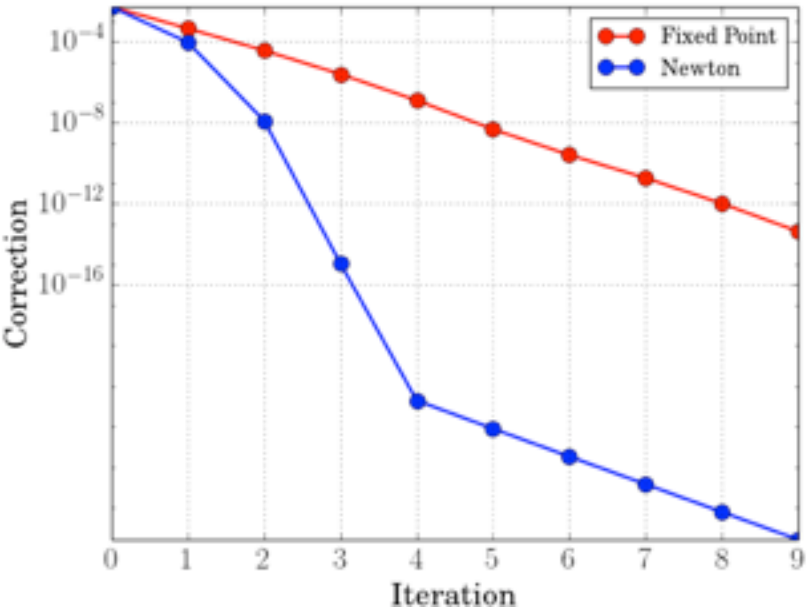
```
for (dof_index q = 0; q < quad.get_num_points(); q++)
{
   Tensor<dim_phys, rank, covariant,
   Tensor<dim_phys, rank, contravariant, double>> grad_vel_q;

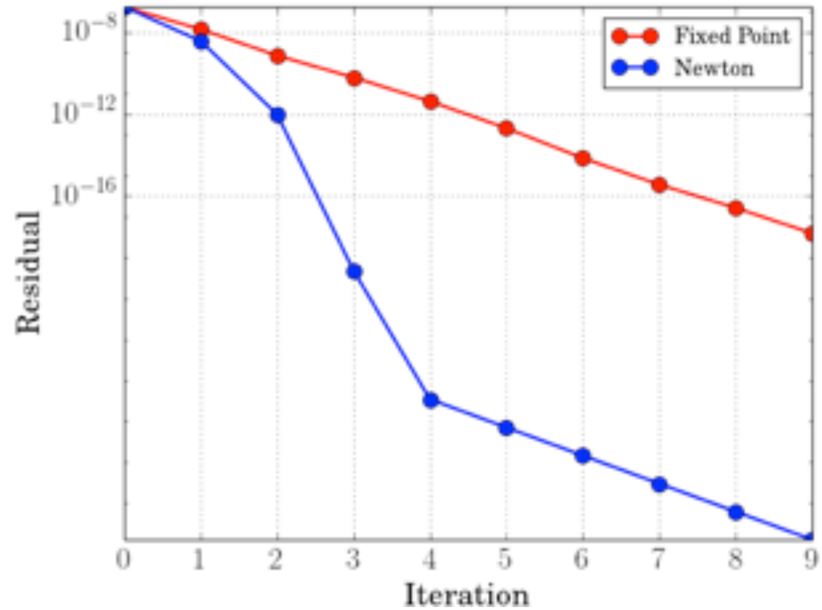
   for (dof_index i = 0; i <local_ndofs; i++){
      auto grad_phi = element->get_gradient(i,q);
      grad_vel_q = grad_vel_q + vel[local_dofs[i]] * grad_phi;}

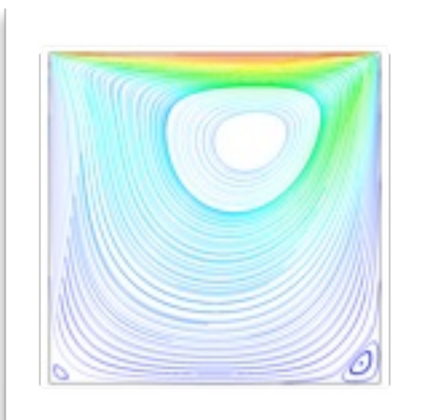
   for (dof_index i = 0; i <local_ndofs; i++){
      for (dof_index j = 0; j <local_ndofs; j++){
         jac_ij = scalar_product(action(
                                    grad_vel_q,
                                           element->get_value(j,q)),
                                    element->get_value(i,q) )*
                                    element->get_w_measures()[q];}}
}
```

Listing 1: Jacobian assemble.

Fluid Dynamics







$$\begin{pmatrix} A + N(\mathbf{u}_k) & B^t \\ B & 0 \end{pmatrix} \begin{pmatrix} \delta \mathbf{u} \\ \delta p \end{pmatrix}_k = -\mathbf{F}(\mathbf{x}_k)$$

$$\begin{pmatrix} A + N(\mathbf{u}_k) + D(\mathbf{u}_k) & B^t \\ B & 0 \end{pmatrix} \begin{pmatrix} \delta \mathbf{u} \\ \delta p \end{pmatrix}_k = -\mathbf{F}(\mathbf{x}_k)$$

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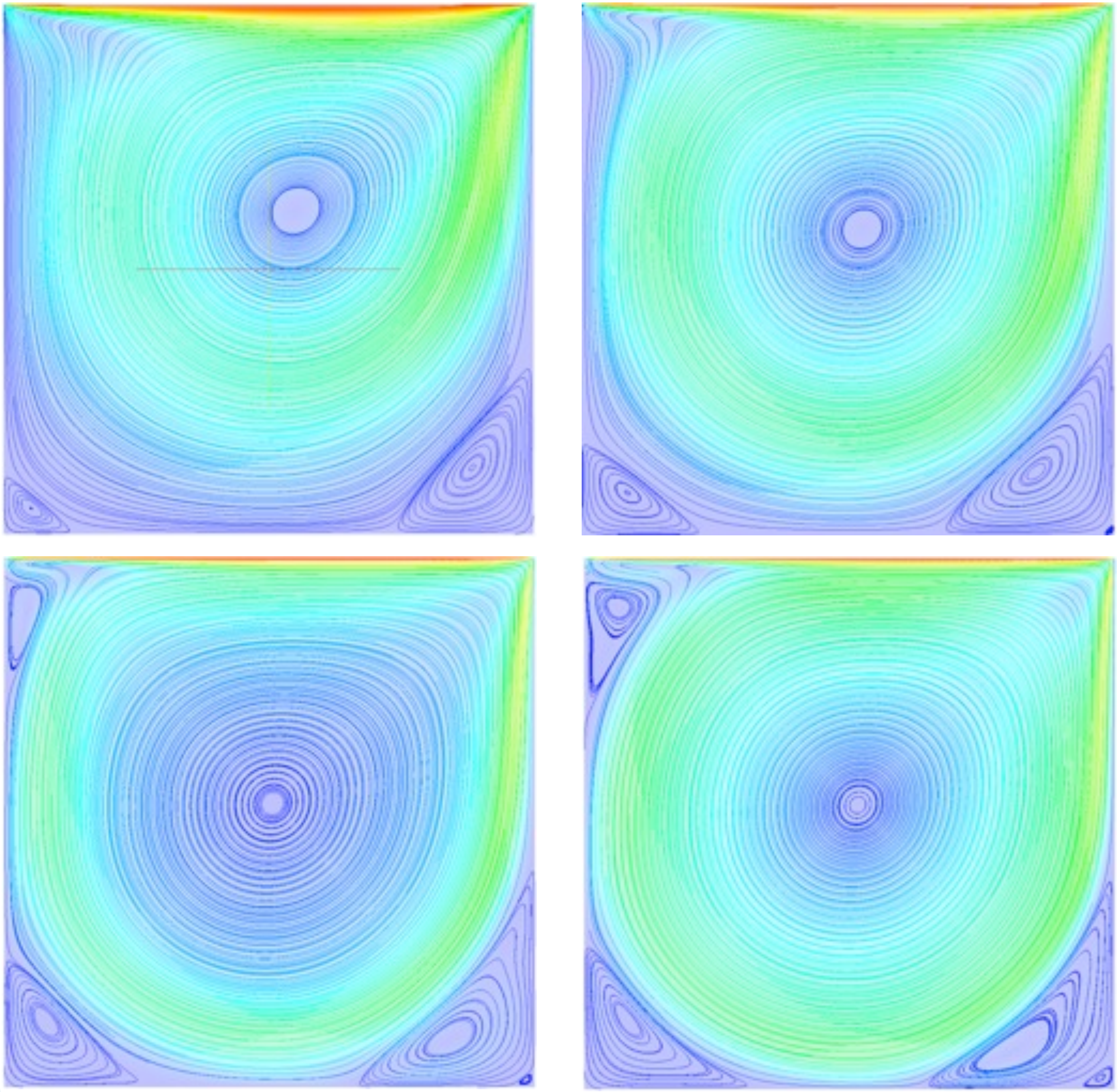

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